



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:07 AM UTC

PDB ID : 1D5L / pdb_00001d5l
Title : CRYSTAL STRUCTURE OF CYANIDE-BOUND HUMAN MYELOPER-
OXIDASE ISOFORM C AT PH 5.5
Authors : Fiedler, T.J.; Davey, C.A.; Fenna, R.E.
Deposited on : 1999-10-07
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

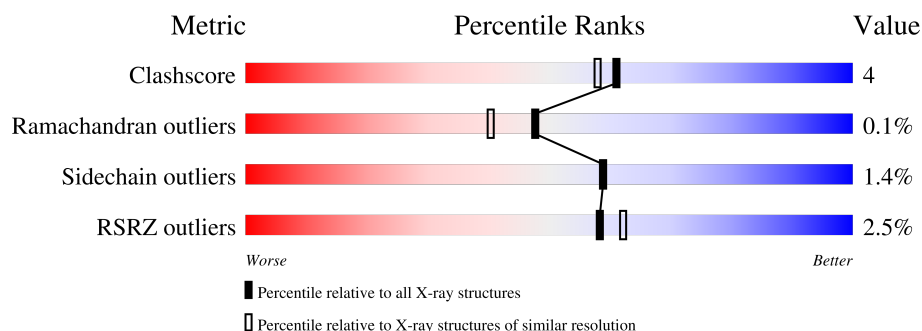
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	104	4% 90% 10%
1	B	104	95% 5%
2	C	466	2% 88% 11%
2	D	466	3% 89% 10%
3	E	6	100%
3	F	6	100%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 10347 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	B	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			

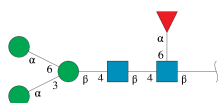
- Molecule 2 is a protein called MYELOPEROXIDASE.

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

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.

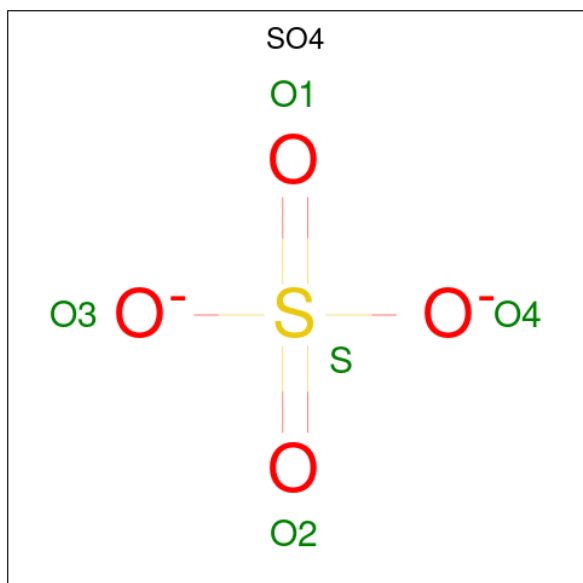


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			71	40	2	29			
3	F	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

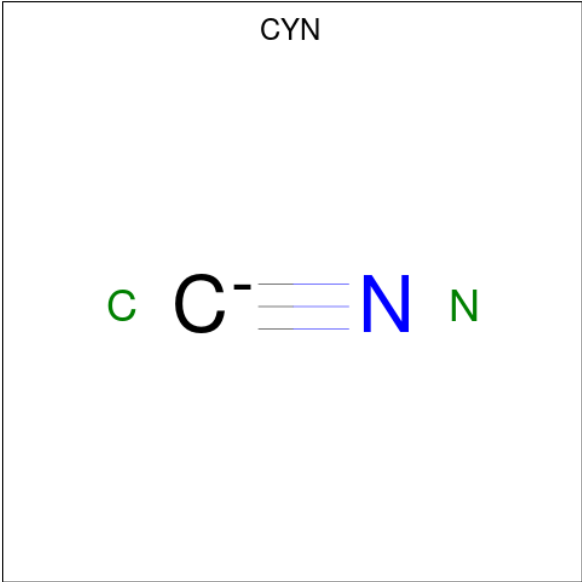
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



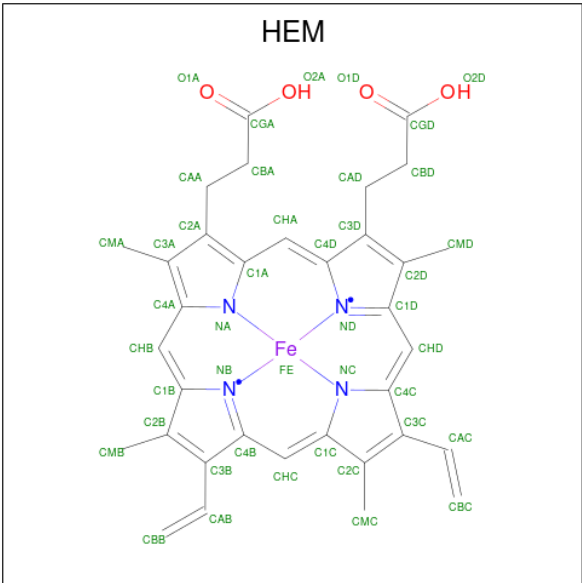
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

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



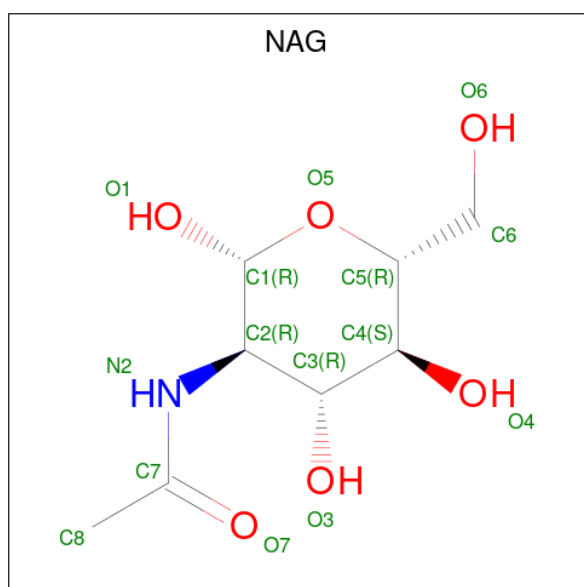
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			2	1	1		
6	C	1	Total	C	N	0	0
			2	1	1		
6	B	1	Total	C	N	0	0
			2	1	1		
6	D	1	Total	C	N	0	0
			2	1	1		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

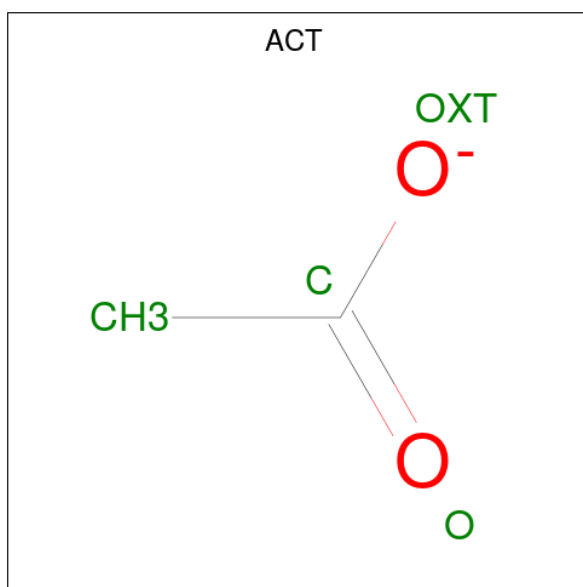


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	94	Total	O	0	0
			94	94		
11	C	340	Total	O	0	0
			340	340		
11	B	106	Total	O	0	0
			106	106		
11	D	326	Total	O	0	0
			326	326		

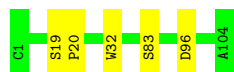
3 Residue-property plots

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

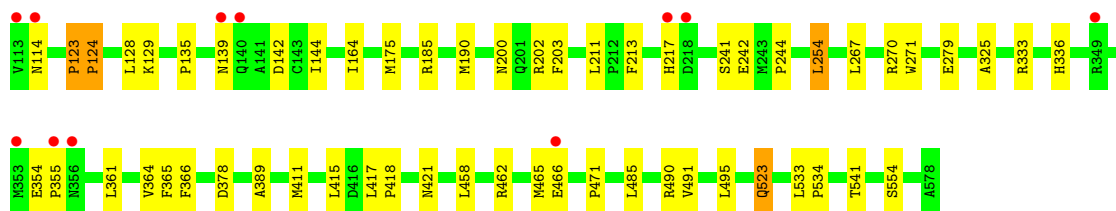
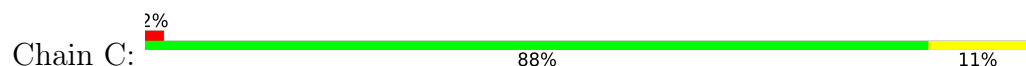
- Molecule 1: MYELOPEROXIDASE



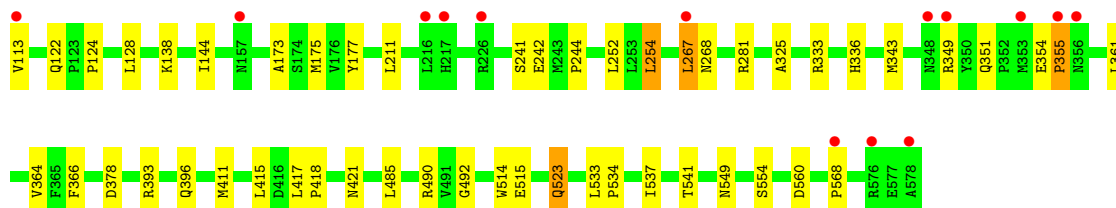
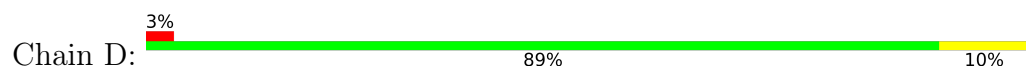
- Molecule 1: MYELOPEROXIDASE



- Molecule 2: MYELOPEROXIDASE



- Molecule 2: MYELOPEROXIDASE



- Molecule 3: 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:  100%

NAG1
NAG2
BMA3
MAN4
MAN5
FUC6

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

Chain F:  100%

NAG1
NAG2
BMA3
MAN4
MAN5
FUC6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.22Å 63.51Å 92.34Å 90.00° 97.43° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.91	Depositor EDS
% Data completeness (in resolution range)	91.3 (30.00-1.90) 96.0 (30.00-1.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.42 (at 1.91Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.172 , 0.215 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10347	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 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACT, HEM, CL, NAG, CYN, CSO, MAN, SO4, BMA, FUC

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	0.75	0/863	0.95	0/1174
1	B	0.73	0/863	0.95	3/1174 (0.3%)
2	C	0.74	0/3811	0.89	2/5168 (0.0%)
2	D	0.70	0/3811	0.88	6/5168 (0.1%)
All	All	0.72	0/9348	0.90	11/12684 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	336	HIS	ND1-CG-CD2	6.72	112.82	106.10
2	D	336	HIS	ND1-CG-CD2	6.23	112.33	106.10
2	C	336	HIS	CG-CD2-NE2	-6.09	101.11	107.20
2	D	336	HIS	CG-CD2-NE2	-6.01	101.19	107.20
1	B	19	SER	CA-C-N	5.29	126.46	119.84
1	B	19	SER	C-N-CA	5.29	126.46	119.84
2	D	492	GLY	CA-C-N	5.15	124.59	119.24
2	D	492	GLY	C-N-CA	5.15	124.59	119.24
2	D	268	ASN	CA-C-N	5.14	124.93	119.28
2	D	268	ASN	C-N-CA	5.14	124.93	119.28
1	B	96	ASP	N-CA-C	-5.02	107.00	113.23

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	8	0
1	B	838	0	798	3	0
2	C	3733	0	3725	38	0
2	D	3733	0	3725	31	0
3	E	71	0	61	0	0
3	F	71	0	61	0	0
4	A	1	0	0	0	0
4	B	1	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	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	1	0
6	D	2	0	0	0	0
7	C	43	0	30	3	0
7	D	43	0	30	3	0
8	C	28	0	26	0	0
8	D	28	0	26	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	C	16	0	12	0	0
10	D	12	0	9	1	0
11	A	94	0	0	2	0
11	B	106	0	0	0	0
11	C	340	0	0	4	0
11	D	326	0	0	3	0
All	All	10347	0	9301	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:465:MET:HE1	2:C:471:PRO:HD3	1.62	0.82
2:C:465:MET:HE3	11:C:995:HOH:O	1.87	0.73
2:D:411:MET:HE2	2:D:415:LEU:HD21	1.77	0.66
2:D:113:VAL:HG21	2:D:122:GLN:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1704:HOH:O	2:C:129:LYS:HD3	1.99	0.61
2:C:333:ARG:HH11	2:C:421:ASN:HD22	1.48	0.60
2:D:568:PRO:HG2	11:D:911:HOH:O	2.00	0.59
7:D:601:HEM:HMC2	7:D:601:HEM:HBC2	1.83	0.59
2:C:333:ARG:HH11	2:C:421:ASN:ND2	1.99	0.59
2:D:411:MET:CE	2:D:415:LEU:HD21	2.34	0.57
2:C:271:TRP:CZ3	2:C:279:GLU:HG3	2.41	0.56
2:C:135:PRO:HG2	11:C:703:HOH:O	2.06	0.55
1:A:4:GLN:HG2	1:A:5:ASP:N	2.20	0.55
7:C:601:HEM:HBC2	7:C:601:HEM:HMC2	1.89	0.55
2:D:241:SER:O	2:D:366:PHE:HA	2.07	0.54
2:D:349:ARG:HG3	2:D:351:GLN:HG2	1.89	0.54
2:C:213:PHE:H	6:C:610:CYN:C	2.20	0.54
2:D:333:ARG:HH11	2:D:421:ASN:ND2	2.04	0.54
2:D:242:GLU:OE1	7:D:601:HEM:HBB2	2.08	0.54
2:D:417:LEU:HB3	2:D:418:PRO:HD3	1.91	0.53
2:C:465:MET:HE1	2:C:471:PRO:CD	2.37	0.52
2:C:242:GLU:OE1	7:C:601:HEM:HBB2	2.09	0.52
2:C:270:ARG:NH1	11:C:704:HOH:O	2.43	0.52
2:C:491:VAL:HB	2:C:495:LEU:HB2	1.92	0.52
2:C:200:ASN:ND2	2:C:202:ARG:H	2.08	0.51
2:C:411:MET:HE2	2:C:415:LEU:HD11	1.92	0.51
2:C:128:LEU:HB2	2:C:144:ILE:HB	1.93	0.51
2:C:200:ASN:HD22	2:C:203:PHE:H	1.57	0.51
2:D:554:SER:HB3	2:D:560:ASP:HB3	1.93	0.51
1:A:70:ARG:HD2	11:A:1719:HOH:O	2.10	0.50
10:D:606:ACT:H1	11:D:991:HOH:O	2.11	0.50
2:D:244:PRO:HB2	2:D:343:MET:SD	2.52	0.50
2:D:534:PRO:HG2	2:D:549:ASN:ND2	2.26	0.50
1:A:83:SER:HB3	2:C:554:SER:O	2.12	0.49
2:C:211:LEU:HD23	2:C:254:LEU:HD13	1.93	0.49
2:D:378:ASP:OD1	2:D:541:THR:HB	2.13	0.48
2:C:417:LEU:HB3	2:C:418:PRO:HD3	1.95	0.48
2:D:523:GLN:H	2:D:523:GLN:CD	2.22	0.48
2:C:200:ASN:HD22	2:C:202:ARG:H	1.59	0.48
2:D:333:ARG:HH11	2:D:421:ASN:HD22	1.61	0.48
1:B:83:SER:HB3	2:D:554:SER:O	2.13	0.47
2:C:354:GLU:HB3	2:C:355:PRO:HA	1.96	0.47
2:D:349:ARG:HE	2:D:351:GLN:HG3	1.80	0.47
2:C:242:GLU:O	2:C:365:PHE:HA	2.15	0.46
1:A:32:TRP:CE2	2:C:325:ALA:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:PRO:HD2	2:C:164:ILE:O	2.17	0.45
2:C:142:ASP:HB3	11:C:945:HOH:O	2.17	0.45
1:B:32:TRP:CE2	2:D:325:ALA:HB2	2.52	0.44
2:C:462:ARG:O	2:C:466:GLU:HG2	2.18	0.44
1:A:84:LEU:HD13	2:C:389:ALA:HA	2.00	0.44
2:C:458:LEU:O	2:C:462:ARG:HG3	2.18	0.44
2:C:523:GLN:CD	2:C:523:GLN:H	2.26	0.44
2:D:533:LEU:HB3	2:D:534:PRO:HD3	2.00	0.44
2:C:485:LEU:HD13	2:C:490:ARG:HA	2.00	0.43
2:D:173:ALA:HA	2:D:175:MET:SD	2.58	0.43
2:C:123:PRO:HA	2:C:124:PRO:HA	1.78	0.43
2:C:533:LEU:N	2:C:534:PRO:CD	2.81	0.43
2:D:354:GLU:HB3	2:D:355:PRO:HA	2.00	0.42
2:C:139:ASN:HB2	2:C:142:ASP:OD1	2.18	0.42
2:C:378:ASP:OD1	2:C:541:THR:HB	2.19	0.42
7:C:601:HEM:HBC2	7:C:601:HEM:CMC	2.49	0.42
2:C:185:ARG:HG3	2:C:190:MET:CE	2.50	0.42
2:D:211:LEU:HD23	2:D:254:LEU:HD13	2.01	0.42
7:D:601:HEM:HBC2	7:D:601:HEM:CMC	2.50	0.42
1:A:40:GLY:HA2	1:B:20:PRO:HD2	2.02	0.41
2:D:514:TRP:CE2	2:D:515:GLU:HG3	2.55	0.41
2:D:177:TYR:OH	2:D:281:ARG:HA	2.20	0.41
2:C:244:PRO:HD3	2:C:364:VAL:O	2.21	0.41
2:D:485:LEU:HD13	2:D:490:ARG:HA	2.03	0.41
2:D:549:ASN:ND2	11:D:706:HOH:O	2.53	0.41
2:C:241:SER:O	2:C:366:PHE:HA	2.21	0.41
2:D:393:ARG:HB2	2:D:396:GLN:HB2	2.03	0.41
1:A:6:LYS:HE3	1:A:7:TYR:CZ	2.57	0.40
2:C:129:LYS:HB3	2:C:129:LYS:HE2	1.78	0.40
2:D:128:LEU:HB2	2:D:144:ILE:HB	2.03	0.40
2:D:252:LEU:HD11	2:D:537:ILE:HA	2.03	0.40
2:D:267:LEU:HA	2:D:267:LEU:HD22	1.84	0.40
2:D:361:LEU:O	2:D:364:VAL:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	99 (97%)	3 (3%)	0	100	100
2	C	463/466 (99%)	453 (98%)	9 (2%)	1 (0%)	43	36
2	D	463/466 (99%)	453 (98%)	10 (2%)	0	100	100
All	All	1130/1140 (99%)	1105 (98%)	24 (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 ⓘ

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%)	404 (98%)	6 (2%)	57	56
All	All	1000/1000 (100%)	986 (99%)	14 (1%)	59	59

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	123	PRO
2	C	124	PRO
2	C	175	MET
2	C	217	HIS
2	C	254	LEU
2	C	267	LEU
2	C	361	LEU
2	C	523	GLN
2	D	124	PRO
2	D	138	LYS
2	D	254	LEU
2	D	267	LEU
2	D	355	PRO
2	D	523	GLN

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	122	GLN
2	C	200	ASN
2	C	409	GLN
2	C	421	ASN
2	C	526	GLN
2	C	540	ASN
1	B	75	GLN
2	D	122	GLN
2	D	421	ASN
2	D	540	ASN
2	D	549	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	D	150	2	3,6,7	0.99	0	1,6,8	1.09	0
2	CSO	C	150	2	3,6,7	0.80	0	1,6,8	1.10	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	D	150	2	-	0/1/5/7	-
2	CSO	C	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

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	0.70	0	17,19,21	0.86	0
3	NAG	E	2	3	14,14,15	0.53	0	17,19,21	0.74	0
3	BMA	E	3	3	11,11,12	0.48	0	15,15,17	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	E	4	3	11,11,12	0.64	0	15,15,17	0.50	0
3	MAN	E	5	3	11,11,12	0.50	0	15,15,17	0.51	0
3	FUC	E	6	3	10,10,11	0.46	0	14,14,16	0.57	0
3	NAG	F	1	3,2	14,14,15	0.51	0	17,19,21	0.97	0
3	NAG	F	2	3	14,14,15	0.44	0	17,19,21	0.76	0
3	BMA	F	3	3	11,11,12	0.34	0	15,15,17	0.60	0
3	MAN	F	4	3	11,11,12	0.67	0	15,15,17	0.61	0
3	MAN	F	5	3	11,11,12	0.53	0	15,15,17	0.49	0
3	FUC	F	6	3	10,10,11	0.61	0	14,14,16	0.43	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.

There are no bond angle outliers.

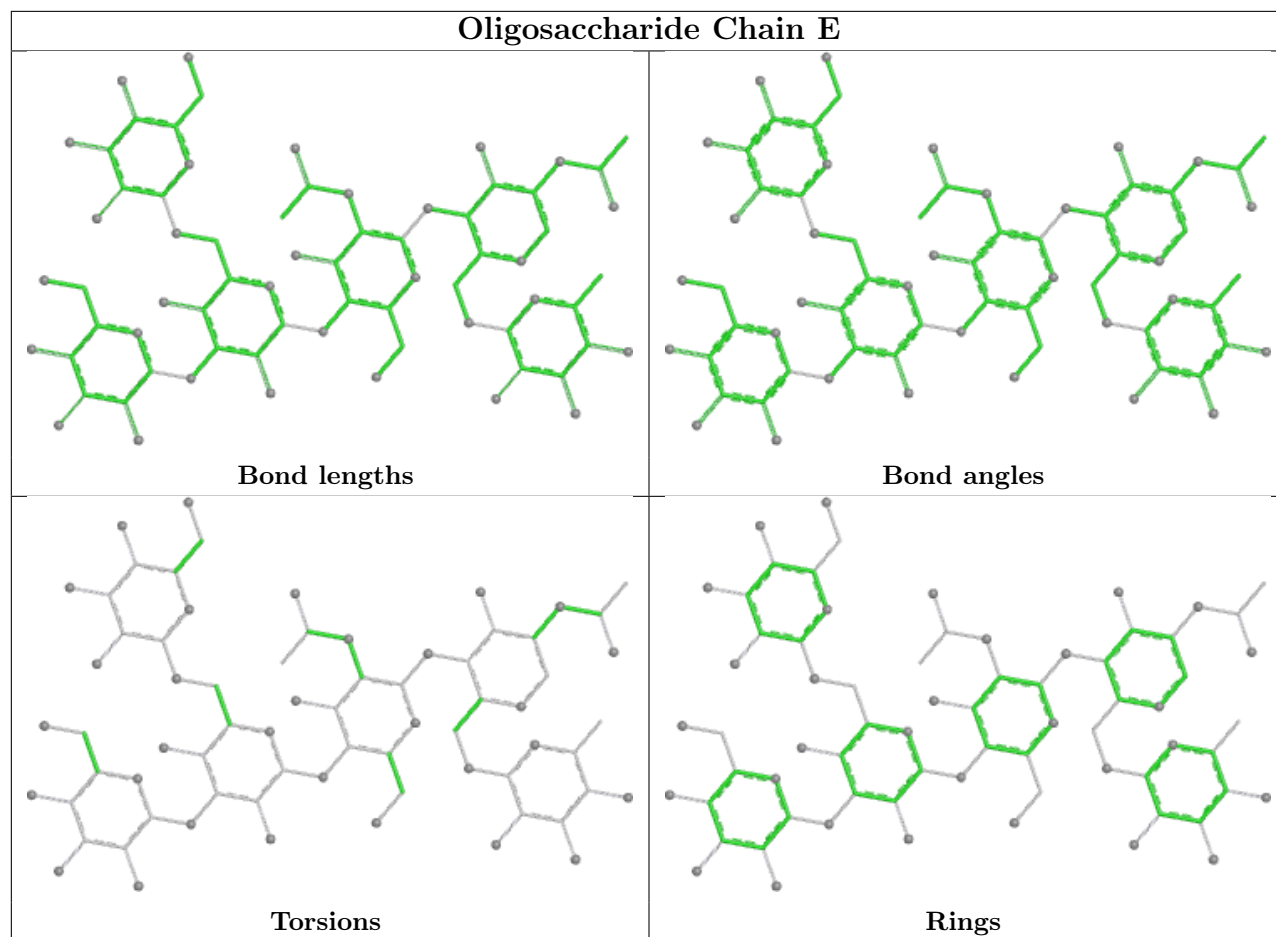
There are no chirality outliers.

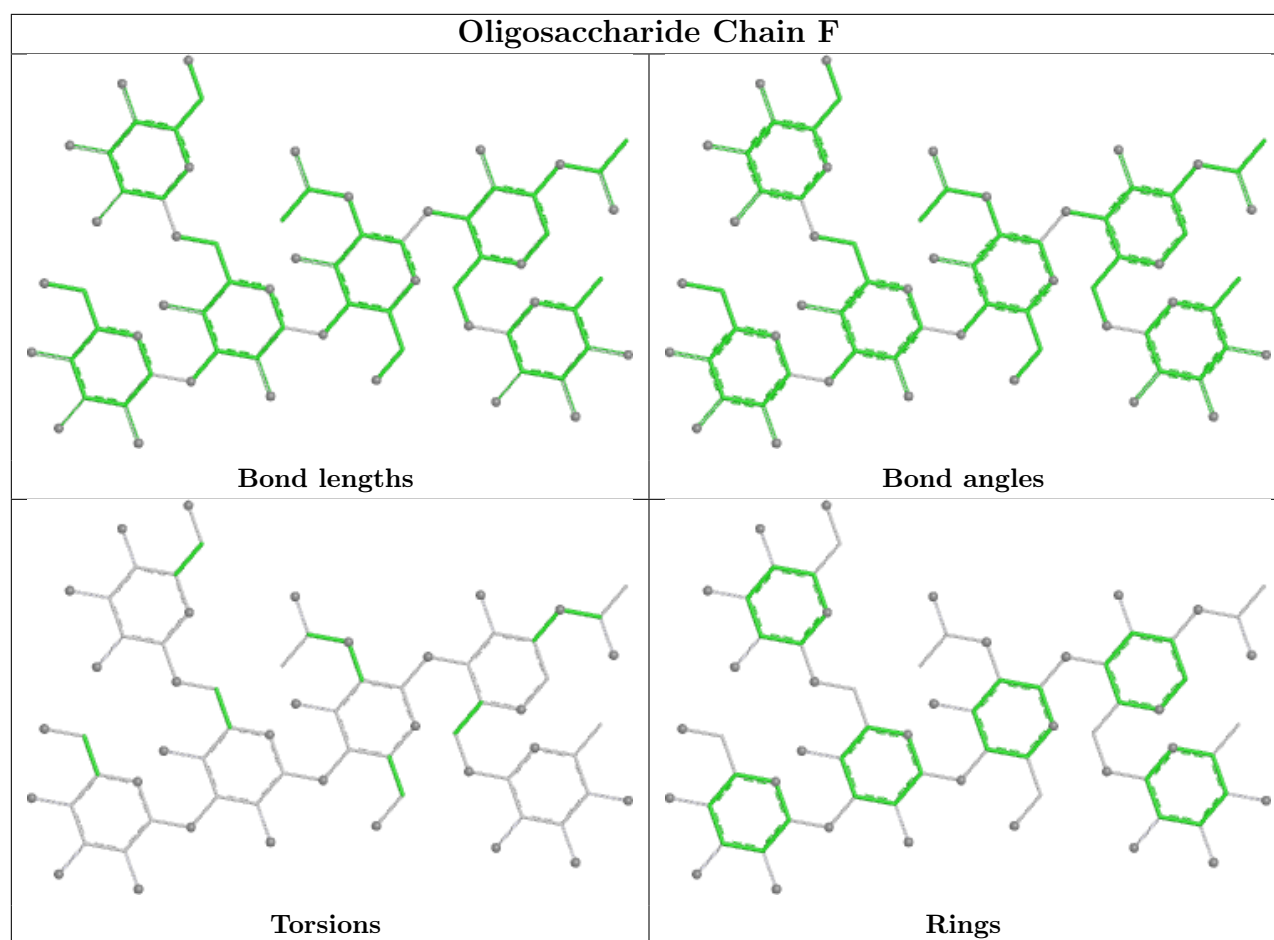
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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
8	NAG	D	602	2	14,14,15	0.52	0	17,19,21	0.82	1 (5%)
6	CYN	B	2602	7	1,1,1	0.18	0	-		
10	ACT	D	607	-	3,3,3	1.39	1 (33%)	3,3,3	1.67	1 (33%)
6	CYN	D	609	-	1,1,1	0.24	0	-		
10	ACT	D	608	-	3,3,3	1.31	1 (33%)	3,3,3	1.69	1 (33%)
10	ACT	C	608	-	3,3,3	1.45	1 (33%)	3,3,3	1.51	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	ACT	C	609	-	3,3,3	1.17	0	3,3,3	1.56	1 (33%)
7	HEM	C	601	6,2	50,50,50	1.06	4 (8%)	67,82,82	0.93	1 (1%)
6	CYN	C	610	-	1,1,1	0.26	0	-		
10	ACT	C	606	-	3,3,3	1.21	0	3,3,3	1.55	1 (33%)
5	SO4	C	605	-	4,4,4	0.35	0	6,6,6	0.12	0
8	NAG	C	602	2	14,14,15	0.86	1 (7%)	17,19,21	0.88	1 (5%)
7	HEM	D	601	6,2	50,50,50	1.08	4 (8%)	67,82,82	0.97	1 (1%)
5	SO4	D	605	-	4,4,4	0.37	0	6,6,6	0.06	0
10	ACT	D	606	-	3,3,3	1.10	0	3,3,3	1.66	1 (33%)
6	CYN	A	1603	7	1,1,1	0.27	0	-		
10	ACT	C	607	-	3,3,3	1.05	0	3,3,3	1.56	1 (33%)
8	NAG	C	603	2	14,14,15	0.47	0	17,19,21	0.72	0
5	SO4	A	1602	-	4,4,4	0.25	0	6,6,6	0.14	0
8	NAG	D	603	2	14,14,15	0.44	0	17,19,21	0.78	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
8	NAG	D	602	2	-	0/6/23/26	0/1/1/1
8	NAG	C	602	2	-	0/6/23/26	0/1/1/1
7	HEM	D	601	6,2	-	4/14/54/54	-
8	NAG	C	603	2	-	0/6/23/26	0/1/1/1
7	HEM	C	601	6,2	-	4/14/54/54	-
8	NAG	D	603	2	-	2/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	601	HEM	CBB-CAB	3.30	1.46	1.30
7	C	601	HEM	CBB-CAB	3.23	1.45	1.30
7	D	601	HEM	CBC-CAC	2.97	1.44	1.30
7	C	601	HEM	CBC-CAC	2.96	1.44	1.30
8	C	602	NAG	C1-C2	2.67	1.56	1.52
7	C	601	HEM	CAB-C3B	-2.33	1.41	1.47
7	D	601	HEM	CAC-C3C	-2.26	1.41	1.47
10	D	607	ACT	O-C	2.20	1.31	1.22
7	C	601	HEM	CAC-C3C	-2.19	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	608	ACT	O-C	2.16	1.31	1.22
7	D	601	HEM	CAB-C3B	-2.07	1.41	1.47
10	D	608	ACT	O-C	2.04	1.31	1.22

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	601	HEM	C3B-C4B-NB	3.95	112.31	109.47
7	C	601	HEM	C3B-C4B-NB	3.14	111.72	109.47
8	D	603	NAG	C2-N2-C7	-2.30	119.82	122.90
10	D	608	ACT	O-C-CH3	-2.28	113.18	122.53
10	D	606	ACT	O-C-CH3	-2.27	113.23	122.53
10	D	607	ACT	O-C-CH3	-2.26	113.24	122.53
8	D	602	NAG	C1-O5-C5	2.25	115.20	112.19
10	C	607	ACT	O-C-CH3	-2.14	113.77	122.53
10	C	609	ACT	O-C-CH3	-2.11	113.89	122.53
10	C	606	ACT	O-C-CH3	-2.11	113.89	122.53
10	C	608	ACT	O-C-CH3	-2.05	114.12	122.53
8	C	602	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 8 short contacts:

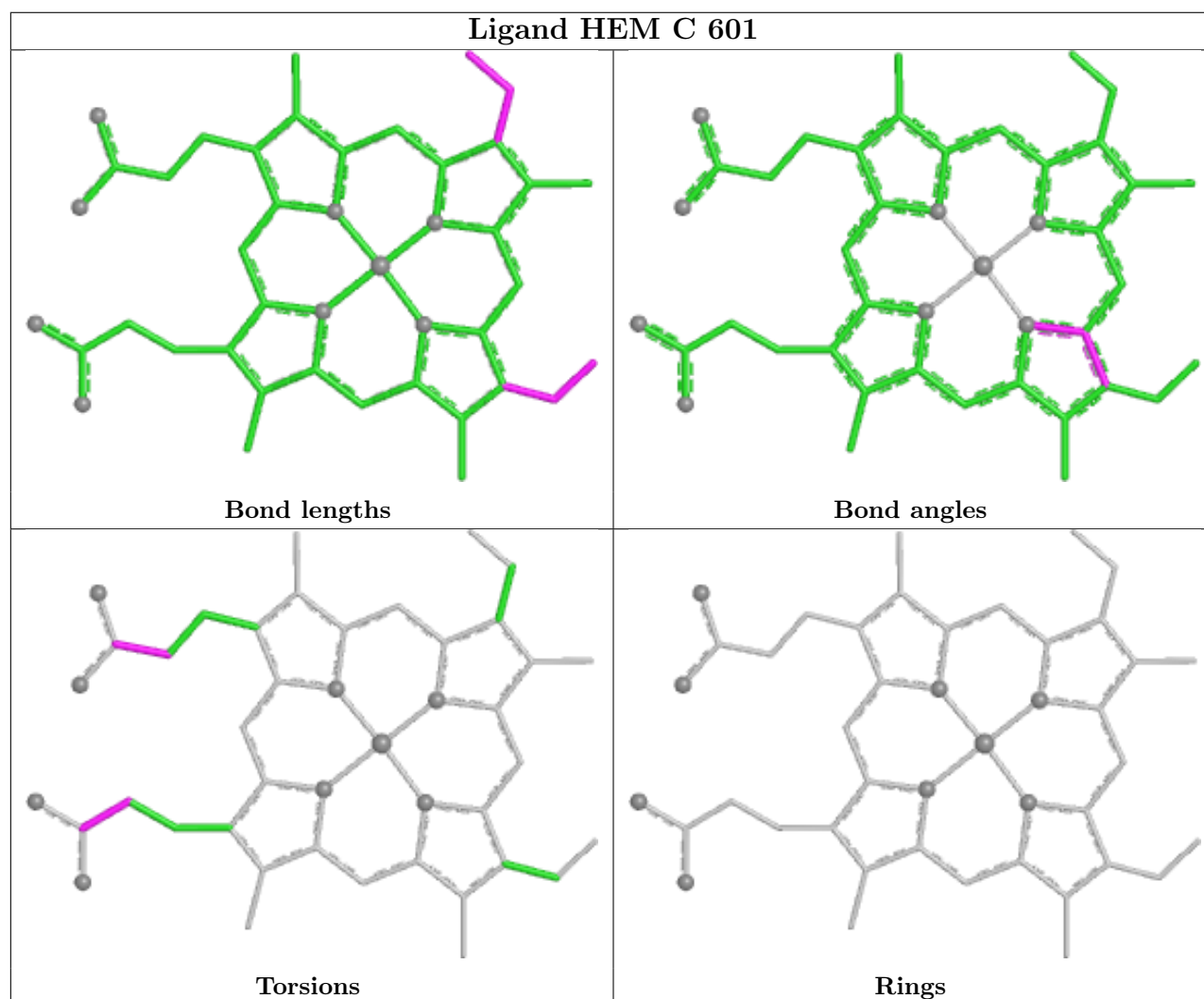
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	601	HEM	3	0
6	C	610	CYN	1	0

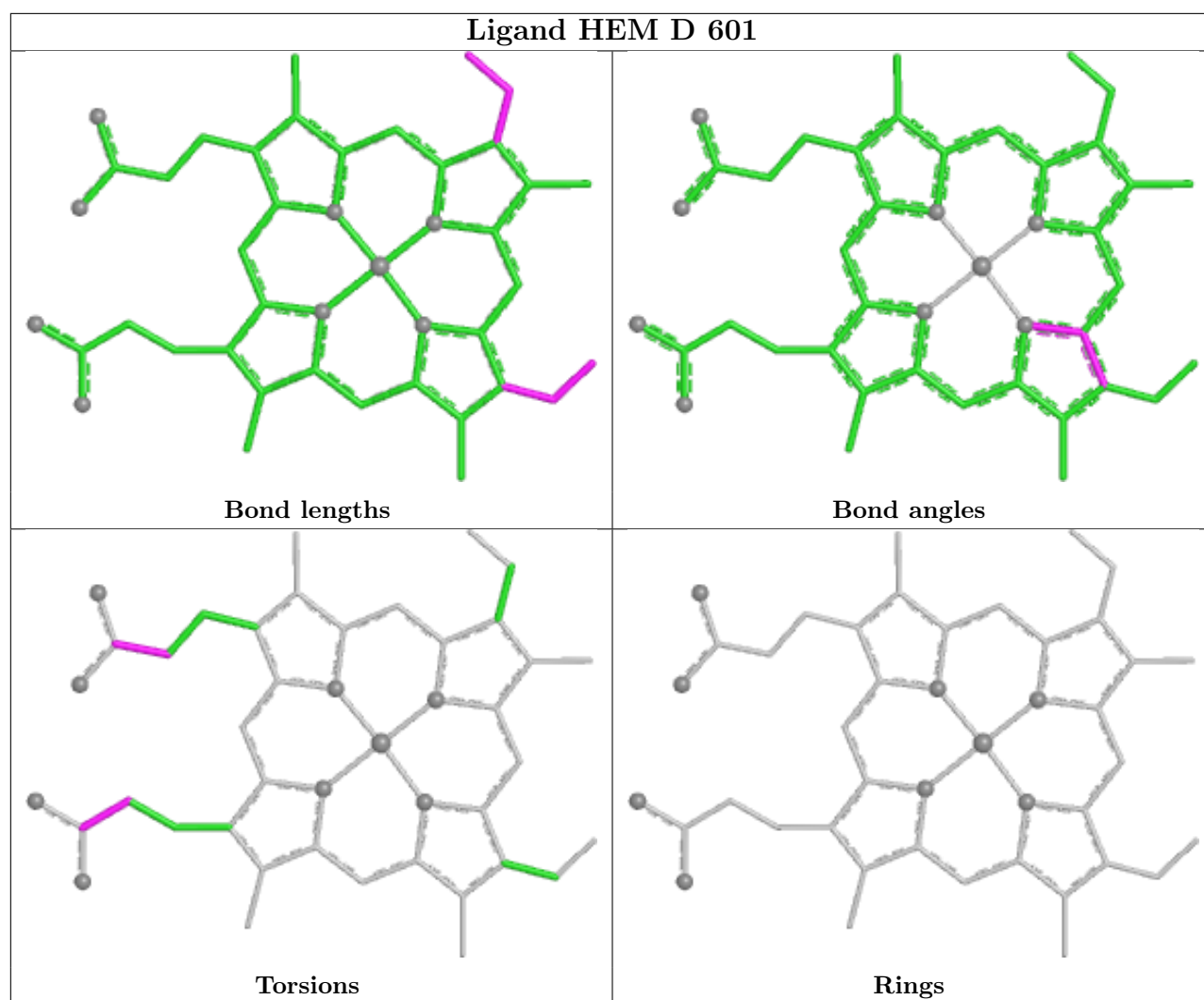
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	601	HEM	3	0
10	D	606	ACT	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	104/104 (100%)	-0.35	4 (3%) 44 47	5, 9, 24, 54	0
1	B	104/104 (100%)	-0.41	0 100 100	6, 10, 20, 28	0
2	C	465/466 (99%)	-0.32	11 (2%) 59 63	4, 10, 24, 40	0
2	D	465/466 (99%)	-0.05	14 (3%) 52 56	5, 13, 30, 53	0
All	All	1138/1140 (99%)	-0.22	29 (2%) 58 62	4, 11, 28, 54	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	113	VAL	7.5
2	C	217	HIS	3.9
2	D	217	HIS	3.8
2	D	349	ARG	3.8
2	C	353	MET	3.3
1	A	4	GLN	3.1
2	D	226	ARG	3.1
2	D	578	ALA	3.0
2	D	267	LEU	3.0
2	D	355	PRO	3.0
2	D	356	ASN	3.0
2	D	113	VAL	2.8
2	D	576	ARG	2.8
1	A	3	GLU	2.7
2	D	348	ASN	2.7
2	C	139	ASN	2.5
2	D	353	MET	2.3
2	D	216	LEU	2.2
2	C	218	ASP	2.2
2	C	114	ASN	2.2
1	A	2	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	355	PRO	2.2
2	D	568	PRO	2.2
2	D	157	ASN	2.2
1	A	1	CYS	2.2
2	C	356	ASN	2.1
2	C	140	GLN	2.1
2	C	466	GLU	2.0
2	C	349	ARG	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.

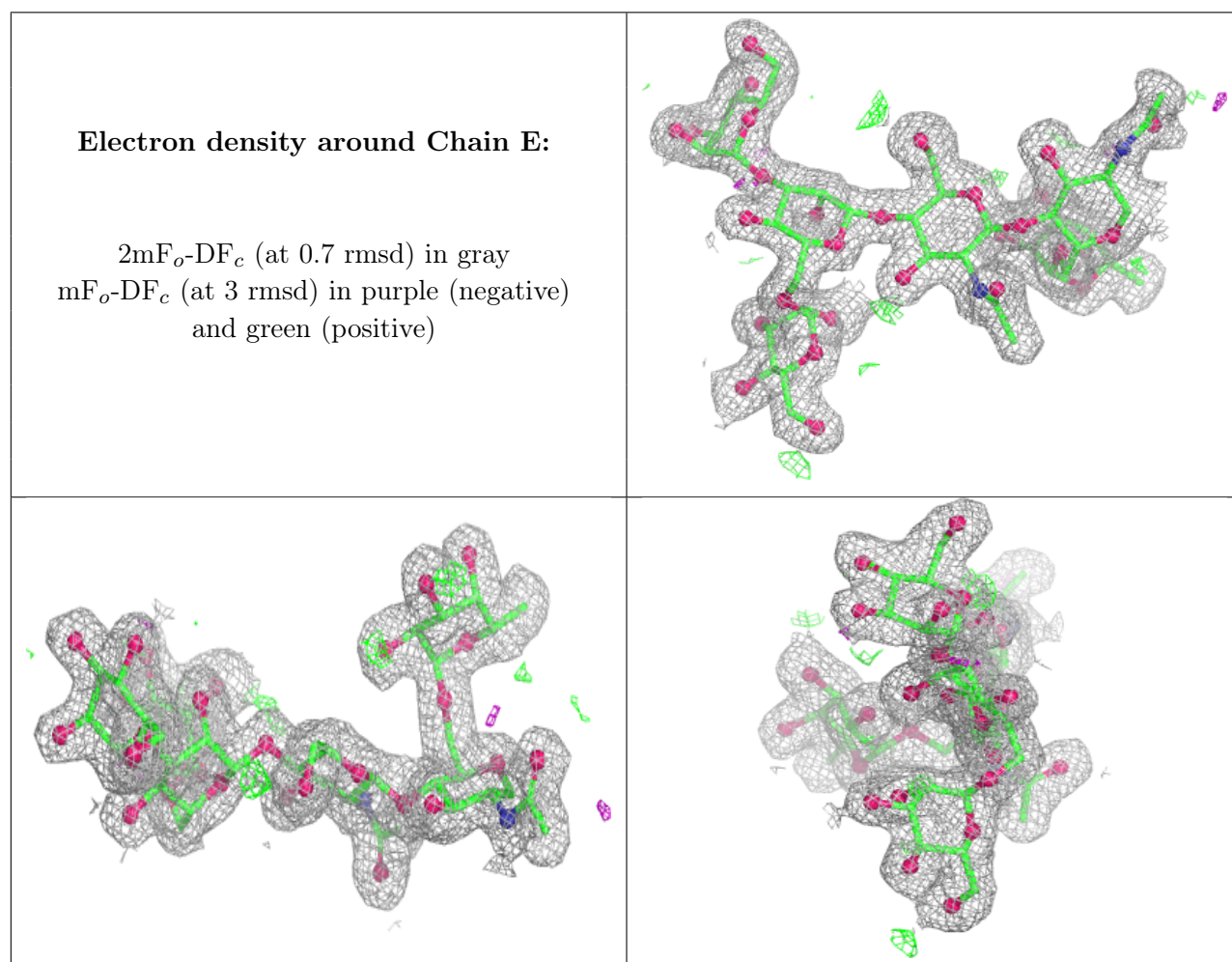
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CSO	C	150	7/8	0.95	0.07	6,9,10,12	0
2	CSO	D	150	7/8	0.95	0.06	5,6,9,13	0

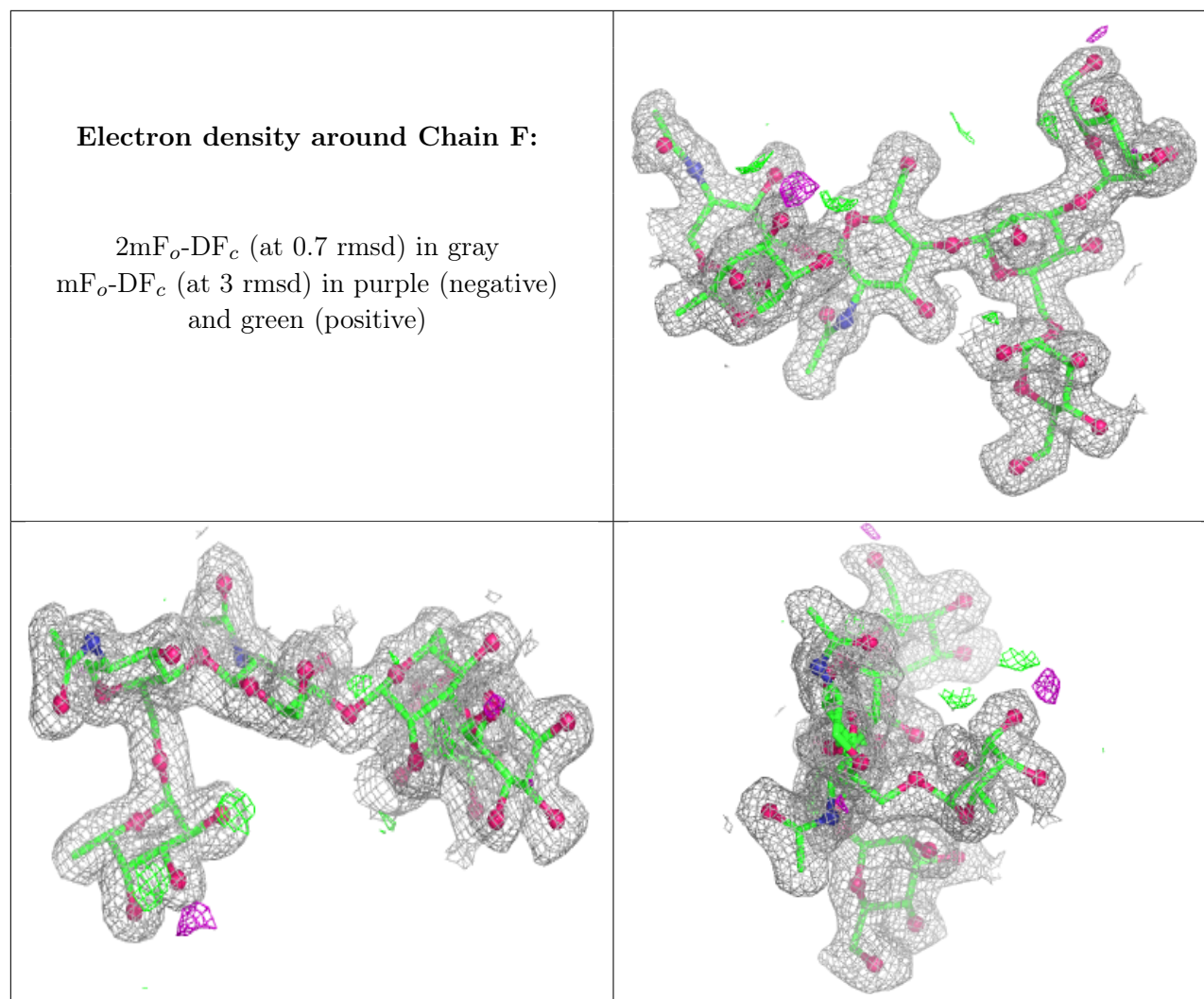
6.3 Carbohydrates [i](#)

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	0.84	0.11	16,21,24,25	0
3	MAN	E	4	11/12	0.92	0.08	18,21,22,26	0
3	FUC	E	6	10/11	0.95	0.06	11,12,13,14	0
3	NAG	E	1	14/15	0.96	0.06	8,10,14,16	0
3	NAG	E	2	14/15	0.96	0.06	6,9,10,11	0
3	BMA	E	3	11/12	0.96	0.06	9,10,13,16	0
3	FUC	F	6	10/11	0.96	0.05	9,12,13,14	0
3	NAG	F	2	14/15	0.97	0.05	5,8,11,12	0
3	BMA	F	3	11/12	0.97	0.05	8,10,11,12	0
3	MAN	E	5	11/12	0.97	0.05	10,12,15,16	0
3	MAN	F	5	11/12	0.97	0.05	8,12,13,13	0
3	NAG	F	1	14/15	0.97	0.06	7,12,17,18	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.





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($\text{\AA}^2$)	Q<0.9
6	CYN	D	609	2/2	0.52	0.18	27,27,27,28	0
10	ACT	D	607	4/4	0.77	0.16	46,48,48,48	0
10	ACT	C	607	4/4	0.78	0.15	17,20,20,23	0
5	SO4	D	605	5/5	0.80	0.20	36,37,37,37	5
10	ACT	C	606	4/4	0.80	0.15	27,29,29,30	0
8	NAG	D	603	14/15	0.81	0.13	33,35,37,40	0
10	ACT	C	609	4/4	0.83	0.22	4,6,7,20	4
6	CYN	C	610	2/2	0.84	0.13	17,17,17,20	0
10	ACT	C	608	4/4	0.84	0.12	23,24,24,24	0

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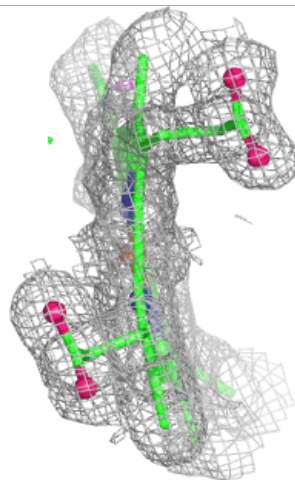
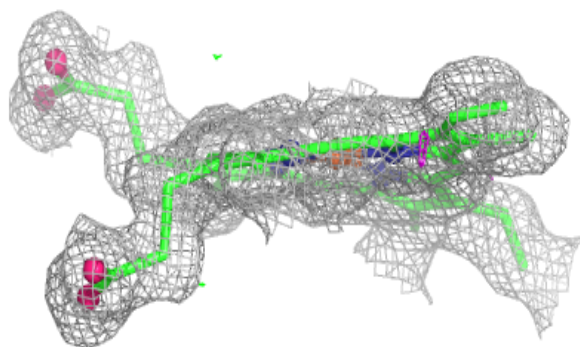
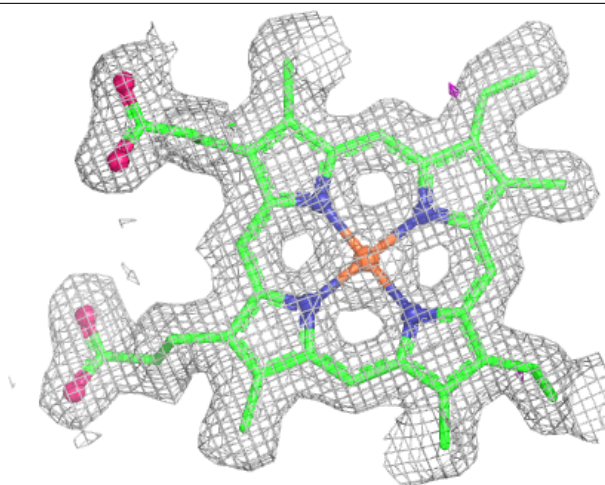
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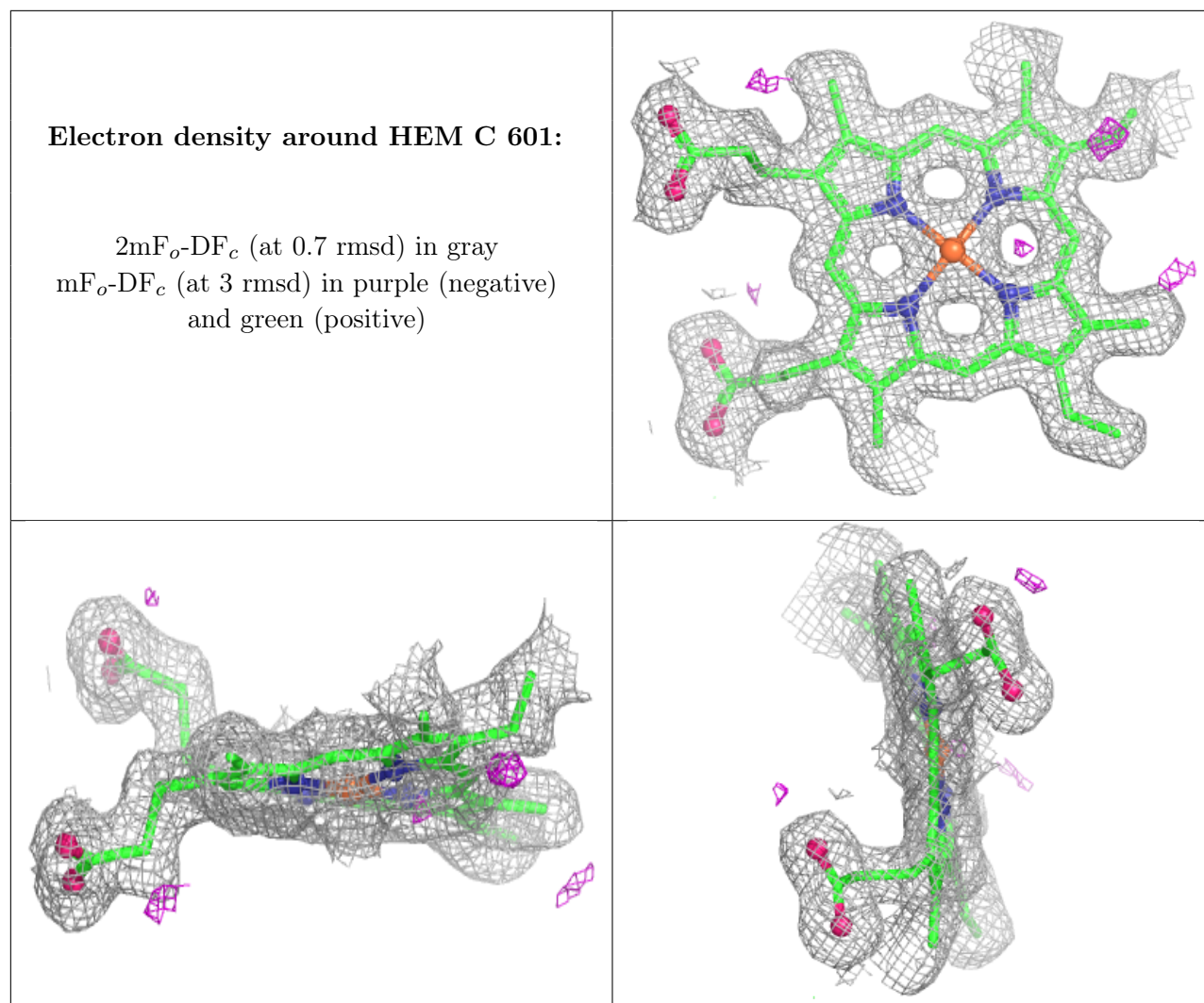
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	ACT	D	606	4/4	0.85	0.14	23,24,25,27	0
8	NAG	C	603	14/15	0.85	0.13	20,26,34,34	0
10	ACT	D	608	4/4	0.87	0.13	29,32,32,33	0
8	NAG	D	602	14/15	0.91	0.09	20,24,28,31	0
8	NAG	C	602	14/15	0.93	0.08	13,16,20,20	0
5	SO4	C	605	5/5	0.96	0.09	26,26,29,31	0
5	SO4	A	1602	5/5	0.97	0.07	25,25,27,28	0
7	HEM	D	601	43/43	0.98	0.05	4,7,8,10	0
6	CYN	B	2602	2/2	0.98	0.06	14,14,14,15	0
7	HEM	C	601	43/43	0.98	0.05	3,7,8,10	0
9	CA	C	604	1/1	0.99	0.02	8,8,8,8	0
6	CYN	A	1603	2/2	0.99	0.05	10,10,10,12	0
4	CL	B	2601	1/1	1.00	0.01	10,10,10,10	0
9	CA	D	604	1/1	1.00	0.02	9,9,9,9	0
4	CL	A	1601	1/1	1.00	0.01	8,8,8,8	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)





6.5 Other polymers [i](#)

There are no such residues in this entry.