Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 10:57 AM EDT

PDB ID	:	4N0U
Title	:	Ternary complex between Neonatal Fc receptor, serum albumin and Fc
Authors	:	Oganesyan, V.; Wu, H.; Dall'Acqua, W.F.
Deposited on	:	2013-10-02
Resolution	:	3.80 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:

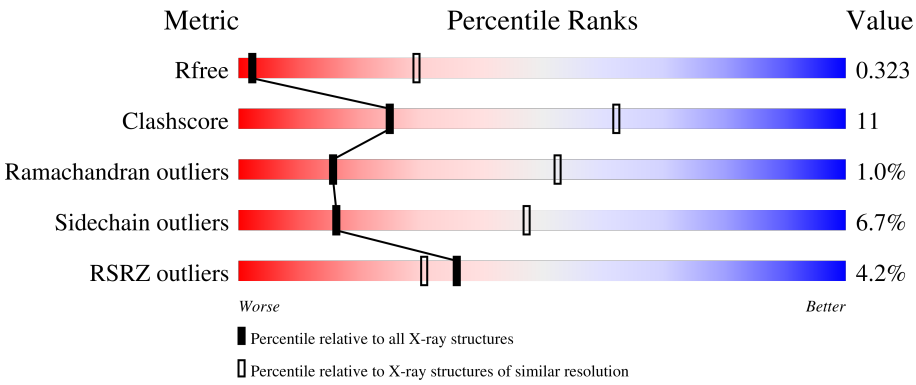
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 <=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	264	6% 76% 21% •
2	B	99	3% 82% 15% •
3	D	583	4% 79% 19% •
4	E	209	2% 62% 34% •
5	C	8	12% 50% 38%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9321 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 IgG receptor FcRn large subunit p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2080	1330	360	382	8	0	0	0

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	829	528	140	158	3	0	0	0

- Molecule 3 is a protein called Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	583	4638	2929	784	884	41	0	0	0

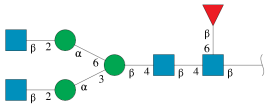
- Molecule 4 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	209	1675	1067	281	322	5	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	252	TYR	MET	engineered mutation	UNP P01857
E	254	THR	SER	engineered mutation	UNP P01857
E	256	GLU	THR	engineered mutation	UNP P01857

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



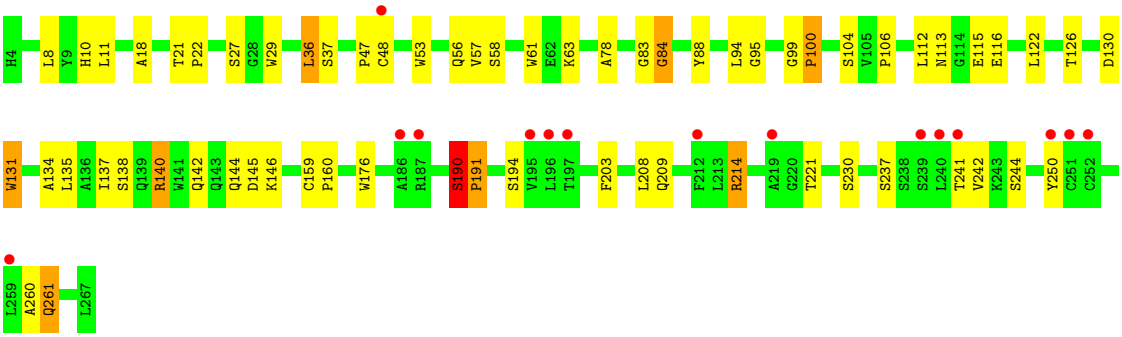
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	C	8	99	56	4	39	0	0	0

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.

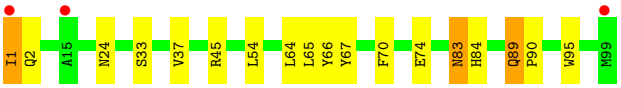
- Molecule 1: IgG receptor FcRn large subunit p51

Chain A:



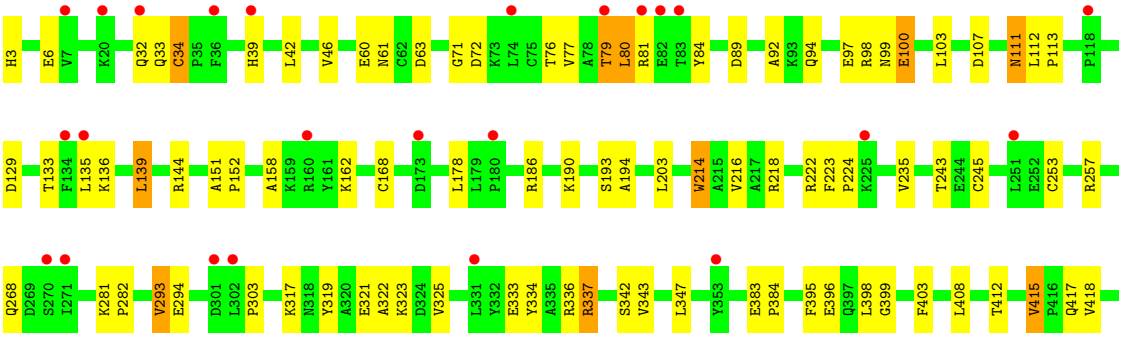
- Molecule 2: Beta-2-microglobulin

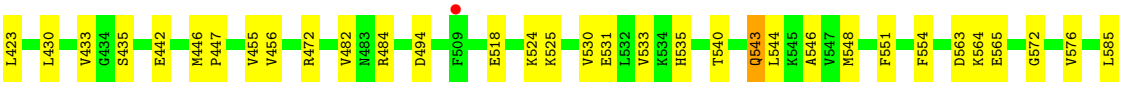
Chain B:



- Molecule 3: Serum albumin

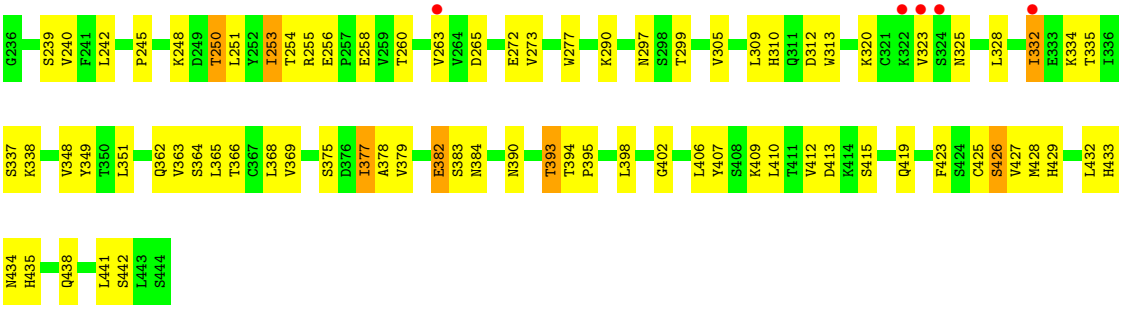
Chain D:





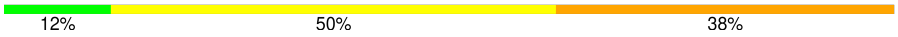
• Molecule 4: Ig gamma-1 chain C region

Chain E:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	153.19Å 153.19Å 146.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.80 45.98 – 3.42	Depositor EDS
% Data completeness (in resolution range)	91.3 (40.00-3.80) 84.2 (45.98-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.282 , 0.303 0.302 , 0.323	Depositor DCC
R_{free} test set	359 reflections (1.77%)	wwPDB-VP
Wilson B-factor (Å^2)	132.2	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.039 for -h,-l,-k 0.039 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9321	wwPDB-VP
Average B, all atoms (Å^2)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, FUL, MAN, 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	0.67	3/2146 (0.1%)	0.71	1/2915 (0.0%)
2	B	0.61	1/852 (0.1%)	0.69	0/1152
3	D	0.51	1/4728 (0.0%)	0.70	0/6377
4	E	0.64	1/1722 (0.1%)	0.74	1/2347 (0.0%)
All	All	0.58	6/9448 (0.1%)	0.71	2/12791 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	TRP	CD2-CE2	5.30	1.47	1.41
2	B	95	TRP	CD2-CE2	5.29	1.47	1.41
1	A	176	TRP	CD2-CE2	5.24	1.47	1.41
3	D	214	TRP	CD2-CE2	5.20	1.47	1.41
4	E	277	TRP	CD2-CE2	5.12	1.47	1.41
1	A	29	TRP	CD2-CE2	5.03	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	253	ILE	CB-CA-C	-6.22	99.17	111.60
1	A	140	ARG	NE-CZ-NH1	5.16	122.88	120.30

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	A	2080	0	1990	66	0
2	B	829	0	794	9	0
3	D	4638	0	4563	71	1
4	E	1675	0	1634	83	0
5	C	99	0	85	3	0
All	All	9321	0	9066	198	1

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 11.

All (198) 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:135:LEU:HD11	4:E:434:ASN:CB	1.49	1.39
4:E:394:THR:O	4:E:406:LEU:HD11	1.40	1.22
4:E:248:LYS:HD3	4:E:255:ARG:NH1	1.61	1.16
1:A:135:LEU:CD1	4:E:434:ASN:HB3	1.78	1.13
1:A:11:LEU:CD1	1:A:94:LEU:HD13	1.82	1.08
1:A:135:LEU:HD11	4:E:434:ASN:HB3	1.06	1.04
3:D:33:GLN:HE21	3:D:112:LEU:CD1	1.72	1.02
4:E:248:LYS:NZ	4:E:255:ARG:HH22	1.56	1.02
1:A:130:ASP:OD1	4:E:434:ASN:ND2	1.93	1.01
1:A:131:TRP:CZ3	4:E:253:ILE:HG12	1.96	1.00
4:E:248:LYS:NZ	4:E:255:ARG:NH2	2.11	0.97
1:A:135:LEU:CD1	4:E:434:ASN:CB	2.40	0.97
1:A:130:ASP:O	4:E:434:ASN:HA	1.68	0.94
4:E:248:LYS:HD3	4:E:255:ARG:HH12	1.18	0.92
4:E:248:LYS:HZ3	4:E:255:ARG:HH22	0.94	0.92
1:A:131:TRP:CZ3	4:E:253:ILE:CG1	2.53	0.91
1:A:11:LEU:HD13	1:A:94:LEU:HD13	1.52	0.91
1:A:115:GLU:OE1	4:E:310:HIS:ND1	2.04	0.90
2:B:83:ASN:HD22	2:B:84:HIS:H	1.20	0.88
1:A:131:TRP:CE3	4:E:253:ILE:HD11	2.09	0.87
1:A:135:LEU:HD11	4:E:434:ASN:CG	2.00	0.82
3:D:33:GLN:HE21	3:D:112:LEU:HD11	1.46	0.80
1:A:131:TRP:HZ3	4:E:253:ILE:HG12	1.47	0.79
3:D:151:ALA:HB3	3:D:152:PRO:HD3	1.65	0.79
3:D:430:LEU:HD23	3:D:456:VAL:HG11	1.66	0.77
3:D:415:VAL:CG1	3:D:415:VAL:O	2.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:248:LYS:CD	4:E:255:ARG:NH1	2.46	0.76
4:E:320:LYS:HE2	4:E:335:THR:OG1	1.87	0.75
4:E:368:LEU:HD13	4:E:407:TYR:CZ	2.22	0.73
1:A:18:ALA:O	1:A:21:THR:HB	1.88	0.73
1:A:11:LEU:HD13	1:A:94:LEU:CD1	2.18	0.73
4:E:248:LYS:CE	4:E:255:ARG:NH2	2.51	0.72
3:D:33:GLN:HE21	3:D:112:LEU:HD12	1.53	0.72
1:A:130:ASP:O	4:E:434:ASN:CA	2.37	0.71
4:E:394:THR:O	4:E:406:LEU:CD1	2.30	0.71
5:C:5:NAG:H82	5:C:5:NAG:O3	1.89	0.71
1:A:11:LEU:HD11	1:A:94:LEU:HD13	1.71	0.71
1:A:131:TRP:CE3	4:E:253:ILE:CG1	2.73	0.71
1:A:36:LEU:HD23	1:A:37:SER:N	2.07	0.70
2:B:83:ASN:HD22	2:B:84:HIS:N	1.90	0.70
1:A:11:LEU:CD1	1:A:94:LEU:CD1	2.65	0.69
1:A:135:LEU:HD11	4:E:434:ASN:HB2	1.67	0.69
4:E:248:LYS:HZ3	4:E:255:ARG:NH2	1.72	0.69
1:A:131:TRP:CZ3	4:E:253:ILE:HD11	2.28	0.67
4:E:379:VAL:HG22	4:E:427:VAL:HG22	1.75	0.67
1:A:131:TRP:HE3	4:E:253:ILE:HD11	1.57	0.67
4:E:309:LEU:HB2	4:E:312:ASP:CG	2.14	0.67
3:D:415:VAL:HG13	3:D:418:VAL:HG23	1.76	0.67
1:A:131:TRP:CZ3	4:E:253:ILE:CD1	2.77	0.67
1:A:131:TRP:CE3	4:E:253:ILE:CD1	2.77	0.67
3:D:77:VAL:O	3:D:80:LEU:HG	1.96	0.66
3:D:540:THR:H	3:D:543:GLN:HE21	1.43	0.65
4:E:378:ALA:HB3	4:E:428:MET:HB2	1.79	0.65
3:D:216:VAL:HG22	3:D:235:VAL:HG21	1.79	0.64
3:D:33:GLN:NE2	3:D:112:LEU:CD1	2.54	0.64
4:E:348:VAL:HG22	4:E:369:VAL:HG13	1.79	0.64
1:A:53:TRP:O	3:D:524:LYS:NZ	2.29	0.63
1:A:88:TYR:HE2	4:E:254:THR:HG23	1.63	0.63
1:A:144:GLN:O	1:A:146:LYS:N	2.31	0.63
3:D:415:VAL:O	3:D:415:VAL:HG13	1.99	0.62
1:A:36:LEU:HD23	1:A:36:LEU:C	2.19	0.62
3:D:81:ARG:NH2	3:D:89:ASP:OD2	2.34	0.61
4:E:365:LEU:HD23	4:E:365:LEU:N	2.16	0.61
3:D:79:THR:O	3:D:81:ARG:N	2.36	0.59
4:E:273:VAL:HG11	4:E:323:VAL:HG13	1.85	0.58
4:E:332:ILE:HG23	4:E:334:LYS:HE2	1.84	0.58
3:D:34:CYS:N	3:D:84:TYR:OH	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:PRO:HB3	1:A:61:TRP:CZ2	2.39	0.58
1:A:241:THR:O	1:A:242:VAL:HG23	2.04	0.58
3:D:417:GLN:HA	3:D:417:GLN:OE1	2.04	0.57
3:D:112:LEU:HD21	3:D:144:ARG:NH1	2.20	0.57
3:D:415:VAL:HG13	3:D:418:VAL:CG2	2.34	0.57
3:D:32:GLN:HE22	3:D:107:ASP:H	1.52	0.56
4:E:273:VAL:CG1	4:E:323:VAL:HG13	2.35	0.56
4:E:375:SER:O	4:E:377:ILE:HG22	2.05	0.56
3:D:293:VAL:HG22	3:D:294:GLU:H	1.71	0.56
3:D:33:GLN:NE2	3:D:112:LEU:HD11	2.18	0.56
1:A:131:TRP:HZ3	4:E:253:ILE:CD1	2.18	0.56
1:A:21:THR:HG23	1:A:22:PRO:HD2	1.88	0.55
1:A:203:PHE:CZ	1:A:208:LEU:HD13	2.42	0.54
3:D:80:LEU:O	3:D:84:TYR:N	2.41	0.54
4:E:290:LYS:NZ	4:E:305:VAL:HG21	2.22	0.54
3:D:60:GLU:O	3:D:61:ASN:HB2	2.08	0.54
4:E:248:LYS:CE	4:E:255:ARG:CZ	2.86	0.54
1:A:131:TRP:HZ3	4:E:253:ILE:CG1	2.07	0.54
1:A:88:TYR:CE2	4:E:254:THR:HG23	2.42	0.53
1:A:94:LEU:HD12	1:A:94:LEU:N	2.24	0.53
4:E:351:LEU:HB2	4:E:366:THR:HB	1.90	0.53
4:E:427:VAL:HG12	4:E:432:LEU:HD11	1.91	0.53
4:E:248:LYS:HE2	4:E:255:ARG:NH2	2.23	0.53
3:D:33:GLN:NE2	3:D:112:LEU:HD12	2.21	0.52
4:E:240:VAL:HG13	4:E:263:VAL:HG22	1.91	0.52
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.90	0.52
3:D:214:TRP:CD1	3:D:343:VAL:HG11	2.45	0.52
3:D:303:PRO:O	3:D:337:ARG:NH1	2.43	0.52
1:A:131:TRP:CE3	4:E:253:ILE:HG13	2.44	0.52
4:E:248:LYS:HZ1	4:E:255:ARG:NH2	2.05	0.51
3:D:531:GLU:O	3:D:535:HIS:HD2	1.93	0.51
3:D:224:PRO:O	3:D:336:ARG:NH1	2.43	0.51
4:E:248:LYS:HE2	4:E:255:ARG:CZ	2.40	0.51
4:E:364:SER:OG	4:E:409:LYS:HE3	2.11	0.50
3:D:551:PHE:O	3:D:554:PHE:HB3	2.12	0.50
1:A:113:ASN:O	2:B:1:ILE:HG22	2.12	0.49
1:A:214:ARG:HG3	1:A:250:TYR:CZ	2.47	0.49
2:B:37:VAL:HB	2:B:66:TYR:CE1	2.48	0.49
3:D:383:GLU:HB3	3:D:384:PRO:HD3	1.93	0.49
1:A:131:TRP:HE3	4:E:253:ILE:CD1	2.23	0.49
3:D:518:GLU:HA	3:D:518:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:395:PHE:O	3:D:398:LEU:O	2.31	0.49
1:A:208:LEU:C	1:A:208:LEU:HD23	2.33	0.49
3:D:218:ARG:HG2	3:D:218:ARG:HH11	1.78	0.49
1:A:53:TRP:O	3:D:524:LYS:CE	2.61	0.49
1:A:134:ALA:O	1:A:138:SER:HB2	2.13	0.48
3:D:347:LEU:HB2	3:D:482:VAL:HG21	1.95	0.48
3:D:415:VAL:O	3:D:415:VAL:HG12	2.10	0.48
4:E:429:HIS:N	4:E:432:LEU:HD12	2.27	0.48
4:E:253:ILE:HA	4:E:310:HIS:CE1	2.47	0.48
4:E:382:GLU:OE2	4:E:426:SER:OG	2.30	0.48
1:A:63:LYS:NZ	3:D:111:ASN:ND2	2.62	0.47
3:D:543:GLN:O	3:D:546:ALA:HB3	2.13	0.47
4:E:242:LEU:HD22	4:E:334:LYS:O	2.14	0.47
4:E:239:SER:O	4:E:263:VAL:HG13	2.14	0.47
1:A:8:LEU:HD23	1:A:95:GLY:HA3	1.97	0.47
1:A:190:SER:OG	1:A:191:PRO:HD2	2.15	0.46
4:E:412:VAL:HG11	4:E:423:PHE:CE2	2.50	0.46
3:D:42:LEU:O	3:D:46:VAL:HG23	2.15	0.46
1:A:203:PHE:CE2	1:A:208:LEU:HD13	2.51	0.46
3:D:194:ALA:HB1	3:D:455:VAL:HG13	1.97	0.46
1:A:63:LYS:NZ	3:D:111:ASN:HD21	2.13	0.46
3:D:342:SER:HB3	3:D:447:PRO:HA	1.98	0.46
4:E:415:SER:O	4:E:419:GLN:HG2	2.15	0.46
4:E:390:ASN:O	4:E:410:LEU:HD12	2.16	0.45
4:E:398:LEU:HD11	4:E:402:GLY:O	2.17	0.45
3:D:408:LEU:HD11	3:D:530:VAL:CG2	2.46	0.45
1:A:130:ASP:O	4:E:434:ASN:C	2.54	0.45
4:E:253:ILE:HA	4:E:310:HIS:NE2	2.32	0.45
4:E:368:LEU:HD13	4:E:407:TYR:CE1	2.52	0.45
5:C:2:NAG:C8	5:C:6:MAN:O3	2.64	0.45
3:D:525:LYS:O	3:D:548:MET:HE1	2.17	0.45
2:B:54:LEU:HD13	2:B:64:LEU:HD22	1.97	0.45
4:E:365:LEU:HB3	4:E:441:LEU:HD23	1.97	0.45
5:C:2:NAG:H83	5:C:6:MAN:O3	2.17	0.45
4:E:240:VAL:HG22	4:E:263:VAL:HG22	1.99	0.44
1:A:112:LEU:O	1:A:113:ASN:C	2.55	0.44
1:A:130:ASP:HB3	4:E:434:ASN:HA	1.99	0.44
4:E:258:GLU:CD	4:E:305:VAL:HG11	2.38	0.44
4:E:337:SER:OG	4:E:338:LYS:N	2.50	0.44
3:D:34:CYS:HB3	3:D:39:HIS:NE2	2.33	0.44
4:E:395:PRO:C	4:E:406:LEU:CD1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:395:PRO:O	4:E:406:LEU:HD12	2.18	0.43
3:D:99:ASN:ND2	3:D:103:LEU:HD11	2.33	0.43
1:A:230:SER:HB3	2:B:67:TYR:CD1	2.54	0.43
3:D:139:LEU:CD1	3:D:158:ALA:HB2	2.49	0.43
3:D:71:GLY:O	3:D:72:ASP:C	2.57	0.43
4:E:297:ASN:O	4:E:299:THR:HG23	2.18	0.43
3:D:322:ALA:HB1	3:D:325:VAL:HB	2.01	0.43
4:E:363:VAL:CG2	4:E:412:VAL:HG22	2.49	0.42
3:D:412:THR:OG1	3:D:423:LEU:HD13	2.19	0.42
4:E:325:ASN:O	4:E:328:LEU:O	2.37	0.42
4:E:250:THR:HG21	4:E:313:TRP:CD1	2.54	0.42
4:E:393:THR:O	4:E:393:THR:CG2	2.68	0.42
1:A:260:ALA:HB3	1:A:261:GLN:NE2	2.34	0.42
2:B:89:GLN:O	2:B:90:PRO:C	2.58	0.42
3:D:544:LEU:HD23	3:D:544:LEU:HA	1.88	0.42
3:D:317:LYS:O	3:D:321:GLU:HG2	2.20	0.42
1:A:78:ALA:HB1	1:A:137:ILE:HD13	2.02	0.42
1:A:214:ARG:HB2	1:A:250:TYR:CE2	2.54	0.42
2:B:54:LEU:HA	2:B:64:LEU:HD13	2.01	0.42
3:D:133:THR:O	3:D:136:LYS:N	2.52	0.42
3:D:203:LEU:HD13	3:D:243:THR:HA	2.00	0.42
3:D:216:VAL:CG2	3:D:235:VAL:HG21	2.46	0.42
3:D:223:PHE:N	3:D:224:PRO:CD	2.83	0.42
3:D:572:GLY:O	3:D:576:VAL:HG23	2.19	0.42
3:D:472:ARG:NH2	3:D:494:ASP:HA	2.35	0.41
3:D:319:TYR:O	3:D:323:LYS:HG2	2.20	0.41
1:A:99:GLY:O	1:A:100:PRO:C	2.59	0.41
3:D:99:ASN:O	3:D:103:LEU:HD12	2.20	0.41
3:D:135:LEU:HD21	3:D:162:LYS:HB2	2.02	0.41
1:A:159:CYS:HB3	1:A:160:PRO:HD3	2.01	0.41
1:A:56:GLN:NE2	1:A:57:VAL:H	2.18	0.41
1:A:83:GLY:O	1:A:84:GLY:O	2.39	0.41
3:D:89:ASP:O	3:D:92:ALA:HB3	2.20	0.41
3:D:97:GLU:HA	3:D:100:GLU:HG3	2.03	0.41
1:A:208:LEU:HD23	1:A:209:GLN:N	2.35	0.41
3:D:333:GLU:HA	3:D:333:GLU:OE1	2.21	0.41
1:A:126:THR:HA	1:A:142:GLN:HE22	1.85	0.41
3:D:281:LYS:HB3	3:D:282:PRO:HD2	2.02	0.40
3:D:399:GLY:O	3:D:403:PHE:HB2	2.21	0.40
1:A:106:PRO:HG2	1:A:122:LEU:HD13	2.03	0.40
3:D:430:LEU:CD2	3:D:456:VAL:HG11	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:248:LYS:CD	4:E:255:ARG:CZ	2.99	0.40
1:A:88:TYR:HE2	4:E:254:THR:CG2	2.31	0.40
3:D:168:CYS:HB2	3:D:178:LEU:HD13	2.03	0.40
1:A:57:VAL:HG12	1:A:58:SER:N	2.36	0.40
4:E:251:LEU:HD22	4:E:435:HIS:ND1	2.36	0.40
3:D:186:ARG:O	3:D:190:LYS:HG2	2.21	0.40
3:D:412:THR:HG21	3:D:533:VAL:HB	2.03	0.40
4:E:245:PRO:HD2	4:E:313:TRP:CH2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:94:GLN:OE1	3:D:333:GLU:OE2[4_544]	2.13	0.07

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	262/264 (99%)	237 (90%)	20 (8%)	5 (2%)	8 42
2	B	97/99 (98%)	93 (96%)	4 (4%)	0	100 100
3	D	581/583 (100%)	534 (92%)	41 (7%)	6 (1%)	15 52
4	E	207/209 (99%)	182 (88%)	24 (12%)	1 (0%)	29 66
All	All	1147/1155 (99%)	1046 (91%)	89 (8%)	12 (1%)	15 52

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	PRO
3	D	80	LEU

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Mol	Chain	Res	Type
3	D	129	ASP
3	D	442	GLU
1	A	84	GLY
1	A	145	ASP
1	A	100	PRO
1	A	190	SER
3	D	111	ASN
3	D	563	ASP
3	D	113	PRO
4	E	377	ILE

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	218/218 (100%)	204 (94%)	14 (6%)	17 48
2	B	94/94 (100%)	86 (92%)	8 (8%)	10 40
3	D	510/510 (100%)	482 (94%)	28 (6%)	21 53
4	E	194/194 (100%)	176 (91%)	18 (9%)	9 35
All	All	1016/1016 (100%)	948 (93%)	68 (7%)	16 47

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	27	SER
1	A	36	LEU
1	A	48	CYS
1	A	104	SER
1	A	116	GLU
1	A	140	ARG
1	A	190	SER
1	A	194	SER
1	A	214	ARG
1	A	221	THR

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Mol	Chain	Res	Type
1	A	237	SER
1	A	244	SER
1	A	261	GLN
2	B	1	ILE
2	B	2	GLN
2	B	33	SER
2	B	45	ARG
2	B	70	PHE
2	B	74	GLU
2	B	83	ASN
2	B	89	GLN
3	D	3	HIS
3	D	6	GLU
3	D	34	CYS
3	D	63	ASP
3	D	76	THR
3	D	79	THR
3	D	98	ARG
3	D	100	GLU
3	D	139	LEU
3	D	193	SER
3	D	222	ARG
3	D	245	CYS
3	D	253	CYS
3	D	257	ARG
3	D	268	GLN
3	D	293	VAL
3	D	334	TYR
3	D	337	ARG
3	D	396	GLU
3	D	415	VAL
3	D	433	VAL
3	D	435	SER
3	D	446	MET
3	D	484	ARG
3	D	543	GLN
3	D	564	LYS
3	D	565	GLU
3	D	585	LEU
4	E	250	THR
4	E	256	GLU
4	E	260	THR

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Mol	Chain	Res	Type
4	E	265	ASP
4	E	272	GLU
4	E	332	ILE
4	E	349	TYR
4	E	362	GLN
4	E	382	GLU
4	E	383	SER
4	E	384	ASN
4	E	393	THR
4	E	413	ASP
4	E	425	CYS
4	E	426	SER
4	E	433	HIS
4	E	438	GLN
4	E	442	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	33	GLN
1	A	56	GLN
1	A	215	ASN
1	A	261	GLN
2	B	83	ASN
3	D	32	GLN
3	D	33	GLN
3	D	99	ASN
3	D	111	ASN
3	D	146	HIS
3	D	535	HIS
3	D	543	GLN
4	E	276	ASN
4	E	361	ASN
4	E	362	GLN
4	E	390	ASN
4	E	418	GLN
4	E	434	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)

8 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	$\#\|Z\| > 2$
5	NAG	C	1	5,4	14,14,15	0.64	0	17,19,21	1.12	2 (11%)
5	NAG	C	2	5	14,14,15	0.77	0	17,19,21	1.38	4 (23%)
5	BMA	C	3	5	11,11,12	0.59	0	15,15,17	0.91	2 (13%)
5	MAN	C	4	5	11,11,12	0.73	0	15,15,17	1.55	3 (20%)
5	NAG	C	5	5	14,14,15	0.63	0	17,19,21	1.50	3 (17%)
5	MAN	C	6	5	11,11,12	0.71	0	15,15,17	1.07	1 (6%)
5	NAG	C	7	5	14,14,15	0.48	0	17,19,21	0.95	0
5	FUL	C	8	5	10,10,11	1.10	1 (10%)	14,14,16	1.08	2 (14%)

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	C	1	5,4	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1
5	MAN	C	4	5	-	0/2/19/22	0/1/1/1
5	NAG	C	5	5	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	C	6	5	-	2/2/19/22	0/1/1/1
5	NAG	C	7	5	-	0/6/23/26	0/1/1/1
5	FUL	C	8	5	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8	FUL	O5-C5	2.50	1.48	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	4	MAN	C1-C2-C3	4.15	115.68	109.64
5	C	5	NAG	O5-C1-C2	-3.45	105.95	111.29
5	C	5	NAG	C3-C4-C5	3.32	116.25	110.23
5	C	4	MAN	O2-C2-C3	-2.88	104.19	110.15
5	C	2	NAG	C1-O5-C5	2.76	115.89	112.19
5	C	1	NAG	O5-C1-C2	-2.65	107.19	111.29
5	C	8	FUL	O2-C2-C1	2.51	114.97	109.22
5	C	2	NAG	O5-C1-C2	-2.45	107.50	111.29
5	C	2	NAG	O7-C7-C8	-2.44	117.70	122.05
5	C	6	MAN	C3-C4-C5	2.31	114.42	110.23
5	C	4	MAN	C1-O5-C5	2.28	115.24	112.19
5	C	8	FUL	O4-C4-C3	-2.23	105.11	110.38
5	C	5	NAG	C4-C3-C2	2.15	114.17	111.02
5	C	2	NAG	O7-C7-N2	2.15	125.78	121.98
5	C	3	BMA	C1-C2-C3	2.14	112.76	109.64
5	C	1	NAG	C1-O5-C5	2.09	114.99	112.19
5	C	3	BMA	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	2	NAG	O5-C5-C6-O6
5	C	6	MAN	O5-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6
5	C	5	NAG	C8-C7-N2-C2
5	C	5	NAG	O7-C7-N2-C2
5	C	6	MAN	C4-C5-C6-O6
5	C	5	NAG	O5-C5-C6-O6

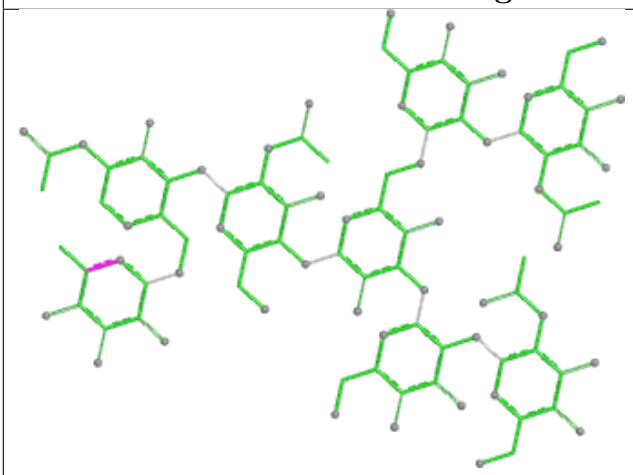
There are no ring outliers.

3 monomers are involved in 3 short contacts:

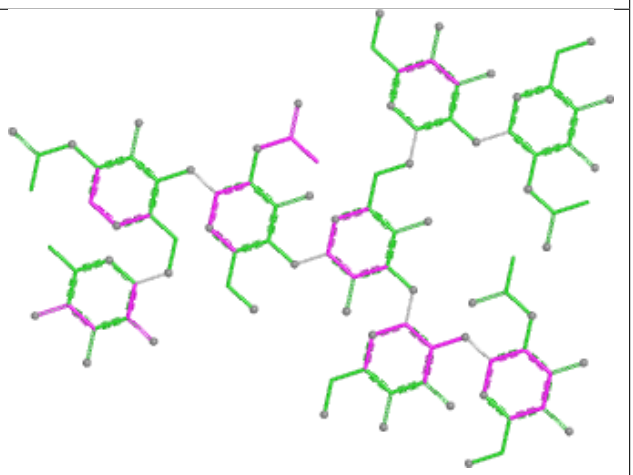
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	5	NAG	1	0
5	C	2	NAG	2	0
5	C	6	MAN	2	0

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

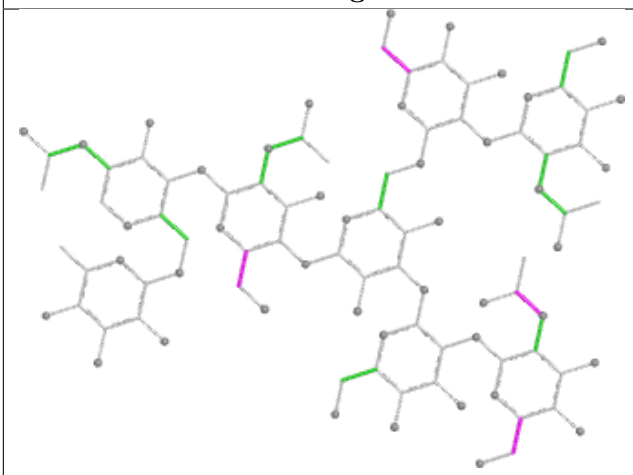
Oligosaccharide Chain C



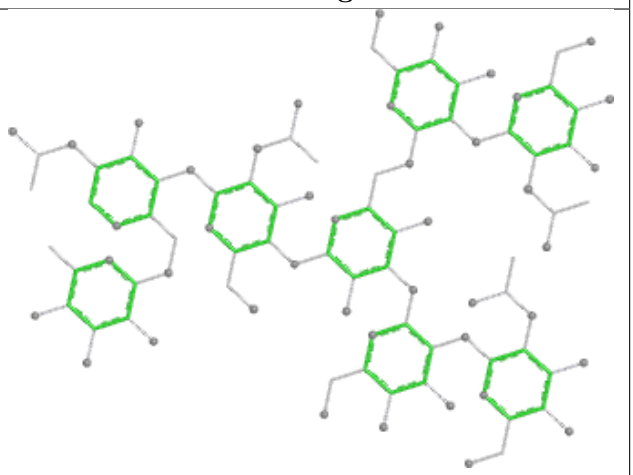
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	264/264 (100%)	0.08	15 (5%)	23	19	73, 125, 307, 373	0
2	B	99/99 (100%)	0.15	3 (3%)	50	40	100, 164, 236, 275	0
3	D	583/583 (100%)	-0.06	25 (4%)	35	30	67, 147, 261, 319	0
4	E	209/209 (100%)	-0.36	5 (2%)	59	50	58, 86, 176, 208	0
All	All	1155/1155 (100%)	-0.06	48 (4%)	36	30	58, 132, 263, 373	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	79	THR	5.5
3	D	82	GLU	5.2
1	A	240	LEU	4.7
1	A	251	CYS	4.4
3	D	39	HIS	3.9
2	B	99	MET	3.7
3	D	301	ASP	3.7
1	A	212	PHE	3.7
3	D	134	PHE	3.5
1	A	241	THR	3.5
3	D	20	LYS	3.2
1	A	187	ARG	3.2
3	D	36	PHE	3.2
1	A	195	VAL	3.1
1	A	196	LEU	3.0
3	D	74	LEU	2.8
4	E	323	VAL	2.8
3	D	7	VAL	2.8
1	A	219	ALA	2.8
1	A	239	SER	2.7
3	D	160	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	252	CYS	2.7
3	D	83	THR	2.7
3	D	173	ASP	2.6
2	B	15	ALA	2.6
3	D	118	PRO	2.5
4	E	322	LYS	2.5
3	D	270	SER	2.4
3	D	32	GLN	2.4
1	A	259	LEU	2.4
1	A	250	TYR	2.4
4	E	263	VAL	2.4
3	D	135	LEU	2.4
1	A	197	THR	2.4
3	D	251	LEU	2.3
1	A	186	ALA	2.3
1	A	48	CYS	2.2
4	E	332	ILE	2.2
3	D	271	ILE	2.1
3	D	509	PHE	2.1
3	D	81	ARG	2.1
3	D	180	PRO	2.1
3	D	225	LYS	2.1
3	D	331	LEU	2.1
3	D	353	TYR	2.1
3	D	302	LEU	2.1
4	E	324	SER	2.0
2	B	1	ILE	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, 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	BMA	C	3	11/12	0.76	0.18	108,112,122,124	0

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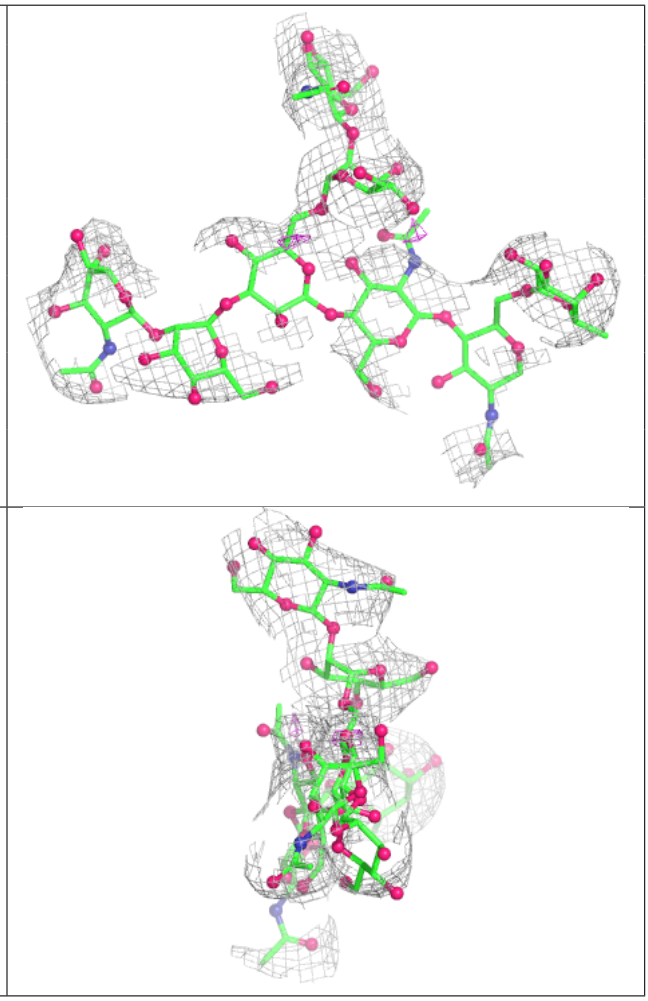
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	C	2	14/15	0.81	0.41	119,126,138,144	0
5	MAN	C	4	11/12	0.82	0.18	121,127,136,136	0
5	NAG	C	7	14/15	0.84	0.29	89,94,101,101	0
5	NAG	C	1	14/15	0.85	0.22	137,149,166,171	0
5	NAG	C	5	14/15	0.87	0.18	105,118,131,134	0
5	MAN	C	6	11/12	0.95	0.23	101,105,111,116	0
5	FUL	C	8	10/11	0.95	0.17	135,146,156,163	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)



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.