Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 01:22 PM EDT

PDB ID	:	1DNU / pdb_00001dnu
Title	:	STRUCTURAL ANALYSES OF HUMAN MYELOPEROXIDASE-THIOCYANATE COMPLEX
Authors	:	Blair-Johnson, M.; Fiedler, T.J.; Fenna, R.E.
Deposited on	:	1999-12-16
Resolution	:	1.85 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:

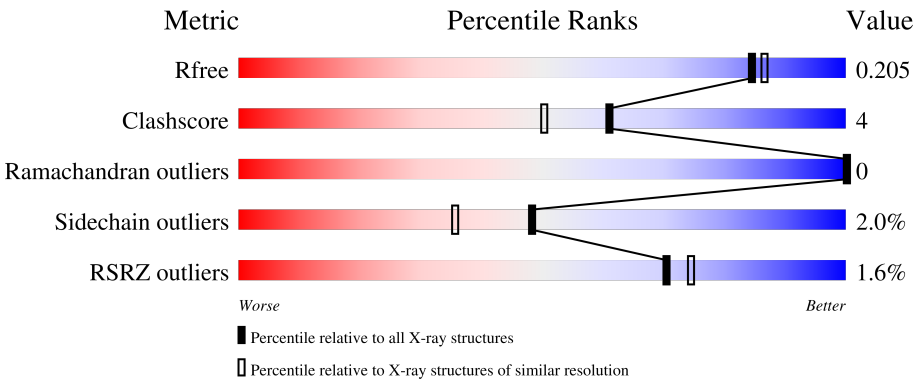
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	104	3%, 92%, 8%
1	B	104	93%, 7%
2	C	466	2%, 88%, 12%
2	D	466	2%, 88%, 12%
3	E	6	83%, 17%

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Mol	Chain	Length	Quality of chain
3	F	6	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	ACY	C	606	-	-	X	-
9	ACY	D	607	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10318 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
			Total	C	N	O	S			
1	A	104	838	529	148	156	5	0	0	0
1	B	104	838	529	148	156	5	0	0	0

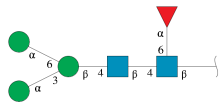
- Molecule 2 is a protein called MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	466	3733	2351	687	668	27	0	0	0
2	D	466	3733	2351	687	668	27	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

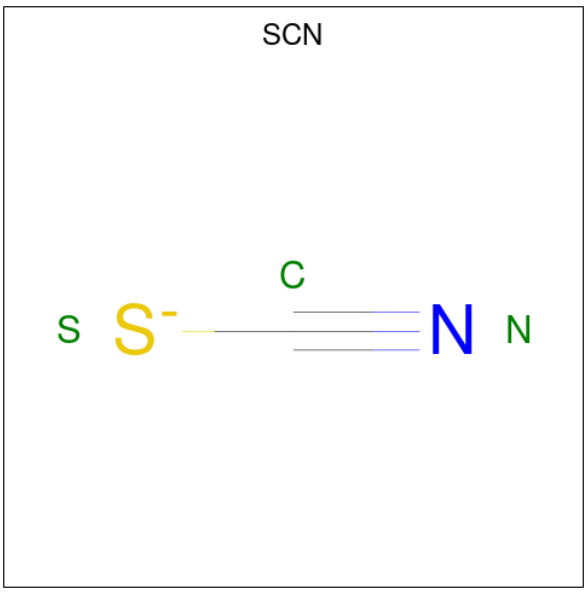
Chain	Residue	Modelled	Actual	Comment	Reference
C	150	CSO	CYS	modified residue	UNP P05164
D	150	CSO	CYS	modified residue	UNP P05164

- Molecule 3 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.



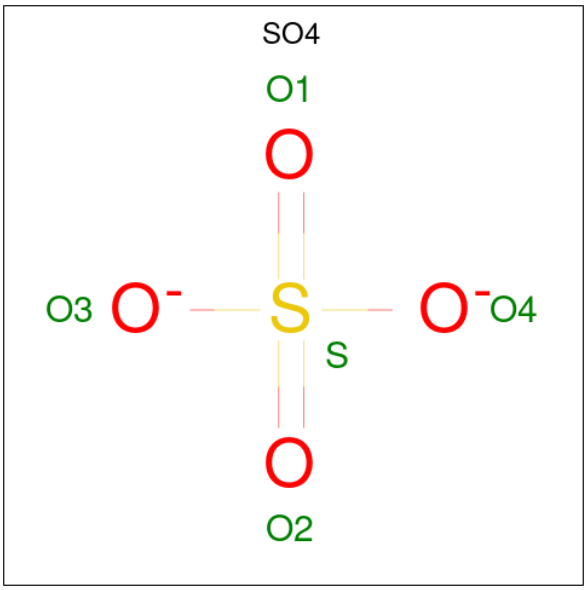
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	6	71	40	2	29	0	0	0
3	F	6	71	40	2	29	0	0	0

- Molecule 4 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



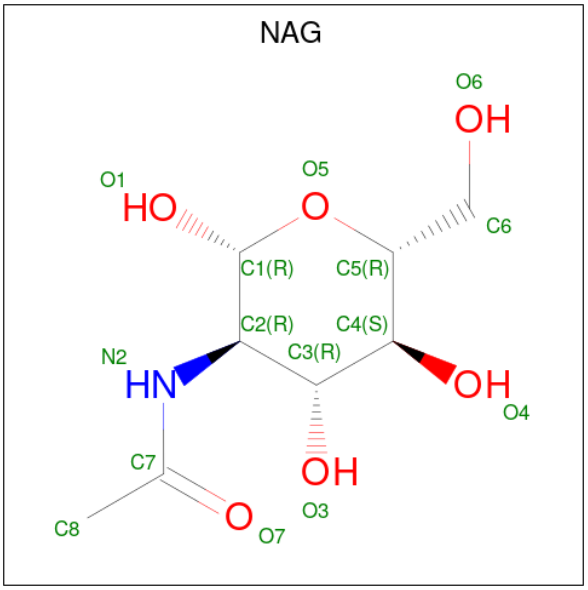
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
4	A	1	3	1	1	1	0	0
			Total	C	N	S		
4	A	1	3	1	1	1	0	0
			Total	C	N	S		
4	B	1	3	1	1	1	0	0
			Total	C	N	S		
4	B	1	3	1	1	1	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
5	A	1	5	4	1		0	0
			Total	O	S			
5	C	1	5	4	1		0	0
			Total	O	S			
5	D	1	5	4	1		0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

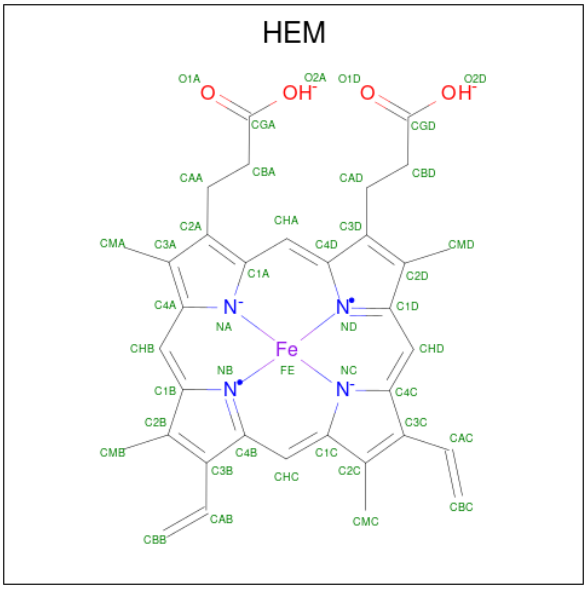


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	C	1	14	8	1	5	0	0
			Total	C	N	O		
6	C	1	14	8	1	5	0	0
			Total	C	N	O		
6	D	1	14	8	1	5	0	0
			Total	C	N	O		
6	D	1	14	8	1	5	0	0

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

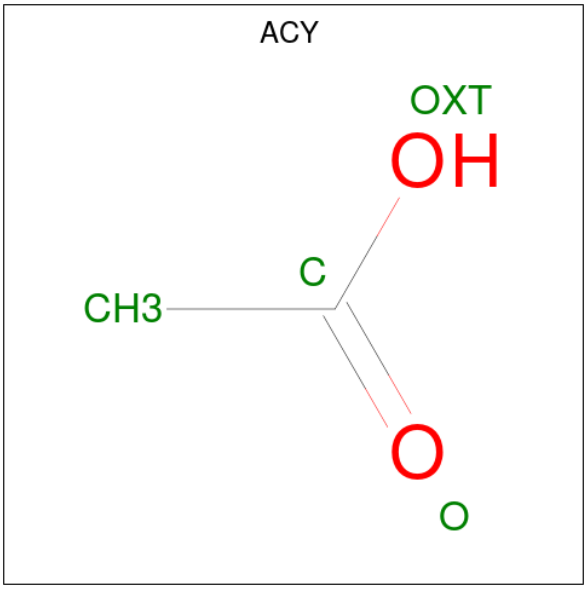
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	C	1	1	1	0	0
			Total	Ca		
7	D	1	1	1	0	0

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 9 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	C	1	4	2	2	0	0
			Total	C	O		
9	C	1	4	2	2	0	0
			Total	C	O		
9	C	1	4	2	2	0	0
			Total	C	O		
9	D	1	4	2	2	0	0
			Total	C	O		
9	D	1	4	2	2	0	0
			Total	C	O		
9	D	1	4	2	2	0	0

- Molecule 10 is water.

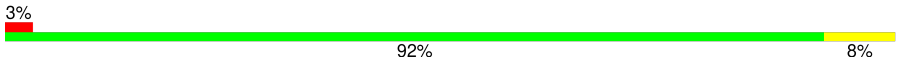
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	96	96	96	0	0
			Total	O		
10	C	329	329	329	0	0
			Total	O		
10	B	104	104	104	0	0
			Total	O		
10	D	310	310	310	0	0

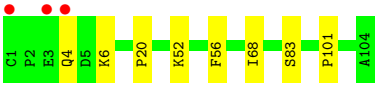
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MYELOPEROXIDASE

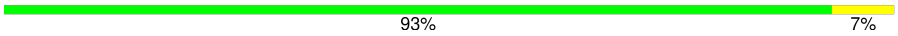
Chain A:

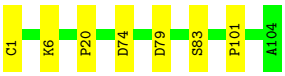




• Molecule 1: MYELOPEROXIDASE

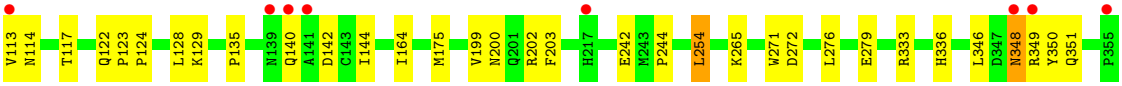
Chain B:





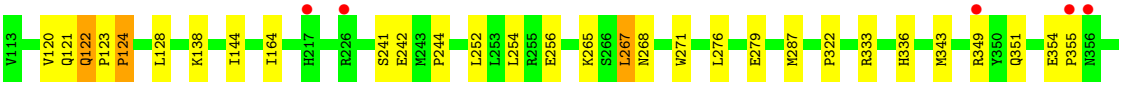
• Molecule 2: MYELOPEROXIDASE

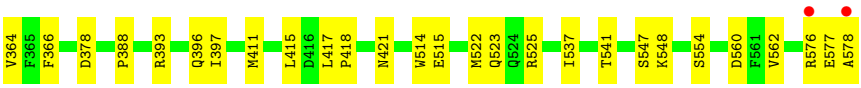
Chain C:



• Molecule 2: MYELOPEROXIDASE

Chain D:



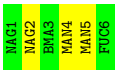


• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 3: 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:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.24Å 63.87Å 92.62Å 90.00° 97.54° 90.00°	Depositor
Resolution (Å)	10.00 – 1.85 10.00 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.7 (10.00-1.85) 97.5 (10.00-1.86)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.51 (at 1.86Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.178 , 0.210 0.172 , 0.205	Depositor DCC
R_{free} test set	5388 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	13.5	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 54.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10318	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: FUC, SCN, NAG, BMA, ACY, MAN, CSO, CA, SO4, HEM

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	0.85	0/863	0.99	1/1174 (0.1%)
1	B	0.79	0/863	0.97	1/1174 (0.1%)
2	C	0.83	0/3811	0.91	3/5168 (0.1%)
2	D	0.80	0/3811	0.91	5/5168 (0.1%)
All	All	0.82	0/9348	0.92	10/12684 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	336	HIS	ND1-CG-CD2	6.95	113.05	106.10
2	D	336	HIS	ND1-CG-CD2	6.34	112.44	106.10
2	D	336	HIS	CG-CD2-NE2	-6.07	101.13	107.20
2	D	397	ILE	N-CA-C	5.73	115.81	110.42
2	C	336	HIS	CG-CD2-NE2	-5.69	101.51	107.20
2	C	272	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	20	PRO	N-CA-C	5.39	120.94	113.98
1	B	74	ASP	CA-CB-CG	5.26	117.86	112.60
2	D	268	ASN	CA-C-N	5.13	124.92	119.28
2	D	268	ASN	C-N-CA	5.13	124.92	119.28

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	838	0	798	5	0
1	B	838	0	798	5	0
2	C	3733	0	3725	39	0
2	D	3733	0	3725	34	0
3	E	71	0	61	0	0
3	F	71	0	61	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
5	A	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	C	28	0	26	0	0
6	D	28	0	26	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	C	43	0	30	2	0
8	D	43	0	30	2	0
9	C	12	0	9	2	0
9	D	12	0	9	2	0
10	A	96	0	0	1	0
10	B	104	0	0	0	0
10	C	329	0	0	2	0
10	D	310	0	0	0	0
All	All	10318	0	9298	78	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (78) 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:C:135:PRO:HG2	10:C:711:HOH:O	1.84	0.77
2:D:525:ARG:HH11	9:D:607:ACY:H2	1.48	0.75
2:C:348:ASN:H	2:C:348:ASN:HD22	1.37	0.71
2:C:465:MET:HE1	2:C:471:PRO:HD3	1.73	0.69
2:D:349:ARG:HG3	2:D:351:GLN:HG2	1.77	0.66
2:C:271:TRP:CZ3	2:C:279:GLU:HG3	2.33	0.63
2:D:265:LYS:HD3	2:D:276:LEU:HD11	1.80	0.62
10:A:302:HOH:O	2:C:129:LYS:HD3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:333:ARG:HH21	2:C:421:ASN:HD22	1.50	0.60
2:C:200:ASN:HD22	2:C:203:PHE:H	1.49	0.59
2:C:128:LEU:HB2	2:C:144:ILE:HB	1.85	0.58
2:C:200:ASN:ND2	2:C:202:ARG:H	2.01	0.58
2:C:200:ASN:HD22	2:C:202:ARG:H	1.51	0.57
2:D:411:MET:CE	2:D:415:LEU:HD21	2.34	0.57
2:C:142:ASP:HB3	10:C:892:HOH:O	2.05	0.57
8:D:601:HEM:HMC2	8:D:601:HEM:HBC2	1.87	0.56
2:D:354:GLU:HB3	2:D:355:PRO:HA	1.90	0.53
2:D:548:LYS:HG2	2:D:562:VAL:HG13	1.90	0.53
2:D:417:LEU:HB3	2:D:418:PRO:HD3	1.92	0.52
2:D:333:ARG:HH21	2:D:421:ASN:HD22	1.57	0.52
2:D:522:MET:HE3	9:D:607:ACY:H1	1.92	0.51
2:D:120:VAL:HG12	2:D:122:GLN:CG	2.41	0.51
2:D:244:PRO:HD3	2:D:364:VAL:O	2.09	0.51
2:C:348:ASN:H	2:C:348:ASN:ND2	2.06	0.50
1:A:101:PRO:HD2	2:C:164:ILE:O	2.12	0.50
2:C:548:LYS:HG2	2:C:562:VAL:HG13	1.93	0.50
2:D:411:MET:HE2	2:D:415:LEU:HD21	1.93	0.50
2:C:265:LYS:HD3	2:C:276:LEU:HD11	1.94	0.49
2:C:333:ARG:HH21	2:C:421:ASN:ND2	2.11	0.48
2:D:242:GLU:OE1	8:D:601:HEM:HBB2	2.13	0.48
2:C:200:ASN:ND2	2:C:203:PHE:H	2.12	0.48
2:C:411:MET:HE2	2:C:415:LEU:HD11	1.95	0.48
1:B:83:SER:HB3	2:D:554:SER:O	2.13	0.47
2:D:267:LEU:HD13	2:D:576:ARG:NE	2.29	0.47
1:B:1:CYS:SG	1:B:20:PRO:HB3	2.55	0.47
1:A:68:ILE:HD13	2:C:464:LEU:HD23	1.96	0.47
2:D:393:ARG:HB2	2:D:396:GLN:HB2	1.97	0.47
2:D:378:ASP:OD1	2:D:541:THR:HB	2.15	0.46
2:D:121:GLN:C	2:D:122:GLN:HG2	2.39	0.46
2:D:333:ARG:HH21	2:D:421:ASN:ND2	2.12	0.46
1:A:83:SER:HB3	2:C:554:SER:O	2.15	0.46
2:C:554:SER:HB3	2:C:560:ASP:HB3	1.97	0.46
2:D:271:TRP:CZ3	2:D:279:GLU:HG3	2.50	0.46
8:C:605:HEM:HBC2	8:C:605:HEM:HMC2	1.98	0.46
2:C:465:MET:HE1	2:C:471:PRO:CD	2.44	0.46
2:C:514:TRP:CE2	2:C:515:GLU:HG3	2.50	0.46
2:C:199:VAL:HG12	2:C:254:LEU:HD21	1.97	0.46
2:C:123:PRO:HB3	9:C:606:ACY:H3	1.98	0.46
2:D:120:VAL:HG12	2:D:122:GLN:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:349:ARG:HG3	2:C:351:GLN:HG2	1.98	0.45
2:D:256:GLU:OE1	2:D:287:MET:HE1	2.17	0.44
2:C:491:VAL:HB	2:C:495:LEU:HB2	1.98	0.44
2:C:485:LEU:HD13	2:C:490:ARG:HA	1.99	0.44
2:D:244:PRO:HB2	2:D:343:MET:SD	2.58	0.44
2:D:349:ARG:HG3	2:D:351:GLN:CG	2.46	0.43
2:C:124:PRO:HA	9:C:606:ACY:CH3	2.49	0.43
2:D:514:TRP:CE2	2:D:515:GLU:HG3	2.54	0.43
2:D:554:SER:HB3	2:D:560:ASP:HB3	2.01	0.43
2:D:252:LEU:HD11	2:D:537:ILE:HA	2.02	0.42
2:C:333:ARG:HD3	2:C:421:ASN:ND2	2.34	0.42
2:C:417:LEU:HB3	2:C:418:PRO:HD3	2.00	0.42
2:C:244:PRO:HD3	2:C:364:VAL:O	2.19	0.42
1:B:79:ASP:O	2:D:388:PRO:HB3	2.19	0.42
2:C:346:LEU:HB3	2:C:350:TYR:HA	2.02	0.42
1:A:68:ILE:CD1	2:C:464:LEU:HD23	2.50	0.42
2:C:123:PRO:HA	2:C:124:PRO:HA	1.84	0.42
1:B:101:PRO:HD2	2:D:164:ILE:O	2.19	0.42
2:D:577:GLU:O	2:D:578:ALA:C	2.63	0.41
1:A:52:LYS:HG3	1:A:56:PHE:C	2.45	0.41
2:D:123:PRO:HA	2:D:124:PRO:HA	1.89	0.41
2:C:242:GLU:OE1	8:C:605:HEM:HBB2	2.21	0.41
2:D:120:VAL:HG12	2:D:122:GLN:HG3	2.03	0.41
2:D:241:SER:O	2:D:366:PHE:HA	2.20	0.41
2:C:113:VAL:HG12	2:C:114:ASN:N	2.35	0.41
2:C:114:ASN:HB3	2:C:117:THR:OG1	2.20	0.41
1:B:6:LYS:HE2	1:B:6:LYS:HB2	1.99	0.41
2:D:128:LEU:HB2	2:D:144:ILE:HB	2.03	0.41
2:C:242:GLU:O	2:C:365:PHE:HA	2.22	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	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
1	B	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
2	C	463/466 (99%)	450 (97%)	13 (3%)	0	100	100
2	D	463/466 (99%)	453 (98%)	10 (2%)	0	100	100
All	All	1130/1140 (99%)	1101 (97%)	29 (3%)	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	90/90 (100%)	88 (98%)	2 (2%)	45	32
1	B	90/90 (100%)	90 (100%)	0	100	100
2	C	410/410 (100%)	400 (98%)	10 (2%)	43	28
2	D	410/410 (100%)	402 (98%)	8 (2%)	48	36
All	All	1000/1000 (100%)	980 (98%)	20 (2%)	48	36

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

Mol	Chain	Res	Type
1	A	4	GLN
1	A	6	LYS
2	C	122	GLN
2	C	140	GLN
2	C	175	MET
2	C	254	LEU
2	C	348	ASN
2	C	361	LEU
2	C	466	GLU
2	C	523	GLN
2	C	547	SER
2	C	558	PRO
2	D	122	GLN

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Mol	Chain	Res	Type
2	D	124	PRO
2	D	138	LYS
2	D	254	LEU
2	D	267	LEU
2	D	322	PRO
2	D	523	GLN
2	D	547	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
2	C	163	GLN
2	C	200	ASN
2	C	206	ASN
2	C	326	ASN
2	C	348	ASN
2	C	421	ASN
2	C	540	ASN
2	D	206	ASN
2	D	348	ASN
2	D	421	ASN
2	D	523	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CSO	C	150	2	3,6,7	0.76	0	1,6,8	1.12	0
2	CSO	D	150	2	3,6,7	0.72	0	1,6,8	1.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSO	C	150	2	-	0/1/5/7	-
2	CSO	D	150	2	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

12 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	E	1	2,3	14,14,15	0.76	0	17,19,21	0.85	0
3	NAG	E	2	3	14,14,15	0.59	0	17,19,21	0.83	0
3	BMA	E	3	3	11,11,12	0.70	0	15,15,17	0.53	0
3	MAN	E	4	3	11,11,12	1.02	0	15,15,17	0.53	0
3	MAN	E	5	3	11,11,12	0.61	0	15,15,17	0.67	1 (6%)
3	FUC	E	6	3	10,10,11	0.62	0	14,14,16	0.48	0
3	NAG	F	1	2,3	14,14,15	0.60	0	17,19,21	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	F	2	3	14,14,15	0.55	0	17,19,21	0.81	1 (5%)
3	BMA	F	3	3	11,11,12	0.57	0	15,15,17	0.58	0
3	MAN	F	4	3	11,11,12	0.88	0	15,15,17	0.66	1 (6%)
3	MAN	F	5	3	11,11,12	0.60	0	15,15,17	0.58	1 (6%)
3	FUC	F	6	3	10,10,11	0.55	0	14,14,16	0.38	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	E	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
3	FUC	E	6	3	-	-	0/1/1/1
3	NAG	F	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	FUC	F	6	3	-	-	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2	NAG	C4-C3-C2	-2.21	107.78	111.02
3	F	4	MAN	C1-O5-C5	2.11	115.01	112.19
3	F	5	MAN	C1-O5-C5	2.09	114.98	112.19
3	E	5	MAN	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

There are no torsion outliers.

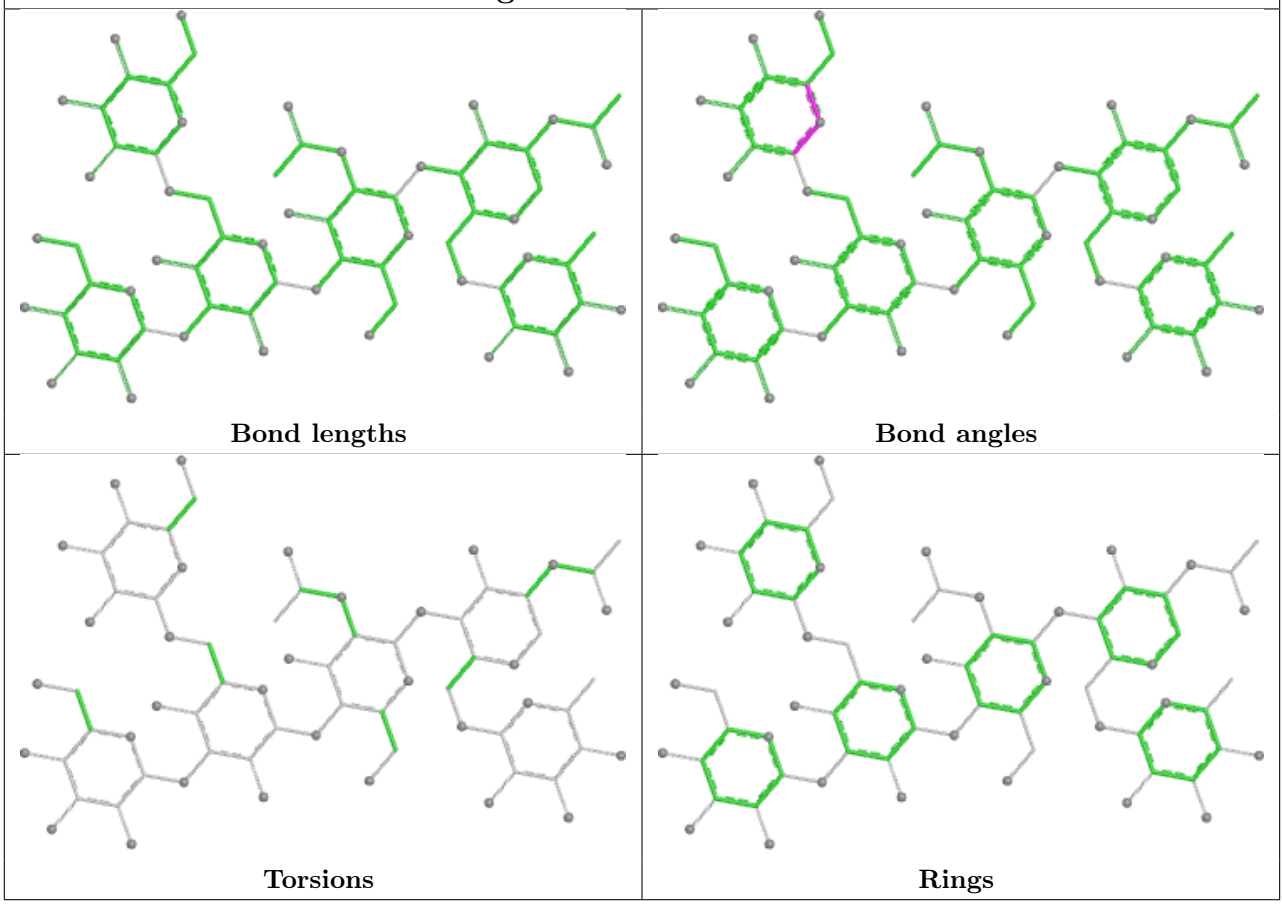
There are no ring outliers.

No monomer is involved in short contacts.

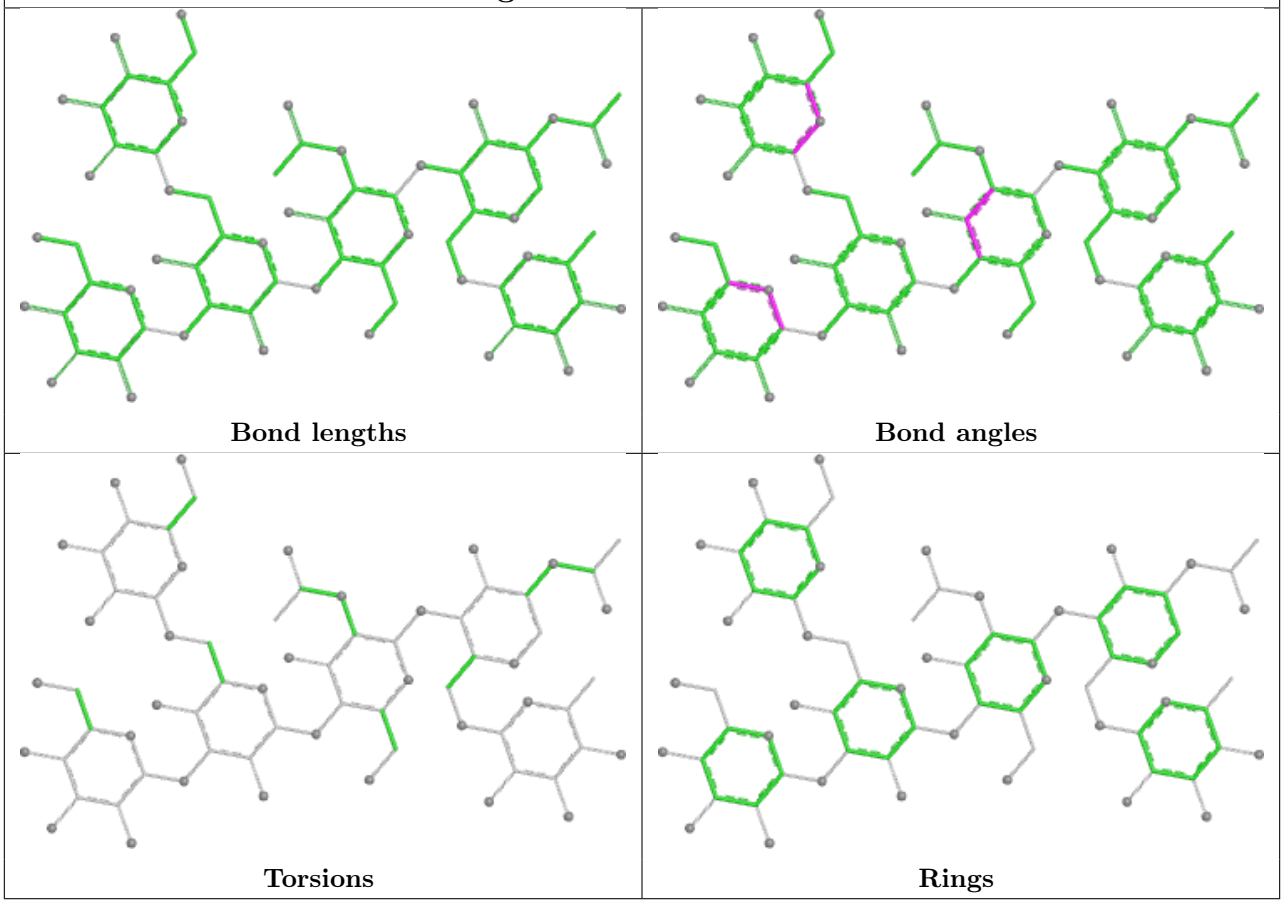
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain E



Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	$\#\|Z\| > 2$
4	SCN	B	201	-	1,2,2	1.69	0	0,1,1	-	-
6	NAG	C	601	2	14,14,15	0.82	1 (7%)	17,19,21	0.99	1 (5%)
9	ACY	D	608	-	3,3,3	1.29	0	3,3,3	1.66	1 (33%)
4	SCN	A	203	-	1,2,2	1.90	0	0,1,1	-	-
4	SCN	B	202	-	1,2,2	1.97	0	0,1,1	-	-
9	ACY	D	606	-	3,3,3	1.31	0	3,3,3	1.62	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SCN	A	201	-	1,2,2	1.55	0	0,1,1	-	-
9	ACY	C	608	-	3,3,3	1.41	1 (33%)	3,3,3	1.61	1 (33%)
9	ACY	D	607	-	3,3,3	1.40	1 (33%)	3,3,3	1.69	1 (33%)
5	SO4	D	605	-	4,4,4	0.45	0	6,6,6	0.12	0
5	SO4	A	202	-	4,4,4	0.27	0	6,6,6	0.08	0
8	HEM	C	605	1,2	50,50,50	1.15	3 (6%)	67,82,82	1.04	2 (2%)
8	HEM	D	601	1,2	50,50,50	1.12	6 (12%)	67,82,82	1.06	1 (1%)
5	SO4	C	604	-	4,4,4	0.46	0	6,6,6	0.17	0
6	NAG	D	602	2	14,14,15	0.68	0	17,19,21	0.68	0
9	ACY	C	606	-	3,3,3	1.16	0	3,3,3	1.59	1 (33%)
6	NAG	C	602	2	14,14,15	0.80	0	17,19,21	0.80	0
9	ACY	C	607	-	3,3,3	1.10	0	3,3,3	1.68	1 (33%)
6	NAG	D	603	2	14,14,15	0.61	0	17,19,21	0.86	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
6	NAG	D	602	2	-	0/6/23/26	0/1/1/1
6	NAG	C	602	2	-	0/6/23/26	0/1/1/1
8	HEM	C	605	1,2	-	5/14/54/54	-
6	NAG	D	603	2	-	0/6/23/26	0/1/1/1
6	NAG	C	601	2	-	0/6/23/26	0/1/1/1
8	HEM	D	601	1,2	-	4/14/54/54	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	601	HEM	CBB-CAB	3.32	1.46	1.30
8	C	605	HEM	CBB-CAB	3.25	1.46	1.30
8	C	605	HEM	CBC-CAC	2.98	1.44	1.30
8	D	601	HEM	CBC-CAC	2.81	1.43	1.30
8	C	605	HEM	CAC-C3C	-2.44	1.40	1.47
9	D	607	ACY	O-C	2.27	1.32	1.22
6	C	601	NAG	C1-C2	2.22	1.55	1.52
9	C	608	ACY	O-C	2.17	1.31	1.22
8	D	601	HEM	CAC-C3C	-2.13	1.41	1.47
8	D	601	HEM	O2A-CGA	-2.07	1.24	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	601	HEM	C2A-C3A	-2.05	1.33	1.38
8	D	601	HEM	O2D-CGD	-2.01	1.24	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	601	HEM	C3B-C4B-NB	4.14	112.44	109.47
8	C	605	HEM	C3B-C4B-NB	3.48	111.97	109.47
6	C	601	NAG	C1-O5-C5	2.86	116.02	112.19
6	D	603	NAG	C1-C2-N2	-2.37	106.69	110.43
9	D	607	ACY	O-C-CH3	-2.30	113.11	122.53
9	C	607	ACY	O-C-CH3	-2.29	113.13	122.53
9	D	608	ACY	O-C-CH3	-2.26	113.26	122.53
9	D	606	ACY	O-C-CH3	-2.21	113.46	122.53
9	C	608	ACY	O-C-CH3	-2.19	113.54	122.53
8	C	605	HEM	C2B-C1B-NB	2.16	112.32	109.84
9	C	606	ACY	O-C-CH3	-2.14	113.75	122.53

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	605	HEM	CAD-CBD-CGD-O2D
8	C	605	HEM	CAA-CBA-CGA-O2A
8	D	601	HEM	CAD-CBD-CGD-O2D
8	C	605	HEM	CAD-CBD-CGD-O1D
8	D	601	HEM	CAD-CBD-CGD-O1D
8	C	605	HEM	CAA-CBA-CGA-O1A
8	D	601	HEM	CAA-CBA-CGA-O1A
8	D	601	HEM	CAA-CBA-CGA-O2A
8	C	605	HEM	C2B-C3B-CAB-CBB

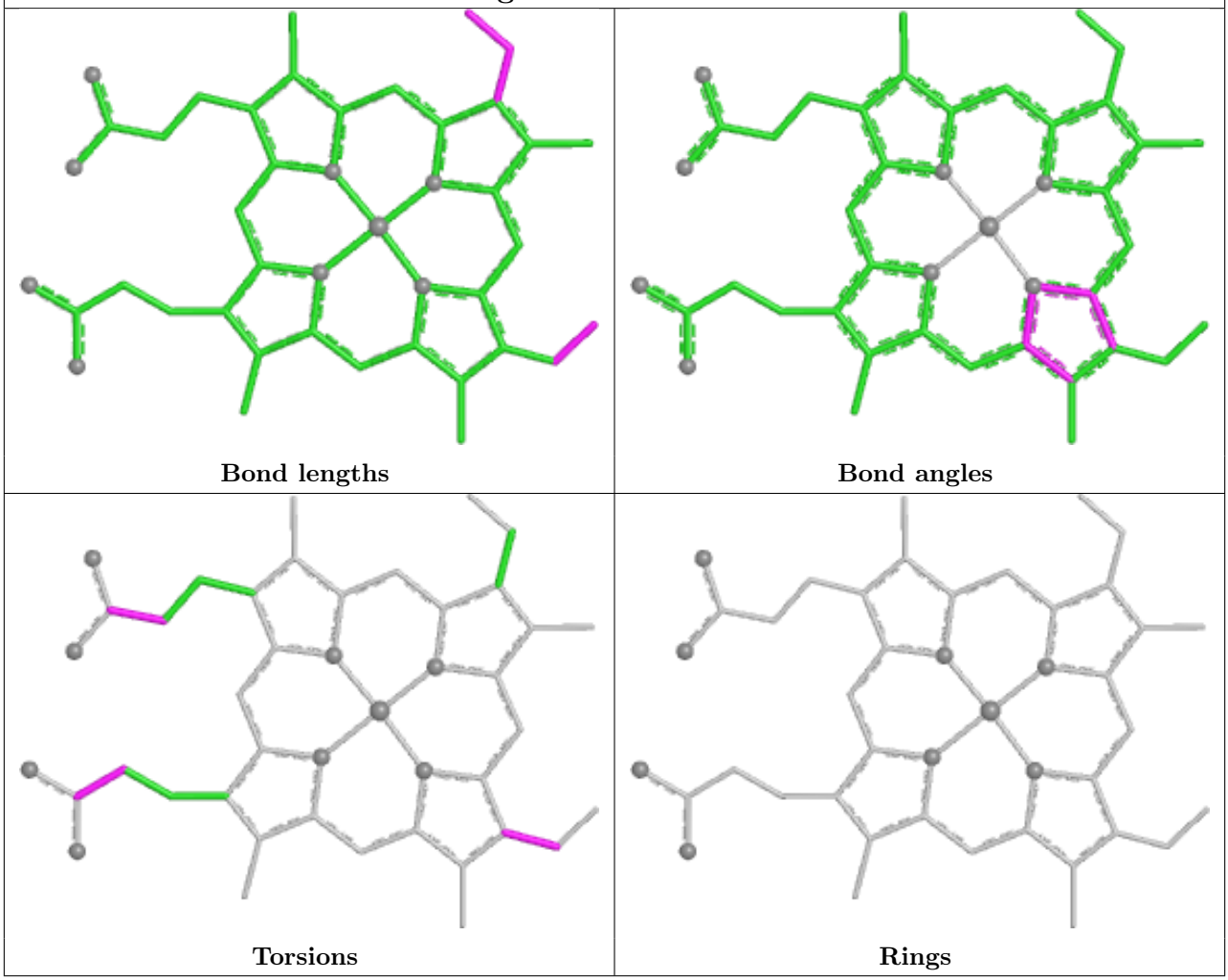
There are no ring outliers.

4 monomers are involved in 8 short contacts:

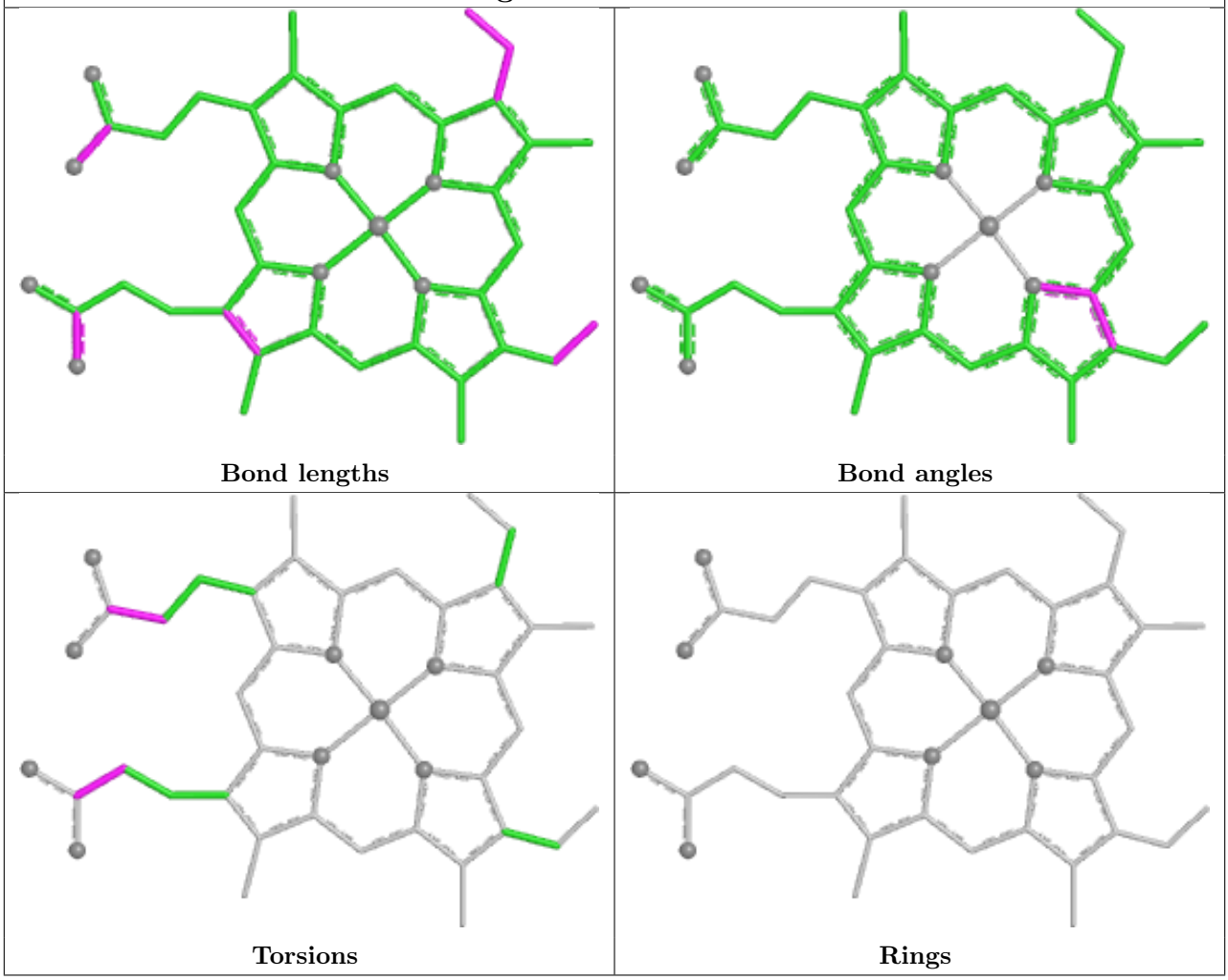
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	607	ACY	2	0
8	C	605	HEM	2	0
8	D	601	HEM	2	0
9	C	606	ACY	2	0

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 HEM C 605



Ligand HEM D 601



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	104/104 (100%)	-0.60	3 (2%) 53 57	6, 9, 23, 46	0
1	B	104/104 (100%)	-0.70	0 100 100	6, 10, 19, 24	0
2	C	465/466 (99%)	-0.56	8 (1%) 69 73	5, 10, 24, 39	0
2	D	465/466 (99%)	-0.45	7 (1%) 72 76	6, 12, 27, 43	0
All	All	1138/1140 (99%)	-0.53	18 (1%) 70 74	5, 11, 25, 46	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	113	VAL	10.0
2	D	217	HIS	5.2
2	C	355	PRO	5.1
2	C	217	HIS	3.9
2	D	355	PRO	3.8
2	D	578	ALA	3.6
1	A	4	GLN	3.5
2	D	349	ARG	2.8
2	C	348	ASN	2.8
1	A	3	GLU	2.8
2	C	140	GLN	2.6
2	C	349	ARG	2.4
2	D	576	ARG	2.4
2	D	356	ASN	2.3
2	D	226	ARG	2.2
1	A	1	CYS	2.1
2	C	141	ALA	2.1
2	C	139	ASN	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CSO	C	150	7/8	0.93	0.06	8,10,11,15	0
2	CSO	D	150	7/8	0.95	0.05	6,8,10,14	0

6.3 Carbohydrates (i)

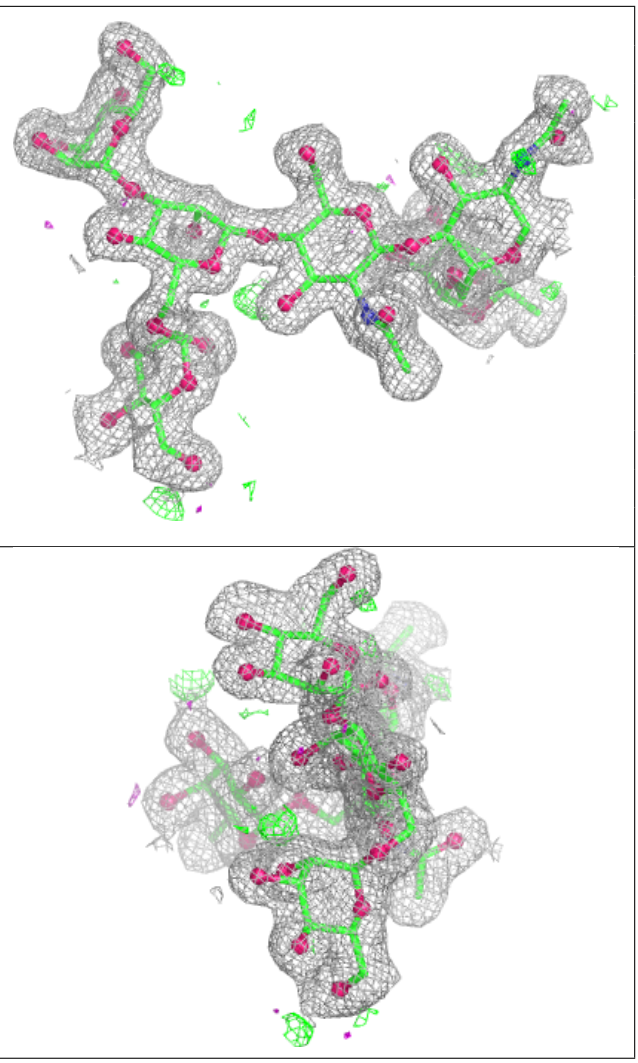
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MAN	F	4	11/12	0.86	0.09	22,24,28,30	0
3	MAN	E	4	11/12	0.90	0.07	24,26,27,27	0
3	NAG	E	1	14/15	0.94	0.06	8,12,16,17	0
3	FUC	E	6	10/11	0.94	0.05	15,16,18,19	0
3	NAG	F	1	14/15	0.94	0.06	10,12,17,20	0
3	BMA	E	3	11/12	0.94	0.07	11,13,16,21	0
3	MAN	E	5	11/12	0.95	0.05	13,15,17,18	0
3	FUC	F	6	10/11	0.95	0.05	14,15,17,18	0
3	NAG	E	2	14/15	0.96	0.05	8,10,11,11	0
3	MAN	F	5	11/12	0.96	0.05	13,14,16,17	0
3	BMA	F	3	11/12	0.96	0.05	10,12,15,19	0
3	NAG	F	2	14/15	0.97	0.04	8,11,12,13	0

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

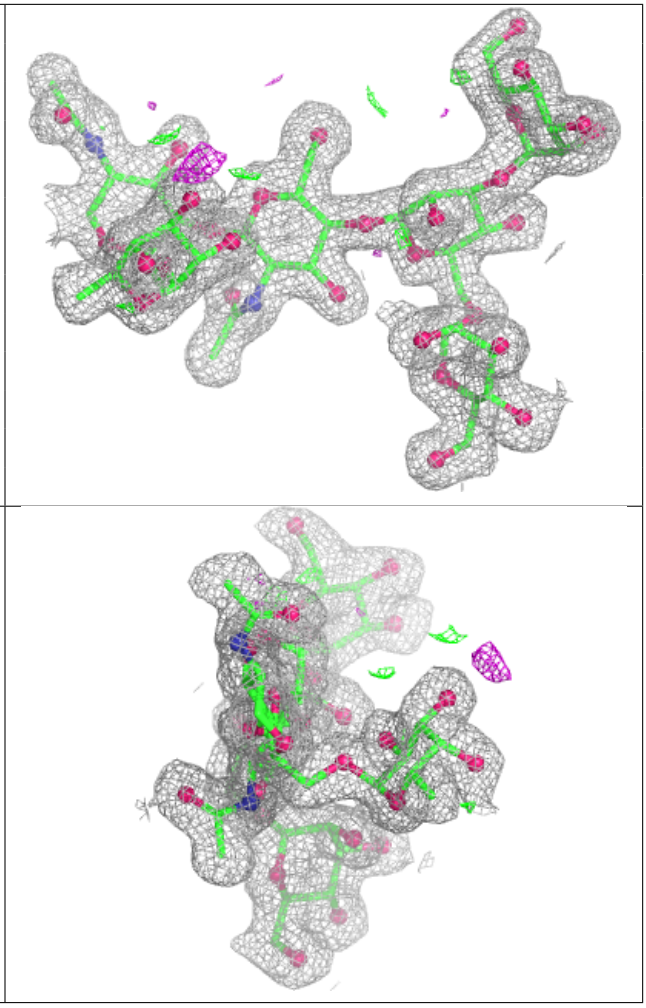
Electron density around Chain E:

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



Electron density around Chain F:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	ACY	D	607	4/4	0.29	0.26	38,38,38,39	0
5	SO4	D	605	5/5	0.51	0.22	46,47,47,47	5
6	NAG	D	603	14/15	0.77	0.11	32,34,37,38	0
9	ACY	C	608	4/4	0.78	0.12	27,28,29,29	0
9	ACY	C	606	4/4	0.78	0.09	27,28,29,30	0
9	ACY	C	607	4/4	0.82	0.11	17,20,20,21	0
9	ACY	D	606	4/4	0.84	0.10	20,21,21,24	0
9	ACY	D	608	4/4	0.85	0.11	30,31,31,32	0
6	NAG	C	602	14/15	0.87	0.11	23,28,36,36	0
6	NAG	D	602	14/15	0.89	0.08	17,24,28,29	0

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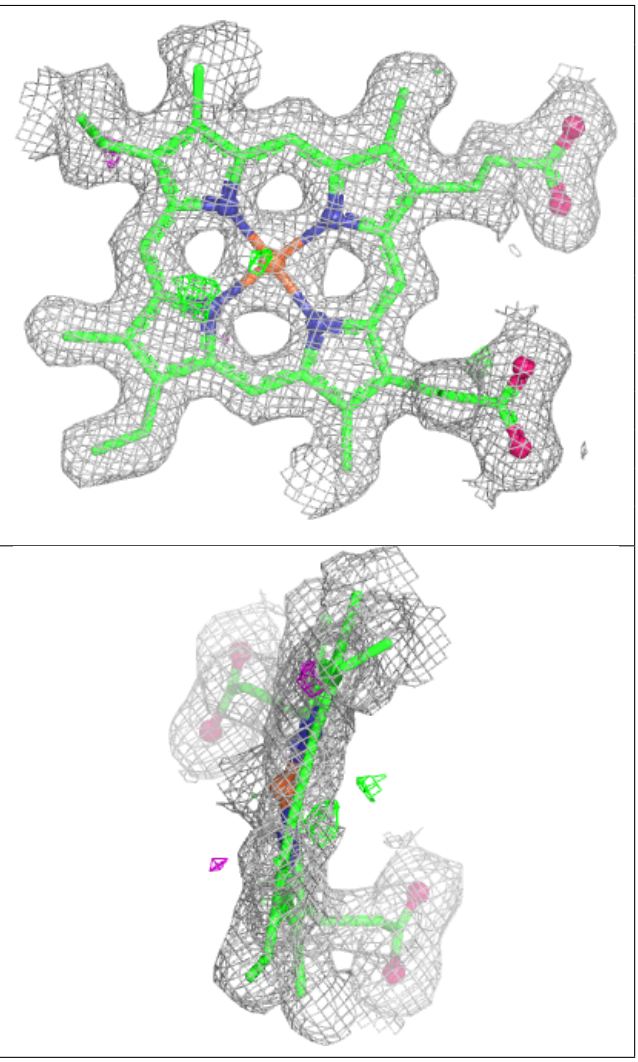
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	C	601	14/15	0.90	0.07	15,17,21,22	0
5	SO4	C	604	5/5	0.94	0.10	27,29,31,33	0
4	SCN	B	202	3/3	0.98	0.05	19,19,19,19	0
5	SO4	A	202	5/5	0.98	0.06	25,25,28,29	0
8	HEM	C	605	43/43	0.98	0.05	4,8,9,10	0
8	HEM	D	601	43/43	0.98	0.05	5,8,10,12	0
4	SCN	A	201	3/3	0.98	0.05	12,12,12,17	0
4	SCN	A	203	3/3	0.99	0.03	15,15,18,20	0
4	SCN	B	201	3/3	0.99	0.05	11,11,16,17	0
7	CA	C	603	1/1	1.00	0.02	10,10,10,10	0
7	CA	D	604	1/1	1.00	0.02	9,9,9,9	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.

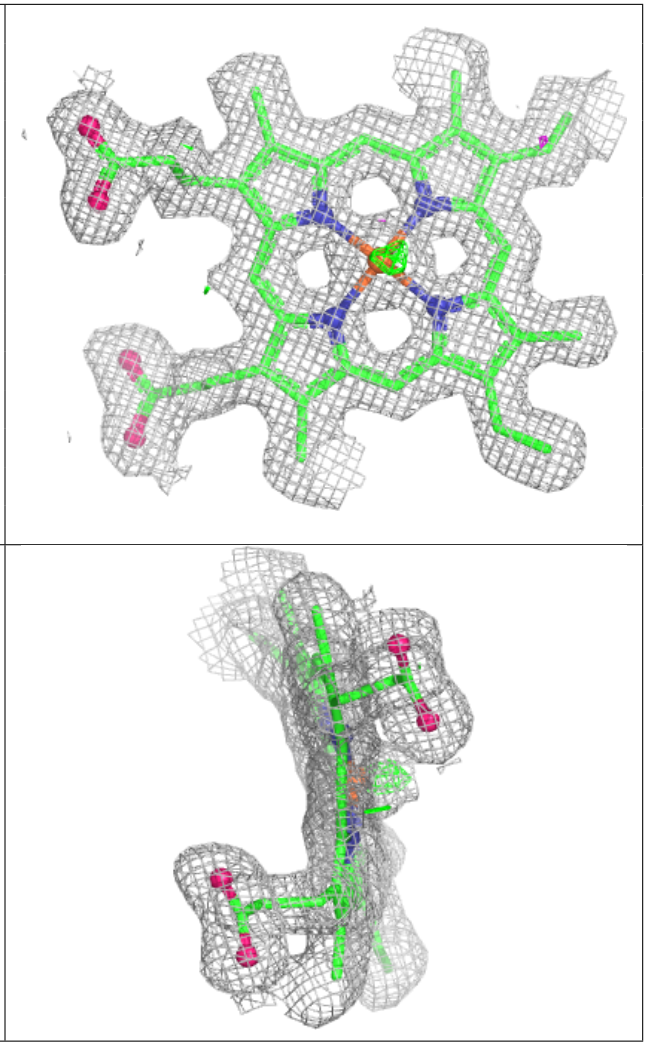
Electron density around HEM C 605:

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 HEM D 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.