Full wwPDB X-ray Structure Validation Report (i)

Mar 6, 2026 – 08:47 PM UTC

PDB ID	:	7LAG / pdb_00007lag
Title	:	CRYSTAL STRUCTURE OF MYELOPEROXIDASE SUBFORM C (MPO) COMPLEX WITH Compound-14 AKA 7-({1-[(3-phenoxyphenyl)methyl]-1H-pyrazol-4-yl}methyl)-3H-[1,2,3]triazolo[4,5-b]pyridin-5-amine
Authors	:	Khan, J.A.
Deposited on	:	2021-01-06
Resolution	:	2.85 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 (i) 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 (i)) were used in the production of this report:

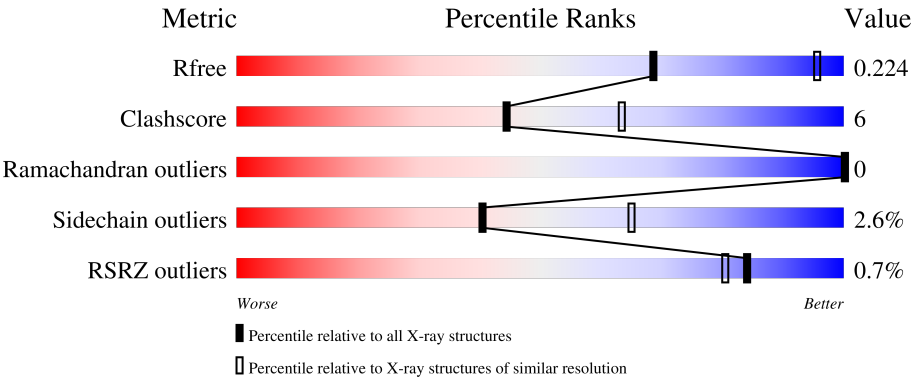
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 <=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	3% 86% 12% ·
1	D	105	% 92% 6% ·
1	F	105	4% 90% 8% ·
1	H	105	88% 10% ·

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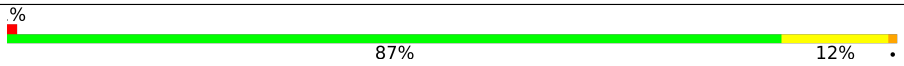
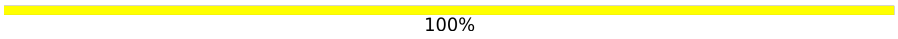
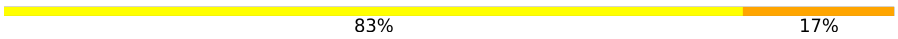
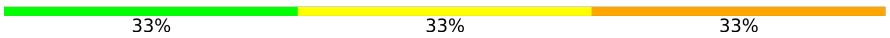
Mol	Chain	Length	Quality of chain
2	B	466	
2	E	466	
2	G	466	
2	I	466	
3	C	2	
3	L	2	
4	J	6	
4	K	6	
4	M	6	
4	N	6	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 18458 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 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	3	0	0
			820	519	145	151	5			
1	D	103	Total	C	N	O	S	3	0	0
			814	517	145	147	5			
1	F	103	Total	C	N	O	S	3	0	0
			821	520	145	151	5			
1	H	103	Total	C	N	O	S	3	0	0
			820	519	145	151	5			

- Molecule 2 is a protein called Isoform H14 of Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	464	Total	C	N	O	S	23	0	0
			3602	2283	639	653	27			
2	E	465	Total	C	N	O	S	30	0	0
			3636	2303	655	651	27			
2	G	464	Total	C	N	O	S	26	0	0
			3620	2295	647	651	27			
2	I	464	Total	C	N	O	S	22	0	0
			3615	2295	641	652	27			

- 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			

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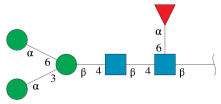
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	L	2	Total C N O 28 16 2 10	0	0	0

- 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.

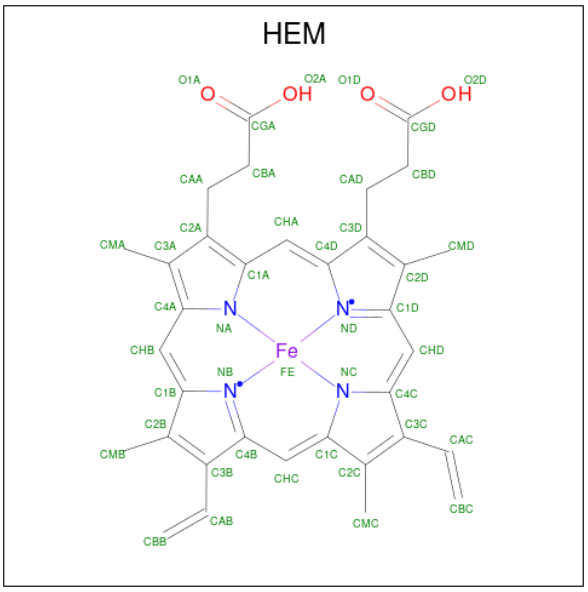


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	J	6	Total C N O 71 40 2 29	0	0	0
4	K	6	Total C N O 71 40 2 29	0	0	0
4	M	6	Total C N O 71 40 2 29	0	0	0
4	N	6	Total C N O 71 40 2 29	0	0	0

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

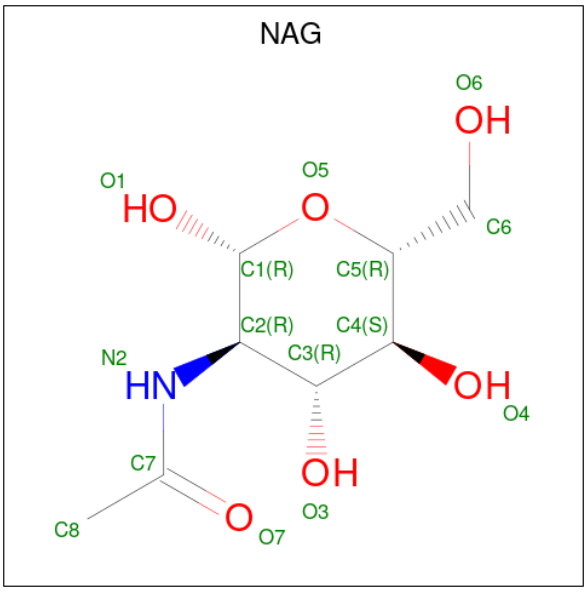
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	I	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: $C_8H_{15}NO_6$).

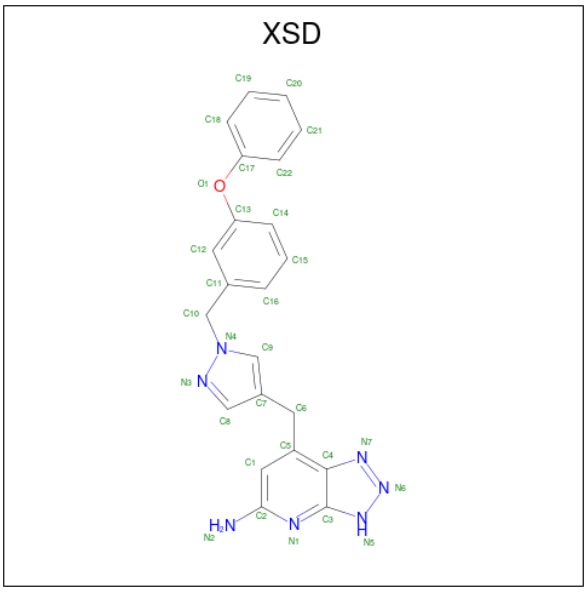


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O 14 8 1 5	0	0
7	E	1	Total C N O 14 8 1 5	0	0
7	G	1	Total C N O 14 8 1 5	0	0
7	I	1	Total C N O 14 8 1 5	0	0
7	I	1	Total C N O 14 8 1 5	0	0

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

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

- Molecule 9 is 7-({1-[(3-phenoxyphenyl)methyl]-1H-pyrazol-4-yl}methyl)-3H-[1,2,3]triazolo[4,5-b]pyridin-5-amine (CCD ID: XSD) (formula: $C_{22}H_{19}N_7O$) (labeled as "Ligand of Interest" by depositor).

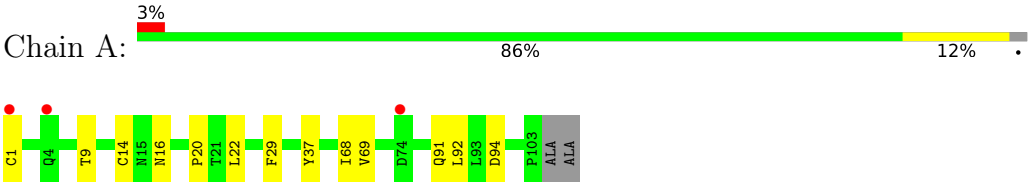


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			30	22	7	1		
9	E	1	Total	C	N	O	0	0
			30	22	7	1		
9	G	1	Total	C	N	O	0	0
			30	22	7	1		
9	I	1	Total	C	N	O	0	0
			30	22	7	1		

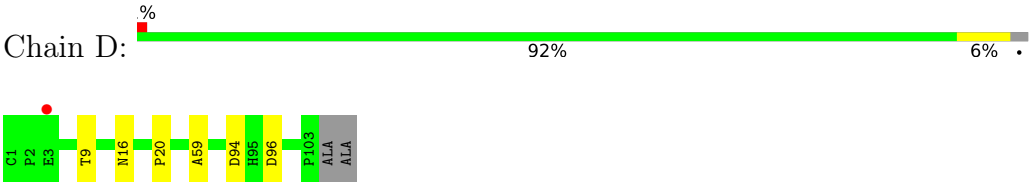
3 Residue-property plots (i)

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.

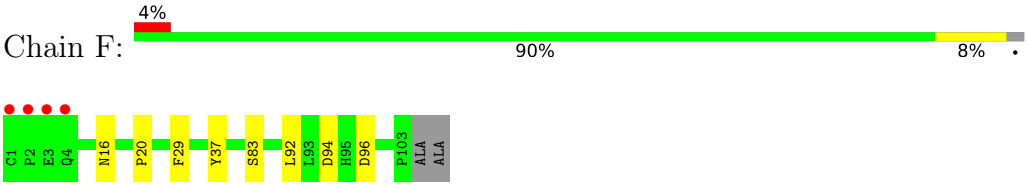
• Molecule 1: Myeloperoxidase light chain



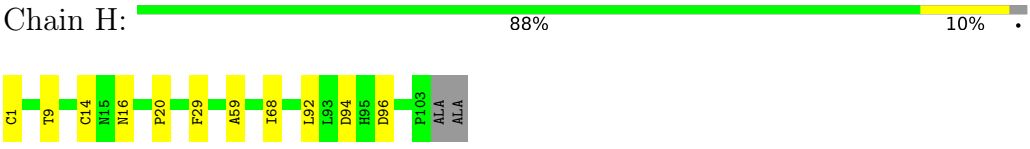
• Molecule 1: Myeloperoxidase light chain



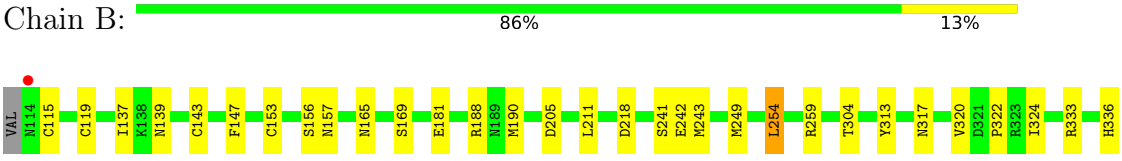
• Molecule 1: Myeloperoxidase light chain

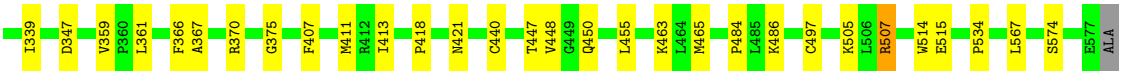


• Molecule 1: Myeloperoxidase light chain



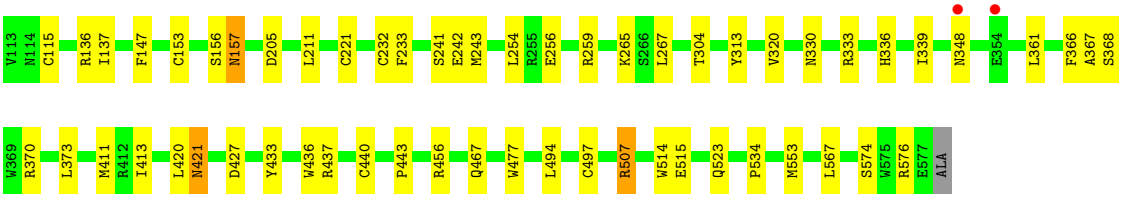
• Molecule 2: Isoform H14 of Myeloperoxidase





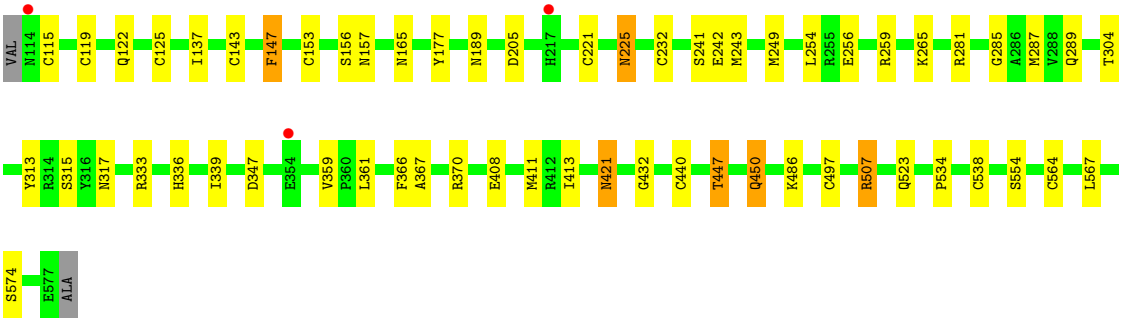
• Molecule 2: Isoform H14 of Myeloperoxidase

Chain E:



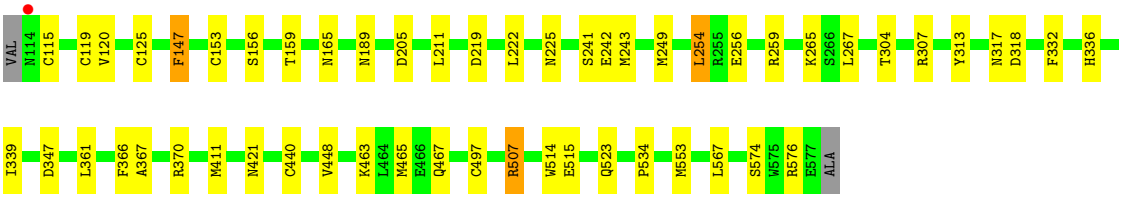
• Molecule 2: Isoform H14 of Myeloperoxidase

Chain G:



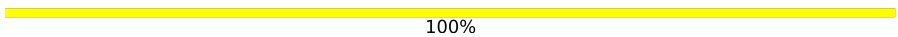
• Molecule 2: Isoform H14 of Myeloperoxidase

Chain I:



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

Chain C:



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

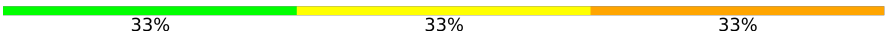
Chain L:

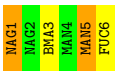
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• 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

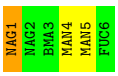
Chain K:





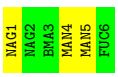
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



• 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 N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	143.46Å 149.89Å 228.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.20 – 2.85 47.20 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.20-2.85) 99.9 (47.20-2.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.193 , 0.235 0.191 , 0.224	Depositor DCC
R_{free} test set	2989 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18458	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MAN, XSD, BMA, HEM, FUC, CL, NAG, CA

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	0.78	0/845	1.20	3/1153 (0.3%)
1	D	0.79	0/839	1.21	2/1145 (0.2%)
1	F	0.80	0/846	1.19	3/1154 (0.3%)
1	H	0.79	0/845	1.20	2/1153 (0.2%)
2	B	0.82	0/3687	1.24	7/5021 (0.1%)
2	E	0.82	0/3721	1.25	8/5064 (0.2%)
2	G	0.84	0/3705	1.24	7/5044 (0.1%)
2	I	0.82	0/3700	1.22	6/5037 (0.1%)
All	All	0.82	0/18188	1.23	38/24771 (0.2%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	157	ASN	CA-CB-CG	6.28	118.88	112.60
1	H	9	THR	N-CA-C	-6.26	102.45	110.53
2	B	407	PHE	CA-C-N	5.95	128.53	120.38
2	B	407	PHE	C-N-CA	5.95	128.53	120.38
2	B	139	ASN	CA-CB-CG	5.81	118.41	112.60
2	I	421	ASN	CA-CB-CG	5.79	118.39	112.60
2	G	225	ASN	N-CA-C	5.64	116.80	107.20
1	A	9	THR	N-CA-C	-5.63	102.94	110.55
2	G	432	GLY	CA-C-N	5.56	128.51	120.79
2	G	432	GLY	C-N-CA	5.56	128.51	120.79
2	E	421	ASN	CA-CB-CG	5.50	118.10	112.60
1	D	96	ASP	N-CA-C	-5.47	106.77	113.50
2	E	420	LEU	CA-C-N	5.45	127.58	120.28
2	E	420	LEU	C-N-CA	5.45	127.58	120.28
2	G	347	ASP	CA-CB-CG	5.45	118.05	112.60
1	F	96	ASP	N-CA-C	-5.44	106.81	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	205	ASP	CA-CB-CG	5.43	118.03	112.60
2	B	205	ASP	CA-CB-CG	5.43	118.03	112.60
1	D	9	THR	N-CA-C	-5.40	103.26	110.55
2	E	205	ASP	CA-CB-CG	5.34	117.94	112.60
2	E	348	ASN	CA-CB-CG	5.34	117.94	112.60
2	B	375	GLY	N-CA-C	5.31	122.65	115.00
2	B	218	ASP	CA-CB-CG	5.30	117.90	112.60
2	B	347	ASP	CA-CB-CG	5.29	117.89	112.60
2	E	427	ASP	CA-CB-CG	5.27	117.87	112.60
1	H	96	ASP	N-CA-C	-5.26	107.03	113.50
2	G	205	ASP	CA-CB-CG	5.19	117.79	112.60
2	I	147	PHE	CA-CB-CG	5.14	118.94	113.80
1	F	37	TYR	CA-C-N	5.14	127.42	120.38
1	F	37	TYR	C-N-CA	5.14	127.42	120.38
2	G	147	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	37	TYR	CA-C-N	5.09	127.36	120.38
1	A	37	TYR	C-N-CA	5.09	127.36	120.38
2	G	421	ASN	CA-CB-CG	5.08	117.68	112.60
2	I	347	ASP	CA-CB-CG	5.07	117.67	112.60
2	I	256	GLU	CB-CG-CD	5.07	121.21	112.60
2	E	256	GLU	CB-CG-CD	5.04	121.17	112.60
2	I	318	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	820	0	774	11	0
1	D	814	0	770	4	0
1	F	821	0	776	6	0
1	H	820	0	774	10	0
2	B	3602	0	3497	44	0
2	E	3636	0	3581	37	0
2	G	3620	0	3550	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	3615	0	3537	44	0
3	C	28	0	25	0	0
3	L	28	0	25	2	0
4	J	71	0	61	5	0
4	K	71	0	61	3	0
4	M	71	0	61	4	0
4	N	71	0	61	5	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
6	B	43	0	30	13	0
6	E	43	0	30	11	0
6	G	43	0	30	9	0
6	I	43	0	30	13	0
7	B	14	0	13	0	0
7	E	14	0	13	4	0
7	G	14	0	13	3	0
7	I	28	0	26	7	0
8	B	1	0	0	0	0
8	E	1	0	0	0	0
8	G	1	0	0	0	0
8	I	1	0	0	0	0
9	B	30	0	0	0	0
9	E	30	0	0	0	0
9	G	30	0	0	0	0
9	I	30	0	0	0	0
All	All	18458	0	17738	194	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 (194) 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:G:317:ASN:HD21	4:M:1:NAG:C1	1.30	1.45
2:I:189:ASN:HD21	7:I:602:NAG:C1	1.30	1.44
2:B:317:ASN:ND2	4:J:1:NAG:C1	1.85	1.39
2:I:317:ASN:HD21	4:N:1:NAG:C1	1.38	1.37
1:D:94:ASP:OD1	6:E:601:HEM:HMD1	1.19	1.32
1:A:94:ASP:OD1	6:B:601:HEM:HMD1	1.26	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:189:ASN:ND2	7:I:602:NAG:C1	2.03	1.20
2:G:317:ASN:ND2	4:M:1:NAG:C1	2.02	1.19
1:F:94:ASP:OD1	6:G:601:HEM:HMD1	1.43	1.19
2:I:317:ASN:ND2	4:N:1:NAG:C1	2.07	1.16
2:I:225:ASN:HD21	7:I:603:NAG:C1	1.64	1.09
2:G:189:ASN:ND2	7:G:602:NAG:C1	2.16	1.08
1:H:94:ASP:OD1	6:I:601:HEM:HMD3	1.52	1.07
2:B:317:ASN:HD21	4:J:1:NAG:C1	1.58	1.04
1:D:94:ASP:OD1	6:E:601:HEM:CMD	2.06	1.03
2:B:242:GLU:OE2	6:B:601:HEM:HMB1	1.59	1.02
2:G:189:ASN:HD21	7:G:602:NAG:C1	1.77	0.97
2:I:242:GLU:OE2	6:I:601:HEM:HMB1	1.63	0.96
2:G:242:GLU:OE2	6:G:601:HEM:HMB1	1.66	0.96
1:A:94:ASP:OD1	6:B:601:HEM:CMD	2.14	0.95
1:H:94:ASP:OD1	6:I:601:HEM:CMD	2.14	0.94
2:I:225:ASN:ND2	7:I:603:NAG:C1	2.33	0.89
6:B:601:HEM:HHC	6:B:601:HEM:HBB2	1.55	0.89
6:I:601:HEM:HBB2	6:I:601:HEM:HHC	1.55	0.88
2:G:440:CYS:HG	2:G:497:CYS:HG	1.09	0.88
2:E:242:GLU:OE2	6:E:601:HEM:HMB1	1.73	0.88
2:E:440:CYS:HG	2:E:497:CYS:HG	1.18	0.84
6:E:601:HEM:HHC	6:E:601:HEM:HBB2	1.61	0.83
6:G:601:HEM:HHC	6:G:601:HEM:HBB2	1.62	0.81
2:G:225:ASN:HD21	3:L:1:NAG:C1	1.92	0.81
1:F:94:ASP:OD1	6:G:601:HEM:CMD	2.28	0.80
2:B:242:GLU:OE2	6:B:601:HEM:CMB	2.30	0.80
2:E:221:CYS:HG	2:E:232:CYS:HG	0.79	0.79
2:G:153:CYS:HG	2:I:153:CYS:HG	0.80	0.78
2:I:440:CYS:HG	2:I:497:CYS:HG	1.18	0.76
2:I:242:GLU:OE2	6:I:601:HEM:CMB	2.33	0.75
7:E:602:NAG:O7	7:E:602:NAG:O3	2.06	0.74
2:G:242:GLU:OE2	6:G:601:HEM:CMB	2.36	0.73
2:B:119:CYS:HG	2:B:143:CYS:HG	0.80	0.72
2:G:256:GLU:HG2	2:G:287:MET:HE1	1.70	0.72
2:G:115:CYS:HG	2:G:125:CYS:HG	0.76	0.72
2:I:317:ASN:CG	4:N:1:NAG:C1	2.62	0.71
2:G:313:TYR:HD1	2:G:507:ARG:HD3	1.54	0.71
2:G:119:CYS:HG	2:G:143:CYS:HG	0.74	0.70
2:B:313:TYR:HD1	2:B:507:ARG:HD3	1.56	0.70
6:E:601:HEM:HBC2	6:E:601:HEM:HMC2	1.72	0.70
2:E:313:TYR:HD1	2:E:507:ARG:HD3	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:317:ASN:CG	4:M:1:NAG:C1	2.66	0.69
2:I:317:ASN:HD21	4:N:1:NAG:C2	2.04	0.69
6:B:601:HEM:HMC1	6:B:601:HEM:HBC2	1.73	0.69
2:I:313:TYR:HD1	2:I:507:ARG:HD3	1.58	0.68
2:B:333:ARG:HH11	2:B:421:ASN:HD22	1.39	0.68
2:G:189:ASN:CG	7:G:602:NAG:C1	2.65	0.68
2:E:243:MET:SD	6:E:601:HEM:CBB	2.82	0.67
2:E:333:ARG:HH11	2:E:421:ASN:HD22	1.40	0.67
2:G:317:ASN:HD21	4:M:1:NAG:C2	2.07	0.66
2:B:243:MET:SD	6:B:601:HEM:CBB	2.83	0.66
2:B:317:ASN:HD22	4:J:1:NAG:C1	2.02	0.66
2:E:242:GLU:OE2	6:E:601:HEM:CMB	2.43	0.66
2:B:243:MET:SD	6:B:601:HEM:HBB1	2.36	0.65
2:E:243:MET:SD	6:E:601:HEM:HBB1	2.35	0.65
2:I:243:MET:SD	6:I:601:HEM:CBB	2.85	0.65
1:H:94:ASP:CG	6:I:601:HEM:HMD3	2.22	0.64
2:B:440:CYS:HG	2:B:497:CYS:CB	2.11	0.63
2:I:225:ASN:HD21	7:I:603:NAG:C2	2.11	0.63
2:I:189:ASN:CG	7:I:602:NAG:C1	2.73	0.61
2:I:243:MET:SD	6:I:601:HEM:HBB1	2.41	0.61
2:I:115:CYS:HG	2:I:125:CYS:HG	0.62	0.60
2:E:333:ARG:HH11	2:E:421:ASN:ND2	2.00	0.60
6:G:601:HEM:HMC1	6:G:601:HEM:HBC2	1.84	0.60
2:B:313:TYR:CD1	2:B:507:ARG:HD3	2.36	0.59
2:G:333:ARG:HH11	2:G:421:ASN:ND2	2.00	0.59
2:B:169:SER:HB2	2:B:324:ILE:HG12	1.84	0.59
2:G:221:CYS:CB	2:G:232:CYS:HG	2.14	0.59
2:I:313:TYR:CD1	2:I:507:ARG:HD3	2.38	0.59
2:G:256:GLU:CG	2:G:287:MET:HE1	2.32	0.58
2:E:313:TYR:CD1	2:E:507:ARG:HD3	2.37	0.58
2:B:317:ASN:ND2	4:J:1:NAG:O5	2.36	0.57
2:G:313:TYR:CD1	2:G:507:ARG:HD3	2.38	0.57
2:E:373:LEU:HD13	7:E:602:NAG:H62	1.86	0.57
2:B:440:CYS:HG	2:B:497:CYS:HB3	1.69	0.57
2:E:221:CYS:CB	2:E:232:CYS:HG	2.17	0.56
2:B:333:ARG:HH11	2:B:421:ASN:ND2	2.01	0.56
2:G:447:THR:HG22	2:G:450:GLN:H	1.70	0.56
7:E:602:NAG:HO3	7:E:602:NAG:C7	2.19	0.56
2:G:333:ARG:HH11	2:G:421:ASN:HD22	1.53	0.55
2:E:456:ARG:HG2	2:I:119:CYS:SG	2.47	0.55
2:G:243:MET:SD	6:G:601:HEM:CBB	2.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:336:HIS:HA	2:E:339:ILE:HD12	1.88	0.54
2:G:336:HIS:HA	2:G:339:ILE:HD12	1.88	0.54
2:I:336:HIS:HA	2:I:339:ILE:HD12	1.88	0.54
2:I:156:SER:HB3	2:I:159:THR:HG22	1.90	0.54
2:B:336:HIS:HA	2:B:339:ILE:HD12	1.89	0.53
1:H:29:PHE:CE1	2:I:165:ASN:HB2	2.44	0.52
6:B:601:HEM:HBC2	6:B:601:HEM:CMC	2.39	0.52
2:E:136:ARG:HG2	2:E:137:ILE:HG13	1.92	0.52
1:A:68:ILE:HD12	2:B:463:LYS:HB3	1.92	0.52
1:A:94:ASP:CG	6:B:601:HEM:HMD1	2.24	0.52
2:B:153:CYS:CB	2:E:153:CYS:HG	2.21	0.51
2:I:211:LEU:HD23	2:I:254:LEU:HD22	1.91	0.51
2:B:505:LYS:NZ	4:K:5:MAN:H61	2.25	0.51
2:B:243:MET:SD	6:B:601:HEM:CAB	2.99	0.51
2:B:447:THR:HG22	2:B:450:GLN:HG3	1.94	0.50
2:I:332:PHE:O	6:I:601:HEM:HAC	2.11	0.50
2:I:440:CYS:CB	2:I:497:CYS:HG	2.24	0.50
2:B:447:THR:HG22	2:B:450:GLN:HE21	1.77	0.49
2:E:440:CYS:CB	2:E:497:CYS:HG	2.24	0.49
2:I:243:MET:SD	6:I:601:HEM:CAB	3.01	0.49
2:I:448:VAL:HB	2:I:465:MET:HG3	1.95	0.48
2:E:241:SER:O	2:E:366:PHE:HA	2.13	0.48
6:G:601:HEM:HBC2	6:G:601:HEM:CMC	2.43	0.48
2:I:241:SER:O	2:I:366:PHE:HA	2.13	0.48
2:G:241:SER:O	2:G:366:PHE:HA	2.13	0.48
2:E:320:VAL:HG22	4:K:1:NAG:H62	1.95	0.48
2:B:211:LEU:HD23	2:B:254:LEU:HD22	1.95	0.48
2:B:241:SER:O	2:B:366:PHE:HA	2.13	0.48
2:E:373:LEU:HD13	7:E:602:NAG:C6	2.44	0.48
2:E:514:TRP:CE2	2:E:515:GLU:HG3	2.49	0.48
1:A:29:PHE:CE1	2:B:165:ASN:HB2	2.49	0.47
2:B:317:ASN:CG	4:J:1:NAG:C1	2.74	0.47
1:H:16:ASN:O	1:H:20:PRO:HA	2.14	0.47
6:E:601:HEM:HBC2	6:E:601:HEM:CMC	2.42	0.47
2:I:317:ASN:OD1	4:N:1:NAG:C1	2.61	0.47
1:H:94:ASP:OD1	6:I:601:HEM:HMD2	2.09	0.47
1:A:69:VAL:HG11	2:B:418:PRO:HG2	1.97	0.47
1:F:92:LEU:HD22	2:G:249:MET:HB3	1.97	0.46
1:H:68:ILE:CD1	2:I:463:LYS:HB3	2.46	0.46
2:E:243:MET:SD	6:E:601:HEM:CAB	3.04	0.46
2:G:243:MET:SD	6:G:601:HEM:HBB1	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:514:TRP:CE2	2:B:515:GLU:HG3	2.51	0.46
1:A:22:LEU:HB3	2:B:322:PRO:HD2	1.98	0.46
2:E:233:PHE:CE2	2:E:368:SER:HB2	2.51	0.46
1:H:59:ALA:HB2	2:I:467:GLN:O	2.16	0.46
1:F:16:ASN:O	1:F:20:PRO:HA	2.16	0.46
2:G:177:TYR:CE2	2:G:281:ARG:HG3	2.51	0.46
2:E:443:PRO:HG2	2:I:120:VAL:HG11	1.97	0.45
6:I:601:HEM:HBC2	6:I:601:HEM:CMC	2.46	0.45
2:E:211:LEU:HD23	2:E:254:LEU:HD22	1.98	0.45
2:B:333:ARG:NH2	6:B:601:HEM:HAD1	2.32	0.45
1:A:91:GLN:HB2	6:B:601:HEM:HMC3	1.97	0.45
2:B:455:LEU:HA	2:B:484:PRO:HD3	1.99	0.45
2:E:330:ASN:OD1	2:E:477:TRP:HB2	2.17	0.45
1:D:16:ASN:O	1:D:20:PRO:HA	2.16	0.45
1:F:83:SER:HB3	2:G:554:SER:O	2.17	0.45
1:A:16:ASN:O	1:A:20:PRO:HA	2.17	0.45
2:E:115:CYS:HB2	2:E:147:PHE:CE1	2.52	0.45
2:B:367:ALA:HB1	2:B:370:ARG:HG3	1.98	0.45
2:I:219:ASP:HB3	2:I:222:LEU:HD12	1.98	0.45
2:B:505:LYS:HZ2	4:K:5:MAN:H61	1.82	0.44
2:B:448:VAL:HB	2:B:465:MET:HG3	1.99	0.44
2:G:225:ASN:ND2	3:L:1:NAG:C1	2.71	0.44
2:E:367:ALA:HB1	2:E:370:ARG:HG3	1.98	0.44
2:I:514:TRP:CE2	2:I:515:GLU:HG3	2.53	0.44
2:E:433:TYR:CZ	2:E:437:ARG:HD3	2.52	0.44
1:A:92:LEU:HD22	2:B:249:MET:HB3	1.99	0.44
2:G:534:PRO:HB2	2:G:567:LEU:HD21	1.99	0.44
2:I:156:SER:CB	2:I:159:THR:HG22	2.48	0.44
2:G:367:ALA:HB1	2:G:370:ARG:HG3	1.98	0.44
2:G:538:CYS:CB	2:G:564:CYS:HG	2.26	0.44
2:B:534:PRO:HB2	2:B:567:LEU:HD21	2.00	0.43
2:B:115:CYS:HB2	2:B:147:PHE:CE1	2.53	0.43
2:E:330:ASN:HA	2:E:333:ARG:HD2	2.00	0.43
2:I:367:ALA:HB1	2:I:370:ARG:HG3	2.00	0.43
2:G:285:GLY:O	2:G:289:GLN:HG3	2.19	0.43
2:G:153:CYS:SG	2:G:156:SER:HB2	2.58	0.43
2:G:115:CYS:HB2	2:G:147:PHE:CE1	2.53	0.43
2:E:534:PRO:HB2	2:E:567:LEU:HD21	2.01	0.43
2:B:333:ARG:NH1	2:B:421:ASN:HD22	2.13	0.42
2:I:115:CYS:HB2	2:I:147:PHE:CE1	2.53	0.42
1:A:1:CYS:SG	1:A:14:CYS:SG	3.13	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:440:CYS:HG	2:G:497:CYS:CB	2.30	0.42
2:G:137:ILE:HG12	2:G:413:ILE:HD11	2.01	0.42
6:I:601:HEM:HBC2	6:I:601:HEM:HMC1	2.02	0.42
2:E:137:ILE:HG12	2:E:413:ILE:HD11	2.01	0.42
2:B:137:ILE:HG12	2:B:413:ILE:HD11	2.01	0.42
1:F:29:PHE:CE1	2:G:165:ASN:HB2	2.55	0.42
1:D:59:ALA:HB2	2:E:467:GLN:O	2.20	0.41
2:G:440:CYS:CB	2:G:497:CYS:HG	2.31	0.41
1:H:92:LEU:HD22	2:I:249:MET:HB3	2.02	0.41
6:E:601:HEM:HBB2	6:E:601:HEM:CHC	2.36	0.41
2:E:153:CYS:SG	2:E:156:SER:HB2	2.61	0.41
2:E:267:LEU:HD22	2:E:576:ARG:HB2	2.03	0.41
2:I:225:ASN:CG	7:I:603:NAG:C1	2.93	0.41
2:E:436:TRP:HB3	2:E:494:LEU:HD11	2.02	0.41
2:E:333:ARG:NH1	2:E:421:ASN:HD22	2.14	0.41
2:B:188:ARG:HB2	2:B:190:MET:HE2	2.03	0.41
1:H:1:CYS:SG	1:H:14:CYS:SG	3.13	0.41
2:I:267:LEU:HD22	2:I:576:ARG:HB2	2.03	0.41
2:I:153:CYS:HB3	2:I:159:THR:HG21	2.03	0.41
2:I:534:PRO:HB2	2:I:567:LEU:HD21	2.02	0.40
2:B:317:ASN:HD22	2:B:320:VAL:HG23	1.86	0.40
2:G:153:CYS:HG	2:I:153:CYS:CB	2.31	0.40
2:B:119:CYS:HG	2:B:143:CYS:CB	2.32	0.40
2:B:153:CYS:SG	2:B:156:SER:HB2	2.62	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	101/105 (96%)	100 (99%)	1 (1%)	0	100	100
1	F	101/105 (96%)	100 (99%)	1 (1%)	0	100	100
1	H	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
2	B	462/466 (99%)	454 (98%)	8 (2%)	0	100	100
2	E	463/466 (99%)	453 (98%)	10 (2%)	0	100	100
2	G	462/466 (99%)	449 (97%)	13 (3%)	0	100	100
2	I	462/466 (99%)	452 (98%)	10 (2%)	0	100	100
All	All	2253/2284 (99%)	2206 (98%)	47 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	87/90 (97%)	87 (100%)	0	100	100
1	D	85/90 (94%)	85 (100%)	0	100	100
1	F	87/90 (97%)	87 (100%)	0	100	100
1	H	87/90 (97%)	87 (100%)	0	100	100
2	B	380/411 (92%)	369 (97%)	11 (3%)	37	61
2	E	390/411 (95%)	380 (97%)	10 (3%)	40	65
2	G	386/411 (94%)	369 (96%)	17 (4%)	25	49
2	I	383/411 (93%)	372 (97%)	11 (3%)	37	61
All	All	1885/2004 (94%)	1836 (97%)	49 (3%)	40	65

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	157	ASN
2	B	181	GLU

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Mol	Chain	Res	Type
2	B	254	LEU
2	B	259	ARG
2	B	304	THR
2	B	359	VAL
2	B	361	LEU
2	B	411	MET
2	B	486	LYS
2	B	507	ARG
2	B	574	SER
2	E	157	ASN
2	E	259	ARG
2	E	265	LYS
2	E	304	THR
2	E	361	LEU
2	E	411	MET
2	E	507	ARG
2	E	523	GLN
2	E	553	MET
2	E	574	SER
2	G	122	GLN
2	G	157	ASN
2	G	254	LEU
2	G	259	ARG
2	G	265	LYS
2	G	304	THR
2	G	315	SER
2	G	359	VAL
2	G	361	LEU
2	G	408	GLU
2	G	411	MET
2	G	447	THR
2	G	450	GLN
2	G	486	LYS
2	G	507	ARG
2	G	523	GLN
2	G	574	SER
2	I	254	LEU
2	I	259	ARG
2	I	265	LYS
2	I	304	THR
2	I	307	ARG
2	I	361	LEU

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Mol	Chain	Res	Type
2	I	411	MET
2	I	507	ARG
2	I	523	GLN
2	I	553	MET
2	I	574	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	121	GLN
2	B	186	ASN
2	B	317	ASN
2	B	421	ASN
2	B	450	GLN
2	B	467	GLN
2	B	540	ASN
2	B	571	ASN
2	E	421	ASN
2	E	467	GLN
2	E	516	ASN
2	E	540	ASN
2	E	563	ASN
2	G	434	ASN
2	G	472	ASN
2	G	540	ASN
1	H	95	HIS
2	I	189	ASN
2	I	225	ASN
2	I	540	ASN
2	I	571	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 (i)

28 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	2,3	14,14,15	1.66	4 (28%)	17,19,21	2.36	6 (35%)
3	NAG	C	2	3	14,14,15	0.79	0	17,19,21	1.15	1 (5%)
4	NAG	J	1	4	14,14,15	0.33	0	17,19,21	0.75	1 (5%)
4	NAG	J	2	4	14,14,15	1.57	3 (21%)	17,19,21	2.15	4 (23%)
4	BMA	J	3	4	11,11,12	1.25	1 (9%)	15,15,17	1.55	5 (33%)
4	MAN	J	4	4	11,11,12	0.90	1 (9%)	15,15,17	1.73	3 (20%)
4	MAN	J	5	4	11,11,12	1.26	1 (9%)	15,15,17	1.50	2 (13%)
4	FUC	J	6	4	10,10,11	1.12	0	14,14,16	1.50	2 (14%)
4	NAG	K	1	2,4	14,14,15	1.24	1 (7%)	17,19,21	4.13	6 (35%)
4	NAG	K	2	4	14,14,15	0.28	0	17,19,21	0.53	0
4	BMA	K	3	4	11,11,12	0.59	0	15,15,17	1.23	3 (20%)
4	MAN	K	4	4	11,11,12	0.38	0	15,15,17	0.75	0
4	MAN	K	5	4	11,11,12	0.44	0	15,15,17	0.83	1 (6%)
4	FUC	K	6	4	10,10,11	0.41	0	14,14,16	0.74	1 (7%)
3	NAG	L	1	3	14,14,15	0.30	0	17,19,21	1.14	2 (11%)
3	NAG	L	2	3	14,14,15	0.28	0	17,19,21	0.62	0
4	NAG	M	1	4	14,14,15	0.40	0	17,19,21	1.08	1 (5%)
4	NAG	M	2	4	14,14,15	0.39	0	17,19,21	0.65	0
4	BMA	M	3	4	11,11,12	0.43	0	15,15,17	0.66	0
4	MAN	M	4	4	11,11,12	0.30	0	15,15,17	0.89	1 (6%)
4	MAN	M	5	4	11,11,12	0.30	0	15,15,17	0.98	1 (6%)
4	FUC	M	6	4	10,10,11	0.34	0	14,14,16	0.47	0
4	NAG	N	1	4	14,14,15	0.29	0	17,19,21	0.70	0
4	NAG	N	2	4	14,14,15	0.30	0	17,19,21	0.49	0
4	BMA	N	3	4	11,11,12	0.27	0	15,15,17	0.67	0
4	MAN	N	4	4	11,11,12	0.31	0	15,15,17	1.11	1 (6%)
4	MAN	N	5	4	11,11,12	0.37	0	15,15,17	0.78	1 (6%)
4	FUC	N	6	4	10,10,11	0.37	0	14,14,16	0.62	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	2,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
4	NAG	J	1	4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	2/2/19/22	0/1/1/1
4	MAN	J	5	4	-	2/2/19/22	0/1/1/1
4	FUC	J	6	4	-	-	0/1/1/1
4	NAG	K	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	1/2/19/22	0/1/1/1
4	MAN	K	4	4	-	2/2/19/22	0/1/1/1
4	MAN	K	5	4	-	2/2/19/22	0/1/1/1
4	FUC	K	6	4	-	-	0/1/1/1
3	NAG	L	1	3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
4	NAG	M	1	4	-	1/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
4	MAN	M	4	4	-	1/2/19/22	0/1/1/1
4	MAN	M	5	4	-	0/2/19/22	0/1/1/1
4	FUC	M	6	4	-	-	0/1/1/1
4	NAG	N	1	4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	BMA	N	3	4	-	0/2/19/22	0/1/1/1
4	MAN	N	4	4	-	1/2/19/22	0/1/1/1
4	MAN	N	5	4	-	0/2/19/22	0/1/1/1
4	FUC	N	6	4	-	-	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	O5-C1	-3.51	1.37	1.43
4	J	2	NAG	O5-C1	-3.28	1.38	1.43
4	J	3	BMA	O5-C1	-2.94	1.38	1.43
4	J	5	MAN	O5-C1	-2.73	1.39	1.43
3	C	1	NAG	C1-C2	-2.61	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	O5-C5	-2.58	1.38	1.43
4	K	1	NAG	O4-C4	2.50	1.49	1.43
4	J	2	NAG	C2-N2	-2.49	1.42	1.46
4	J	4	MAN	O5-C1	-2.21	1.40	1.43
4	J	2	NAG	O7-C7	-2.21	1.18	1.23
3	C	1	NAG	C2-N2	-2.09	1.42	1.46

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	1	NAG	O5-C1-C2	-10.65	94.81	111.29
4	K	1	NAG	C1-O5-C5	10.63	126.43	112.19
4	J	2	NAG	C1-O5-C5	5.82	119.99	112.19
3	C	1	NAG	C1-O5-C5	-5.78	104.44	112.19
4	K	1	NAG	C4-C3-C2	5.45	119.01	111.02
4	J	2	NAG	O5-C1-C2	-4.76	103.92	111.29
3	C	1	NAG	C1-C2-N2	-4.61	103.17	110.43
4	J	5	MAN	C1-O5-C5	4.03	117.58	112.19
4	N	4	MAN	C1-O5-C5	3.95	117.49	112.19
4	J	6	FUC	O5-C1-C2	-3.74	101.87	110.79
4	M	1	NAG	O5-C1-C2	-3.63	105.67	111.29
4	J	4	MAN	C1-O5-C5	3.62	117.04	112.19
3	C	1	NAG	O5-C1-C2	-3.58	105.75	111.29
4	M	5	MAN	C1-O5-C5	3.48	116.85	112.19
4	K	1	NAG	C3-C4-C5	-3.48	103.92	110.23
3	L	1	NAG	O5-C1-C2	-3.37	106.08	111.29
4	J	5	MAN	O4-C4-C3	-3.25	102.72	110.38
3	C	2	NAG	O5-C1-C2	-3.18	106.38	111.29
4	M	4	MAN	C1-O5-C5	3.17	116.43	112.19
4	J	4	MAN	C2-C3-C4	-3.16	105.30	110.86
3	C	1	NAG	O4-C4-C5	-2.88	102.23	109.32
4	K	3	BMA	C1-O5-C5	2.81	115.96	112.19
4	J	3	BMA	O5-C1-C2	-2.81	104.10	110.79
4	J	3	BMA	O5-C5-C4	-2.73	104.19	110.83
4	N	5	MAN	C1-O5-C5	2.72	115.83	112.19
4	K	1	NAG	C2-N2-C7	-2.66	119.33	122.90
4	J	4	MAN	O4-C4-C3	-2.62	104.20	110.38
3	L	1	NAG	C1-C2-N2	-2.58	106.36	110.43
4	J	3	BMA	C1-O5-C5	2.48	115.51	112.19
4	K	3	BMA	C1-C2-C3	2.43	113.18	109.64
4	K	6	FUC	C1-O5-C5	2.35	118.51	112.97
4	K	5	MAN	C1-O5-C5	2.21	115.15	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	2	NAG	C3-C4-C5	-2.20	106.25	110.23
4	K	1	NAG	O4-C4-C5	2.17	114.68	109.32
4	J	3	BMA	O5-C5-C6	-2.16	103.45	107.66
4	J	6	FUC	C6-C5-C4	-2.14	109.16	113.08
4	J	2	NAG	C6-C5-C4	-2.13	107.79	113.02
4	J	1	NAG	O5-C1-C2	-2.13	108.00	111.29
3	C	1	NAG	C3-C4-C5	-2.12	106.39	110.23
3	C	1	NAG	O3-C3-C2	-2.12	105.00	109.40
4	J	3	BMA	O4-C4-C3	-2.11	105.41	110.38
4	K	3	BMA	O5-C5-C6	-2.00	103.77	107.66

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	J	4	MAN	C4-C5-C6-O6
4	J	4	MAN	O5-C5-C6-O6
4	K	5	MAN	C4-C5-C6-O6
4	K	5	MAN	O5-C5-C6-O6
4	K	4	MAN	O5-C5-C6-O6
4	J	5	MAN	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	J	5	MAN	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	M	4	MAN	O5-C5-C6-O6
4	N	4	MAN	O5-C5-C6-O6
4	K	3	BMA	C4-C5-C6-O6
4	K	4	MAN	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	5	MAN	2	0
4	N	1	NAG	5	0
3	L	1	NAG	2	0
4	K	1	NAG	1	0

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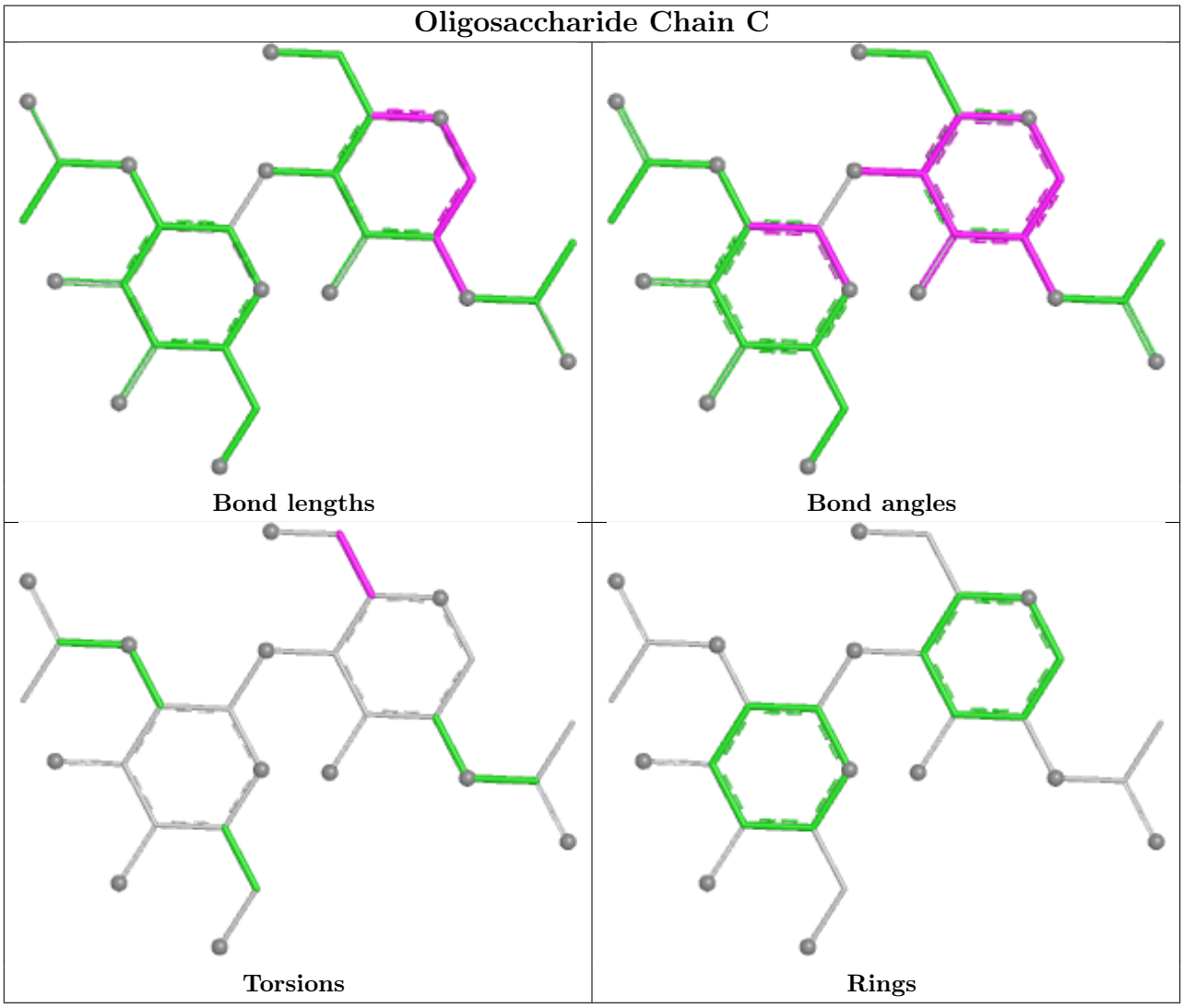
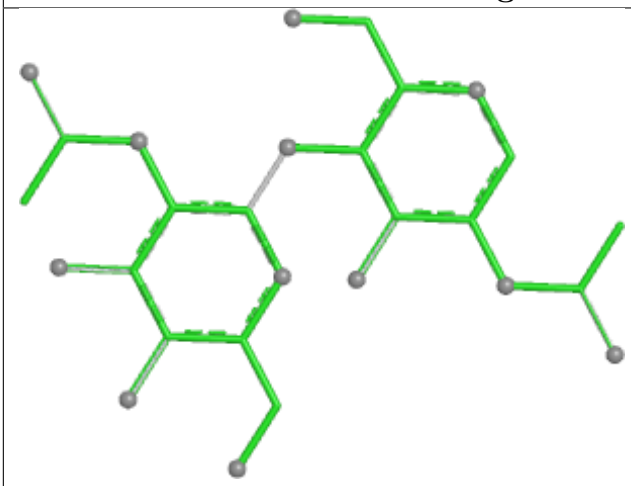
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	1	NAG	4	0
4	J	1	NAG	5	0

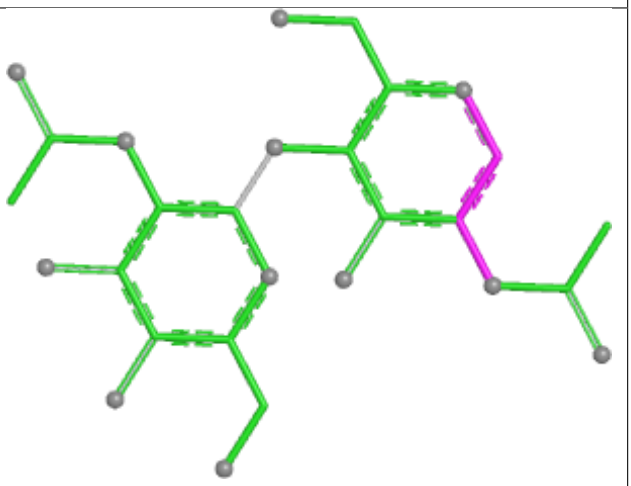
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



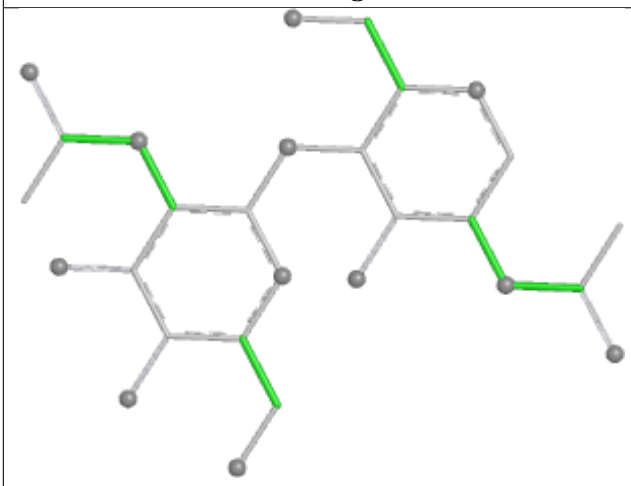
Oligosaccharide Chain L



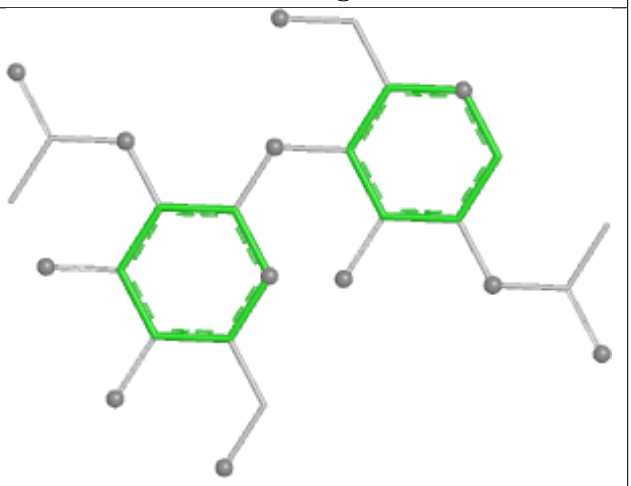
Bond lengths



Bond angles

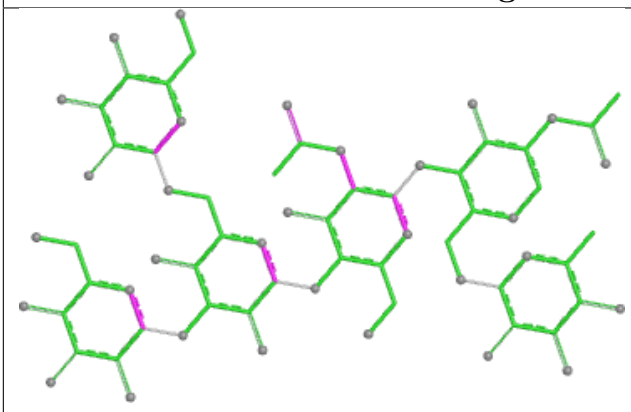


Torsions

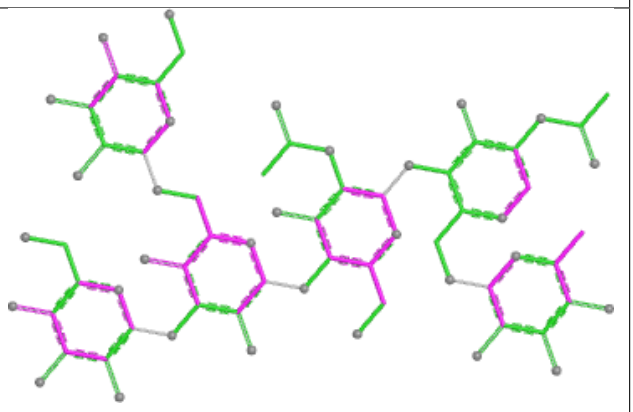


Rings

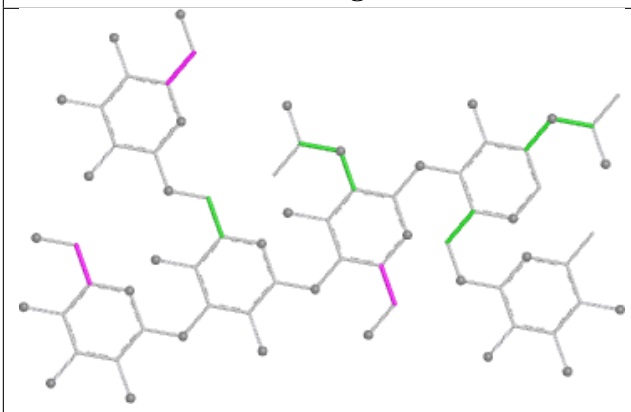
Oligosaccharide Chain J



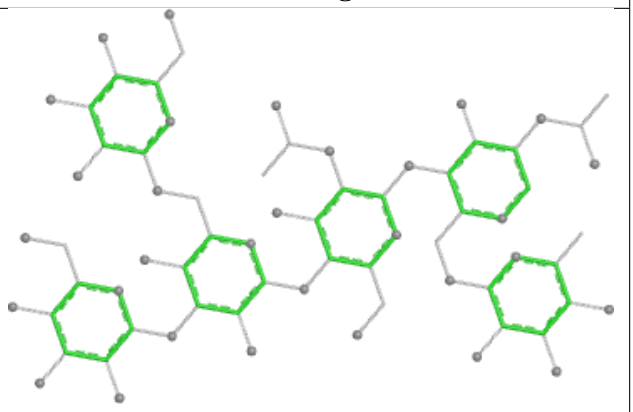
Bond lengths



Bond angles

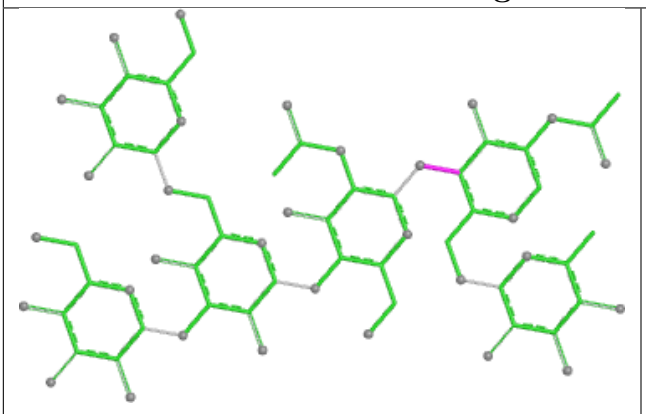


Torsions

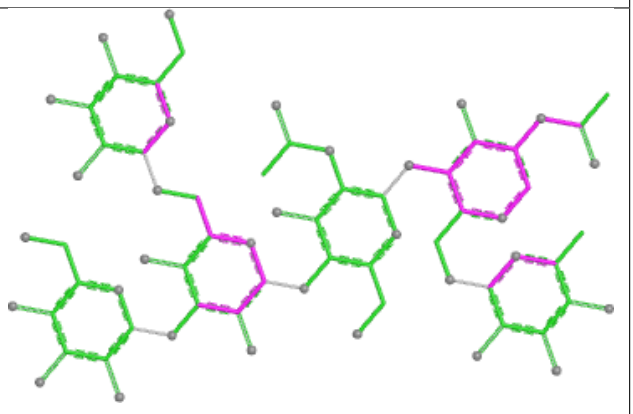


Rings

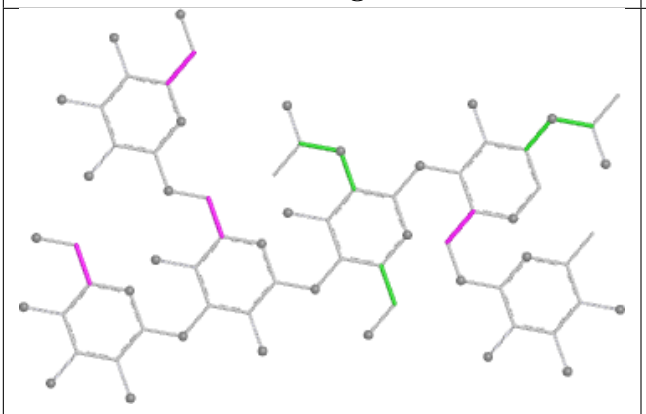
Oligosaccharide Chain K



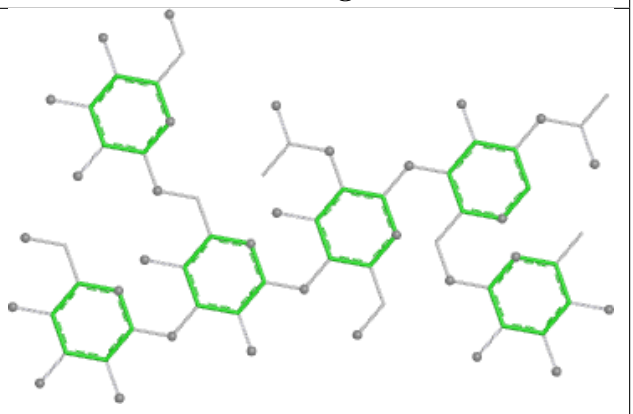
Bond lengths



Bond angles

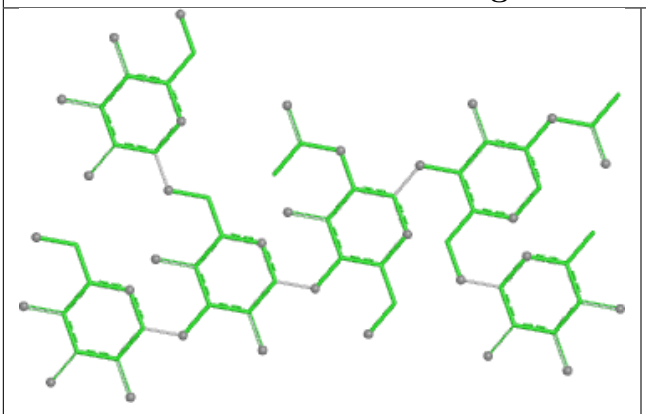


Torsions

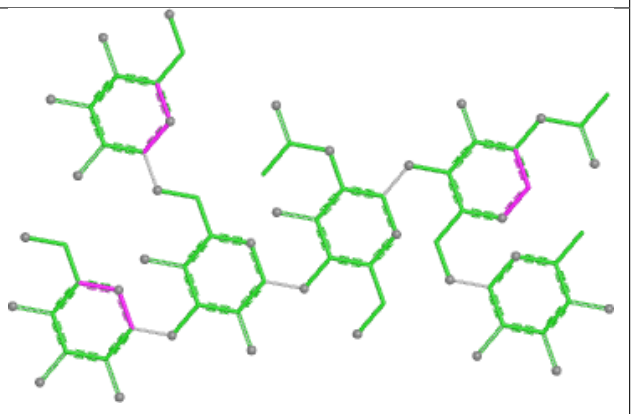


Rings

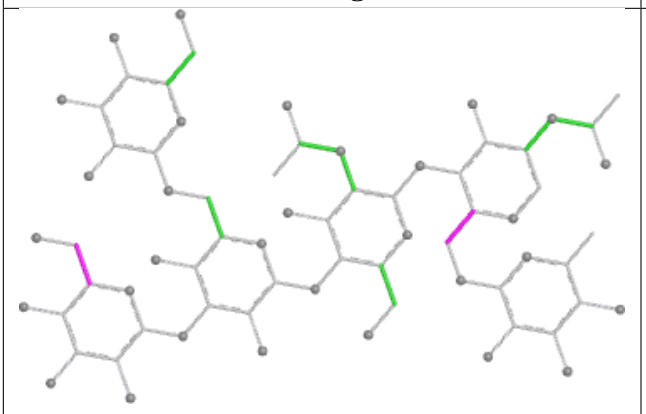
Oligosaccharide Chain M



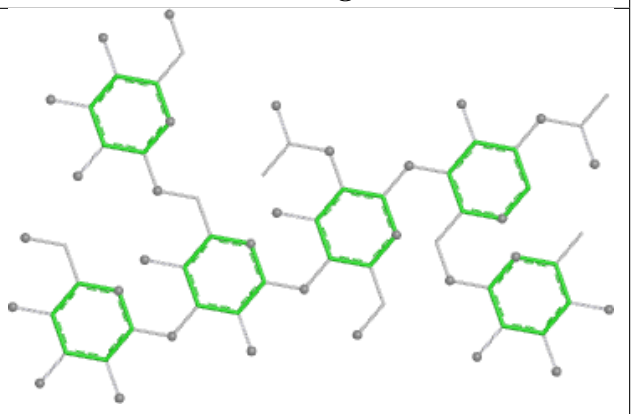
Bond lengths



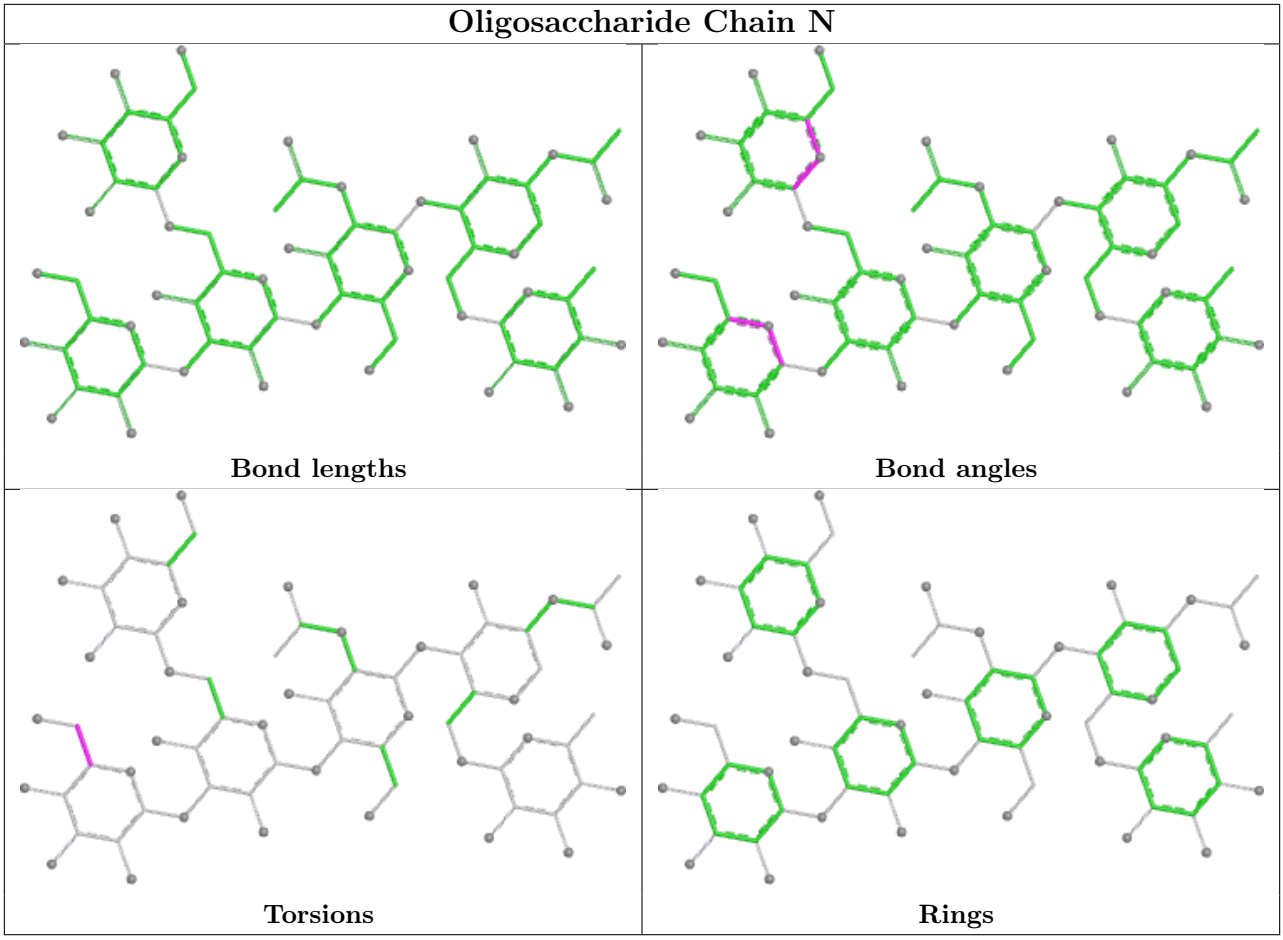
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
9	XSD	E	604	-	34,34,34	1.87	2 (5%)	41,47,47	2.01	5 (12%)
7	NAG	B	602	2	14,14,15	1.00	1 (7%)	17,19,21	1.68	3 (17%)
7	NAG	E	602	2	14,14,15	0.58	0	17,19,21	1.76	5 (29%)
9	XSD	G	605	-	34,34,34	1.36	1 (2%)	41,47,47	1.91	4 (9%)
7	NAG	I	603	-	14,14,15	0.26	0	17,19,21	0.76	1 (5%)
6	HEM	E	601	2	50,50,50	1.40	7 (14%)	67,82,82	1.70	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	G	602	-	14,14,15	0.30	0	17,19,21	0.83	1 (5%)
6	HEM	I	601	2	50,50,50	1.21	7 (14%)	67,82,82	1.69	18 (26%)
6	HEM	B	601	2	50,50,50	1.34	7 (14%)	67,82,82	1.65	18 (26%)
9	XSD	I	605	-	34,34,34	1.46	2 (5%)	41,47,47	2.11	5 (12%)
9	XSD	B	605	-	34,34,34	2.09	2 (5%)	41,47,47	2.03	4 (9%)
6	HEM	G	601	2	50,50,50	1.43	7 (14%)	67,82,82	1.77	19 (28%)
7	NAG	I	602	-	14,14,15	0.29	0	17,19,21	0.84	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	XSD	E	604	-	-	1/12/12/12	0/5/5/5
7	NAG	B	602	2	-	2/6/23/26	0/1/1/1
7	NAG	E	602	2	-	3/6/23/26	0/1/1/1
9	XSD	G	605	-	-	1/12/12/12	0/5/5/5
7	NAG	I	603	-	-	0/6/23/26	0/1/1/1
6	HEM	E	601	2	-	5/14/54/54	-
7	NAG	G	602	-	-	0/6/23/26	0/1/1/1
6	HEM	I	601	2	-	5/14/54/54	-
6	HEM	B	601	2	-	5/14/54/54	-
9	XSD	I	605	-	-	0/12/12/12	0/5/5/5
9	XSD	B	605	-	-	0/12/12/12	0/5/5/5
6	HEM	G	601	2	-	5/14/54/54	-
7	NAG	I	602	-	-	0/6/23/26	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	605	XSD	C3-N5	11.72	1.44	1.35
9	E	604	XSD	C3-N5	9.84	1.42	1.35
9	I	605	XSD	C3-N5	7.79	1.41	1.35
9	G	605	XSD	C3-N5	7.33	1.40	1.35
6	B	601	HEM	C1B-NB	-3.76	1.33	1.40
6	E	601	HEM	C1B-NB	-3.70	1.33	1.40
6	E	601	HEM	C3B-C2B	-3.57	1.29	1.37
9	E	604	XSD	C4-N7	3.47	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	601	HEM	C4D-ND	-3.46	1.34	1.40
6	B	601	HEM	C4D-ND	-3.27	1.34	1.40
6	G	601	HEM	C1B-NB	-3.06	1.34	1.40
6	G	601	HEM	C3C-C2C	3.02	1.43	1.37
6	G	601	HEM	C3B-C2B	-2.96	1.31	1.37
6	E	601	HEM	CHA-C1A	-2.93	1.32	1.39
6	I	601	HEM	C2A-C3A	-2.86	1.31	1.38
6	B	601	HEM	CHA-C1A	-2.77	1.33	1.39
6	B	601	HEM	C1D-ND	-2.59	1.33	1.38
6	E	601	HEM	C4B-NB	-2.53	1.33	1.38
6	G	601	HEM	C1A-C2A	-2.51	1.39	1.44
6	G	601	HEM	CHA-C1A	-2.50	1.33	1.39
9	B	605	XSD	C4-N7	2.49	1.43	1.38
6	E	601	HEM	C1A-C2A	-2.49	1.39	1.44
6	G	601	HEM	C3B-C4B	2.48	1.49	1.44
6	E	601	HEM	C4D-ND	-2.44	1.36	1.40
9	I	605	XSD	C4-N7	2.40	1.43	1.38
6	I	601	HEM	C1B-NB	-2.32	1.36	1.40
6	I	601	HEM	C3D-C2D	-2.31	1.31	1.36
6	I	601	HEM	C1D-ND	-2.25	1.34	1.38
6	B	601	HEM	CHB-C4A	-2.17	1.34	1.39
6	E	601	HEM	O2A-CGA	2.16	1.37	1.30
6	B	601	HEM	CBA-CGA	2.14	1.55	1.50
6	I	601	HEM	CHA-C1A	-2.09	1.34	1.39
6	I	601	HEM	C1D-C2D	2.08	1.48	1.44
6	I	601	HEM	C3B-C4B	2.07	1.48	1.44
6	B	601	HEM	C3B-C2B	-2.07	1.33	1.37
7	B	602	NAG	C2-N2	-2.02	1.42	1.46

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	605	XSD	C3-N5-N6	-10.21	105.52	111.18
9	B	605	XSD	C3-N5-N6	-8.94	106.22	111.18
9	E	604	XSD	C3-N5-N6	-8.59	106.41	111.18
9	G	605	XSD	C3-N5-N6	-8.34	106.56	111.18
9	B	605	XSD	N5-C3-N1	7.21	131.57	125.64
9	E	604	XSD	N5-C3-N1	7.12	131.51	125.64
9	G	605	XSD	N5-C3-N1	6.94	131.36	125.64
9	I	605	XSD	N5-C3-N1	6.06	130.63	125.64
9	I	605	XSD	C4-C3-N1	-4.45	122.18	126.55
9	B	605	XSD	C4-C3-N1	-4.39	122.25	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	604	XSD	C4-C3-N1	-4.18	122.45	126.55
6	G	601	HEM	CHA-C4D-C3D	-4.14	117.60	125.23
9	G	605	XSD	C4-C3-N1	-4.10	122.53	126.55
6	B	601	HEM	CHA-C4D-ND	4.04	129.36	124.37
6	E	601	HEM	CHA-C4D-ND	4.00	129.32	124.37
7	B	602	NAG	O5-C1-C2	-3.98	105.13	111.29
6	B	601	HEM	CHA-C4D-C3D	-3.97	117.92	125.23
6	E	601	HEM	O2D-CGD-O1D	-3.90	113.30	123.33
6	G	601	HEM	CHA-C4D-ND	3.83	129.11	124.37
6	I	601	HEM	CHA-C4D-C3D	-3.83	118.16	125.23
6	I	601	HEM	CHA-C4D-ND	3.74	129.00	124.37
6	I	601	HEM	O2D-CGD-O1D	-3.71	113.79	123.33
6	I	601	HEM	C4A-NA-C1A	-3.65	99.86	105.82
6	I	601	HEM	CMD-C2D-C1D	3.65	130.74	125.03
7	E	602	NAG	O5-C1-C2	-3.62	105.69	111.29
7	B	602	NAG	C4-C3-C2	-3.55	105.81	111.02
6	G	601	HEM	CBD-CAD-C3D	-3.51	102.83	112.53
6	E	601	HEM	CMB-C2B-C1B	3.44	130.42	125.03
6	G	601	HEM	CMD-C2D-C1D	3.37	130.30	125.03
6	E	601	HEM	C2A-C1A-NA	3.34	113.85	110.15
6	B	601	HEM	CBD-CAD-C3D	-3.33	103.32	112.53
6	E	601	HEM	CHA-C4D-C3D	-3.27	119.19	125.23
6	B	601	HEM	C2A-C1A-NA	3.24	113.74	110.15
6	G	601	HEM	C2A-C1A-NA	3.14	113.64	110.15
6	I	601	HEM	O2A-CGA-O1A	-3.13	115.28	123.33
6	G	601	HEM	C4A-NA-C1A	-3.11	100.75	105.82
6	G	601	HEM	O2A-CGA-O1A	-3.07	115.42	123.33
6	E	601	HEM	C4A-NA-C1A	-3.07	100.81	105.82
6	B	601	HEM	CHD-C1D-ND	3.03	127.69	124.42
6	B	601	HEM	C4A-NA-C1A	-3.01	100.92	105.82
6	E	601	HEM	CBD-CAD-C3D	-2.94	104.40	112.53
7	E	602	NAG	C2-N2-C7	-2.93	118.98	122.90
7	I	602	NAG	C1-O5-C5	2.92	116.11	112.19
7	G	602	NAG	C1-O5-C5	2.90	116.07	112.19
7	E	602	NAG	C3-C4-C5	-2.77	105.21	110.23
6	I	601	HEM	CMB-C2B-C1B	2.75	129.33	125.03
6	I	601	HEM	C2A-C1A-NA	2.69	113.14	110.15
6	G	601	HEM	O2D-CGD-O1D	-2.68	116.45	123.33
7	I	603	NAG	C1-O5-C5	2.67	115.77	112.19
6	G	601	HEM	CHD-C1D-ND	2.67	127.29	124.42
6	B	601	HEM	CBA-CAA-C2A	-2.66	105.19	112.53
6	I	601	HEM	CBA-CAA-C2A	-2.66	105.19	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	601	HEM	CBA-CAA-C2A	-2.61	105.33	112.53
7	E	602	NAG	C1-C2-N2	2.59	114.51	110.43
6	E	601	HEM	CMD-C2D-C1D	2.55	129.02	125.03
7	E	602	NAG	C4-C3-C2	-2.51	107.34	111.02
6	G	601	HEM	C3D-C4D-ND	2.47	112.88	110.17
6	I	601	HEM	C1A-CHA-C4D	-2.46	120.45	126.25
6	B	601	HEM	CMA-C3A-C4A	2.45	129.14	125.42
6	G	601	HEM	CAD-C3D-C4D	2.42	128.91	124.70
6	G	601	HEM	CMB-C2B-C1B	2.39	128.76	125.03
6	G	601	HEM	C1A-CHA-C4D	-2.35	120.71	126.25
6	B	601	HEM	CMB-C2B-C1B	2.35	128.71	125.03
6	E	601	HEM	CMB-C2B-C3B	-2.33	122.78	128.43
9	G	605	XSD	C3-C4-N7	-2.33	107.51	109.31
6	I	601	HEM	C3C-C2C-C1C	-2.32	104.85	107.05
6	G	601	HEM	C4C-C3C-C2C	-2.31	104.81	106.81
9	E	604	XSD	C6-C7-C9	2.30	128.75	126.47
9	B	605	XSD	C3-C4-N7	-2.30	107.53	109.31
6	B	601	HEM	O2D-CGD-O1D	-2.29	117.45	123.33
6	E	601	HEM	O2D-CGD-CBD	2.28	121.20	114.00
7	B	602	NAG	C2-N2-C7	-2.27	119.86	122.90
6	I	601	HEM	CBD-CAD-C3D	-2.27	106.26	112.53
6	E	601	HEM	C3A-C4A-NA	2.27	113.77	110.14
6	E	601	HEM	CHB-C1B-NB	2.27	127.17	124.37
6	I	601	HEM	CMA-C3A-C4A	2.26	128.86	125.42
6	E	601	HEM	CAA-CBA-CGA	2.25	119.63	113.67
6	B	601	HEM	C3A-C4A-NA	2.23	113.72	110.14
6	B	601	HEM	C1A-CHA-C4D	-2.23	121.00	126.25
9	I	605	XSD	C6-C7-C9	2.22	128.66	126.47
6	B	601	HEM	CMD-C2D-C1D	2.22	128.50	125.03
6	E	601	HEM	C1A-CHA-C4D	-2.21	121.05	126.25
6	I	601	HEM	C3A-C4A-NA	2.20	113.66	110.14
6	B	601	HEM	CAD-C3D-C4D	2.18	128.50	124.70
6	B	601	HEM	C3D-C4D-ND	2.18	112.56	110.17
6	G	601	HEM	CMB-C2B-C3B	-2.17	123.17	128.43
6	G	601	HEM	CBA-CAA-C2A	-2.16	106.56	112.53
9	E	604	XSD	C3-C4-N7	-2.14	107.66	109.31
6	E	601	HEM	CHB-C1B-C2B	-2.14	120.87	126.95
6	I	601	HEM	C2B-C1B-NB	2.11	112.26	109.84
6	G	601	HEM	C4C-CHD-C1D	-2.11	121.54	126.02
9	I	605	XSD	C3-C4-N7	-2.10	107.68	109.31
6	B	601	HEM	CHB-C1B-NB	2.09	126.95	124.37
6	I	601	HEM	O2A-CGA-CBA	2.07	120.54	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	601	HEM	O2A-CGA-O1A	-2.06	118.04	123.33
6	E	601	HEM	C3C-C2C-C1C	-2.06	105.10	107.05
6	E	601	HEM	O2A-CGA-CBA	2.05	120.48	114.00
6	E	601	HEM	CAB-C3B-C2B	-2.05	121.77	128.43
6	I	601	HEM	CMB-C2B-C3B	-2.04	123.48	128.43
6	E	601	HEM	CHD-C1D-ND	2.04	126.62	124.42
6	G	601	HEM	O2D-CGD-CBD	2.03	120.42	114.00
6	B	601	HEM	CHB-C1B-C2B	-2.02	121.20	126.95
6	I	601	HEM	CHB-C1B-C2B	-2.01	121.23	126.95
6	G	601	HEM	C3A-C4A-NA	2.01	113.36	110.14

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	602	NAG	C8-C7-N2-C2
7	E	602	NAG	O7-C7-N2-C2
7	E	602	NAG	O5-C5-C6-O6
6	B	601	HEM	C4B-C3B-CAB-CBB
6	E	601	HEM	C4B-C3B-CAB-CBB
6	G	601	HEM	C4B-C3B-CAB-CBB
6	I	601	HEM	C4B-C3B-CAB-CBB
7	B	602	NAG	C4-C5-C6-O6
6	G	601	HEM	CAA-CBA-CGA-O1A
6	I	601	HEM	CAA-CBA-CGA-O1A
6	I	601	HEM	CAD-CBD-CGD-O1D
6	B	601	HEM	CAD-CBD-CGD-O1D
6	G	601	HEM	CAA-CBA-CGA-O2A
6	E	601	HEM	CAD-CBD-CGD-O1D
6	E	601	HEM	CAD-CBD-CGD-O2D
6	I	601	HEM	CAA-CBA-CGA-O2A
6	G	601	HEM	CAD-CBD-CGD-O2D
6	B	601	HEM	CAA-CBA-CGA-O1A
6	G	601	HEM	CAD-CBD-CGD-O1D
6	B	601	HEM	CAD-CBD-CGD-O2D
6	B	601	HEM	CAA-CBA-CGA-O2A
6	I	601	HEM	CAD-CBD-CGD-O2D
6	E	601	HEM	CAA-CBA-CGA-O2A
6	E	601	HEM	CAA-CBA-CGA-O1A
7	B	602	NAG	O5-C5-C6-O6
9	E	604	XSD	N4-C10-C11-C12
9	G	605	XSD	N4-C10-C11-C16

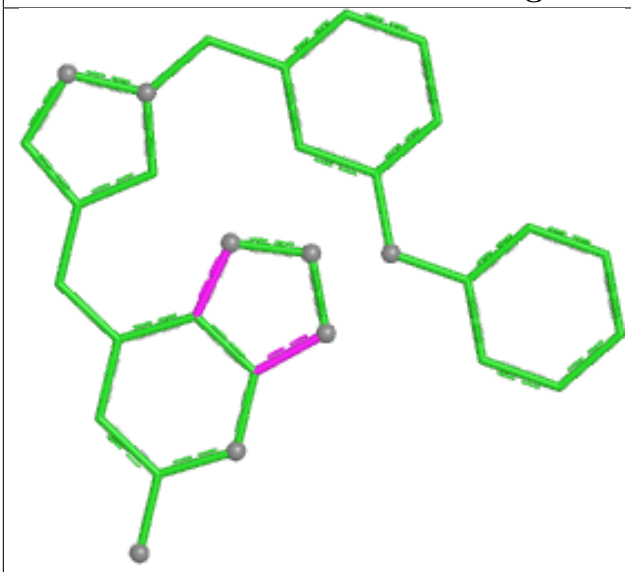
There are no ring outliers.

8 monomers are involved in 60 short contacts:

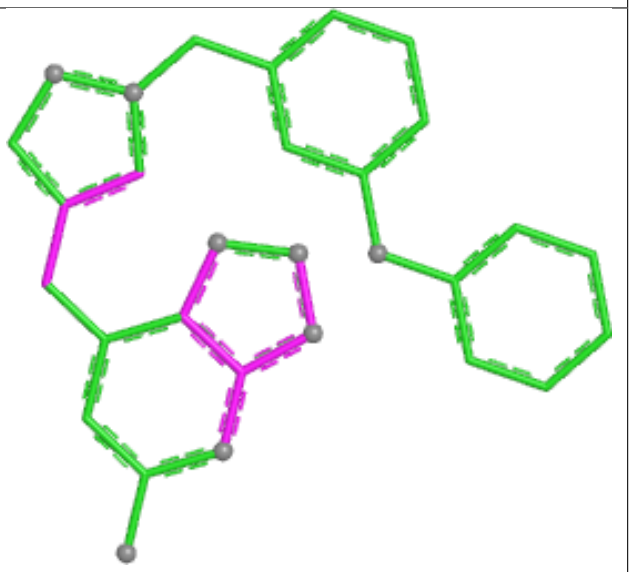
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	602	NAG	4	0
7	I	603	NAG	4	0
6	E	601	HEM	11	0
7	G	602	NAG	3	0
6	I	601	HEM	13	0
6	B	601	HEM	13	0
6	G	601	HEM	9	0
7	I	602	NAG	3	0

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

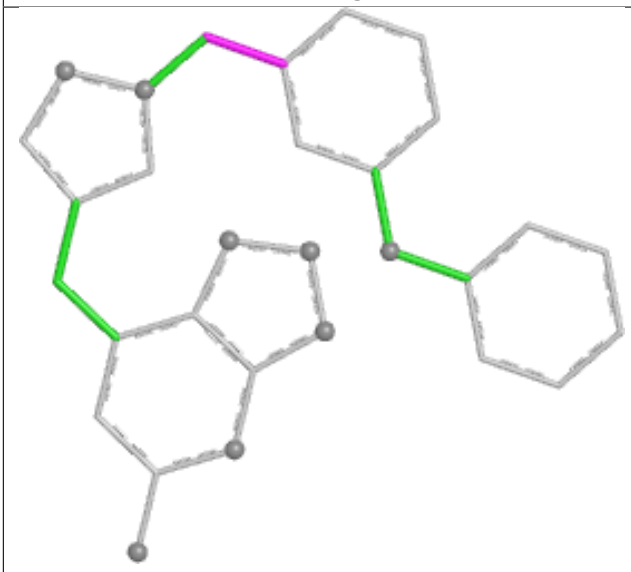
Ligand XSD E 604



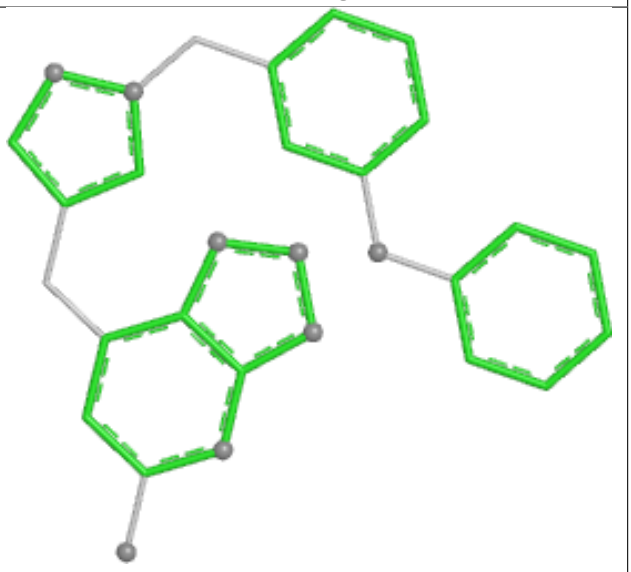
Bond lengths



Bond angles

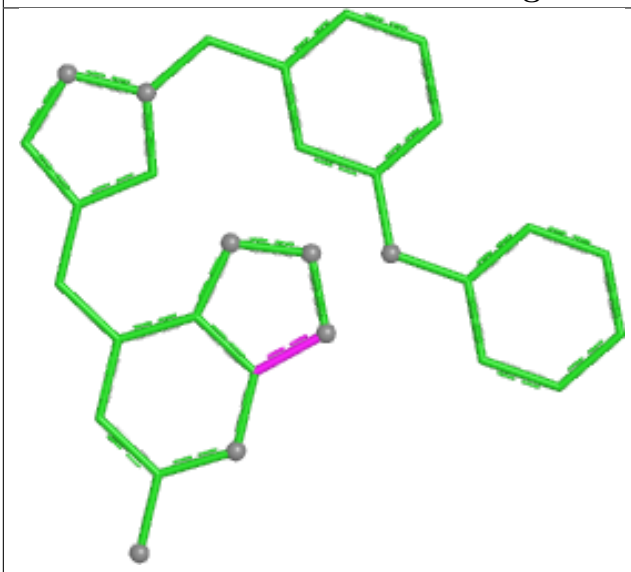


Torsions

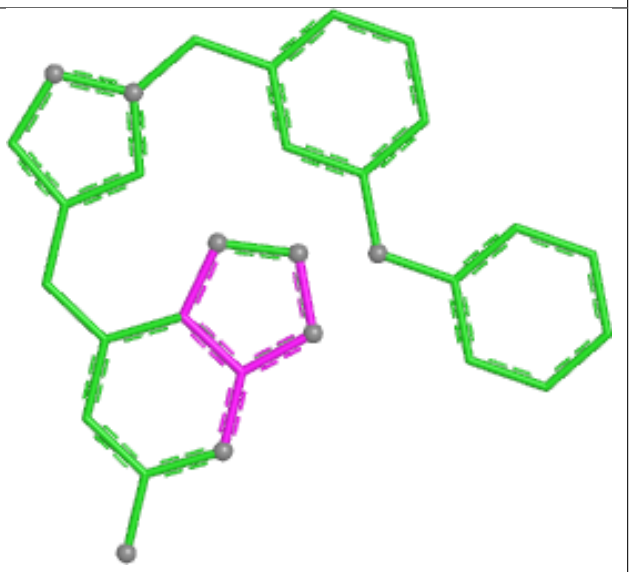


Rings

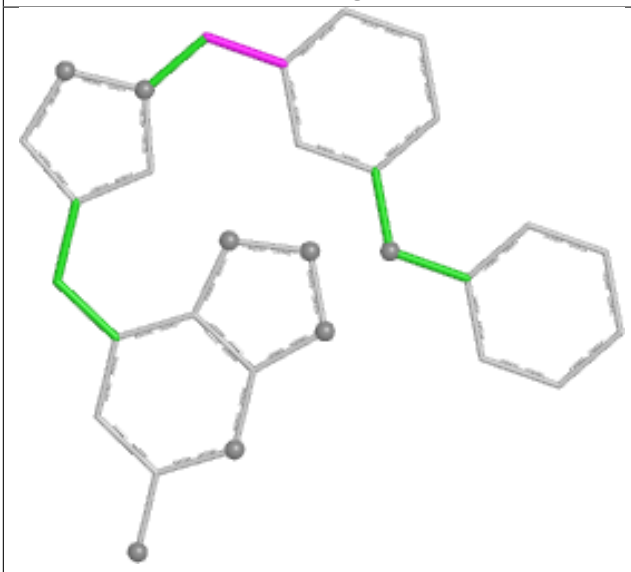
Ligand XSD G 605



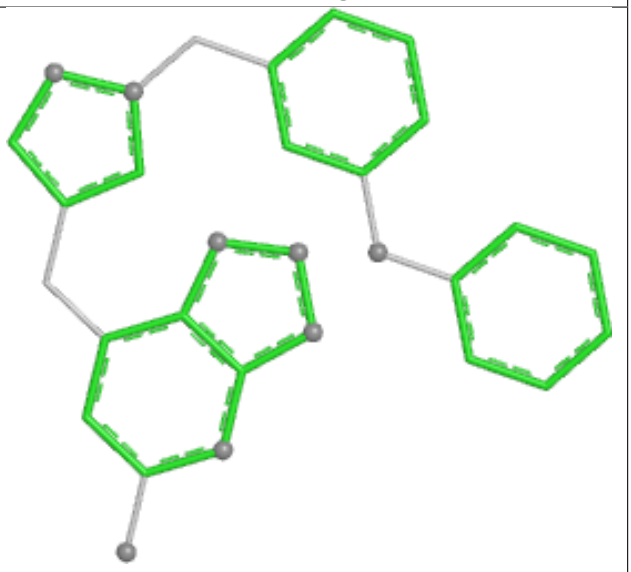
Bond lengths



Bond angles

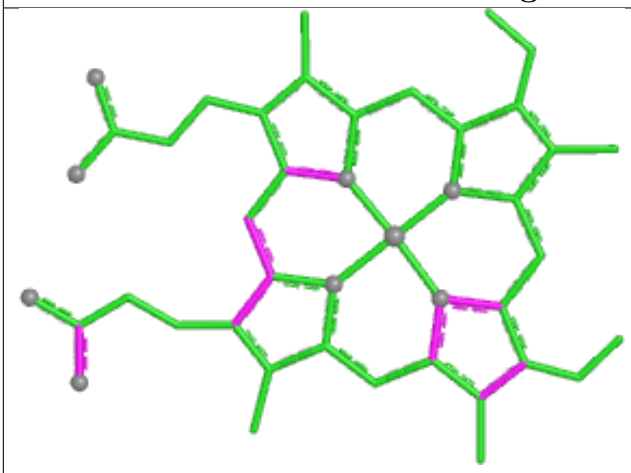


Torsions

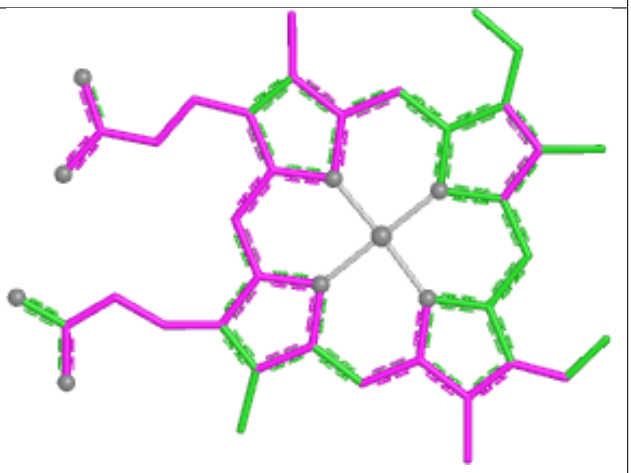


Rings

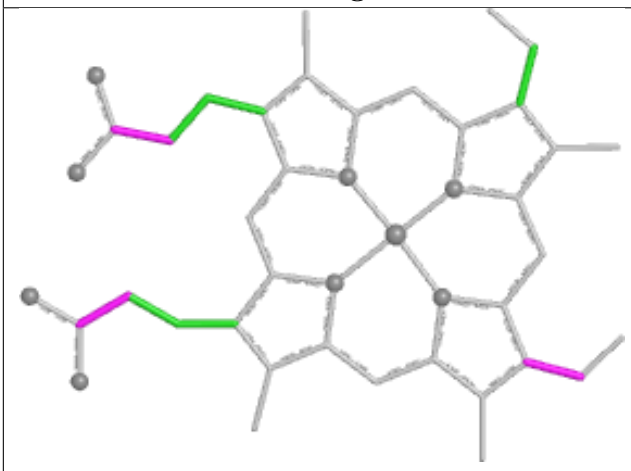
Ligand HEM E 601



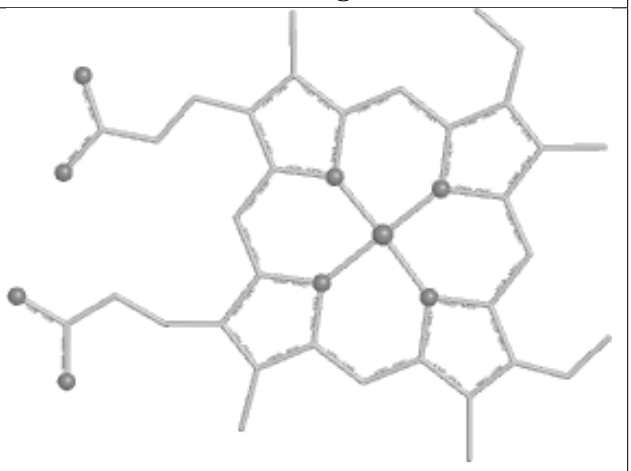
Bond lengths



Bond angles

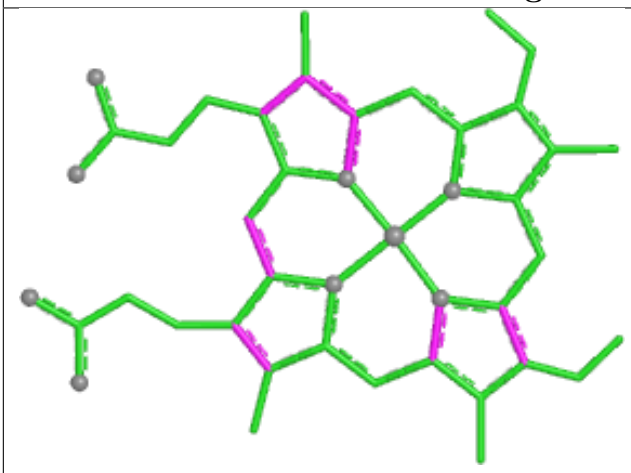


Torsions



Rings

Ligand HEM I 601



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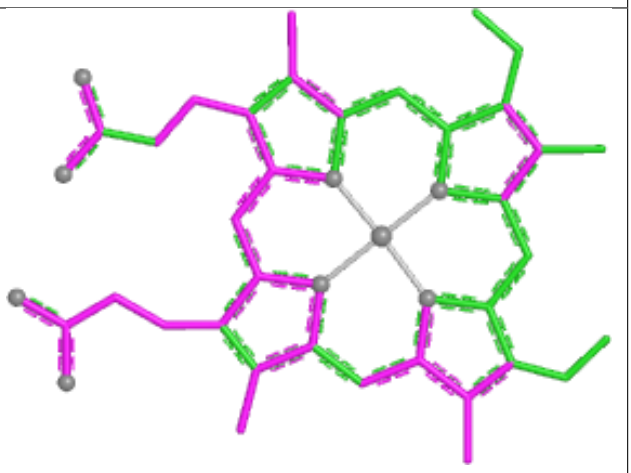
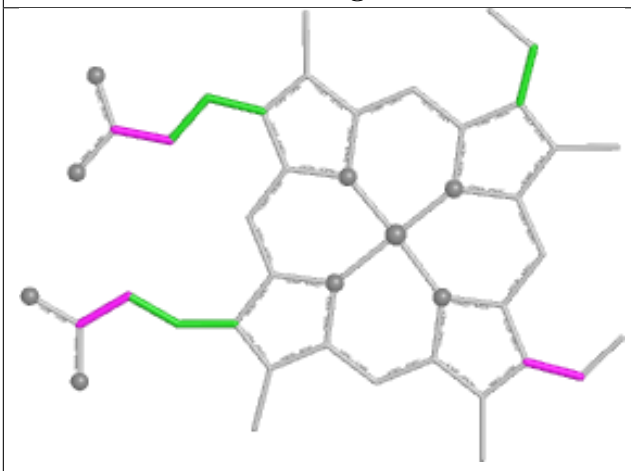
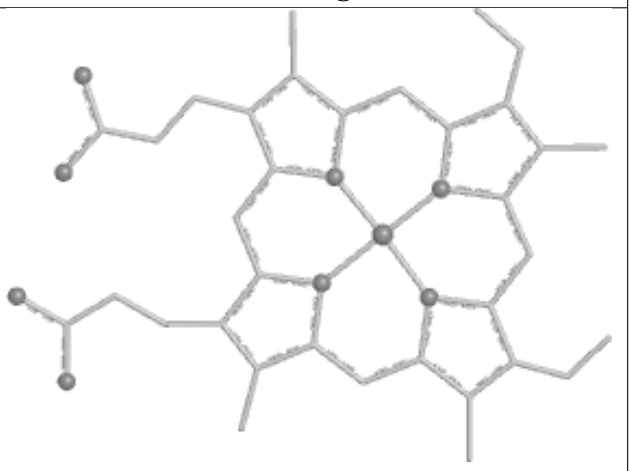


Bond angles

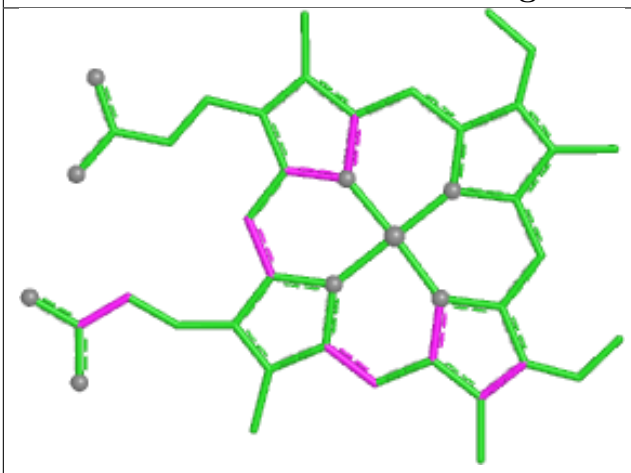


Torsions

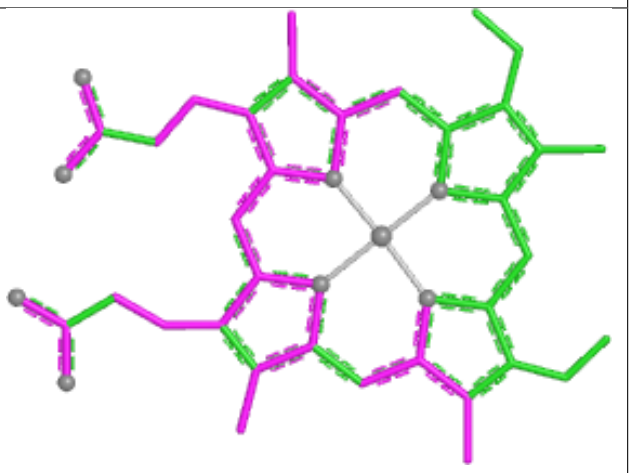


Rings

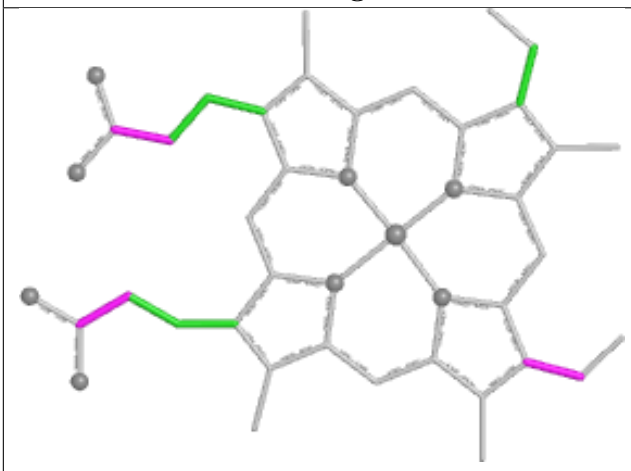
Ligand HEM B 601



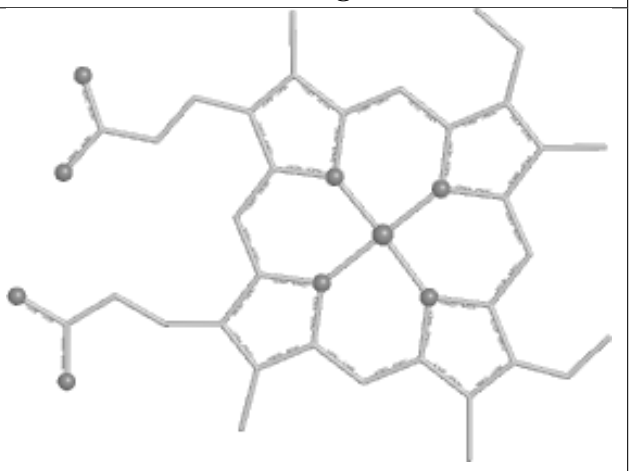
Bond lengths



Bond angles

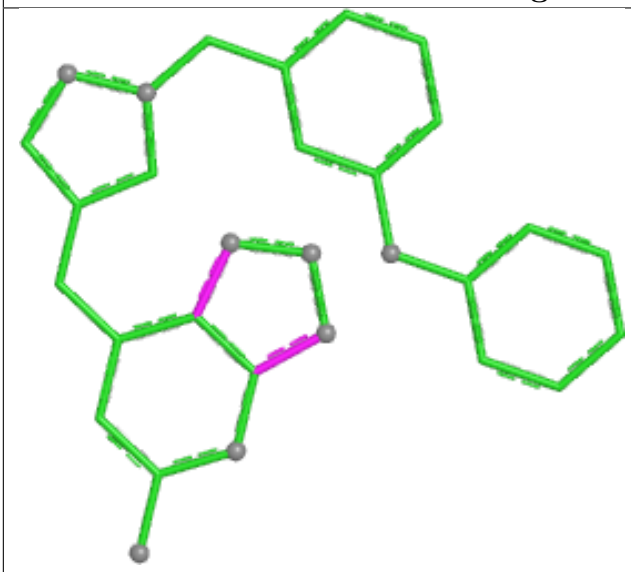


Torsions

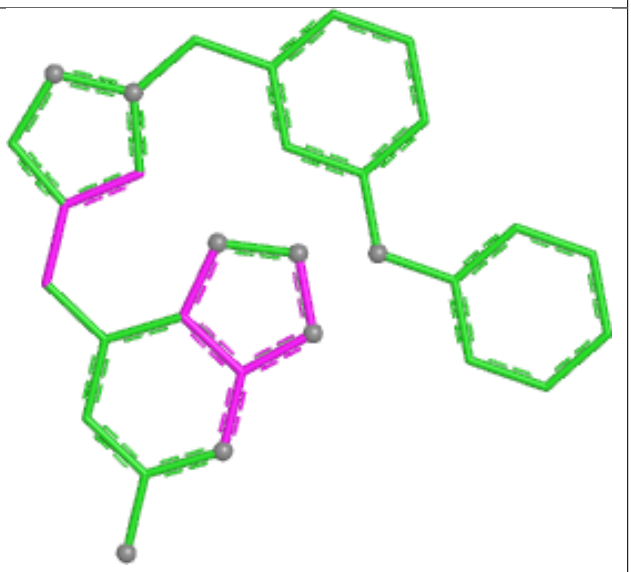


Rings

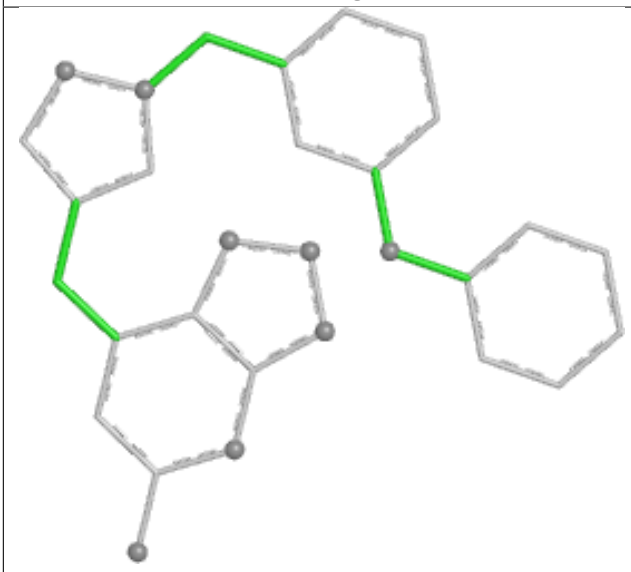
Ligand XSD I 605



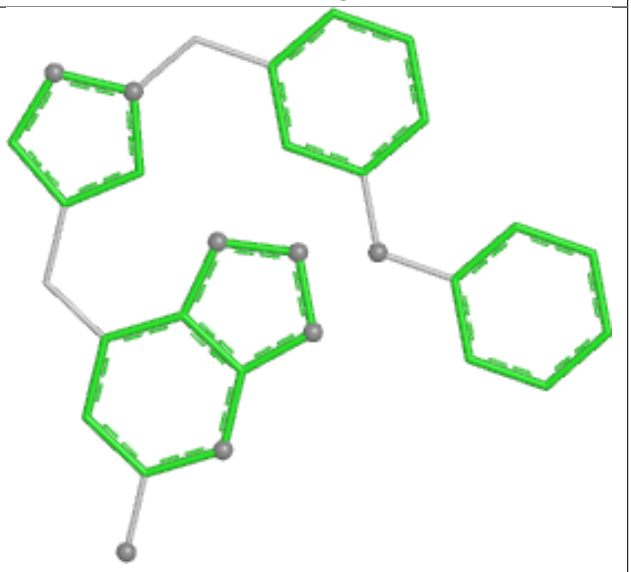
Bond lengths



Bond angles

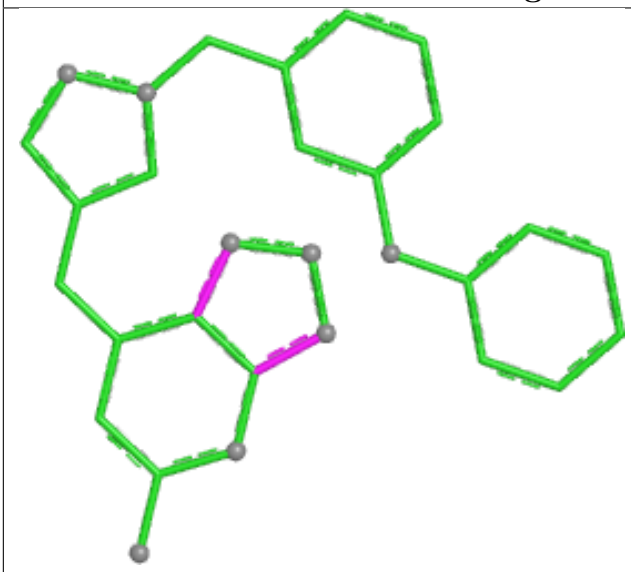


Torsions

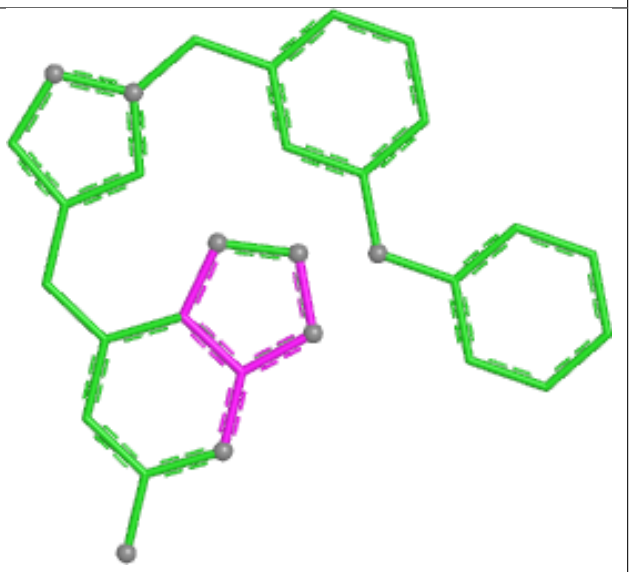


Rings

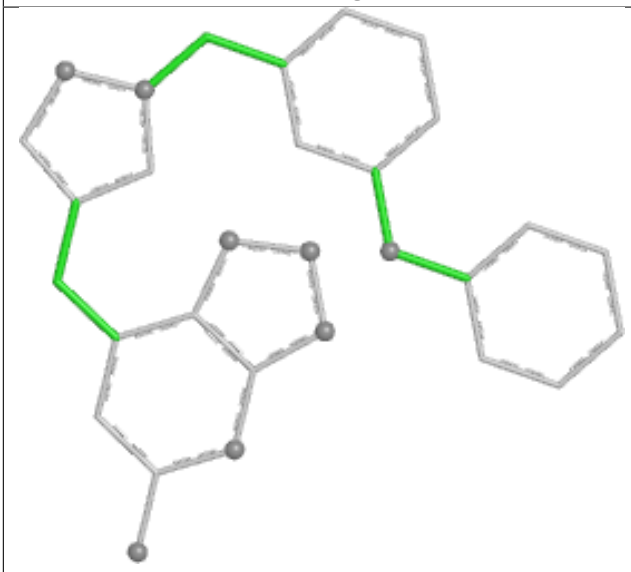
Ligand XSD B 605



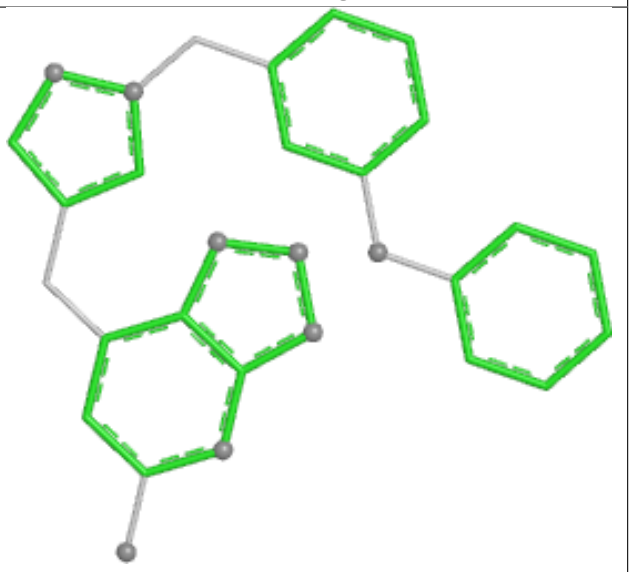
Bond lengths



Bond angles

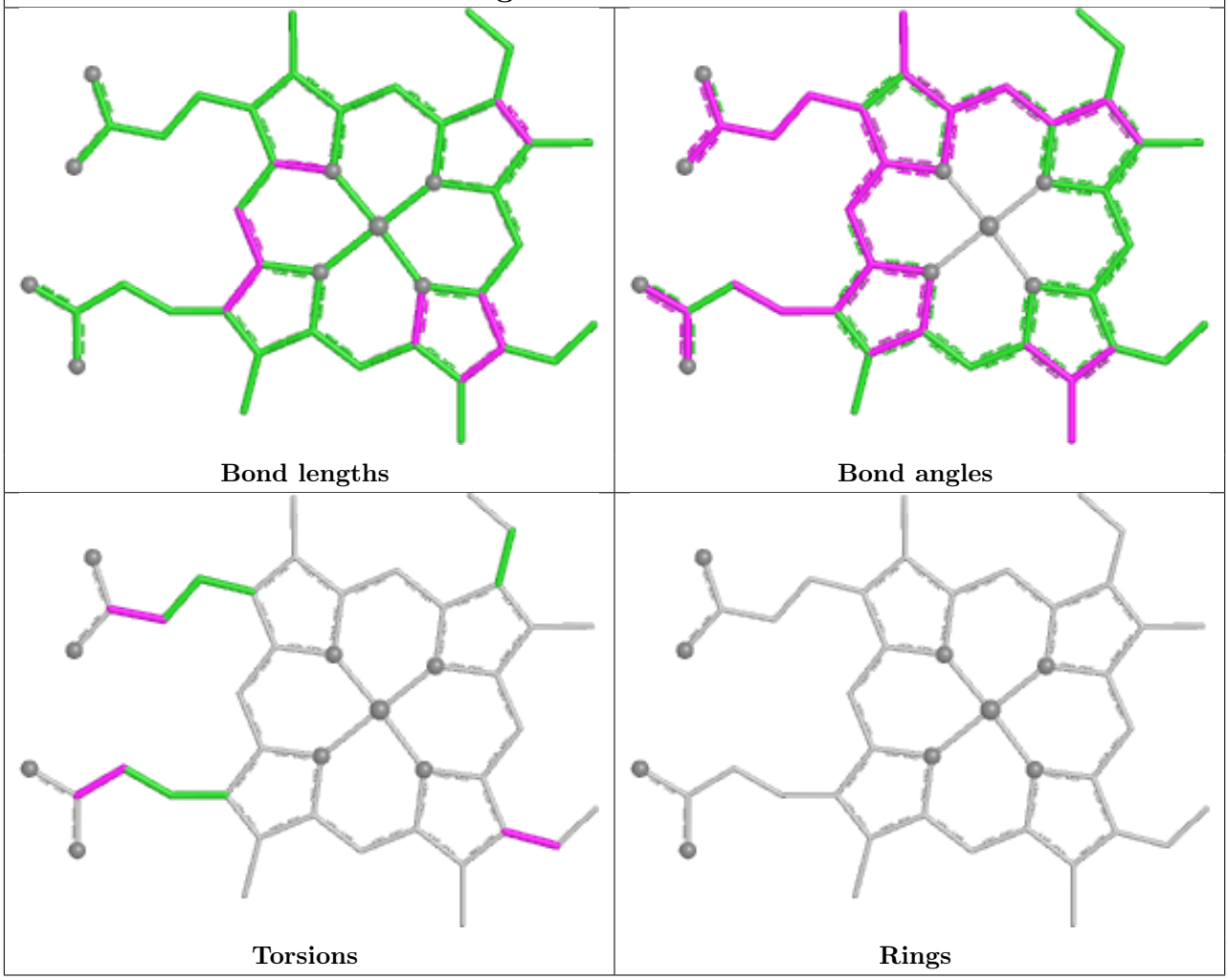


Torsions



Rings

Ligand HEM G 601



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, 95^{th} 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%)	-0.19	3 (2%) 53 45	27, 40, 65, 90	1 (0%)
1	D	103/105 (98%)	-0.28	1 (0%) 79 74	26, 38, 62, 86	1 (0%)
1	F	103/105 (98%)	-0.31	4 (3%) 43 34	26, 39, 63, 94	1 (0%)
1	H	103/105 (98%)	-0.38	0 100 100	22, 37, 65, 69	1 (0%)
2	B	464/466 (99%)	-0.27	1 (0%) 91 91	23, 44, 64, 89	8 (1%)
2	E	465/466 (99%)	-0.31	2 (0%) 88 87	20, 41, 62, 76	11 (2%)
2	G	464/466 (99%)	-0.31	3 (0%) 85 82	23, 41, 62, 75	7 (1%)
2	I	464/466 (99%)	-0.28	1 (0%) 91 91	24, 41, 62, 78	9 (1%)
All	All	2269/2284 (99%)	-0.29	15 (0%) 84 80	20, 41, 63, 94	39 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	114	ASN	4.7
2	I	114	ASN	3.5
1	F	3	GLU	2.8
1	A	4	GLN	2.7
1	D	3	GLU	2.6
1	A	74	ASP	2.6
2	E	354	GLU	2.5
1	F	4	GLN	2.4
2	E	348	ASN	2.4
1	F	1	CYS	2.3
1	F	2	PRO	2.2
2	G	217	HIS	2.2
1	A	1	CYS	2.2
2	G	114	ASN	2.1
2	G	354	GLU	2.0

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

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

6.3 Carbohydrates (i)

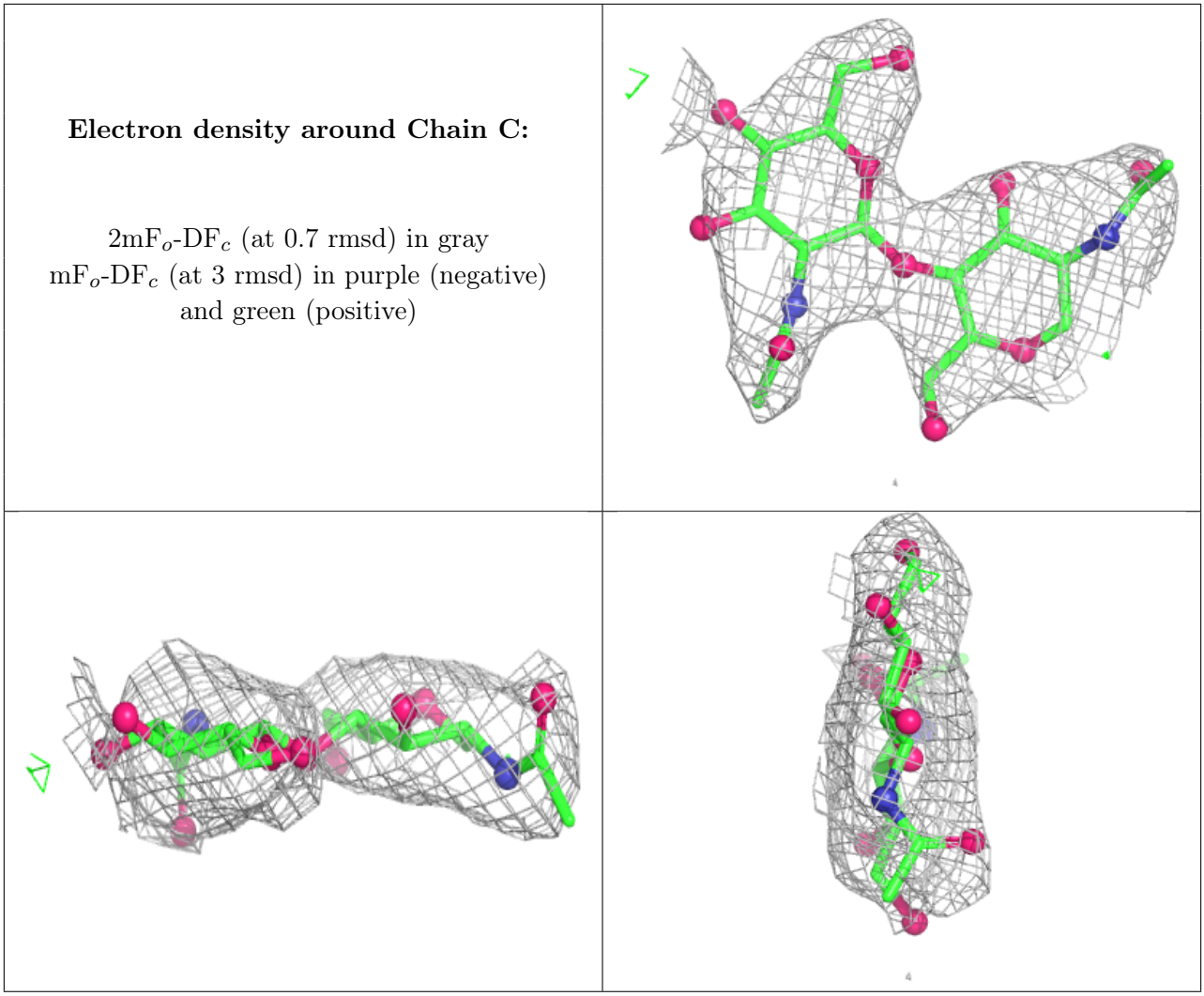
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	-	-	79,84,87,90	0
3	NAG	C	2	14/15	-	-	93,95,97,97	0
3	NAG	L	2	14/15	0.54	0.14	75,79,84,85	0
4	MAN	N	4	11/12	0.73	0.13	54,61,65,67	0
4	MAN	K	4	11/12	0.75	0.12	61,65,75,79	0
3	NAG	L	1	14/15	0.76	0.17	59,63,69,76	0
4	MAN	M	4	11/12	0.78	0.12	53,59,63,68	0
4	MAN	J	4	11/12	0.82	0.10	53,58,64,68	0
4	MAN	N	5	11/12	0.82	0.11	38,40,45,45	0
4	BMA	K	3	11/12	0.86	0.10	35,38,44,53	0
4	MAN	K	5	11/12	0.87	0.09	40,42,45,48	0
4	FUC	K	6	10/11	0.88	0.11	38,42,44,44	0
4	MAN	J	5	11/12	0.88	0.10	36,38,41,42	0
4	NAG	J	1	14/15	0.89	0.10	32,34,39,46	0
4	NAG	K	2	14/15	0.89	0.10	25,31,34,37	0
4	NAG	M	1	14/15	0.89	0.10	32,35,42,44	0
4	FUC	J	6	10/11	0.90	0.09	37,43,44,44	0
4	MAN	M	5	11/12	0.91	0.09	38,43,45,49	0
4	FUC	M	6	10/11	0.91	0.09	34,35,38,38	0
4	FUC	N	6	10/11	0.91	0.08	37,40,41,42	0
4	BMA	M	3	11/12	0.92	0.08	36,41,46,47	0
4	NAG	K	1	14/15	0.92	0.08	31,39,44,44	0
4	NAG	N	2	14/15	0.92	0.09	24,33,37,38	0
4	BMA	J	3	11/12	0.93	0.09	32,36,40,46	0
4	BMA	N	3	11/12	0.93	0.08	34,38,42,48	0
4	NAG	M	2	14/15	0.93	0.09	23,29,34,37	0
4	NAG	J	2	14/15	0.93	0.08	25,33,38,40	0
4	NAG	N	1	14/15	0.93	0.10	35,38,44,48	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.

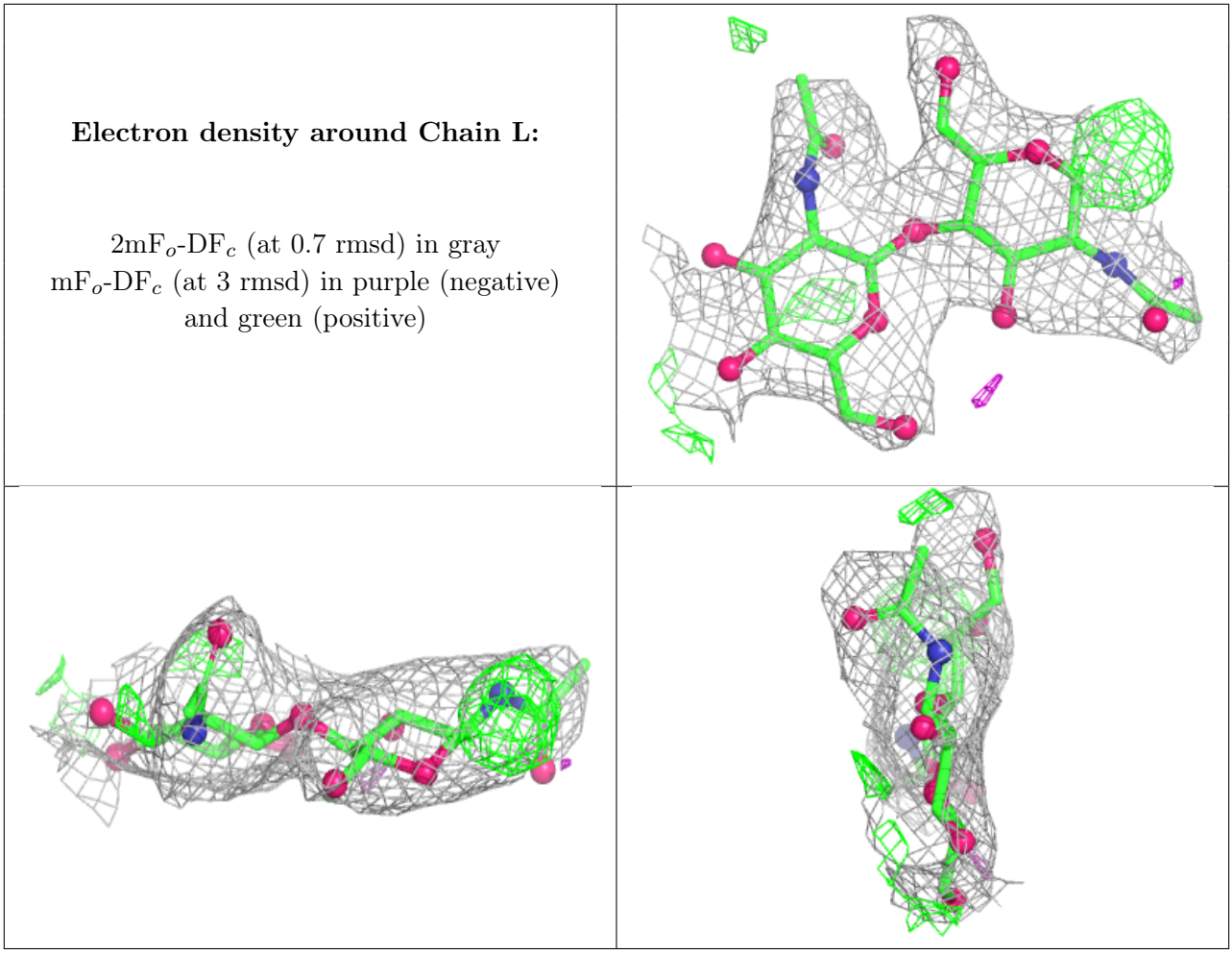
Electron density around Chain C:

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



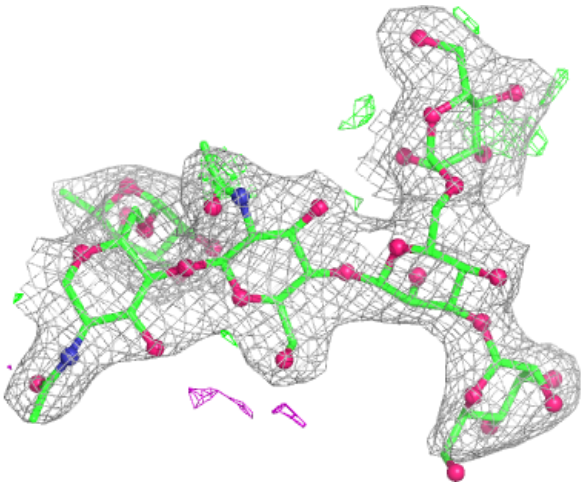
Electron density around Chain L:

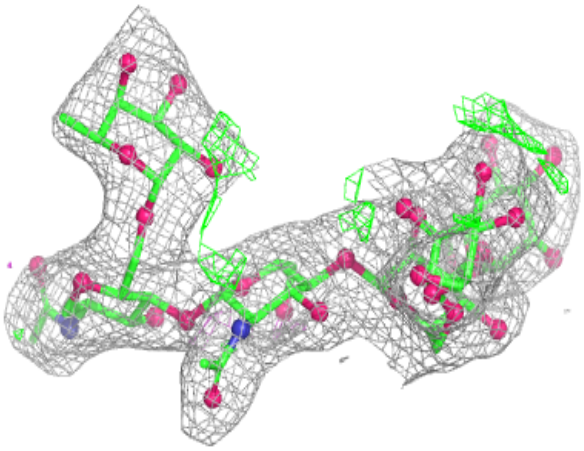
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

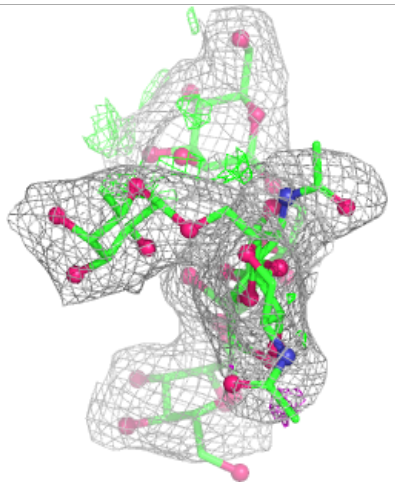


Electron density around Chain J:

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

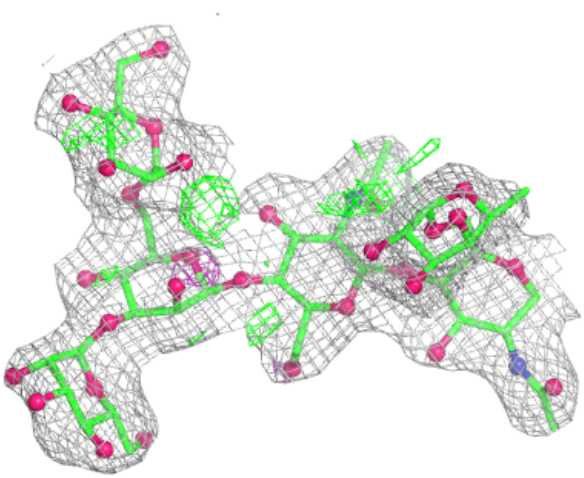


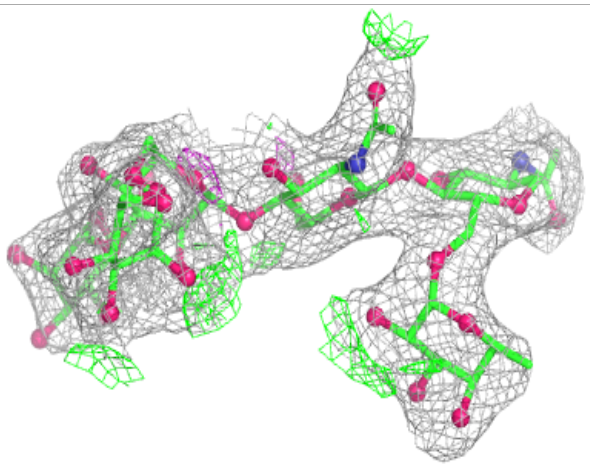


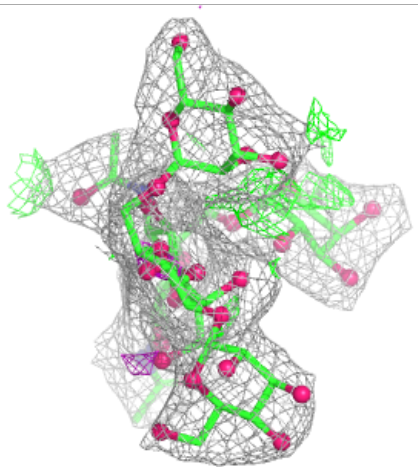


Electron density around Chain K:

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

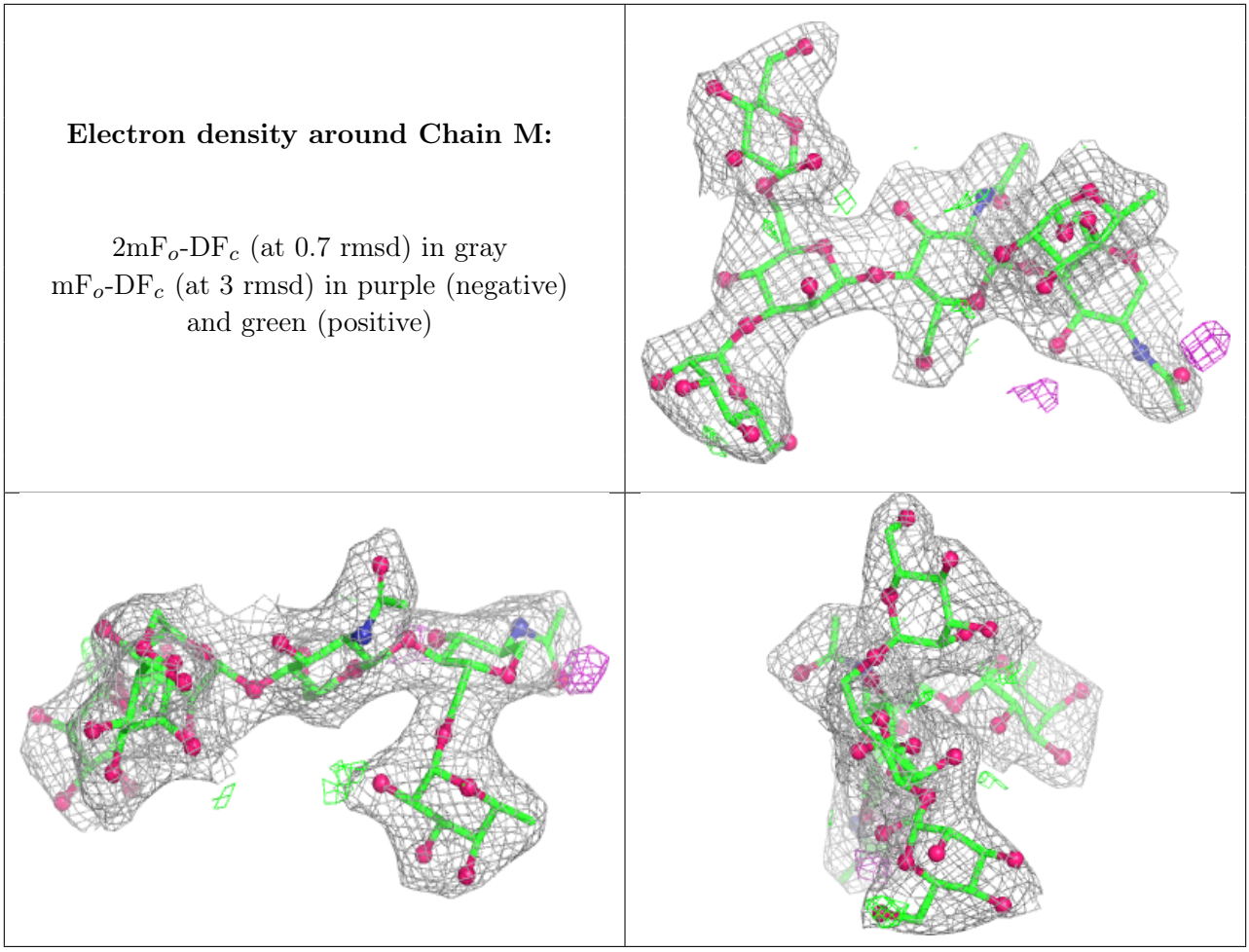






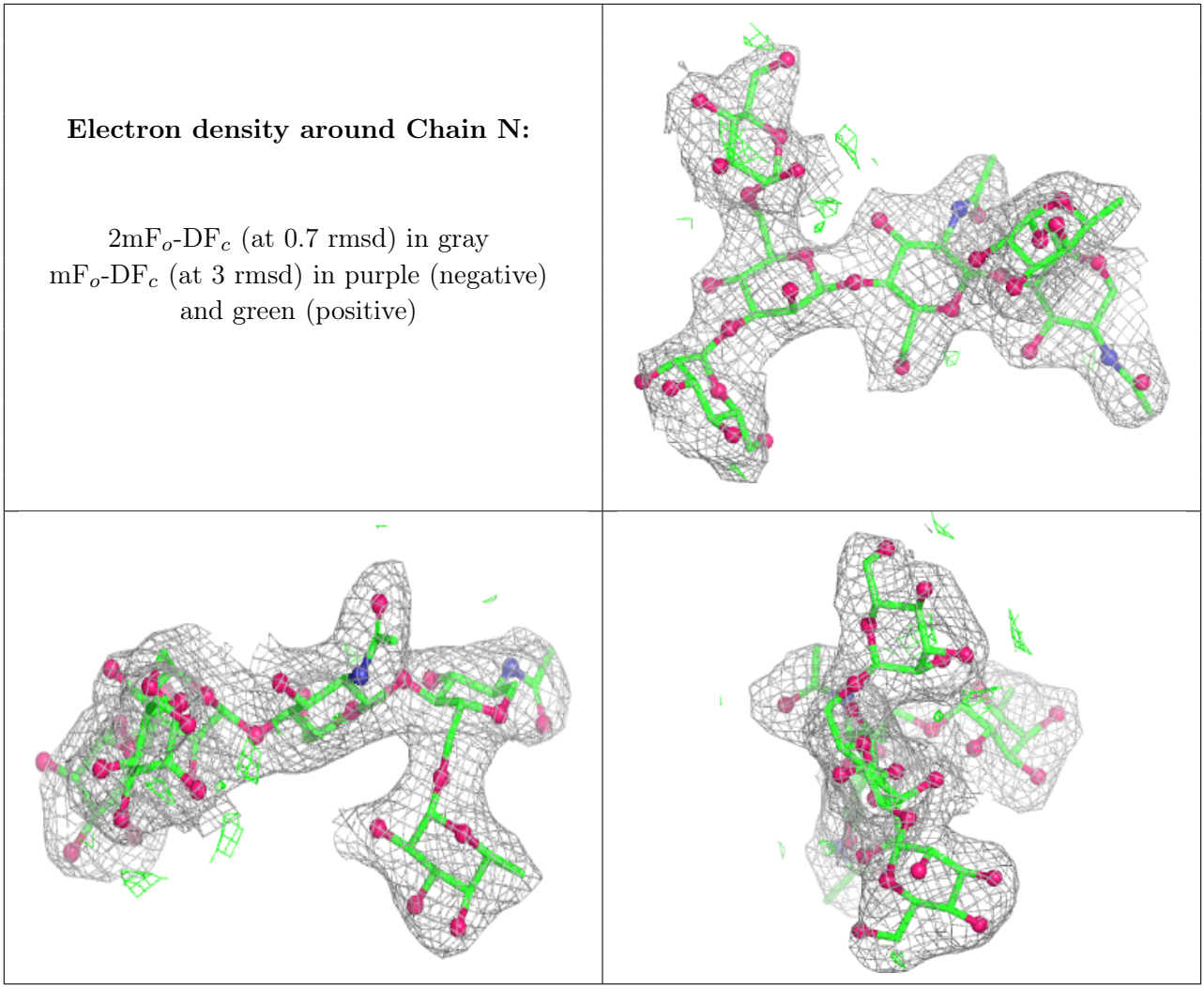
Electron density around Chain M:

$2mF_o$-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 N:

$2mF_o$-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, 95^{th} 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	I	603	14/15	0.72	0.21	89,91,93,93	0
7	NAG	E	602	14/15	0.78	0.18	75,80,84,88	0
7	NAG	G	602	14/15	0.79	0.14	55,65,70,70	0
7	NAG	I	602	14/15	0.83	0.13	57,61,63,65	0
7	NAG	B	602	14/15	0.83	0.10	49,69,72,73	0
9	XSD	B	605	30/30	0.91	0.10	41,48,57,59	0
9	XSD	I	605	30/30	0.91	0.09	38,43,60,62	0
9	XSD	G	605	30/30	0.92	0.09	43,51,57,59	0
9	XSD	E	604	30/30	0.93	0.09	37,46,57,59	0

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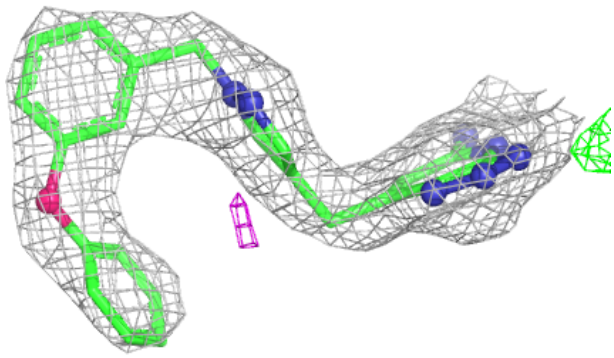
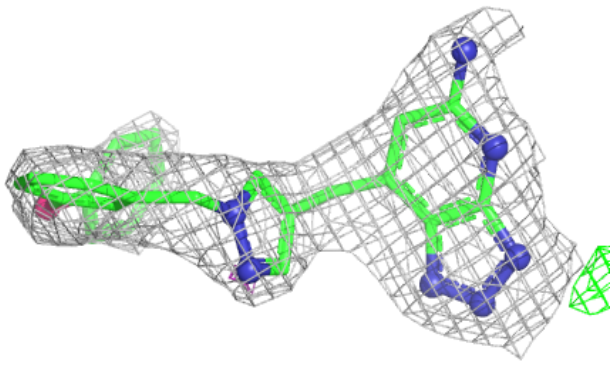
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	G	604	1/1	0.95	0.17	43,43,43,43	0
5	CL	B	604	1/1	0.95	0.15	54,54,54,54	0
6	HEM	E	601	43/43	0.97	0.07	31,32,35,50	0
6	HEM	G	601	43/43	0.97	0.08	32,33,37,52	0
6	HEM	I	601	43/43	0.97	0.08	33,35,39,53	0
6	HEM	B	601	43/43	0.97	0.07	32,33,36,47	0
5	CL	A	201	1/1	0.98	0.06	31,31,31,31	0
5	CL	F	201	1/1	0.98	0.08	31,31,31,31	0
8	CA	G	603	1/1	0.99	0.03	34,34,34,34	0
8	CA	B	603	1/1	1.00	0.02	36,36,36,36	0
8	CA	I	604	1/1	1.00	0.05	32,32,32,32	0
8	CA	E	603	1/1	1.00	0.02	32,32,32,32	0

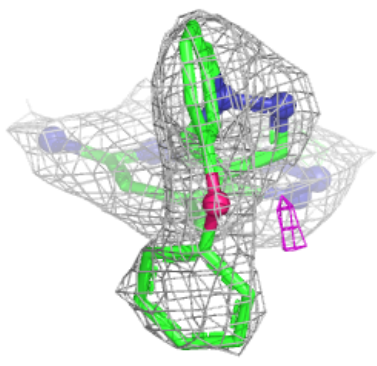
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XSD B 605:

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

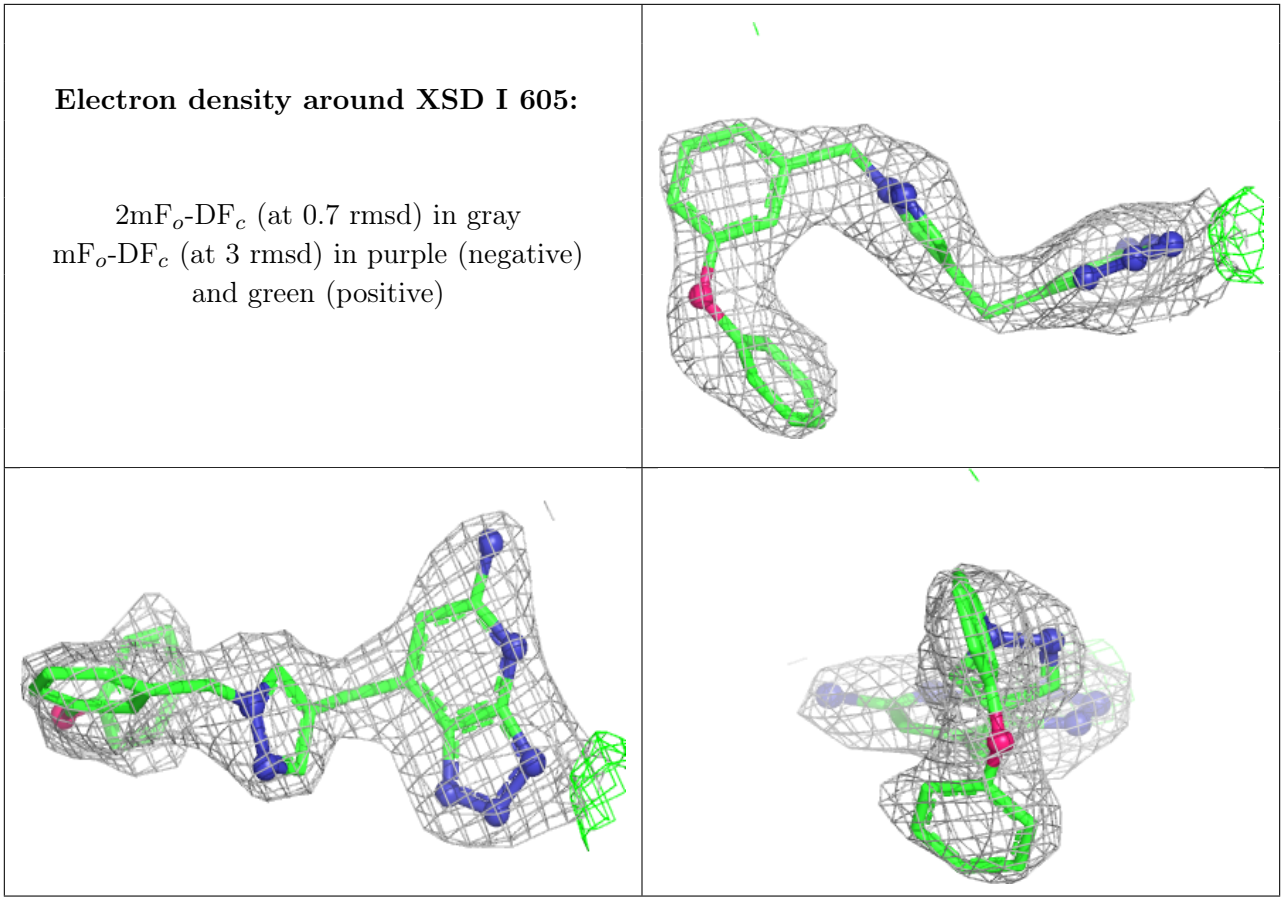






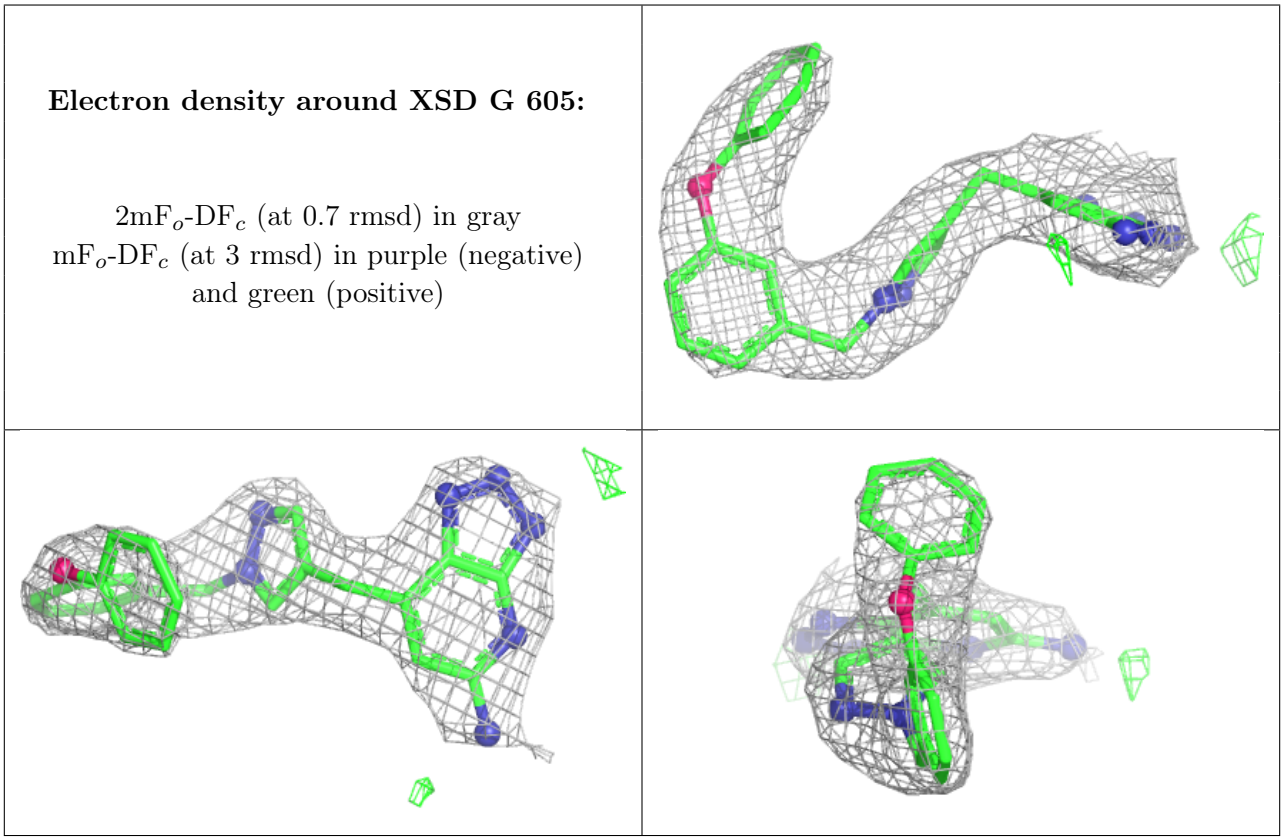
Electron density around XSD I 605:

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



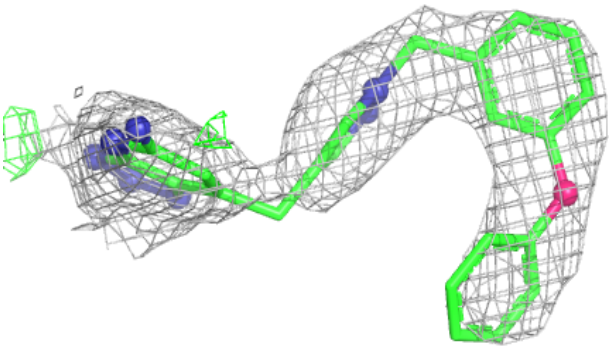
Electron density around XSD G 605:

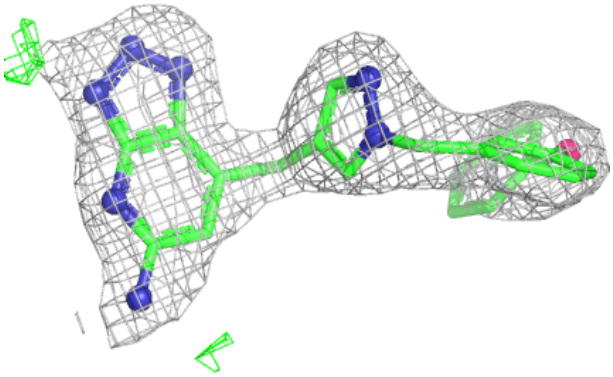
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

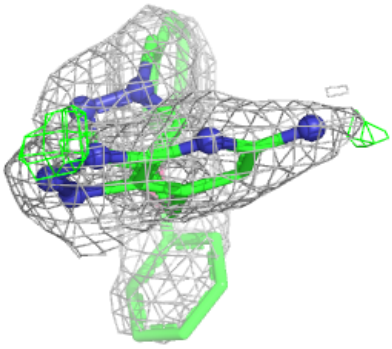


Electron density around XSD E 604:

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

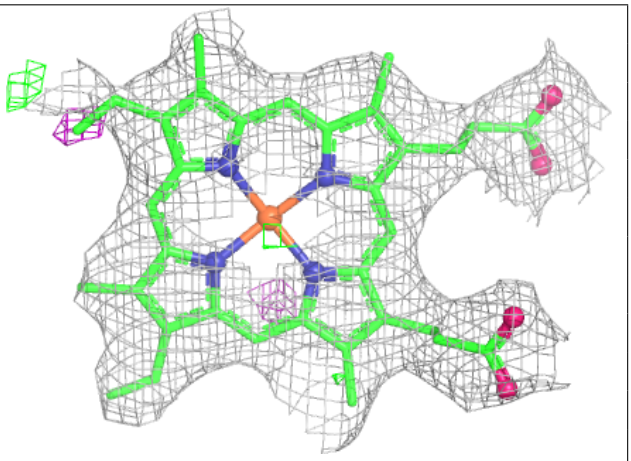


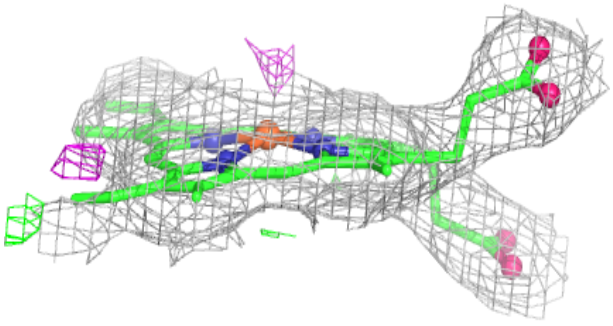


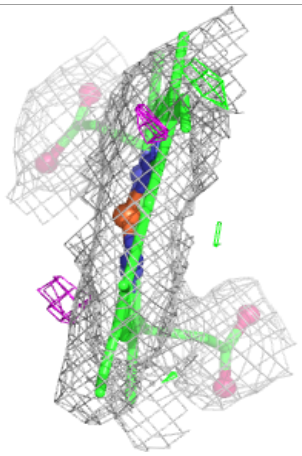


Electron density around HEM E 601:

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

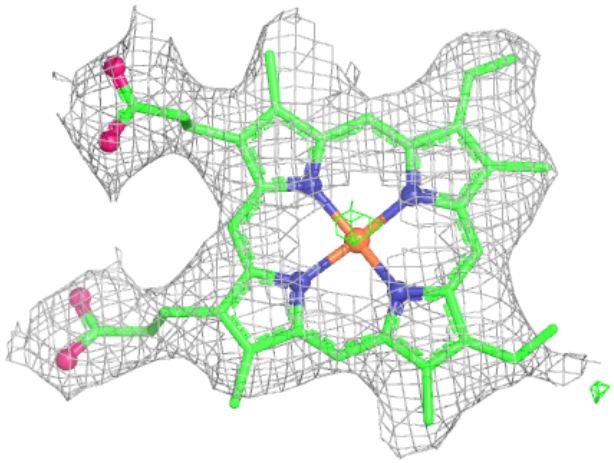


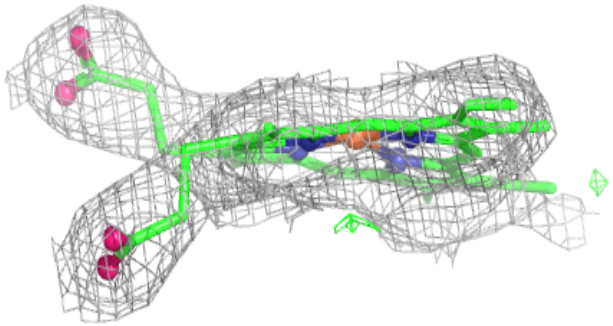


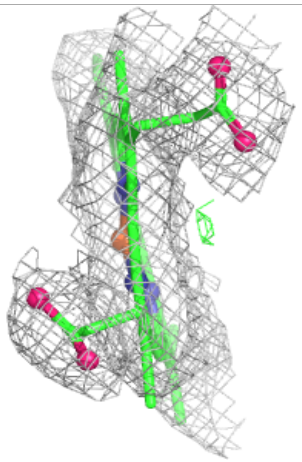


Electron density around HEM G 601:

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

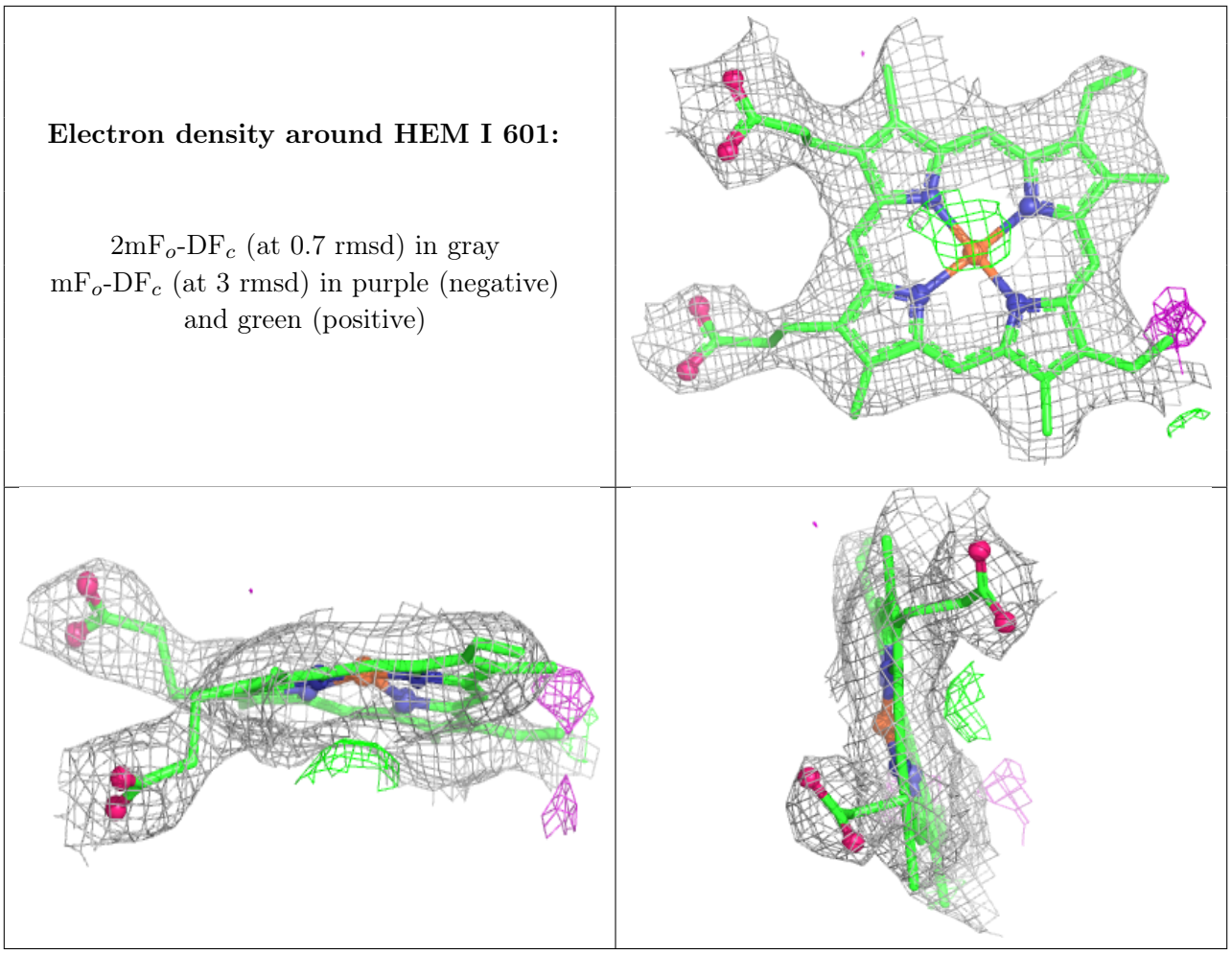






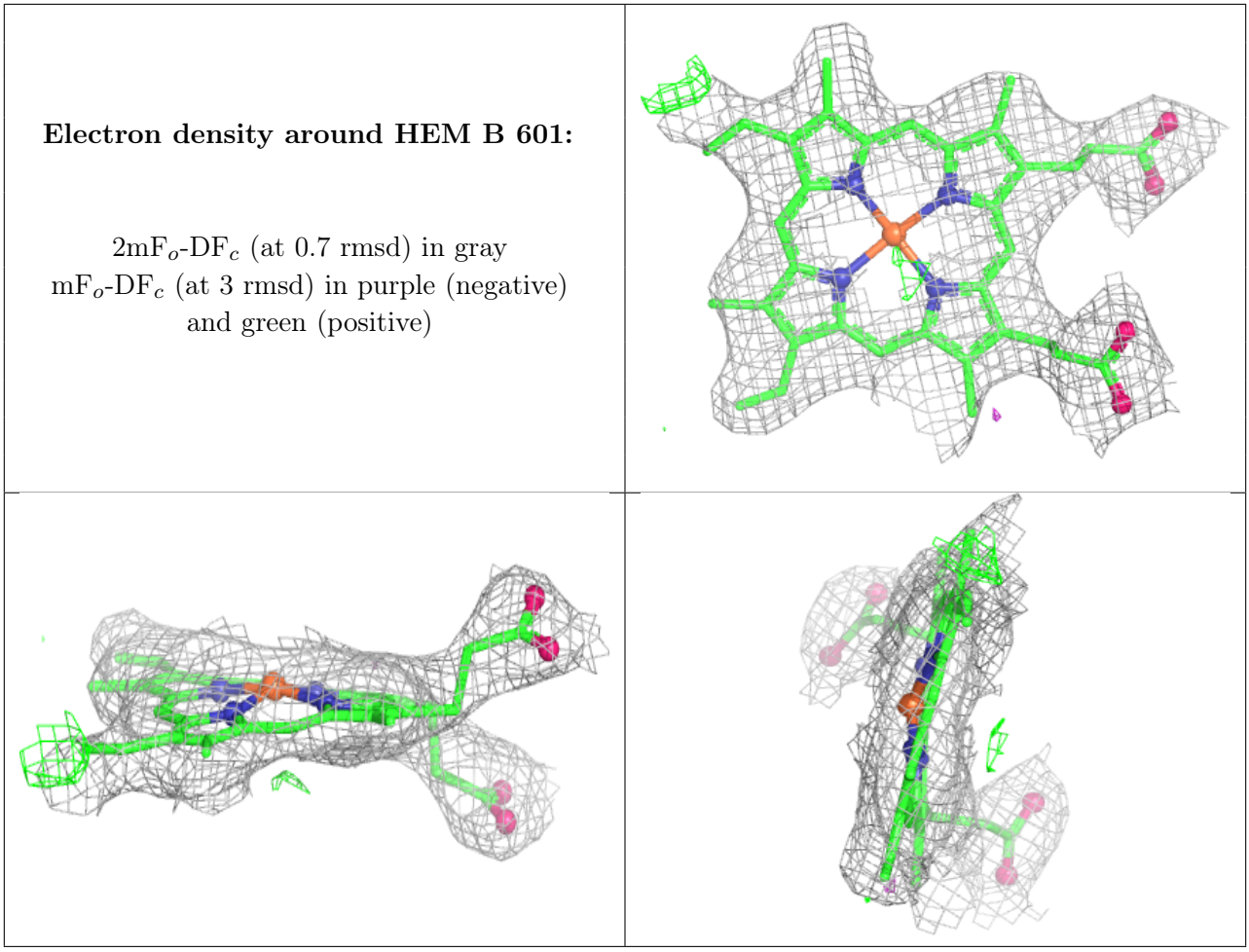
Electron density around HEM I 601:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.