Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 10:11 am GMT

PDB ID	:	5LBV
Title	:	Structural basis of zika and dengue virus potent antibody cross-neutralization
Authors	:	Barba-Spaeth, G.
Deposited on	:	2016-06-17
Resolution	:	2.20 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

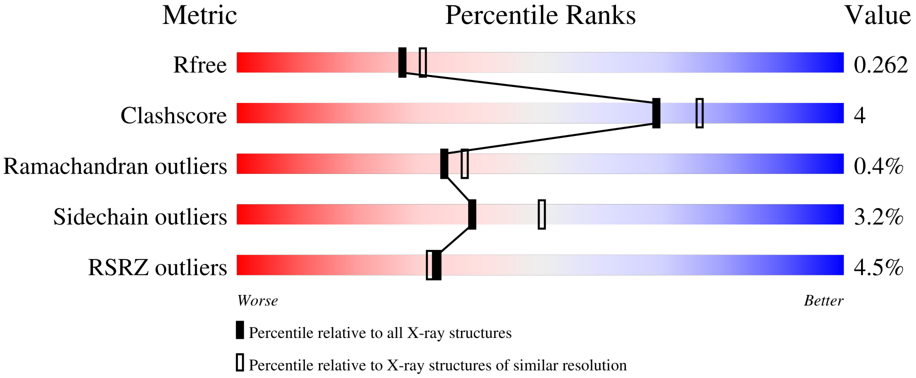
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

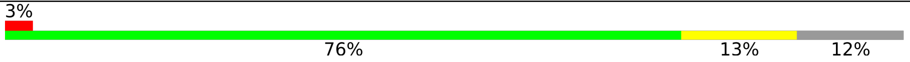
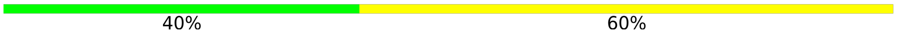
The reported resolution of this entry is 2.20 Å.

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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	447	
1	B	447	
2	C	5	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6074 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 protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	2961	1850	514	573	24	0	0	0
1	B	394	3011	1882	525	578	26	0	0	0

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	GLY	-	expression tag	UNP A0A120IIH9
A	410	PRO	-	expression tag	UNP A0A120IIH9
A	411	PHE	-	expression tag	UNP A0A120IIH9
A	412	GLU	-	expression tag	UNP A0A120IIH9
A	413	ASP	-	expression tag	UNP A0A120IIH9
A	414	ASP	-	expression tag	UNP A0A120IIH9
A	415	ASP	-	expression tag	UNP A0A120IIH9
A	416	ASP	-	expression tag	UNP A0A120IIH9
A	417	LYS	-	expression tag	UNP A0A120IIH9
A	418	ALA	-	expression tag	UNP A0A120IIH9
A	419	GLY	-	expression tag	UNP A0A120IIH9
A	420	TRP	-	expression tag	UNP A0A120IIH9
A	421	SER	-	expression tag	UNP A0A120IIH9
A	422	HIS	-	expression tag	UNP A0A120IIH9
A	423	PRO	-	expression tag	UNP A0A120IIH9
A	424	GLN	-	expression tag	UNP A0A120IIH9
A	425	PHE	-	expression tag	UNP A0A120IIH9
A	426	GLU	-	expression tag	UNP A0A120IIH9
A	427	LYS	-	expression tag	UNP A0A120IIH9
A	428	GLY	-	expression tag	UNP A0A120IIH9
A	429	GLY	-	expression tag	UNP A0A120IIH9
A	430	GLY	-	expression tag	UNP A0A120IIH9
A	431	SER	-	expression tag	UNP A0A120IIH9
A	432	GLY	-	expression tag	UNP A0A120IIH9
A	433	GLY	-	expression tag	UNP A0A120IIH9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	434	GLY	-	expression tag	UNP A0A120IIH9
A	435	SER	-	expression tag	UNP A0A120IIH9
A	436	GLY	-	expression tag	UNP A0A120IIH9
A	437	GLY	-	expression tag	UNP A0A120IIH9
A	438	GLY	-	expression tag	UNP A0A120IIH9
A	439	SER	-	expression tag	UNP A0A120IIH9
A	440	TRP	-	expression tag	UNP A0A120IIH9
A	441	SER	-	expression tag	UNP A0A120IIH9
A	442	HIS	-	expression tag	UNP A0A120IIH9
A	443	PRO	-	expression tag	UNP A0A120IIH9
A	444	GLN	-	expression tag	UNP A0A120IIH9
A	445	PHE	-	expression tag	UNP A0A120IIH9
A	446	GLU	-	expression tag	UNP A0A120IIH9
A	447	LYS	-	expression tag	UNP A0A120IIH9
B	409	GLY	-	expression tag	UNP A0A120IIH9
B	410	PRO	-	expression tag	UNP A0A120IIH9
B	411	PHE	-	expression tag	UNP A0A120IIH9
B	412	GLU	-	expression tag	UNP A0A120IIH9
B	413	ASP	-	expression tag	UNP A0A120IIH9
B	414	ASP	-	expression tag	UNP A0A120IIH9
B	415	ASP	-	expression tag	UNP A0A120IIH9
B	416	ASP	-	expression tag	UNP A0A120IIH9
B	417	LYS	-	expression tag	UNP A0A120IIH9
B	418	ALA	-	expression tag	UNP A0A120IIH9
B	419	GLY	-	expression tag	UNP A0A120IIH9
B	420	TRP	-	expression tag	UNP A0A120IIH9
B	421	SER	-	expression tag	UNP A0A120IIH9
B	422	HIS	-	expression tag	UNP A0A120IIH9
B	423	PRO	-	expression tag	UNP A0A120IIH9
B	424	GLN	-	expression tag	UNP A0A120IIH9
B	425	PHE	-	expression tag	UNP A0A120IIH9
B	426	GLU	-	expression tag	UNP A0A120IIH9
B	427	LYS	-	expression tag	UNP A0A120IIH9
B	428	GLY	-	expression tag	UNP A0A120IIH9
B	429	GLY	-	expression tag	UNP A0A120IIH9
B	430	GLY	-	expression tag	UNP A0A120IIH9
B	431	SER	-	expression tag	UNP A0A120IIH9
B	432	GLY	-	expression tag	UNP A0A120IIH9
B	433	GLY	-	expression tag	UNP A0A120IIH9
B	434	GLY	-	expression tag	UNP A0A120IIH9
B	435	SER	-	expression tag	UNP A0A120IIH9
B	436	GLY	-	expression tag	UNP A0A120IIH9

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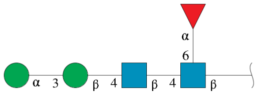
Chain	Residue	Modelled	Actual	Comment	Reference
B	437	GLY	-	expression tag	UNP A0A120IIH9
B	438	GLY	-	expression tag	UNP A0A120IIH9
B	439	SER	-	expression tag	UNP A0A120IIH9
B	440	TRP	-	expression tag	UNP A0A120IIH9
B	441	SER	-	expression tag	UNP A0A120IIH9
B	442	HIS	-	expression tag	UNP A0A120IIH9
B	443	PRO	-	expression tag	UNP A0A120IIH9
B	444	GLN	-	expression tag	UNP A0A120IIH9
B	445	PHE	-	expression tag	UNP A0A120IIH9
B	446	GLU	-	expression tag	UNP A0A120IIH9
B	447	LYS	-	expression tag	UNP A0A120IIH9

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	5	Total C N O 60 34 2 24	0	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0

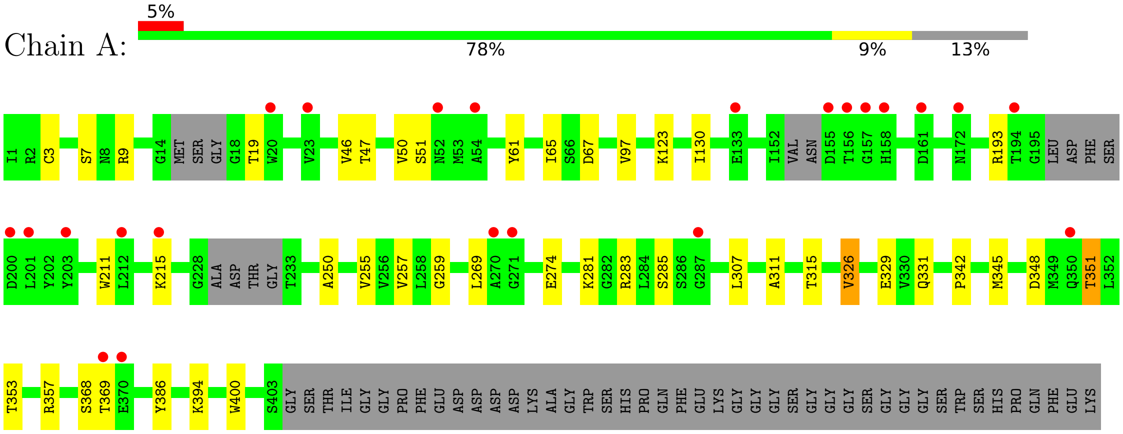
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	17	Total O 17 17	0	0
4	B	24	Total O 24 24	0	0

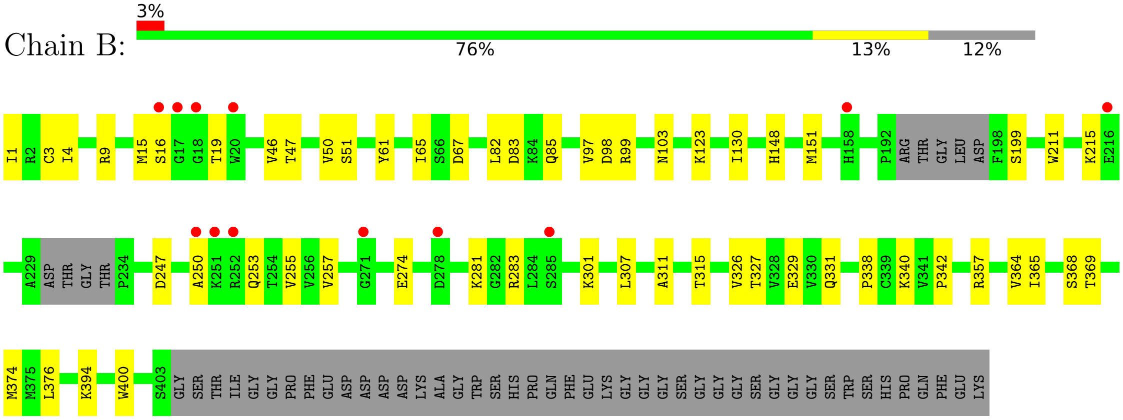
3 Residue-property plots

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.

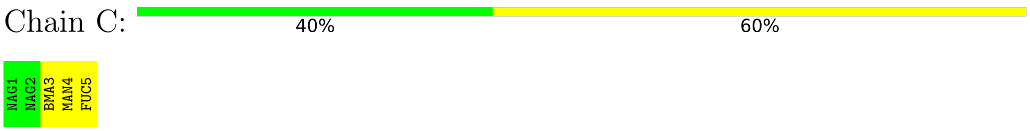
- Molecule 1: envelope protein E



- Molecule 1: envelope protein E



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



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	64.63Å 213.57Å 124.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.55 – 2.20 38.55 – 2.20	Depositor EDS
% Data completeness (in resolution range)	66.4 (38.55-2.20) 66.1 (38.55-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.207 , 0.239 0.227 , 0.262	Depositor DCC
R_{free} test set	1466 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6074	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: NA, FUC, 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	0.50	0/3019	0.74	0/4088
1	B	0.52	0/3074	0.73	0/4162
All	All	0.51	0/6093	0.73	0/8250

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	2961	0	2876	20	0
1	B	3011	0	2936	25	0
2	C	60	0	52	0	0
3	B	1	0	0	0	0
4	A	17	0	0	0	0
4	B	24	0	0	0	0
All	All	6074	0	5864	44	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 4.

All (44) 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:B:97:VAL:HG11	1:B:250:ALA:HA	1.50	0.94
1:A:97:VAL:HG11	1:A:250:ALA:HA	1.55	0.86
1:B:65:ILE:HG12	1:B:257:VAL:HG13	1.62	0.81
1:B:99:ARG:HA	1:B:103:ASN:HD22	1.54	0.73
1:A:65:ILE:HG12	1:A:257:VAL:HG23	1.81	0.62
1:B:47:THR:HG22	1:B:283:ARG:HH11	1.67	0.60
1:B:211:TRP:CD1	1:B:274:GLU:HG2	2.36	0.60
1:B:315:THR:HG23	1:B:331:GLN:HB2	1.88	0.56
1:B:338:PRO:HA	1:B:365:ILE:O	2.06	0.55
1:B:326:VAL:HG21	1:B:400:TRP:CE2	2.41	0.54
1:A:315:THR:HG23	1:A:331:GLN:HB2	1.88	0.54
1:B:50:VAL:HG21	1:B:130:ILE:HG12	1.90	0.54
1:B:311:ALA:HB2	1:B:394:LYS:HD2	1.92	0.52
1:A:326:VAL:HG13	1:A:400:TRP:CZ2	2.44	0.52
1:B:1:ILE:HD11	1:B:151:MET:HB2	1.91	0.52
1:A:311:ALA:HB2	1:A:394:LYS:HD2	1.93	0.50
1:A:61:TYR:CZ	1:A:123:LYS:HB3	2.47	0.50
1:A:326:VAL:HG13	1:A:400:TRP:CH2	2.46	0.49
1:B:61:TYR:CZ	1:B:123:LYS:HB3	2.47	0.49
1:B:51:SER:HA	1:B:281:LYS:HG2	1.94	0.49
1:A:348:ASP:OD2	1:A:351:THR:HB	2.12	0.48
1:A:47:THR:HG22	1:A:283:ARG:HH11	1.79	0.48
1:A:51:SER:HA	1:A:281:LYS:HG2	1.95	0.47
1:B:374:MET:HE1	1:B:376:LEU:HB3	1.96	0.47
1:B:340:LYS:HA	1:B:364:VAL:HG12	1.97	0.46
1:B:99:ARG:HE	1:B:103:ASN:HB3	1.81	0.45
1:A:3:CYS:HB3	1:A:9:ARG:HG3	1.98	0.45
1:B:65:ILE:HD13	1:B:255:VAL:HG22	1.99	0.45
1:B:3:CYS:HB3	1:B:9:ARG:HG3	1.99	0.45
1:A:7:SER:HB2	1:B:98:ASP:OD1	2.16	0.45
1:A:351:THR:HG22	1:A:353:THR:H	1.83	0.44
1:A:211:TRP:CD1	1:A:274:GLU:HG2	2.52	0.43
1:A:345:MET:HA	1:A:386:TYR:O	2.18	0.43
1:B:4:ILE:HG21	1:B:327:THR:HG21	2.00	0.42
1:A:257:VAL:HG12	1:A:259:GLY:H	1.85	0.42
1:B:247:ASP:HA	1:B:253:GLN:HG3	2.02	0.42
1:B:326:VAL:HG22	1:B:400:TRP:CZ2	2.56	0.41
1:A:50:VAL:HG21	1:A:130:ILE:HG23	2.03	0.41
1:A:211:TRP:CD2	1:A:269:LEU:HD13	2.56	0.41
1:A:307:LEU:HG	1:A:342:PRO:HG3	2.03	0.41
1:B:148:HIS:HB2	1:B:329:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:HD13	1:A:255:VAL:HG22	2.02	0.40
1:B:307:LEU:HG	1:B:342:PRO:HG3	2.03	0.40
1:B:82:LEU:O	1:B:85:GLN:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	380/447 (85%)	374 (98%)	5 (1%)	1 (0%)	41	46
1	B	388/447 (87%)	378 (97%)	8 (2%)	2 (0%)	29	31
All	All	768/894 (86%)	752 (98%)	13 (2%)	3 (0%)	34	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ARG
1	B	16	SER
1	B	15	MET

5.3.2 Protein sidechains ⓘ

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	321/367 (88%)	310 (97%)	11 (3%)	37 47
1	B	329/367 (90%)	319 (97%)	10 (3%)	41 53
All	All	650/734 (89%)	629 (97%)	21 (3%)	39 50

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

Mol	Chain	Res	Type
1	A	19	THR
1	A	46	VAL
1	A	67	ASP
1	A	215	LYS
1	A	285	SER
1	A	326	VAL
1	A	329	GLU
1	A	351	THR
1	A	357	ARG
1	A	368	SER
1	A	369	THR
1	B	19	THR
1	B	46	VAL
1	B	67	ASP
1	B	83	ASP
1	B	199	SER
1	B	215	LYS
1	B	301	LYS
1	B	357	ARG
1	B	368	SER
1	B	369	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	208	ASN
1	B	103	ASN
1	B	163	ASN
1	B	208	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

5 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	$\#\|Z\| > 2$
2	NAG	C	1	2,1	14,14,15	0.28	0	17,19,21	0.66	0
2	NAG	C	2	2	14,14,15	0.35	0	17,19,21	0.72	0
2	BMA	C	3	2	11,11,12	0.38	0	15,15,17	1.41	1 (6%)
2	MAN	C	4	2	11,11,12	0.35	0	15,15,17	1.32	1 (6%)
2	FUC	C	5	2	10,10,11	0.39	0	14,14,16	0.95	1 (7%)

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	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	1/1/1/1
2	FUC	C	5	2	-	-	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(°)	Ideal(°)
2	C	4	MAN	C1-O5-C5	4.89	118.82	112.19
2	C	3	BMA	C1-O5-C5	3.38	116.77	112.19
2	C	5	FUC	C3-C4-C5	2.07	113.00	109.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

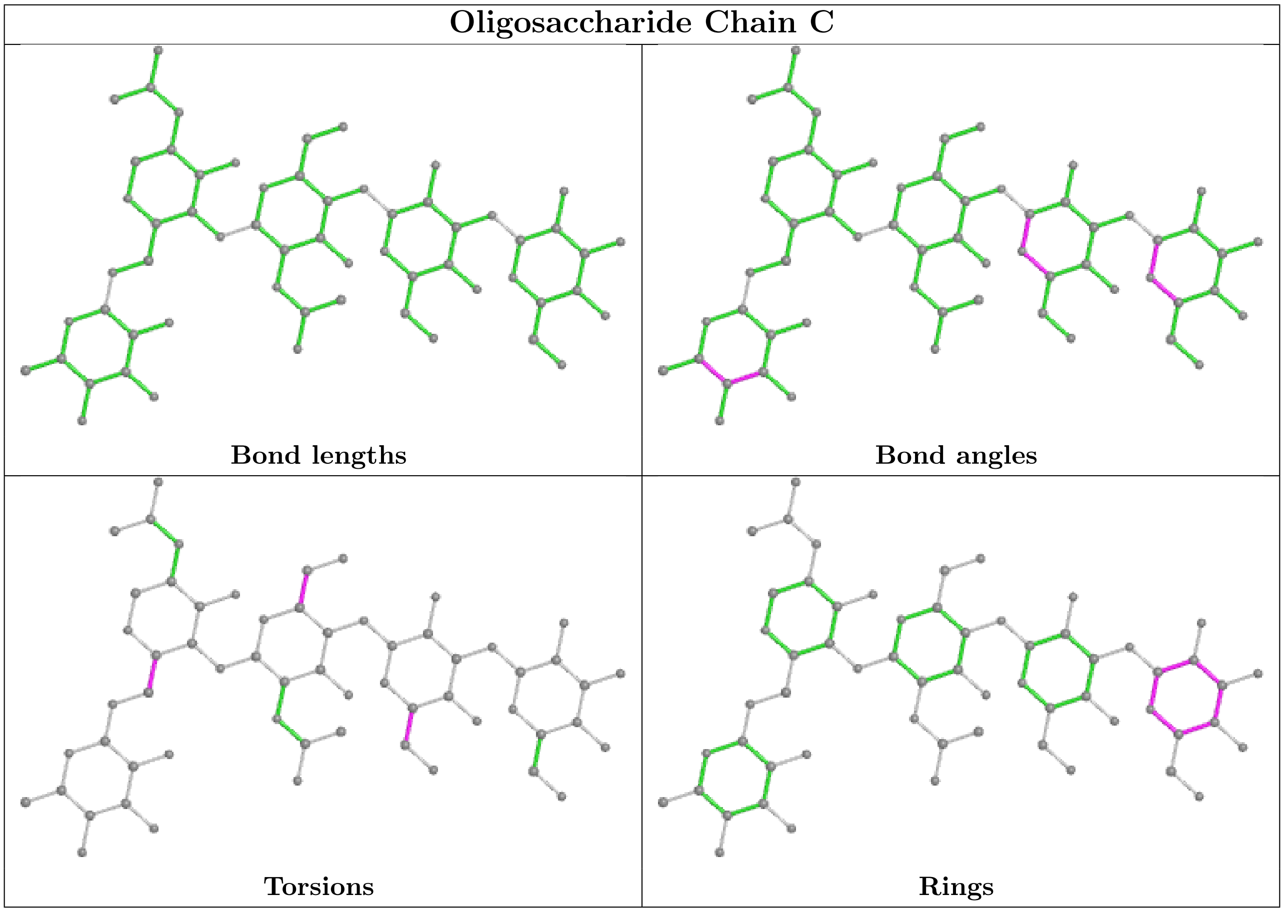
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

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



Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	390/447 (87%)	0.31	23 (5%)	22	21	34, 68, 103, 125	0
1	B	394/447 (88%)	0.04	12 (3%)	50	48	28, 54, 93, 120	0
All	All	784/894 (87%)	0.18	35 (4%)	33	32	28, 61, 100, 125	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	GLY	5.1
1	A	52	ASN	4.7
1	B	271	GLY	4.2
1	B	17	GLY	3.9
1	A	23	VAL	3.8
1	B	251	LYS	3.8
1	A	156	THR	3.7
1	A	20	TRP	3.5
1	A	157	GLY	3.4
1	B	250	ALA	3.2
1	B	216	GLU	3.2
1	A	172	ASN	3.2
1	A	215	LYS	3.1
1	A	200	ASP	3.0
1	A	133	GLU	3.0
1	B	252	ARG	3.0
1	B	16	SER	2.9
1	A	287	GLY	2.9
1	B	278	ASP	2.6
1	A	369	THR	2.5
1	B	18	GLY	2.5
1	A	270	ALA	2.4
1	A	370	GLU	2.4
1	A	212	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	194	THR	2.3
1	B	20	TRP	2.3
1	B	158	HIS	2.2
1	A	155	ASP	2.1
1	A	161	ASP	2.1
1	B	285	SER	2.1
1	A	350	GLN	2.1
1	A	203	TYR	2.1
1	A	54	ALA	2.1
1	A	158	HIS	2.0
1	A	201	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

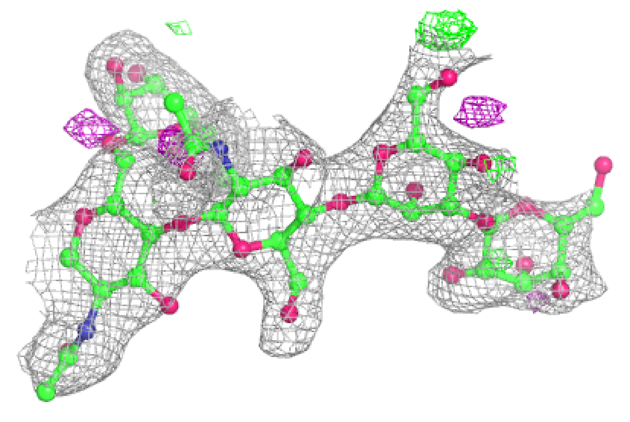
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

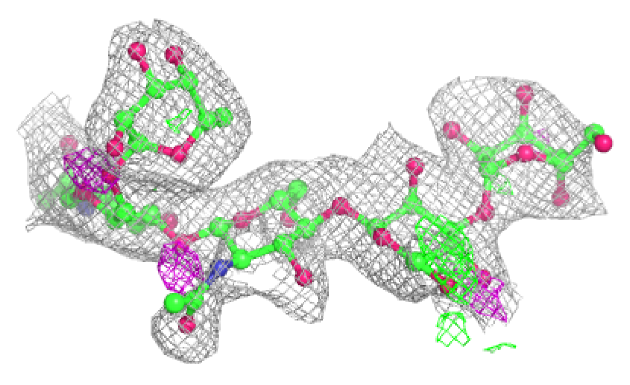
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	NAG	C	2	14/15	0.82	0.19	70,74,82,83	0
2	MAN	C	4	11/12	0.85	0.26	82,88,89,89	0
2	BMA	C	3	11/12	0.89	0.15	67,72,77,80	0
2	FUC	C	5	10/11	0.89	0.15	64,71,74,75	0
2	NAG	C	1	14/15	0.90	0.14	75,78,80,81	0

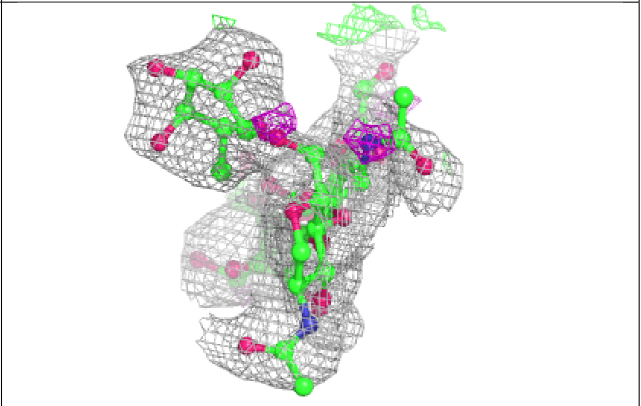
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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 ⓘ

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
3	NA	B	506	1/1	0.94	0.08	51,51,51,51	0

6.5 Other polymers ⓘ

There are no such residues in this entry.