



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 04:37 AM JST

PDB ID : 7ENU
Title : Crystal structure of iron-saturated C-terminal half of lactoferrin produced proteolytically using pepsin at 2.32Å resolution
Authors : Singh, J.; Maurya, A.; Viswanathan, V.; Singh, P.K.; Sharma, P.; Sharma, S.; Singh, T.P.
Deposited on : 2021-04-19
Resolution : 2.32 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

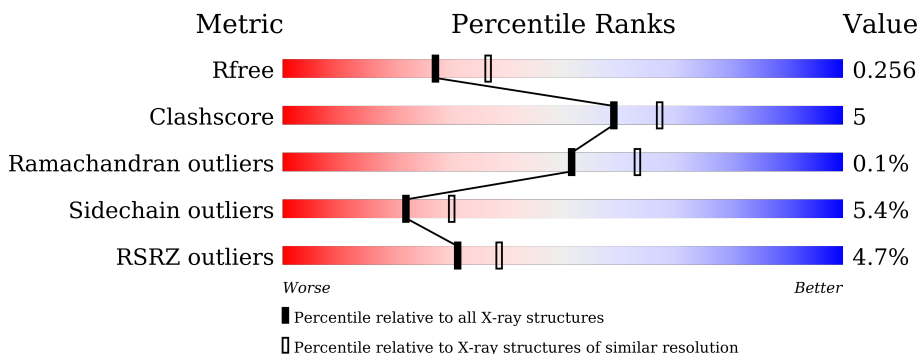
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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.



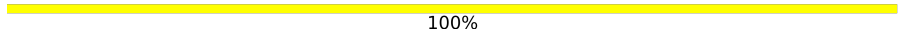

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	348	
1	B	348	
2	D	2	
2	F	2	
2	G	2	
3	E	3	

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Mol	Chain	Length	Quality of chain
4	H	4	 100%
5	C	5	 40% 60%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5652 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 Lactotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	348	Total 2657	C 1655	N 465	O 516	S 21	0	0	0
1	B	348	Total 2657	C 1655	N 465	O 516	S 21	0	0	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	F	2	Total 28	C 16	N 2	O 10	0	0	0
2	D	2	Total 28	C 16	N 2	O 10	0	0	0
2	G	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	3	Total 39	C 22	N 2	O 15	0	0	0

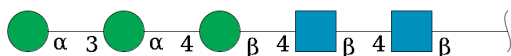
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-beta-D-mannopyranos

e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	H	4	50	28	2	20	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

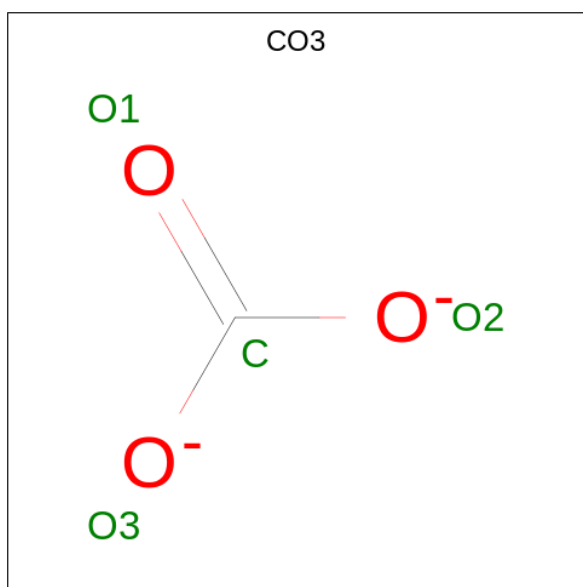


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	C	5	61	34	2	25	0	0	0

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Fe	0	0
			1	1		
6	B	1	Total	Fe	0	0
			1	1		

- Molecule 7 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 1 3	0	0
7	B	1	Total C O 4 1 3	0	0

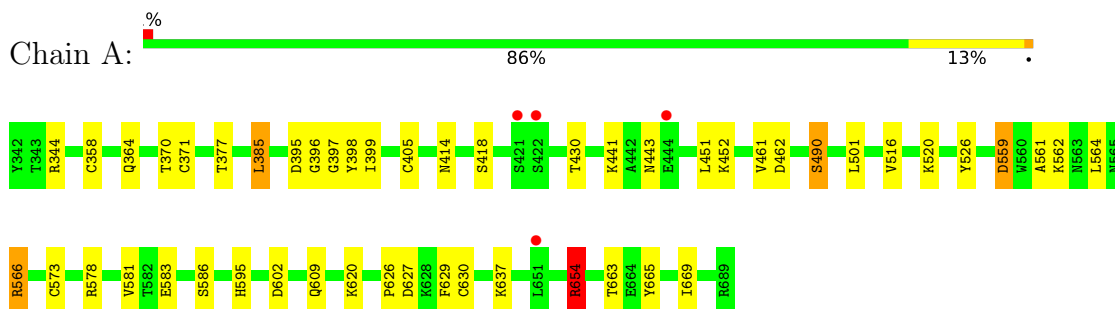
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	46	Total O 46 46	0	0
8	B	48	Total O 48 48	0	0

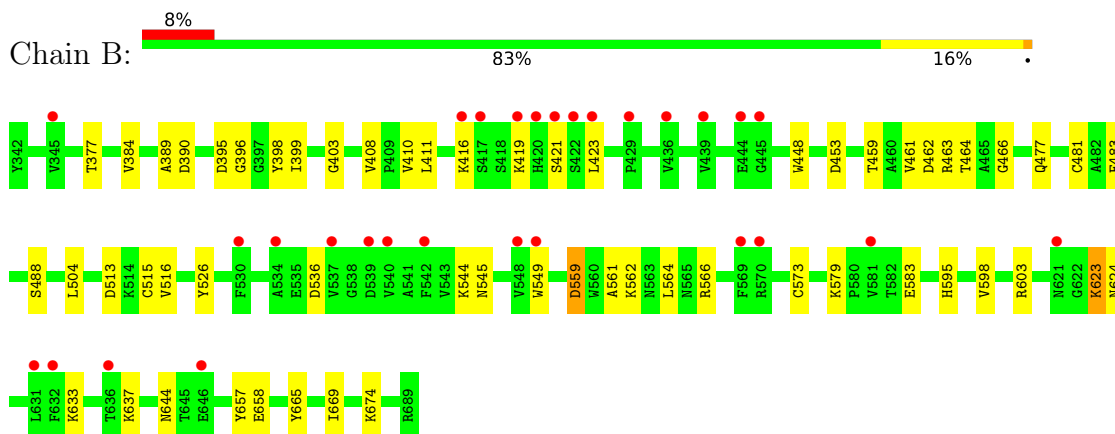
3 Residue-property plots i

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.

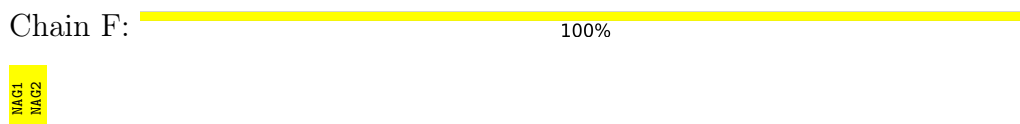
- Molecule 1: Lactotransferrin



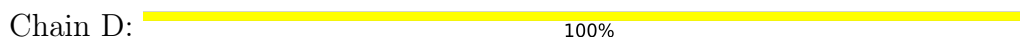
- Molecule 1: Lactotransferrin



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




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



MAG1
MAG2

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

Chain G:  100%MAG1
MAG2

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

Chain E:  100%MAG1
MAG2
BMA3

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

Chain H:  100%MAG1
MAG2
BMA3
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  40% 60%MAG1
MAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.67Å 82.03Å 112.14Å 90.00° 129.62° 90.00°	Depositor
Resolution (Å)	77.75 – 2.32 77.63 – 2.32	Depositor EDS
% Data completeness (in resolution range)	98.8 (77.75-2.32) 98.8 (77.63-2.32)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.32Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.203 , 0.249 0.209 , 0.256	Depositor DCC
R_{free} test set	2275 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtrriage
Anisotropy	0.187	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5652	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: MAN, NAG, BMA, CO3, FE

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	0.70	0/2707	0.85	1/3669 (0.0%)
1	B	0.72	0/2707	0.85	0/3669
All	All	0.71	0/5414	0.85	1/7338 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	370	THR	CA-CB-OG1	-5.42	97.61	109.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	490	SER	Peptide

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	2657	0	2581	25	0
1	B	2657	0	2581	26	0
2	D	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
3	E	39	0	34	0	0
4	H	50	0	43	0	0
5	C	61	0	52	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	4	0	0	1	0
7	B	4	0	0	0	0
8	A	46	0	0	0	0
8	B	48	0	0	1	0
All	All	5652	0	5366	51	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 5.

All (51) 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)
1:B:481:CYS:HB2	8:B:841:HOH:O	1.63	0.97
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.34	0.62
1:B:453:ASP:O	1:B:488:SER:HB3	2.03	0.58
1:B:526:TYR:CE2	1:B:544:LYS:HE2	2.38	0.58
1:A:385:LEU:HD11	1:A:405:CYS:HB3	1.85	0.57
1:B:513:ASP:O	1:B:516:VAL:HG12	2.04	0.57
1:A:377:THR:HG21	1:A:398:TYR:CD2	2.41	0.55
1:A:665:TYR:CE2	1:A:669:ILE:HD11	2.43	0.54
1:B:377:THR:HG21	1:B:398:TYR:CD2	2.45	0.52
1:B:623:LYS:HB2	1:B:624:ASN:OD1	2.09	0.51
1:B:390:ASP:OD1	1:B:603:ARG:NE	2.37	0.51
1:B:464:THR:HG23	1:B:665:TYR:CZ	2.46	0.50
1:A:561:ALA:HA	1:A:564:LEU:HD12	1.95	0.48
1:B:396:GLY:HA2	1:B:399:ILE:HD12	1.95	0.48
1:A:358:CYS:C	1:A:371:CYS:SG	2.93	0.47
1:A:397:GLY:HA3	1:A:462:ASP:O	2.14	0.47
1:A:626:PRO:HA	1:A:630:CYS:SG	2.55	0.47
1:B:395:ASP:OD2	1:B:463:ARG:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:GLY:HA2	1:A:399:ILE:HD12	1.97	0.45
1:A:665:TYR:CZ	1:A:669:ILE:HD11	2.52	0.45
1:A:566:ARG:HB2	1:A:581:VAL:HG21	1.99	0.45
1:B:408:VAL:O	1:B:598:VAL:HA	2.17	0.44
1:B:665:TYR:CZ	1:B:669:ILE:HD11	2.52	0.44
1:B:549:TRP:CE3	1:B:566:ARG:NH1	2.85	0.44
1:A:654:ARG:HE	1:A:654:ARG:HB2	1.59	0.44
1:B:395:ASP:HA	1:B:595:HIS:CD2	2.53	0.43
5:C:4:MAN:O2	5:C:4:MAN:H62	2.19	0.43
1:A:559:ASP:HA	1:A:562:LYS:HD3	1.99	0.43
1:B:384:VAL:HA	1:B:389:ALA:O	2.19	0.43
1:B:403:GLY:HA3	1:B:657:TYR:CG	2.53	0.43
5:C:3:BMA:C3	5:C:4:MAN:O5	2.67	0.42
1:B:448:TRP:HE1	1:B:477:GLN:HE22	1.67	0.42
1:A:414:ASN:OD1	1:A:430:THR:HA	2.20	0.42
1:A:418:SER:HA	5:C:2:NAG:O6	2.19	0.42
1:A:516:VAL:HG13	1:A:516:VAL:O	2.20	0.42
1:A:344:ARG:HG2	1:B:674:LYS:O	2.19	0.42
1:A:559:ASP:OD1	1:A:559:ASP:N	2.52	0.41
1:A:344:ARG:HD3	1:B:481:CYS:SG	2.61	0.41
1:A:364:GLN:HG3	1:A:629:PHE:HB2	2.02	0.41
1:B:461:VAL:O	1:B:462:ASP:HB2	2.21	0.41
1:B:410:VAL:HG12	1:B:411:LEU:HG	2.03	0.41
1:B:483:PHE:CD1	1:B:483:PHE:C	2.94	0.41
1:A:451:LEU:HD23	1:A:451:LEU:HA	1.91	0.41
1:B:561:ALA:HA	1:B:564:LEU:CD1	2.51	0.41
1:A:490:SER:HB2	1:A:501:LEU:HA	2.03	0.40
1:A:461:VAL:O	1:A:462:ASP:HB2	2.22	0.40
1:B:559:ASP:HA	1:B:562:LYS:HE3	2.03	0.40
1:A:443:ASN:O	1:A:578:ARG:NH2	2.54	0.40
1:A:526:TYR:CZ	7:A:702:CO3:O1	2.74	0.40
1:B:459:THR:OG1	1:B:466:GLY:HA3	2.22	0.40
1:B:579:LYS:HD3	1:B:583:GLU:HG2	2.04	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	346/348 (99%)	326 (94%)	19 (6%)	1 (0%)	41	50
1	B	346/348 (99%)	319 (92%)	27 (8%)	0	100	100
All	All	692/696 (99%)	645 (93%)	46 (7%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	654	ARG

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	289/289 (100%)	273 (94%)	16 (6%)	21	29
1	B	289/289 (100%)	274 (95%)	15 (5%)	23	32
All	All	578/578 (100%)	547 (95%)	31 (5%)	22	30

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	385	LEU
1	A	441	LYS
1	A	452	LYS
1	A	520	LYS
1	A	559	ASP

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Mol	Chain	Res	Type
1	A	566	ARG
1	A	573	CYS
1	A	583	GLU
1	A	586	SER
1	A	602	ASP
1	A	609	GLN
1	A	620	LYS
1	A	627	ASP
1	A	637	LYS
1	A	654	ARG
1	A	663	THR
1	B	416	LYS
1	B	419	LYS
1	B	421	SER
1	B	423	LEU
1	B	504	LEU
1	B	515	CYS
1	B	536	ASP
1	B	545	ASN
1	B	559	ASP
1	B	573	CYS
1	B	623	LYS
1	B	633	LYS
1	B	637	LYS
1	B	644	ASN
1	B	658	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	363	GLN
1	A	468	ASN
1	A	613	HIS
1	B	468	ASN
1	B	613	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

18 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
5	NAG	C	1	1,5	14,14,15	0.38	0	17,19,21	2.12	5 (29%)
5	NAG	C	2	5	14,14,15	0.50	0	17,19,21	1.94	2 (11%)
5	BMA	C	3	5	11,11,12	0.69	0	15,15,17	1.31	3 (20%)
5	MAN	C	4	5	11,11,12	0.87	0	15,15,17	2.23	4 (26%)
5	MAN	C	5	5	11,11,12	0.71	0	15,15,17	1.57	2 (13%)
2	NAG	D	1	2,1	14,14,15	0.44	0	17,19,21	1.76	3 (17%)
2	NAG	D	2	2	14,14,15	0.38	0	17,19,21	1.23	2 (11%)
3	NAG	E	1	1,3	14,14,15	0.57	0	17,19,21	2.13	5 (29%)
3	NAG	E	2	3	14,14,15	0.54	0	17,19,21	1.39	3 (17%)
3	BMA	E	3	3	11,11,12	0.72	0	15,15,17	2.57	5 (33%)
2	NAG	F	1	2,1	14,14,15	0.47	0	17,19,21	1.01	1 (5%)
2	NAG	F	2	2	14,14,15	0.80	1 (7%)	17,19,21	1.70	4 (23%)
2	NAG	G	1	2,1	14,14,15	0.37	0	17,19,21	1.31	3 (17%)
2	NAG	G	2	2	14,14,15	0.42	0	17,19,21	1.75	4 (23%)
4	NAG	H	1	1,4	14,14,15	0.42	0	17,19,21	2.11	3 (17%)
4	NAG	H	2	4	14,14,15	0.37	0	17,19,21	2.53	6 (35%)
4	BMA	H	3	4	11,11,12	0.71	0	15,15,17	2.28	5 (33%)
4	MAN	H	4	4	11,11,12	0.59	0	15,15,17	1.59	2 (13%)

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
5	NAG	C	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	BMA	C	3	5	-	2/2/19/22	0/1/1/1
5	MAN	C	4	5	-	2/2/19/22	0/1/1/1
5	MAN	C	5	5	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	MAN	H	4	4	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NAG	C1-C2	2.05	1.55	1.52

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2	NAG	C1-O5-C5	8.44	123.63	112.19
5	C	4	MAN	C1-O5-C5	7.04	121.73	112.19
3	E	3	BMA	C1-O5-C5	6.80	121.40	112.19
4	H	1	NAG	C1-O5-C5	6.46	120.95	112.19
5	C	1	NAG	C1-O5-C5	6.33	120.77	112.19
5	C	2	NAG	C1-O5-C5	5.82	120.08	112.19
3	E	1	NAG	O5-C5-C6	-5.61	98.40	107.20
4	H	3	BMA	C1-C2-C3	5.23	116.10	109.67
2	D	1	NAG	C1-O5-C5	4.86	118.77	112.19
4	H	4	MAN	C1-O5-C5	4.60	118.42	112.19
2	G	2	NAG	O5-C1-C2	4.37	118.18	111.29
3	E	3	BMA	O5-C1-C2	4.07	117.05	110.77
3	E	1	NAG	C1-O5-C5	4.03	117.65	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	3	BMA	O5-C1-C2	3.82	116.66	110.77
5	C	5	MAN	O5-C5-C6	3.77	113.12	107.20
2	D	1	NAG	C3-C4-C5	3.71	116.85	110.24
3	E	3	BMA	C1-C2-C3	3.70	114.21	109.67
5	C	1	NAG	C3-C4-C5	3.51	116.50	110.24
4	H	2	NAG	O5-C5-C6	-3.51	101.71	107.20
2	F	2	NAG	O5-C5-C6	3.40	112.54	107.20
2	G	1	NAG	C1-O5-C5	3.34	116.72	112.19
4	H	1	NAG	C3-C4-C5	3.26	116.05	110.24
3	E	1	NAG	O6-C6-C5	-3.24	100.17	111.29
2	F	2	NAG	O5-C1-C2	3.22	116.38	111.29
5	C	3	BMA	O4-C4-C5	3.20	117.24	109.30
2	G	2	NAG	C1-O5-C5	3.07	116.35	112.19
5	C	5	MAN	C1-O5-C5	2.94	116.17	112.19
3	E	3	BMA	C2-C3-C4	-2.89	105.90	110.89
2	G	2	NAG	O5-C5-C6	2.88	111.71	107.20
4	H	1	NAG	C2-N2-C7	2.87	126.99	122.90
3	E	2	NAG	C1-O5-C5	2.85	116.05	112.19
2	F	2	NAG	C2-N2-C7	2.82	126.92	122.90
5	C	1	NAG	O3-C3-C4	-2.80	103.87	110.35
4	H	3	BMA	O4-C4-C5	2.79	116.23	109.30
2	F	2	NAG	C4-C3-C2	2.74	115.04	111.02
5	C	4	MAN	O5-C5-C6	2.71	111.46	107.20
2	D	2	NAG	C1-O5-C5	2.70	115.85	112.19
4	H	3	BMA	C3-C4-C5	-2.68	105.45	110.24
5	C	2	NAG	O4-C4-C3	-2.66	104.19	110.35
4	H	2	NAG	C3-C4-C5	2.63	114.93	110.24
3	E	2	NAG	O5-C1-C2	2.57	115.35	111.29
5	C	1	NAG	O5-C5-C4	2.48	116.87	110.83
5	C	4	MAN	C2-C3-C4	2.33	114.94	110.89
2	D	2	NAG	C4-C3-C2	-2.29	107.66	111.02
3	E	3	BMA	C3-C4-C5	-2.29	106.16	110.24
2	G	1	NAG	O4-C4-C3	-2.27	105.10	110.35
4	H	2	NAG	C1-C2-N2	2.23	114.29	110.49
2	F	1	NAG	C4-C3-C2	2.18	114.22	111.02
5	C	3	BMA	C1-O5-C5	2.18	115.14	112.19
4	H	2	NAG	O5-C1-C2	2.17	114.72	111.29
2	D	1	NAG	O5-C5-C4	2.17	116.10	110.83
3	E	1	NAG	O5-C5-C4	2.12	115.98	110.83
4	H	4	MAN	C2-C3-C4	2.11	114.55	110.89
5	C	4	MAN	C1-C2-C3	2.11	112.26	109.67
3	E	2	NAG	C1-C2-N2	-2.11	106.88	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	NAG	C6-C5-C4	-2.11	108.07	113.00
2	G	2	NAG	O5-C5-C4	-2.10	105.72	110.83
3	E	1	NAG	O5-C1-C2	-2.08	108.00	111.29
4	H	3	BMA	O5-C5-C4	-2.07	105.79	110.83
2	G	1	NAG	O5-C5-C6	2.04	110.40	107.20
5	C	3	BMA	C1-C2-C3	2.00	112.13	109.67
4	H	2	NAG	O4-C4-C3	-2.00	105.72	110.35

There are no chirality outliers.

All (24) torsion outliers are listed below:

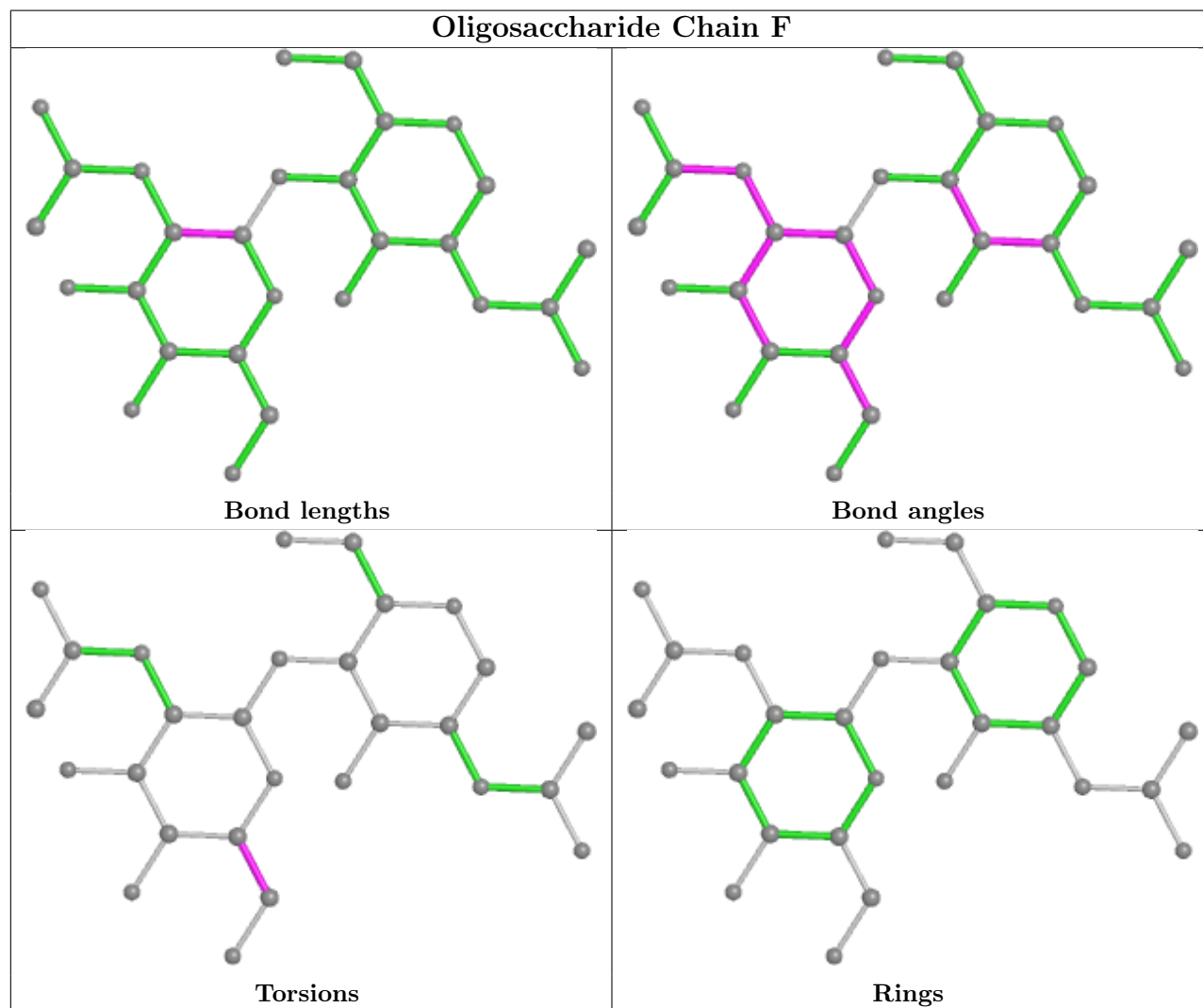
Mol	Chain	Res	Type	Atoms
4	H	4	MAN	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
4	H	4	MAN	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
5	C	4	MAN	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
5	C	3	BMA	O5-C5-C6-O6
5	C	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
5	C	3	BMA	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
5	C	4	MAN	C4-C5-C6-O6

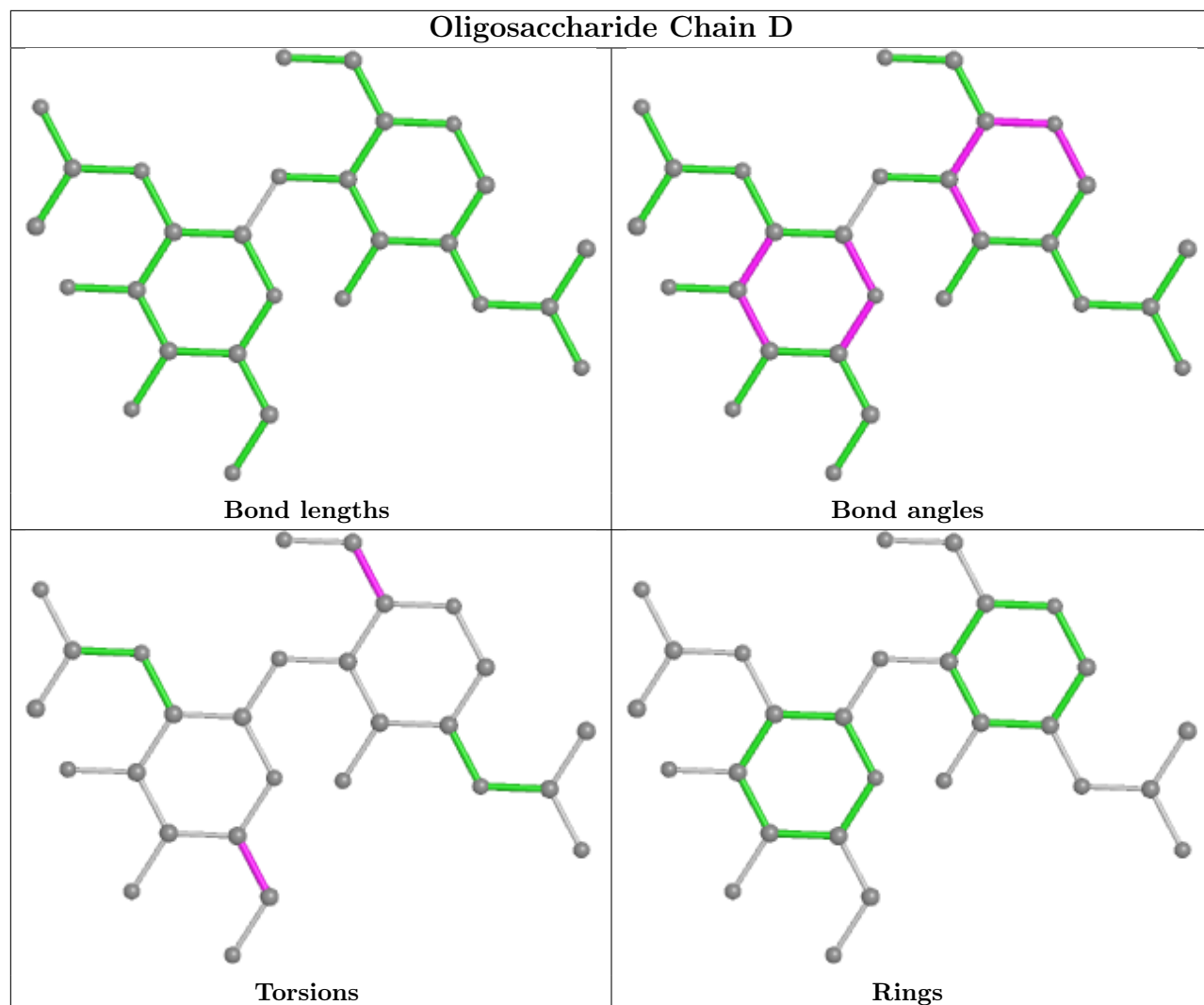
There are no ring outliers.

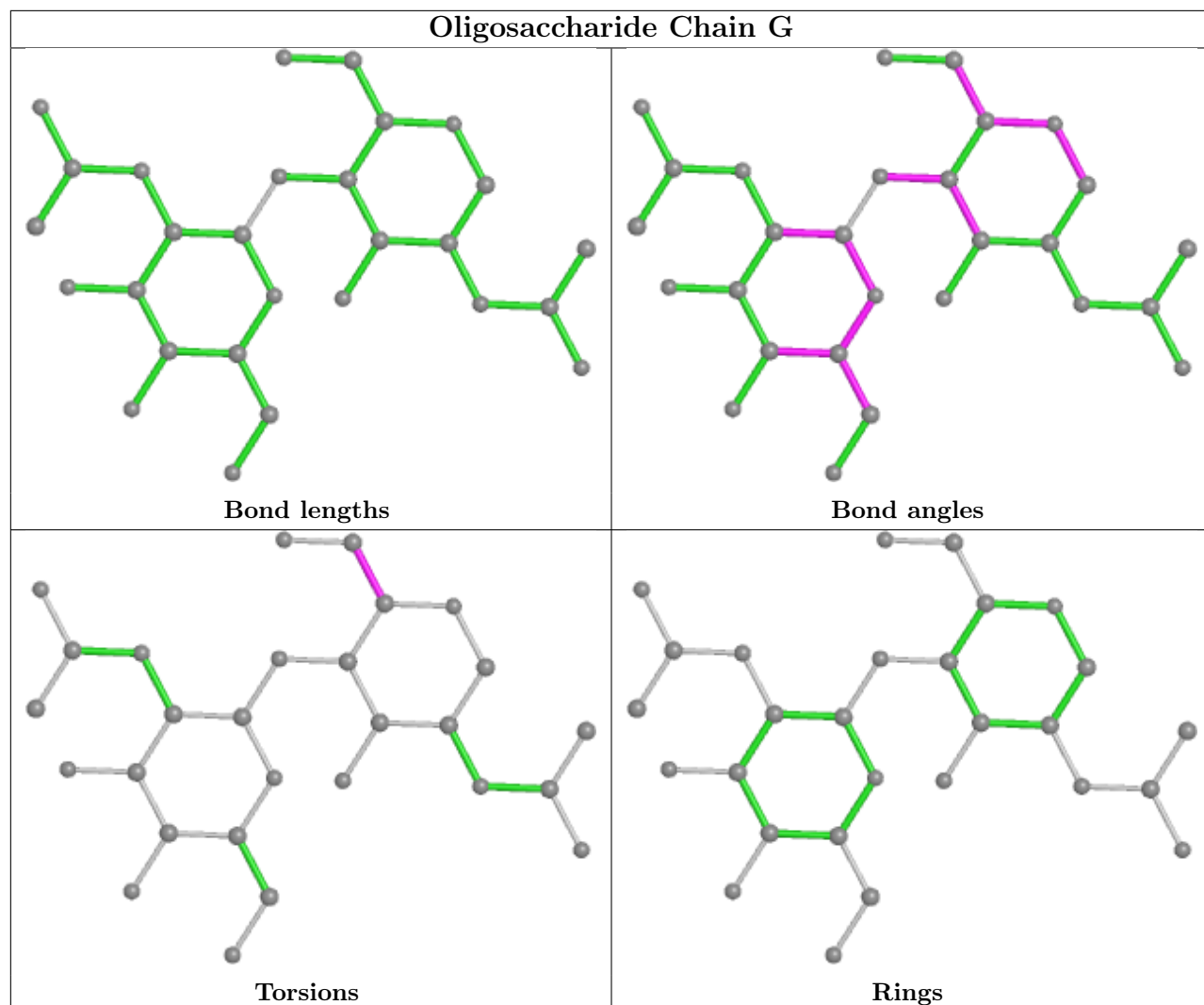
3 monomers are involved in 3 short contacts:

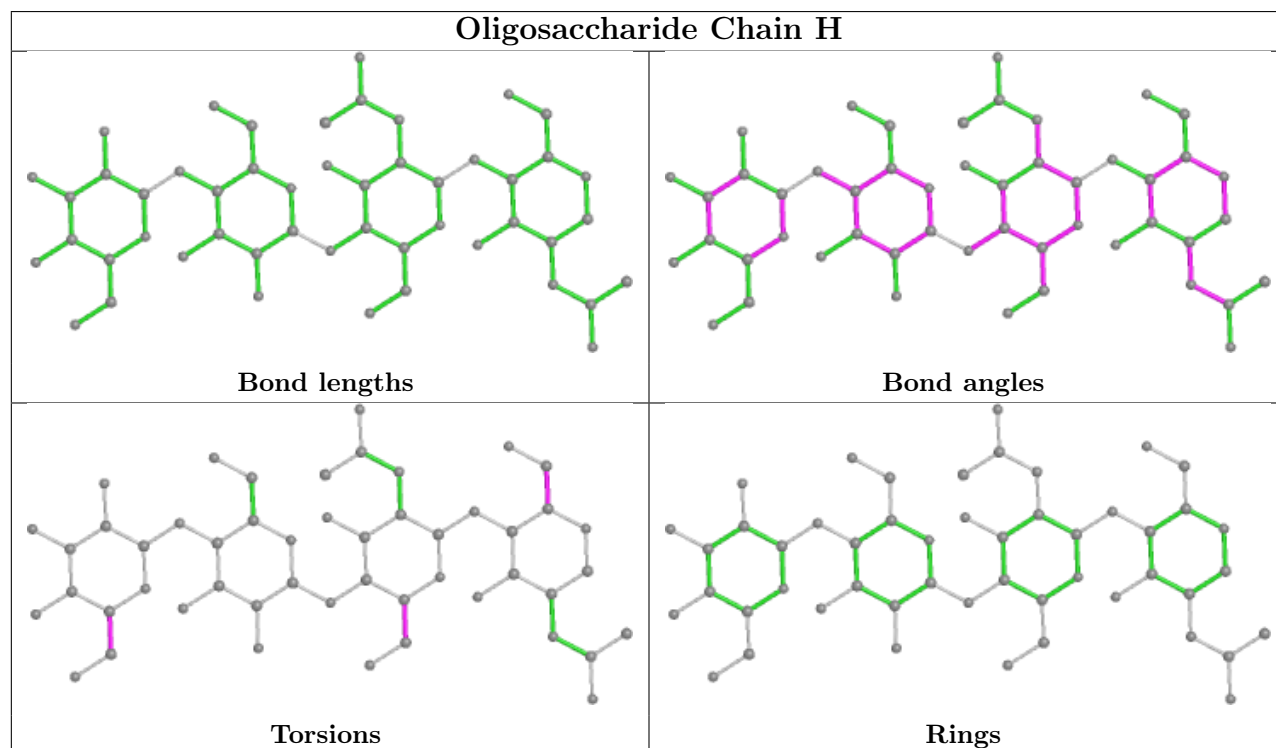
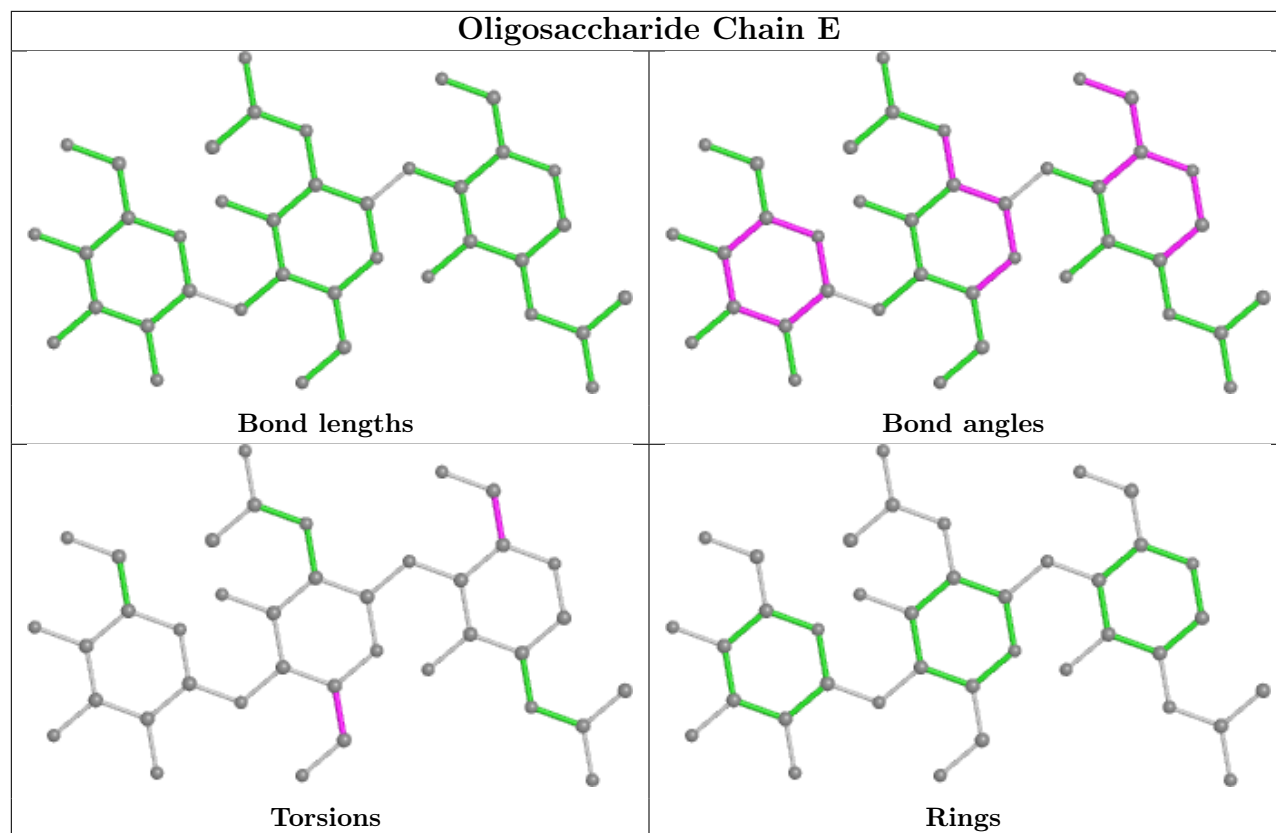
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	4	MAN	2	0
5	C	3	BMA	1	0
5	C	2	NAG	1	0

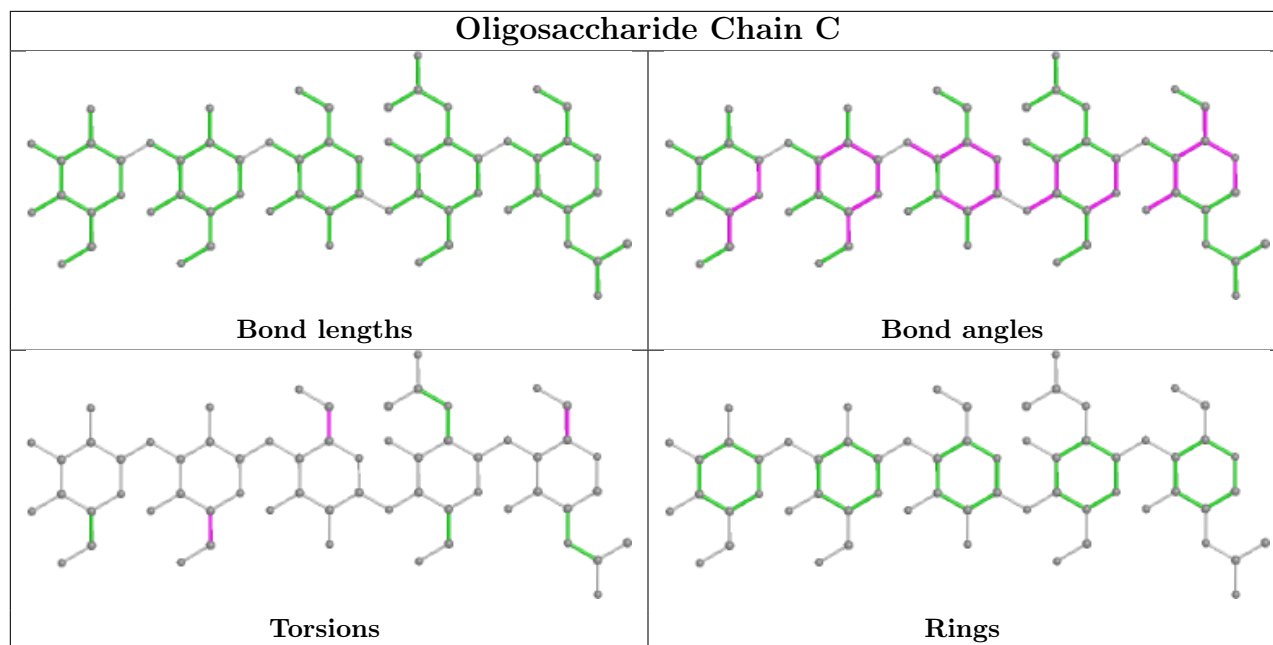
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CO3	A	702	6	2,3,3	0.47	0	2,3,3	0.26	0
7	CO3	B	702	6	2,3,3	0.50	0	2,3,3	0.49	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	702	CO3	1	0

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	348/348 (100%)	0.33	4 (1%) 80 85	47, 74, 119, 152	0
1	B	348/348 (100%)	0.52	29 (8%) 11 15	49, 77, 119, 159	0
All	All	696/696 (100%)	0.42	33 (4%) 31 38	47, 75, 119, 159	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	419	LYS	5.8
1	B	420	HIS	5.6
1	B	421	SER	4.3
1	B	621	ASN	4.3
1	B	530	PHE	3.9
1	A	422	SER	3.6
1	B	422	SER	3.4
1	B	445	GLY	3.3
1	B	548	VAL	2.9
1	B	542	PHE	2.8
1	B	534	ALA	2.7
1	B	537	VAL	2.7
1	B	539	ASP	2.6
1	B	444	GLU	2.6
1	B	632	PHE	2.6
1	B	569	PHE	2.6
1	B	631	LEU	2.5
1	B	439	VAL	2.5
1	B	423	LEU	2.5
1	B	646	GLU	2.4
1	A	651	LEU	2.4
1	B	636	THR	2.3
1	B	416	LYS	2.3
1	B	436	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	549	TRP	2.2
1	B	570	ARG	2.2
1	B	429	PRO	2.2
1	B	417	SER	2.2
1	B	581	VAL	2.2
1	A	421	SER	2.1
1	A	444	GLU	2.1
1	B	345	VAL	2.0
1	B	540	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

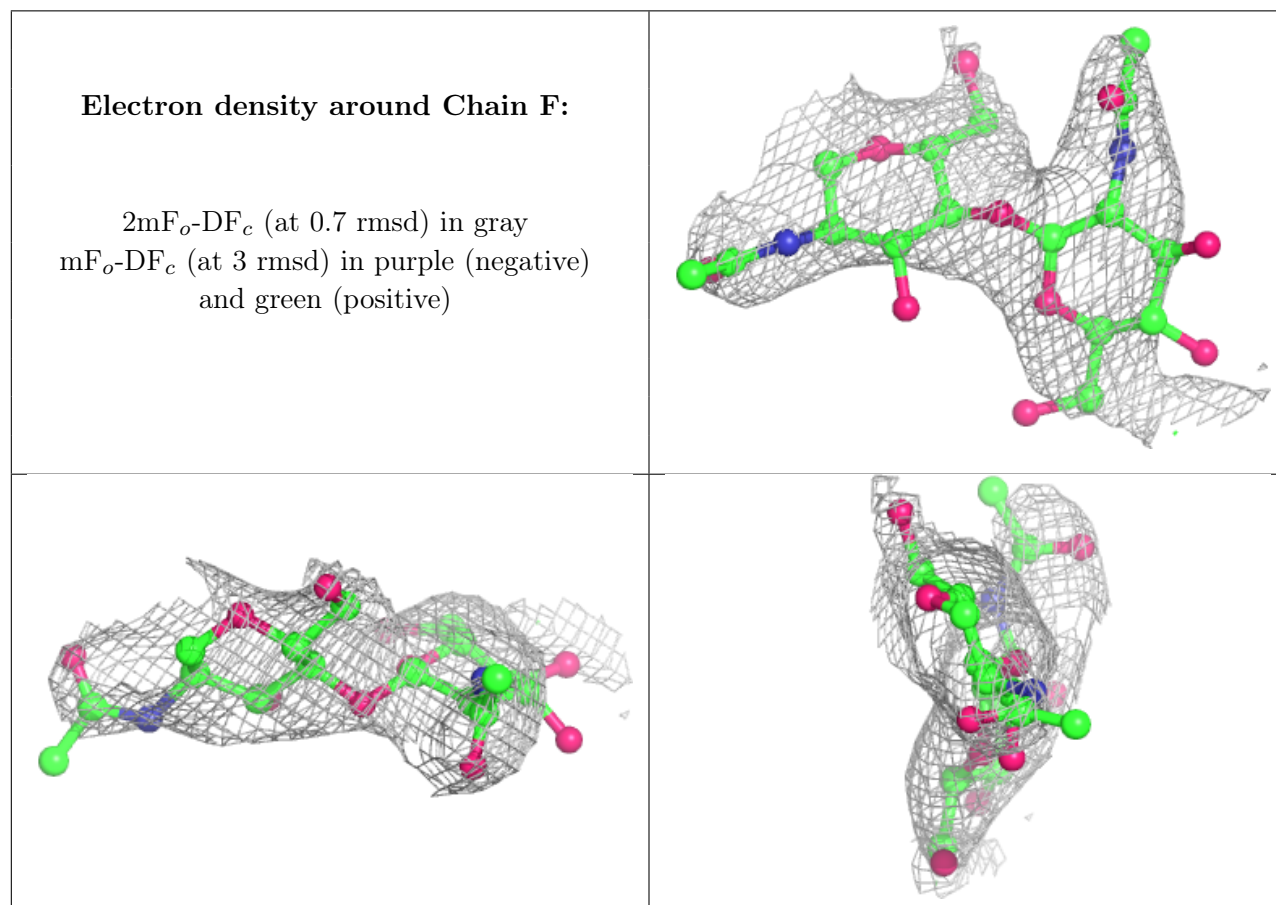
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [\(i\)](#)

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

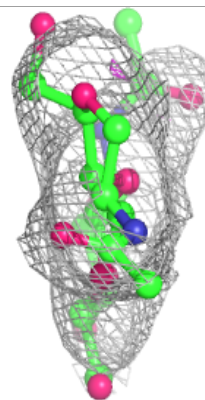
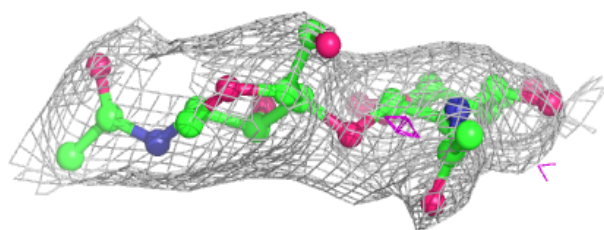
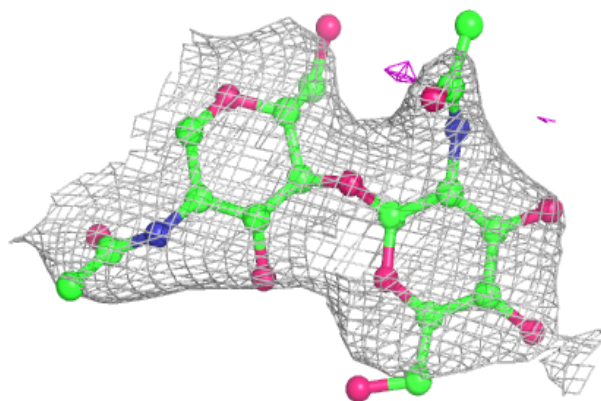
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	C	4	11/12	0.55	0.19	143,176,184,193	0
4	MAN	H	4	11/12	0.62	0.23	179,201,207,208	0
3	BMA	E	3	11/12	0.69	0.23	151,170,182,182	0
5	MAN	C	5	11/12	0.72	0.21	99,132,166,168	0
4	BMA	H	3	11/12	0.76	0.17	151,165,180,186	0
5	BMA	C	3	11/12	0.76	0.15	128,157,165,168	0
2	NAG	F	2	14/15	0.83	0.27	124,151,168,168	0
2	NAG	G	2	14/15	0.83	0.28	144,158,164,165	0
2	NAG	F	1	14/15	0.87	0.24	125,147,158,162	0
3	NAG	E	2	14/15	0.89	0.13	91,105,133,166	0
2	NAG	D	2	14/15	0.90	0.23	102,131,139,141	0
5	NAG	C	2	14/15	0.93	0.13	95,114,130,143	0
2	NAG	G	1	14/15	0.93	0.12	78,92,97,127	0
4	NAG	H	2	14/15	0.94	0.14	92,105,114,140	0
4	NAG	H	1	14/15	0.95	0.14	82,92,94,99	0
3	NAG	E	1	14/15	0.95	0.15	69,76,86,88	0
2	NAG	D	1	14/15	0.96	0.12	91,100,108,113	0
5	NAG	C	1	14/15	0.97	0.14	83,91,99,112	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.

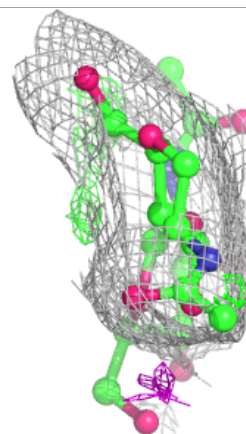
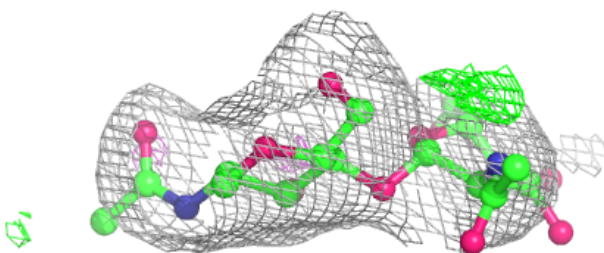
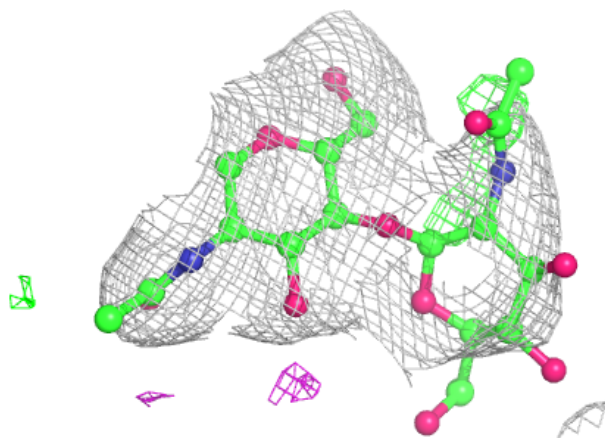


Electron density around Chain D:

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

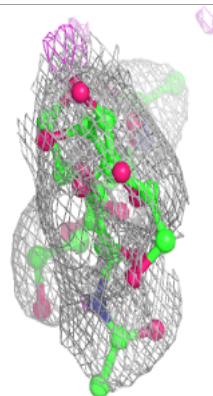
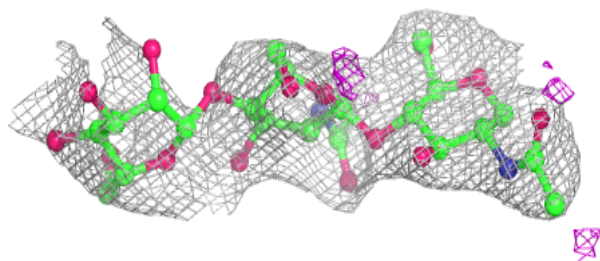
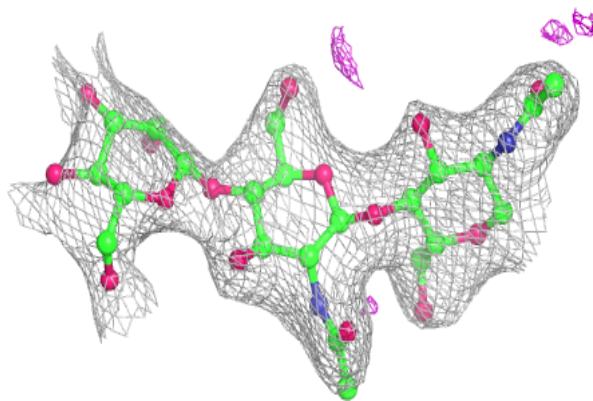
**Electron density around Chain G:**

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

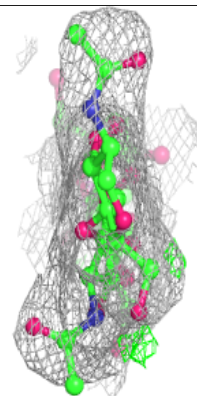
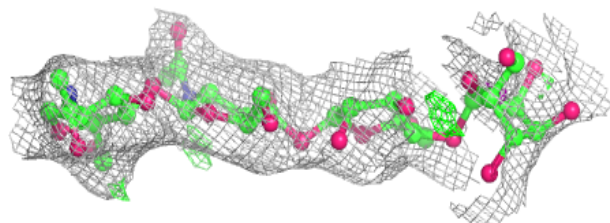
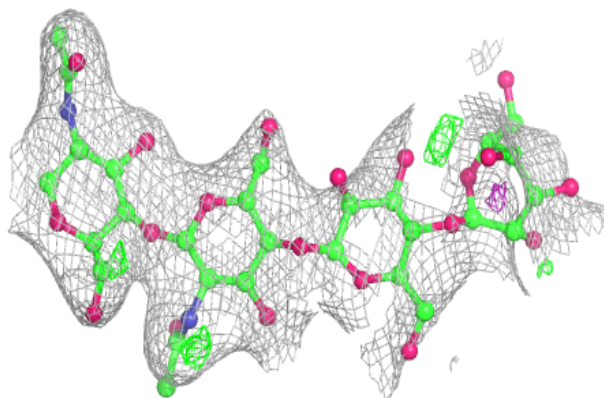


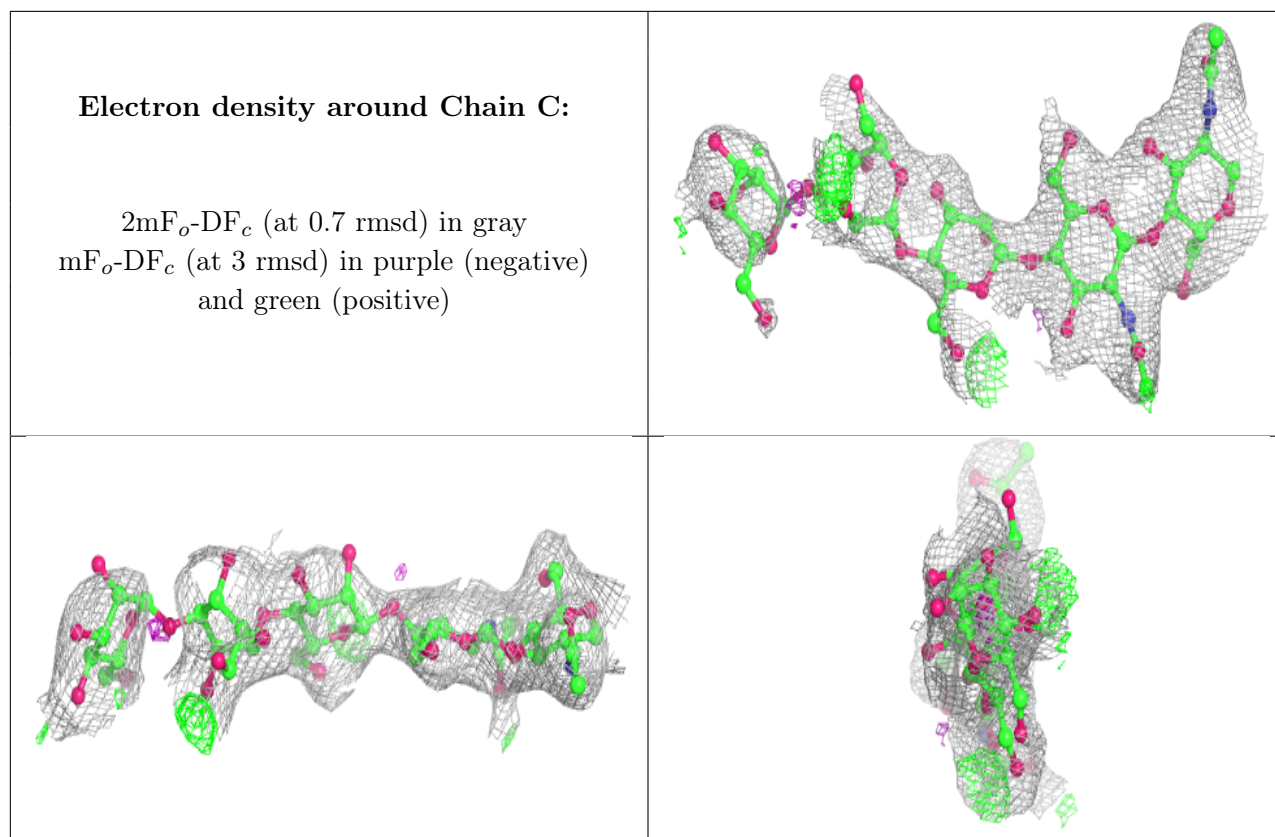
Electron density around Chain E:

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

**Electron density around Chain H:**

$2mF_o-DF_c$ (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	FE	A	701	1/1	0.98	0.18	77,77,77,77	0
7	CO3	B	702	4/4	0.98	0.11	48,50,50,53	0
7	CO3	A	702	4/4	0.99	0.10	63,63,65,71	0
6	FE	B	701	1/1	0.99	0.11	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.