



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2021 – 10:08 AM JST

PDB ID : 7EVQ
Title : Crystal structure of C-terminal half of lactoferrin obtained by limited proteolysis using pepsin at 2.6 Å resolution
Authors : Viswanathan, V.; Singh, J.; Sharma, P.; Sharma, S.; Singh, T.P.
Deposited on : 2021-05-21
Resolution : 2.60 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 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	:	2.19
buster-report	:	1.1.7 (2018)
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)	:	2.19

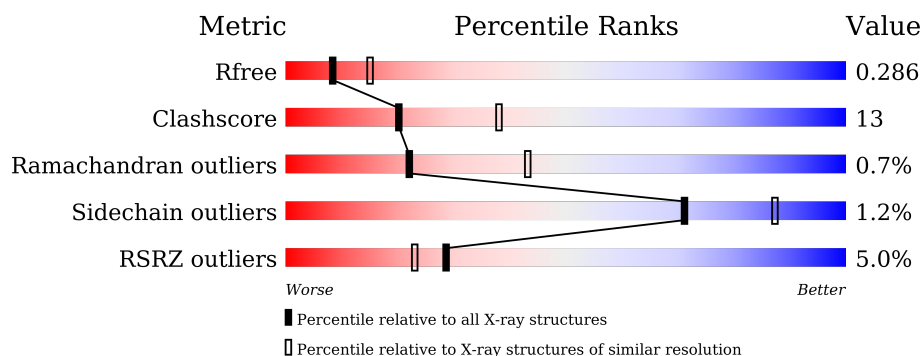
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	<div> <div>3%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	B	348	<div> <div>7%</div> <div>70%</div> <div>27%</div> <div>..</div> </div>
2	C	3	<div> <div>67%</div> <div>33%</div> </div>
2	D	3	<div> <div>100%</div> </div>
2	E	3	<div> <div>100%</div> </div>
2	F	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>

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
5	NAG	A	703	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5593 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
1	A	348	Total	C	N	O	S	0	0	0
			2657	1655	465	516	21			
1	B	348	Total	C	N	O	S	0	0	0
			2657	1655	465	516	21			

- Molecule 2 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.



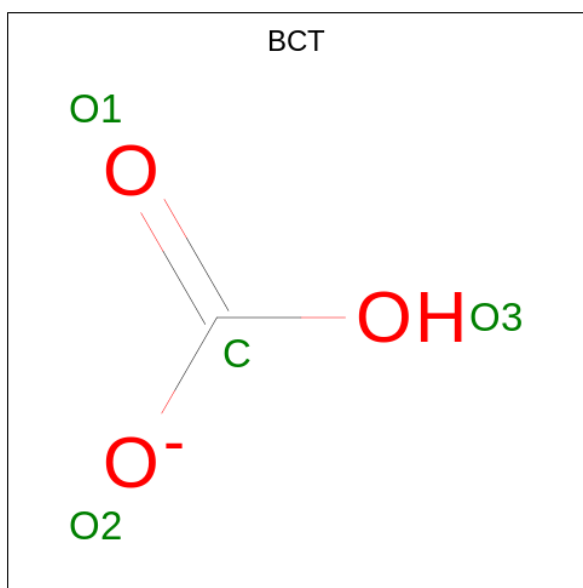
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

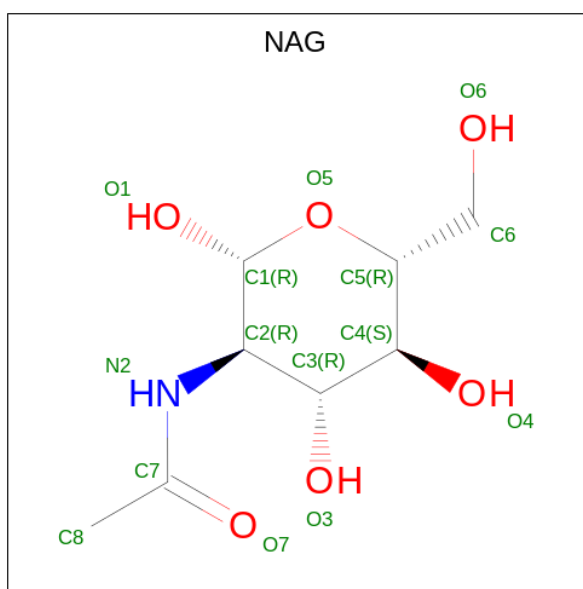
- Molecule 4 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃) (labeled as

"Ligand of Interest" by depositor).



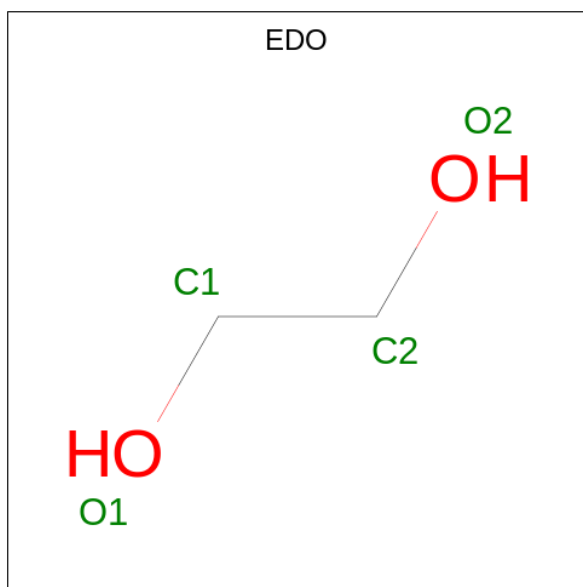
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	1	3		
4	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

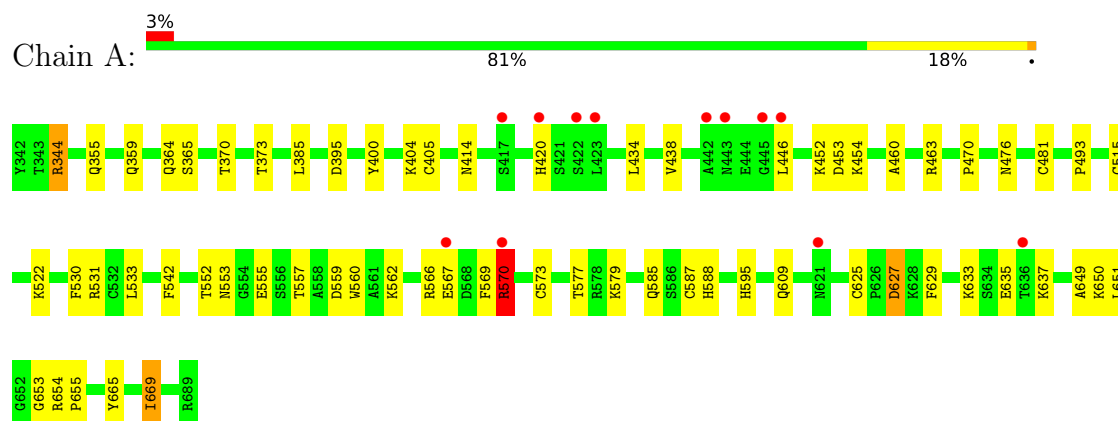
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	57	Total	O	0	0
			57	57		
7	B	24	Total	O	0	0
			24	24		

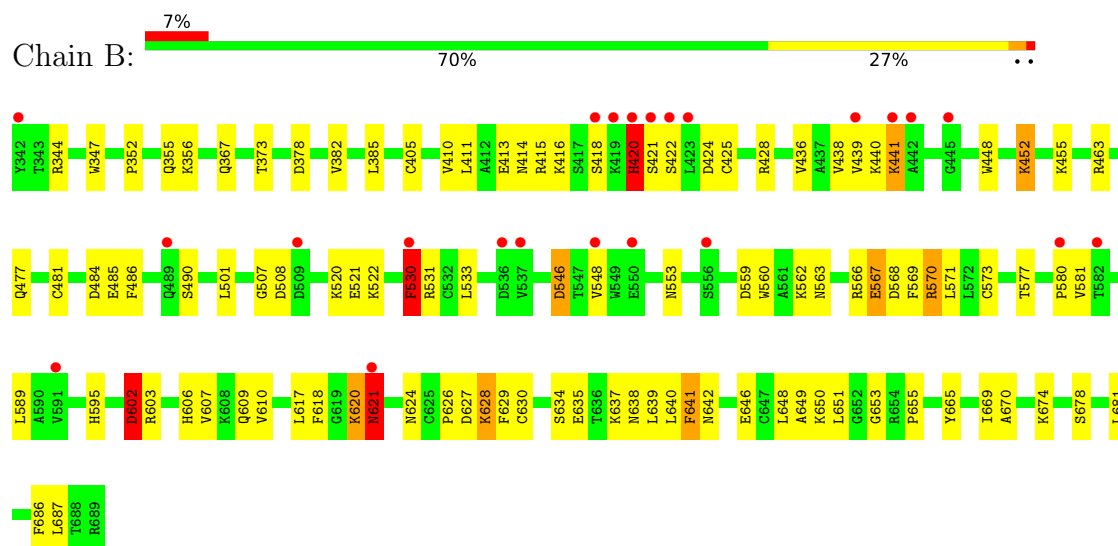
3 Residue-property plots [i](#)

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.

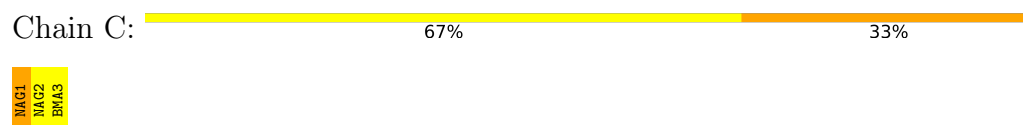
• Molecule 1: Lactotransferrin



• Molecule 1: Lactotransferrin



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




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

Chain D:  100%

MAG1
MAG2
BMA3

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

Chain F:  33% 33% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.25Å 81.69Å 110.23Å 90.00° 129.91° 90.00°	Depositor
Resolution (Å)	45.12 – 2.60 67.08 – 2.60	Depositor EDS
% Data completeness (in resolution range)	65.2 (45.12-2.60) 65.0 (67.08-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.227 , 0.284 0.230 , 0.286	Depositor DCC
R_{free} test set	1026 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5593	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, NAG, BCT, BMA, EDO

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	0.48	1/2707 (0.0%)	0.74	7/3669 (0.2%)
1	B	0.52	2/2707 (0.1%)	0.83	11/3669 (0.3%)
All	All	0.50	3/5414 (0.1%)	0.79	18/7338 (0.2%)

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	2
1	B	0	4
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	570	ARG	CZ-NH1	10.16	1.46	1.33
1	B	567	GLU	CD-OE2	5.33	1.31	1.25
1	B	452	LYS	CD-CE	5.17	1.64	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	628	LYS	CA-CB-CG	-11.77	87.50	113.40
1	A	570	ARG	NE-CZ-NH1	11.13	125.86	120.30
1	A	627	ASP	CB-CG-OD2	-10.86	108.53	118.30
1	B	420	HIS	CB-CA-C	-10.27	89.86	110.40
1	A	570	ARG	CG-CD-NE	-9.82	91.18	111.80
1	A	625	CYS	C-N-CD	-8.22	102.53	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	669	ILE	CG1-CB-CG2	-6.94	96.13	111.40
1	B	621	ASN	N-CA-CB	-6.82	98.32	110.60
1	B	567	GLU	OE1-CD-OE2	6.69	131.33	123.30
1	B	530	PHE	CB-CG-CD2	-6.67	116.13	120.80
1	A	570	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	441	LYS	CD-CE-NZ	-6.05	97.78	111.70
1	B	356	LYS	CA-CB-CG	-5.65	100.96	113.40
1	B	602	ASP	CB-CG-OD1	-5.60	113.26	118.30
1	B	628	LYS	CD-CE-NZ	5.42	124.17	111.70
1	A	481	CYS	CA-CB-SG	5.32	123.58	114.00
1	B	620	LYS	C-N-CA	5.14	134.55	121.70
1	B	420	HIS	N-CA-CB	5.03	119.66	110.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	570	ARG	Sidechain
1	A	627	ASP	Sidechain
1	B	420	HIS	Sidechain,Peptide
1	B	530	PHE	Sidechain
1	B	621	ASN	Sidechain

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	45	0
1	B	2657	0	2581	93	0
2	C	39	0	34	1	0
2	D	39	0	34	1	0
2	E	39	0	34	0	0
2	F	39	0	34	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	1	0	0
4	B	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	14	0	13	2	0
5	B	14	0	13	0	0
6	A	4	0	6	0	0
7	A	57	0	0	1	0
7	B	24	0	0	1	0
All	All	5593	0	5331	136	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 13.

All (136) 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:570:ARG:HH21	1:B:580:PRO:HA	1.16	1.07
1:B:570:ARG:NH2	1:B:580:PRO:HA	1.78	0.97
1:A:569:PHE:O	1:A:570:ARG:HD3	1.67	0.95
1:B:570:ARG:NH2	1:B:581:VAL:H	1.66	0.94
1:B:436:VAL:HA	1:B:589:LEU:HD23	1.50	0.93
1:B:441:LYS:HE2	1:B:568:ASP:HA	1.50	0.93
1:B:567:GLU:OE1	1:B:570:ARG:NH1	2.02	0.93
1:B:530:PHE:CE1	1:B:548:VAL:HA	2.11	0.85
1:A:452:LYS:HD2	1:A:453:ASP:HB2	1.57	0.85
1:B:570:ARG:HH22	1:B:581:VAL:H	1.23	0.85
1:A:569:PHE:C	1:A:570:ARG:HD3	1.97	0.84
1:B:567:GLU:HA	1:B:570:ARG:NH1	1.94	0.83
1:A:569:PHE:O	1:A:570:ARG:CD	2.27	0.83
1:B:638:ASN:OD1	1:B:642:ASN:HA	1.80	0.80
1:B:567:GLU:HA	1:B:570:ARG:HH11	1.47	0.79
1:B:530:PHE:HE1	1:B:548:VAL:HA	1.45	0.79
1:A:573:CYS:SG	1:A:577:THR:OG1	2.42	0.78
1:B:418:SER:HG	2:F:2:NAG:HO6	1.27	0.78
1:B:627:ASP:C	1:B:628:LYS:HG2	2.02	0.78
1:B:635:GLU:OE1	1:B:637:LYS:NZ	2.15	0.77
1:B:570:ARG:NH2	1:B:580:PRO:CA	2.51	0.73
1:B:570:ARG:HH21	1:B:580:PRO:CA	1.99	0.71
1:B:425:CYS:HA	1:B:428:ARG:HD3	1.73	0.70
1:B:618:PHE:CD1	1:B:629:PHE:HB3	2.26	0.70
1:B:570:ARG:NH2	1:B:581:VAL:N	2.39	0.69
1:B:344:ARG:HG2	1:B:367:GLN:O	1.93	0.69
1:B:448:TRP:NE1	1:B:477:GLN:OE1	2.24	0.68
1:B:571:LEU:HD22	1:B:581:VAL:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:LYS:HG2	1:B:621:ASN:OD1	1.94	0.68
1:B:617:LEU:HB3	1:B:618:PHE:CD2	2.30	0.67
1:B:635:GLU:HB2	1:B:637:LYS:HE2	1.77	0.66
1:B:620:LYS:HD2	1:B:646:GLU:HA	1.76	0.66
1:B:570:ARG:HD3	1:B:580:PRO:HA	1.79	0.65
1:A:609:GLN:NE2	7:A:802:HOH:O	2.30	0.64
1:B:641:PHE:N	1:B:641:PHE:CD1	2.65	0.64
1:B:355:GLN:OE1	1:B:373:THR:OG1	2.13	0.64
1:B:546:ASP:N	1:B:546:ASP:OD1	2.29	0.64
1:B:352:PRO:HA	1:B:355:GLN:HB3	1.80	0.63
1:B:573:CYS:SG	1:B:577:THR:OG1	2.57	0.63
1:B:531:ARG:HG3	1:B:560:TRP:CD2	2.34	0.62
1:B:650:LYS:HG2	1:B:651:LEU:H	1.64	0.62
1:B:624:ASN:OD1	1:B:628:LYS:HB2	1.99	0.62
1:B:603:ARG:O	1:B:607:VAL:HG23	1.99	0.62
1:B:626:PRO:HA	1:B:630:CYS:SG	2.41	0.61
1:A:553:ASN:OD1	1:A:566:ARG:HG3	2.00	0.60
1:B:440:LYS:HG2	1:B:533:LEU:HD11	1.84	0.60
1:B:571:LEU:HD13	1:B:581:VAL:HG12	1.84	0.59
1:B:606:HIS:O	1:B:610:VAL:HG23	2.01	0.59
1:A:355:GLN:O	1:A:359:GLN:HG2	2.03	0.58
1:A:414:ASN:HD22	1:A:649:ALA:HB2	1.69	0.58
1:A:460:ALA:HB3	1:A:463:ARG:HD3	1.85	0.58
1:A:385:LEU:HD21	1:A:405:CYS:HB3	1.85	0.57
1:B:602:ASP:OD1	1:B:602:ASP:N	2.32	0.55
1:B:641:PHE:N	1:B:641:PHE:HD1	2.04	0.55
1:A:365:SER:HA	2:C:1:NAG:H81	1.90	0.54
1:A:476:ASN:OD1	5:A:703:NAG:H2	2.09	0.53
1:A:633:LYS:HZ3	1:A:635:GLU:HA	1.72	0.53
1:A:567:GLU:O	1:A:570:ARG:NH1	2.42	0.53
1:A:653:GLY:O	1:A:655:PRO:HD3	2.08	0.53
1:B:567:GLU:OE1	1:B:570:ARG:CZ	2.57	0.52
1:B:452:LYS:HD2	1:B:486:PHE:O	2.08	0.52
1:B:378:ASP:O	1:B:382:VAL:HG23	2.09	0.52
1:A:370:THR:HG21	1:B:481:CYS:SG	2.50	0.52
1:B:508:ASP:OD2	1:B:520:LYS:NZ	2.41	0.51
1:B:410:VAL:HG12	1:B:411:LEU:HG	1.92	0.51
1:B:553:ASN:OD1	1:B:566:ARG:HG3	2.11	0.51
1:A:650:LYS:O	1:A:651:LEU:HD23	2.11	0.51
1:B:439:VAL:HG22	1:B:570:ARG:O	2.11	0.51
1:B:484:ASP:OD2	1:B:485:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:VAL:HG12	1:B:533:LEU:CD2	2.42	0.50
1:A:569:PHE:O	1:A:570:ARG:HD2	2.08	0.50
1:B:385:LEU:HD21	1:B:405:CYS:HB3	1.94	0.50
1:B:413:GLU:HG3	1:B:595:HIS:O	2.12	0.49
1:B:570:ARG:HD3	1:B:580:PRO:CA	2.41	0.49
1:B:428:ARG:HH22	1:B:646:GLU:CD	2.16	0.49
1:B:411:LEU:HB3	1:B:648:LEU:HB3	1.95	0.49
1:A:364:GLN:HG3	1:A:629:PHE:HB2	1.95	0.49
1:B:522:LYS:HG3	1:B:531:ARG:NH1	2.27	0.48
1:B:606:HIS:O	1:B:609:GLN:HG2	2.12	0.48
1:B:415:ARG:NH1	7:B:801:HOH:O	2.46	0.48
1:A:355:GLN:HG3	1:A:373:THR:OG1	2.13	0.48
1:B:617:LEU:HB3	1:B:618:PHE:CE2	2.48	0.48
1:B:634:SER:HB2	1:B:639:LEU:HB2	1.95	0.48
1:A:493:PRO:HA	1:A:515:CYS:SG	2.55	0.47
1:B:414:ASN:HD22	1:B:649:ALA:HB2	1.79	0.47
1:B:507:GLY:N	1:B:521:GLU:OE1	2.42	0.47
1:A:522:LYS:HD2	1:A:531:ARG:NH2	2.30	0.47
1:A:635:GLU:O	1:A:637:LYS:NZ	2.47	0.47
1:A:434:LEU:HD22	1:A:588:HIS:CG	2.49	0.47
1:B:627:ASP:O	1:B:628:LYS:NZ	2.45	0.47
1:B:424:ASP:O	1:B:428:ARG:HG3	2.14	0.46
1:B:530:PHE:HZ	1:B:548:VAL:HG13	1.80	0.46
1:B:639:LEU:O	1:B:641:PHE:N	2.46	0.46
1:A:579:LYS:HD2	1:A:587:CYS:HB2	1.97	0.46
1:B:440:LYS:HD3	1:B:569:PHE:CE2	2.51	0.45
1:B:455:LYS:HE2	1:B:455:LYS:HB3	1.61	0.45
1:B:438:VAL:HG12	1:B:533:LEU:HD23	1.98	0.45
1:A:585:GLN:OE1	2:D:1:NAG:H81	2.17	0.45
1:B:570:ARG:CD	1:B:580:PRO:HA	2.46	0.44
1:A:438:VAL:HG12	1:A:533:LEU:CD2	2.47	0.44
1:B:416:LYS:HA	1:B:646:GLU:OE2	2.17	0.44
1:B:686:PHE:HD2	1:B:687:LEU:HD23	1.82	0.44
1:B:570:ARG:HG3	1:B:571:LEU:H	1.82	0.44
1:B:678:SER:HB3	1:B:681:LEU:HB2	1.99	0.44
1:A:552:THR:O	1:A:555:GLU:HG2	2.17	0.44
1:B:686:PHE:CD2	1:B:687:LEU:HD23	2.53	0.43
1:B:653:GLY:O	1:B:655:PRO:HD3	2.19	0.43
1:B:670:ALA:O	1:B:674:LYS:HG3	2.18	0.43
1:A:476:ASN:ND2	5:A:703:NAG:H61	2.33	0.43
1:A:470:PRO:HB3	1:A:542:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:PHE:HD1	1:B:629:PHE:O	2.02	0.43
1:B:665:TYR:CZ	1:B:669:ILE:HD11	2.54	0.43
1:A:446:LEU:HD13	1:A:454:LYS:HE2	2.01	0.43
1:B:570:ARG:HH21	1:B:581:VAL:N	2.12	0.43
1:A:530:PHE:HD1	1:A:560:TRP:HZ3	1.67	0.42
1:A:452:LYS:CD	1:A:453:ASP:HB2	2.40	0.42
1:A:438:VAL:HG12	1:A:533:LEU:HD23	2.01	0.42
1:A:452:LYS:HD2	1:A:453:ASP:CB	2.41	0.42
1:B:490:SER:HB2	1:B:501:LEU:HA	2.02	0.42
1:A:665:TYR:CE2	1:A:669:ILE:HD11	2.54	0.42
1:B:347:TRP:CD1	1:B:640:LEU:HD22	2.55	0.41
1:B:463:ARG:HB3	4:B:703:BCT:C	2.50	0.41
1:A:654:ARG:N	1:A:654:ARG:HD2	2.35	0.41
1:B:562:LYS:HG3	1:B:563:ASN:ND2	2.36	0.41
1:B:650:LYS:HG2	1:B:651:LEU:N	2.31	0.41
1:B:522:LYS:HG3	1:B:531:ARG:HH11	1.85	0.41
1:B:420:HIS:O	1:B:422:SER:N	2.53	0.41
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.56	0.41
1:A:344:ARG:HD2	1:B:674:LYS:O	2.20	0.41
1:B:415:ARG:NH1	1:B:546:ASP:OD2	2.54	0.41
1:A:665:TYR:O	1:A:669:ILE:HG13	2.21	0.40
1:A:400:TYR:CZ	1:A:404:LYS:HE2	2.56	0.40
1:A:557:THR:HA	1:A:562:LYS:HB3	2.03	0.40
1:B:441:LYS:HE2	1:B:567:GLU:O	2.21	0.40
1:A:522:LYS:NZ	1:A:531:ARG:HH21	2.20	0.40
1:A:567:GLU:HA	1:A:570:ARG:NH1	2.37	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%)	18 (5%)	2 (1%)	25	47
1	B	346/348 (99%)	320 (92%)	23 (7%)	3 (1%)	17	35
All	All	692/696 (99%)	646 (93%)	41 (6%)	5 (1%)	22	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	421	SER
1	B	559	ASP
1	A	420	HIS
1	A	559	ASP
1	B	420	HIS

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	289/289 (100%)	288 (100%)	1 (0%)	92	98
1	B	289/289 (100%)	283 (98%)	6 (2%)	53	77
All	All	578/578 (100%)	571 (99%)	7 (1%)	71	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	ARG
1	B	420	HIS
1	B	530	PHE
1	B	546	ASP
1	B	570	ARG
1	B	602	ASP
1	B	641	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	563	ASN
1	B	642	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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$
2	NAG	C	1	1,2	14,14,15	0.66	1 (7%)	17,19,21	0.71	0
2	NAG	C	2	2	14,14,15	0.25	0	17,19,21	2.12	2 (11%)
2	BMA	C	3	2	11,11,12	1.35	2 (18%)	15,15,17	1.15	1 (6%)
2	NAG	D	1	1,2	14,14,15	0.53	0	17,19,21	0.65	0
2	NAG	D	2	2	14,14,15	0.81	1 (7%)	17,19,21	0.93	1 (5%)
2	BMA	D	3	2	11,11,12	1.08	1 (9%)	15,15,17	2.37	3 (20%)
2	NAG	E	1	1,2	14,14,15	0.25	0	17,19,21	1.16	1 (5%)
2	NAG	E	2	2	14,14,15	0.51	0	17,19,21	1.03	2 (11%)
2	BMA	E	3	2	11,11,12	0.60	0	15,15,17	1.79	2 (13%)
2	NAG	F	1	1,2	14,14,15	0.40	0	17,19,21	0.59	0
2	NAG	F	2	2	14,14,15	0.65	1 (7%)	17,19,21	0.81	1 (5%)
2	BMA	F	3	2	11,11,12	1.29	1 (9%)	15,15,17	1.76	3 (20%)

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	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	BMA	F	3	2	-	2/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	BMA	C1-C2	3.63	1.60	1.52
2	C	3	BMA	O5-C1	-3.02	1.38	1.43
2	C	3	BMA	O5-C5	2.41	1.48	1.43
2	D	3	BMA	C4-C5	2.18	1.57	1.53
2	D	2	NAG	O5-C1	-2.16	1.40	1.43
2	F	2	NAG	C1-C2	2.12	1.55	1.52
2	C	1	NAG	O5-C1	-2.03	1.40	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	8.04	123.08	112.19
2	D	3	BMA	O5-C1-C2	6.72	121.15	110.77
2	E	3	BMA	C1-O5-C5	5.92	120.22	112.19
2	F	3	BMA	C3-C4-C5	4.15	117.63	110.24
2	D	3	BMA	C1-C2-C3	4.10	114.70	109.67
2	E	1	NAG	C1-O5-C5	4.00	117.61	112.19
2	D	3	BMA	C1-O5-C5	3.45	116.87	112.19
2	F	3	BMA	O2-C2-C3	-3.02	104.09	110.14
2	D	2	NAG	C1-O5-C5	2.89	116.11	112.19
2	F	2	NAG	C1-O5-C5	2.59	115.70	112.19
2	F	3	BMA	O3-C3-C4	-2.50	104.58	110.35
2	E	3	BMA	O2-C2-C3	-2.33	105.48	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C3-C4-C5	2.23	114.21	110.24
2	C	3	BMA	C1-C2-C3	2.19	112.36	109.67
2	E	2	NAG	C1-O5-C5	2.19	115.16	112.19
2	E	2	NAG	C3-C4-C5	2.16	114.09	110.24

There are no chirality outliers.

All (16) torsion outliers are listed below:

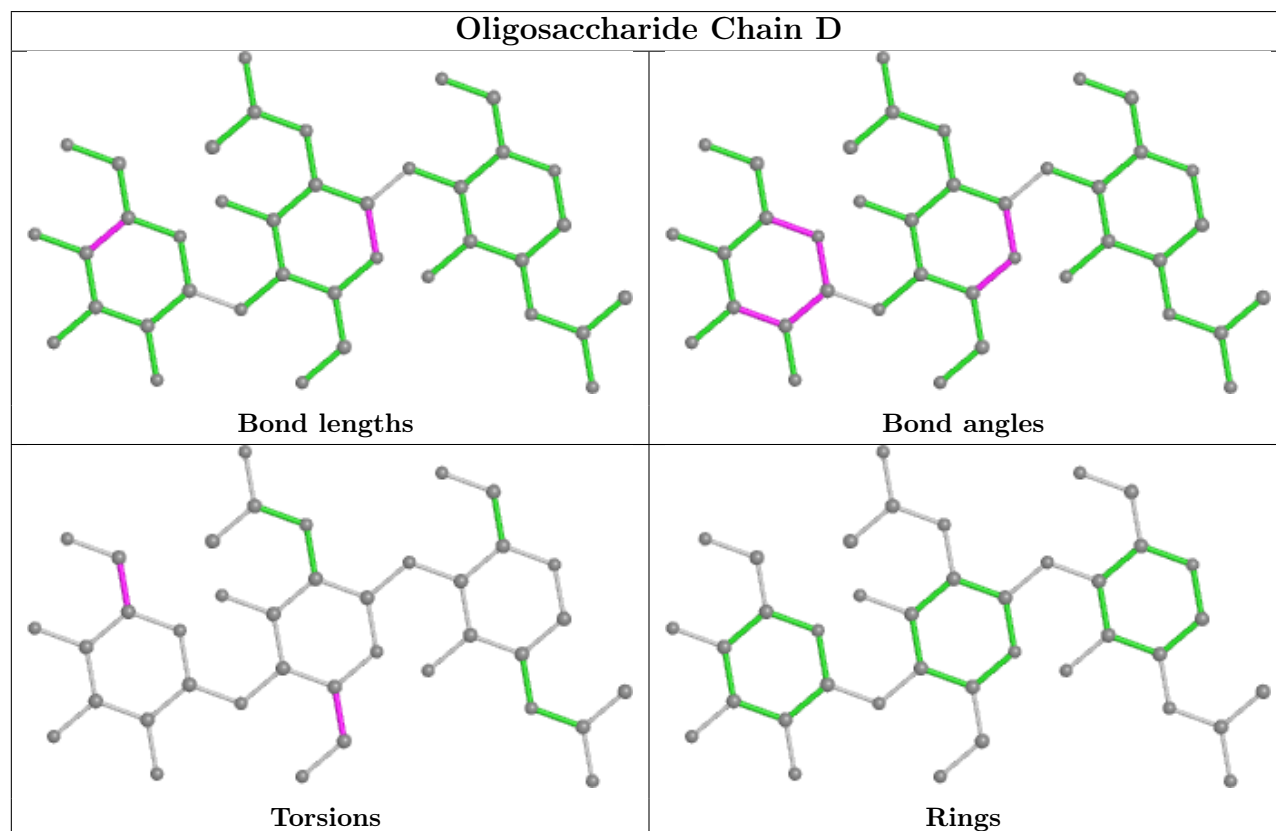
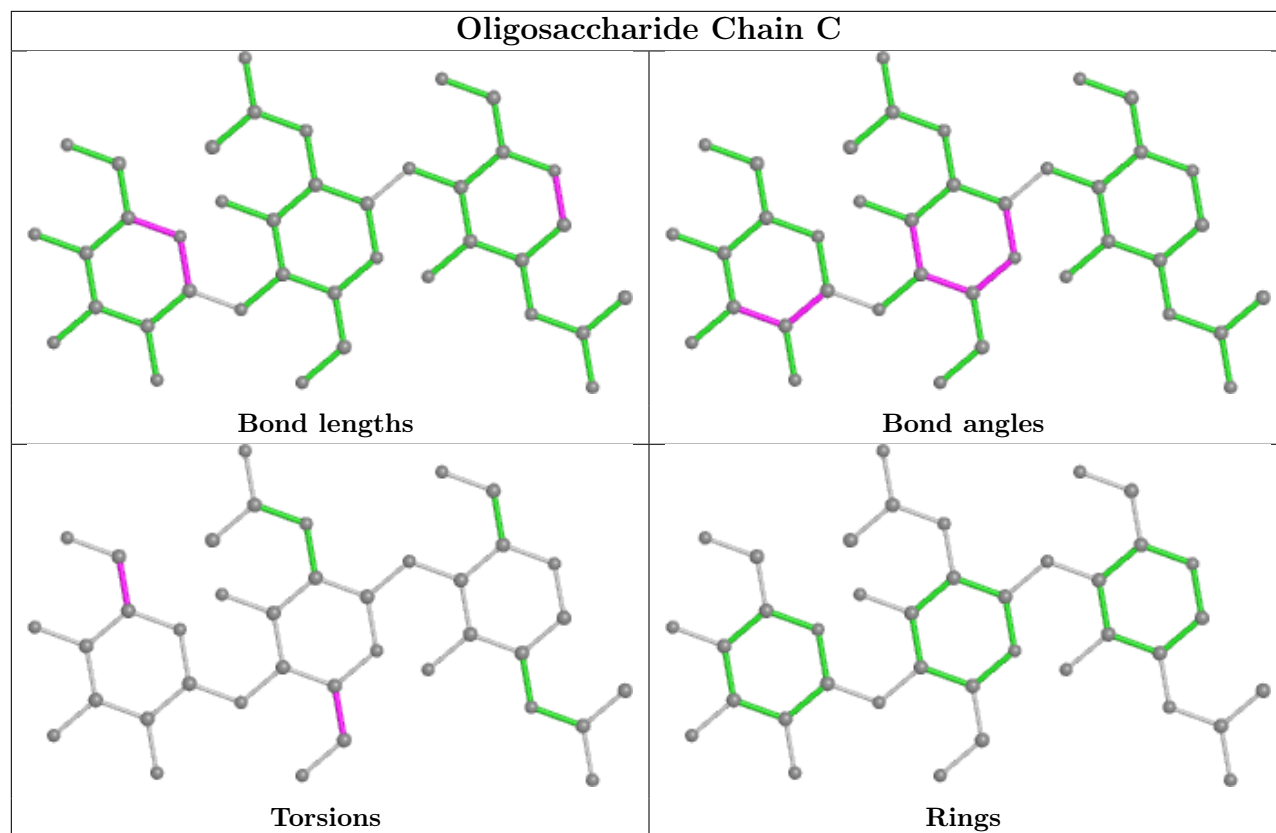
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	F	3	BMA	C4-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6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

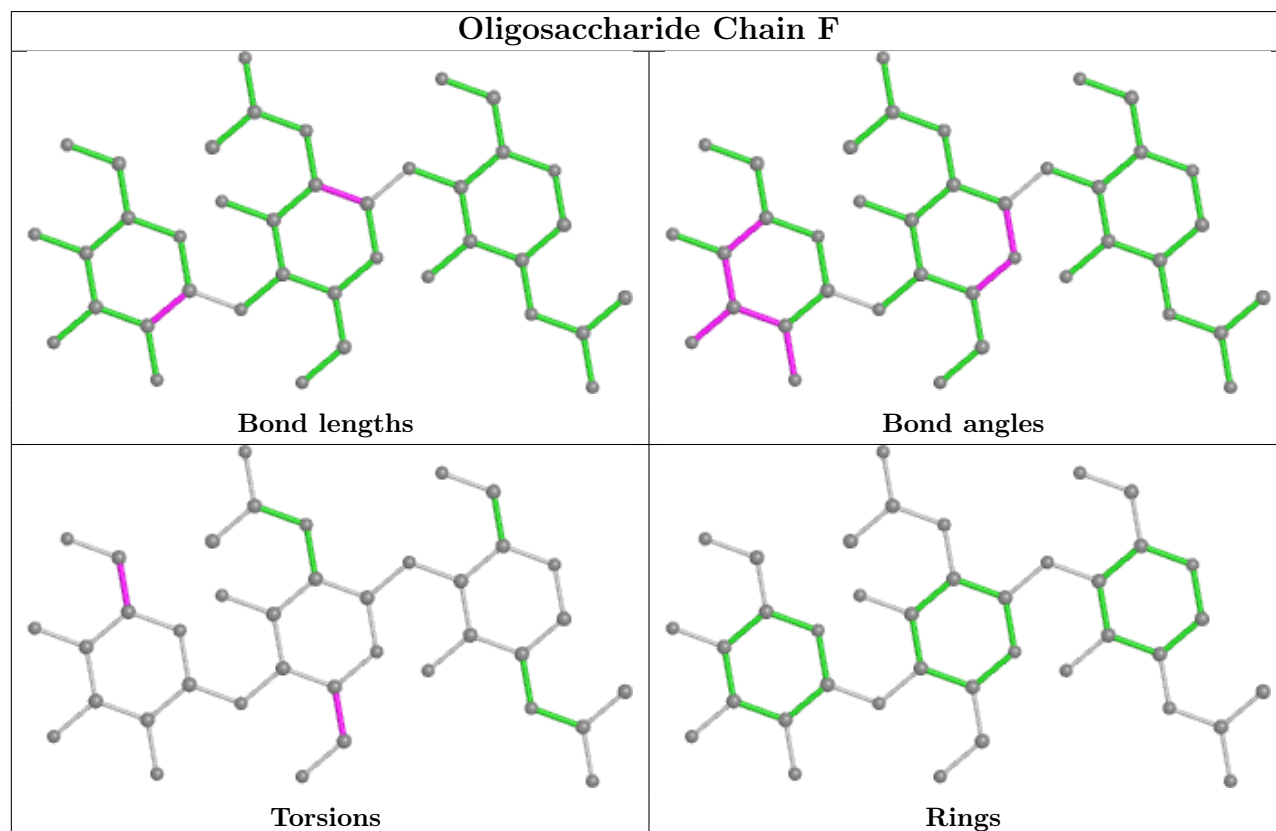
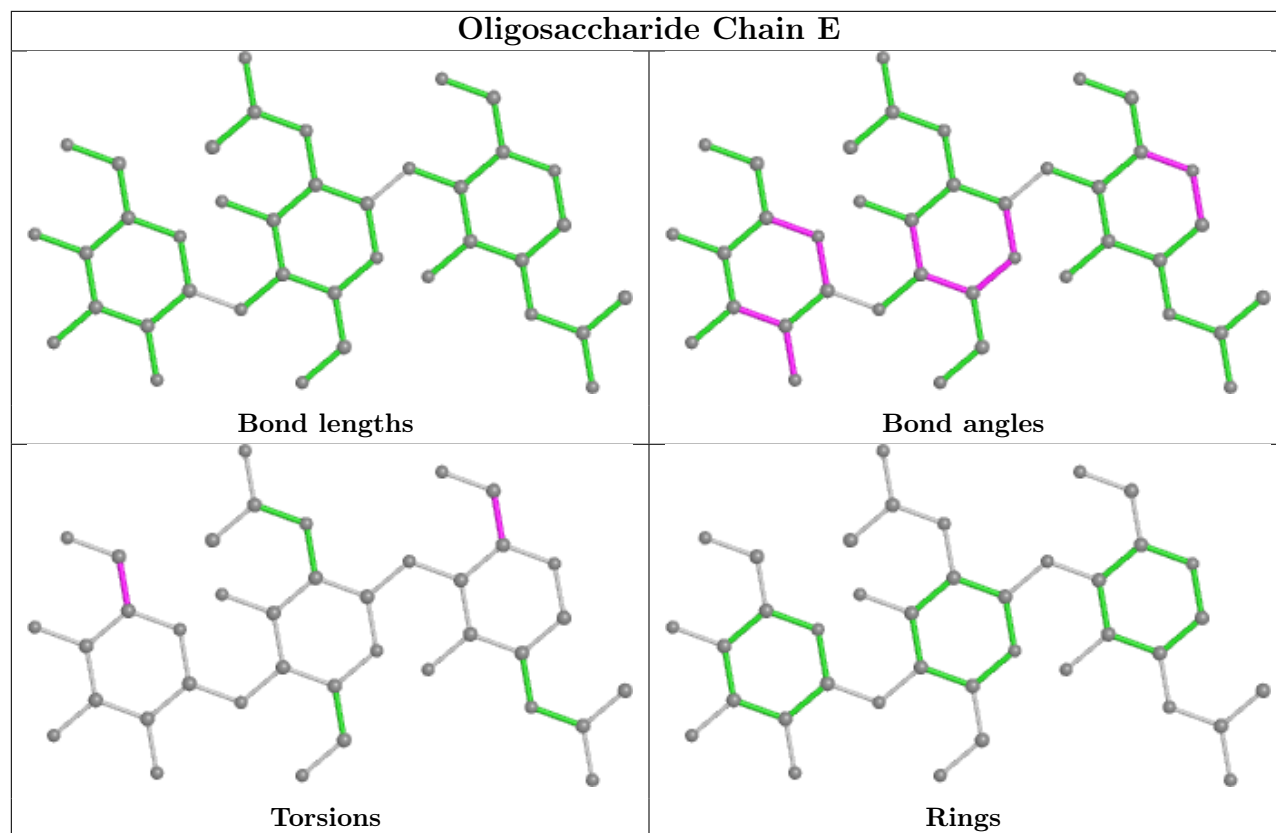
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	F	2	NAG	1	0
2	D	1	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

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
5	NAG	A	703	1	14,14,15	1.02	1 (7%)	17,19,21	1.11	1 (5%)
4	BCT	A	702	3	0,3,3	0.00	-	0,3,3	0.00	-
5	NAG	B	701	1	14,14,15	0.48	0	17,19,21	0.52	0
4	BCT	B	703	3	0,3,3	0.00	-	0,3,3	0.00	-
6	EDO	A	704	-	3,3,3	0.48	0	2,2,2	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	704	-	-	0/1/1/1	-
5	NAG	B	701	1	-	2/6/23/26	0/1/1/1
5	NAG	A	703	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	703	NAG	O5-C1	3.19	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	703	NAG	C1-O5-C5	4.25	117.95	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

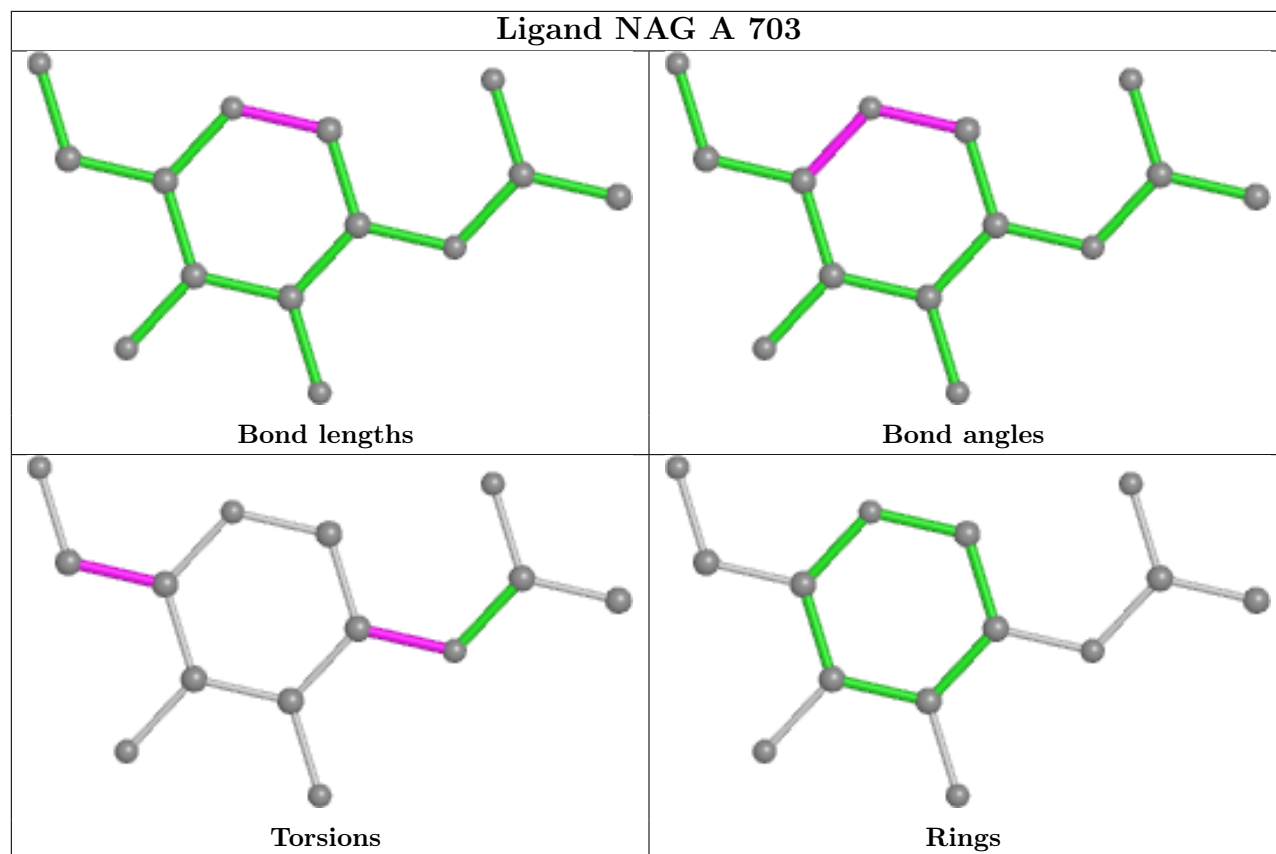
Mol	Chain	Res	Type	Atoms
5	B	701	NAG	C1-C2-N2-C7
5	A	703	NAG	C4-C5-C6-O6
5	A	703	NAG	C3-C2-N2-C7
5	B	701	NAG	C3-C2-N2-C7

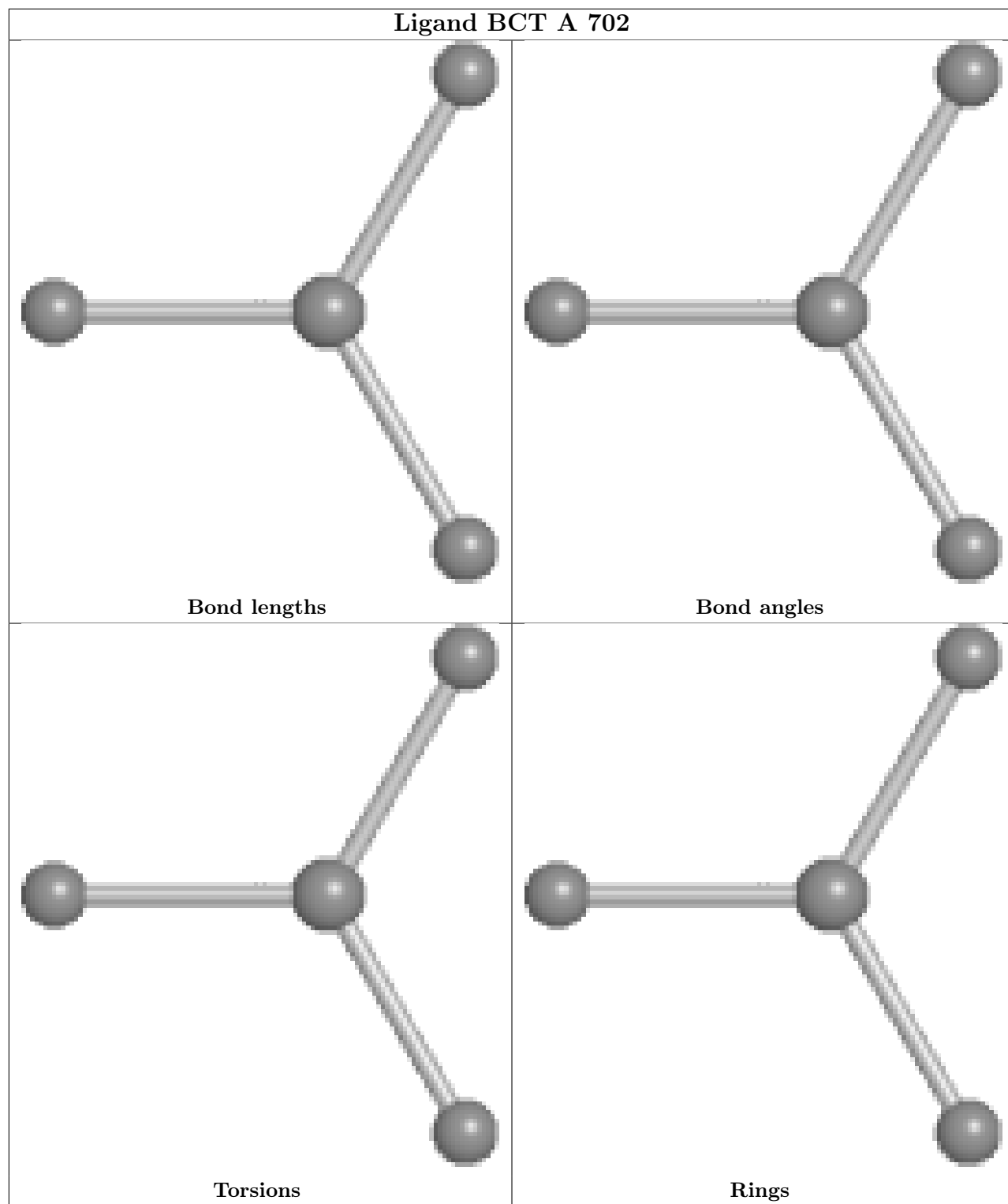
There are no ring outliers.

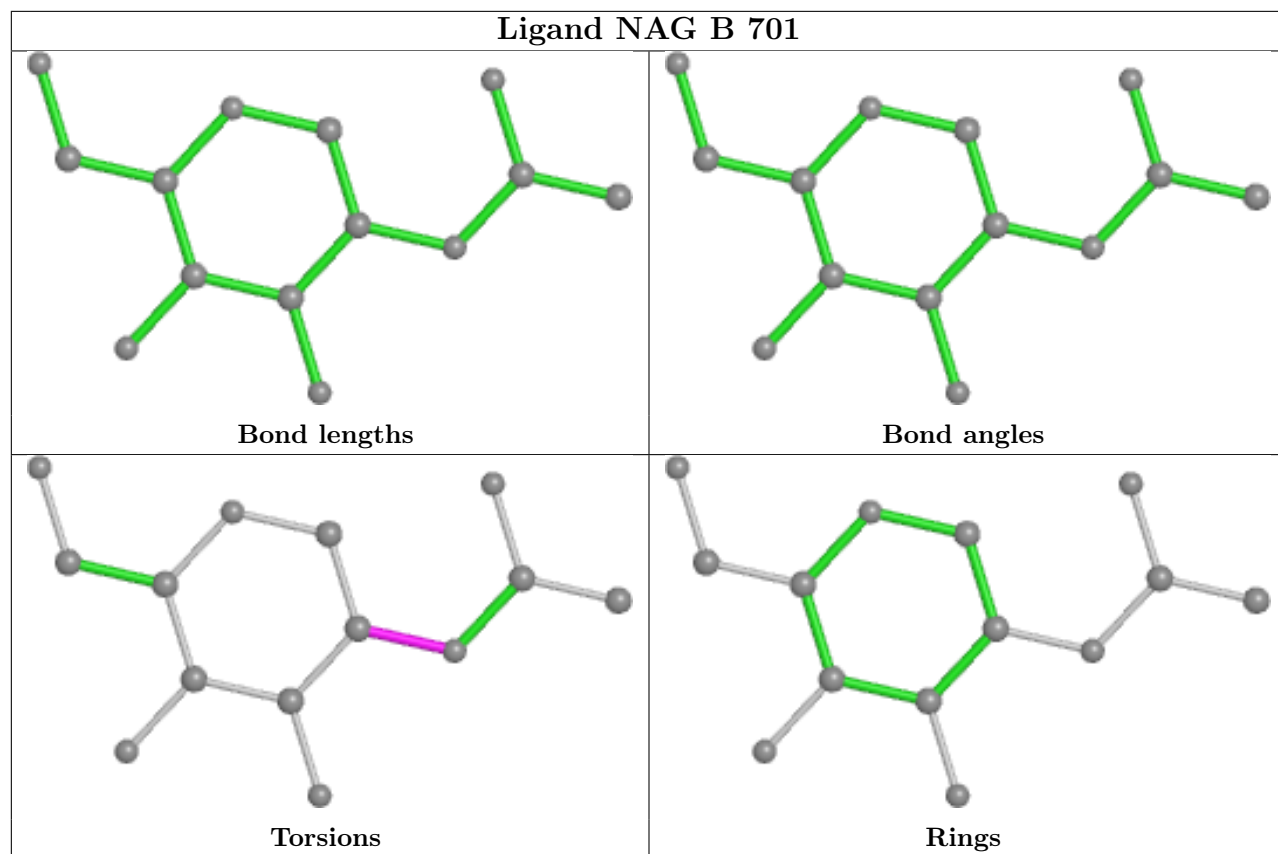
2 monomers are involved in 3 short contacts:

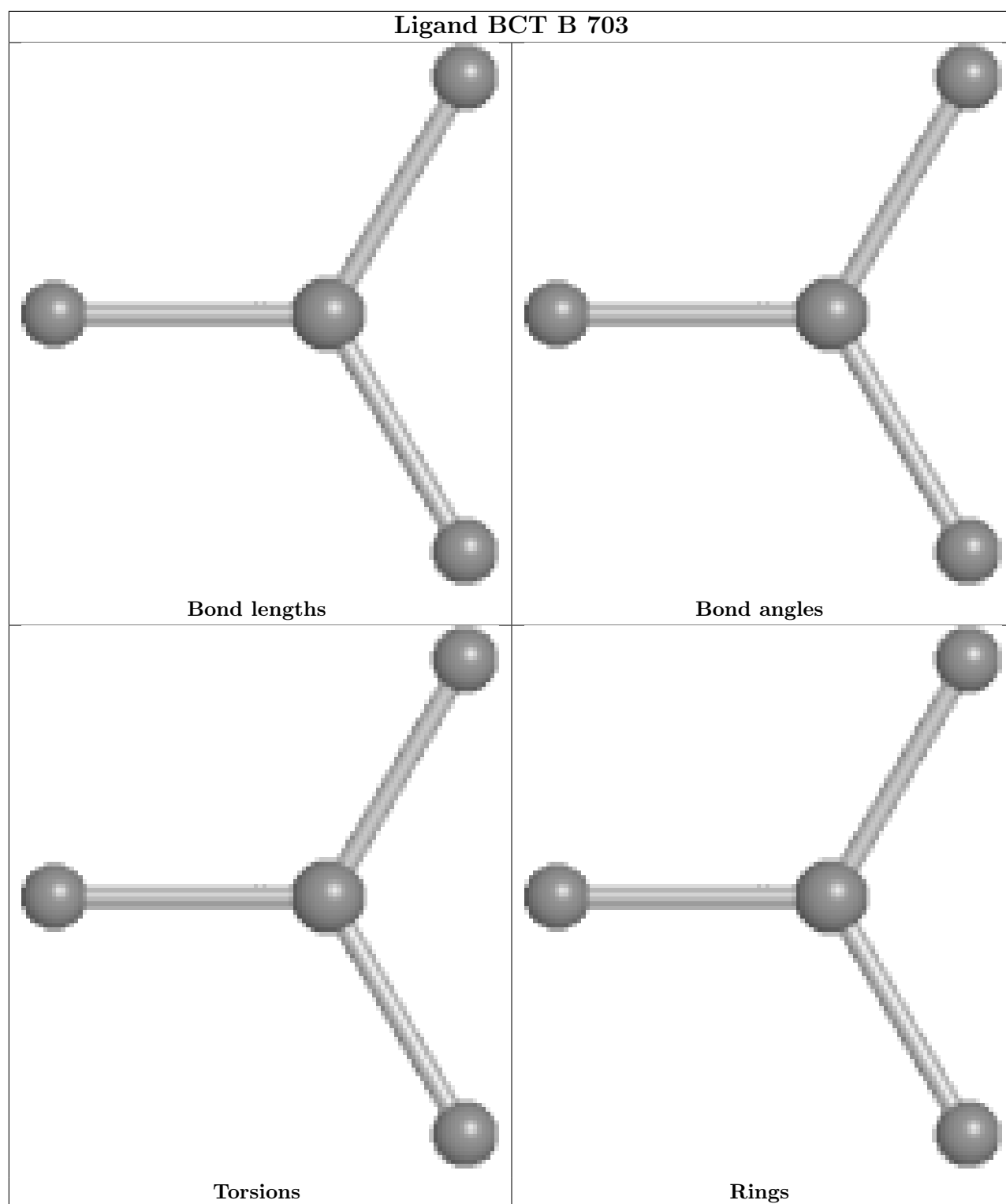
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	703	NAG	2	0
4	B	703	BCT	1	0

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 ⓘ

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%)	0.10	12 (3%) 45 38	11, 38, 80, 112	0
1	B	348/348 (100%)	0.42	23 (6%) 18 13	21, 60, 107, 160	0
All	All	696/696 (100%)	0.26	35 (5%) 28 23	11, 47, 97, 160	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	420	HIS	10.1
1	A	422	SER	5.7
1	B	419	LYS	5.1
1	B	421	SER	5.0
1	A	621	ASN	4.9
1	A	636	THR	4.2
1	B	580	PRO	4.1
1	B	442	ALA	4.1
1	B	441	LYS	4.0
1	B	422	SER	3.6
1	A	442	ALA	3.5
1	B	548	VAL	3.3
1	A	443	ASN	3.2
1	A	445	GLY	3.2
1	B	582	THR	3.2
1	B	445	GLY	3.1
1	B	439	VAL	3.0
1	B	418	SER	2.8
1	B	509	ASP	2.8
1	B	621	ASN	2.8
1	B	556	SER	2.8
1	B	537	VAL	2.7
1	A	423	LEU	2.6
1	B	591	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	536	ASP	2.5
1	B	530	PHE	2.5
1	A	567	GLU	2.4
1	B	423	LEU	2.4
1	A	570	ARG	2.2
1	A	420	HIS	2.2
1	B	550	GLU	2.1
1	B	342	TYR	2.1
1	A	446	LEU	2.1
1	B	489	GLN	2.1
1	A	417	SER	2.1

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](#)

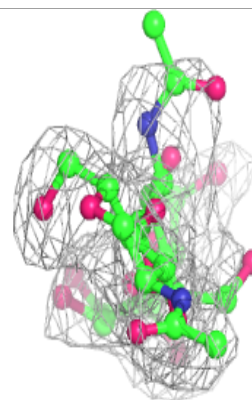
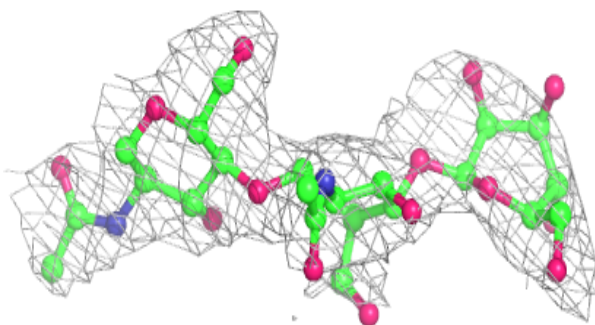
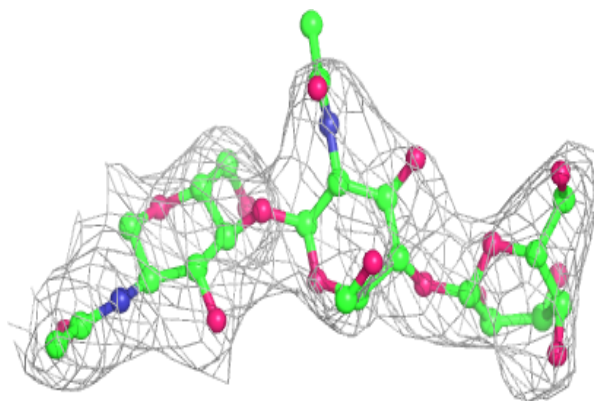
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	F	3	11/12	0.70	0.19	74,100,116,117	0
2	NAG	E	2	14/15	0.76	0.33	92,122,149,154	0
2	BMA	E	3	11/12	0.82	0.24	136,154,161,163	0
2	BMA	D	3	11/12	0.84	0.15	43,61,85,87	0
2	NAG	E	1	14/15	0.85	0.24	77,91,111,114	0
2	BMA	C	3	11/12	0.86	0.17	77,95,107,110	0
2	NAG	C	2	14/15	0.86	0.25	61,82,103,104	0
2	NAG	D	2	14/15	0.87	0.21	45,74,85,89	0
2	NAG	F	2	14/15	0.90	0.23	65,87,105,113	0
2	NAG	D	1	14/15	0.92	0.16	42,58,72,80	0
2	NAG	C	1	14/15	0.92	0.14	32,43,60,66	0
2	NAG	F	1	14/15	0.94	0.21	57,79,85,87	0

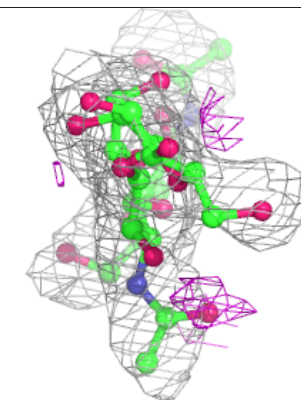
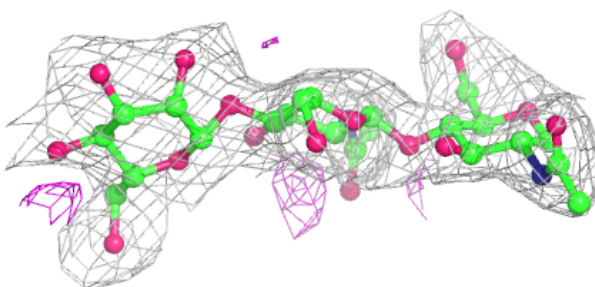
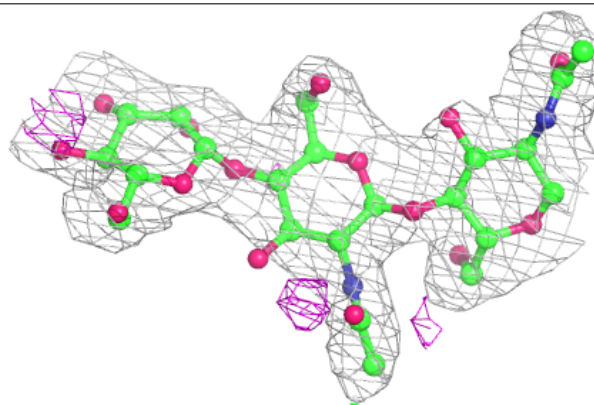
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

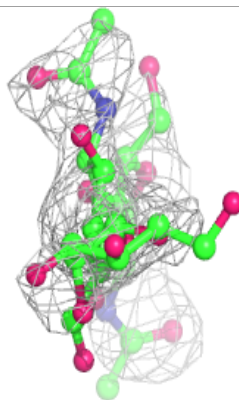
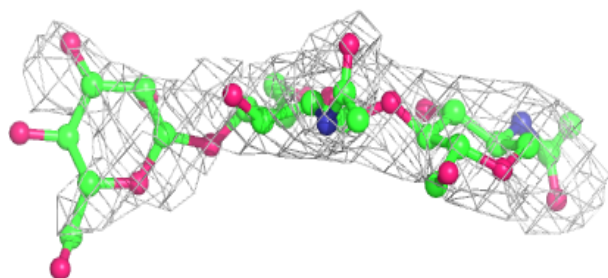
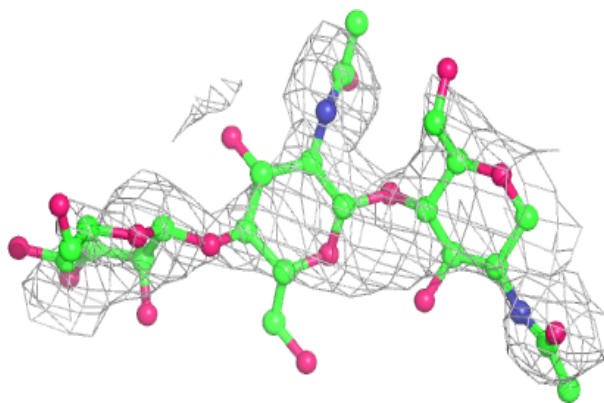
**Electron density around Chain D:**

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

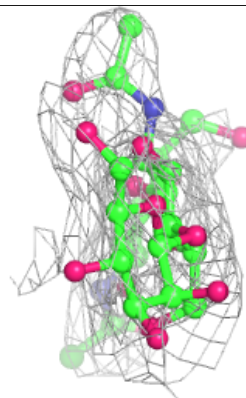
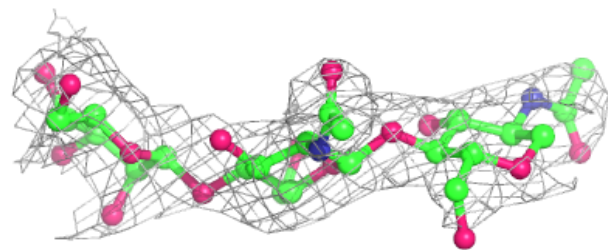
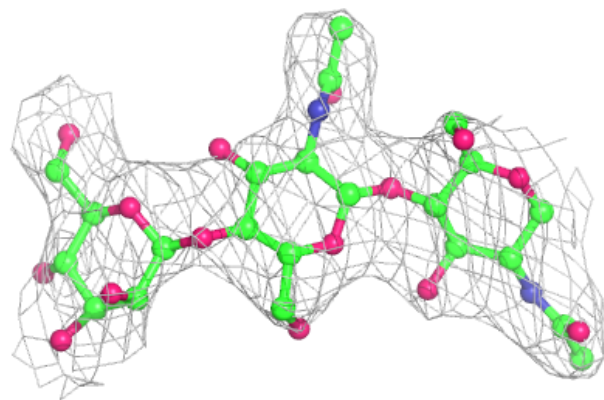


Electron density around Chain E:

$2mF_o-DF_c$ (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 ⓘ

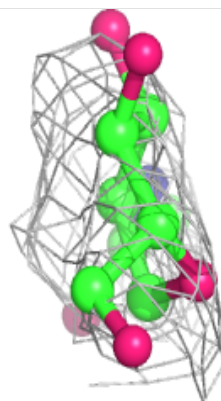
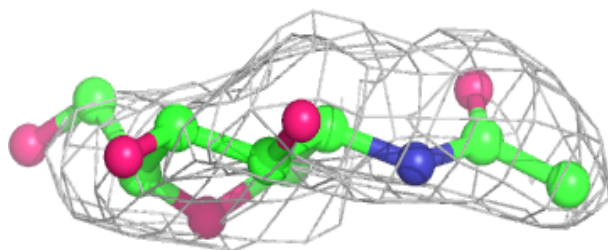
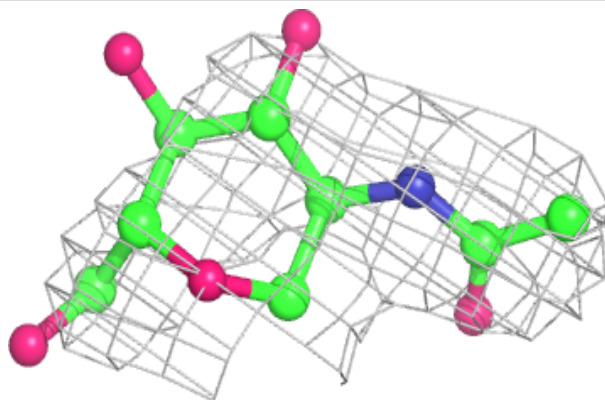
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	NAG	A	703	14/15	0.73	0.40	84,100,114,115	0
6	EDO	A	704	4/4	0.86	0.12	47,52,67,68	0
5	NAG	B	701	14/15	0.88	0.17	49,59,69,81	0
3	FE	B	702	1/1	0.97	0.12	51,51,51,51	0
4	BCT	B	703	4/4	0.98	0.11	33,33,35,43	0
3	FE	A	701	1/1	0.98	0.11	28,28,28,28	0
4	BCT	A	702	4/4	0.99	0.15	9,12,19,26	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.

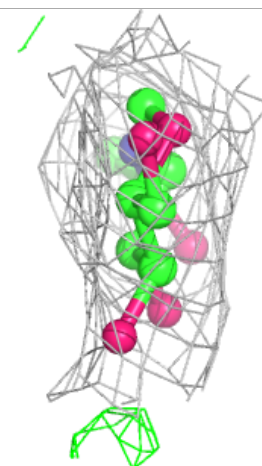
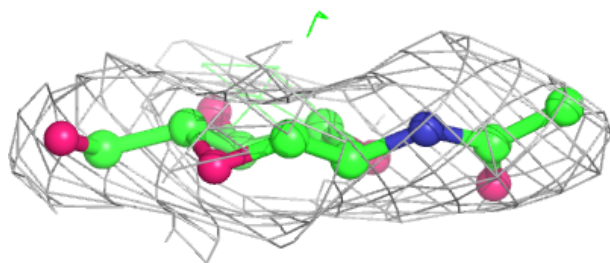
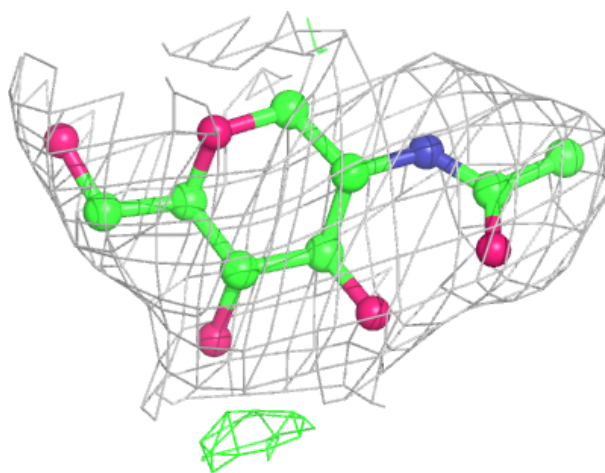
Electron density around NAG A 703:

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



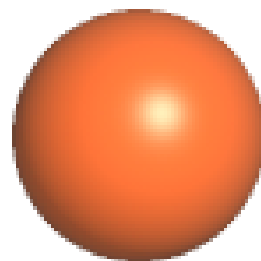
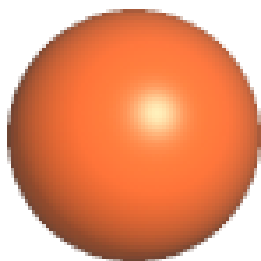
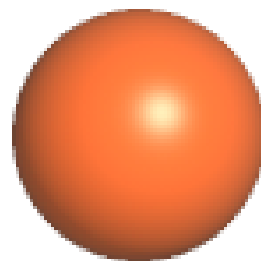
Electron density around NAG B 701:

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



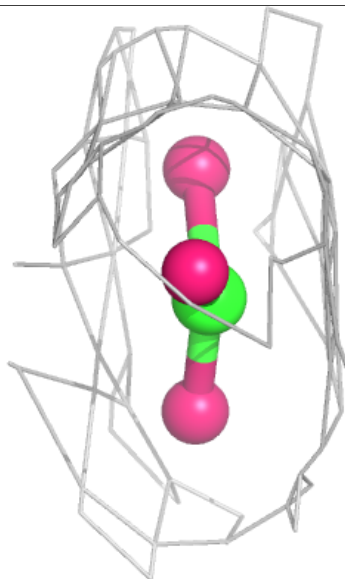
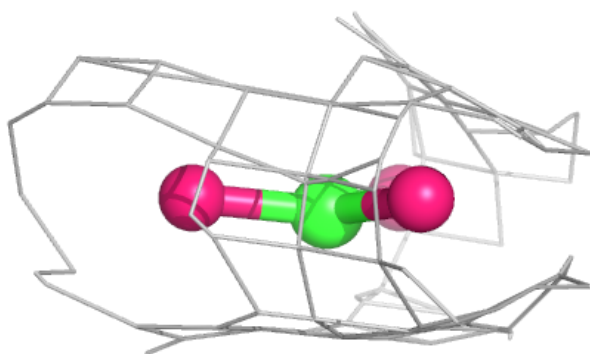
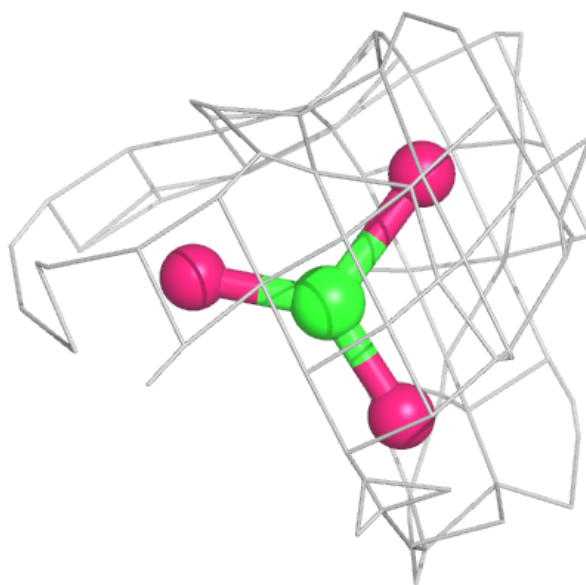
Electron density around FE B 702:

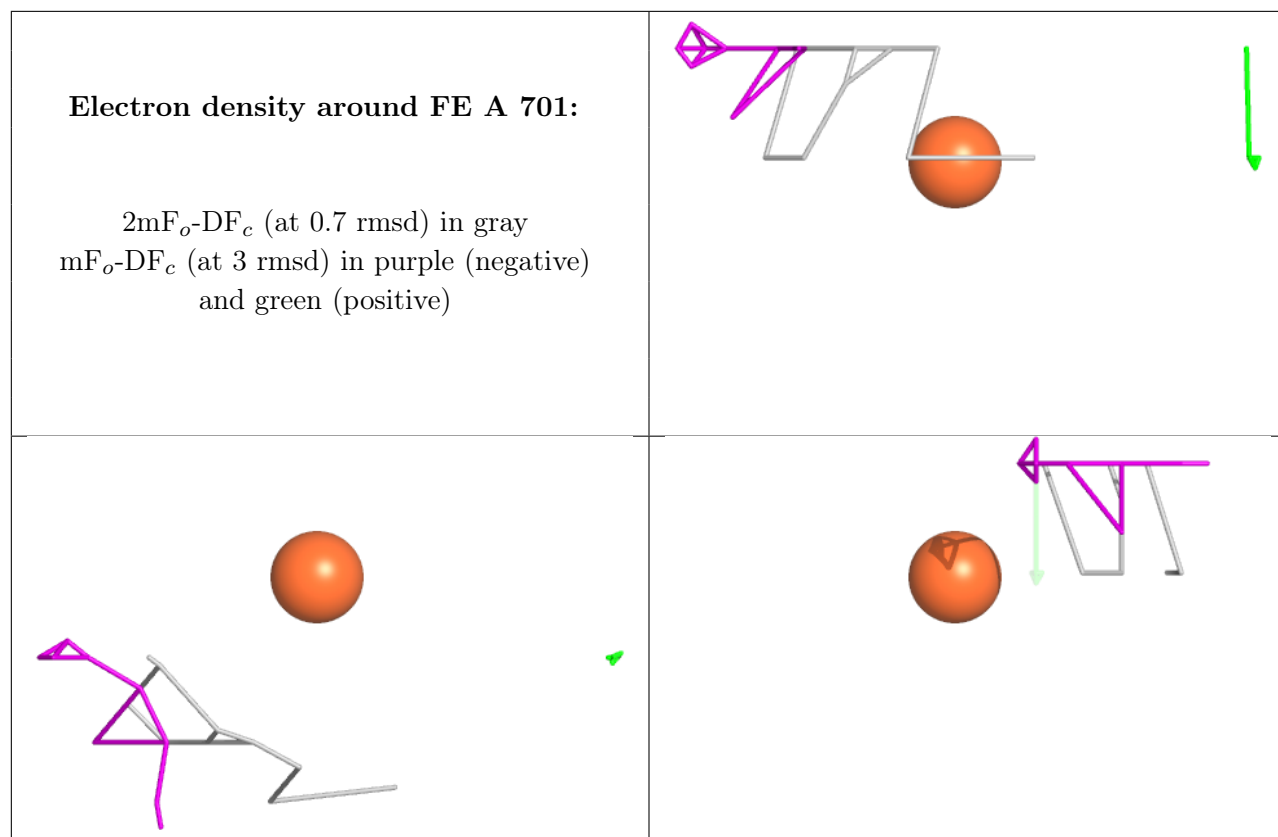
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

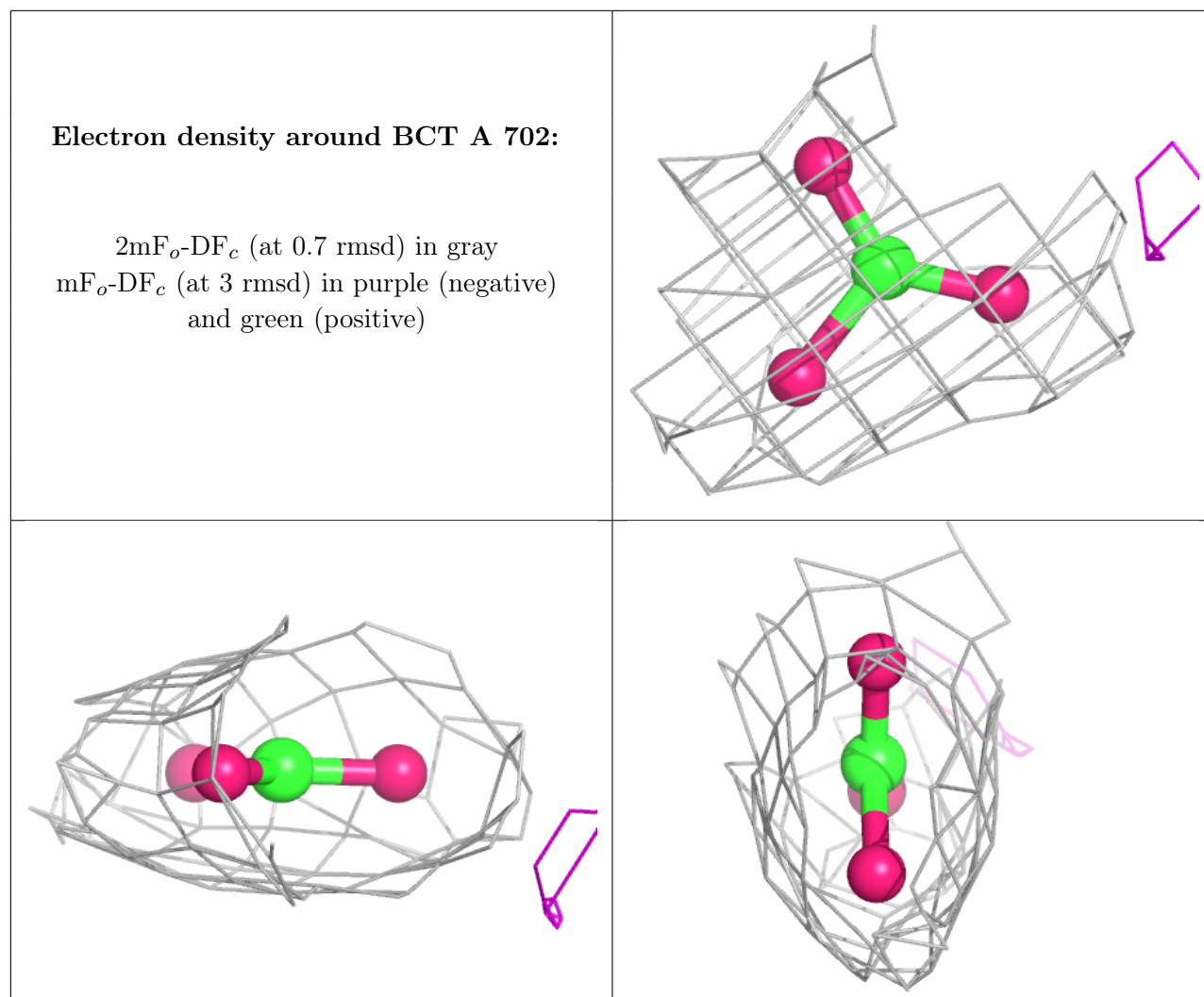


Electron density around BCT B 703:

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







6.5 Other polymers ⓘ

There are no such residues in this entry.