Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 06:41 AM EDT

PDB ID	:	3TYG
Title	:	Crystal structure of broad and potent HIV-1 neutralizing antibody PGT128 in complex with a glycosylated engineered gp120 outer domain with miniV3 (eODmV3)
Authors	:	Pejchal, R.; Huang, P.S.; Schief, W.R.; Stanfield, R.L.; Wilson, I.A.
Deposited on	:	2011-09-25
Resolution	:	3.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

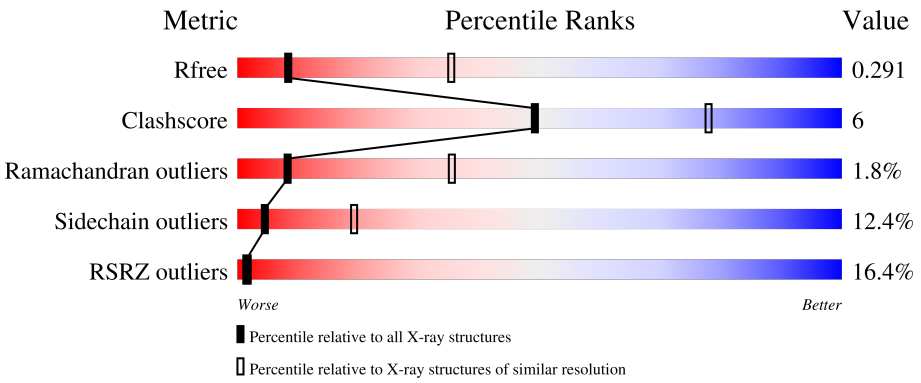
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	199	28%, 64%, 16%, •, 17%
2	L	211	5%, 74%, 22%, • •
3	H	239	13%, 75%, 20%, • •
4	B	10	20%, 80%
5	C	7	43%, 57%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4715 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 gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	165	1239	761	220	251	7	0	0	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	linker	UNP P04578
A	10	ALA	-	linker	UNP P04578
A	11	PRO	-	linker	UNP P04578
A	12	PRO	-	linker	UNP P04578
A	13	PRO	-	linker	UNP P04578
A	14	HIS	-	linker	UNP P04578
A	23	ILE	LEU	engineered mutation	UNP P04578
A	48	ILE	-	linker	UNP P04578
A	49	ALA	-	linker	UNP P04578
A	50	ARG	-	linker	UNP P04578
A	51	CYS	-	linker	UNP P04578
A	52	GLN	-	linker	UNP P04578
A	53	ILE	-	linker	UNP P04578
A	54	ALA	-	linker	UNP P04578
A	55	GLY	-	linker	UNP P04578
A	56	THR	-	linker	UNP P04578
A	86	SER	THR	engineered mutation	UNP P04578
A	88	CYS	ILE	engineered mutation	UNP P04578
A	108	PRO	LYS	engineered mutation	UNP Q75760
A	175	ASP	ASN	engineered mutation	UNP P04578
A	191	GLY	-	expression tag	UNP P04578
A	192	THR	-	expression tag	UNP P04578
A	193	LYS	-	expression tag	UNP P04578
A	194	HIS	-	expression tag	UNP P04578
A	195	HIS	-	expression tag	UNP P04578
A	196	HIS	-	expression tag	UNP P04578
A	197	HIS	-	expression tag	UNP P04578

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Chain	Residue	Modelled	Actual	Comment	Reference
A	198	HIS	-	expression tag	UNP P04578
A	199	HIS	-	expression tag	UNP P04578

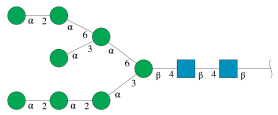
- Molecule 2 is a protein called PGT128 light chain, Ig lambda-2 chain C regions.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	207	1527	958	254	311	4	0	0	0

- Molecule 3 is a protein called PGT128 heavy chain, Ig gamma-1 chain C region.

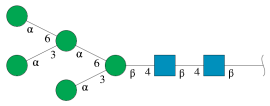
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	234	1750	1115	293	336	6	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	B	10	116	64	2	50	0	0	0

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



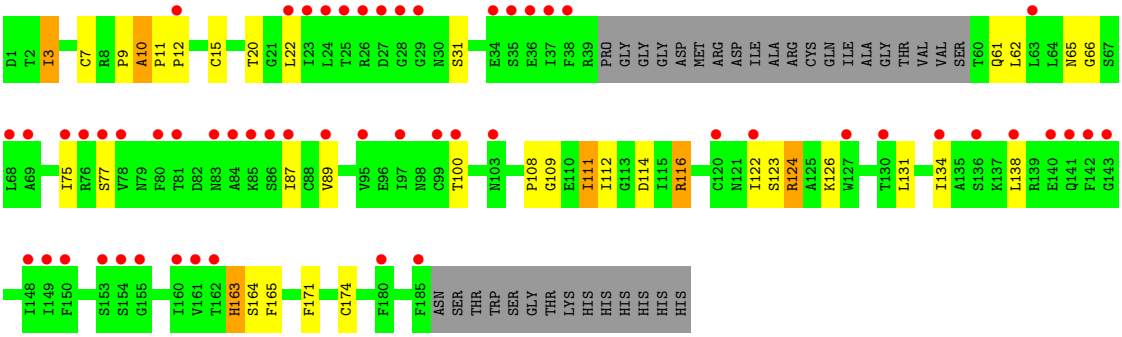
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	C	7	83	46	2	35	0	0	0

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.

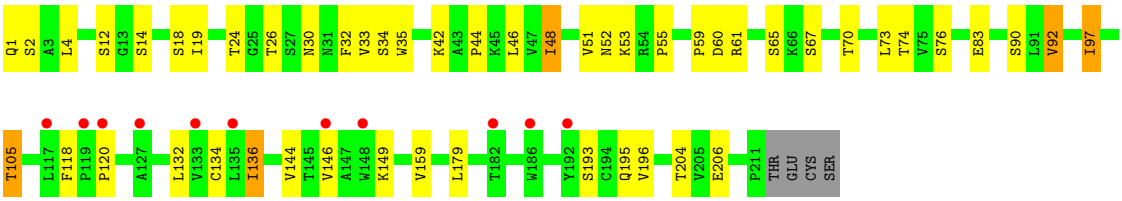
- Molecule 1: Envelope glycoprotein gp160

Chain A:



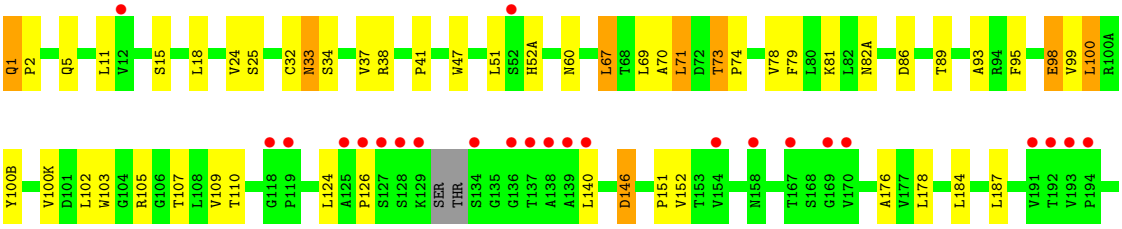
- Molecule 2: PGT128 light chain, Ig lambda-2 chain C regions

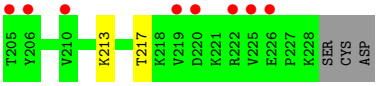
Chain L:



- Molecule 3: PGT128 heavy chain, Ig gamma-1 chain C region

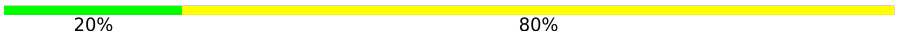
Chain H:





• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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

Chain B:



• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.79Å 73.51Å 241.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 3.25 49.70 – 3.07	Depositor EDS
% Data completeness (in resolution range)	89.9 (49.70-3.25) 79.0 (49.70-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.207 , 0.257 0.232 , 0.291	Depositor DCC
R_{free} test set	420 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.8	Xtriage
Anisotropy	1.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 110.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4715	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: PCA, BMA, 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	0.43	0/1259	0.70	0/1713
2	L	0.46	0/1558	0.71	0/2132
3	H	0.45	0/1794	0.70	0/2464
All	All	0.45	0/4611	0.70	0/6309

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	A	1239	0	1164	18	0
2	L	1527	0	1479	17	0
3	H	1750	0	1686	23	0
4	B	116	0	97	0	0
5	C	83	0	70	3	0
All	All	4715	0	4496	54	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 6.

All (54) 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:7:CYS:HA	1:A:174:CYS:HB2	1.46	0.94
1:A:10:ALA:HB1	1:A:11:PRO:HA	1.48	0.93
3:H:73:THR:HG21	5:C:3:BMA:O2	1.90	0.72
2:L:30:ASN:HD22	2:L:32:PHE:H	1.39	0.70
1:A:7:CYS:HA	1:A:174:CYS:CB	2.23	0.66
3:H:34:SER:HB2	3:H:95:PHE:O	1.96	0.66
1:A:114:ASP:HA	3:H:100(B):TYR:O	1.97	0.65
1:A:10:ALA:CB	1:A:11:PRO:HA	2.25	0.64
2:L:26:THR:HG22	2:L:90:SER:CB	2.29	0.63
2:L:35:TRP:HB2	2:L:48:ILE:HG22	1.79	0.62
3:H:18:LEU:HD13	3:H:109:VAL:HG11	1.81	0.61
1:A:20:THR:HG21	1:A:66:GLY:H	1.67	0.59
3:H:70:ALA:HB3	3:H:79:PHE:HB2	1.85	0.59
1:A:112:ILE:HG22	3:H:100:LEU:HD21	1.86	0.56
1:A:164:SER:HB2	1:A:171:PHE:CZ	2.41	0.56
3:H:176:ALA:HA	3:H:187:LEU:HB3	1.89	0.55
3:H:38:ARG:HH12	3:H:86:ASP:HA	1.73	0.53
2:L:26:THR:HG22	2:L:90:SER:HB2	1.91	0.53
2:L:32:PHE:HE1	3:H:98:GLU:HB2	1.74	0.53
3:H:126:PRO:HG3	3:H:140:LEU:HB3	1.92	0.51
1:A:131:LEU:HA	1:A:134:ILE:HD12	1.92	0.51
3:H:99:VAL:O	3:H:100(B):TYR:HD2	1.93	0.51
1:A:3:ILE:HG23	1:A:124:ARG:HG2	1.92	0.51
1:A:163:HIS:CE1	1:A:165:PHE:HB3	2.46	0.50
1:A:75:ILE:HG22	1:A:89:VAL:HA	1.92	0.50
1:A:11:PRO:HD2	1:A:12:PRO:HD3	1.94	0.50
3:H:93:ALA:HB1	3:H:100(K):VAL:HG13	1.96	0.48
3:H:73:THR:HG23	3:H:74:PRO:HD3	1.96	0.48
1:A:123:SER:HB3	1:A:126:LYS:HB2	1.96	0.48
3:H:37:VAL:HG22	3:H:47:TRP:HA	1.96	0.48
2:L:83:GLU:HG3	2:L:105:THR:HA	1.96	0.47
2:L:146:VAL:HG22	2:L:196:VAL:HG13	1.98	0.46
2:L:92:VAL:HG21	2:L:97:ILE:HG13	1.99	0.45
2:L:136:ILE:HG12	2:L:196:VAL:HG21	2.00	0.43
2:L:118:PHE:CD1	3:H:124:LEU:HB3	2.54	0.43
2:L:59:PRO:HB2	2:L:61:ARG:HG2	2.00	0.43
3:H:2:PRO:HB2	3:H:102:LEU:HD22	2.00	0.43
3:H:32:CYS:SG	5:C:1:NAG:H61	2.59	0.43
1:A:108:PRO:HA	1:A:109:GLY:HA2	1.82	0.43
3:H:52(A):HIS:NE2	3:H:71:LEU:HB3	2.34	0.42
2:L:4:LEU:HD22	2:L:26:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:33:ASN:HA	3:H:100:LEU:HB2	2.02	0.42
1:A:77:SER:HB2	1:A:87:ILE:HG23	2.02	0.42
2:L:46:LEU:HD23	2:L:55:PRO:HG3	2.01	0.41
3:H:1:PCA:HB2	3:H:2:PRO:HD3	2.02	0.41
5:C:4:MAN:H61	5:C:6:MAN:H2	1.67	0.41
3:H:67:LEU:HD11	3:H:69:LEU:HG	2.03	0.41
2:L:18:SER:HB3	2:L:76:SER:HA	2.02	0.41
2:L:149:LYS:HB2	2:L:193:SER:HB2	2.03	0.41
2:L:120:PRO:HD3	2:L:132:LEU:HG	2.02	0.41
3:H:2:PRO:HA	3:H:25:SER:O	2.21	0.41
2:L:44:PRO:HD2	3:H:103:TRP:CE3	2.56	0.41
1:A:62:LEU:HB2	1:A:163:HIS:CE1	2.56	0.40
1:A:111:ILE:H	1:A:111:ILE:HD13	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	161/199 (81%)	135 (84%)	20 (12%)	6 (4%)	3 19
2	L	205/211 (97%)	186 (91%)	18 (9%)	1 (0%)	29 62
3	H	230/239 (96%)	206 (90%)	20 (9%)	4 (2%)	9 36
All	All	596/649 (92%)	527 (88%)	58 (10%)	11 (2%)	8 35

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	15	CYS
1	A	116	ARG
1	A	163	HIS

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Mol	Chain	Res	Type
3	H	146	ASP
3	H	100	LEU
1	A	10	ALA
1	A	31	SER
2	L	51	VAL
3	H	41	PRO
3	H	151	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	A	139/175 (79%)	129 (93%)	10 (7%)	14	41
2	L	171/176 (97%)	143 (84%)	28 (16%)	2	10
3	H	192/202 (95%)	168 (88%)	24 (12%)	4	19
All	All	502/553 (91%)	440 (88%)	62 (12%)	4	19

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	22	LEU
1	A	61	GLN
1	A	65	ASN
1	A	100	THR
1	A	111	ILE
1	A	116	ARG
1	A	122	ILE
1	A	124	ARG
1	A	138	LEU
2	L	2	SER
2	L	12	SER
2	L	14	SER
2	L	19	ILE
2	L	24	THR

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Mol	Chain	Res	Type
2	L	33	VAL
2	L	34	SER
2	L	42	LYS
2	L	48	ILE
2	L	52	ASN
2	L	53	LYS
2	L	60	ASP
2	L	65	SER
2	L	67	SER
2	L	70	THR
2	L	73	LEU
2	L	74	THR
2	L	92	VAL
2	L	97	ILE
2	L	105	THR
2	L	134	CYS
2	L	136	ILE
2	L	144	VAL
2	L	159	VAL
2	L	179	LEU
2	L	195	GLN
2	L	204	THR
2	L	206	GLU
3	H	5	GLN
3	H	11	LEU
3	H	15	SER
3	H	24	VAL
3	H	33	ASN
3	H	51	LEU
3	H	60	ASN
3	H	67	LEU
3	H	71	LEU
3	H	73	THR
3	H	78	VAL
3	H	81	LYS
3	H	82(A)	ASN
3	H	89	THR
3	H	98	GLU
3	H	105	ARG
3	H	107	THR
3	H	110	THR
3	H	146	ASP

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Mol	Chain	Res	Type
3	H	152	VAL
3	H	178	LEU
3	H	184	LEU
3	H	213	LYS
3	H	217	THR

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

Mol	Chain	Res	Type
2	L	30	ASN
2	L	195	GLN
3	H	179	GLN
3	H	209	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PCA	L	1	2	7,8,9	1.43	2 (28%)	9,10,12	2.17	4 (44%)
3	PCA	H	1	3	7,8,9	0.68	0	9,10,12	2.45	4 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PCA	L	1	2	-	0/0/11/13	0/1/1/1
3	PCA	H	1	3	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1	PCA	CG-CD	2.44	1.57	1.50
2	L	1	PCA	CB-CG	2.32	1.58	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1	PCA	CB-CA-C	5.13	119.77	112.70
2	L	1	PCA	CB-CA-C	4.62	119.06	112.70
3	H	1	PCA	O-C-CA	-2.79	117.46	124.78
2	L	1	PCA	OE-CD-CG	2.75	131.57	126.76
3	H	1	PCA	CB-CA-N	2.71	111.07	103.30
3	H	1	PCA	CA-N-CD	-2.36	105.51	113.58
2	L	1	PCA	CA-N-CD	-2.23	105.95	113.58
2	L	1	PCA	O-C-CA	-2.08	119.33	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	PCA	1	0

5.5 Carbohydrates (i)

17 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	B	1	1,4	14,14,15	0.31	0	17,19,21	0.89	1 (5%)
4	MAN	B	10	4	11,11,12	0.34	0	15,15,17	0.92	2 (13%)
4	NAG	B	2	4	14,14,15	0.33	0	17,19,21	0.91	1 (5%)
4	BMA	B	3	4	11,11,12	0.42	0	15,15,17	0.62	0
4	MAN	B	4	4	11,11,12	0.43	0	15,15,17	1.07	1 (6%)
4	MAN	B	5	4	11,11,12	0.48	0	15,15,17	1.04	2 (13%)
4	MAN	B	6	4	11,11,12	0.48	0	15,15,17	1.20	1 (6%)
4	MAN	B	7	4	11,11,12	0.28	0	15,15,17	1.12	1 (6%)
4	MAN	B	8	4	11,11,12	0.37	0	15,15,17	1.27	1 (6%)
4	MAN	B	9	4	11,11,12	0.33	0	15,15,17	0.76	0
5	NAG	C	1	5,1	14,14,15	0.31	0	17,19,21	0.87	1 (5%)
5	NAG	C	2	5	14,14,15	0.31	0	17,19,21	2.39	4 (23%)
5	BMA	C	3	5	11,11,12	0.43	0	15,15,17	1.23	2 (13%)
5	MAN	C	4	5	11,11,12	0.43	0	15,15,17	0.88	1 (6%)
5	MAN	C	5	5	11,11,12	0.43	0	15,15,17	0.86	1 (6%)
5	MAN	C	6	5	11,11,12	0.46	0	15,15,17	0.82	1 (6%)
5	MAN	C	7	5	11,11,12	0.33	0	15,15,17	1.31	2 (13%)

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	B	1	1,4	-	0/6/23/26	0/1/1/1
4	MAN	B	10	4	-	1/2/19/22	0/1/1/1
4	NAG	B	2	4	-	1/6/23/26	0/1/1/1
4	BMA	B	3	4	-	0/2/19/22	0/1/1/1
4	MAN	B	4	4	-	1/2/19/22	0/1/1/1
4	MAN	B	5	4	-	0/2/19/22	0/1/1/1
4	MAN	B	6	4	-	0/2/19/22	0/1/1/1
4	MAN	B	7	4	-	0/2/19/22	0/1/1/1
4	MAN	B	8	4	-	0/2/19/22	0/1/1/1
4	MAN	B	9	4	-	1/2/19/22	0/1/1/1
5	NAG	C	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	C	2	5	-	1/6/23/26	0/1/1/1
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1
5	MAN	C	4	5	-	2/2/19/22	0/1/1/1
5	MAN	C	5	5	-	0/2/19/22	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	MAN	C	7	5	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	2	NAG	C1-C2-N2	8.37	124.79	110.49
4	B	8	MAN	C1-O5-C5	4.51	118.30	112.19
4	B	4	MAN	C1-O5-C5	3.85	117.41	112.19
4	B	6	MAN	C1-C2-C3	3.64	114.14	109.67
4	B	7	MAN	C1-O5-C5	3.55	117.00	112.19
5	C	7	MAN	C1-O5-C5	3.43	116.83	112.19
5	C	4	MAN	C1-O5-C5	2.96	116.20	112.19
5	C	3	BMA	O3-C3-C2	2.80	115.36	109.99
4	B	2	NAG	O5-C1-C2	-2.77	106.91	111.29
4	B	1	NAG	C1-O5-C5	2.58	115.69	112.19
5	C	2	NAG	C1-O5-C5	2.56	115.66	112.19
5	C	5	MAN	C1-C2-C3	2.49	112.72	109.67
5	C	2	NAG	O5-C1-C2	-2.46	107.41	111.29
4	B	5	MAN	O2-C2-C3	-2.44	105.24	110.14
5	C	7	MAN	O5-C1-C2	-2.42	107.03	110.77
5	C	3	BMA	O3-C3-C4	2.39	115.88	110.35
4	B	10	MAN	C1-O5-C5	2.29	115.30	112.19
5	C	2	NAG	C4-C3-C2	-2.22	107.77	111.02
4	B	5	MAN	C1-O5-C5	2.18	115.14	112.19
4	B	10	MAN	C1-C2-C3	2.13	112.29	109.67
5	C	1	NAG	C1-C2-N2	2.12	114.11	110.49
5	C	6	MAN	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1	NAG	C8-C7-N2-C2
5	C	1	NAG	O7-C7-N2-C2
5	C	4	MAN	O5-C5-C6-O6
5	C	4	MAN	C4-C5-C6-O6
5	C	6	MAN	O5-C5-C6-O6
5	C	1	NAG	C1-C2-N2-C7
5	C	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	B	4	MAN	O5-C5-C6-O6
4	B	10	MAN	O5-C5-C6-O6
5	C	7	MAN	O5-C5-C6-O6
4	B	2	NAG	O5-C5-C6-O6
4	B	9	MAN	C4-C5-C6-O6
5	C	6	MAN	C4-C5-C6-O6

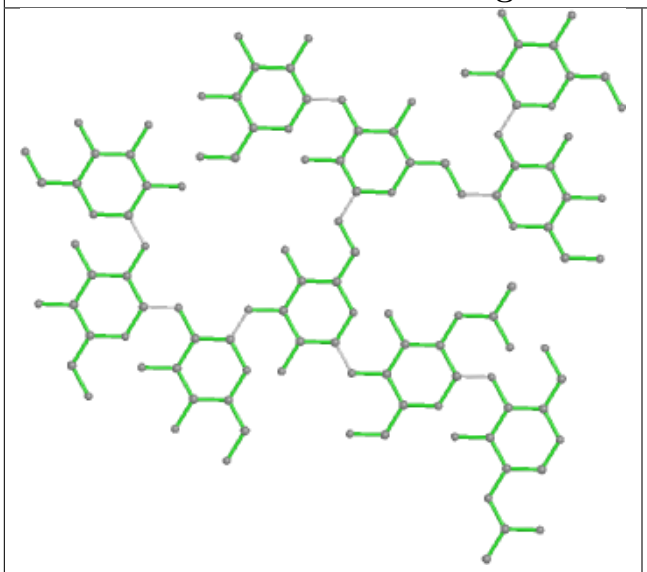
There are no ring outliers.

4 monomers are involved in 3 short contacts:

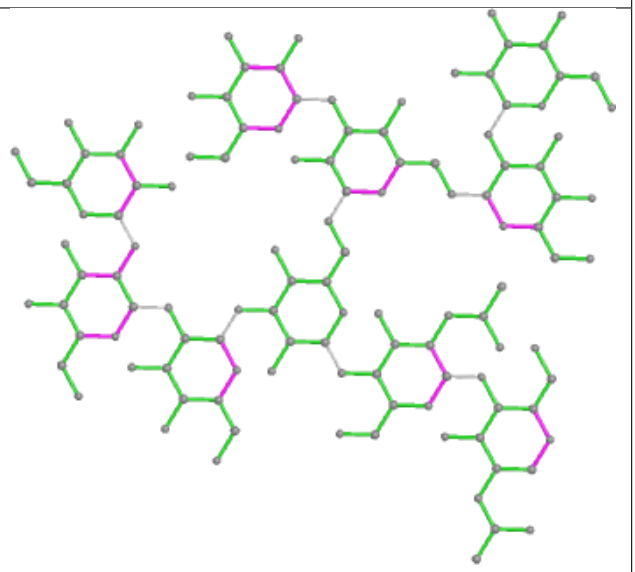
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1	NAG	1	0
5	C	4	MAN	1	0
5	C	6	MAN	1	0
5	C	3	BMA	1	0

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

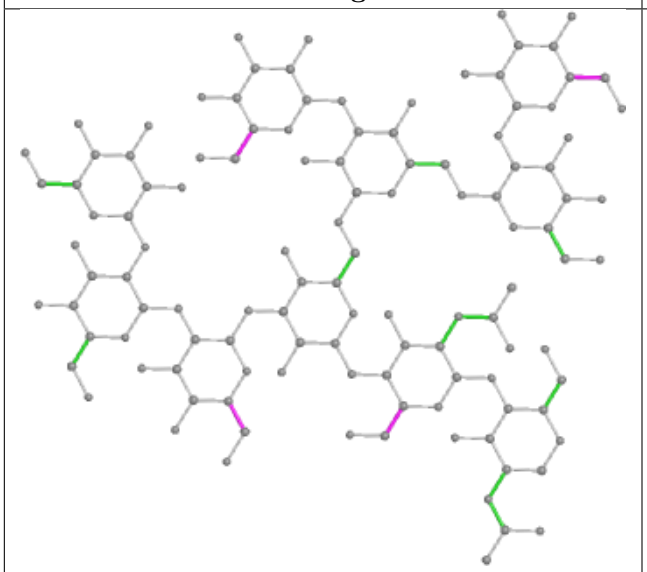
Oligosaccharide Chain B



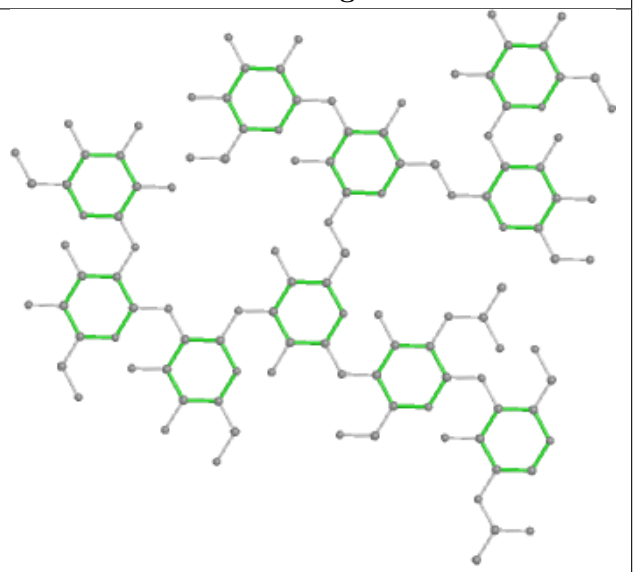
Bond lengths



Bond angles

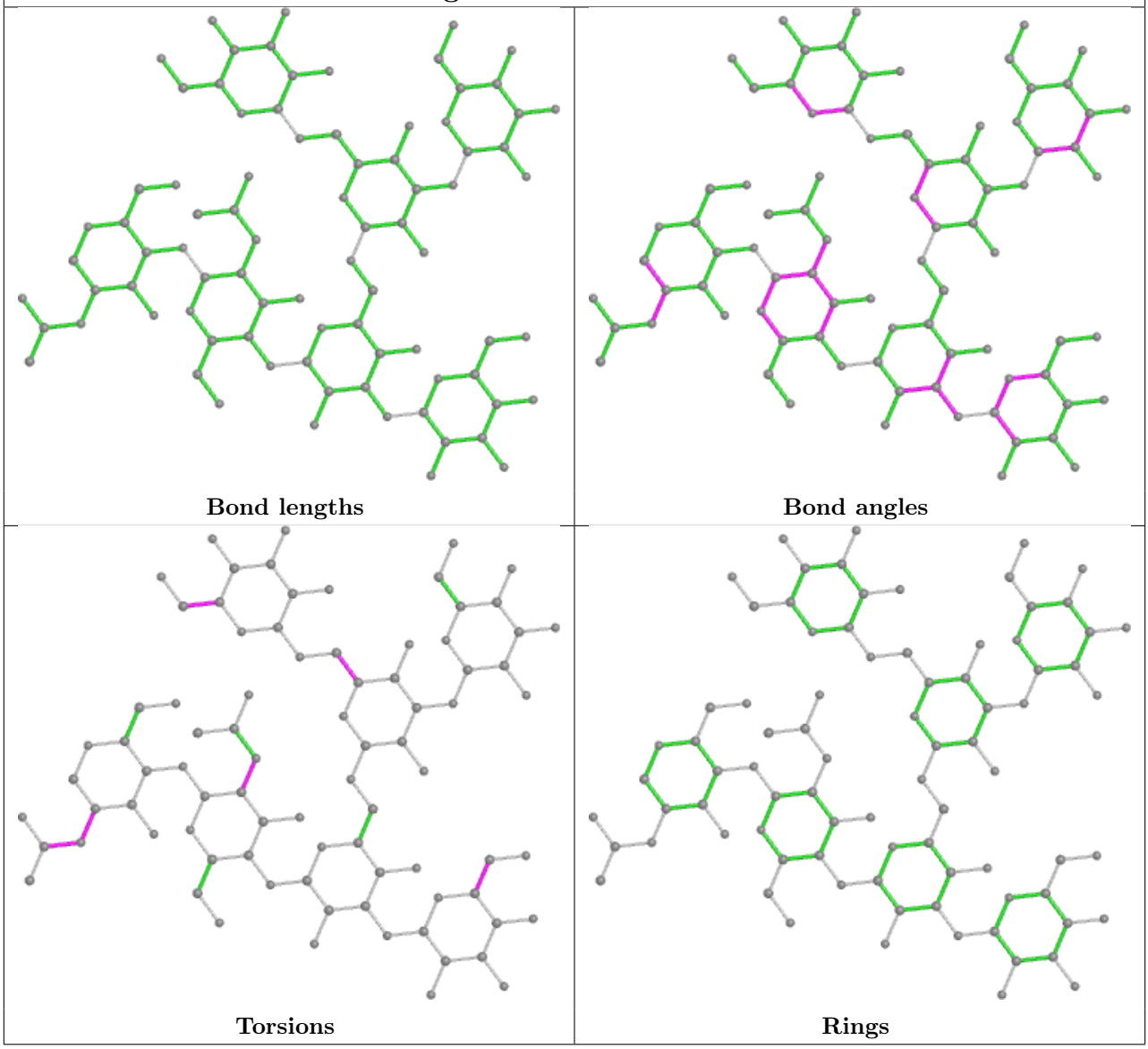


Torsions



Rings

Oligosaccharide Chain C



5.6 Ligand geometry (i)

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	165/199 (82%)	1.75	56 (33%)	0	0	72, 172, 206, 212	0
2	L	206/211 (97%)	0.39	11 (5%)	26	24	32, 76, 168, 183	0
3	H	233/239 (97%)	0.80	32 (13%)	3	3	42, 87, 181, 208	0
All	All	604/649 (93%)	0.92	99 (16%)	1	2	32, 130, 198, 212	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	ILE	14.3
3	H	128	SER	14.2
3	H	129	LYS	12.1
1	A	24	LEU	7.4
3	H	127	SER	7.1
1	A	141	GLN	6.9
3	H	139	ALA	6.8
1	A	161	VAL	6.7
3	H	193	VAL	6.4
1	A	77	SER	6.3
1	A	36	GLU	6.3
1	A	154	SER	6.2
1	A	80	PHE	6.1
1	A	25	THR	6.0
1	A	83	ASN	5.7
3	H	154	VAL	5.7
1	A	63	LEU	5.5
3	H	219	VAL	5.4
3	H	126	PRO	5.4
3	H	134	SER	5.4
1	A	29	GLY	5.4
2	L	120	PRO	5.3
1	A	68	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
3	H	140	LEU	5.1
3	H	137	THR	4.9
3	H	205	THR	4.7
1	A	38	PHE	4.7
1	A	150	PHE	4.6
1	A	149	ILE	4.5
1	A	35	SER	4.3
3	H	225	VAL	4.1
1	A	75	ILE	4.0
3	H	210	VAL	3.9
1	A	28	GLY	3.9
1	A	84	ALA	3.9
3	H	220	ASP	3.9
1	A	87	ILE	3.7
1	A	76	ARG	3.7
1	A	34	GLU	3.7
1	A	86	SER	3.6
3	H	226	GLU	3.6
3	H	136	GLY	3.6
1	A	69	ALA	3.6
2	L	192	TYR	3.6
1	A	120	CYS	3.6
1	A	97	ILE	3.5
2	L	117	LEU	3.5
1	A	23	ILE	3.4
3	H	169	GLY	3.4
1	A	22	LEU	3.4
1	A	148	ILE	3.4
1	A	78	VAL	3.4
1	A	127	TRP	3.4
1	A	140	GLU	3.3
3	H	222	ARG	3.3
1	A	95	VAL	3.2
2	L	148	TRP	3.2
1	A	153	SER	3.2
1	A	130	THR	3.2
1	A	26	ARG	3.1
2	L	146	VAL	3.0
3	H	170	VAL	3.0
2	L	186	TRP	2.9
3	H	138	ALA	2.9
1	A	155	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	142	PHE	2.8
1	A	122	ILE	2.8
3	H	191	VAL	2.8
3	H	192	THR	2.8
3	H	194	PRO	2.8
1	A	185	PHE	2.7
2	L	127	ALA	2.6
3	H	167	THR	2.6
1	A	160	ILE	2.5
3	H	52	SER	2.5
1	A	12	PRO	2.5
2	L	133	VAL	2.4
1	A	27	ASP	2.4
3	H	119	PRO	2.4
2	L	182	THR	2.4
1	A	81	THR	2.3
1	A	143	GLY	2.3
3	H	118	GLY	2.3
1	A	138	LEU	2.2
2	L	119	PRO	2.2
1	A	162	THR	2.2
1	A	99	CYS	2.2
3	H	12	VAL	2.2
1	A	85	LYS	2.2
1	A	89	VAL	2.2
1	A	100	THR	2.1
1	A	134	ILE	2.1
3	H	206	TYR	2.1
1	A	136	SER	2.1
1	A	180	PHE	2.1
1	A	103	ASN	2.0
3	H	158	ASN	2.0
2	L	135	LEU	2.0
3	H	125	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	PCA	L	1	8/9	0.89	0.22	76,78,81,83	0
3	PCA	H	1	8/9	0.89	0.28	89,92,94,94	0

6.3 Carbohydrates (i)

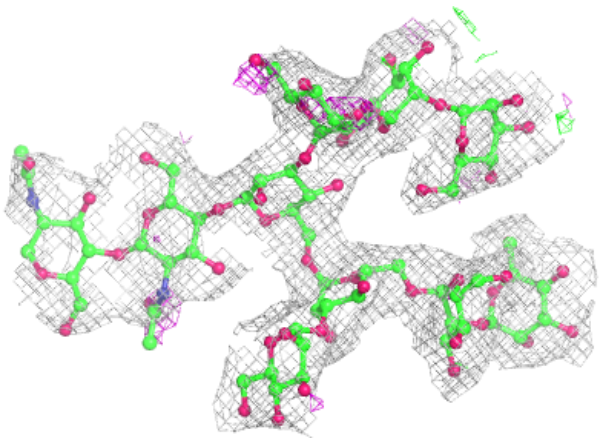
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

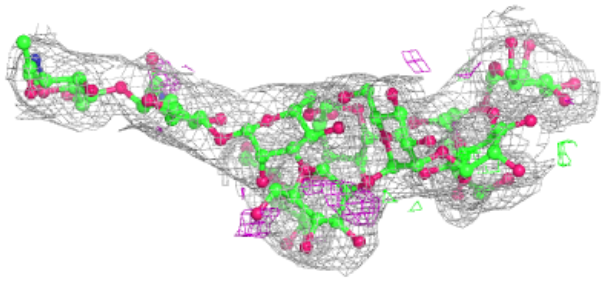
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	C	7	11/12	0.73	0.30	79,83,85,85	0
5	MAN	C	6	11/12	0.79	0.26	100,105,107,108	0
5	MAN	C	5	11/12	0.85	0.24	95,96,97,99	0
4	NAG	B	2	14/15	0.87	0.20	73,79,90,92	0
4	MAN	B	10	11/12	0.87	0.19	98,104,105,106	0
5	BMA	C	3	11/12	0.87	0.24	63,74,79,82	0
4	NAG	B	1	14/15	0.89	0.23	87,95,101,102	0
4	MAN	B	4	11/12	0.90	0.19	58,71,78,81	0
5	MAN	C	4	11/12	0.91	0.21	84,90,95,99	0
4	MAN	B	7	11/12	0.91	0.17	69,78,86,96	0
4	MAN	B	6	11/12	0.92	0.26	52,54,57,58	0
4	BMA	B	3	11/12	0.93	0.25	67,70,74,77	0
5	NAG	C	1	14/15	0.94	0.21	35,39,49,50	0
4	MAN	B	5	11/12	0.95	0.25	38,41,54,54	0
4	MAN	B	8	11/12	0.95	0.17	61,68,70,71	0
5	NAG	C	2	14/15	0.95	0.23	39,45,57,59	0
4	MAN	B	9	11/12	0.95	0.25	46,55,59,60	0

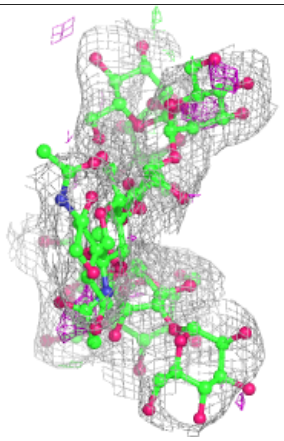
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

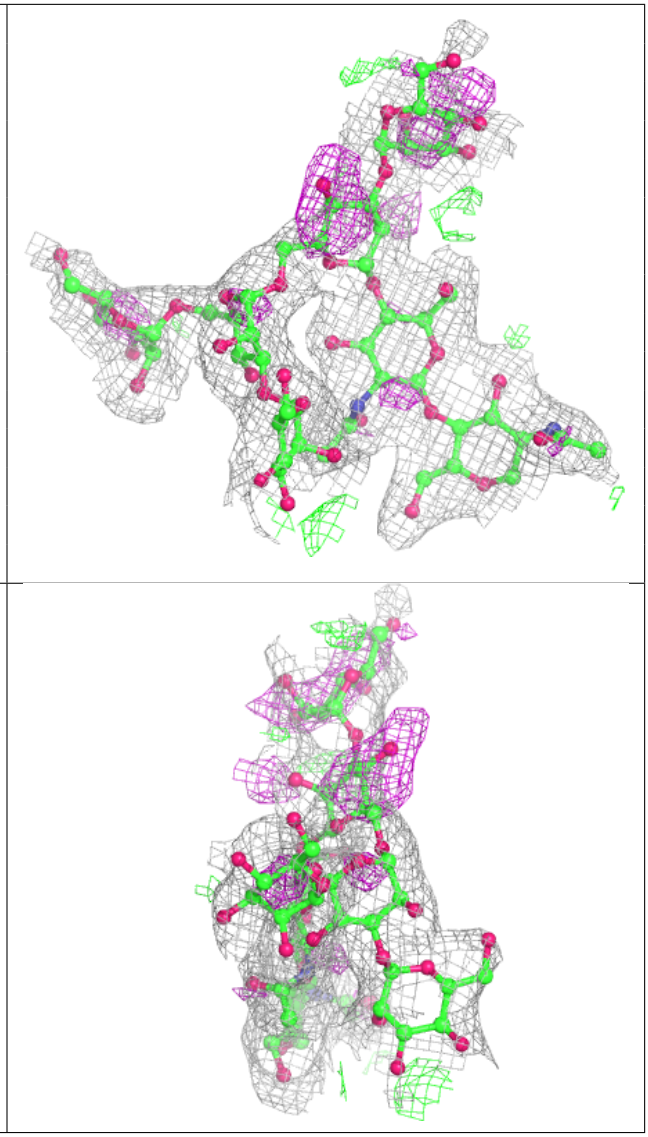






Electron density around Chain C:

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



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.