Full wwPDB X-ray Structure Validation Report (i)

Mar 29, 2023 – 04:31 pm BST

PDB ID	:	8CEM
Title	:	Structure of bovine native C3, re-refinement
Authors	:	Andersen, G.R.; Fredslund, F.
Deposited on	:	2023-02-02
Resolution	:	3.00 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 (1)) were used in the production of this report:

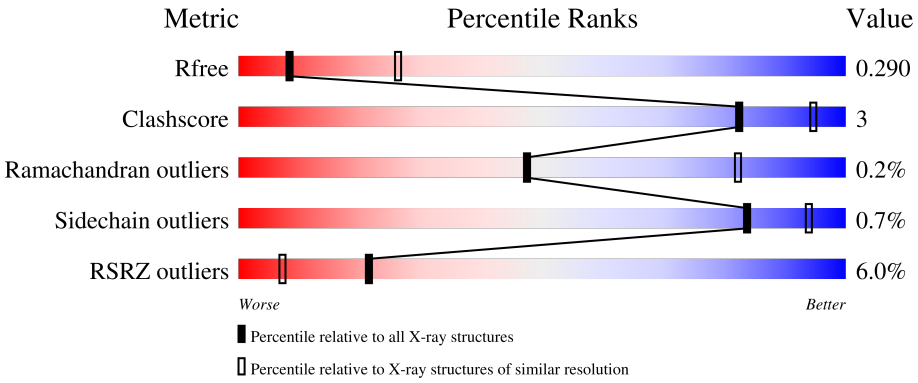
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	E	643	12% 90% 9%
1	F	643	6% 93% 6%
2	A	992	3% 89% 9%
2	B	992	5% 90% 8%
3	C	3	100%

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Mol	Chain	Length	Quality of chain
3	D	3	33% 67%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25695 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.

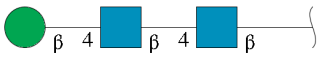
- Molecule 1 is a protein called Complement C3 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	640	Total	C	N	O	S	0	0	0
			5012	3185	861	953	13			
1	F	639	Total	C	N	O	S	0	0	0
			5005	3180	860	952	13			

- Molecule 2 is a protein called Complement C3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	975	Total	C	N	O	S	0	0	0
			7804	4938	1331	1492	43			
2	B	974	Total	C	N	O	S	0	0	0
			7796	4932	1330	1491	43			

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



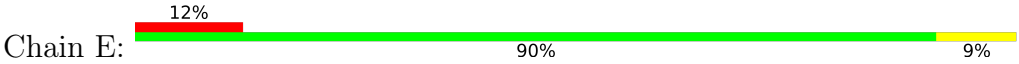
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

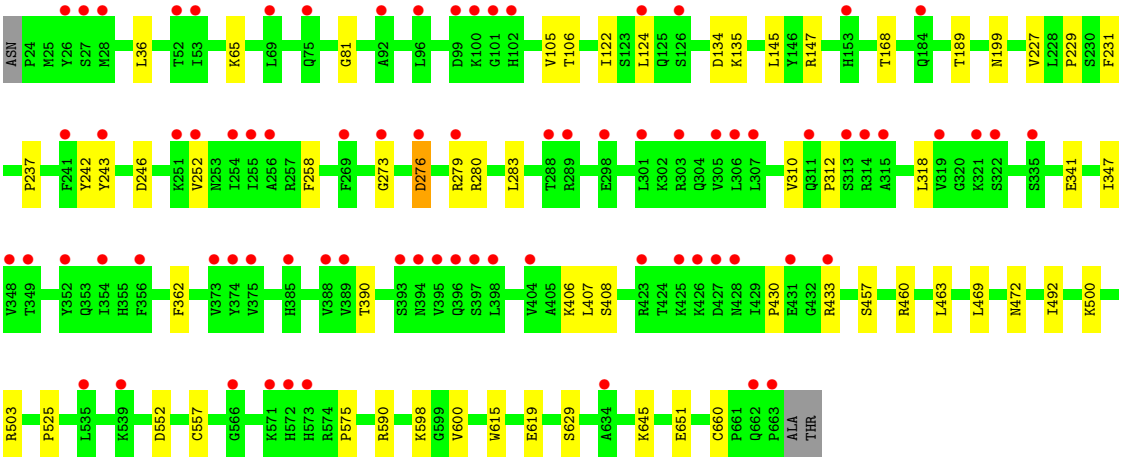
3 Residue-property plots (i)

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: Complement C3 beta chain

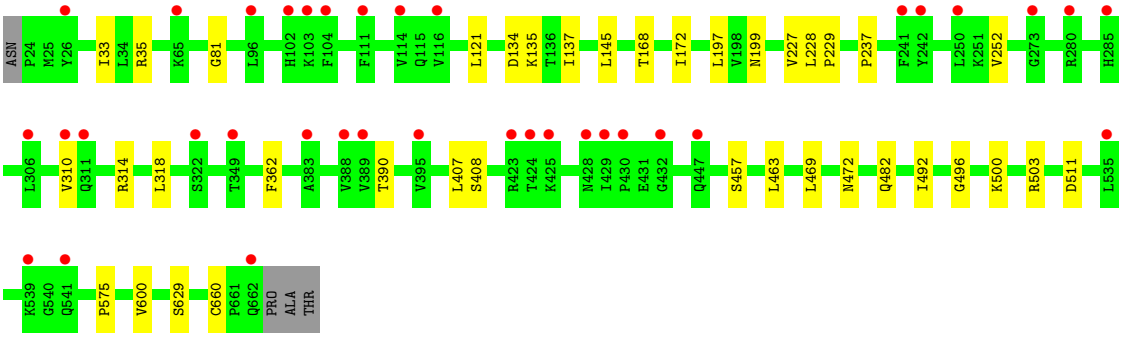
Chain E:





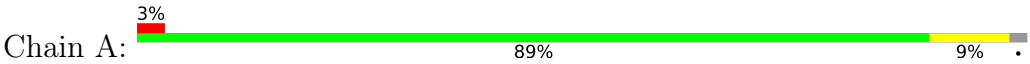
• Molecule 1: Complement C3 beta chain

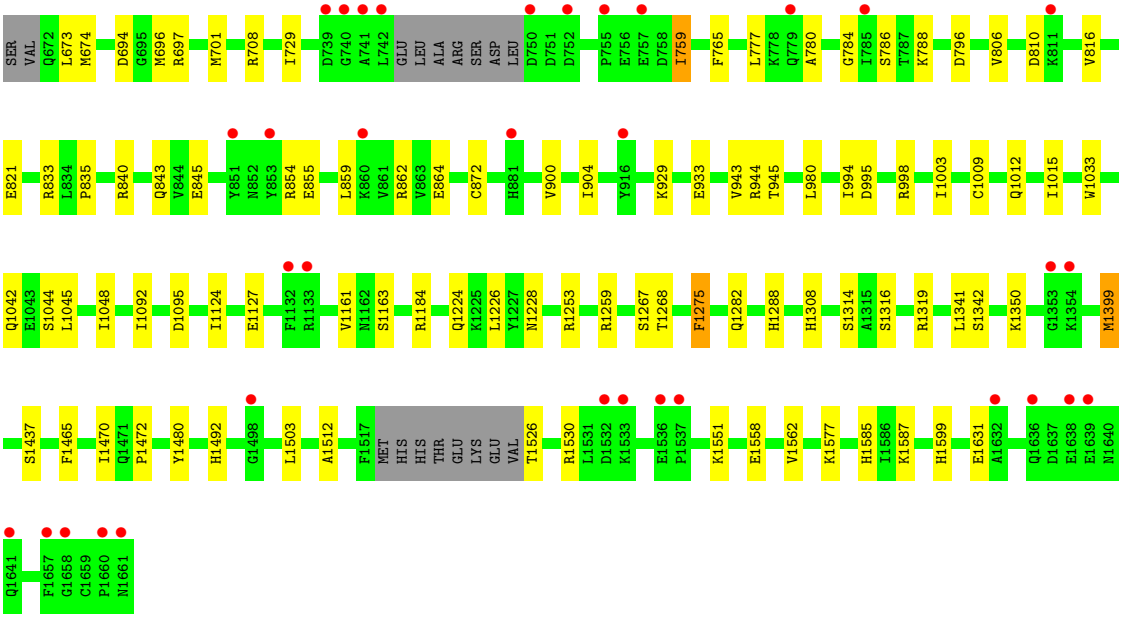
Chain F:



• Molecule 2: Complement C3 alpha chain

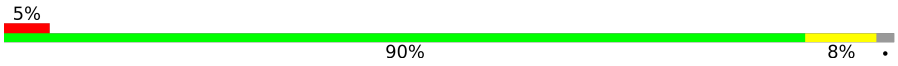
Chain A:

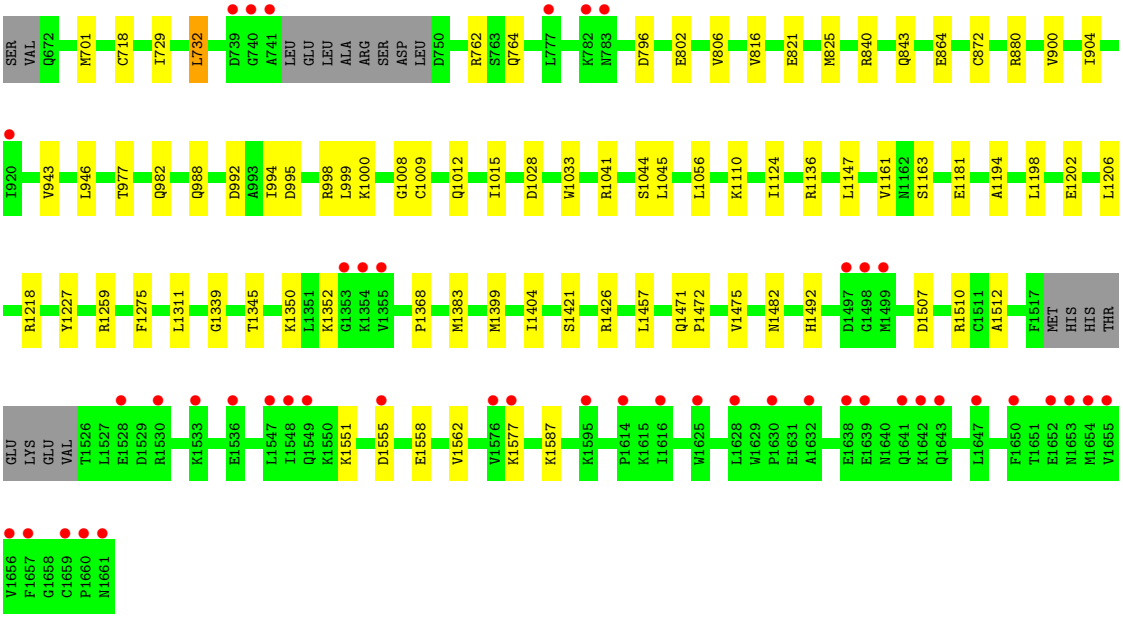




• Molecule 2: Complement C3 alpha chain

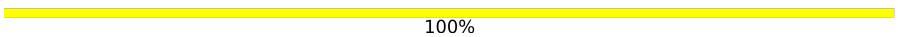
Chain B:





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

Chain C:



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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	254.25Å 246.86Å 113.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.85 – 3.00 37.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (37.85-3.00) 97.2 (37.85-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.259 , 0.284 0.263 , 0.290	Depositor DCC
R_{free} test set	1392 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	68.4	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	25695	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.36% 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: BMA, 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	E	0.32	0/5113	0.61	1/6945 (0.0%)
1	F	0.31	0/5105	0.60	1/6933 (0.0%)
2	A	0.36	0/7953	0.68	4/10749 (0.0%)
2	B	0.36	0/7945	0.68	6/10738 (0.1%)
All	All	0.34	0/26116	0.65	12/35365 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	276	ASP	CB-CG-OD1	6.43	124.09	118.30
2	A	1480	TYR	CB-CG-CD2	6.37	124.83	121.00
2	B	732	LEU	CA-CB-CG	6.30	129.80	115.30
2	A	1470	ILE	C-N-CA	6.29	137.43	121.70
2	B	1275	PHE	CB-CG-CD1	5.53	124.67	120.80
2	A	1275	PHE	CB-CG-CD1	5.34	124.54	120.80
2	B	999	LEU	CA-CB-CG	5.29	127.47	115.30
2	B	1457	LEU	CA-CB-CG	5.06	126.93	115.30
2	A	1095	ASP	CB-CG-OD1	5.05	122.85	118.30
2	B	1352	LYS	CA-CB-CG	5.03	124.47	113.40
2	B	1311	LEU	CA-CB-CG	5.00	126.81	115.30
1	F	228	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

There are no planarity outliers.

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	E	5012	0	5071	32	0
1	F	5005	0	5064	20	0
2	A	7804	0	7756	47	0
2	B	7796	0	7745	39	0
3	C	39	0	34	0	0
3	D	39	0	34	0	0
All	All	25695	0	25704	130	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 3.

All (130) 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:E:135:LYS:HB2	1:E:600:VAL:HG11	1.63	0.81
2:B:1041:ARG:O	2:B:1045:LEU:HD23	1.96	0.65
1:F:135:LYS:HB2	1:F:600:VAL:HG11	1.82	0.60
2:A:854:ARG:HH11	2:A:859:LEU:HD21	1.67	0.60
2:A:994:ILE:HG23	2:A:1044:SER:HB3	1.85	0.59
1:F:227:VAL:HG12	1:F:229:PRO:HD3	1.85	0.58
1:F:310:VAL:HG21	1:F:318:LEU:HD21	1.85	0.58
1:F:575:PRO:HB3	2:B:796:ASP:HA	1.84	0.58
1:E:575:PRO:HB3	2:A:796:ASP:HA	1.84	0.58
1:E:310:VAL:HG21	1:E:318:LEU:HD21	1.86	0.58
1:E:457:SER:HB3	1:E:472:ASN:HB2	1.85	0.57
2:B:1136:ARG:HG2	2:B:1181:GLU:HB3	1.84	0.57
2:B:994:ILE:HG23	2:B:1044:SER:HB3	1.86	0.57
2:A:1512:ALA:HB1	2:A:1587:LYS:HE2	1.87	0.57
2:B:843:GLN:HG3	2:B:900:VAL:HG22	1.86	0.56
2:A:862:ARG:NH2	2:A:864:GLU:OE2	2.36	0.56
1:E:341:GLU:HB2	2:A:759:ILE:HG13	1.88	0.56
2:A:843:GLN:HG3	2:A:900:VAL:HG22	1.88	0.55
2:A:980:LEU:HB3	2:A:1342:SER:HB2	1.90	0.54
2:B:992:ASP:HB2	2:B:998:ARG:HB3	1.89	0.54
1:E:65:LYS:HE2	1:E:106:THR:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1472:PRO:HB3	2:A:1492:HIS:HB2	1.89	0.54
2:A:777:LEU:HD22	2:A:786:SER:HB3	1.89	0.53
2:A:1267:SER:OG	2:A:1268:THR:N	2.41	0.53
2:A:1526:THR:O	2:A:1530:ARG:NH1	2.41	0.53
2:A:1551:LYS:HB2	2:A:1558:GLU:HB2	1.89	0.53
1:E:36:LEU:HB2	1:E:124:LEU:HG	1.90	0.53
2:B:872:CYS:HB3	2:B:900:VAL:HB	1.89	0.53
1:F:137:ILE:HG22	1:F:600:VAL:HG13	1.90	0.53
1:E:227:VAL:HG12	1:E:229:PRO:HD3	1.91	0.53
2:B:1350:LYS:HE2	2:B:1555:ASP:HB2	1.90	0.53
2:B:1471:GLN:NE2	2:B:1555:ASP:OD1	2.42	0.53
1:E:430:PRO:HD2	1:E:433:ARG:HD2	1.91	0.52
2:B:1472:PRO:HB3	2:B:1492:HIS:HB2	1.90	0.52
2:B:762:ARG:NH1	2:B:764:GLN:O	2.43	0.52
2:B:943:VAL:HG21	2:B:1259:ARG:HB2	1.91	0.52
2:B:1124:ILE:HG23	2:B:1399:MET:HG3	1.92	0.52
1:E:645:LYS:NZ	1:E:651:GLU:OE1	2.40	0.51
1:F:457:SER:HB3	1:F:472:ASN:HB2	1.91	0.51
1:F:81:GLY:O	1:F:503:ARG:NH1	2.44	0.51
2:A:845:GLU:HB2	2:A:1503:LEU:HD21	1.93	0.51
2:B:1551:LYS:HB2	2:B:1558:GLU:HB2	1.93	0.50
1:F:362:PHE:HB2	1:F:629:SER:HB3	1.94	0.50
2:A:943:VAL:HG21	2:A:1259:ARG:HB2	1.93	0.50
1:F:168:THR:HB	1:F:199:ASN:HD22	1.76	0.50
2:A:777:LEU:HD21	2:A:788:LYS:HB2	1.94	0.49
1:E:81:GLY:O	1:E:503:ARG:NH1	2.45	0.49
2:A:1562:VAL:HG13	2:A:1577:LYS:HA	1.93	0.49
2:B:1421:SER:O	2:B:1426:ARG:NH2	2.42	0.49
1:F:237:PRO:HA	1:F:252:VAL:HA	1.95	0.49
2:B:1000:LYS:HA	2:B:1015:ILE:HD11	1.94	0.49
2:B:1202:GLU:HA	2:B:1206:LEU:HD12	1.95	0.49
2:A:929:LYS:NZ	2:A:1437:SER:O	2.46	0.49
2:A:1124:ILE:HG23	2:A:1399:MET:HG3	1.94	0.48
2:B:946:LEU:O	2:B:1339:GLY:N	2.46	0.48
1:E:105:VAL:HG13	1:E:122:ILE:HD13	1.94	0.48
2:A:945:THR:HG21	2:A:1253:ARG:HG2	1.95	0.48
2:B:995:ASP:HB3	2:B:998:ARG:HB2	1.95	0.48
1:E:237:PRO:HA	1:E:252:VAL:HA	1.97	0.47
1:F:197:LEU:HD11	2:B:1008:GLY:HA2	1.96	0.47
1:E:590:ARG:NH2	2:A:810:ASP:OD1	2.47	0.47
1:F:35:ARG:HH22	1:F:496:GLY:HA3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1042:GLN:HA	2:A:1045:LEU:HD12	1.95	0.47
2:B:1147:LEU:HD23	2:B:1194:ALA:HB1	1.96	0.47
1:F:134:ASP:HB3	1:F:145:LEU:HB2	1.97	0.47
1:F:172:ILE:HD13	2:B:1056:LEU:HD12	1.97	0.46
2:A:696:MET:HA	2:A:729:ILE:HD11	1.96	0.46
1:F:390:THR:HG23	1:F:407:LEU:HD22	1.98	0.46
1:E:390:THR:HG23	1:E:407:LEU:HD22	1.96	0.46
2:A:806:VAL:HG22	2:A:816:VAL:HG22	1.98	0.45
2:A:1127:GLU:OE2	2:A:1184:ARG:NH2	2.49	0.45
1:F:463:LEU:HD11	1:F:469:LEU:HD13	1.98	0.45
1:E:598:LYS:HE3	2:A:821:GLU:OE2	2.15	0.45
1:E:463:LEU:HD11	1:E:469:LEU:HD13	1.99	0.45
2:A:1599:HIS:ND1	2:A:1631:GLU:OE2	2.49	0.45
2:B:701:MET:SD	2:B:701:MET:N	2.89	0.45
1:F:492:ILE:HD12	1:F:500:LYS:HB3	1.98	0.45
1:E:600:VAL:HG22	2:A:765:PHE:CD1	2.51	0.45
2:A:1226:LEU:HD13	2:A:1267:SER:HB3	2.00	0.44
1:F:314:ARG:HD2	1:F:314:ARG:HA	1.73	0.44
2:A:1161:VAL:HG12	2:A:1163:SER:H	1.82	0.44
2:A:1048:ILE:HB	2:A:1092:ILE:HG13	2.00	0.44
2:A:780:ALA:HB1	2:A:784:GLY:HA2	1.99	0.44
2:A:995:ASP:HB3	2:A:998:ARG:HB2	2.00	0.44
2:B:806:VAL:HG22	2:B:816:VAL:HG22	1.99	0.44
2:B:1161:VAL:HG12	2:B:1163:SER:H	1.83	0.44
2:A:1224:GLN:O	2:A:1228:ASN:ND2	2.51	0.44
2:B:864:GLU:OE2	2:B:880:ARG:HD3	2.18	0.44
2:A:673:LEU:HD12	2:A:674:MET:HG3	1.98	0.44
2:A:1282:GLN:HG3	2:A:1288:HIS:HD2	1.82	0.44
1:E:147:ARG:HG2	1:E:189:THR:HA	2.00	0.44
1:E:134:ASP:HB3	1:E:145:LEU:HB2	2.00	0.43
2:A:1003:ILE:HG12	2:A:1268:THR:HG22	1.98	0.43
2:A:840:ARG:HD3	2:A:904:ILE:HG13	2.00	0.43
2:B:982:GLN:OE1	2:B:988:GLN:HB2	2.18	0.43
2:A:835:PRO:HB3	2:A:1465:PHE:HZ	1.84	0.43
2:B:802:GLU:HG3	2:B:821:GLU:HG2	2.00	0.43
2:B:729:ILE:HA	2:B:732:LEU:HB3	2.01	0.43
2:A:694:ASP:HA	2:A:697:ARG:HG3	2.00	0.42
1:F:33:ILE:HG12	1:F:121:LEU:HD23	2.01	0.42
1:E:273:GLY:HA2	1:E:283:LEU:HG	2.01	0.42
2:A:777:LEU:HD23	2:A:777:LEU:HA	1.85	0.42
2:A:944:ARG:HB2	2:A:1341:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:PHE:HA	1:E:258:PHE:HA	2.01	0.42
1:E:406:LYS:HD2	1:E:460:ARG:HB2	2.01	0.42
2:B:1404:ILE:HG23	2:B:1475:VAL:HG22	2.00	0.42
2:A:1308:HIS:HB3	2:A:1319:ARG:HD3	2.01	0.42
2:B:1562:VAL:HG13	2:B:1577:LYS:HA	2.02	0.41
1:E:279:ARG:NH1	1:E:280:ARG:O	2.53	0.41
2:B:977:THR:HA	2:B:1345:THR:HA	2.02	0.41
2:B:1368:PRO:HA	2:B:1383:MET:HG2	2.01	0.41
1:E:242:TYR:HD2	1:E:347:ILE:HG23	1.85	0.41
1:E:525:PRO:HB3	1:E:615:TRP:HB3	2.02	0.41
2:A:872:CYS:HB3	2:A:900:VAL:HB	2.02	0.41
1:E:492:ILE:HD12	1:E:500:LYS:HB3	2.02	0.41
2:A:1003:ILE:HB	2:A:1015:ILE:HD12	2.02	0.41
1:E:243:TYR:HB2	1:E:246:ASP:HB2	2.03	0.41
2:B:1147:LEU:HD11	2:B:1198:LEU:HD11	2.02	0.41
2:A:833:ARG:HA	2:A:833:ARG:HD2	1.91	0.41
2:B:1507:ASP:HA	2:B:1510:ARG:HB3	2.02	0.41
1:E:276:ASP:HB3	1:E:279:ARG:HB3	2.03	0.41
1:E:310:VAL:HG12	1:E:312:PRO:HD2	2.03	0.41
1:E:362:PHE:HB2	1:E:629:SER:HB3	2.03	0.41
1:F:482:GLN:NE2	1:F:511:ASP:OD1	2.51	0.41
1:E:168:THR:HB	1:E:199:ASN:HD22	1.86	0.40
2:A:933:GLU:OE1	2:A:1585:HIS:NE2	2.47	0.40
2:B:840:ARG:HD3	2:B:904:ILE:HG13	2.02	0.40
2:B:1110:LYS:HA	2:B:1110:LYS:HD3	1.90	0.40
2:B:1227:TYR:CE2	2:B:1482:ASN:HB2	2.57	0.40
2:B:1512:ALA:HB1	2:B:1587:LYS:HE2	2.03	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	E	638/643 (99%)	615 (96%)	23 (4%)	0	100 100
1	F	637/643 (99%)	617 (97%)	20 (3%)	0	100 100
2	A	969/992 (98%)	925 (96%)	39 (4%)	5 (0%)	29 68
2	B	968/992 (98%)	933 (96%)	35 (4%)	0	100 100
All	All	3212/3270 (98%)	3090 (96%)	117 (4%)	5 (0%)	47 82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1350	LYS
2	A	759	ILE
2	A	1314	SER
2	A	855	GLU
2	A	1399	MET

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	E	564/566 (100%)	559 (99%)	5 (1%)	78 92
1	F	563/566 (100%)	561 (100%)	2 (0%)	91 97
2	A	861/877 (98%)	854 (99%)	7 (1%)	81 93
2	B	860/877 (98%)	853 (99%)	7 (1%)	81 93
All	All	2848/2886 (99%)	2827 (99%)	21 (1%)	84 94

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	408	SER
1	E	552	ASP
1	E	557	CYS
1	E	619	GLU
1	E	660	CYS
2	A	701	MET

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Mol	Chain	Res	Type
2	A	708	ARG
2	A	1009	CYS
2	A	1012	GLN
2	A	1033	TRP
2	A	1275	PHE
2	A	1316	SER
1	F	408	SER
1	F	660	CYS
2	B	718	CYS
2	B	825	MET
2	B	1009	CYS
2	B	1012	GLN
2	B	1028	ASP
2	B	1033	TRP
2	B	1218	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	672	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	$\#\|Z\|>2$
3	NAG	C	1	3,2	14,14,15	0.35	0	17,19,21	0.94	1 (5%)
3	NAG	C	2	3	14,14,15	0.34	0	17,19,21	0.84	1 (5%)
3	BMA	C	3	3	11,11,12	1.17	1 (9%)	15,15,17	0.97	1 (6%)
3	NAG	D	1	3,2	14,14,15	0.37	0	17,19,21	0.92	0
3	NAG	D	2	3	14,14,15	0.72	1 (7%)	17,19,21	0.63	0
3	BMA	D	3	3	11,11,12	1.13	1 (9%)	15,15,17	1.06	1 (6%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	BMA	C2-C3	2.38	1.56	1.52
3	D	3	BMA	C2-C3	2.27	1.55	1.52
3	D	2	NAG	O5-C1	2.23	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3	BMA	C1-O5-C5	2.95	116.19	112.19
3	C	2	NAG	C1-O5-C5	2.91	116.14	112.19
3	C	1	NAG	O4-C4-C5	-2.62	102.78	109.30
3	C	3	BMA	C1-O5-C5	2.56	115.67	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6

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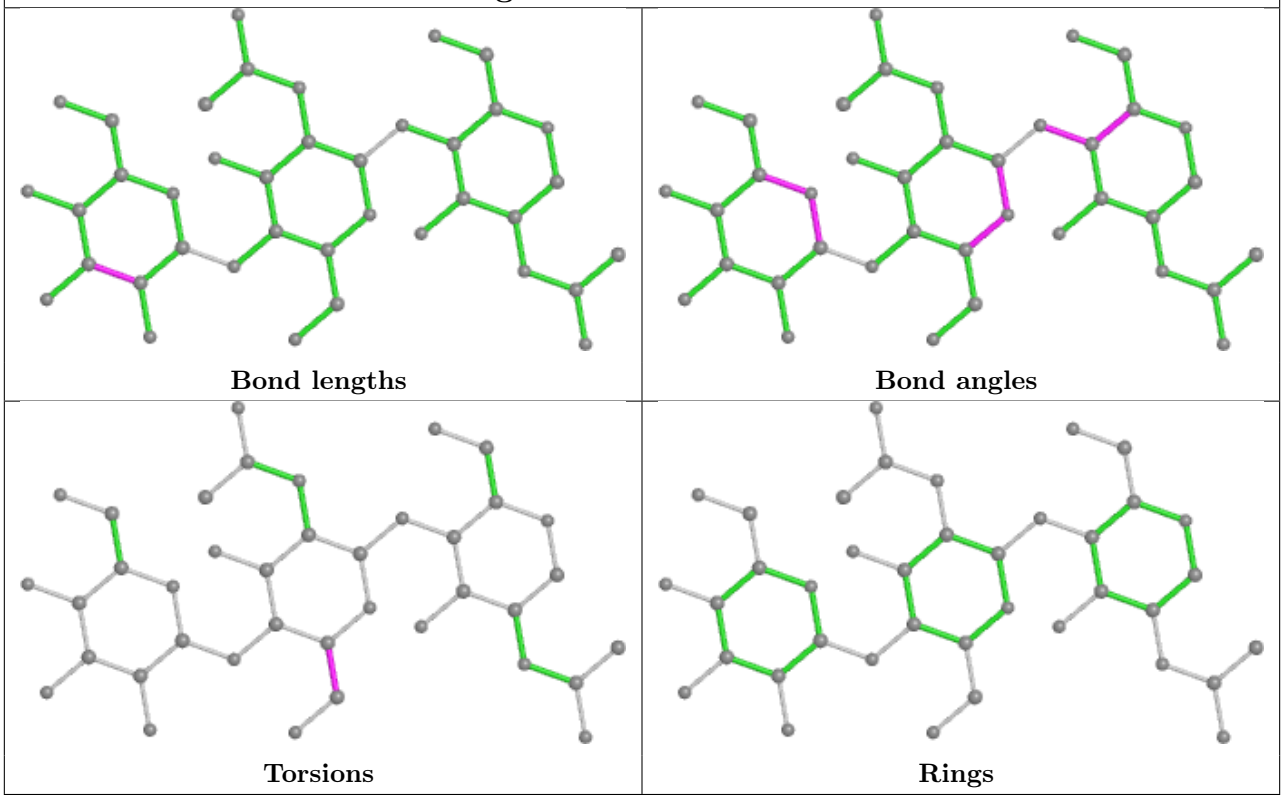
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6

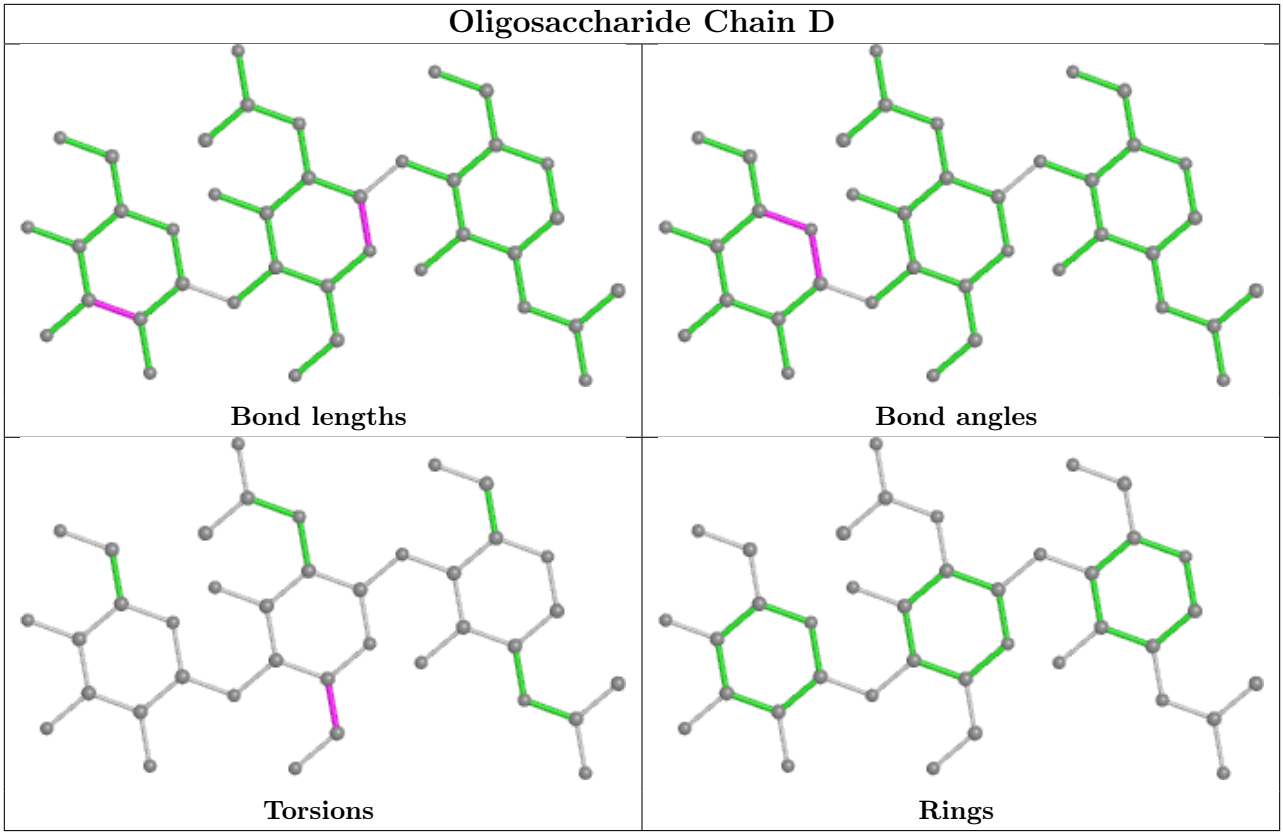
There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry

There are no ligands in this entry.

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	E	640/643 (99%)	0.63	78 (12%) 4 1	68, 146, 198, 230	0
1	F	639/643 (99%)	0.25	36 (5%) 24 8	61, 129, 165, 205	0
2	A	975/992 (98%)	-0.01	34 (3%) 44 18	35, 80, 168, 214	0
2	B	974/992 (98%)	0.01	46 (4%) 31 11	28, 76, 192, 248	0
All	All	3228/3270 (98%)	0.18	194 (6%) 21 7	28, 110, 187, 248	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	663	PRO	6.1
1	E	102	HIS	5.7
2	B	1353	GLY	5.5
2	B	1654	MET	5.2
1	E	395	VAL	5.1
2	A	752	ASP	5.1
2	A	742	LEU	5.0
2	B	1497	ASP	4.9
2	A	741	ALA	4.8
1	E	254	ILE	4.7
1	E	389	VAL	4.7
1	E	398	LEU	4.6
1	E	349	THR	4.6
2	B	1660	PRO	4.5
1	F	662	GLN	4.4
2	B	1577	LYS	4.3
2	A	1354	LYS	4.2
1	E	662	GLN	4.2
1	E	301	LEU	4.2
1	F	310	VAL	4.2
1	E	100	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	423	ARG	4.0
2	B	1659	CYS	4.0
1	E	252	VAL	4.0
1	E	276	ASP	4.0
1	E	307	LEU	4.0
1	E	373	VAL	4.0
1	E	374	TYR	4.0
2	A	1133	ARG	4.0
2	B	1632	ALA	3.9
2	B	1595	LYS	3.8
2	B	1616	ILE	3.8
1	E	289	ARG	3.8
1	E	279	ARG	3.8
2	B	1650	PHE	3.7
1	E	313	SER	3.6
1	F	535	LEU	3.6
2	A	1661	ASN	3.6
1	E	425	LYS	3.6
1	E	306	LEU	3.6
2	B	782	LYS	3.6
1	E	352	TYR	3.5
1	E	256	ALA	3.5
1	E	288	THR	3.4
2	B	1630	PRO	3.4
2	A	757	GLU	3.4
1	E	298	GLU	3.4
2	A	1632	ALA	3.4
1	F	311	GLN	3.4
1	E	385	HIS	3.4
1	E	397	SER	3.4
2	B	1639	GLU	3.4
2	A	740	GLY	3.3
2	A	1657	PHE	3.3
2	A	1353	GLY	3.3
1	E	375	VAL	3.3
1	E	426	LYS	3.2
2	A	750	ASP	3.2
2	A	881	HIS	3.2
2	A	853	TYR	3.1
1	E	428	ASN	3.1
2	A	916	TYR	3.1
2	A	1660	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	1499	MET	3.1
2	A	1536	GLU	3.1
1	E	396	GLN	3.1
2	B	1642	LYS	3.1
1	E	393	SER	3.1
1	E	431	GLU	3.1
2	B	1533	LYS	3.0
2	B	1547	LEU	3.0
2	A	1638	GLU	3.0
2	B	1643	GLN	3.0
2	B	1647	LEU	3.0
1	F	388	VAL	3.0
1	E	303	ARG	3.0
1	F	280	ARG	3.0
2	B	741	ALA	3.0
1	E	92	ALA	2.9
1	F	429	ILE	2.9
1	F	96	LEU	2.9
1	E	26	TYR	2.9
1	F	389	VAL	2.9
2	B	1530	ARG	2.9
1	E	255	ILE	2.9
1	F	273	GLY	2.9
2	A	1532	ASP	2.9
2	B	1641	GLN	2.9
1	F	306	LEU	2.9
2	B	1656	VAL	2.9
2	B	1657	PHE	2.9
1	E	311	GLN	2.8
1	F	26	TYR	2.8
1	E	321	LYS	2.8
1	E	634	ALA	2.8
2	B	1498	GLY	2.8
2	B	1661	ASN	2.8
1	E	124	LEU	2.8
2	A	1636	GLN	2.7
1	F	395	VAL	2.7
2	B	1652	GLU	2.7
2	A	851	TYR	2.7
2	B	1655	VAL	2.7
2	B	1354	LYS	2.6
1	E	404	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	269	PHE	2.6
1	E	354	ILE	2.6
1	F	111	PHE	2.6
1	F	430	PRO	2.6
1	F	65	LYS	2.6
1	E	535	LEU	2.6
2	B	1576	VAL	2.6
1	E	153	HIS	2.5
1	E	101	GLY	2.5
1	F	432	GLY	2.5
1	E	273	GLY	2.5
1	F	103	LYS	2.5
1	F	250	LEU	2.5
1	F	541	GLN	2.5
1	E	433	ARG	2.5
2	A	755	PRO	2.5
2	B	739	ASP	2.5
1	E	571	LYS	2.5
1	E	75	GLN	2.4
1	E	126	SER	2.4
1	E	356	PHE	2.4
1	F	241	PHE	2.4
1	E	184	GLN	2.4
1	F	539	LYS	2.4
1	E	566	GLY	2.4
1	E	314	ARG	2.4
1	F	104	PHE	2.4
2	A	785	ILE	2.4
1	E	388	VAL	2.4
1	E	305	VAL	2.4
2	B	1638	GLU	2.4
2	A	1537	PRO	2.3
1	F	425	LYS	2.3
2	B	1548	ILE	2.3
2	B	1625	TRP	2.3
1	E	322	SER	2.3
1	F	428	ASN	2.3
1	E	96	LEU	2.3
1	F	349	THR	2.3
2	B	1614	PRO	2.3
1	E	27	SER	2.3
1	F	423	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	424	THR	2.3
2	B	777	LEU	2.2
2	B	920	ILE	2.2
1	E	394	ASN	2.2
2	A	1498	GLY	2.2
2	B	783	ASN	2.2
1	E	69	LEU	2.2
2	A	1658	GLY	2.2
2	B	1528	GLU	2.2
1	F	383	ALA	2.2
2	A	779	GLN	2.2
1	F	285	HIS	2.2
2	A	1533	LYS	2.2
1	E	243	TYR	2.2
2	A	860	LYS	2.2
1	E	53	ILE	2.1
1	F	322	SER	2.1
1	E	539	LYS	2.1
1	E	348	VAL	2.1
1	F	447	GLN	2.1
2	A	739	ASP	2.1
2	A	811	LYS	2.1
2	A	1132	PHE	2.1
1	F	102	HIS	2.1
2	B	1549	GLN	2.1
2	B	1536	GLU	2.1
2	B	1653	ASN	2.1
1	E	335	SER	2.1
1	E	427	ASP	2.1
1	E	573	HIS	2.1
2	B	740	GLY	2.1
1	F	242	TYR	2.1
1	F	116	VAL	2.1
1	E	572	HIS	2.1
2	A	1639	GLU	2.0
1	E	52	THR	2.0
1	F	114	VAL	2.0
2	A	1641	GLN	2.0
2	B	1628	LEU	2.0
1	E	99	ASP	2.0
1	E	319	VAL	2.0
2	B	1355	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	1555	ASP	2.0
1	E	315	ALA	2.0
1	E	28	MET	2.0
1	E	241	PHE	2.0
1	E	251	LYS	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)

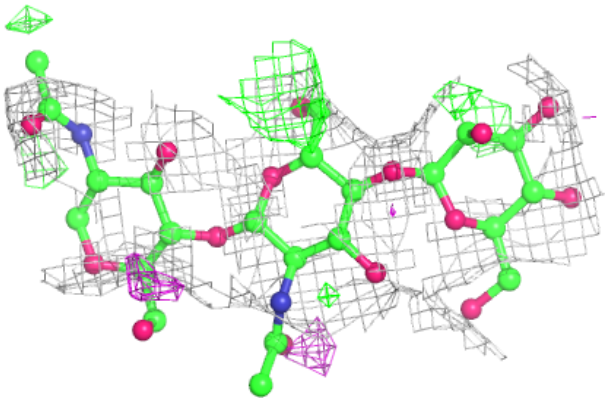
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

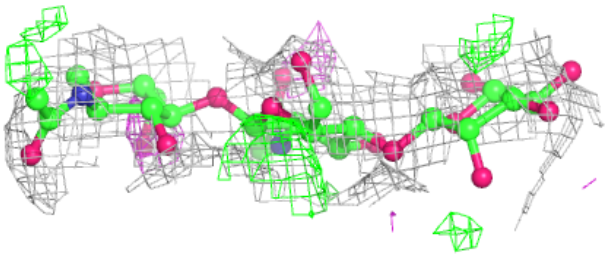
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	C	3	11/12	0.65	0.32	127,149,168,170	0
3	BMA	D	3	11/12	0.76	0.23	103,137,148,152	0
3	NAG	C	2	14/15	0.80	0.35	135,157,175,179	0
3	NAG	C	1	14/15	0.82	0.24	87,123,149,149	0
3	NAG	D	2	14/15	0.85	0.26	99,131,153,153	0
3	NAG	D	1	14/15	0.93	0.16	86,105,122,134	0

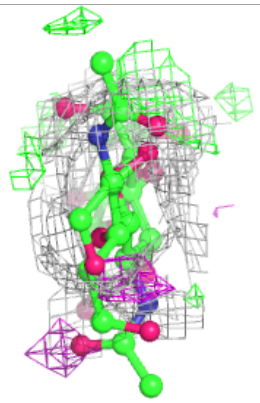
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

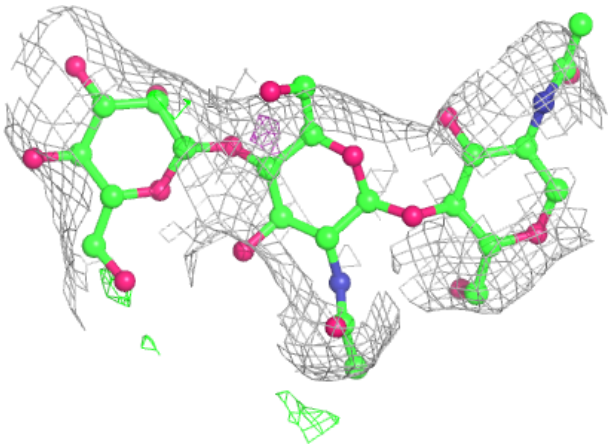


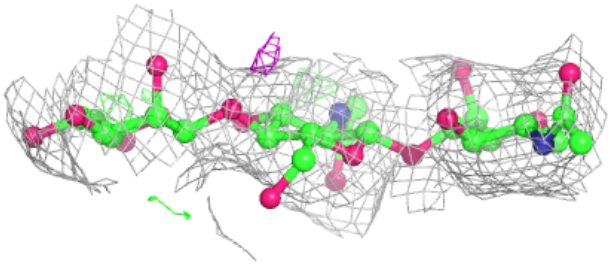


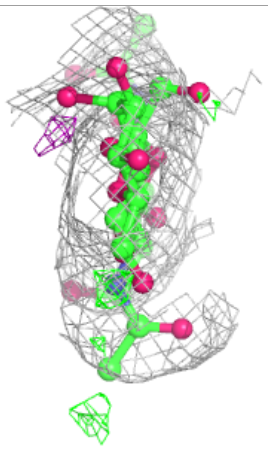


Electron density around Chain D:

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







6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.