Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 02:15 AM EDT

PDB ID	:	1DNW / pdb_00001dnw
Title	:	HUMAN MYELOPEROXIDASE-CYANIDE-THIOCYANATE COMPLEX
Authors	:	Blair-Johnson, M.; Fiedler, T.J.; Fenna, R.E.
Deposited on	:	1999-12-16
Resolution	:	1.90 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:

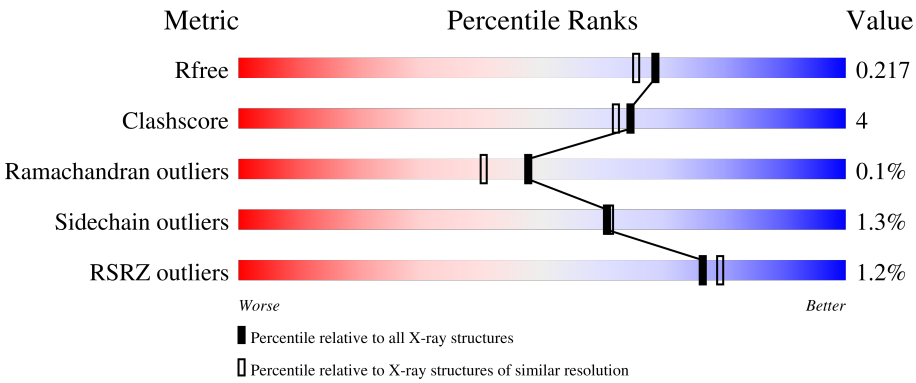
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	2% 88% 12%
1	B	104	89% 11%
2	C	466	% 86% 13% •
2	D	466	% 86% 14%
3	E	6	100%

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Mol	Chain	Length	Quality of chain
3	F	6	83% 17%

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
4	SCN	B	203	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 10349 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

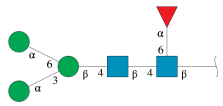
- Molecule 2 is a protein called MYELOPEROXIDASE.

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:

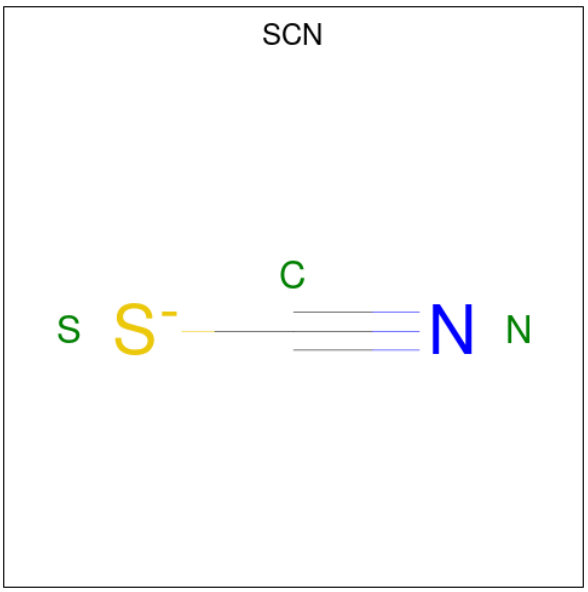
Chain	Residue	Modelled	Actual	Comment	Reference
C	150	CSO	CYS	modified residue	UNP P05164
D	150	CSO	CYS	modified residue	UNP P05164

- 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.



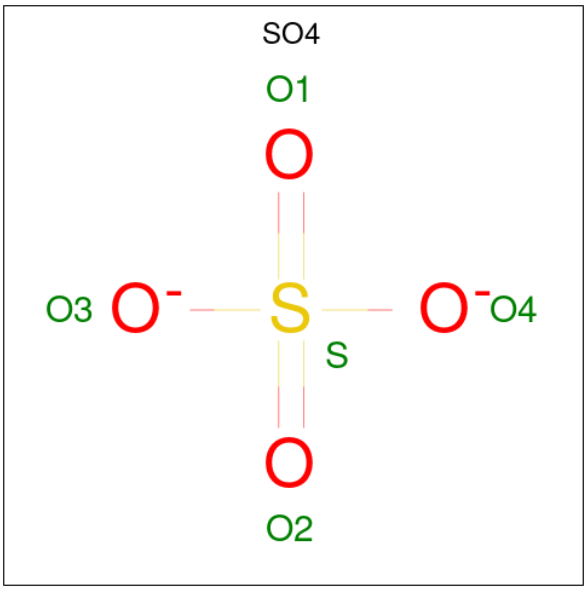
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	6	71	40	2	29	0	0	0
3	F	6	71	40	2	29	0	0	0

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



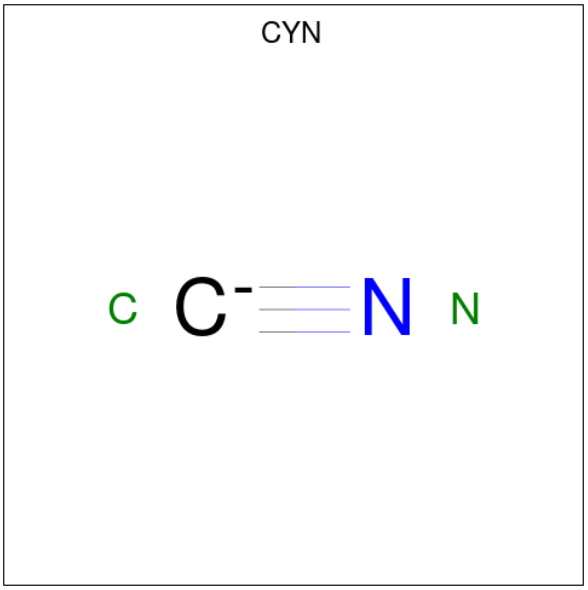
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
4	A	1	3	1	1	1	0	0
4	C	1	3	1	1	1	0	0
4	B	1	3	1	1	1	0	0
4	B	1	3	1	1	1	0	0

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



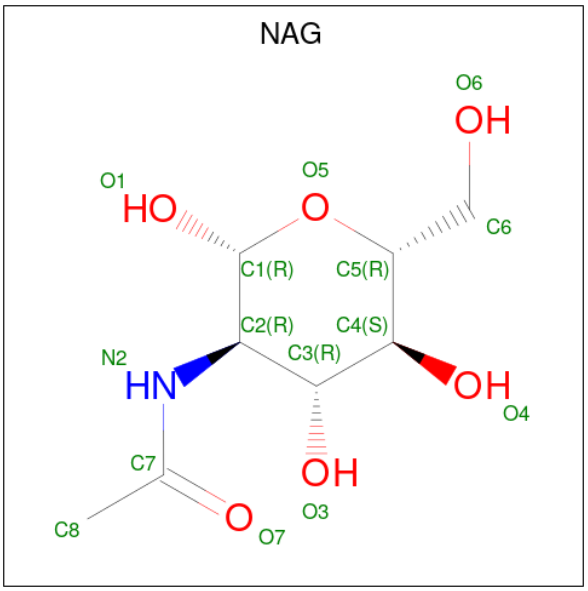
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	C	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0

- Molecule 6 is CYANIDE ION (CCD ID: CYN) (formula: CN).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
6	A	1	2	1	1	0	0
			Total	C	N		
6	C	1	2	1	1	0	0
			Total	C	N		
6	B	1	2	1	1	0	0
			Total	C	N		
6	D	1	2	1	1	0	0

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

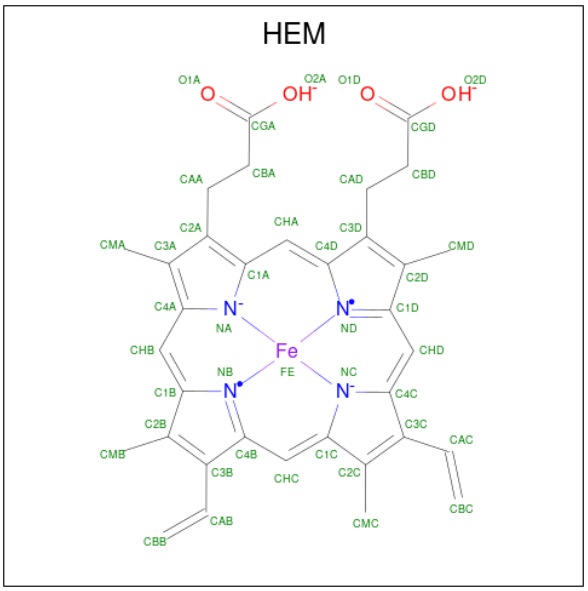


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	C	1	14	8	1	5	0	0
			Total	C	N	O		
7	C	1	14	8	1	5	0	0
			Total	C	N	O		
7	D	1	14	8	1	5	0	0
			Total	C	N	O		
7	D	1	14	8	1	5	0	0

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

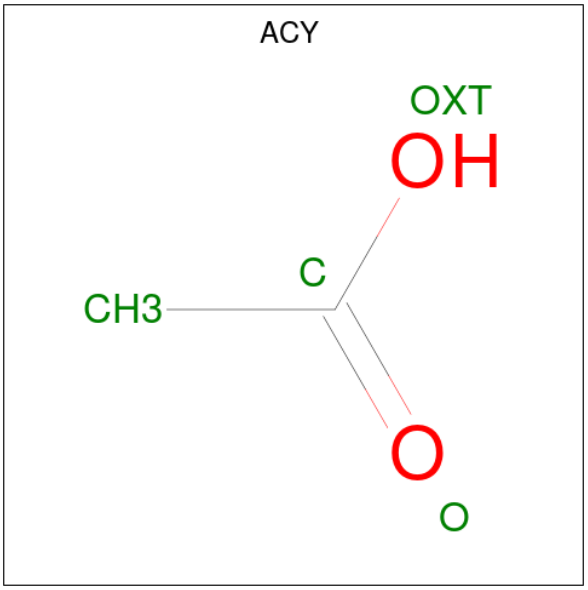
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
8	C	1	1	1	0	0
			Total	Ca		
8	D	1	1	1	0	0

- Molecule 9 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		
9	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
9	D	1	43	34	1	4	4	0	0

- Molecule 10 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



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

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

- Molecule 11 is water.

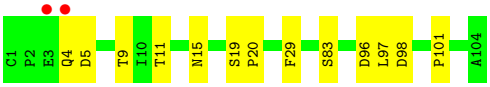
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	96	96	96	0	0
			Total	O		
11	C	339	339	339	0	0
			Total	O		
11	B	100	100	100	0	0
			Total	O		
11	D	327	327	327	0	0

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:

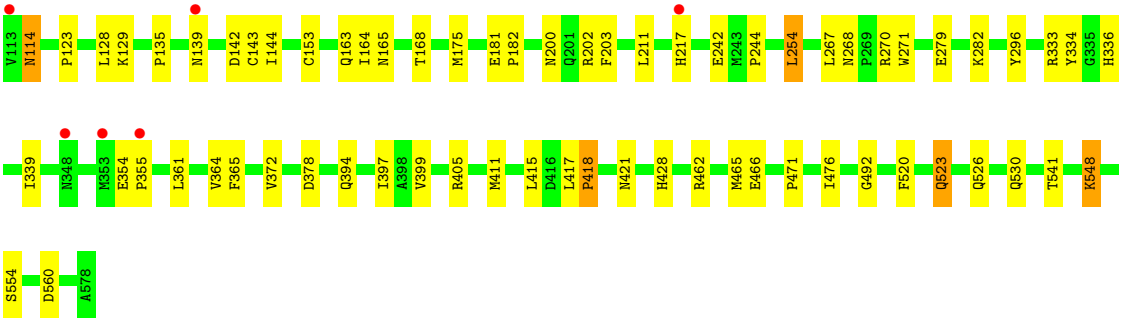


- Molecule 1: MYELOPEROXIDASE

Chain B:

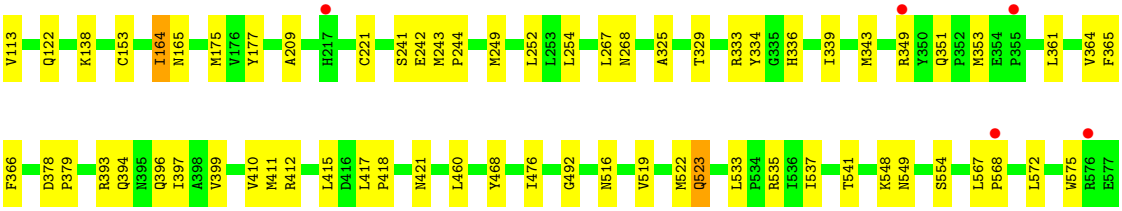
- Molecule 2: MYELOPEROXIDASE

Chain C:

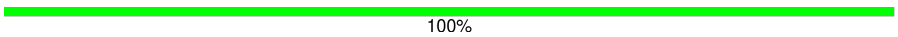


- Molecule 2: MYELOPEROXIDASE

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	111.26Å 63.77Å 92.60Å 90.00° 97.51° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 10.00 – 1.91	Depositor EDS
% Data completeness (in resolution range)	93.4 (10.00-1.90) 91.8 (10.00-1.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.74 (at 1.91Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.224 0.188 , 0.217	Depositor DCC
R_{free} test set	4686 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	17.1	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 62.9	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	0.94	EDS
Total number of atoms	10349	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: CYN, NAG, SO4, SCN, CA, MAN, FUC, HEM, BMA, CSO, ACY

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	0.51	0/863	1.10	8/1174 (0.7%)
1	B	0.49	0/863	1.10	7/1174 (0.6%)
2	C	0.50	0/3811	1.03	19/5168 (0.4%)
2	D	0.52	1/3811 (0.0%)	1.03	22/5168 (0.4%)
All	All	0.51	1/9348 (0.0%)	1.04	56/12684 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	353	MET	SD-CE	5.59	1.93	1.79

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	397	ILE	N-CA-C	7.83	117.78	110.42
2	D	268	ASN	CA-C-N	7.75	127.81	119.28
2	D	268	ASN	C-N-CA	7.75	127.81	119.28
1	B	19	SER	CA-C-N	7.72	129.49	119.84
1	B	19	SER	C-N-CA	7.72	129.49	119.84
1	B	96	ASP	N-CA-C	-7.38	104.42	113.50
2	C	397	ILE	N-CA-C	7.29	117.28	110.42
2	D	476	ILE	N-CA-C	7.26	117.98	110.36
1	A	20	PRO	N-CA-C	7.22	123.30	113.98
1	A	96	ASP	N-CA-C	-7.21	104.61	113.41
2	D	399	VAL	N-CA-C	6.76	118.79	109.80
2	C	153	CYS	CA-C-N	6.72	127.12	119.93
2	C	153	CYS	C-N-CA	6.72	127.12	119.93
1	A	98	ASP	N-CA-C	6.72	119.53	108.99
2	C	372	VAL	N-CA-C	6.69	116.82	110.53
2	D	339	ILE	N-CA-C	6.51	117.44	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	399	VAL	N-CA-C	6.45	118.38	109.80
2	D	153	CYS	CA-C-N	6.36	126.70	119.83
2	D	153	CYS	C-N-CA	6.36	126.70	119.83
2	C	476	ILE	N-CA-C	6.30	116.98	110.36
1	B	98	ASP	N-CA-C	6.27	118.83	108.99
2	D	468	TYR	N-CA-C	6.07	120.76	113.23
2	C	336	HIS	CB-CG-CD2	-6.06	123.32	131.20
1	B	67	GLU	N-CA-C	5.87	119.63	112.23
2	C	492	GLY	CA-C-N	5.86	125.34	119.24
2	C	492	GLY	C-N-CA	5.86	125.34	119.24
2	C	268	ASN	CA-C-N	5.85	125.71	119.28
2	C	268	ASN	C-N-CA	5.85	125.71	119.28
1	A	19	SER	CA-C-N	5.70	125.40	119.82
1	A	19	SER	C-N-CA	5.70	125.40	119.82
2	D	410	VAL	N-CA-C	5.66	117.65	111.77
2	C	296	TYR	N-CA-C	5.62	118.49	111.24
1	A	97	LEU	N-CA-C	5.55	120.03	112.04
1	B	9	THR	N-CA-C	-5.55	103.06	110.55
2	D	209	ALA	N-CA-C	5.45	118.34	110.28
1	B	15	ASN	N-CA-C	-5.42	105.27	111.07
2	D	549	ASN	N-CA-C	-5.40	102.29	110.28
2	D	548	LYS	N-CA-C	-5.39	102.50	110.48
2	D	492	GLY	CA-C-N	5.24	125.29	119.32
2	D	492	GLY	C-N-CA	5.24	125.29	119.32
2	D	243	MET	CA-C-N	5.22	126.37	119.84
2	D	243	MET	C-N-CA	5.22	126.37	119.84
2	C	339	ILE	N-CA-C	5.18	115.77	109.30
2	C	143	CYS	N-CA-C	5.16	115.16	107.88
2	C	336	HIS	CG-CD2-NE2	-5.15	102.05	107.20
2	D	164	ILE	N-CA-C	5.13	115.87	108.48
2	D	412	ARG	N-CA-C	5.12	117.60	111.71
2	C	548	LYS	N-CA-C	-5.11	103.65	110.55
2	D	334	TYR	N-CA-C	-5.10	105.85	111.71
2	C	334	TYR	N-CA-C	-5.08	105.87	111.71
2	D	177	TYR	N-CA-C	5.07	119.52	113.23
1	A	9	THR	N-CA-C	-5.04	104.02	110.53
2	C	405	ARG	N-CA-C	5.03	118.95	112.41
2	D	336	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	A	15	ASN	N-CA-C	-5.01	105.82	111.28
2	C	394	GLN	N-CA-C	5.01	118.49	112.38

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	6	0
2	C	3733	0	3724	36	0
2	D	3733	0	3724	32	0
3	E	71	0	61	0	0
3	F	71	0	61	0	0
4	A	3	0	0	0	0
4	B	6	0	0	2	0
4	C	3	0	0	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
6	A	2	0	0	1	0
6	B	2	0	0	1	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
7	C	28	0	26	0	0
7	D	28	0	26	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	C	43	0	30	1	0
9	D	43	0	30	1	0
10	C	12	0	9	0	0
10	D	12	0	9	1	0
11	A	96	0	0	1	0
11	B	100	0	0	1	0
11	C	339	0	0	6	0
11	D	327	0	0	1	0
All	All	10349	0	9296	73	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 (73) 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:333:ARG:HH21	2:C:421:ASN:HD22	1.31	0.75
2:C:333:ARG:HH21	2:C:421:ASN:ND2	1.85	0.74
2:C:465:MET:HE3	11:C:997:HOH:O	1.90	0.71
11:A:302:HOH:O	2:C:129:LYS:HD3	1.92	0.69
2:C:200:ASN:HD22	2:C:203:PHE:H	1.41	0.67
4:C:605:SCN:S	11:C:1009:HOH:O	2.54	0.66
2:D:244:PRO:HB2	2:D:343:MET:SD	2.39	0.63
2:C:465:MET:HE1	2:C:471:PRO:HD3	1.80	0.62
2:D:349:ARG:HG3	2:D:351:GLN:HG2	1.82	0.62
2:C:211:LEU:HD23	2:C:254:LEU:HD13	1.82	0.61
2:D:411:MET:HE2	2:D:415:LEU:HD21	1.82	0.60
2:C:200:ASN:ND2	2:C:203:PHE:H	2.01	0.58
2:D:241:SER:O	2:D:366:PHE:HA	2.04	0.58
1:A:4:GLN:HG2	1:A:5:ASP:N	2.18	0.57
2:C:200:ASN:ND2	2:C:202:ARG:H	2.02	0.57
2:C:139:ASN:HB3	11:C:939:HOH:O	2.04	0.56
2:C:354:GLU:HB3	2:C:355:PRO:HA	1.87	0.56
2:C:411:MET:HE2	2:C:415:LEU:HD11	1.89	0.55
2:C:135:PRO:HG2	11:C:703:HOH:O	2.07	0.54
2:C:271:TRP:CZ3	2:C:279:GLU:HG3	2.44	0.53
2:D:244:PRO:HD3	2:D:364:VAL:O	2.07	0.53
2:D:113:VAL:HG21	2:D:122:GLN:HB2	1.89	0.53
1:B:83:SER:HB3	2:D:554:SER:O	2.10	0.52
1:A:83:SER:HB3	2:C:554:SER:O	2.09	0.52
2:C:244:PRO:HD3	2:C:364:VAL:O	2.08	0.52
2:D:393:ARG:HB2	2:D:396:GLN:HB2	1.91	0.52
2:C:200:ASN:HD22	2:C:202:ARG:H	1.56	0.51
2:D:333:ARG:HH21	2:D:421:ASN:ND2	2.09	0.51
4:B:203:SCN:C	2:D:242:GLU:HG3	2.41	0.50
2:C:417:LEU:HB3	2:C:418:PRO:HD3	1.92	0.50
2:D:417:LEU:HB3	2:D:418:PRO:HD3	1.94	0.50
4:B:203:SCN:N	6:B:204:CYN:N	2.60	0.50
2:D:349:ARG:HE	2:D:351:GLN:HG3	1.76	0.50
1:B:101:PRO:HD2	2:D:164:ILE:O	2.12	0.49
2:D:523:GLN:H	2:D:523:GLN:CD	2.21	0.49
1:A:101:PRO:HD2	2:C:164:ILE:O	2.13	0.49
2:D:572:LEU:O	2:D:575:TRP:HB2	2.13	0.49
2:C:333:ARG:HD3	2:C:421:ASN:ND2	2.28	0.49
1:A:29:PHE:CE2	2:C:165:ASN:HB2	2.47	0.48
2:D:411:MET:CE	2:D:415:LEU:HD21	2.43	0.48
6:A:203:CYN:C	9:C:607:HEM:ND	2.77	0.48
2:D:252:LEU:HD11	2:D:537:ILE:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:242:GLU:OE1	9:D:601:HEM:HBB2	2.14	0.47
1:B:29:PHE:CZ	2:D:329:THR:HG21	2.50	0.47
2:C:128:LEU:HB2	2:C:144:ILE:HB	1.96	0.47
2:D:249:MET:HE1	2:D:533:LEU:HD11	1.98	0.46
2:D:535:ARG:NH2	2:D:567:LEU:O	2.49	0.45
1:A:11:THR:O	2:C:168:THR:HG22	2.16	0.45
2:C:270:ARG:NH2	11:C:704:HOH:O	2.49	0.45
2:D:394:GLN:HB3	2:D:460:LEU:HD22	1.99	0.45
2:C:462:ARG:O	2:C:466:GLU:HG2	2.18	0.44
2:D:522:MET:HG3	10:D:607:ACY:H1	2.00	0.44
2:D:378:ASP:HB2	2:D:379:PRO:HD3	2.00	0.44
2:C:378:ASP:OD1	2:C:541:THR:HB	2.18	0.44
1:B:32:TRP:CE2	2:D:325:ALA:HB2	2.53	0.43
2:C:282:LYS:HG2	2:C:520:PHE:CZ	2.54	0.43
2:D:361:LEU:O	2:D:364:VAL:HG22	2.19	0.42
2:C:526:GLN:NE2	2:C:530:GLN:HE21	2.17	0.42
2:C:548:LYS:HD2	2:C:560:ASP:HA	2.00	0.42
2:C:139:ASN:HB2	2:C:142:ASP:OD1	2.19	0.42
2:D:221:CYS:HA	2:D:366:PHE:O	2.19	0.42
2:D:568:PRO:HG2	11:D:875:HOH:O	2.19	0.42
2:C:114:ASN:HA	11:C:886:HOH:O	2.20	0.42
1:B:1:CYS:HB2	11:B:340:HOH:O	2.20	0.41
2:C:242:GLU:O	2:C:365:PHE:HA	2.20	0.41
2:C:333:ARG:NH2	2:C:421:ASN:HD22	2.08	0.41
2:D:242:GLU:O	2:D:365:PHE:HA	2.20	0.41
2:D:516:ASN:HB3	2:D:519:VAL:CG2	2.50	0.41
2:C:163:GLN:HG2	2:C:428:HIS:NE2	2.35	0.41
2:C:181:GLU:HB2	2:C:182:PRO:HD3	2.02	0.41
2:C:523:GLN:CD	2:C:523:GLN:H	2.28	0.41
1:B:29:PHE:CE2	2:D:165:ASN:HB2	2.56	0.41
2:D:378:ASP:OD1	2:D:541:THR:HB	2.21	0.41

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%)	100 (98%)	2 (2%)	0	100	100
1	B	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
2	C	463/466 (99%)	451 (97%)	11 (2%)	1 (0%)	43	36
2	D	463/466 (99%)	450 (97%)	13 (3%)	0	100	100
All	All	1130/1140 (99%)	1101 (97%)	28 (2%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	114	ASN

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%)	90 (100%)	0	100	100
1	B	90/90 (100%)	90 (100%)	0	100	100
2	C	410/410 (100%)	402 (98%)	8 (2%)	48	46
2	D	410/410 (100%)	405 (99%)	5 (1%)	63	63
All	All	1000/1000 (100%)	987 (99%)	13 (1%)	61	61

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	123	PRO
2	C	175	MET
2	C	217	HIS
2	C	254	LEU
2	C	267	LEU
2	C	361	LEU
2	C	418	PRO

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Mol	Chain	Res	Type
2	C	523	GLN
2	D	138	LYS
2	D	175	MET
2	D	254	LEU
2	D	267	LEU
2	D	523	GLN

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

Mol	Chain	Res	Type
1	A	54	ASN
2	C	122	GLN
2	C	200	ASN
2	C	326	ASN
2	C	392	ASN
2	C	409	GLN
2	C	421	ASN
2	C	526	GLN
2	C	530	GLN
1	B	54	ASN
1	B	75	GLN
2	D	122	GLN
2	D	133	ASN
2	D	540	ASN

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	0.72	0	1,6,8	0.49	0
2	CSO	D	150	2	3,6,7	0.67	0	1,6,8	1.31	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	3,2	14,14,15	0.56	0	17,19,21	0.88	0
3	NAG	E	2	3	14,14,15	0.41	0	17,19,21	0.75	0
3	BMA	E	3	3	11,11,12	0.35	0	15,15,17	0.44	0
3	MAN	E	4	3	11,11,12	0.52	0	15,15,17	0.59	0
3	MAN	E	5	3	11,11,12	0.44	0	15,15,17	0.55	0
3	FUC	E	6	3	10,10,11	0.43	0	14,14,16	0.47	0
3	NAG	F	1	3,2	14,14,15	0.48	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	0.46	0	17,19,21	0.99	2 (11%)
3	BMA	F	3	3	11,11,12	0.45	0	15,15,17	0.56	0
3	MAN	F	4	3	11,11,12	0.43	0	15,15,17	0.67	0
3	MAN	F	5	3	11,11,12	0.48	0	15,15,17	0.54	0
3	FUC	F	6	3	10,10,11	0.48	0	14,14,16	0.55	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	3,2	-	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	3,2	-	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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2	NAG	C4-C3-C2	-2.63	107.16	111.02
3	F	2	NAG	C2-N2-C7	-2.38	119.71	122.90

There are no chirality outliers.

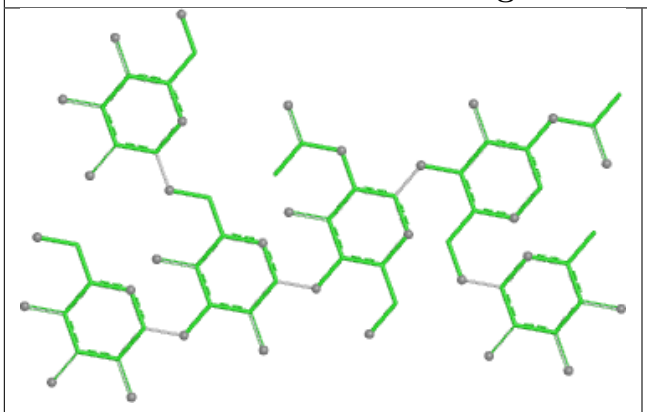
There are no torsion outliers.

There are no ring outliers.

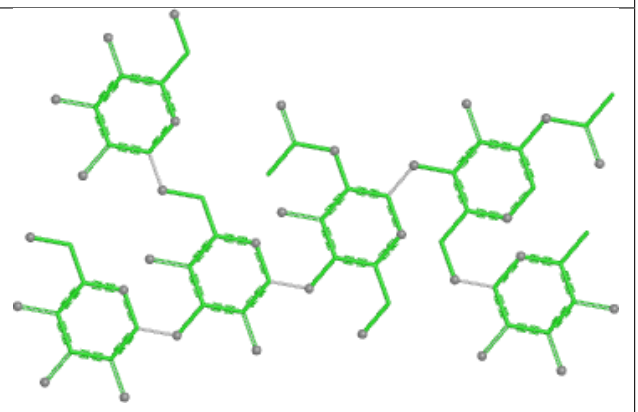
No monomer is involved in short contacts.

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

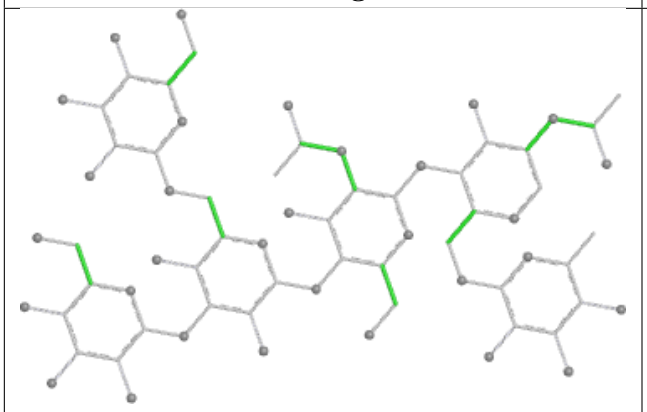
Oligosaccharide Chain E



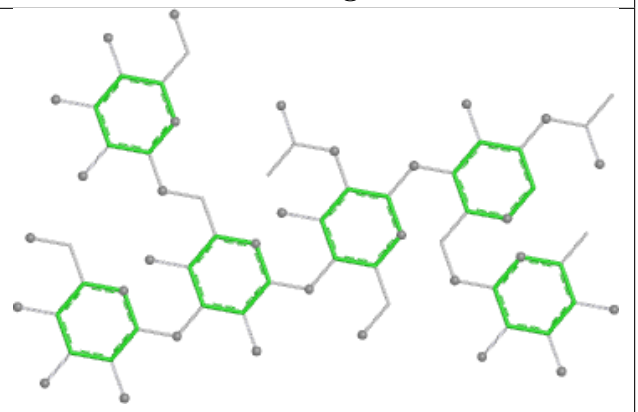
Bond lengths



Bond angles

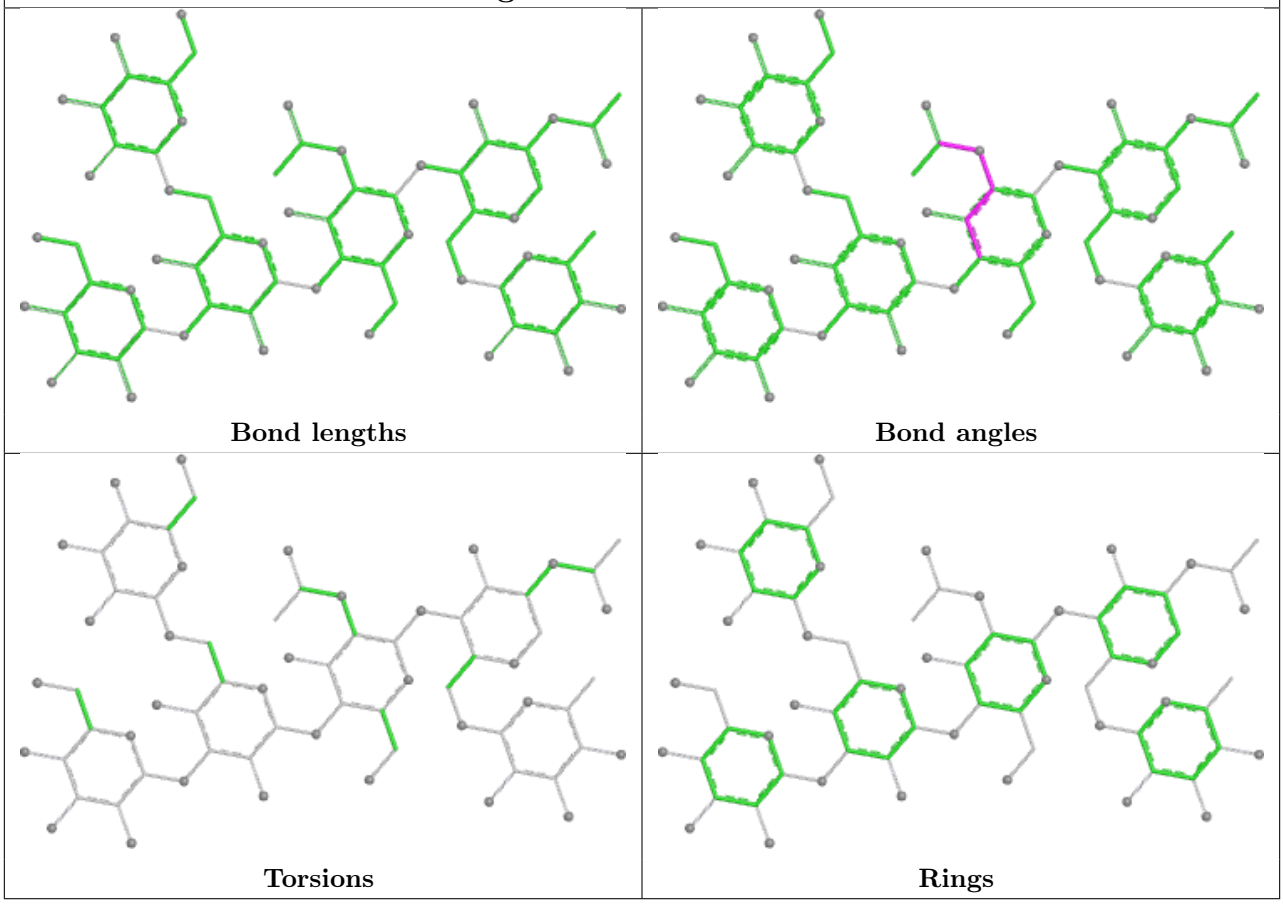


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	C	605	-	1,2,2	1.77	0	0,1,1	-	-
10	ACY	C	609	-	3,3,3	1.25	1 (33%)	3,3,3	1.68	1 (33%)
4	SCN	B	201	-	1,2,2	1.56	0	0,1,1	-	-
6	CYN	B	204	-	1,1,1	0.30	0	-		
7	NAG	D	603	2	14,14,15	0.55	0	17,19,21	0.65	0
5	SO4	C	604	-	4,4,4	0.44	0	6,6,6	0.20	0
5	SO4	B	202	-	4,4,4	0.74	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SCN	B	203	-	1,2,2	1.72	0	0,1,1	-	-
10	ACY	C	608	-	3,3,3	1.38	1 (33%)	3,3,3	1.62	1 (33%)
6	CYN	D	605	-	1,1,1	0.24	0	-		
4	SCN	A	201	-	1,2,2	1.30	0	0,1,1	-	-
7	NAG	C	602	2	14,14,15	0.44	0	17,19,21	0.77	0
5	SO4	A	202	-	4,4,4	0.40	0	6,6,6	0.06	0
7	NAG	C	601	2	14,14,15	0.48	0	17,19,21	0.92	1 (5%)
6	CYN	C	606	-	1,1,1	0.14	0	-		
9	HEM	C	607	2	50,50,50	1.17	4 (8%)	67,82,82	1.16	2 (2%)
10	ACY	D	608	-	3,3,3	1.39	1 (33%)	3,3,3	1.58	1 (33%)
10	ACY	D	606	-	3,3,3	1.34	1 (33%)	3,3,3	1.64	1 (33%)
6	CYN	A	203	-	1,1,1	0.33	0	-		
7	NAG	D	602	2	14,14,15	0.54	0	17,19,21	0.79	0
10	ACY	C	610	-	3,3,3	1.48	1 (33%)	3,3,3	1.56	1 (33%)
10	ACY	D	607	-	3,3,3	1.62	1 (33%)	3,3,3	1.70	1 (33%)
9	HEM	D	601	2	50,50,50	1.21	4 (8%)	67,82,82	1.31	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	D	602	2	-	0/6/23/26	0/1/1/1
7	NAG	C	601	2	-	0/6/23/26	0/1/1/1
7	NAG	C	602	2	-	0/6/23/26	0/1/1/1
7	NAG	D	603	2	-	2/6/23/26	0/1/1/1
9	HEM	C	607	2	-	4/14/54/54	-
9	HEM	D	601	2	-	4/14/54/54	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	601	HEM	CBB-CAB	3.25	1.46	1.30
9	D	601	HEM	CBC-CAC	2.80	1.43	1.30
9	C	607	HEM	CBB-CAB	2.78	1.43	1.30
9	C	607	HEM	CAC-C3C	-2.78	1.40	1.47
9	D	601	HEM	CAC-C3C	-2.63	1.40	1.47
9	C	607	HEM	CBC-CAC	2.62	1.43	1.30
10	D	607	ACY	O-C	2.55	1.33	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	607	HEM	CAB-C3B	-2.38	1.41	1.47
9	D	601	HEM	CAB-C3B	-2.36	1.41	1.47
10	C	610	ACY	O-C	2.32	1.32	1.22
10	C	608	ACY	O-C	2.22	1.32	1.22
10	D	608	ACY	O-C	2.09	1.31	1.22
10	D	606	ACY	O-C	2.05	1.31	1.22
10	C	609	ACY	O-C	2.00	1.31	1.22

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	601	HEM	C4B-C3B-C2B	-4.26	103.36	107.28
9	D	601	HEM	C3B-C4B-NB	4.26	112.53	109.47
9	C	607	HEM	C3B-C4B-NB	4.20	112.48	109.47
9	D	601	HEM	CMB-C2B-C1B	-3.01	120.33	125.03
9	D	601	HEM	C3B-C2B-C1B	2.89	108.58	106.41
7	C	601	NAG	C2-N2-C7	-2.65	119.35	122.90
9	C	607	HEM	CMA-C3A-C4A	2.43	129.12	125.42
10	D	607	ACY	O-C-CH3	-2.31	113.04	122.53
10	C	609	ACY	O-C-CH3	-2.29	113.12	122.53
10	D	606	ACY	O-C-CH3	-2.24	113.36	122.53
9	D	601	HEM	CMA-C3A-C4A	2.23	128.81	125.42
10	C	608	ACY	O-C-CH3	-2.19	113.56	122.53
10	D	608	ACY	O-C-CH3	-2.14	113.77	122.53
10	C	610	ACY	O-C-CH3	-2.11	113.87	122.53

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	603	NAG	C4-C5-C6-O6
7	D	603	NAG	O5-C5-C6-O6
9	C	607	HEM	CAD-CBD-CGD-O2D
9	D	601	HEM	CAD-CBD-CGD-O1D
9	D	601	HEM	CAD-CBD-CGD-O2D
9	C	607	HEM	CAD-CBD-CGD-O1D
9	C	607	HEM	CAA-CBA-CGA-O1A
9	C	607	HEM	CAA-CBA-CGA-O2A
9	D	601	HEM	CAA-CBA-CGA-O2A
9	D	601	HEM	CAA-CBA-CGA-O1A

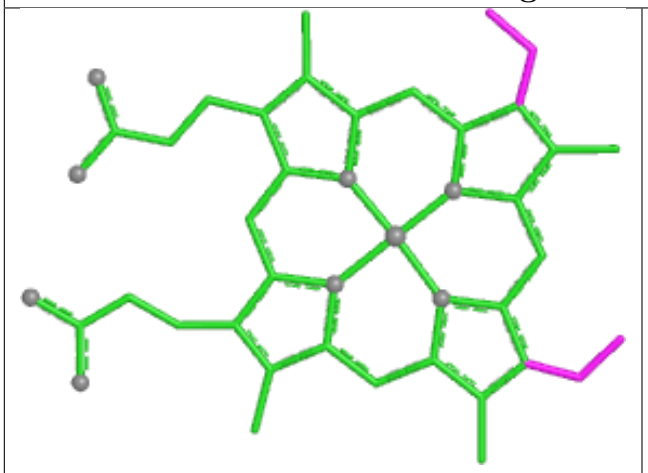
There are no ring outliers.

7 monomers are involved in 6 short contacts:

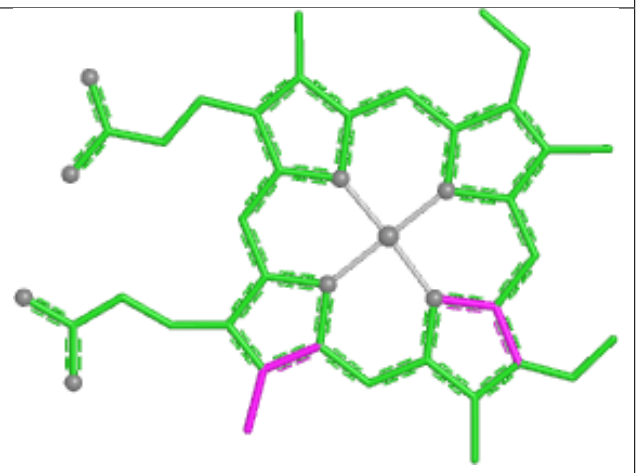
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	605	SCN	1	0
6	B	204	CYN	1	0
4	B	203	SCN	2	0
9	C	607	HEM	1	0
6	A	203	CYN	1	0
10	D	607	ACY	1	0
9	D	601	HEM	1	0

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

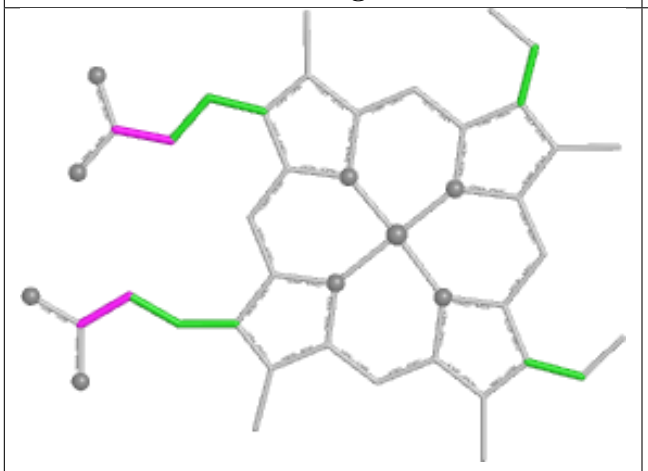
Ligand HEM C 607



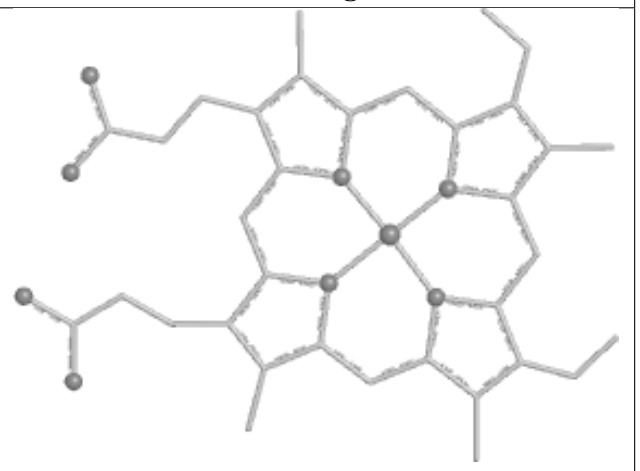
Bond lengths



Bond angles

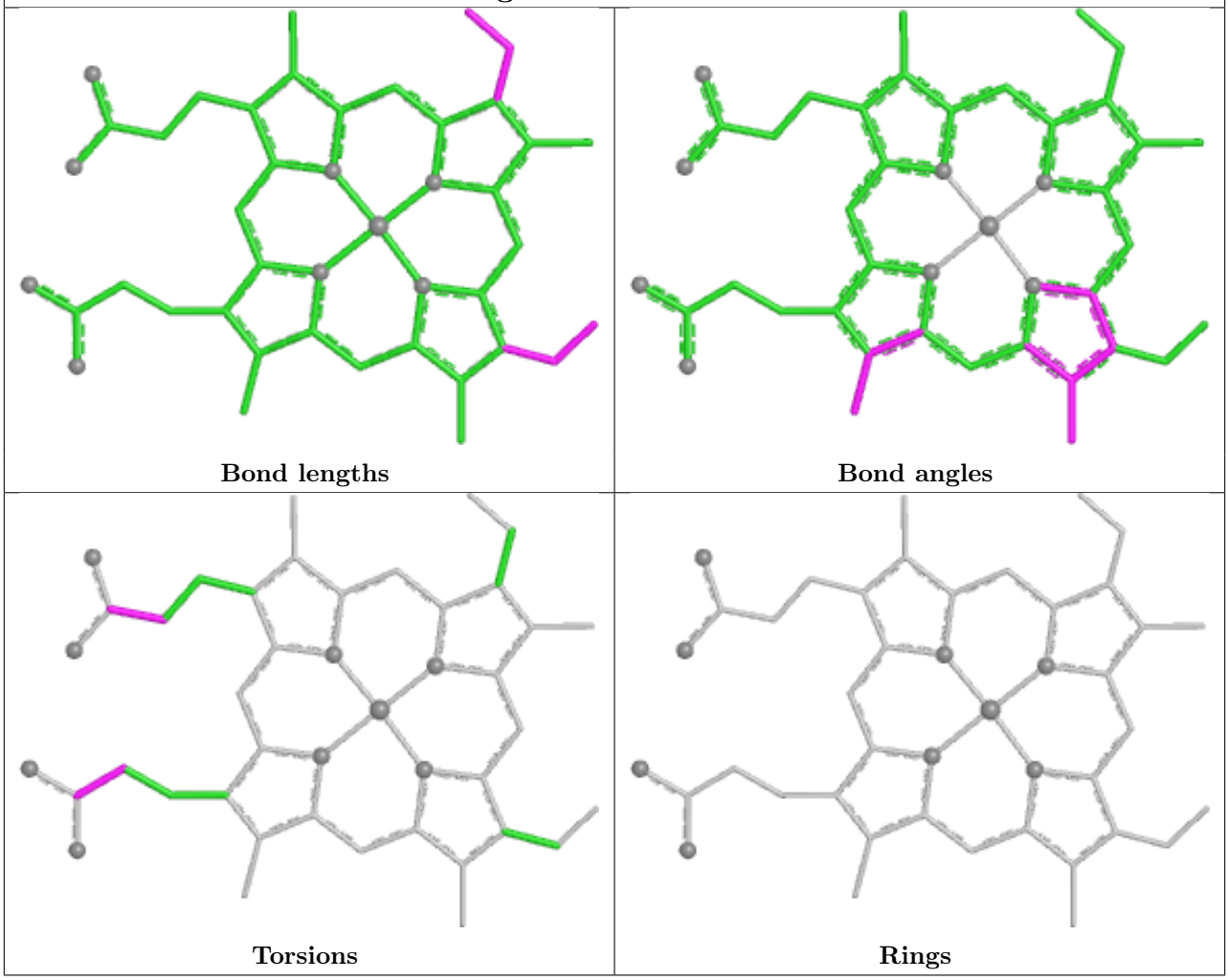


Torsions



Rings

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%)	-0.38	2 (1%) 66 70	6, 11, 23, 38	0
1	B	104/104 (100%)	-0.40	0 100 100	7, 12, 21, 26	0
2	C	465/466 (99%)	-0.31	6 (1%) 75 78	5, 13, 24, 33	0
2	D	465/466 (99%)	-0.18	6 (1%) 75 78	6, 15, 27, 35	0
All	All	1138/1140 (99%)	-0.27	14 (1%) 76 79	5, 13, 26, 38	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	113	VAL	6.2
2	C	217	HIS	4.7
2	D	217	HIS	4.3
2	C	355	PRO	3.6
2	D	355	PRO	3.4
1	A	3	GLU	2.9
2	D	349	ARG	2.9
2	C	139	ASN	2.2
2	D	576	ARG	2.2
2	D	568	PRO	2.2
2	C	353	MET	2.1
2	C	348	ASN	2.1
2	D	578	ALA	2.1
1	A	4	GLN	2.0

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	0.94	0.06	8,9,10,12	0
2	CSO	D	150	7/8	0.94	0.06	7,10,10,14	0

6.3 Carbohydrates (i)

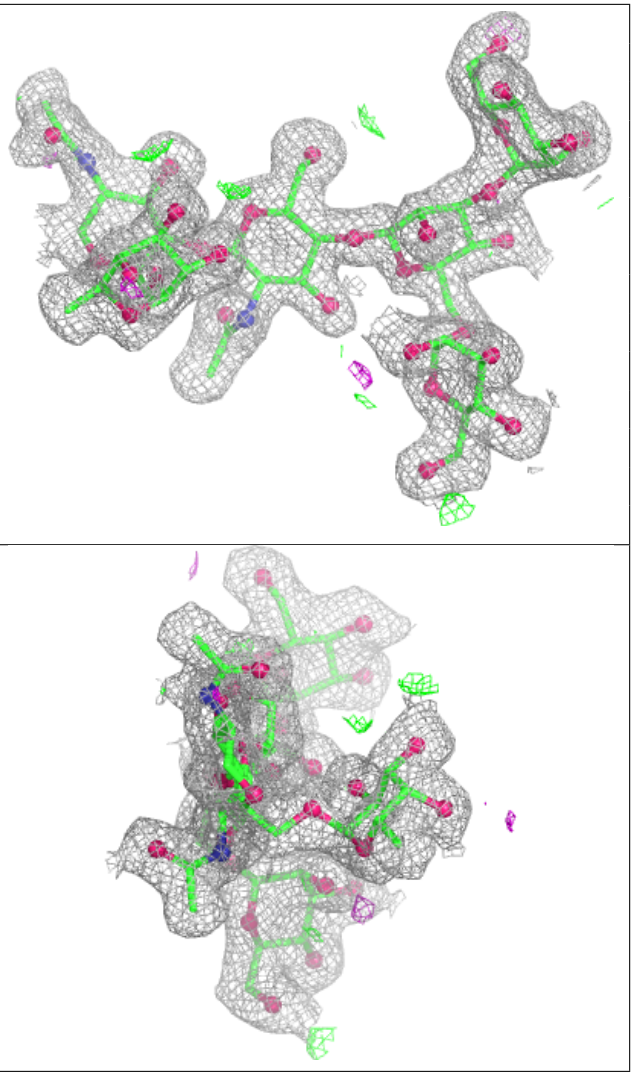
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.87	0.09	20,23,25,26	0
3	MAN	F	5	11/12	0.91	0.07	14,15,16,16	0
3	MAN	E	4	11/12	0.92	0.07	21,23,24,24	0
3	NAG	F	1	14/15	0.93	0.06	11,13,18,20	0
3	BMA	E	3	11/12	0.94	0.06	12,13,15,19	0
3	FUC	F	6	10/11	0.94	0.06	14,15,16,18	0
3	NAG	E	2	14/15	0.95	0.05	9,10,12,12	0
3	MAN	E	5	11/12	0.95	0.05	13,14,15,15	0
3	NAG	E	1	14/15	0.95	0.05	9,11,16,17	0
3	FUC	E	6	10/11	0.96	0.04	13,15,16,16	0
3	NAG	F	2	14/15	0.96	0.05	9,10,13,13	0
3	BMA	F	3	11/12	0.96	0.05	12,13,14,17	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.

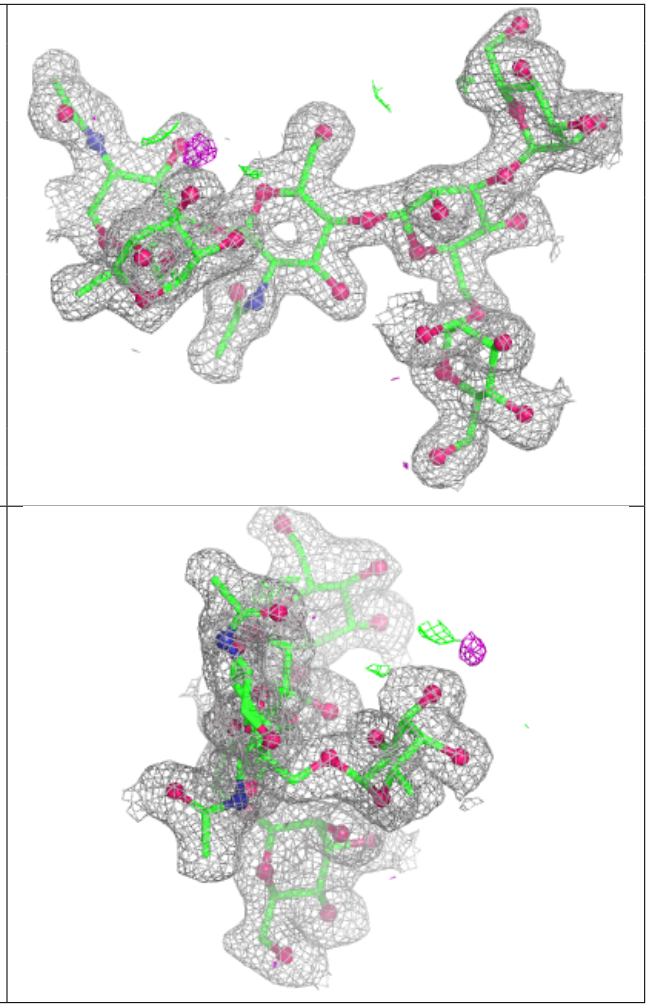
Electron density around Chain E:

$2mF_o$-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
6	CYN	D	605	2/2	0.62	0.27	11,11,11,14	0
10	ACY	C	609	4/4	0.74	0.12	26,26,27,27	0
10	ACY	C	608	4/4	0.76	0.09	28,29,29,29	0
7	NAG	D	603	14/15	0.80	0.10	26,29,30,33	0
6	CYN	C	606	2/2	0.80	0.11	21,21,21,24	0
5	SO4	B	202	5/5	0.80	0.23	55,55,56,57	0
10	ACY	D	606	4/4	0.81	0.10	25,25,25,28	0
10	ACY	D	607	4/4	0.81	0.12	33,36,36,38	0
10	ACY	C	610	4/4	0.87	0.08	26,26,26,26	0
7	NAG	C	602	14/15	0.88	0.09	22,25,31,31	0

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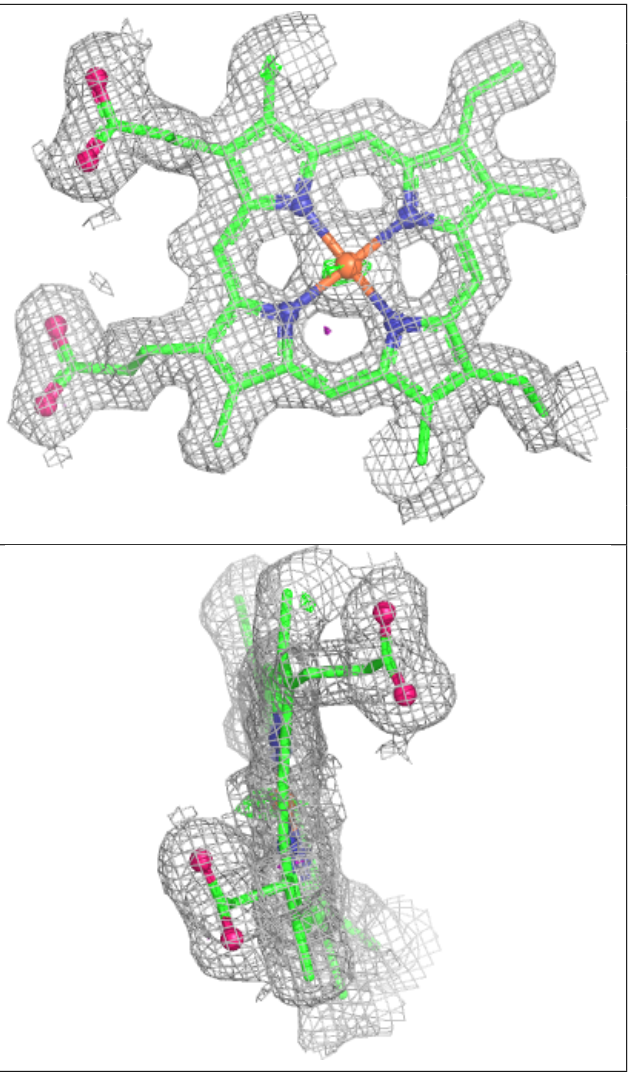
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CYN	A	203	2/2	0.89	0.10	12,12,12,15	0
7	NAG	C	601	14/15	0.90	0.07	14,19,22,23	0
10	ACY	D	608	4/4	0.90	0.10	29,29,29,31	0
7	NAG	D	602	14/15	0.91	0.08	17,21,25,26	0
6	CYN	B	204	2/2	0.93	0.08	18,18,18,18	0
5	SO4	C	604	5/5	0.93	0.09	27,27,29,29	0
4	SCN	C	605	3/3	0.94	0.08	19,19,20,21	0
4	SCN	A	201	3/3	0.96	0.06	3,3,4,12	0
4	SCN	B	203	3/3	0.97	0.08	26,26,26,28	0
9	HEM	D	601	43/43	0.97	0.06	6,10,14,14	0
8	CA	D	604	1/1	0.98	0.03	8,8,8,8	0
9	HEM	C	607	43/43	0.98	0.05	4,9,10,12	0
5	SO4	A	202	5/5	0.98	0.06	25,26,27,28	0
8	CA	C	603	1/1	0.99	0.03	7,7,7,7	0
4	SCN	B	201	3/3	0.99	0.04	5,5,5,10	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 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)



Electron density around HEM C 607:

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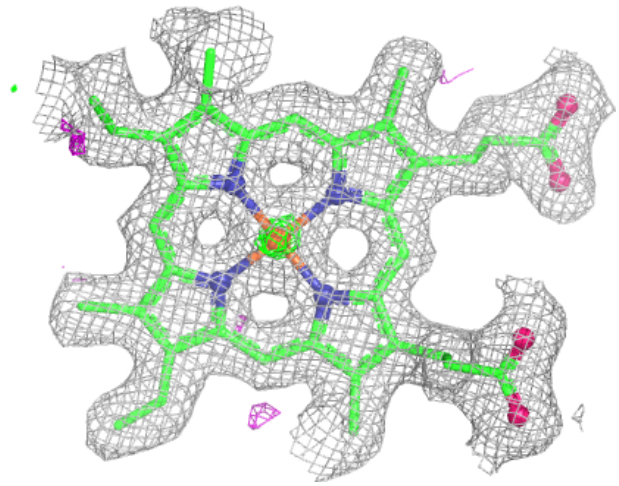
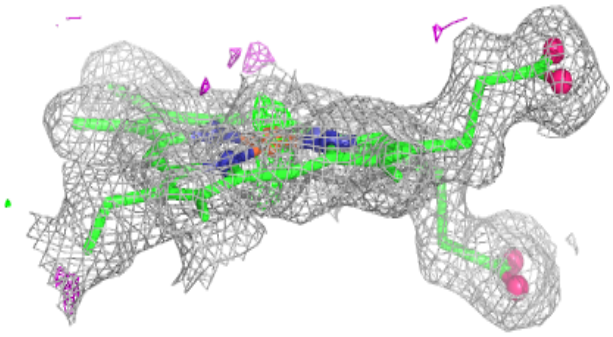
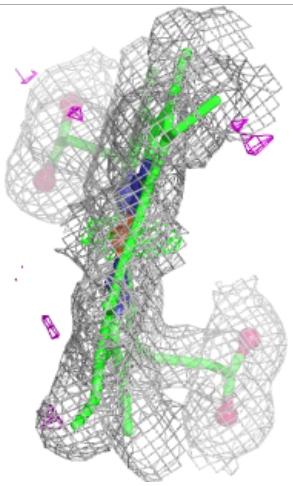
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.