



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:22 AM UTC

PDB ID : 7EVQ / pdb_00007evq
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 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

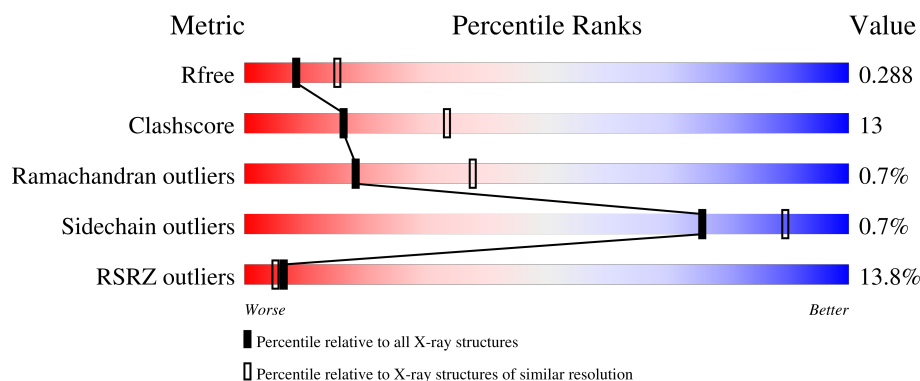
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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	8% 82% 18%
1	B	348	19% 69% 28% ..
2	C	3	100%
2	D	3	100%
2	E	3	100%

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Mol	Chain	Length	Quality of chain
2	F	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCT	B	703	-	X	-	-

2 Entry composition

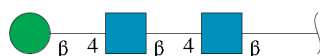
There are 7 unique types of molecules in this entry. The entry contains 5593 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.



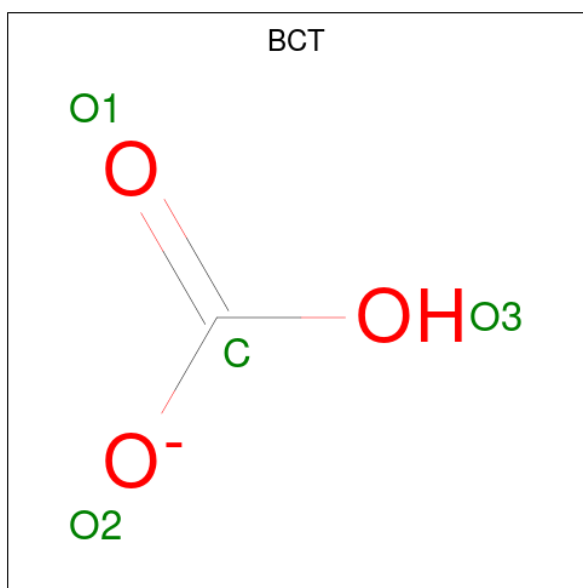
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is FE (III) ION (CCD ID: 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		

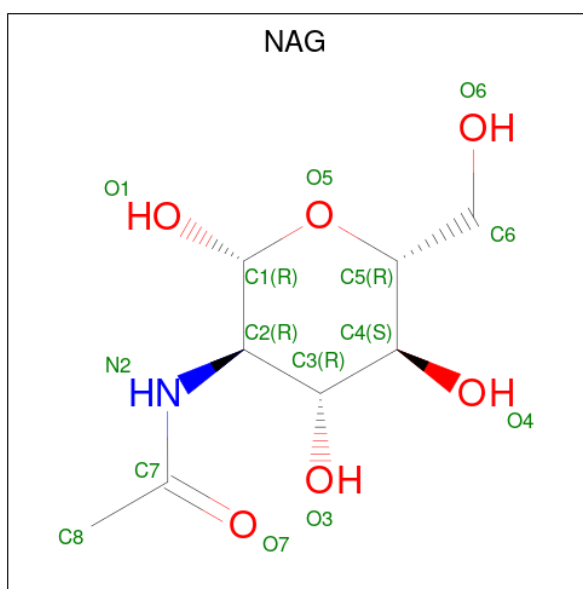
- Molecule 4 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃) (labeled as "Ligand

of Interest" by depositor).



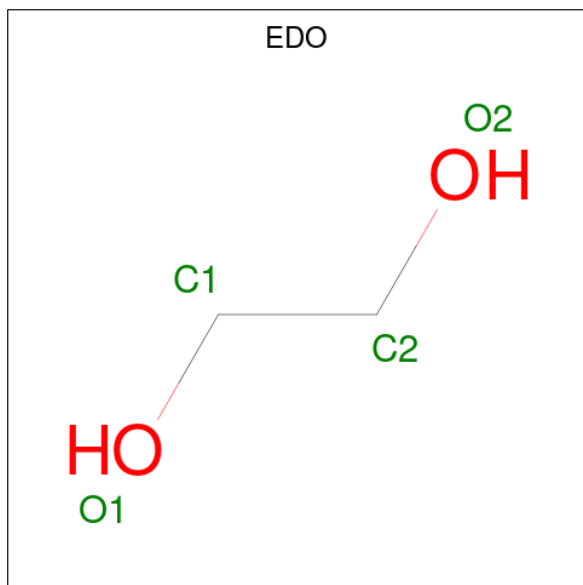
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	1	3		
4	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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 (CCD ID: EDO) (formula: C₂H₆O₂).



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

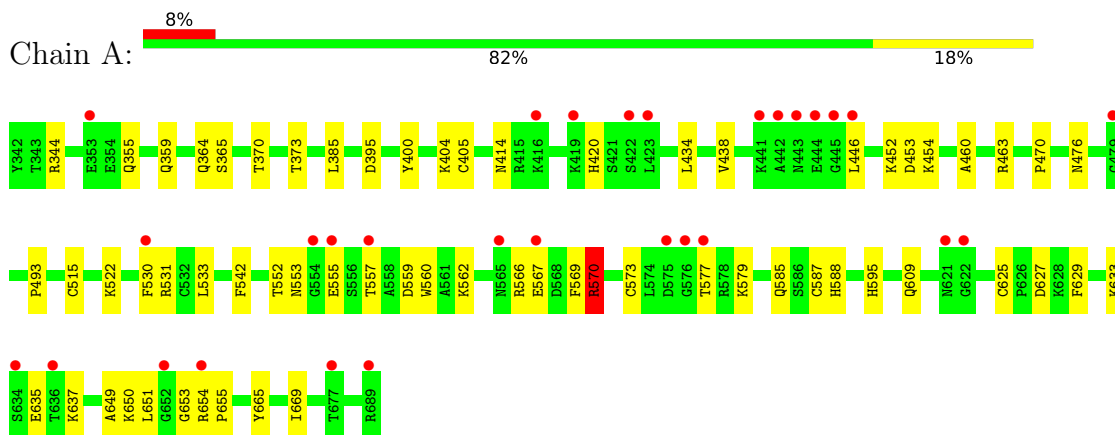
- Molecule 7 is water.

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

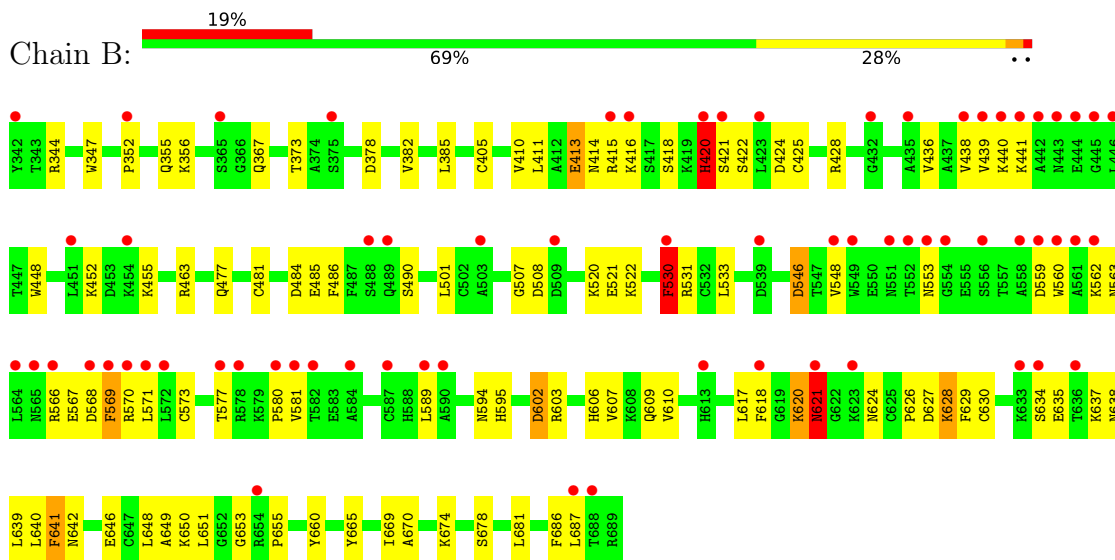
3 Residue-property plots

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



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 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 45.12 – 2.60	Depositor EDS
% Data completeness (in resolution range)	65.2 (45.12-2.60) 64.9 (45.12-2.60)	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 0.231 , 0.288	Depositor DCC
R_{free} test set	1026 reflections (3.17%)	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 , 56.0	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	0.88	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: EDO, BMA, BCT, FE, NAG

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	0.42	1/2707 (0.0%)	0.69	2/3669 (0.1%)
1	B	0.50	0/2707	0.90	12/3669 (0.3%)
All	All	0.46	1/5414 (0.0%)	0.80	14/7338 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	570	ARG	CZ-NH1	9.64	1.46	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	628	LYS	CA-CB-CG	-13.30	87.50	114.10
1	B	420	HIS	CB-CA-C	-10.33	89.86	110.42
1	A	570	ARG	CG-CD-NE	-9.46	91.18	112.00
1	A	625	CYS	C-N-CD	-8.22	102.53	120.60
1	B	620	LYS	CA-C-N	7.52	134.55	123.12
1	B	620	LYS	C-N-CA	7.52	134.55	123.12
1	B	356	LYS	CA-CB-CG	-6.57	100.96	114.10
1	B	530	PHE	CB-CA-C	-6.13	101.51	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	413	GLU	CA-C-N	-5.78	112.43	122.37
1	B	413	GLU	C-N-CA	-5.78	112.43	122.37
1	B	621	ASN	N-CA-CB	-5.57	98.32	110.29
1	B	420	HIS	N-CA-CB	5.43	119.66	110.49
1	B	569	PHE	CA-C-N	-5.43	112.36	121.75
1	B	569	PHE	C-N-CA	-5.43	112.36	121.75

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	46	0
1	B	2657	0	2581	97	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
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	141	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 (141) 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:A:569:PHE:C	1:A:570:ARG:HD3	1.97	0.90
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: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:627:ASP:C	1:B:628:LYS:HG2	2.02	0.82
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:428:ARG:HH22	1:B:646:GLU:CD	2.16	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:594:ASN:O	1:B:660:TYR:OH	2.26	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:569:PHE:C	1:A:570:ARG:CD	2.77	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:640:LEU:C	1:B:641:PHE:CD1	2.96	0.43
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:GLU:CD	1:B:570:ARG:HH11	2.27	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:B:626:PRO:O	1:B:627:ASP:C	2.65	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%)	21	42
1	B	346/348 (99%)	320 (92%)	23 (7%)	3 (1%)	14	30
All	All	692/696 (99%)	646 (93%)	41 (6%)	5 (1%)	18	38

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%)	289 (100%)	0	100	100
1	B	289/289 (100%)	285 (99%)	4 (1%)	59	81
All	All	578/578 (100%)	574 (99%)	4 (1%)	76	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	420	HIS
1	B	546	ASP
1	B	602	ASP
1	B	641	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	GLN
1	A	367	GLN
1	A	588	HIS
1	A	594	ASN
1	A	638	ASN
1	B	360	GLN
1	B	563	ASN
1	B	594	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	0.65	0	17,19,21	0.73	0
2	NAG	C	2	2	14,14,15	0.25	0	17,19,21	2.14	2 (11%)
2	BMA	C	3	2	11,11,12	1.33	2 (18%)	15,15,17	0.99	0
2	NAG	D	1	1,2	14,14,15	0.50	0	17,19,21	0.67	0
2	NAG	D	2	2	14,14,15	0.82	2 (14%)	17,19,21	0.94	1 (5%)
2	BMA	D	3	2	11,11,12	1.05	1 (9%)	15,15,17	1.88	3 (20%)
2	NAG	E	1	1,2	14,14,15	0.26	0	17,19,21	1.19	1 (5%)
2	NAG	E	2	2	14,14,15	0.49	0	17,19,21	1.04	2 (11%)
2	BMA	E	3	2	11,11,12	0.60	0	15,15,17	1.77	2 (13%)
2	NAG	F	1	1,2	14,14,15	0.40	0	17,19,21	0.61	0
2	NAG	F	2	2	14,14,15	0.70	1 (7%)	17,19,21	0.82	1 (5%)
2	BMA	F	3	2	11,11,12	1.24	1 (9%)	15,15,17	1.71	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	3.47	1.60	1.52
2	C	3	BMA	O5-C1	-2.86	1.38	1.43
2	C	3	BMA	O5-C5	2.51	1.48	1.43
2	F	2	NAG	C1-C2	2.32	1.55	1.52
2	D	3	BMA	C4-C5	2.16	1.57	1.53
2	D	2	NAG	C1-C2	2.16	1.55	1.52
2	D	2	NAG	O5-C1	-2.04	1.40	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	8.13	123.08	112.19
2	E	3	BMA	C1-O5-C5	5.99	120.22	112.19
2	D	3	BMA	O5-C1-C2	4.34	121.15	110.79
2	F	3	BMA	C3-C4-C5	4.08	117.64	110.23
2	E	1	NAG	C1-O5-C5	4.05	117.61	112.19
2	D	3	BMA	C1-O5-C5	3.49	116.87	112.19
2	D	3	BMA	C1-C2-C3	3.48	114.70	109.64
2	D	2	NAG	C1-O5-C5	2.93	116.11	112.19
2	F	3	BMA	O2-C2-C3	-2.92	104.10	110.15
2	F	2	NAG	C1-O5-C5	2.62	115.70	112.19
2	F	3	BMA	O3-C3-C4	-2.46	104.58	110.38
2	E	3	BMA	O2-C2-C3	-2.26	105.48	110.15
2	E	2	NAG	C1-O5-C5	2.22	115.16	112.19
2	C	2	NAG	C3-C4-C5	2.20	114.21	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C3-C4-C5	2.13	114.10	110.23

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	C4-C5-C6-O6
2	D	3	BMA	O5-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	F	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-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

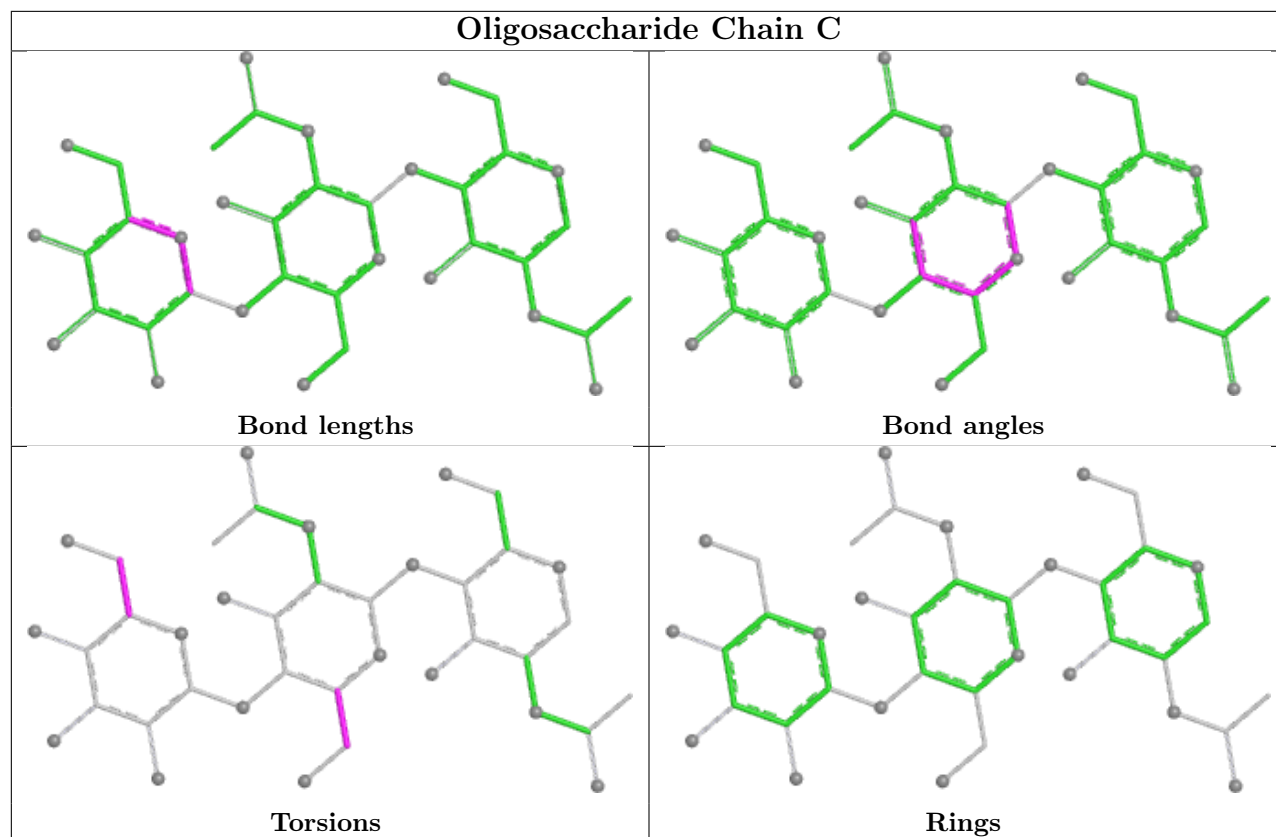
There are no ring outliers.

3 monomers are involved in 3 short contacts:

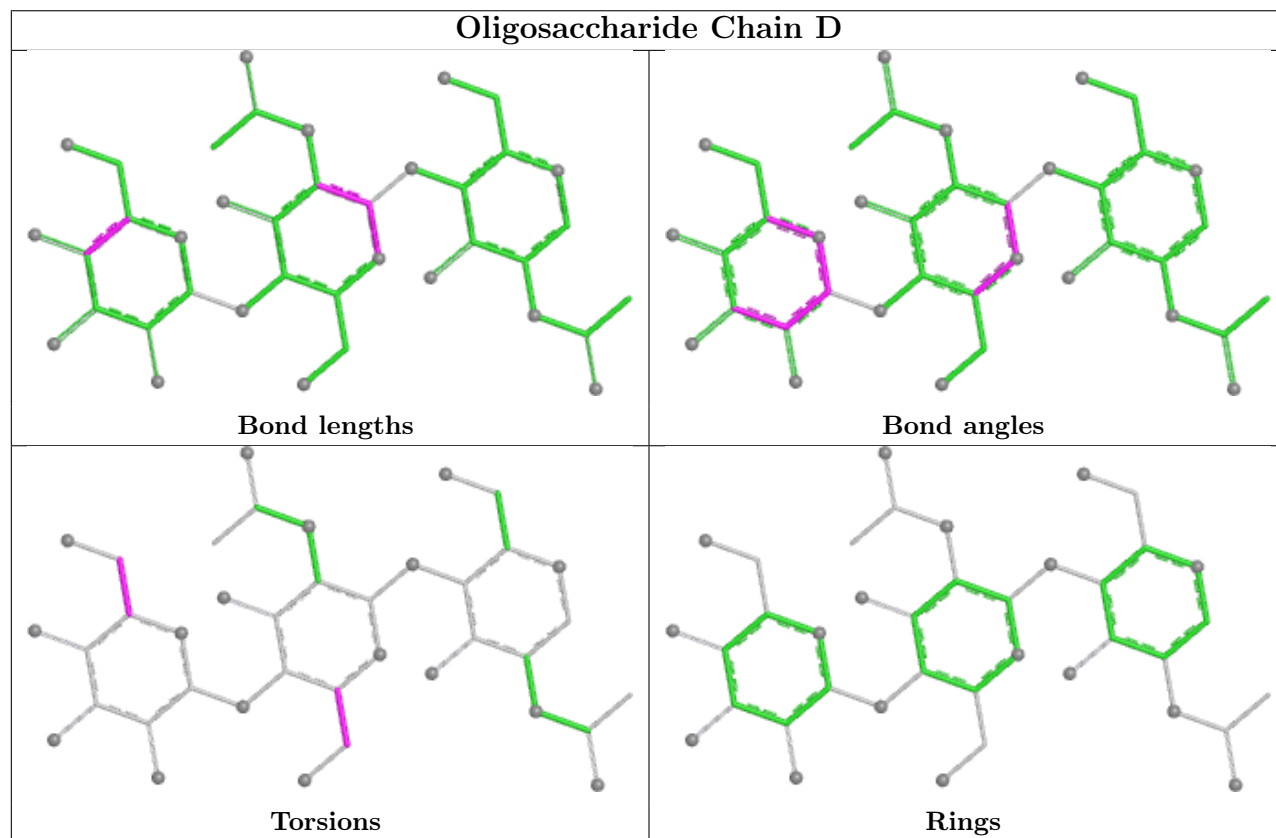
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	D	1	NAG	1	0
2	F	2	NAG	1	0

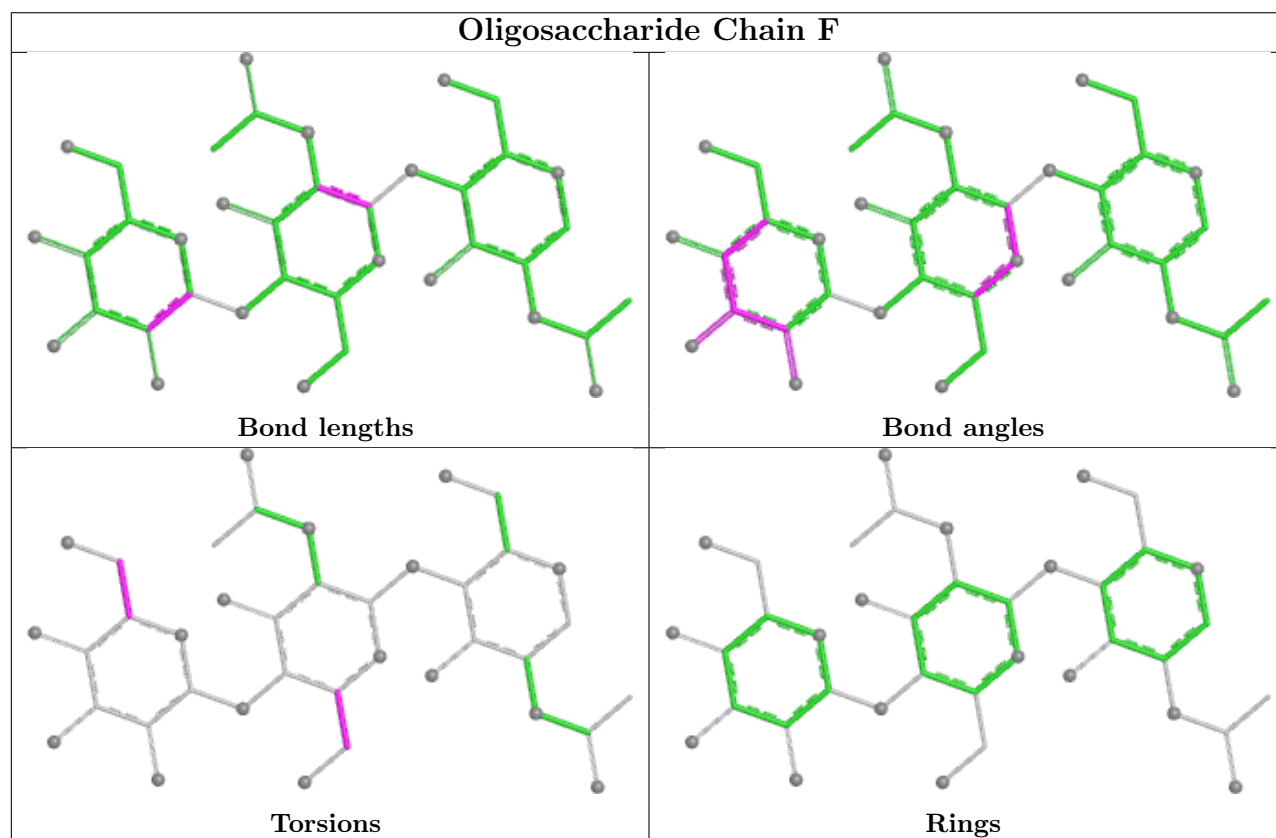
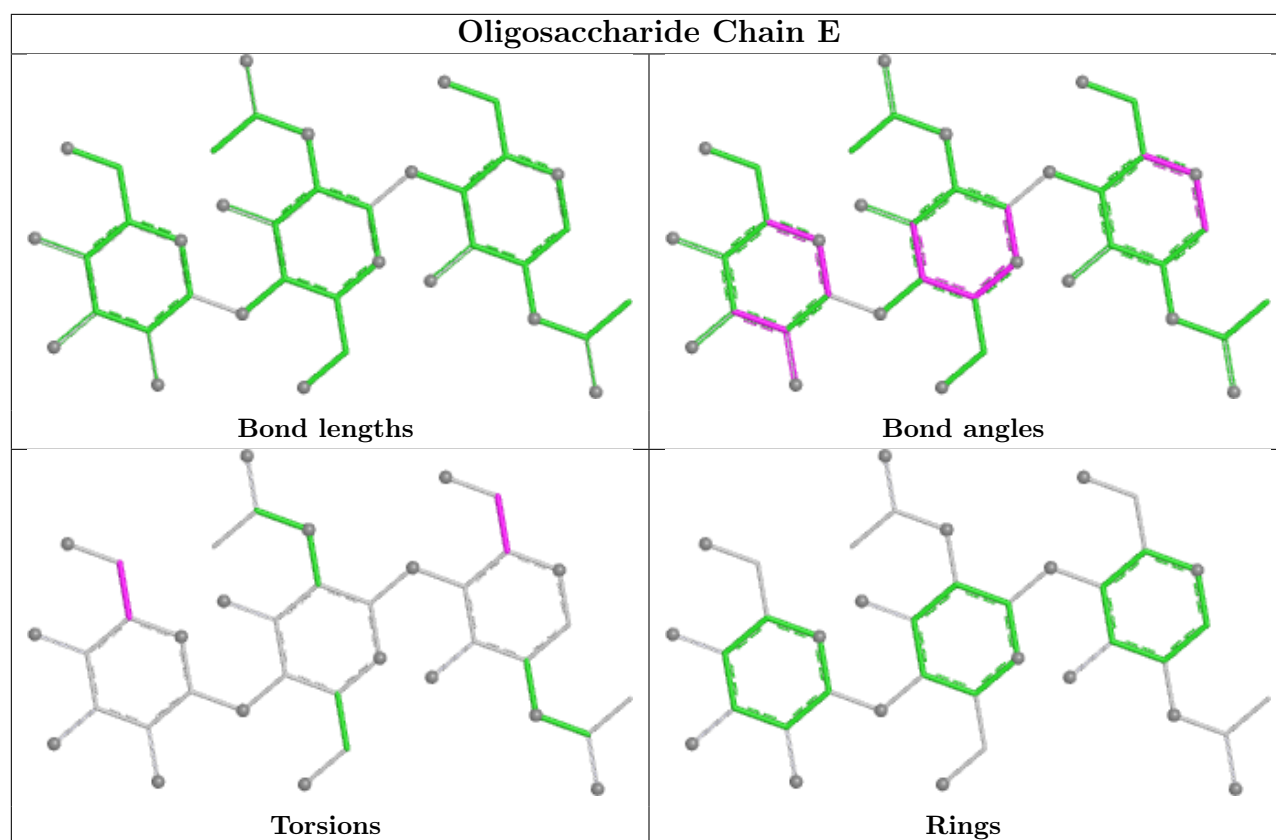
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C



Oligosaccharide Chain D





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	1.01	2 (14%)	17,19,21	1.13	1 (5%)
6	EDO	A	704	-	3,3,3	0.44	0	2,2,2	0.31	0
4	BCT	B	703	3	3,3,3	3.36	1 (33%)	2,3,3	2.92	2 (100%)
5	NAG	B	701	1	14,14,15	0.51	0	17,19,21	0.53	0
4	BCT	A	702	3	3,3,3	1.13	0	2,3,3	3.99	1 (50%)

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	B	701	1	-	1/6/23/26	0/1/1/1
6	EDO	A	704	-	-	0/1/1/1	-
5	NAG	A	703	1	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	BCT	O1-C	5.58	1.44	1.25
5	A	703	NAG	O5-C1	3.05	1.48	1.43
5	A	703	NAG	C1-C2	2.18	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	BCT	O2-C-O1	5.34	133.32	119.68
5	A	703	NAG	C1-O5-C5	4.30	117.95	112.19
4	B	703	BCT	O2-C-O1	-3.56	110.56	119.68
4	B	703	BCT	O3-C-O1	-2.08	114.35	119.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

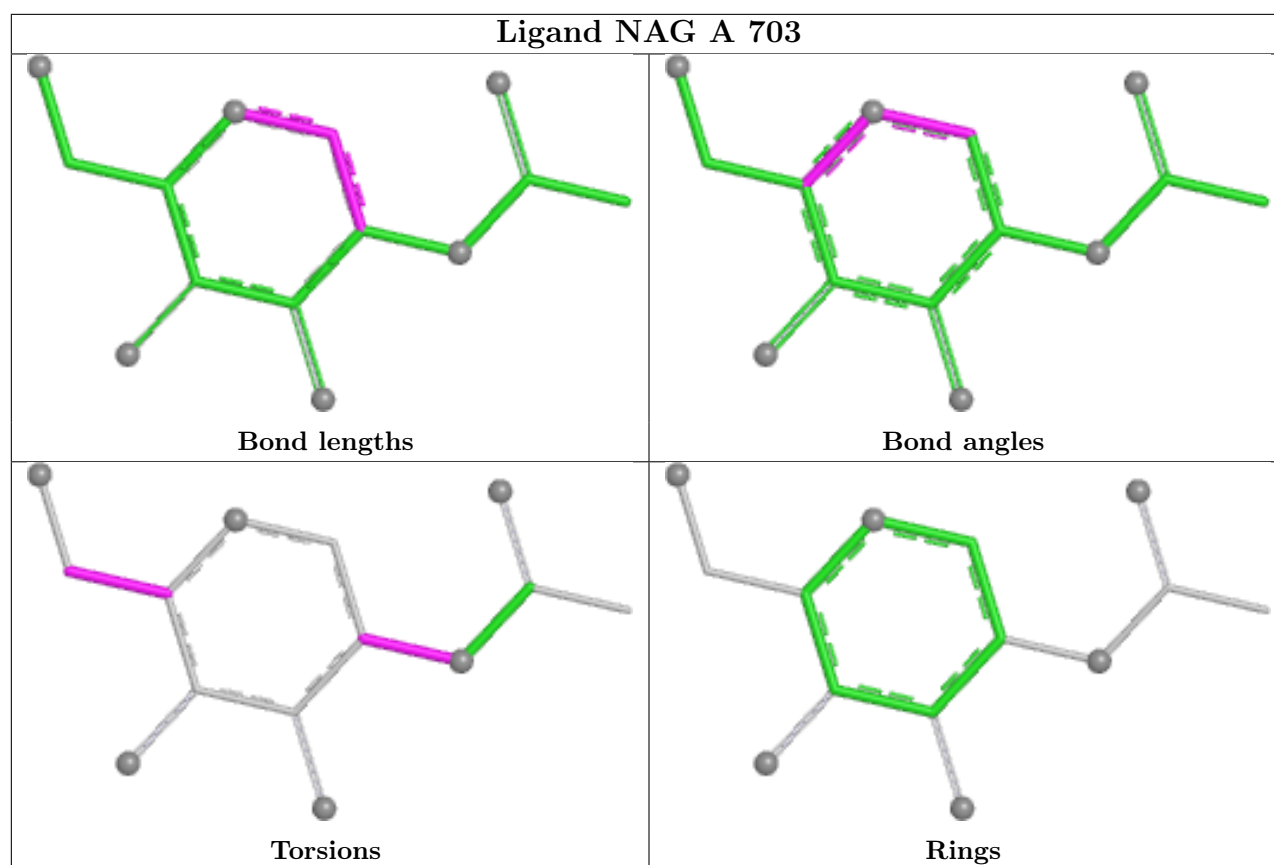
Mol	Chain	Res	Type	Atoms
5	A	703	NAG	C4-C5-C6-O6
5	A	703	NAG	C1-C2-N2-C7
5	A	703	NAG	C3-C2-N2-C7
5	B	701	NAG	C3-C2-N2-C7
5	A	703	NAG	O5-C5-C6-O6

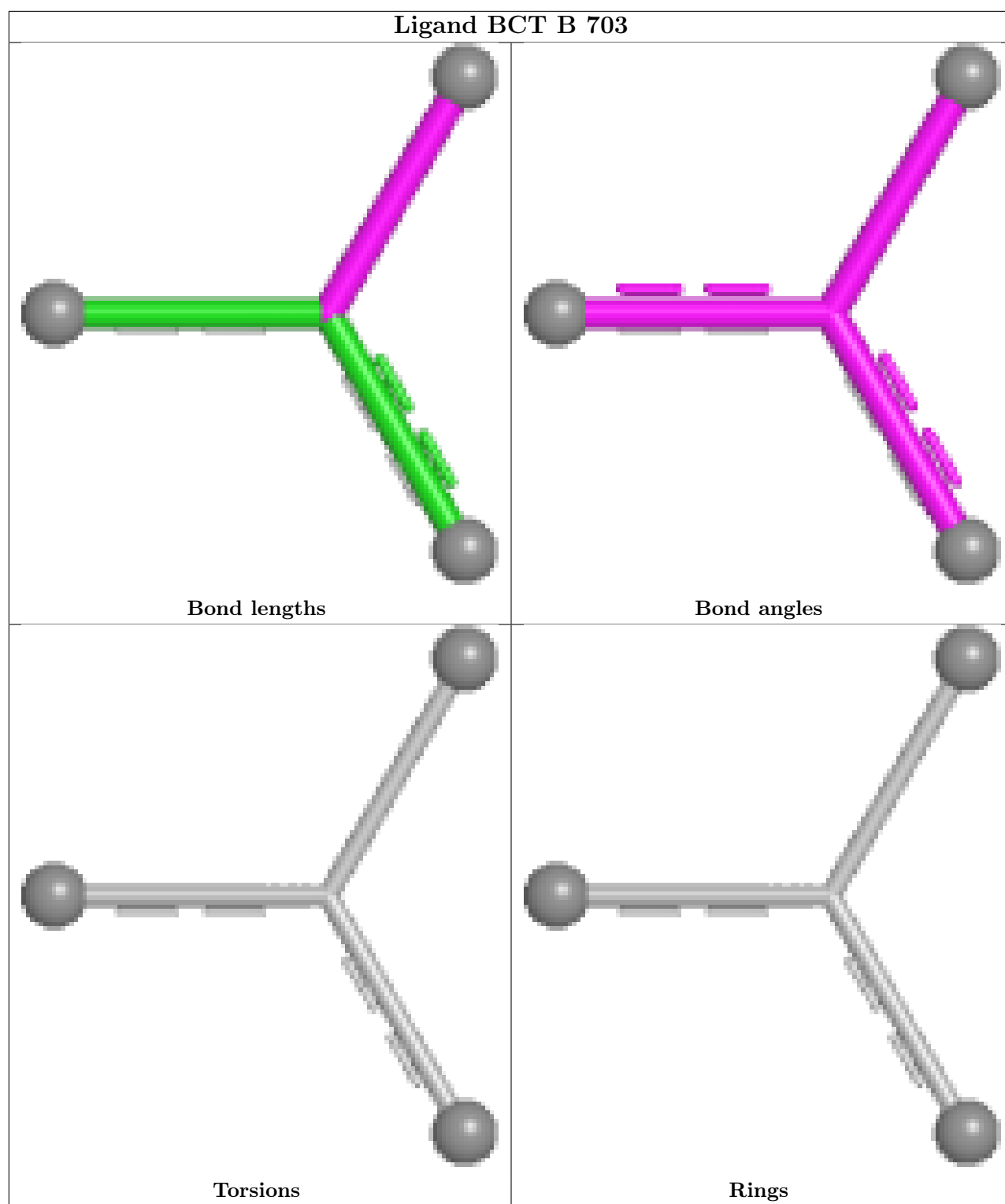
There are no ring outliers.

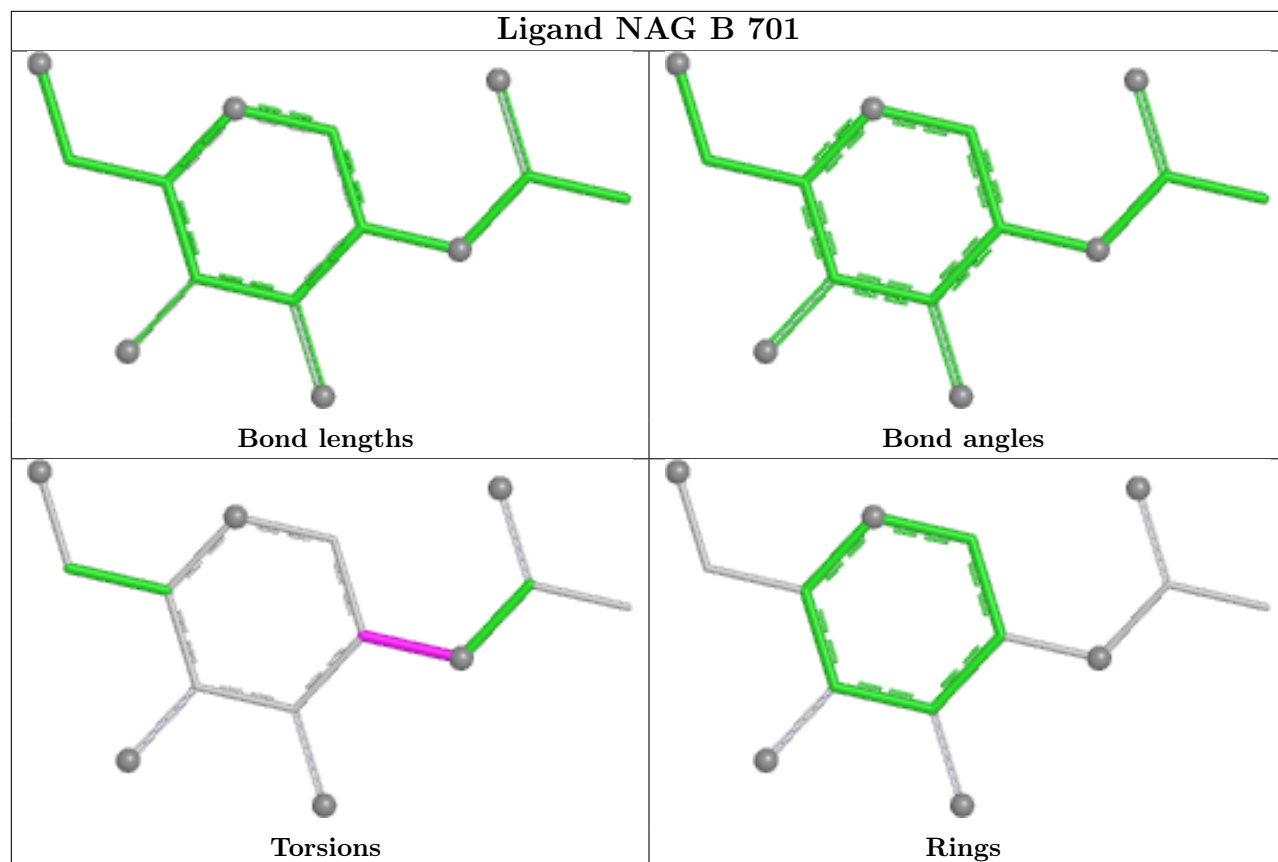
2 monomers are involved in 3 short contacts:

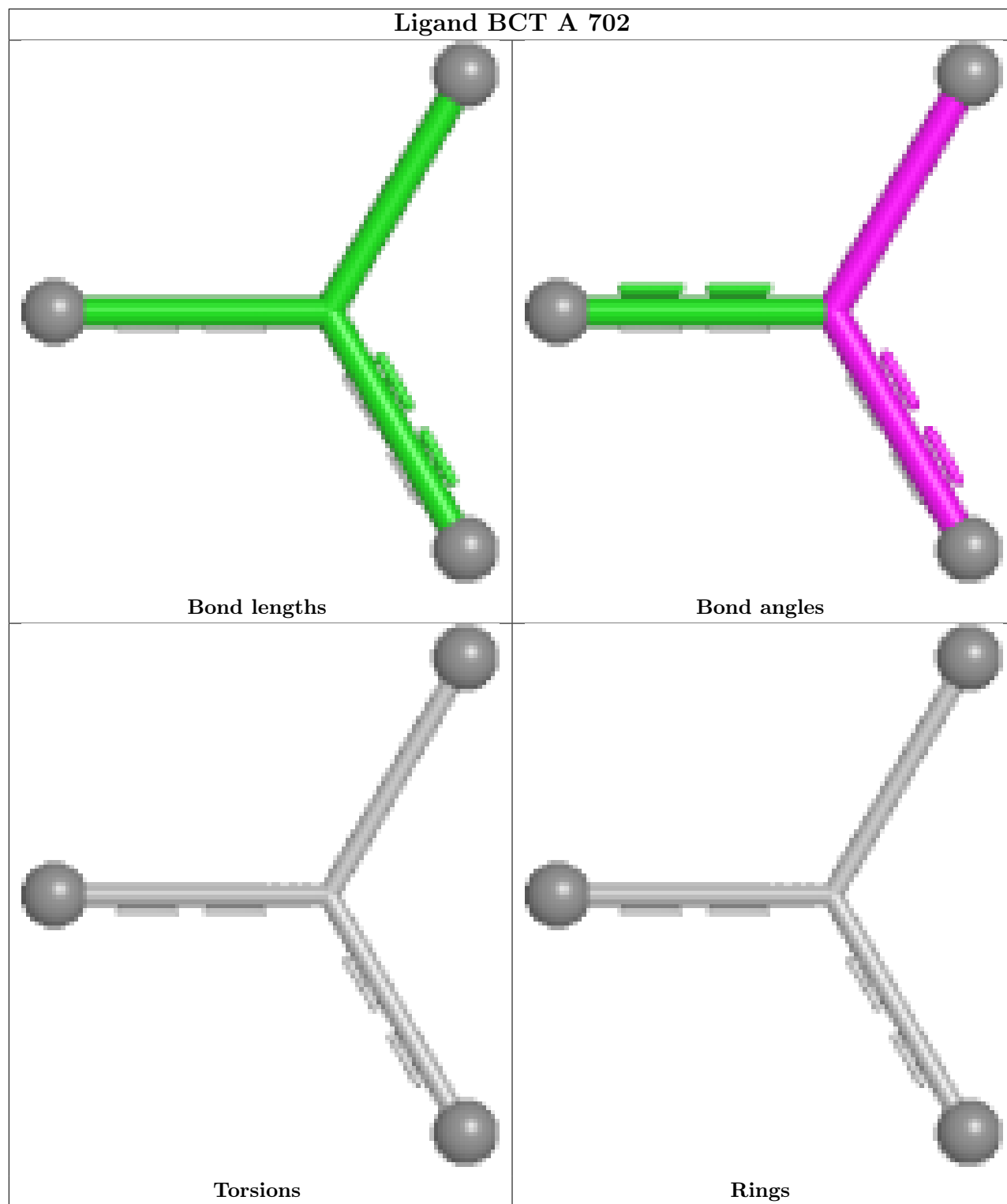
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	703	NAG	2	0
4	B	703	BCT	1	0

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%)	0.58	29 (8%)	17	13	11, 38, 80, 112	0
1	B	348/348 (100%)	1.14	67 (19%)	3	2	21, 60, 107, 160	0
All	All	696/696 (100%)	0.86	96 (13%)	6	5	11, 47, 97, 160	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	442	ALA	6.9
1	B	439	VAL	4.9
1	A	636	THR	4.9
1	B	441	LYS	4.8
1	B	342	TYR	4.3
1	B	621	ASN	4.1
1	B	572	LEU	3.9
1	A	442	ALA	3.9
1	B	549	TRP	3.9
1	B	548	VAL	3.8
1	B	552	THR	3.8
1	A	422	SER	3.7
1	B	566	ARG	3.6
1	B	420	HIS	3.5
1	A	677	THR	3.5
1	B	569	PHE	3.4
1	A	577	THR	3.4
1	B	577	THR	3.4
1	A	555	GLU	3.4
1	B	636	THR	3.4
1	B	445	GLY	3.3
1	B	435	ALA	3.3
1	A	443	ASN	3.2
1	A	557	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	530	PHE	3.2
1	A	446	LEU	3.2
1	A	554	GLY	3.2
1	B	578	ARG	3.1
1	B	580	PRO	3.1
1	B	571	LEU	3.1
1	B	556	SER	3.1
1	B	568	ASP	3.0
1	B	558	ALA	3.0
1	B	554	GLY	3.0
1	B	446	LEU	2.9
1	B	451	LEU	2.9
1	B	564	LEU	2.9
1	A	621	ASN	2.9
1	B	489	GLN	2.9
1	B	421	SER	2.8
1	B	443	ASN	2.8
1	B	590	ALA	2.8
1	B	618	PHE	2.8
1	B	654	ARG	2.8
1	B	553	ASN	2.8
1	A	441	LYS	2.8
1	B	581	VAL	2.8
1	A	423	LEU	2.7
1	A	654	ARG	2.7
1	B	440	LYS	2.7
1	A	689	ARG	2.7
1	B	613	HIS	2.6
1	B	551	ASN	2.6
1	A	445	GLY	2.6
1	A	622	GLY	2.6
1	B	438	VAL	2.6
1	B	561	ALA	2.6
1	B	634	SER	2.5
1	B	509	ASP	2.5
1	A	479	GLY	2.5
1	B	352	PRO	2.5
1	A	530	PHE	2.4
1	B	687	LEU	2.4
1	B	582	THR	2.4
1	B	688	THR	2.4
1	B	565	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	454	LYS	2.4
1	B	560	TRP	2.4
1	B	562	LYS	2.3
1	A	353	GLU	2.3
1	B	488	SER	2.3
1	B	559	ASP	2.3
1	B	415	ARG	2.3
1	B	503	ALA	2.3
1	A	567	GLU	2.2
1	B	539	ASP	2.2
1	B	444	GLU	2.2
1	A	652	GLY	2.2
1	B	623	LYS	2.2
1	B	375	SER	2.2
1	B	633	LYS	2.1
1	B	589	LEU	2.1
1	A	634	SER	2.1
1	B	423	LEU	2.1
1	A	444	GLU	2.1
1	B	570	ARG	2.1
1	A	416	LYS	2.1
1	A	419	LYS	2.1
1	A	565	ASN	2.1
1	B	587	CYS	2.1
1	A	575	ASP	2.1
1	B	365	SER	2.1
1	B	584	ALA	2.1
1	B	432	GLY	2.1
1	A	576	GLY	2.0
1	B	416	LYS	2.0

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

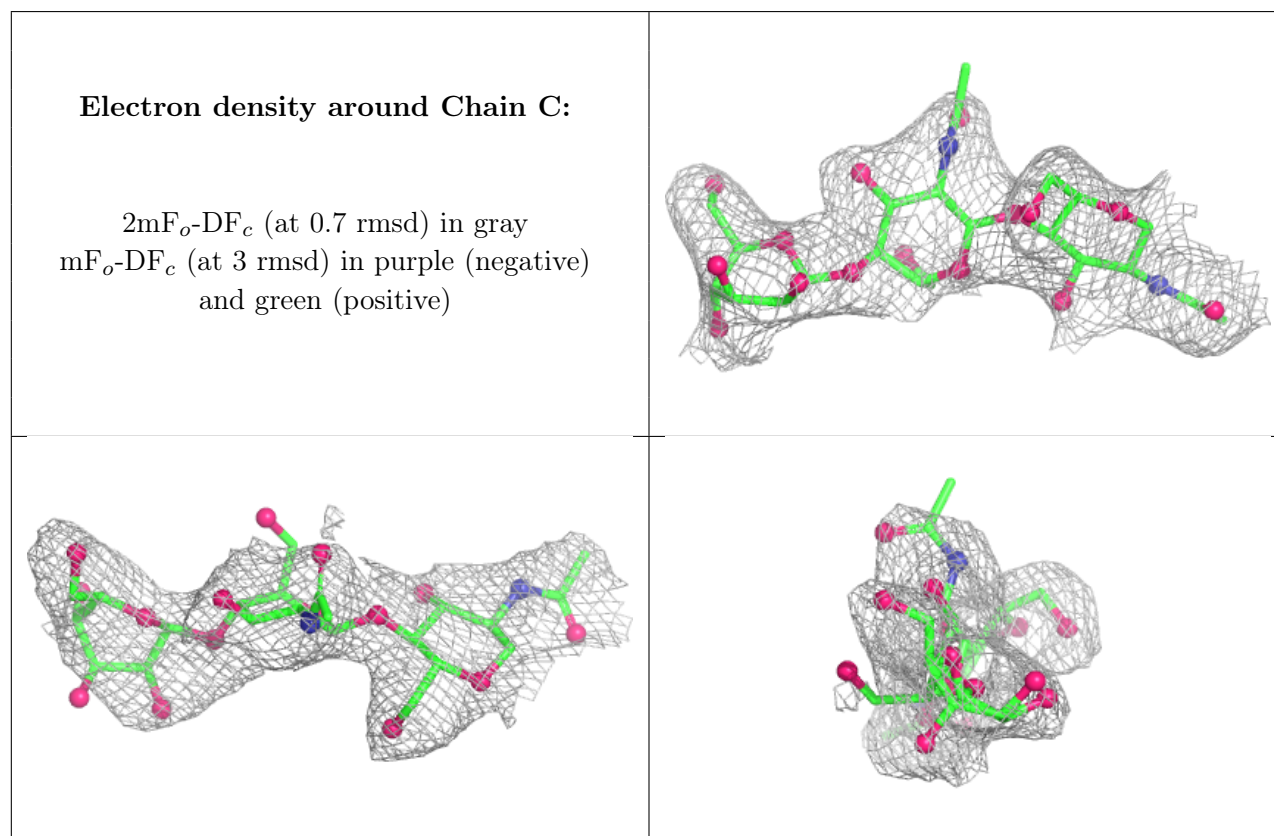
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

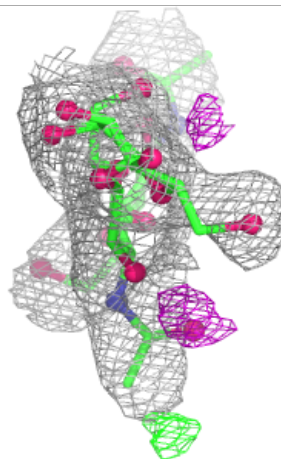
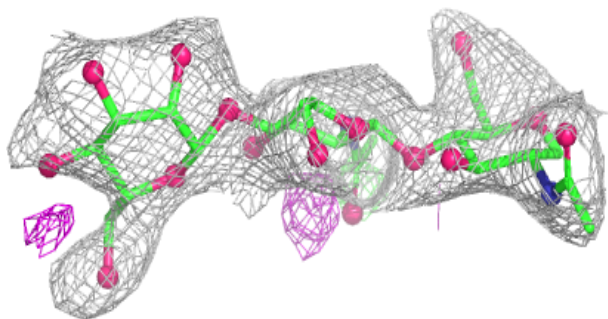
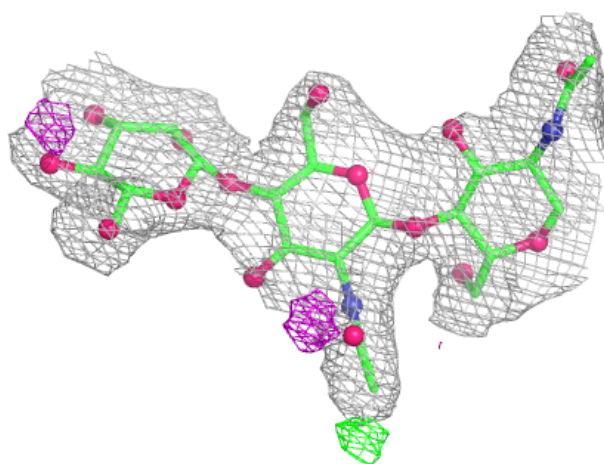
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	E	3	11/12	0.43	0.17	136,154,161,163	0
2	BMA	F	3	11/12	0.53	0.17	74,100,116,117	0
2	NAG	E	2	14/15	0.61	0.19	92,122,149,154	0
2	BMA	C	3	11/12	0.62	0.14	77,95,107,110	0
2	NAG	D	2	14/15	0.71	0.16	45,74,85,89	0
2	NAG	E	1	14/15	0.76	0.16	77,91,111,114	0
2	BMA	D	3	11/12	0.76	0.12	43,61,85,87	0
2	NAG	F	2	14/15	0.82	0.12	65,87,105,113	0
2	NAG	C	2	14/15	0.82	0.14	61,82,103,104	0
2	NAG	C	1	14/15	0.87	0.10	32,43,60,66	0
2	NAG	F	1	14/15	0.87	0.12	57,79,85,87	0
2	NAG	D	1	14/15	0.88	0.11	42,58,72,80	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.



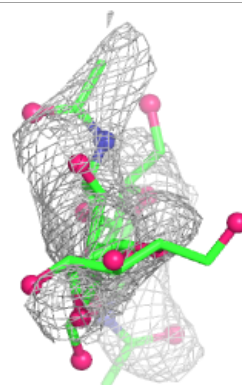
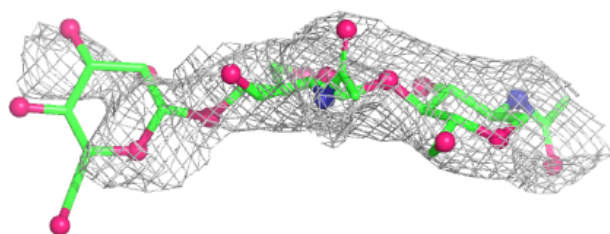
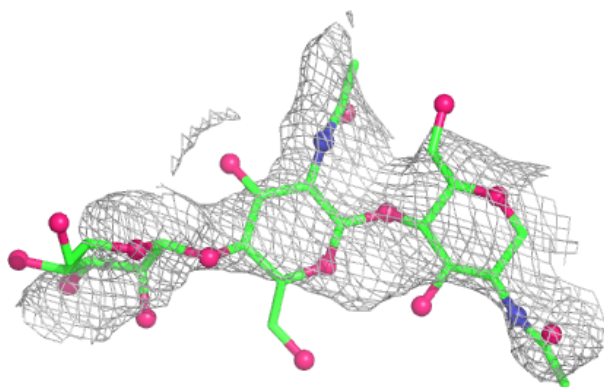
Electron density around Chain D:

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

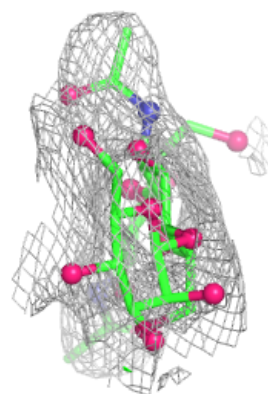
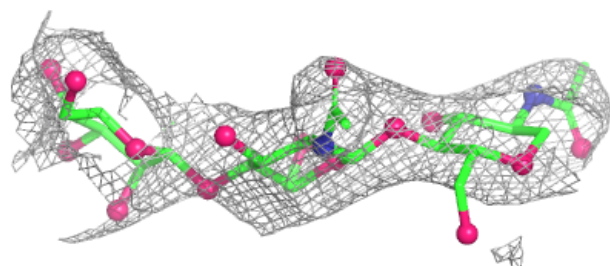
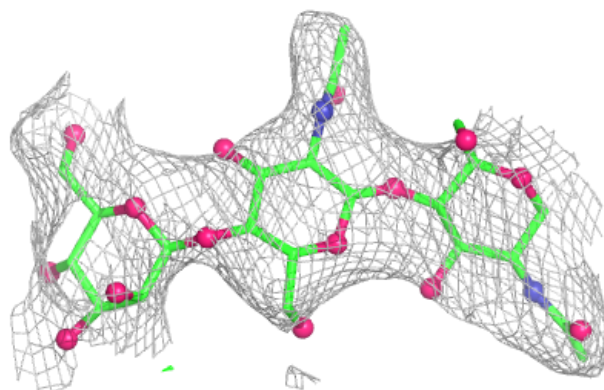


Electron density around Chain E:

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

**Electron density around Chain F:**

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



6.4 Ligands [i](#)

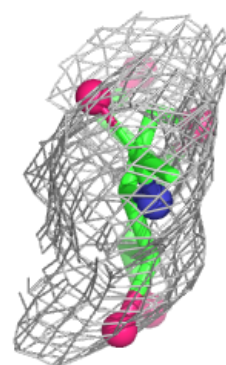
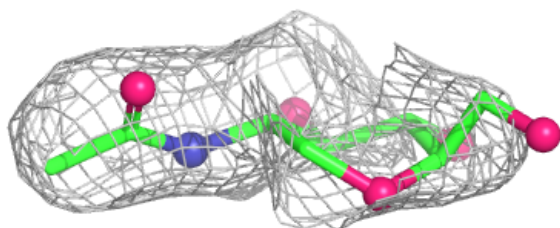
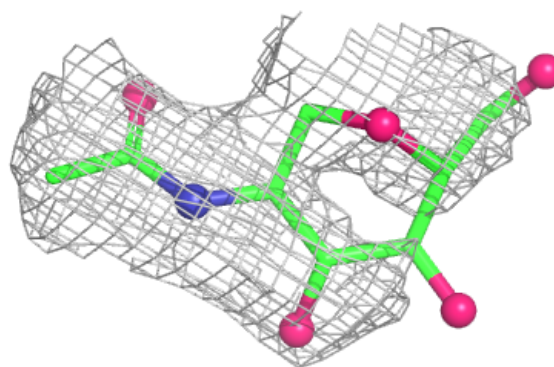
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	703	14/15	0.53	0.19	84,100,114,115	0
5	NAG	B	701	14/15	0.64	0.15	49,59,69,81	0
6	EDO	A	704	4/4	0.75	0.15	47,52,67,68	0
4	BCT	B	703	4/4	0.88	0.09	33,33,35,43	0
4	BCT	A	702	4/4	0.98	0.06	9,12,19,26	0
3	FE	B	702	1/1	0.99	0.03	51,51,51,51	0
3	FE	A	701	1/1	0.99	0.02	28,28,28,28	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.

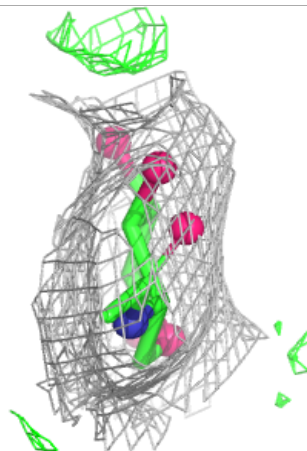
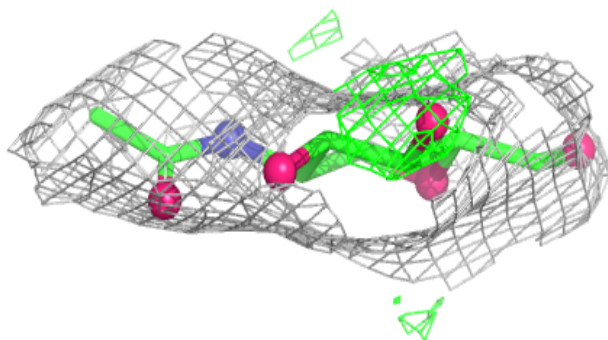
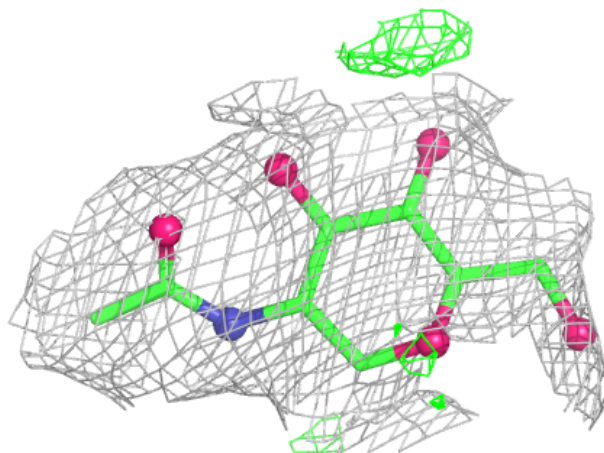
Electron density around NAG A 703:

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



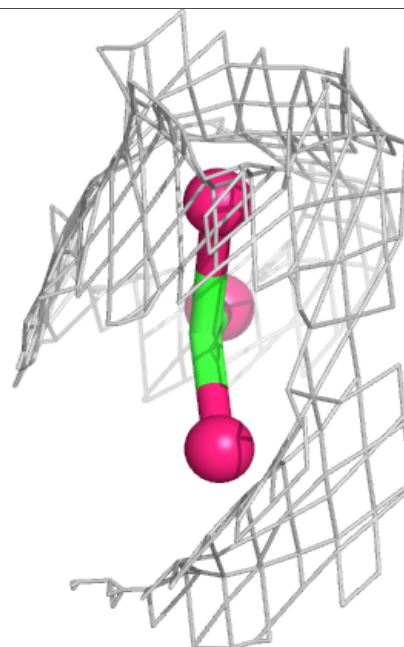
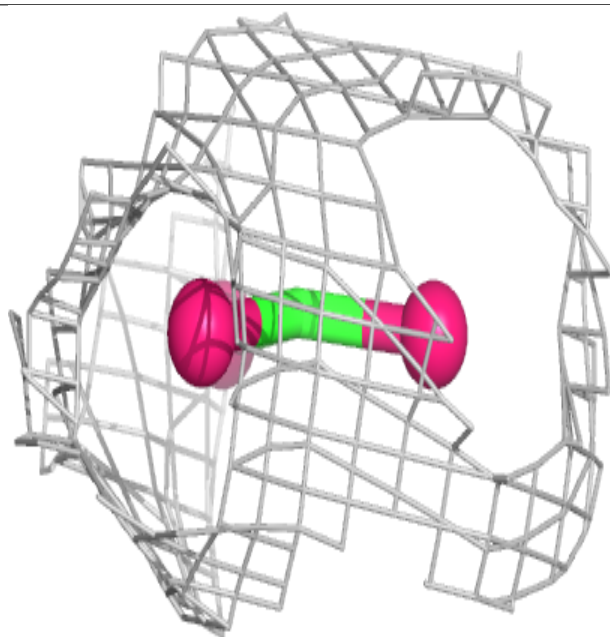
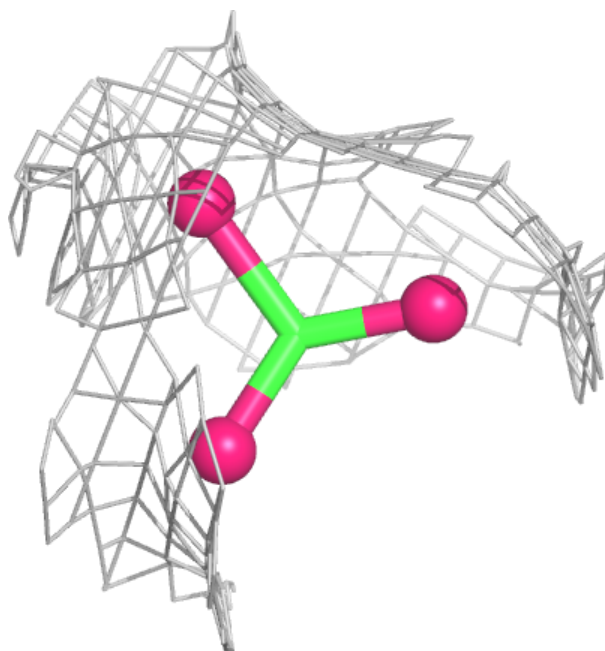
Electron density around NAG B 701:

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



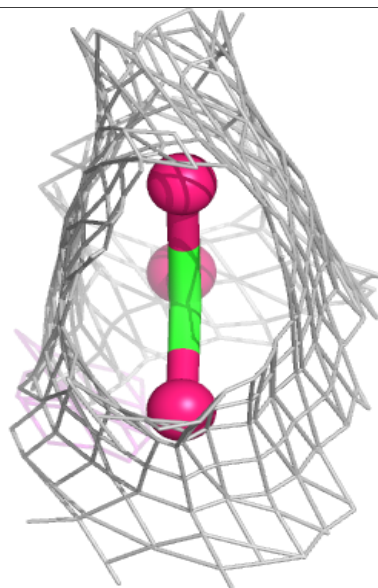
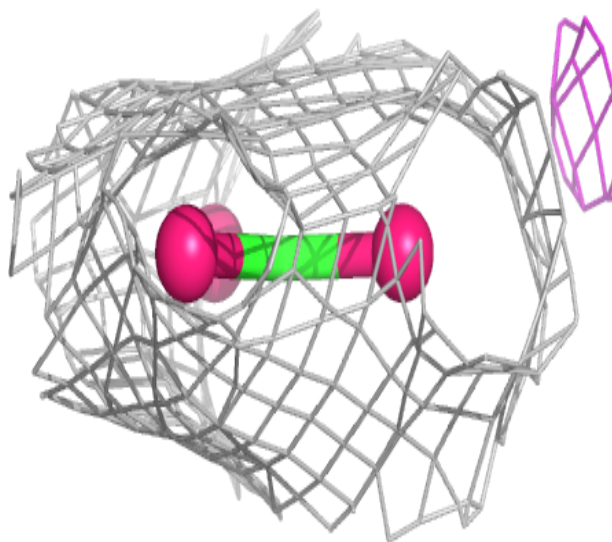
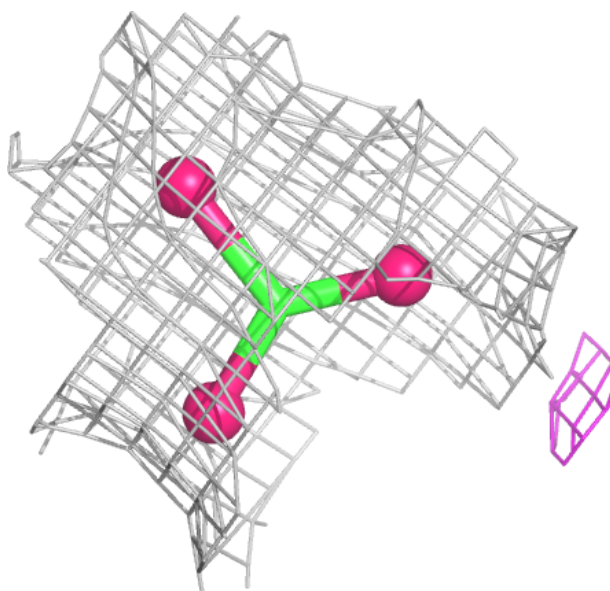
Electron density around BCT B 703:

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



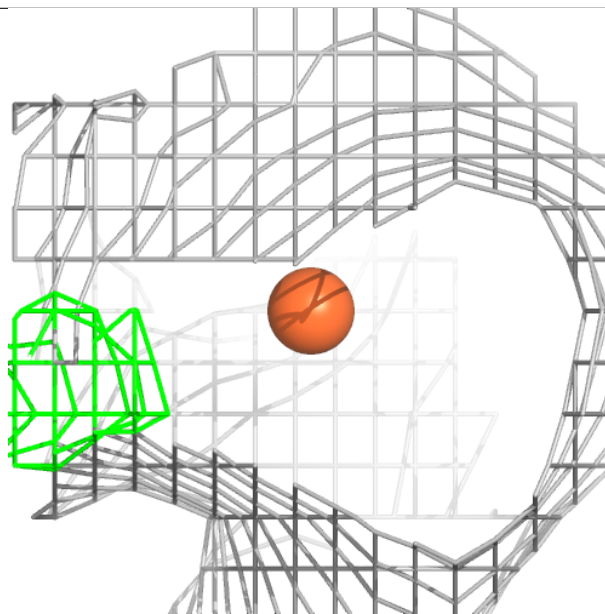
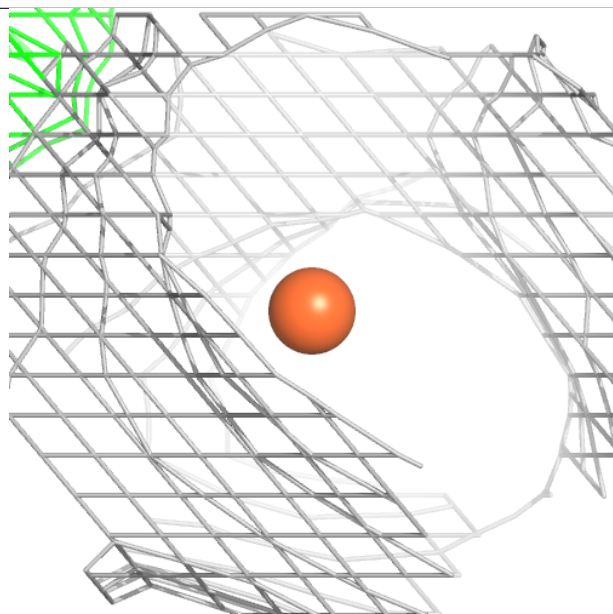
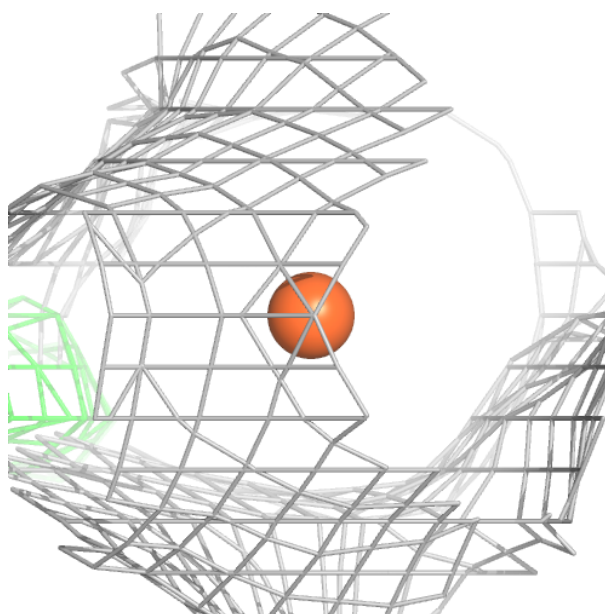
Electron density around BCT A 702:

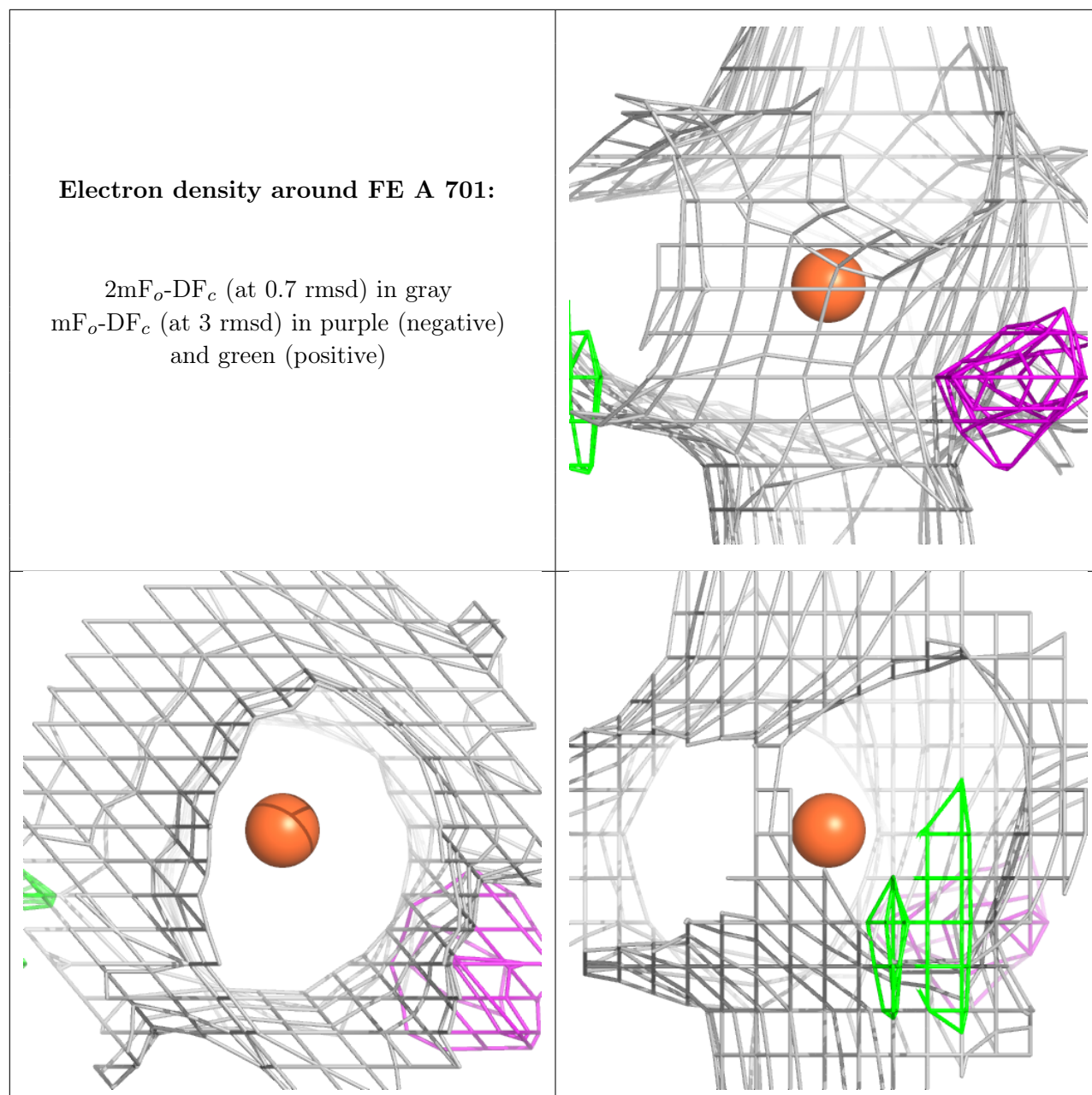
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.