Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 09:39 AM EDT

PDB ID	:	3K7N
Title	:	Structures of two elapid snake venom metalloproteases with distinct activities highlight the disulfide patterns in the D domain of ADAMalysin family proteins
Authors	:	Guan, H.H.; Huang, Y.W.; Wu, W.G.; Chen, C.J.
Deposited on	:	2009-10-13
Resolution	:	2.30 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:

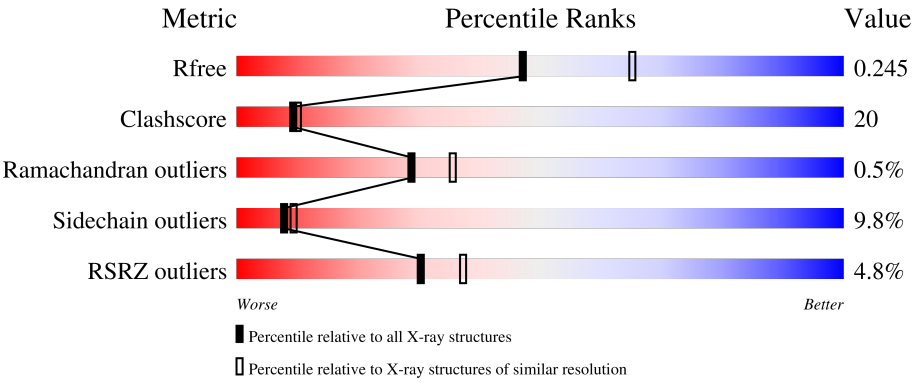
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	397	5%, 66%, 24%, 8%
2	B	3	33%, 67%
3	C	3	33%, 67%

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
2	FUC	B	3	-	-	-	X

2 Entry composition

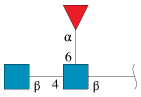
There are 6 unique types of molecules in this entry. The entry contains 3264 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 K-like.

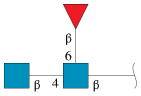
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3067	1907	538	584	38			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Ca 3 3	0	0

- Molecule 6 is water.

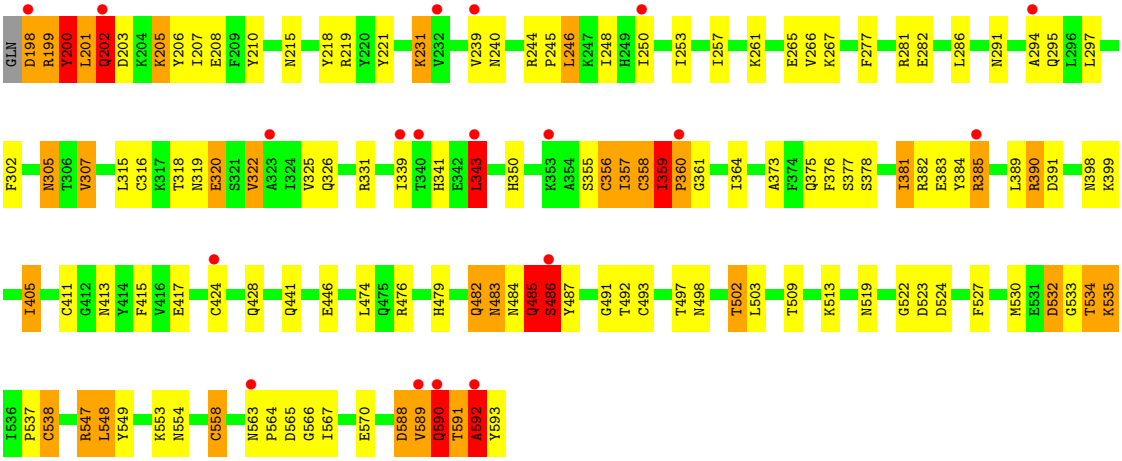
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	117	Total O 117 117	0	0

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: K-like

Chain A:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	63.00Å 63.00Å 273.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.36 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.30) 99.3 (29.36-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.241 0.236 , 0.245	Depositor DCC
R_{free} test set	2512 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3264	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, ZN, FUL, FUC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.34	17/3128 (0.5%)	1.34	31/4233 (0.7%)

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	1	12

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	558	CYS	C-N	10.68	1.58	1.34
1	A	424	CYS	CB-SG	10.62	2.00	1.82
1	A	486	SER	C-N	8.57	1.53	1.34
1	A	411	CYS	CB-SG	7.70	1.95	1.82
1	A	231	LYS	CD-CE	7.62	1.70	1.51
1	A	549	TYR	CD2-CE2	7.07	1.50	1.39
1	A	316	CYS	CB-SG	6.64	1.93	1.82
1	A	486	SER	CB-OG	6.58	1.50	1.42
1	A	538	CYS	CB-SG	6.52	1.93	1.82
1	A	570	GLU	CD-OE2	6.08	1.32	1.25
1	A	486	SER	CA-CB	5.63	1.61	1.52
1	A	231	LYS	CB-CG	5.61	1.67	1.52
1	A	446	GLU	CG-CD	5.45	1.60	1.51
1	A	261	LYS	CE-NZ	5.44	1.62	1.49
1	A	320	GLU	CG-CD	5.37	1.60	1.51
1	A	570	GLU	CD-OE1	5.23	1.31	1.25
1	A	218	TYR	CE2-CZ	-5.10	1.31	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	486	SER	O-C-N	-19.66	91.25	122.70
1	A	485	GLN	O-C-N	17.19	150.20	122.70
1	A	487	TYR	N-CA-CB	-16.82	80.32	110.60
1	A	558	CYS	O-C-N	-14.39	99.68	122.70
1	A	547	ARG	NE-CZ-NH2	-12.84	113.88	120.30
1	A	485	GLN	CA-C-N	-10.73	93.59	117.20
1	A	487	TYR	N-CA-C	10.34	138.91	111.00
1	A	486	SER	CB-CA-C	9.46	128.07	110.10
1	A	200	TYR	CB-CA-C	8.72	127.85	110.40
1	A	547	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	A	331	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	A	202	GLN	N-CA-C	7.86	132.23	111.00
1	A	487	TYR	CB-CA-C	7.41	125.23	110.40
1	A	485	GLN	N-CA-C	7.01	129.93	111.00
1	A	231	LYS	CD-CE-NZ	-6.75	96.18	111.70
1	A	441	GLN	O-C-N	-6.60	112.14	122.70
1	A	359	ILE	CB-CA-C	6.43	124.45	111.60
1	A	547	ARG	CG-CD-NE	-6.38	98.39	111.80
1	A	358	CYS	N-CA-C	-6.28	94.05	111.00
1	A	331	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	548	LEU	CB-CG-CD2	6.00	121.21	111.00
1	A	343	LEU	CB-CG-CD2	-5.82	101.11	111.00
1	A	592	ALA	N-CA-C	5.72	126.45	111.00
1	A	201	LEU	C-N-CA	5.60	135.70	121.70
1	A	307	VAL	CB-CA-C	5.49	121.83	111.40
1	A	266	VAL	CB-CA-C	5.34	121.54	111.40
1	A	390	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	532	ASP	N-CA-C	5.23	125.13	111.00
1	A	405	ILE	CB-CA-C	-5.21	101.19	111.60
1	A	524	ASP	CB-CA-C	5.11	120.62	110.40
1	A	343	LEU	CB-CG-CD1	5.08	119.63	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	486	SER	CA

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	200	TYR	Peptide
1	A	356	CYS	Peptide
1	A	357	ILE	Peptide
1	A	359	ILE	Peptide
1	A	485	GLN	Peptide
1	A	486	SER	Mainchain,Peptide
1	A	558	CYS	Mainchain
1	A	588	ASP	Peptide
1	A	590	GLN	Peptide
1	A	591	THR	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	3067	0	2987	120	0
2	B	38	0	34	2	0
3	C	38	0	34	1	0
4	A	1	0	0	0	0
5	A	3	0	0	0	0
6	A	117	0	0	3	0
All	All	3264	0	3055	123	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 20.

All (123) 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:A:592:ALA:HA	1:A:593:TYR:CD1	1.82	1.14
1:A:592:ALA:HA	1:A:593:TYR:HD1	1.08	1.14
1:A:240:ASN:HD21	1:A:250:ILE:H	0.94	0.93
1:A:207:ILE:HD11	1:A:248:ILE:HG12	1.53	0.90
1:A:295:GLN:NE2	1:A:339:ILE:HD12	1.86	0.90
1:A:281:ARG:HE	1:A:291:ASN:HD21	1.18	0.90
1:A:325:VAL:HG21	1:A:339:ILE:HD13	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASN:ND2	1:A:250:ILE:H	1.72	0.88
1:A:590:GLN:HA	1:A:592:ALA:HB3	1.54	0.88
1:A:295:GLN:HE22	1:A:339:ILE:HG23	1.40	0.87
1:A:590:GLN:CA	1:A:592:ALA:HB3	2.08	0.84
1:A:295:GLN:HE22	1:A:339:ILE:HD12	1.43	0.79
1:A:240:ASN:HD21	1:A:250:ILE:N	1.78	0.79
3:C:1:NAG:O5	3:C:3:FUL:H2	1.83	0.78
1:A:532:ASP:OD2	1:A:534:THR:HG23	1.84	0.78
1:A:530:MET:O	1:A:533:GLY:HA2	1.84	0.76
1:A:201:LEU:H	1:A:202:GLN:CB	2.01	0.73
1:A:215:ASN:HD21	1:A:219:ARG:HE	1.37	0.73
1:A:482:GLN:O	1:A:485:GLN:HB2	1.92	0.69
1:A:364:ILE:HD13	1:A:373:ALA:HB3	1.73	0.69
1:A:357:ILE:HG22	1:A:358:CYS:HA	1.76	0.67
1:A:530:MET:O	1:A:533:GLY:CA	2.43	0.67
1:A:207:ILE:CD1	1:A:248:ILE:HG12	2.25	0.67
1:A:295:GLN:NE2	1:A:339:ILE:HG23	2.08	0.67
1:A:359:ILE:O	1:A:375:GLN:NE2	2.28	0.67
1:A:281:ARG:HE	1:A:291:ASN:ND2	1.92	0.66
1:A:405:ILE:HD13	1:A:417:GLU:HG2	1.78	0.66
1:A:405:ILE:HD11	1:A:415:PHE:CE1	2.32	0.64
1:A:486:SER:HB3	1:A:493:CYS:SG	2.38	0.64
1:A:547:ARG:NH1	1:A:563:ASN:OD1	2.31	0.63
1:A:590:GLN:HA	1:A:592:ALA:CB	2.27	0.63
1:A:199:ARG:HB3	1:A:202:GLN:HB2	1.80	0.63
1:A:547:ARG:HD2	6:A:101:HOH:O	1.99	0.62
1:A:201:LEU:H	1:A:202:GLN:HB2	1.63	0.62
1:A:208:GLU:HB3	1:A:253:ILE:CD1	2.29	0.62
1:A:282:GLU:OE2	1:A:319:ASN:HB3	1.98	0.62
1:A:297:LEU:HD21	1:A:339:ILE:HD11	1.82	0.61
1:A:497:THR:HG23	1:A:509:THR:HG22	1.84	0.60
1:A:405:ILE:HD11	1:A:415:PHE:HE1	1.64	0.59
1:A:265:GLU:OE2	1:A:267:LYS:HE2	2.01	0.59
2:B:2:NAG:H82	2:B:3:FUC:H63	1.84	0.59
1:A:277:PHE:CE2	1:A:322:VAL:HG22	2.37	0.59
1:A:246:LEU:HD21	1:A:381:ILE:HD11	1.84	0.58
1:A:358:CYS:C	1:A:359:ILE:HD12	2.24	0.58
1:A:563:ASN:HD22	1:A:567:ILE:HD12	1.69	0.57
1:A:199:ARG:HB3	1:A:201:LEU:N	2.19	0.57
1:A:364:ILE:HD13	1:A:373:ALA:CB	2.34	0.57
1:A:325:VAL:HG21	1:A:339:ILE:CD1	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ILE:HG12	1:A:377:SER:HB2	1.87	0.57
1:A:486:SER:CB	1:A:493:CYS:SG	2.93	0.56
1:A:482:GLN:HG2	1:A:493:CYS:SG	2.46	0.56
1:A:589:VAL:HG12	1:A:592:ALA:HB2	1.88	0.55
1:A:198:ASP:O	1:A:199:ARG:HD3	2.06	0.55
1:A:206:TYR:CZ	1:A:399:LYS:HG3	2.43	0.54
1:A:305:ASN:HD22	1:A:305:ASN:H	1.56	0.54
1:A:207:ILE:HD12	1:A:207:ILE:N	2.23	0.53
1:A:201:LEU:H	1:A:202:GLN:CA	2.22	0.53
1:A:358:CYS:O	1:A:359:ILE:HD12	2.08	0.53
1:A:207:ILE:HD11	1:A:248:ILE:CG1	2.32	0.52
1:A:405:ILE:CD1	1:A:417:GLU:HG2	2.38	0.52
1:A:257:ILE:HD12	1:A:257:ILE:N	2.25	0.52
1:A:356:CYS:HB3	1:A:357:ILE:HG12	1.90	0.52
1:A:527:PHE:CD2	1:A:535:LYS:HE3	2.45	0.52
1:A:239:VAL:HG11	1:A:250:ILE:HD12	1.91	0.52
1:A:319:ASN:OD1	1:A:320:GLU:HG3	2.09	0.52
1:A:246:LEU:HD21	1:A:381:ILE:CD1	2.41	0.51
1:A:265:GLU:OE2	1:A:267:LYS:CE	2.59	0.51
1:A:282:GLU:HB2	1:A:318:THR:O	2.11	0.51
1:A:563:ASN:OD1	1:A:566:GLY:HA3	2.11	0.50
1:A:305:ASN:H	1:A:305:ASN:ND2	2.09	0.50
1:A:200:TYR:O	1:A:203:ASP:N	2.39	0.50
1:A:200:TYR:O	1:A:203:ASP:HB2	2.10	0.49
1:A:215:ASN:ND2	1:A:219:ARG:HE	2.08	0.49
1:A:250:ILE:HD13	1:A:343:LEU:HD21	1.95	0.49
1:A:208:GLU:HB3	1:A:253:ILE:HD11	1.94	0.49
1:A:305:ASN:HD22	1:A:305:ASN:N	2.09	0.49
1:A:350:HIS:ND1	1:A:383:GLU:OE1	2.42	0.48
1:A:523:ASP:OD1	1:A:523:ASP:C	2.51	0.48
1:A:302:PHE:H	1:A:326:GLN:NE2	2.11	0.48
1:A:221:TYR:OH	1:A:231:LYS:HD2	2.14	0.47
1:A:364:ILE:HD11	1:A:373:ALA:O	2.14	0.47
2:B:2:NAG:H4	2:B:3:FUC:H61	1.96	0.47
1:A:497:THR:CG2	1:A:509:THR:HG22	2.44	0.47
1:A:356:CYS:HA	1:A:357:ILE:HD13	1.97	0.46
1:A:563:ASN:HA	1:A:564:PRO:HD2	1.74	0.46
1:A:390:ARG:CZ	1:A:391:ASP:OD2	2.64	0.46
1:A:246:LEU:HD13	1:A:384:TYR:CD2	2.51	0.46
1:A:498:ASN:O	1:A:502:THR:HG23	2.16	0.46
1:A:356:CYS:HB3	1:A:377:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ASN:HB3	1:A:538:CYS:SG	2.56	0.45
1:A:590:GLN:C	1:A:592:ALA:HB3	2.36	0.45
1:A:565:ASP:HB2	1:A:566:GLY:HA2	1.98	0.45
1:A:360:PRO:HG2	1:A:361:GLY:H	1.82	0.44
1:A:210:TYR:O	1:A:294:ALA:HA	2.16	0.44
1:A:208:GLU:HB3	1:A:253:ILE:HD13	1.98	0.44
1:A:205:LYS:HB2	1:A:205:LYS:HE2	1.23	0.44
1:A:482:GLN:CG	1:A:493:CYS:SG	3.05	0.44
1:A:563:ASN:ND2	1:A:567:ILE:H	2.15	0.44
1:A:239:VAL:CG1	1:A:250:ILE:HD12	2.47	0.43
1:A:405:ILE:HD12	6:A:24:HOH:O	2.18	0.43
1:A:522:GLY:CA	1:A:537:PRO:HA	2.48	0.43
1:A:199:ARG:HD2	1:A:201:LEU:HB3	2.00	0.43
1:A:201:LEU:HD21	1:A:385:ARG:NH1	2.34	0.43
1:A:589:VAL:CG1	1:A:592:ALA:HB2	2.49	0.43
1:A:325:VAL:CG2	1:A:339:ILE:HD13	2.37	0.43
1:A:277:PHE:CD2	1:A:322:VAL:HG22	2.53	0.43
1:A:530:MET:O	1:A:533:GLY:HA3	2.18	0.43
1:A:590:GLN:C	1:A:590:GLN:HE21	2.22	0.43
1:A:376:PHE:HB2	1:A:381:ILE:HD11	2.00	0.42
1:A:199:ARG:HB3	1:A:202:GLN:CB	2.47	0.42
1:A:474:LEU:HD13	1:A:491:GLY:HA3	2.01	0.42
1:A:305:ASN:ND2	1:A:305:ASN:N	2.65	0.42
1:A:199:ARG:HB3	1:A:201:LEU:H	1.83	0.42
1:A:244:ARG:HB3	1:A:245:PRO:HD3	2.02	0.41
1:A:297:LEU:HD21	1:A:339:ILE:CD1	2.48	0.41
1:A:503:LEU:HD11	1:A:567:ILE:HG21	2.00	0.41
1:A:357:ILE:HG13	1:A:378:SER:H	1.85	0.41
1:A:341:HIS:HD2	1:A:364:ILE:O	2.03	0.41
1:A:325:VAL:HG11	1:A:339:ILE:HD13	2.01	0.40
1:A:476:ARG:HH21	1:A:479:HIS:HD2	1.69	0.40
1:A:590:GLN:CB	1:A:592:ALA:HB3	2.52	0.40
1:A:483:ASN:O	1:A:484:ASN:HB2	2.21	0.40
1:A:244:ARG:NH1	6:A:65:HOH:O	2.39	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	394/397 (99%)	371 (94%)	21 (5%)	2 (0%)	29 35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	592	ALA
1	A	360	PRO

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	346/347 (100%)	312 (90%)	34 (10%)	8 9

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	202	GLN
1	A	205	LYS
1	A	246	LEU
1	A	286	LEU
1	A	305	ASN
1	A	307	VAL
1	A	315	LEU
1	A	322	VAL

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Mol	Chain	Res	Type
1	A	343	LEU
1	A	355	SER
1	A	381	ILE
1	A	382	ARG
1	A	385	ARG
1	A	389	LEU
1	A	398	ASN
1	A	413	ASN
1	A	428	GLN
1	A	482	GLN
1	A	483	ASN
1	A	485	GLN
1	A	486	SER
1	A	492	THR
1	A	502	THR
1	A	513	LYS
1	A	534	THR
1	A	535	LYS
1	A	548	LEU
1	A	553	LYS
1	A	554	ASN
1	A	588	ASP
1	A	589	VAL
1	A	590	GLN
1	A	591	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	ASN
1	A	223	ASN
1	A	240	ASN
1	A	291	ASN
1	A	293	ASN
1	A	295	GLN
1	A	305	ASN
1	A	326	GLN
1	A	341	HIS
1	A	346	ASN
1	A	375	GLN
1	A	413	ASN
1	A	428	GLN

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Mol	Chain	Res	Type
1	A	441	GLN
1	A	479	HIS
1	A	499	GLN
1	A	590	GLN

5.3.3 RNA (i)

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)

6 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	B	1	1,2	14,14,15	0.70	0	17,19,21	2.19	4 (23%)
2	NAG	B	2	2	14,14,15	0.79	1 (7%)	17,19,21	2.01	5 (29%)
2	FUC	B	3	2	10,10,11	0.88	0	14,14,16	1.89	4 (28%)
3	NAG	C	1	1,3	14,14,15	0.62	0	17,19,21	2.04	4 (23%)
3	NAG	C	2	3	14,14,15	1.15	2 (14%)	17,19,21	2.11	5 (29%)
3	FUL	C	3	3	10,10,11	1.26	1 (10%)	14,14,16	2.32	5 (35%)

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	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	FUC	B	3	2	-	-	0/1/1/1
3	NAG	C	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	FUL	C	3	3	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C1-C2	3.08	1.56	1.52
3	C	2	NAG	C3-C2	2.43	1.57	1.52
3	C	3	FUL	C1-C2	2.39	1.57	1.52
2	B	2	NAG	C1-C2	2.01	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	C1-O5-C5	5.91	120.20	112.19
3	C	1	NAG	C1-O5-C5	5.36	119.45	112.19
2	B	2	NAG	C1-C2-N2	4.95	118.95	110.49
3	C	2	NAG	C1-O5-C5	4.94	118.88	112.19
2	B	1	NAG	C2-N2-C7	-4.59	116.36	122.90
3	C	3	FUL	C1-C2-C3	4.36	115.03	109.67
3	C	1	NAG	C4-C3-C2	4.31	117.34	111.02
3	C	3	FUL	C1-O5-C5	4.30	122.52	112.78
2	B	3	FUC	O5-C1-C2	3.73	116.53	110.77
3	C	2	NAG	O5-C1-C2	3.66	117.07	111.29
2	B	2	NAG	C1-O5-C5	3.63	117.12	112.19
3	C	3	FUL	O5-C1-C2	3.53	116.23	110.77
2	B	1	NAG	O4-C4-C3	-3.24	102.87	110.35
3	C	2	NAG	C2-N2-C7	3.14	127.37	122.90
2	B	3	FUC	C1-O5-C5	3.05	119.70	112.78
3	C	2	NAG	C1-C2-N2	-2.89	105.55	110.49
3	C	3	FUL	O5-C5-C4	2.86	114.66	109.52
3	C	2	NAG	O3-C3-C2	2.77	115.21	109.47
2	B	2	NAG	C2-N2-C7	2.62	126.63	122.90
3	C	1	NAG	O5-C1-C2	-2.48	107.38	111.29
2	B	3	FUC	O2-C2-C1	2.47	114.21	109.15
2	B	3	FUC	O5-C5-C4	2.46	113.93	109.52
2	B	2	NAG	O5-C1-C2	-2.43	107.45	111.29
3	C	3	FUL	O2-C2-C1	2.38	114.03	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	NAG	C1-C2-N2	-2.36	106.46	110.49
2	B	1	NAG	O5-C5-C4	2.14	116.03	110.83
2	B	2	NAG	O7-C7-C8	-2.09	118.17	122.06

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C1-C2-N2-C7
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C3-C2-N2-C7

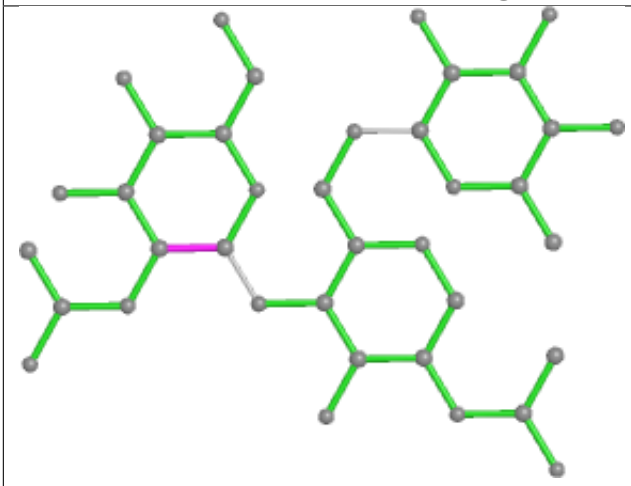
There are no ring outliers.

4 monomers are involved in 3 short contacts:

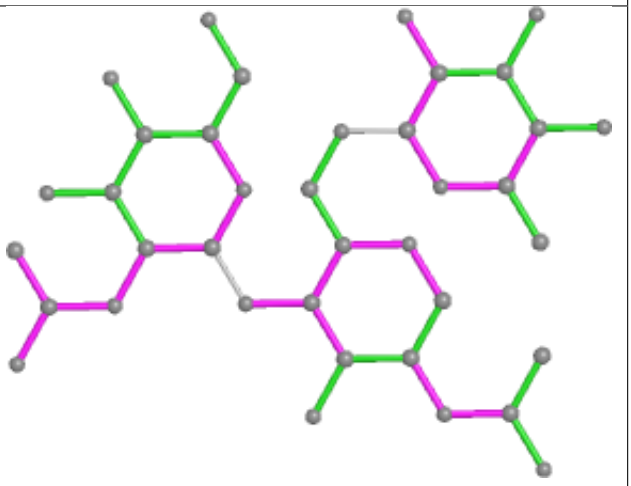
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	2	0
2	B	3	FUC	2	0
3	C	1	NAG	1	0
3	C	3	FUL	1	0

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

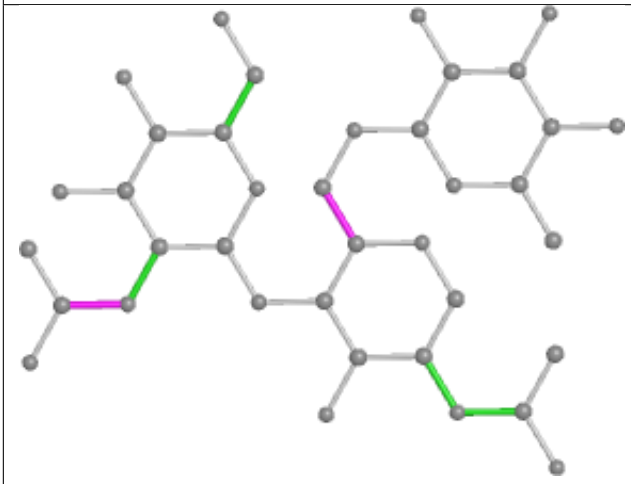
Oligosaccharide Chain B



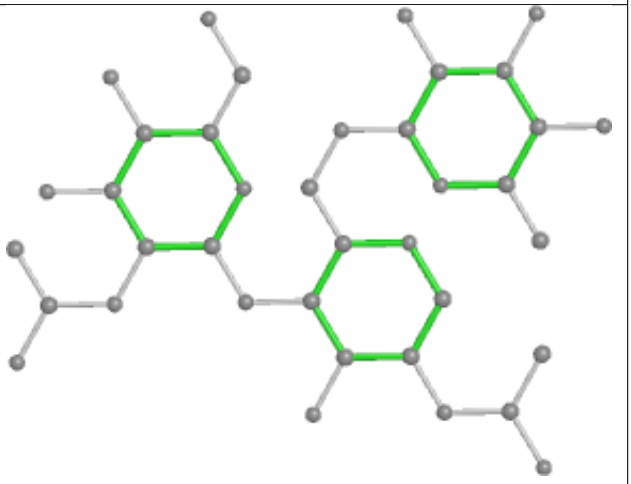
Bond lengths



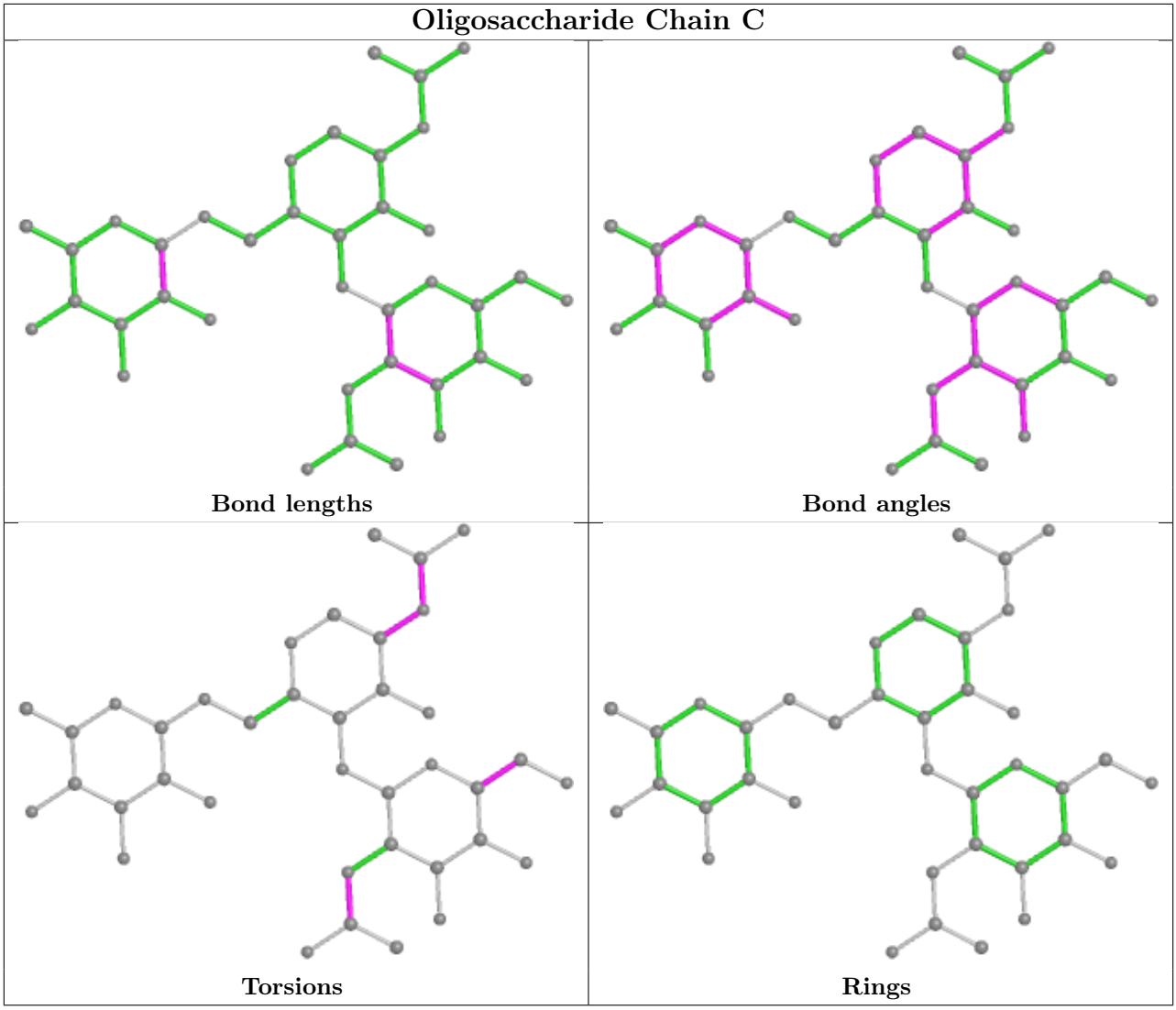
Bond angles



Torsions



Rings



5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 95^{th} 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	396/397 (99%)	0.08	19 (4%) 30 37	29, 48, 79, 115	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	486	SER	6.2
1	A	339	ILE	3.4
1	A	590	GLN	3.3
1	A	592	ALA	3.3
1	A	239	VAL	2.9
1	A	563	ASN	2.8
1	A	340	THR	2.7
1	A	250	ILE	2.7
1	A	294	ALA	2.6
1	A	360	PRO	2.5
1	A	323	ALA	2.4
1	A	343	LEU	2.4
1	A	385	ARG	2.4
1	A	232	VAL	2.1
1	A	589	VAL	2.1
1	A	198	ASP	2.1
1	A	424	CYS	2.1
1	A	353	LYS	2.0
1	A	202	GLN	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 (i)

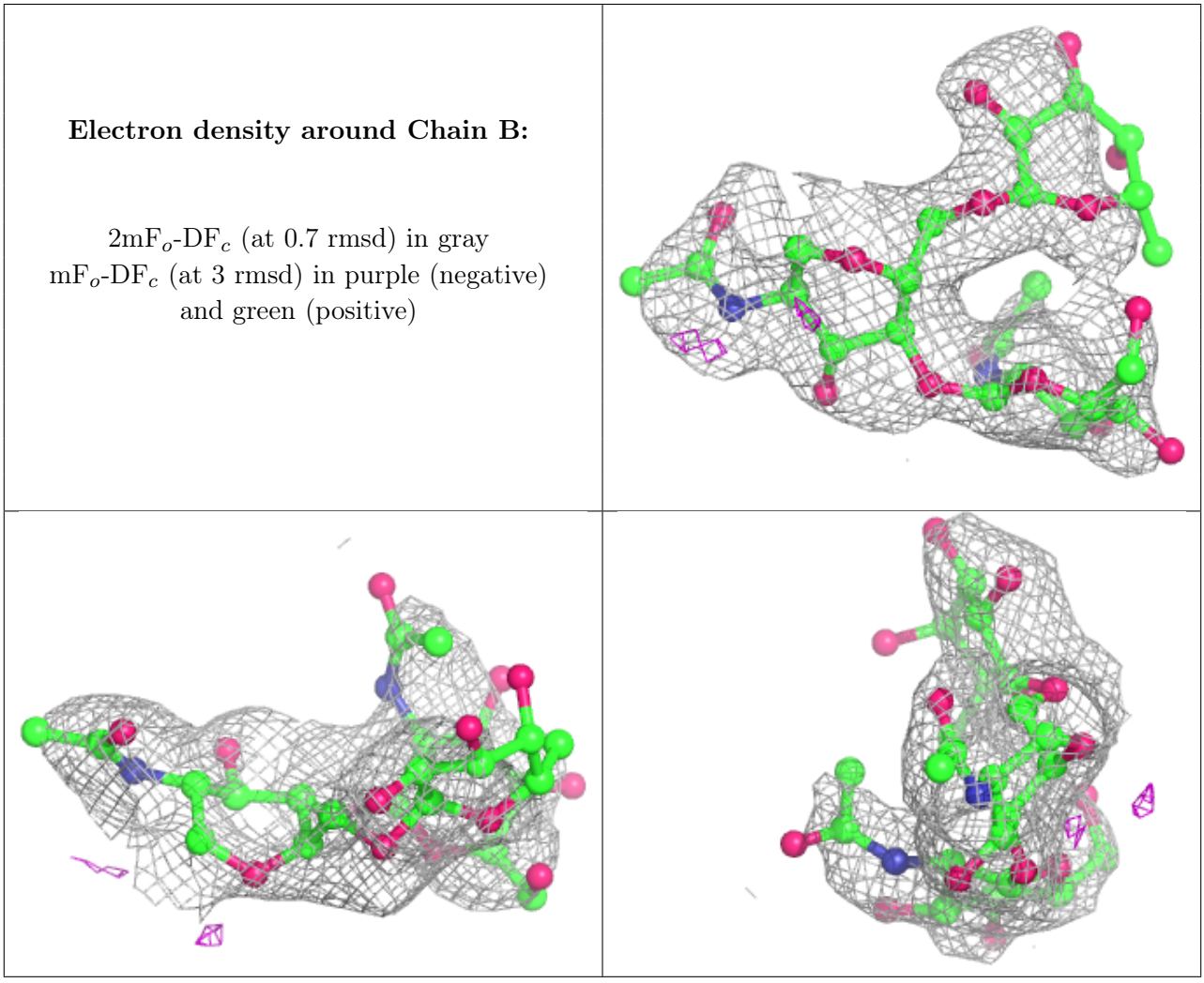
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	C	2	14/15	0.49	0.39	129,132,134,134	0
3	FUL	C	3	10/11	0.54	0.38	133,134,135,135	0
2	FUC	B	3	10/11	0.65	0.58	125,128,129,129	0
3	NAG	C	1	14/15	0.72	0.20	78,86,95,98	0
2	NAG	B	2	14/15	0.86	0.39	123,126,128,129	0
2	NAG	B	1	14/15	0.88	0.23	75,83,97,98	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.

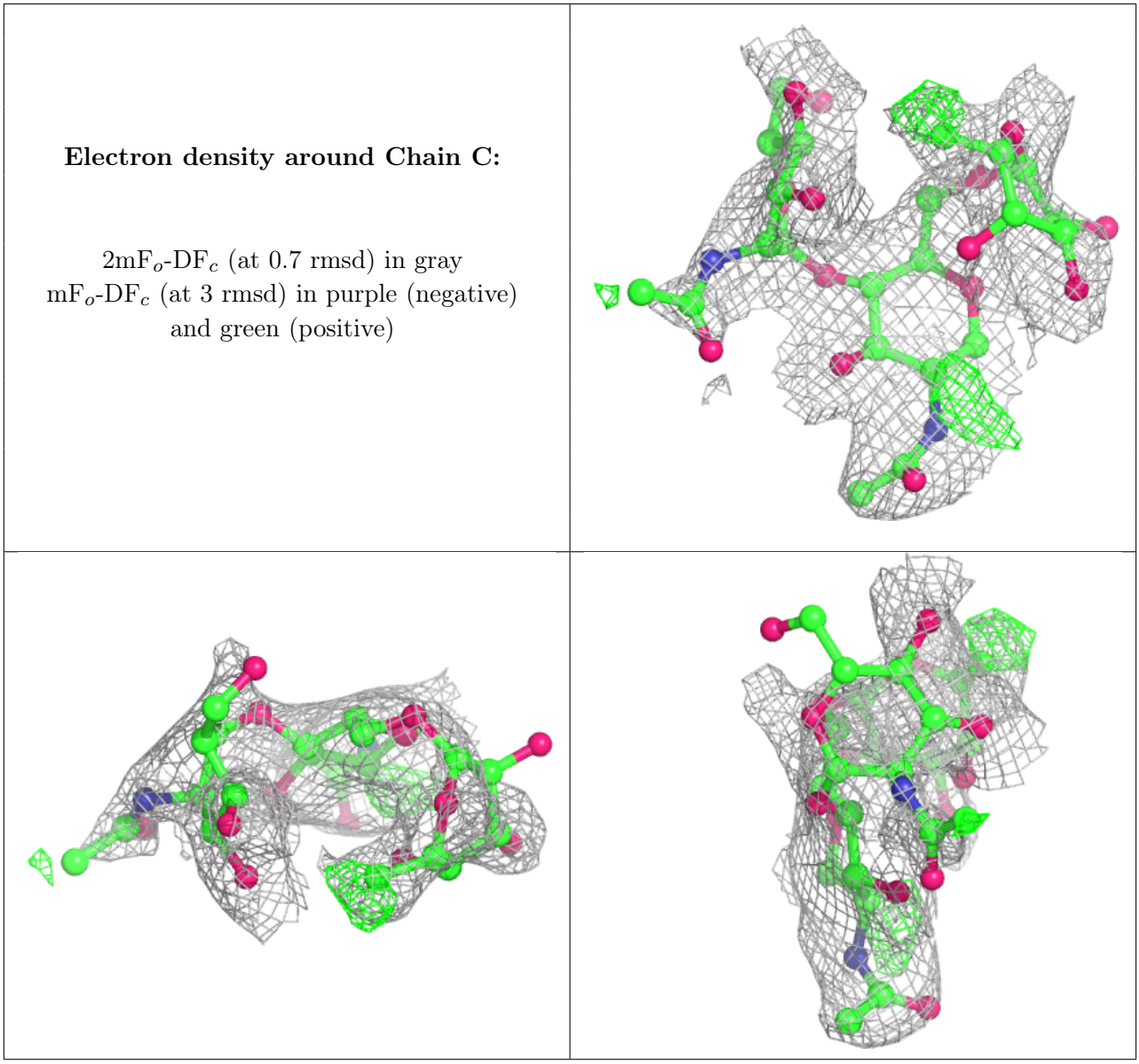
Electron density around Chain B:

$2mF_o$-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 C:

$2mF_o$-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, 95^{th} 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
4	ZN	A	704	1/1	0.96	0.17	51,51,51,51	0
5	CA	A	702	1/1	0.98	0.05	37,37,37,37	0
5	CA	A	703	1/1	0.98	0.13	46,46,46,46	0
5	CA	A	701	1/1	0.99	0.06	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.