Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 05:58 PM EST

PDB ID	:	1C82
Title	:	MECHANISM OF HYALURONAN BINDING AND DEGRADATION: STRUCTURE OF STREPTOCOCCUS PNEUMONIAE HYALURONATE LYASE IN COMPLEX WITH HYALURONIC ACID DISACCHARIDE AT 1.7 A RESOLUTION
Authors	:	Ponnuraj, K.; Jedrzejas, M.J.
Deposited on	:	2000-04-05
Resolution	:	1.70 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 (i) 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 (i)) were used in the production of this report:

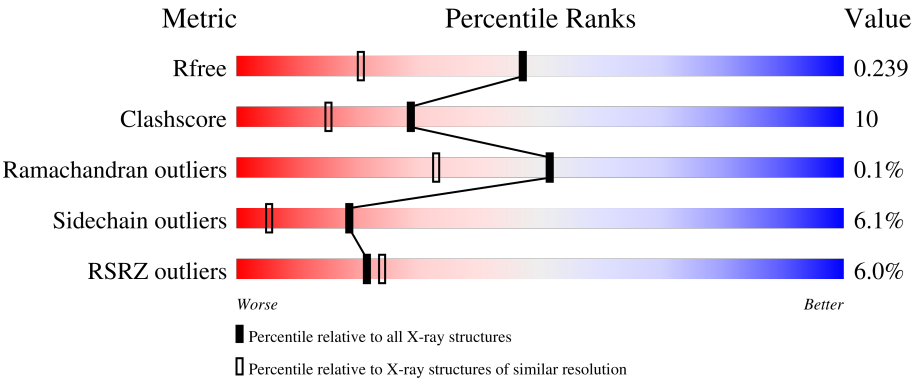
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	731	6% 78% 18%
2	B	2	50% 50%
2	C	2	100%

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	NA	A	906	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6407 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.

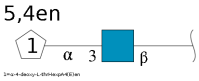
- Molecule 1 is a protein called HYALURONATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total	C	N	O	S	0	0	0
			5770	3629	966	1153	22			

There are 7 discrepancies between the modelled and reference sequences:

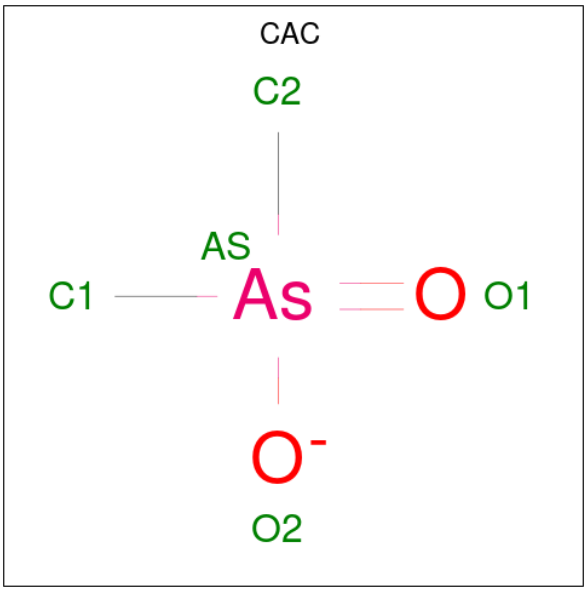
Chain	Residue	Modelled	Actual	Comment	Reference
A	731	VAL	GLY	SEE REMARK 999	UNP Q54873
A	893	HIS	-	expression tag	UNP Q54873
A	894	HIS	-	expression tag	UNP Q54873
A	895	HIS	-	expression tag	UNP Q54873
A	896	HIS	-	expression tag	UNP Q54873
A	897	HIS	-	expression tag	UNP Q54873
A	898	HIS	-	expression tag	UNP Q54873

- Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1 -3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			26	14	1	11			
2	C	2	Total	C	N	O	0	0	0
			26	14	1	11			

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total As C O 5 1 2 2	0	0
3	A	1	Total As C O 5 1 2 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Na 2 2	0	0

- Molecule 5 is water.

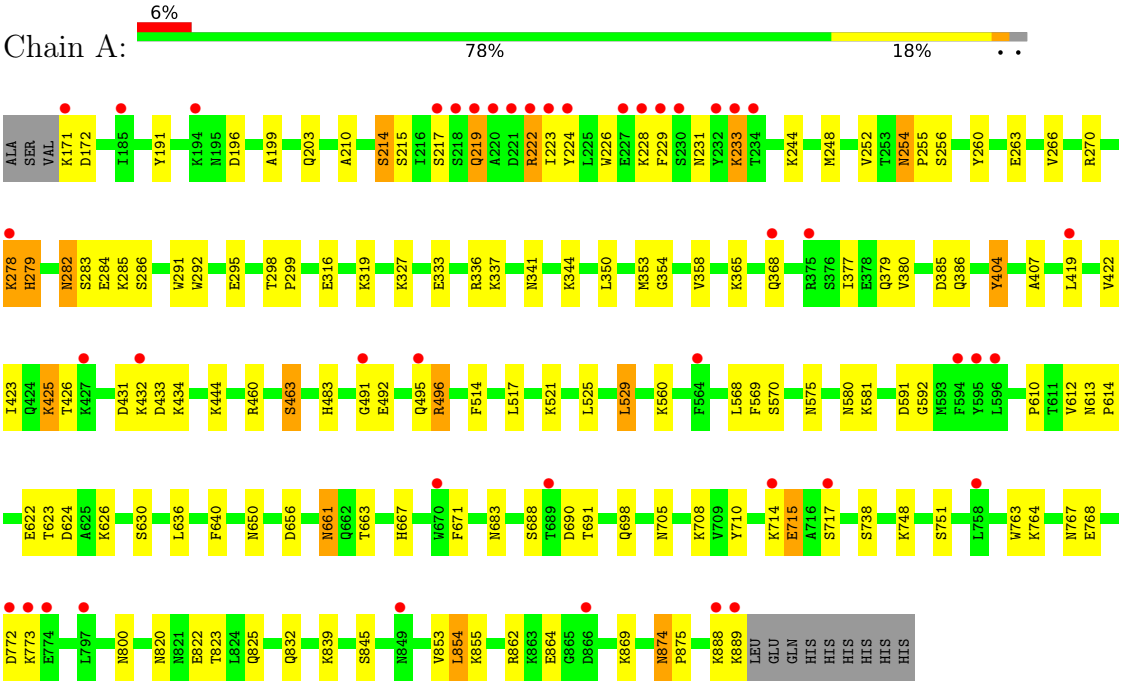
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	573	Total O 573 573	0	0

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: HYALURONATE LYASE

Chain A:

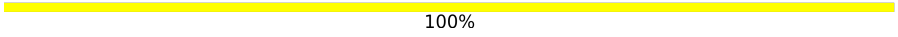


• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.55Å 104.19Å 99.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.70 36.15 – 1.70	Depositor EDS
% Data completeness (in resolution range)	90.2 (40.00-1.70) 90.2 (36.15-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.22 (at 1.70Å)	Xtriage
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.215 , 0.257 0.205 , 0.239	Depositor DCC
R_{free} test set	2870 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6407	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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, NA, CAC, GCD

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	0.36	0/5889	0.61	0/7953

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5770	0	5586	111	0
2	B	26	0	19	1	0
2	C	26	0	19	0	0
3	A	10	0	0	1	0
4	A	2	0	0	0	0
5	A	573	0	0	11	0
All	All	6407	0	5624	111	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 10.

All (111) 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:219:GLN:HB3	1:A:222:ARG:HB3	1.42	1.02
1:A:613:ASN:H	1:A:698:GLN:HE22	1.09	0.98
1:A:222:ARG:HG3	1:A:223:ILE:N	1.80	0.95
1:A:219:GLN:CB	1:A:222:ARG:HB3	2.04	0.87
1:A:560:LYS:HD3	5:A:1165:HOH:O	1.74	0.87
1:A:862:ARG:HD3	1:A:864:GLU:OE1	1.81	0.81
1:A:266:VAL:O	1:A:270:ARG:HG3	1.83	0.77
1:A:283:SER:O	1:A:327:LYS:HE3	1.85	0.77
1:A:219:GLN:NE2	1:A:222:ARG:H	1.86	0.73
1:A:650:ASN:HD21	1:A:832:GLN:HE22	1.36	0.72
1:A:222:ARG:HG3	1:A:224:TYR:H	1.57	0.69
1:A:327:LYS:HE2	5:A:1331:HOH:O	1.91	0.69
1:A:229:PHE:HE2	1:A:244:LYS:HE3	1.58	0.66
1:A:219:GLN:HB2	1:A:222:ARG:H	1.60	0.66
1:A:217:SER:O	1:A:219:GLN:HG3	1.97	0.65
1:A:217:SER:HB2	1:A:219:GLN:HG2	1.78	0.65
1:A:820:ASN:HD22	1:A:825:GLN:HG2	1.60	0.65
1:A:425:LYS:HD2	5:A:1223:HOH:O	1.98	0.64
1:A:613:ASN:N	1:A:698:GLN:HE22	1.90	0.63
1:A:219:GLN:NE2	1:A:222:ARG:N	2.46	0.63
1:A:521:LYS:HE3	1:A:525:LEU:HG	1.81	0.63
1:A:630:SER:H	3:A:907:CAC:C1	2.13	0.61
1:A:705:ASN:HB3	5:A:1173:HOH:O	2.01	0.61
1:A:422:VAL:HA	5:A:1224:HOH:O	2.01	0.60
1:A:219:GLN:HE21	1:A:222:ARG:N	2.00	0.60
1:A:282:ASN:ND2	1:A:285:LYS:HG2	2.17	0.60
1:A:254:ASN:ND2	1:A:256:SER:H	2.00	0.59
1:A:254:ASN:C	1:A:254:ASN:HD22	2.06	0.59
1:A:708:LYS:HE3	1:A:710:TYR:OH	2.03	0.58
1:A:581:LYS:HB3	1:A:768:GLU:HB2	1.85	0.58
1:A:219:GLN:HE21	1:A:222:ARG:H	1.51	0.57
1:A:492:GLU:O	1:A:496:ARG:HB3	2.04	0.57
1:A:764:LYS:HA	1:A:767:ASN:O	2.06	0.56
1:A:217:SER:C	1:A:219:GLN:H	2.09	0.56
1:A:222:ARG:HG2	1:A:224:TYR:O	2.07	0.55
1:A:354:GLY:HA3	1:A:377:ILE:HD11	1.88	0.55
1:A:341:ASN:N	1:A:341:ASN:OD1	2.40	0.54
1:A:431:ASP:HB2	1:A:434:LYS:HG3	1.90	0.54
1:A:845:SER:HB2	1:A:853:VAL:HG23	1.89	0.53
1:A:222:ARG:HG3	1:A:223:ILE:H	1.70	0.53
1:A:233:LYS:HB2	1:A:233:LYS:NZ	2.24	0.53
1:A:460:ARG:O	1:A:463:SER:HB2	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:SER:HG	1:A:226:TRP:HD1	1.57	0.52
1:A:282:ASN:HD21	1:A:285:LYS:HG2	1.74	0.52
1:A:822:GLU:HG2	1:A:823:THR:HG23	1.90	0.52
1:A:386:GLN:NE2	5:A:1555:HOH:O	2.42	0.52
1:A:344:LYS:HE3	1:A:379:GLN:OE1	2.10	0.51
1:A:222:ARG:CG	1:A:224:TYR:H	2.22	0.51
1:A:874:ASN:C	1:A:874:ASN:HD22	2.14	0.51
1:A:278:LYS:HA	1:A:278:LYS:NZ	2.26	0.51
1:A:683:ASN:ND2	5:A:1065:HOH:O	2.38	0.50
1:A:661:ASN:C	1:A:661:ASN:HD22	2.14	0.50
1:A:613:ASN:H	1:A:698:GLN:NE2	1.93	0.50
1:A:624:ASP:OD1	1:A:690:ASP:HB3	2.10	0.50
1:A:278:LYS:HA	1:A:278:LYS:HZ3	1.76	0.50
1:A:336:ARG:NH1	1:A:341:ASN:O	2.44	0.49
1:A:229:PHE:CE2	1:A:244:LYS:HE3	2.44	0.49
1:A:354:GLY:O	1:A:358:VAL:HB	2.12	0.49
1:A:610:PRO:HG3	1:A:763:TRP:CE2	2.47	0.49
1:A:172:ASP:OD1	1:A:365:LYS:NZ	2.45	0.49
1:A:217:SER:OG	1:A:222:ARG:NH2	2.43	0.48
1:A:354:GLY:CA	1:A:377:ILE:HD11	2.44	0.48
1:A:650:ASN:HD21	1:A:832:GLN:NE2	2.09	0.47
1:A:483:HIS:NE2	1:A:529:LEU:HG	2.28	0.47
1:A:491:GLY:O	1:A:495:GLN:HG3	2.13	0.47
1:A:210:ALA:O	1:A:214:SER:HB3	2.14	0.47
1:A:219:GLN:HB2	1:A:222:ARG:N	2.26	0.47
1:A:854:LEU:O	1:A:855:LYS:HD3	2.14	0.46
1:A:219:GLN:HG3	1:A:219:GLN:H	1.48	0.46
1:A:233:LYS:HB2	1:A:233:LYS:HZ3	1.80	0.46
1:A:191:TYR:OH	1:A:199:ALA:HA	2.15	0.46
1:A:254:ASN:ND2	1:A:254:ASN:C	2.68	0.46
1:A:661:ASN:ND2	1:A:663:THR:OG1	2.47	0.46
1:A:222:ARG:HG3	1:A:224:TYR:N	2.28	0.45
1:A:640:PHE:CD1	1:A:875:PRO:HG2	2.52	0.45
1:A:248:MET:O	1:A:252:VAL:HG23	2.17	0.45
1:A:570:SER:HA	1:A:636:LEU:HB3	1.99	0.45
1:A:316:GLU:H	1:A:316:GLU:CD	2.19	0.44
1:A:521:LYS:HA	1:A:521:LYS:HD2	1.79	0.44
1:A:568:LEU:HD23	1:A:592:GLY:HA2	2.00	0.44
1:A:663:THR:HB	1:A:688:SER:HB3	2.00	0.44
1:A:298:THR:HB	1:A:299:PRO:HD3	1.99	0.44
1:A:350:LEU:O	1:A:353:MET:HB3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:LYS:HD2	1:A:853:VAL:HG23	2.00	0.43
1:A:623:THR:HA	1:A:691:THR:O	2.18	0.43
1:A:278:LYS:HG2	1:A:279:HIS:NE2	2.33	0.43
1:A:714:LYS:NZ	5:A:1587:HOH:O	2.50	0.43
1:A:292:TRP:CD2	2:B:1:NAG:H5	2.54	0.43
1:A:419:LEU:HB3	1:A:423:ILE:HD12	2.00	0.43
1:A:671:PHE:CD1	1:A:671:PHE:N	2.86	0.43
1:A:282:ASN:HD22	1:A:284:GLU:H	1.66	0.42
1:A:708:LYS:NZ	1:A:715:GLU:HG3	2.34	0.42
1:A:404:TYR:CD1	1:A:407:ALA:HB3	2.54	0.42
1:A:229:PHE:HE2	1:A:244:LYS:CE	2.29	0.42
1:A:217:SER:CB	1:A:222:ARG:HE	2.32	0.42
1:A:667:HIS:HD2	5:A:1052:HOH:O	2.01	0.42
1:A:514:PHE:CD1	1:A:517:LEU:HD12	2.54	0.42
1:A:580:ASN:O	1:A:581:LYS:HB2	2.20	0.42
1:A:203:GLN:HG3	5:A:1245:HOH:O	2.19	0.42
1:A:422:VAL:O	1:A:426:THR:HG23	2.20	0.41
1:A:708:LYS:HZ3	1:A:715:GLU:HG3	1.84	0.41
1:A:764:LYS:HD2	1:A:772:ASP:HB3	2.03	0.41
1:A:612:VAL:O	1:A:614:PRO:HD3	2.21	0.41
1:A:640:PHE:HB3	1:A:656:ASP:HB2	2.03	0.41
1:A:569:PHE:CE2	1:A:575:ASN:HB3	2.55	0.41
1:A:591:ASP:OD2	1:A:622:GLU:OE2	2.39	0.41
1:A:255:PRO:HA	1:A:260:TYR:CG	2.56	0.40
1:A:738:SER:O	1:A:800:ASN:HA	2.21	0.40
1:A:291:TRP:O	1:A:295:GLU:HG3	2.21	0.40
1:A:661:ASN:C	1:A:661:ASN:ND2	2.75	0.40
1:A:244:LYS:HE2	5:A:1724:HOH:O	2.21	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	717/731 (98%)	679 (95%)	37 (5%)	1 (0%)	51 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ASN

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	637/649 (98%)	598 (94%)	39 (6%)	18 5

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	LYS
1	A	196	ASP
1	A	214	SER
1	A	219	GLN
1	A	222	ARG
1	A	228	LYS
1	A	233	LYS
1	A	254	ASN
1	A	263	GLU
1	A	278	LYS
1	A	279	HIS
1	A	282	ASN
1	A	286	SER
1	A	319	LYS
1	A	333	GLU
1	A	337	LYS
1	A	368	GLN
1	A	380	VAL
1	A	385	ASP
1	A	404	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	425	LYS
1	A	432	LYS
1	A	433	ASP
1	A	444	LYS
1	A	463	SER
1	A	496	ARG
1	A	529	LEU
1	A	626	LYS
1	A	661	ASN
1	A	715	GLU
1	A	717	SER
1	A	748	LYS
1	A	751	SER
1	A	773	LYS
1	A	854	LEU
1	A	869	LYS
1	A	874	ASN
1	A	888	LYS
1	A	889	LYS

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	202	ASN
1	A	219	GLN
1	A	237	ASN
1	A	254	ASN
1	A	282	ASN
1	A	349	ASN
1	A	368	GLN
1	A	386	GLN
1	A	418	GLN
1	A	661	ASN
1	A	667	HIS
1	A	698	GLN
1	A	788	GLN
1	A	820	ASN
1	A	825	GLN
1	A	832	GLN
1	A	874	ASN

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)

4 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	2	15,15,15	1.81	4 (26%)	21,21,21	1.05	2 (9%)
2	GCD	B	2	2	10,11,12	3.63	4 (40%)	13,15,17	3.15	6 (46%)
2	NAG	C	1	2	15,15,15	2.72	6 (40%)	21,21,21	0.91	0
2	GCD	C	2	2	10,11,12	3.99	7 (70%)	13,15,17	3.20	8 (61%)

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	2	-	0/6/26/26	0/1/1/1
2	GCD	B	2	2	-	4/4/17/20	0/1/1/1
2	NAG	C	1	2	-	2/6/26/26	0/1/1/1
2	GCD	C	2	2	-	0/4/17/20	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GCD	O5-C5	9.82	1.51	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	GCD	O5-C5	9.58	1.51	1.37
2	C	1	NAG	C2-N2	5.93	1.55	1.45
2	C	2	GCD	O6A-C6	4.73	1.35	1.22
2	C	1	NAG	C7-N2	4.21	1.48	1.34
2	B	1	NAG	C2-N2	4.08	1.52	1.45
2	C	1	NAG	O5-C1	3.98	1.52	1.42
2	B	2	GCD	O5-C1	3.92	1.51	1.45
2	C	2	GCD	O5-C1	3.58	1.50	1.45
2	C	1	NAG	O5-C5	3.46	1.52	1.44
2	B	2	GCD	C3-C4	3.31	1.54	1.50
2	C	2	GCD	C5-C6	3.21	1.56	1.48
2	B	1	NAG	O5-C1	2.88	1.50	1.42
2	B	1	NAG	O5-C5	2.84	1.51	1.44
2	C	1	NAG	C3-C2	2.81	1.58	1.53
2	B	1	NAG	C7-N2	2.70	1.43	1.34
2	B	2	GCD	O6A-C6	2.54	1.29	1.22
2	C	2	GCD	O2-C2	2.51	1.48	1.43
2	C	2	GCD	O6B-C6	-2.47	1.23	1.30
2	C	1	NAG	O1-C1	2.40	1.47	1.39
2	C	2	GCD	C1-C2	2.03	1.56	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	GCD	O5-C5-C4	-6.96	118.93	124.81
2	C	2	GCD	C2-C3-C4	6.38	121.04	112.32
2	B	2	GCD	O3-C3-C4	4.95	120.46	109.31
2	C	2	GCD	C3-C4-C5	-4.63	113.77	121.60
2	C	2	GCD	C1-C2-C3	-4.44	104.20	109.67
2	B	2	GCD	C2-C3-C4	4.24	118.11	112.32
2	C	2	GCD	O6B-C6-O6A	4.14	133.09	123.61
2	B	2	GCD	C1-C2-C3	-3.25	105.67	109.67
2	B	2	GCD	O5-C5-C6	3.19	116.31	111.52
2	B	2	GCD	O6B-C6-O6A	3.02	130.52	123.61
2	C	2	GCD	O2-C2-C1	2.97	115.24	109.15
2	C	2	GCD	O3-C3-C2	-2.94	104.31	109.42
2	C	2	GCD	O5-C5-C4	2.54	126.96	124.81
2	C	2	GCD	O6B-C6-C5	-2.48	108.02	114.20
2	B	1	NAG	C2-N2-C7	-2.12	118.02	123.18
2	B	1	NAG	C8-C7-N2	-2.04	112.65	116.10

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	GCD	O5-C5-C6-O6B
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	B	2	GCD	O5-C5-C6-O6A
2	B	2	GCD	C4-C5-C6-O6B
2	B	2	GCD	C4-C5-C6-O6A

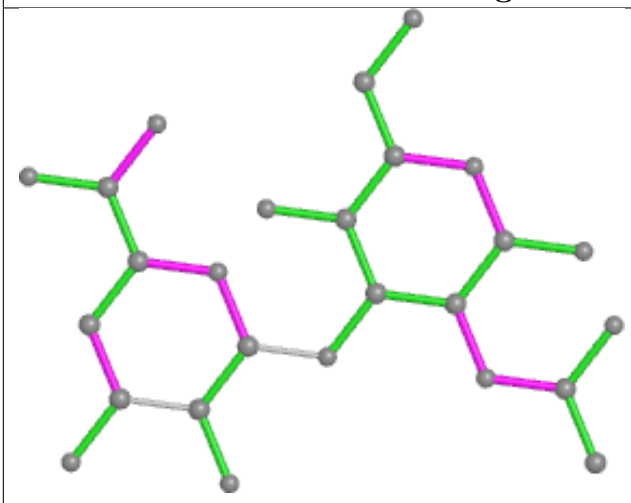
There are no ring outliers.

1 monomer is involved in 1 short contact:

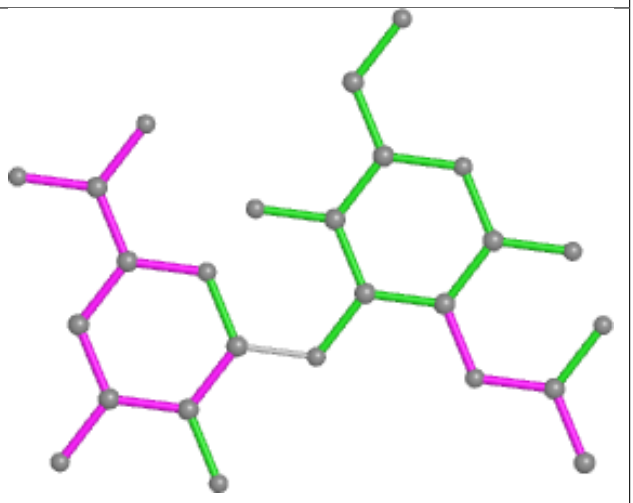
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0

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

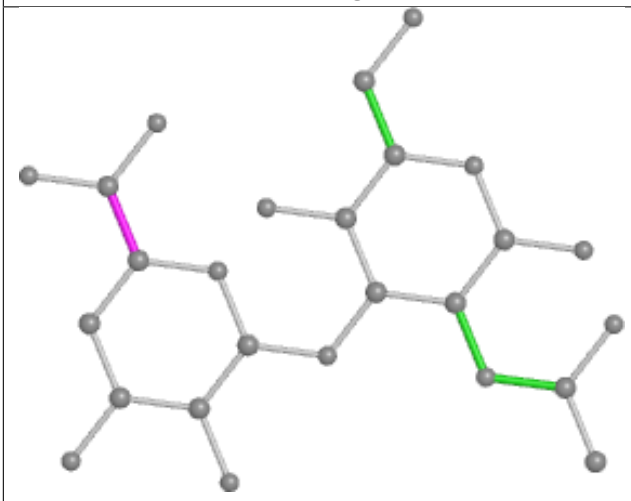
Oligosaccharide Chain B



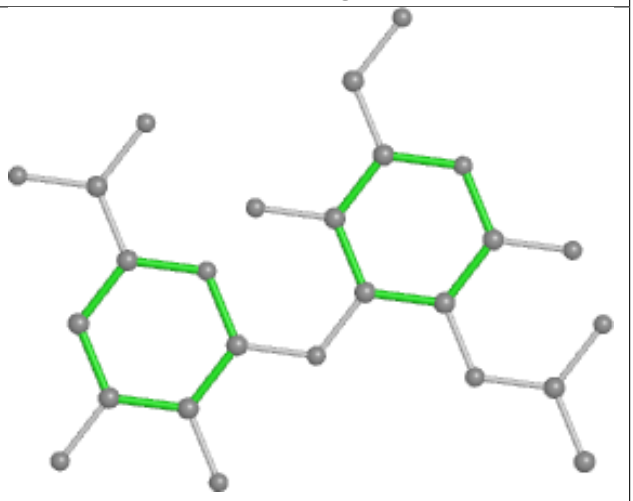
Bond lengths



Bond angles

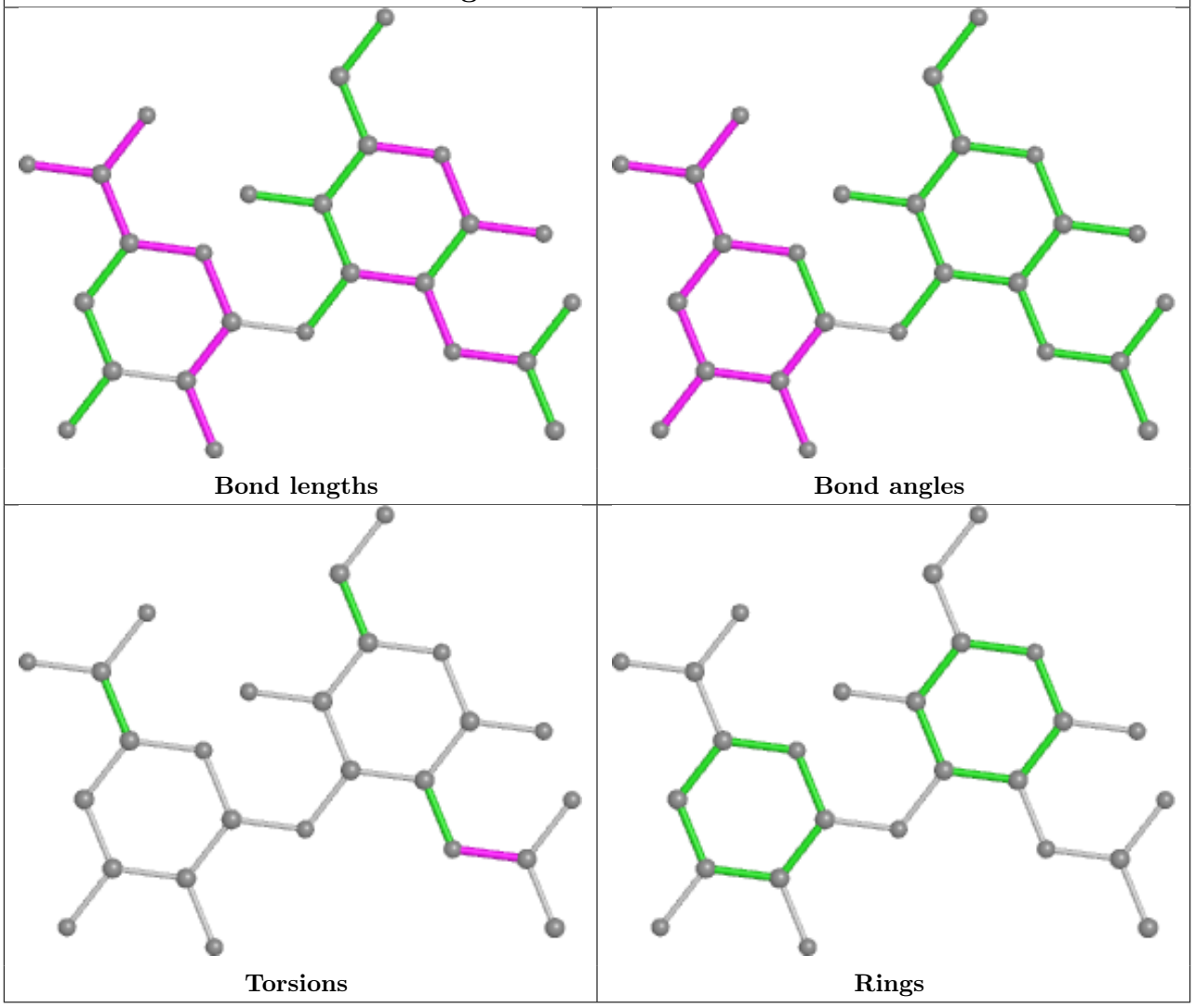


Torsions



Rings

Oligosaccharide Chain C



5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CAC	A	905	4	0,4,4	-	-	0,6,6	-	-
3	CAC	A	907	4	0,4,4	-	-	0,6,6	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	907	CAC	1	0

5.7 Other polymers

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, 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	719/731 (98%)	0.31	43 (5%)	21	24	16, 26, 47, 79	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	GLN	7.3
1	A	221	ASP	6.8
1	A	223	ILE	6.3
1	A	222	ARG	5.4
1	A	224	TYR	4.8
1	A	427	LYS	4.4
1	A	866	ASP	3.6
1	A	233	LYS	3.5
1	A	491	GLY	3.5
1	A	218	SER	3.4
1	A	432	LYS	3.4
1	A	594	PHE	3.4
1	A	220	ALA	3.2
1	A	230	SER	3.2
1	A	229	PHE	3.0
1	A	689	THR	2.9
1	A	232	TYR	2.9
1	A	797	LEU	2.8
1	A	185	ILE	2.7
1	A	596	LEU	2.7
1	A	171	LYS	2.7
1	A	773	LYS	2.7
1	A	234	THR	2.6
1	A	217	SER	2.5
1	A	368	GLN	2.5
1	A	849	ASN	2.4
1	A	758	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	717	SER	2.4
1	A	375	ARG	2.3
1	A	595	TYR	2.3
1	A	564	PHE	2.3
1	A	889	LYS	2.3
1	A	194	LYS	2.3
1	A	228	LYS	2.3
1	A	227	GLU	2.3
1	A	495	GLN	2.2
1	A	774	GLU	2.2
1	A	714	LYS	2.2
1	A	772	ASP	2.1
1	A	278	LYS	2.1
1	A	888	LYS	2.0
1	A	670	TRP	2.0
1	A	419	LEU	2.0

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

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

6.3 Carbohydrates (i)

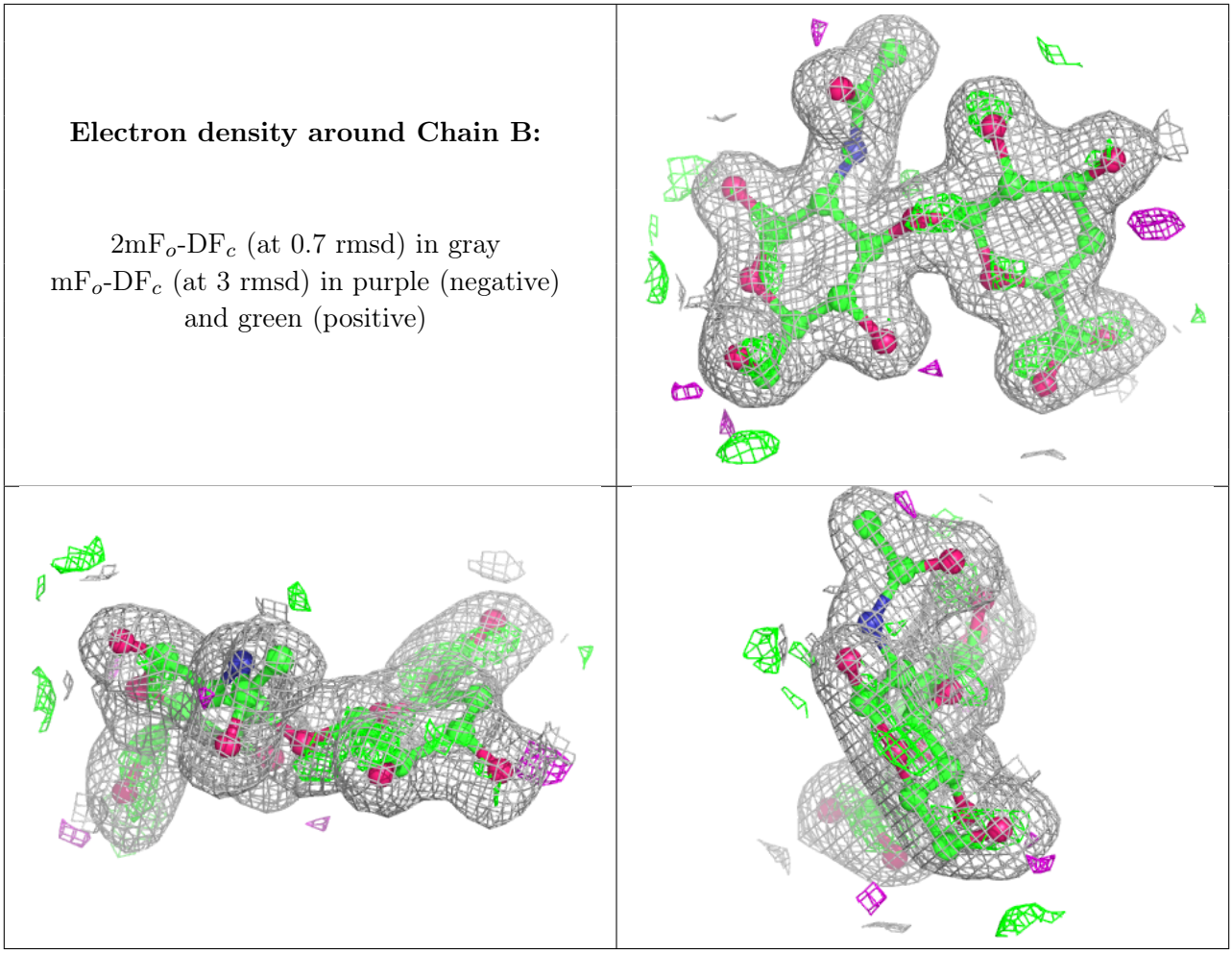
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	NAG	C	1	15/15	0.64	0.29	33,44,48,51	0
2	GCD	C	2	11/12	0.85	0.14	41,43,44,45	0
2	GCD	B	2	11/12	0.90	0.23	33,39,44,46	0
2	NAG	B	1	15/15	0.94	0.17	20,36,41,41	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.

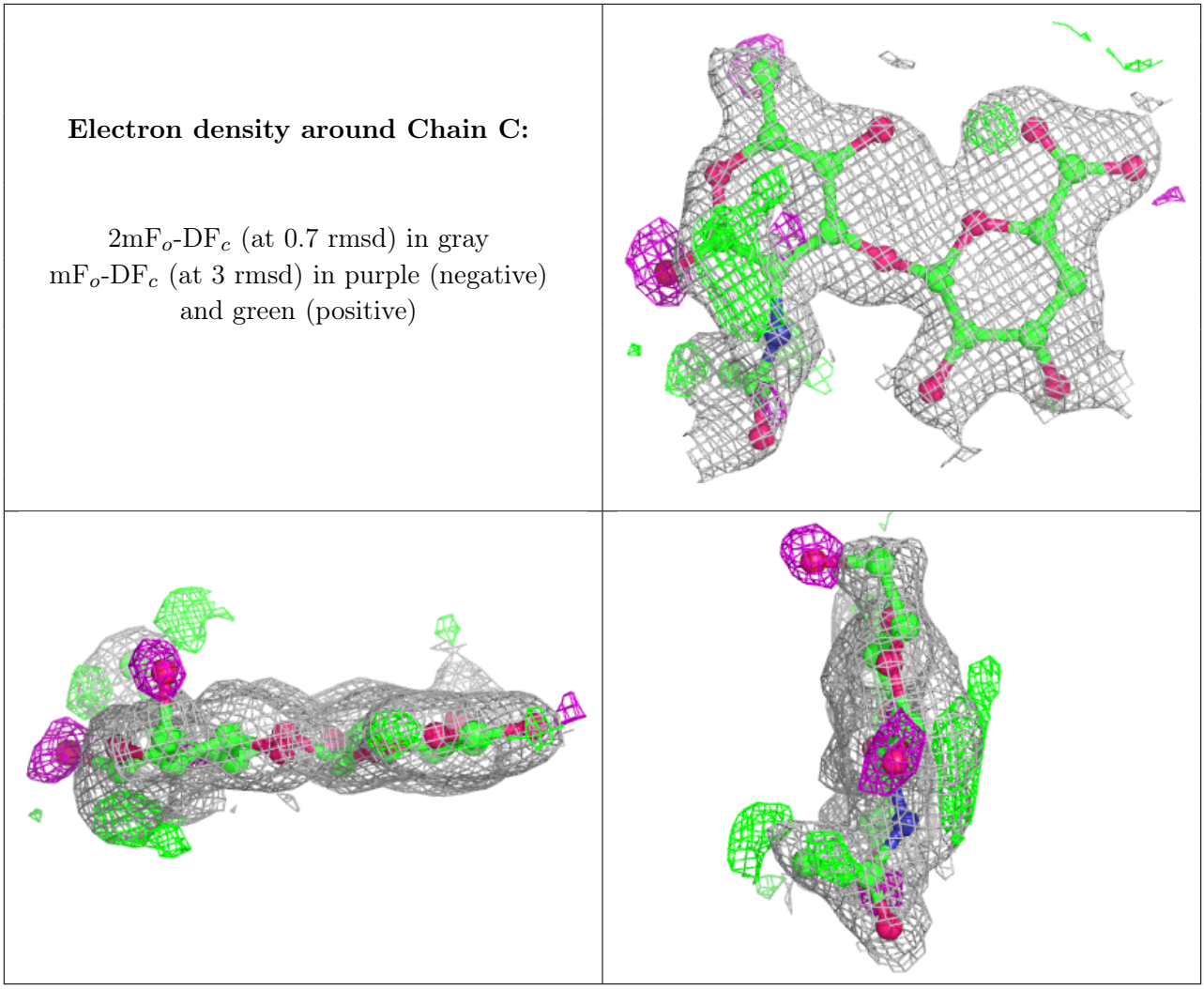
Electron density around Chain B:

$2mF_o$-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	NA	A	906	1/1	0.79	0.57	20,20,20,20	0
4	NA	A	908	1/1	0.88	0.55	20,20,20,20	0
3	CAC	A	907	5/5	0.92	0.34	39,40,41,42	0
3	CAC	A	905	5/5	0.96	0.32	39,40,41,42	0

6.5 Other polymers

There are no such residues in this entry.