



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 11:42 AM BST

PDB ID : 6MEI
Title : Crystal structure of broadly neutralizing antibody HEPC3 in complex with Hepatitis C virus envelope glycoprotein E2 ectodomain
Authors : Flyak, A.I.; Bjorkman, P.J.
Deposited on : 2018-09-06
Resolution : 2.90 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 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 : 2.13.1
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) : 2.13.1

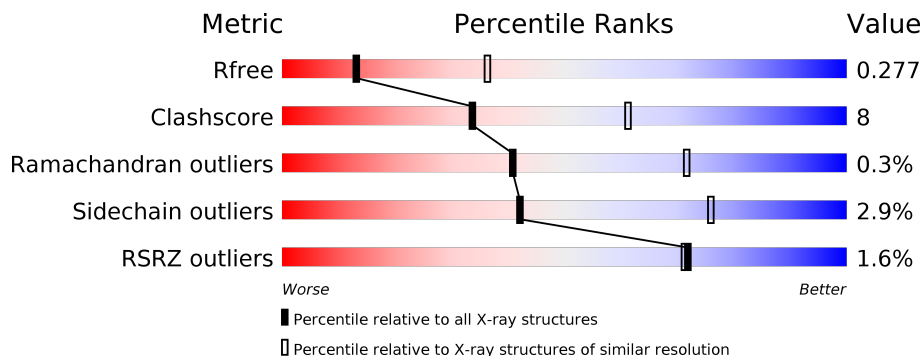
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	270	
2	H	241	
3	L	214	
4	A	2	
5	B	3	
5	D	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	BR	H	301	-	-	X	-

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 5589 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 E2 glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	238	1859	1176	331	333	19	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	646	ILE	-	expression tag	UNP A0A2P0NE26
C	647	GLY	-	expression tag	UNP A0A2P0NE26
C	648	HIS	-	expression tag	UNP A0A2P0NE26
C	649	HIS	-	expression tag	UNP A0A2P0NE26
C	650	HIS	-	expression tag	UNP A0A2P0NE26
C	651	HIS	-	expression tag	UNP A0A2P0NE26
C	652	HIS	-	expression tag	UNP A0A2P0NE26
C	653	HIS	-	expression tag	UNP A0A2P0NE26

- Molecule 2 is a protein called antibody HEPC3 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	228	1701	1068	286	338	9	0	0	0

- Molecule 3 is a protein called antibody HEPC3 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	214	1642	1020	282	334	6	0	0	0

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



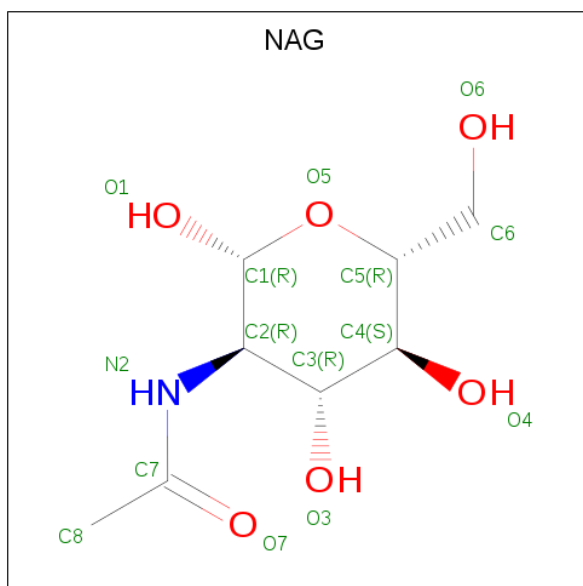
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	A	2	28	16	2	10	0	0	0

- Molecule 5 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
			Total	C	N	O			
5	B	3	39	22	2	15	0	0	0
5	D	3	39	22	2	15	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	C	1	14	8	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	3	Total	Br	0	0
			3	3		
7	L	1	Total	Br	0	0
			1	1		
7	C	3	Total	Br	0	0
			3	3		

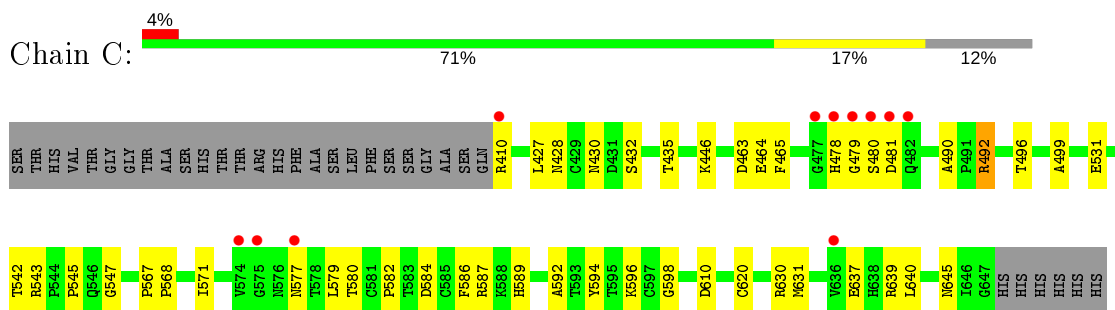
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	67	Total	O	0	0
			67	67		
8	H	64	Total	O	0	0
			64	64		
8	L	73	Total	O	0	0
			73	73		

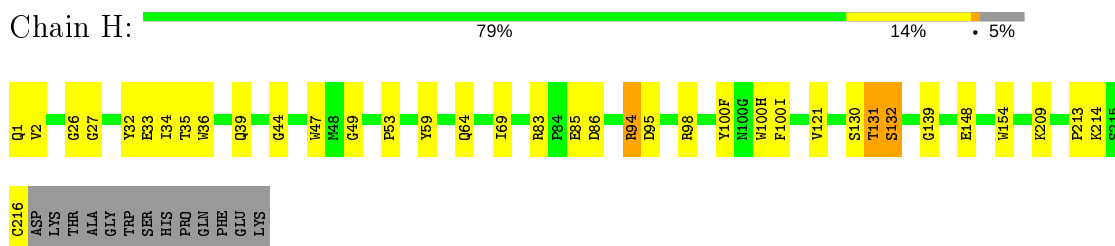
3 Residue-property plots [i](#)

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.

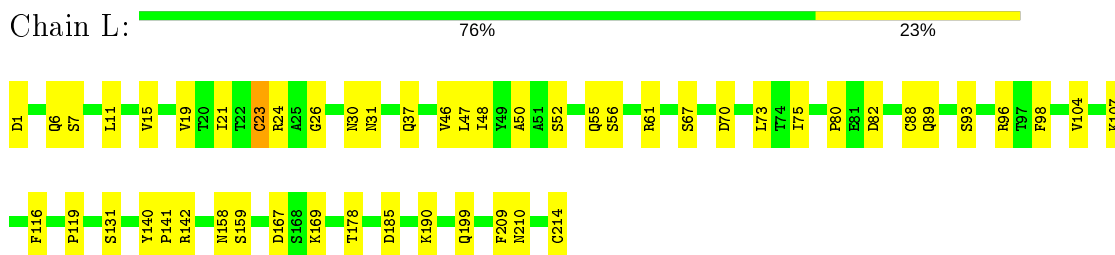
- Molecule 1: E2 glycoprotein



- Molecule 2: antibody HEPC3 Heavy Chain




- Molecule 3: antibody HEPC3 Light Chain



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



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  33% 67%

MAG1
MAG2
BMA3

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  67% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.81Å 75.79Å 174.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.00 – 2.90 87.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (87.00-2.90) 98.6 (87.00-2.90)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.208 , 0.277 0.208 , 0.277	Depositor DCC
R_{free} test set	947 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtrriage
Anisotropy	0.422	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 28.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5589	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, BR

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	C	0.35	0/1925	0.55	0/2636
2	H	0.37	0/1742	0.55	0/2375
3	L	0.36	0/1675	0.53	0/2273
All	All	0.36	0/5342	0.54	0/7284

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 [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	C	1859	0	1719	27	0
2	H	1701	0	1659	26	0
3	L	1642	0	1593	35	0
4	A	28	0	25	1	0
5	B	39	0	34	0	0
5	D	39	0	34	0	0
6	C	70	0	65	5	0
7	C	3	0	0	2	0
7	H	3	0	0	2	0
7	L	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	67	0	0	9	1
8	H	64	0	0	5	0
8	L	73	0	0	8	0
All	All	5589	0	5129	88	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 8.

All (88) 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)
3:L:24:ARG:NH1	8:L:402:HOH:O	1.89	1.02
3:L:169:LYS:NZ	8:L:403:HOH:O	2.03	0.91
3:L:131:SER:O	8:L:401:HOH:O	1.89	0.89
6:C:702:NAG:O7	8:C:801:HOH:O	1.93	0.85
3:L:26:GLY:HA3	7:L:301:BR:BR	2.32	0.84
2:H:86:ASP:OD1	8:H:401:HOH:O	1.98	0.81
1:C:543:ARG:NH2	1:C:567:PRO:O	2.15	0.79
8:H:458:HOH:O	3:L:214:CYS:SG	2.45	0.74
2:H:132:SER:O	2:H:132:SER:OG	2.05	0.74
1:C:630:ARG:HD2	1:C:637:GLU:OE2	1.89	0.73
3:L:185:ASP:OD2	8:L:404:HOH:O	2.08	0.72
1:C:645:ASN:O	8:C:802:HOH:O	2.08	0.72
2:H:213:PRO:O	8:H:402:HOH:O	2.07	0.71
3:L:47:LEU:HD12	3:L:48:ILE:HG13	1.72	0.71
3:L:6:GLN:HG3	3:L:23:CYS:SG	2.31	0.71
3:L:67:SER:O	8:L:405:HOH:O	2.10	0.69
2:H:148:GLU:OE2	8:H:403:HOH:O	2.11	0.68
3:L:1:ASP:O	8:L:406:HOH:O	2.11	0.67
4:A:1:NAG:H61	4:A:2:NAG:H82	1.77	0.67
3:L:55:GLN:NE2	8:L:410:HOH:O	2.27	0.67
1:C:543:ARG:NH1	1:C:598:GLY:O	2.28	0.66
1:C:496:THR:H	6:C:703:NAG:H62	1.62	0.64
1:C:446:LYS:NZ	2:H:53:PRO:O	2.33	0.62
1:C:545:PRO:O	8:C:803:HOH:O	2.16	0.61
3:L:55:GLN:OE1	3:L:56:SER:N	2.33	0.61
3:L:46:VAL:HG13	3:L:55:GLN:HG3	1.81	0.61
3:L:167:ASP:OD2	3:L:169:LYS:HG2	2.00	0.60
6:C:702:NAG:H2	8:C:801:HOH:O	2.00	0.60
3:L:199:GLN:OE1	8:L:408:HOH:O	2.16	0.60
3:L:37:GLN:HB2	3:L:47:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:24:ARG:NH2	3:L:70:ASP:OD2	2.36	0.57
2:H:35:THR:HG21	2:H:100(I):PHE:CE1	2.40	0.57
1:C:594:TYR:O	1:C:598:GLY:N	2.26	0.56
3:L:190:LYS:HE3	3:L:210:ASN:HB3	1.87	0.56
1:C:430:ASN:OD1	1:C:432:SER:OG	2.25	0.55
1:C:410:ARG:NH1	8:C:812:HOH:O	2.39	0.54
6:C:703:NAG:H4	7:C:715:BR:BR	2.63	0.54
1:C:531:GLU:OE1	8:C:804:HOH:O	2.18	0.54
2:H:1:GLN:HG3	2:H:26:GLY:O	2.09	0.53
2:H:83:ARG:HB3	2:H:85:GLU:OE1	2.09	0.53
1:C:568:PRO:HB2	1:C:580:THR:HG22	1.92	0.51
3:L:61:ARG:NH2	3:L:82:ASP:OD1	2.44	0.51
3:L:93:SER:O	3:L:96:ARG:NH1	2.44	0.51
2:H:2:VAL:HG12	2:H:27:GLY:HA3	1.92	0.50
2:H:2:VAL:HG22	7:H:301:BR:BR	2.67	0.50
2:H:214:LYS:HE2	3:L:119:PRO:HG2	1.94	0.49
1:C:620:CYS:HB2	7:C:714:BR:BR	2.67	0.49
2:H:32:TYR:HD1	2:H:94:ARG:NH1	2.11	0.49
2:H:59:TYR:HB2	2:H:64:GLN:HG3	1.94	0.49
1:C:465:PHE:HA	1:C:577:ASN:OD1	2.14	0.48
3:L:19:VAL:HG22	3:L:75:ILE:HB	1.95	0.48
2:H:148:GLU:OE1	8:H:405:HOH:O	2.20	0.46
1:C:490:ALA:HB1	1:C:568:PRO:HG3	1.96	0.46
1:C:586:PHE:HA	1:C:589:HIS:O	2.16	0.46
1:C:446:LYS:HA	1:C:446:LYS:HD3	1.77	0.45
1:C:478:HIS:NE2	1:C:492:ARG:HB2	2.32	0.45
2:H:33:GLU:HG2	2:H:95:ASP:O	2.16	0.45
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.52	0.45
2:H:98:ARG:NH2	7:H:301:BR:BR	3.02	0.45
1:C:428:ASN:ND2	1:C:499:ALA:O	2.49	0.44
3:L:30:ASN:HB3	3:L:31:ASN:H	1.66	0.44
2:H:100(F):TYR:OH	3:L:31:ASN:ND2	2.49	0.44
2:H:131:THR:HG22	2:H:132:SER:N	2.33	0.44
1:C:610:ASP:OD1	8:C:806:HOH:O	2.21	0.44
3:L:140:TYR:CG	3:L:141:PRO:HA	2.52	0.43
3:L:89:GLN:HB2	3:L:98:PHE:CD1	2.53	0.43
1:C:542:THR:O	1:C:547:GLY:HA3	2.17	0.43
1:C:596:LYS:NZ	8:C:819:HOH:O	2.49	0.43
3:L:158:ASN:N	3:L:158:ASN:OD1	2.50	0.43
3:L:15:VAL:CG2	3:L:80:PRO:HD3	2.48	0.43
2:H:130:SER:HA	3:L:116:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100(H):TRP:CD1	3:L:46:VAL:HG11	2.53	0.42
1:C:427:LEU:HA	1:C:427:LEU:HD12	1.77	0.42
6:C:712:NAG:O4	8:C:807:HOH:O	2.22	0.42
3:L:159:SER:HA	3:L:178:THR:O	2.19	0.42
3:L:11:LEU:O	3:L:104:VAL:HA	2.20	0.42
2:H:121:VAL:O	2:H:209:LYS:HE3	2.20	0.41
2:H:34:ILE:HD13	2:H:34:ILE:HA	1.83	0.41
1:C:479:GLY:O	1:C:481:ASP:N	2.53	0.41
2:H:36:TRP:CD1	2:H:69:ILE:HD13	2.55	0.41
3:L:119:PRO:HB3	3:L:209:PHE:CE1	2.55	0.41
1:C:637:GLU:OE2	1:C:639:ARG:NH1	2.45	0.41
2:H:139:GLY:HA2	2:H:154:TRP:CH2	2.56	0.41
1:C:589:HIS:HB3	1:C:592:ALA:HB2	2.03	0.41
3:L:21:ILE:HD12	3:L:73:LEU:HD23	2.03	0.41
3:L:50:ALA:O	3:L:52:SER:N	2.50	0.41
1:C:571:ILE:HD11	1:C:579:LEU:HB3	2.02	0.40
2:H:39:GLN:HG3	2:H:44:GLY:O	2.21	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)
8:C:811:HOH:O	8:C:817:HOH:O[4_455]	2.15	0.05

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	C	236/270 (87%)	217 (92%)	17 (7%)	2 (1%)	19	51
2	H	226/241 (94%)	212 (94%)	14 (6%)	0	100	100
3	L	212/214 (99%)	205 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	674/725 (93%)	634 (94%)	38 (6%)	2 (0%)	41 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	480	SER
1	C	582	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	C	200/226 (88%)	192 (96%)	8 (4%)	31 65
2	H	192/203 (95%)	188 (98%)	4 (2%)	53 81
3	L	188/188 (100%)	183 (97%)	5 (3%)	44 77
All	All	580/617 (94%)	563 (97%)	17 (3%)	42 76

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	435	THR
1	C	463	ASP
1	C	464	GLU
1	C	492	ARG
1	C	584	ASP
1	C	587	ARG
1	C	631	MET
1	C	640	LEU
2	H	94	ARG
2	H	131	THR
2	H	132	SER
2	H	216	CYS
3	L	7	SER
3	L	23	CYS

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Mol	Chain	Res	Type
3	L	88	CYS
3	L	107	LYS
3	L	142	ARG

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

Mol	Chain	Res	Type
3	L	199	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](#)

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
4	NAG	A	1	1,4	14,14,15	0.32	0	17,19,21	1.08	1 (5%)
4	NAG	A	2	4	14,14,15	0.37	0	17,19,21	0.86	0
5	NAG	B	1	1,5	14,14,15	0.37	0	17,19,21	1.04	1 (5%)
5	NAG	B	2	5	14,14,15	0.41	0	17,19,21	0.95	1 (5%)
5	BMA	B	3	5	11,11,12	0.90	0	15,15,17	0.72	0
5	NAG	D	1	1,5	14,14,15	0.37	0	17,19,21	1.13	0
5	NAG	D	2	5	14,14,15	0.42	0	17,19,21	0.66	0
5	BMA	D	3	5	11,11,12	0.94	1 (9%)	15,15,17	0.82	0

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
4	NAG	A	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
5	NAG	B	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	B	2	5	-	3/6/23/26	0/1/1/1
5	BMA	B	3	5	-	2/2/19/22	0/1/1/1
5	NAG	D	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2	5	-	0/6/23/26	0/1/1/1
5	BMA	D	3	5	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	3	BMA	C1-C2	2.18	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	NAG	O5-C5-C6	3.05	111.98	107.20
4	A	1	NAG	C2-N2-C7	2.71	126.76	122.90
5	B	2	NAG	O5-C5-C6	2.19	110.63	107.20

There are no chirality outliers.

All (8) torsion outliers are listed below:

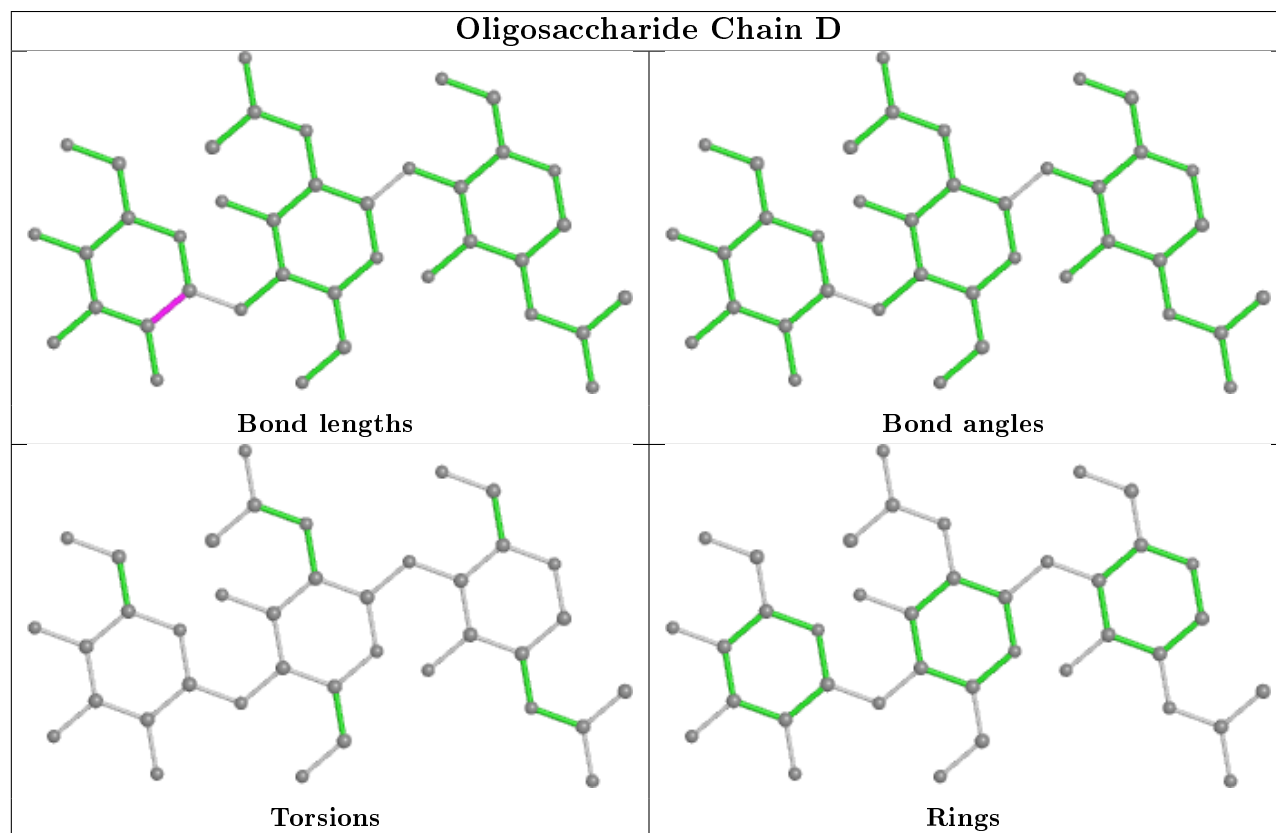
Mol	Chain	Res	Type	Atoms
4	A	2	NAG	C8-C7-N2-C2
4	A	2	NAG	O7-C7-N2-C2
5	B	2	NAG	C8-C7-N2-C2
5	B	2	NAG	O5-C5-C6-O6
5	B	3	BMA	C4-C5-C6-O6
5	B	2	NAG	O7-C7-N2-C2
5	B	3	BMA	O5-C5-C6-O6
5	B	1	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	NAG	1	0
4	A	2	NAG	1	0

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



5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	C	713	1	14,14,15	0.24	0	17,19,21	0.68	0
6	NAG	C	703	1	14,14,15	0.30	0	17,19,21	0.87	0
6	NAG	C	701	1	14,14,15	0.35	0	17,19,21	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	712	1	14,14,15	0.34	0	17,19,21	1.43	2 (11%)
6	NAG	C	702	1	14,14,15	0.29	0	17,19,21	0.82	0

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
6	NAG	C	713	1	-	3/6/23/26	0/1/1/1
6	NAG	C	703	1	-	0/6/23/26	0/1/1/1
6	NAG	C	701	1	-	4/6/23/26	0/1/1/1
6	NAG	C	712	1	-	2/6/23/26	0/1/1/1
6	NAG	C	702	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	712	NAG	C1-O5-C5	-3.86	106.96	112.19
6	C	712	NAG	C2-N2-C7	2.72	126.77	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	713	NAG	C8-C7-N2-C2
6	C	713	NAG	O7-C7-N2-C2
6	C	712	NAG	C8-C7-N2-C2
6	C	712	NAG	O7-C7-N2-C2
6	C	701	NAG	C8-C7-N2-C2
6	C	701	NAG	C1-C2-N2-C7
6	C	701	NAG	O7-C7-N2-C2
6	C	701	NAG	C3-C2-N2-C7
6	C	713	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	703	NAG	2	0
6	C	712	NAG	1	0
6	C	702	NAG	2	0

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	C	238/270 (88%)	-0.11	11 (4%) 32 29	16, 30, 71, 96	0
2	H	228/241 (94%)	-0.54	0 100 100	14, 27, 39, 76	0
3	L	214/214 (100%)	-0.57	0 100 100	16, 29, 42, 78	0
All	All	680/725 (93%)	-0.40	11 (1%) 72 71	14, 28, 52, 96	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	480	SER	4.8
1	C	574	VAL	4.6
1	C	575	GLY	4.2
1	C	479	GLY	2.8
1	C	577	ASN	2.8
1	C	636	VAL	2.8
1	C	410	ARG	2.8
1	C	478	HIS	2.7
1	C	482	GLN	2.2
1	C	477	GLY	2.2
1	C	481	ASP	2.1

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

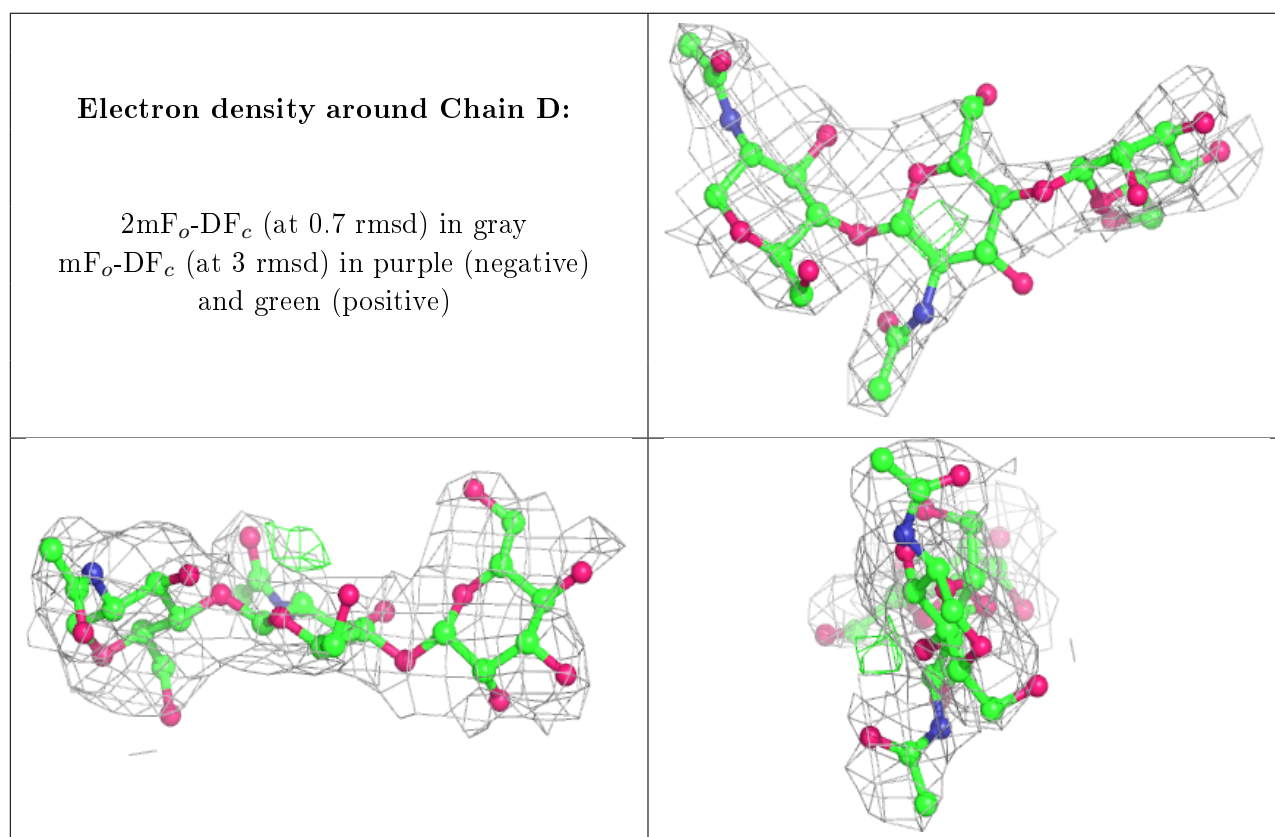
There are no non-standard protein/DNA/RNA residues in this entry.

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(\AA^2)	Q<0.9
5	BMA	D	3	11/12	0.71	0.22	82,93,96,99	0
5	BMA	B	3	11/12	0.73	0.22	64,77,81,83	0
5	NAG	D	2	14/15	0.75	0.28	56,78,92,94	0
4	NAG	A	2	14/15	0.85	0.22	44,61,69,70	0
5	NAG	B	2	14/15	0.88	0.25	46,58,71,77	0
5	NAG	B	1	14/15	0.91	0.19	26,40,47,55	0
5	NAG	D	1	14/15	0.92	0.15	31,45,58,68	0
4	NAG	A	1	14/15	0.93	0.15	23,39,56,57	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.



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	C	701	14/15	0.83	0.28	44,56,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	C	712	14/15	0.83	0.15	49,56,61,65	0
6	NAG	C	713	14/15	0.84	0.34	66,73,79,96	0
6	NAG	C	702	14/15	0.84	0.21	40,57,77,83	0
7	BR	L	301	1/1	0.94	0.06	77,77,77,77	0
6	NAG	C	703	14/15	0.94	0.24	38,42,53,58	0
7	BR	H	303	1/1	0.97	0.04	44,44,44,44	0
7	BR	C	716	1/1	0.98	0.05	57,57,57,57	0
7	BR	C	715	1/1	0.98	0.13	66,66,66,66	0
7	BR	C	714	1/1	0.98	0.06	51,51,51,51	0
7	BR	H	301	1/1	0.99	0.05	53,53,53,53	0
7	BR	H	302	1/1	0.99	0.02	40,40,40,40	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.