

Full wwPDB X-ray Structure Validation Report (i)

Mar 21, 2024 - 04:09 PM EDT

PDB ID	:	8W0W
Title	:	Crystal structure of broadly neutralizing antibody hcab64 in complex with
		Hepatitis C virus envelope glycoprotein E2 ectodomain
Authors	:	Flyak, A.I.; Wilcox, X.E.
Deposited on	:	2024-02-14
Resolution	:	2.13 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:

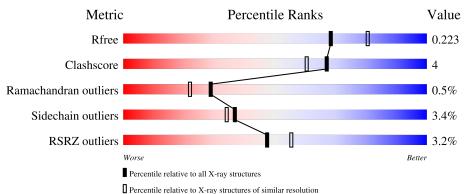
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.13 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	С	262	4% 73% 10% • 16%	6					
2	Н	237	85% 7%	5%					
3	L	215	^{2%} 92%	7% •					
4	А	5	40% 60%						
5	В	2	100%						

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Mol	Chain	Length	Quality of chain					
5	D	2	50%	50%				
5	Е	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	MAN	А	4	-	-	-	Х



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2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5508 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 Envelope glycoprotein E2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	С	221	Total 1738	C 1105	N 306	O 308	S 19	0	0	0

• Molecule 2 is a protein called hcab64 Fab Heavy Chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	Н	224	Total	С	Ν	0	S	0	0	0
			1688	1053	292	334	9			Ĵ

• Molecule 3 is a protein called hcab64 Fab Light Chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	L	213	Total 1641	C 1029	N 278	O 330	S 4	0	0	0

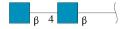
• Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mo	l Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
4	А	5	Total 61	C 34	N 2	0 25	0	0	0

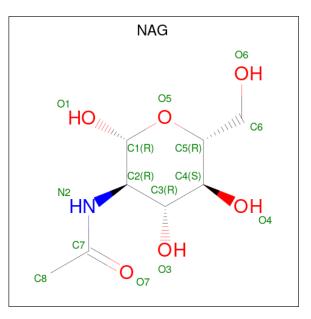
• Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	В	2	Total C N O 28 16 2 10	0	0	0
5	D	2	Total C N O 28 16 2 10	0	0	0
5	Е	2	Total C N O 28 16 2 10	0	0	0

• Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	С	86	Total O 86 86	0	0
7	Н	107	Total O 107 107	0	0

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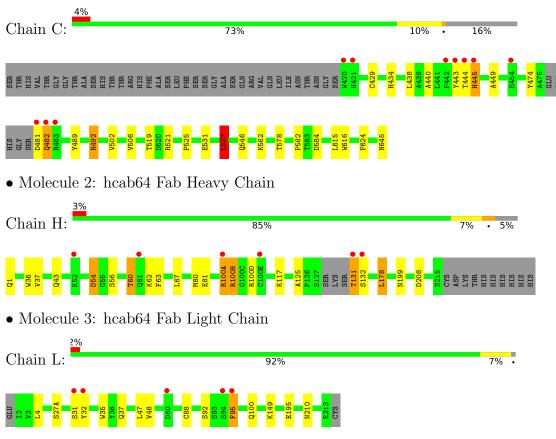
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	75	Total O 75 75	0	0



3 Residue-property plots (i)

• Molecule 1: Envelope glycoprotein E2

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.



 \bullet Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose nose



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

Chain B:

NAG1 NAG2

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

Chain D:	50%	50%

NAG1 NAG2

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

Chain E:	100%
NAG2 NAG2	



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	68.68Å 88.23Å 174.71Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.99 - 2.13	Depositor
Resolution (A)	53.99 - 2.13	EDS
% Data completeness	98.8 (53.99-2.13)	Depositor
(in resolution range)	98.8 (53.99-2.13)	EDS
R _{merge}	0.16	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.85 (at 2.12 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
D D.	0.195 , 0.224	Depositor
R, R_{free}	0.195 , 0.223	DCC
R_{free} test set	2967 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	40.4	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , 43.7	EDS
L-test for twinning ²	$ \langle L \rangle = 0.48, \langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5508	wwPDB-VP
Average B, all atoms $(Å^2)$	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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, MAN

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	Bo	nd angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	С	0.50	0/1802	0.67	1/2469~(0.0%)
2	Н	0.49	0/1726	0.65	1/2349~(0.0%)
3	L	0.53	0/1679	0.66	0/2281
All	All	0.51	0/5207	0.66	2/7099~(0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	С	537	LEU	CA-CB-CG	-5.64	102.33	115.30
2	Н	178	LEU	CA-CB-CG	5.49	127.92	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	С	1738	0	1604	15	0
2	Н	1688	0	1650	18	0
3	L	1641	0	1586	8	0
4	А	61	0	52	0	0
5	В	28	0	25	0	0
5	D	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Е	28	0	25	1	0
6	С	28	0	26	1	0
7	С	86	0	0	2	1
7	Н	107	0	0	7	1
7	L	75	0	0	1	1
All	All	5508	0	4993	40	2

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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 4.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:117:LYS:NZ	7:H:303:HOH:O	1.86	1.08
2:H:208:ASP:OD1	7:H:301:HOH:O	1.81	0.96
2:H:125:ALA:O	7:H:302:HOH:O	1.83	0.95
1:C:531:GLU:OE2	2:H:100(B):ARG:NE	2.01	0.92
2:H:81:GLU:OE2	7:H:304:HOH:O	1.89	0.91
2:H:43:GLN:O	7:H:305:HOH:O	2.01	0.78
1:C:449:ALA:HB1	6:C:702:NAG:H83	1.69	0.73
1:C:474:TYR:OH	7:C:801:HOH:O	2.08	0.72
1:C:584:ASP:OD1	7:C:802:HOH:O	2.10	0.70
2:H:54:ASP:HB3	2:H:56:SER:H	1.59	0.66
1:C:444:THR:O	1:C:445:HIS:HB2	1.98	0.62
2:H:60:THR:HG23	2:H:62:LYS:H	1.64	0.61
2:H:100(D):ARG:NH2	7:H:306:HOH:O	2.22	0.60
1:C:506:VAL:HG21	1:C:537:LEU:HD22	1.82	0.59
2:H:100(A):ARG:HG2	2:H:100(B):ARG:HD3	1.83	0.59
3:L:100:GLN:NE2	7:L:302:HOH:O	2.30	0.59
3:L:32:TYR:HB2	3:L:92:SER:HB3	1.85	0.58
2:H:1:GLN:OE1	2:H:1:GLN:N	2.29	0.57
3:L:149:LYS:NZ	3:L:195:GLU:OE2	2.37	0.57
2:H:36:TRP:CE2	2:H:80:MET:HB2	2.39	0.56
3:L:35:TRP:HB2	3:L:48:VAL:HG22	1.86	0.56
2:H:131:THR:N	7:H:308:HOH:O	2.41	0.53
1:C:481:ASP:OD2	1:C:492:ARG:NH1	2.35	0.53
1:C:502:VAL:HG21	1:C:537:LEU:HD13	1.91	0.52
1:C:429:CYS:HB3	1:C:438:LEU:HD21	1.93	0.49
1:C:562:LYS:NZ	5:E:1:NAG:O6	2.39	0.46
1:C:440:ALA:HB3	1:C:616:TRP:CD1	2.51	0.46
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:67:LEU:HD11	2:H:80:MET:HG2	2.00	0.43
2:H:60:THR:HG23	2:H:62:LYS:N	2.33	0.43
2:H:54:ASP:HB3	2:H:56:SER:HB2	2.00	0.42
3:L:4:LEU:HD23	3:L:88:CYS:SG	2.59	0.42
1:C:624:PHE:CZ	1:C:645:ASN:HB2	2.54	0.42
2:H:131:THR:HG22	2:H:132:SER:H	1.83	0.42
3:L:95:PHE:C	3:L:95:PHE:CD1	2.92	0.42
3:L:95:PHE:C	3:L:95:PHE:HD1	2.23	0.42
1:C:482:GLN:HA	1:C:489:TYR:HE1	1.85	0.41
1:C:615:LEU:HD23	1:C:615:LEU:HA	1.79	0.41
1:C:519:THR:HG22	1:C:525:PRO:HA	2.03	0.41
2:H:60:THR:HG22	2:H:63:PHE:HD1	1.87	0.40

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All (2) 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)
7:C:868:HOH:O	7:C:875:HOH:O[4_445]	1.86	0.34
7:H:382:HOH:O	7:L:372:HOH:O[4_444]	2.04	0.16

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	\mathbf{C}	217/262~(83%)	205~(94%)	10~(5%)	2(1%)	17 10
2	Η	220/237~(93%)	215~(98%)	5(2%)	0	100 100
3	L	211/215~(98%)	205~(97%)	5(2%)	1 (0%)	29 22
All	All	648/714~(91%)	625~(96%)	20 (3%)	3(0%)	29 22

All (3) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	С	445	HIS
3	L	31	SER
1	С	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	С	187/219~(85%)	179~(96%)	8 (4%)		29	25
2	Н	193/206~(94%)	185 (96%)	8 (4%)		30	27
3	L	185/187~(99%)	182 (98%)	3~(2%)		62	65
All	All	565/612~(92%)	546 (97%)	19 (3%)		37	34

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	434	HIS
1	С	443	TYR
1	С	482	GLN
1	С	492	ARG
1	С	521	ARG
1	С	537	LEU
1	C C	546	GLN
1		578	THR
2	Н	37	VAL
2	Н	54	ASP
2	Н	60	THR
2	Н	100(A)	ARG
2	Н	100(B)	ARG
2	Н	131	THR
2	Н	178	LEU
2	Н	199	ASN
3	L	27(A)	SER
3	L	95	PHE
3	L	210	ASN



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	Н	3	GLN
2	Н	164	HIS
2	Н	171	GLN
2	Н	199	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)

11 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	Turne	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	NAG	А	1	4,1	14,14,15	0.35	0	17,19,21	0.95	0
4	NAG	А	2	4	14,14,15	0.27	0	17,19,21	0.81	0
4	BMA	А	3	4	11,11,12	0.88	1 (9%)	$15,\!15,\!17$	1.87	2 (13%)
4	MAN	А	4	4	11,11,12	0.78	0	$15,\!15,\!17$	1.30	2 (13%)
4	MAN	А	5	4	11,11,12	0.88	0	$15,\!15,\!17$	1.55	4 (26%)
5	NAG	В	1	1,5	14,14,15	0.36	0	17,19,21	0.95	1 (5%)
5	NAG	В	2	5	14,14,15	0.47	0	$17,\!19,\!21$	1.20	2 (11%)
5	NAG	D	1	1,5	$14,\!14,\!15$	0.50	0	$17,\!19,\!21$	1.02	0
5	NAG	D	2	5	$14,\!14,\!15$	0.50	0	$17,\!19,\!21$	1.06	1 (5%)
5	NAG	Е	1	1,5	14,14,15	0.32	0	17,19,21	1.00	0
5	NAG	Е	2	5	14,14,15	0.39	0	17,19,21	1.00	2 (11%)



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	А	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	А	2	4	-	0/6/23/26	0/1/1/1
4	BMA	А	3	4	-	2/2/19/22	0/1/1/1
4	MAN	А	4	4	-	0/2/19/22	0/1/1/1
4	MAN	А	5	4	-	0/2/19/22	0/1/1/1
5	NAG	В	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	В	2	5	-	2/6/23/26	0/1/1/1
5	NAG	D	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	D	2	5	-	2/6/23/26	0/1/1/1
5	NAG	Е	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Е	2	5	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	3	BMA	C2-C3	2.23	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	3	BMA	C1-O5-C5	4.68	118.54	112.19
4	А	3	BMA	O5-C5-C6	3.76	113.10	107.20
5	D	2	NAG	O5-C5-C6	3.28	112.35	107.20
4	А	5	MAN	C1-O5-C5	3.21	116.54	112.19
5	В	2	NAG	C2-N2-C7	-2.65	119.13	122.90
4	А	4	MAN	C2-C3-C4	2.31	114.90	110.89
4	А	5	MAN	C1-C2-C3	2.31	112.51	109.67
5	В	2	NAG	O5-C5-C6	2.27	110.77	107.20
4	А	4	MAN	C1-O5-C5	2.20	115.17	112.19
4	А	5	MAN	O5-C1-C2	2.12	114.04	110.77
5	Ε	2	NAG	O5-C5-C6	2.08	110.46	107.20
4	А	5	MAN	C2-C3-C4	2.06	114.46	110.89
5	Ε	2	NAG	C2-N2-C7	2.04	125.80	122.90
5	В	1	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
4	А	3	BMA	O5-C5-C6-O6
5	Е	2	NAG	C4-C5-C6-O6
5	Е	2	NAG	O5-C5-C6-O6
4	А	3	BMA	C4-C5-C6-O6
5	В	2	NAG	C8-C7-N2-C2
5	D	1	NAG	C4-C5-C6-O6
5	D	2	NAG	C8-C7-N2-C2
5	В	2	NAG	O7-C7-N2-C2
5	D	2	NAG	O7-C7-N2-C2
5	D	1	NAG	C3-C2-N2-C7
5	D	1	NAG	O5-C5-C6-O6

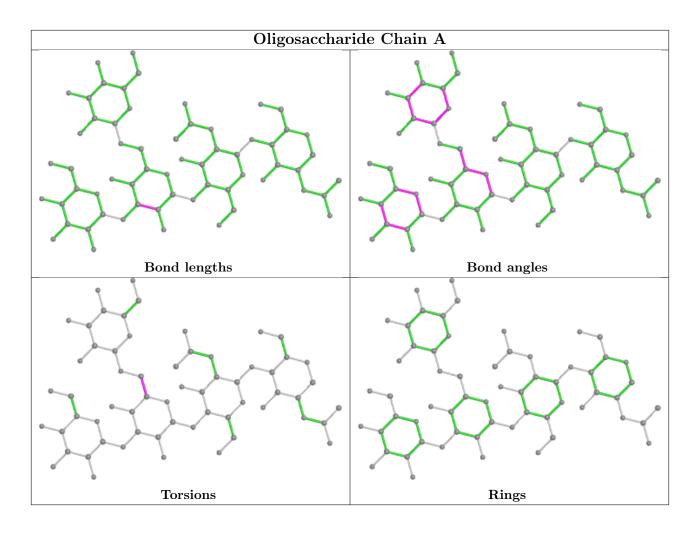
There are no ring outliers.

1 monomer is involved in 1 short contact:

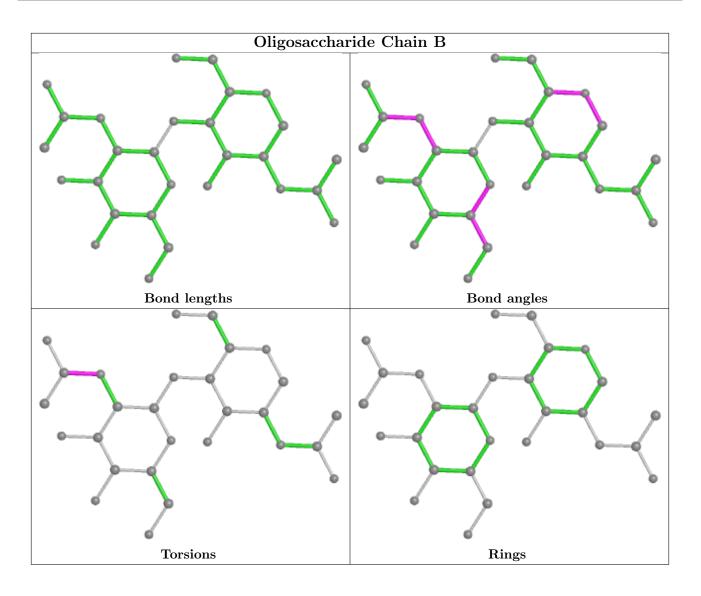
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Ε	1	NAG	1	0

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

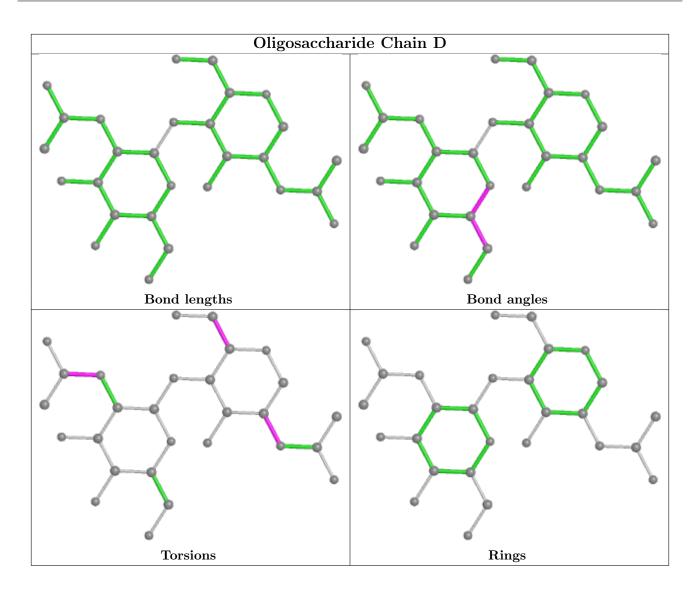




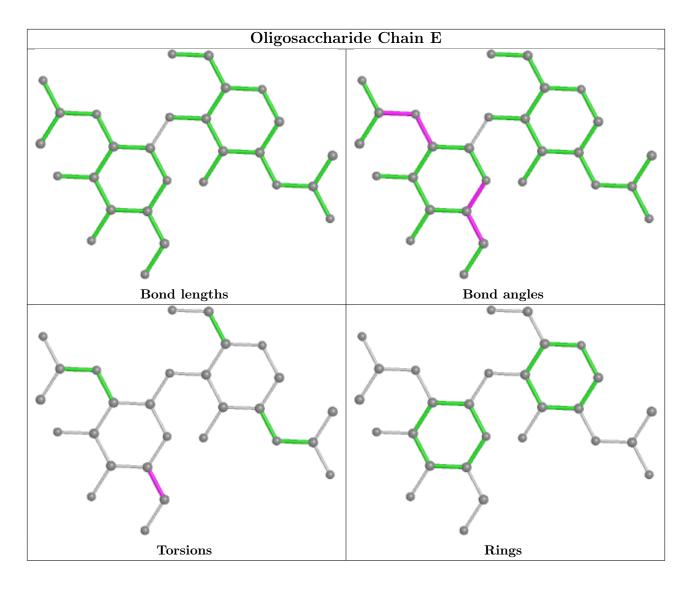












5.6 Ligand geometry (i)

2 ligands 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 Cha	Chain	Res	Link	Bo	Bond lengths			Bond angles		
IVIOI		Ullaili	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
6	NAG	С	701	1	14,14,15	0.35	0	$17,\!19,\!21$	1.23	1 (5%)	
6	NAG	С	702	1	14,14,15	0.56	0	17,19,21	1.07	2 (11%)	



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	С	701	1	-	0/6/23/26	0/1/1/1
6	NAG	С	702	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	С	701	NAG	C1-O5-C5	2.79	115.97	112.19
6	С	702	NAG	O5-C5-C6	2.35	110.88	107.20
6	С	702	NAG	C2-N2-C7	-2.16	119.83	122.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	С	702	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

ſ	Mol	Chain	Res	Type	Clashes	Symm-Clashes
ſ	6	С	702	NAG	1	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, 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	С	221/262~(84%)	0.48	10 (4%) 33 40	30, 42, 74, 98	0
2	Н	224/237 (94%)	0.44	6 (2%) 54 61	27, 44, 76, 94	0
3	L	213/215~(99%)	0.36	5 (2%) 60 67	29, 49, 78, 88	0
All	All	658/714~(92%)	0.43	21 (3%) 47 55	27, 45, 78, 98	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	443	TYR	7.5
1	С	481	ASP	6.2
1	С	420	TRP	5.9
1	С	445	HIS	4.3
2	Н	132	SER	4.2
1	С	444	THR	3.6
3	L	95	PHE	3.3
1	С	421	HIS	3.1
1	С	483	ARG	3.0
1	С	454	GLU	2.7
3	L	32	TYR	2.7
2	Н	131	THR	2.7
2	Н	61	GLN	2.7
2	Н	100(A)	ARG	2.7
3	L	94	SER	2.6
3	L	31	SER	2.4
1	С	482	GLN	2.3
3	L	60	ASP	2.3
1	С	442	PHE	2.2
2	Н	52	LYS	2.2
2	Н	100(E)	CYS	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.

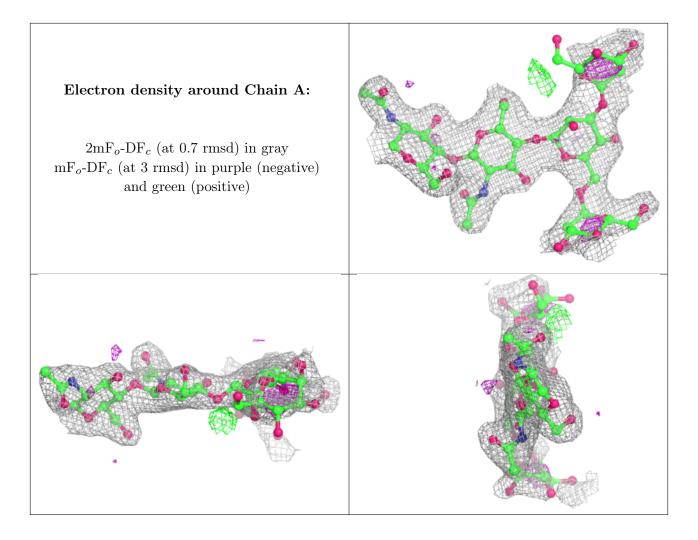
6.3 Carbohydrates (i)

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, 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.

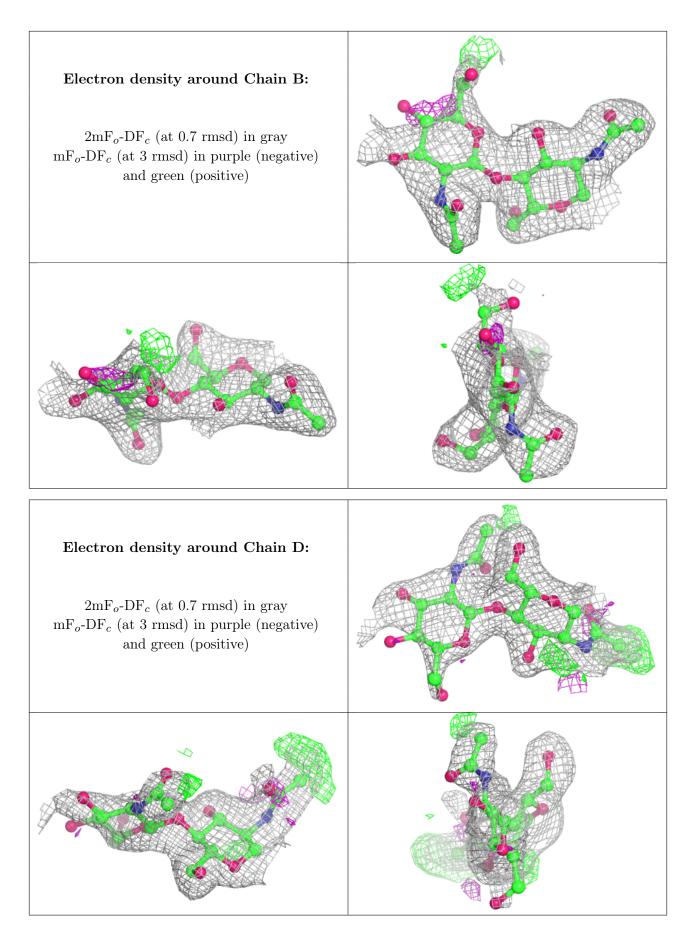
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q<0.9
4	MAN	А	5	11/12	0.59	0.38	91,93,96,96	0
4	MAN	А	4	11/12	0.60	0.48	$93,\!95,\!96,\!98$	0
5	NAG	D	2	14/15	0.78	0.33	59,80,86,91	0
5	NAG	D	1	14/15	0.80	0.12	56, 59, 70, 75	0
5	NAG	В	2	14/15	0.80	0.23	68,73,80,85	0
4	BMA	А	3	11/12	0.86	0.24	85,89,91,92	0
5	NAG	Е	2	14/15	0.90	0.21	62,72,78,79	0
4	NAG	А	2	14/15	0.93	0.16	55,65,75,79	0
5	NAG	Е	1	14/15	0.95	0.13	47,54,61,65	0
4	NAG	А	1	14/15	0.96	0.14	48,52,59,61	0
5	NAG	В	1	14/15	0.97	0.11	46,54,68,69	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.

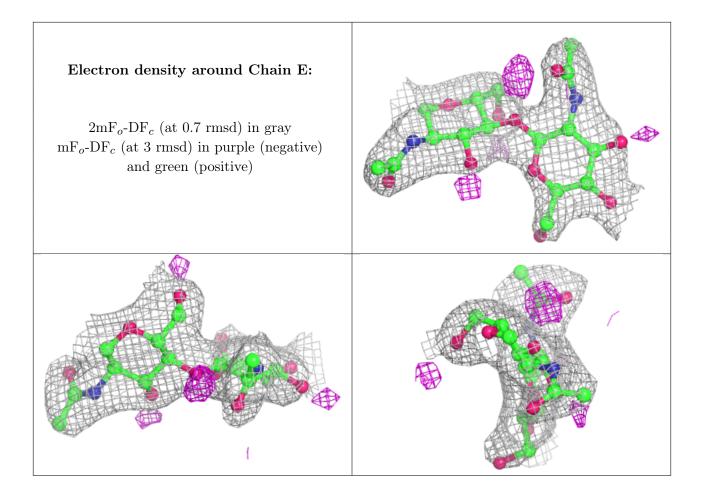












6.4 Ligands (i)

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, 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
6	NAG	С	702	14/15	0.77	0.34	$67,\!77,\!89,\!95$	0
6	NAG	С	701	14/15	0.88	0.33	72,76,78,81	0

6.5 Other polymers (i)

There are no such residues in this entry.

