



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 12:03 PM BST

PDB ID : 6OAI  
Title : Crystal structure of P[6] rotavirus vp8\* complexed with LNFPI  
Authors : Xu, S.; Liu, Y.; Jiang, X.; Kennedy, M.A.  
Deposited on : 2019-03-16  
Resolution : 1.90 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](mailto: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.

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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

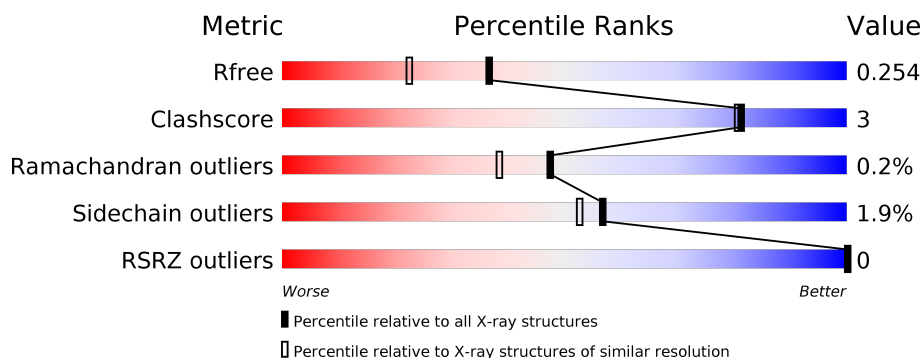
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	A	159	<div> <div>95%</div> <div>5%</div> </div>
1	B	159	<div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	C	159	<div> <div>95%</div> <div>..</div> <div>..</div> </div>
1	D	159	<div> <div>93%</div> <div>6%</div> <div>..</div> </div>
2	E	5	<div> <div>100%</div> </div>

## 2 Entry composition [i](#)

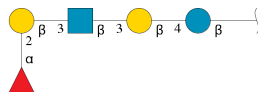
There are 3 unique types of molecules in this entry. The entry contains 5394 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Protease-sensitive outer capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1303	833	214	253	3			
1	B	158	Total	C	N	O	S	0	0	0
			1295	827	213	252	3			
1	C	158	Total	C	N	O	S	0	0	0
			1295	827	213	252	3			
1	D	158	Total	C	N	O	S	0	0	0
			1295	827	213	252	3			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			58	32	1	25			

- Molecule 3 is water.

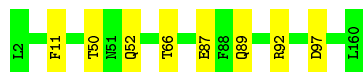
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		
3	B	42	Total	O	0	0
			42	42		
3	C	36	Total	O	0	0
			36	36		
3	D	30	Total	O	0	0
			30	30		

### 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: Protease-sensitive outer capsid protein

Chain A: 



- Molecule 1: Protease-sensitive outer capsid protein

Chain B: 



- Molecule 1: Protease-sensitive outer capsid protein

Chain C: 



- Molecule 1: Protease-sensitive outer capsid protein

Chain D: 



- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain E: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.69Å 75.87Å 74.93Å 90.00° 91.86° 90.00°	Depositor
Resolution (Å)	45.95 – 1.90 45.91 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (45.95-1.90) 97.2 (45.91-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.195 , 0.250 0.203 , 0.254	Depositor DCC
$R_{free}$ test set	2342 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.3	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-l,-k 0.000 for -h,l,k 0.031 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5394	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, GAL, NAG, FUC

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	0.83	1/1339 (0.1%)	0.81	2/1826 (0.1%)
1	B	0.86	0/1331	0.81	1/1815 (0.1%)
1	C	0.84	1/1331 (0.1%)	0.84	1/1815 (0.1%)
1	D	0.82	0/1331	0.83	0/1815
All	All	0.84	2/5332 (0.0%)	0.82	4/7271 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	GLU	CD-OE1	7.71	1.34	1.25
1	C	123	ASP	C-O	5.09	1.33	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	92	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	92	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	92	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	92	ARG	NE-CZ-NH1	5.17	122.89	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	82	SER	Mainchain

## 5.2 Too-close contacts ⓘ

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	1303	0	1247	3	0
1	B	1295	0	1236	20	0
1	C	1295	0	1236	2	0
1	D	1295	0	1236	4	0
2	E	58	0	50	0	0
3	A	40	0	0	0	0
3	B	42	0	0	1	0
3	C	36	0	0	0	0
3	D	30	0	0	0	0
All	All	5394	0	5005	27	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 3.

All (27) 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:92:ARG:HD3	3:B:316:HOH:O	1.87	0.74
1:B:113:PHE:CD1	1:B:156:ILE:HD13	2.24	0.73
1:A:66:THR:H	1:B:89:GLN:HE22	1.43	0.66
1:B:12:LYS:HE3	1:B:131:SER:O	2.02	0.59
1:B:103:PHE:CE1	1:B:110:VAL:HG13	2.39	0.58
1:A:89:GLN:HE22	1:B:66:THR:H	1.52	0.58
1:B:83:ASN:ND2	1:B:85:SER:H	2.02	0.58
1:B:25:ASN:HD22	1:B:25:ASN:H	1.54	0.54
1:B:113:PHE:CD1	1:B:156:ILE:CD1	2.90	0.54
1:B:25:ASN:HD22	1:B:25:ASN:N	2.07	0.53
1:B:2:LEU:CD2	1:B:144:ILE:HD11	2.40	0.51
1:C:25:ASN:HD22	1:C:25:ASN:C	2.12	0.50
1:B:113:PHE:CE1	1:B:156:ILE:CD1	2.96	0.48
1:C:39:TRP:HB2	1:C:81:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ASN:ND2	1:B:25:ASN:N	2.61	0.48
1:B:39:TRP:HB2	1:B:81:ARG:HG2	1.97	0.47
1:B:83:ASN:HD22	1:B:85:SER:H	1.63	0.47
1:B:39:TRP:CZ2	1:B:84:VAL:HB	2.51	0.45
1:B:113:PHE:CG	1:B:156:ILE:HD13	2.51	0.44
1:D:11:PHE:O	1:D:13:PRO:HD3	2.18	0.44
1:B:2:LEU:HD21	1:B:144:ILE:HD11	2.00	0.43
1:D:43:LEU:O	1:D:76:PHE:HA	2.18	0.43
1:B:30:LEU:HD12	1:B:137:ILE:CD1	2.50	0.42
1:B:25:ASN:ND2	1:B:25:ASN:H	2.17	0.42
1:D:144:ILE:HA	1:D:145:PRO:HD2	1.88	0.41
1:A:50:THR:O	1:A:52:GLN:HG2	2.20	0.41
1:D:39:TRP:HB2	1:D:81:ARG:HG2	2.03	0.41

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	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
1	B	156/159 (98%)	150 (96%)	5 (3%)	1 (1%)	25	15
1	C	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
1	D	156/159 (98%)	148 (95%)	8 (5%)	0	100	100
All	All	625/636 (98%)	599 (96%)	25 (4%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	107	TYR



### 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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	149/149 (100%)	147 (99%)	2 (1%)	69	68
1	B	148/149 (99%)	145 (98%)	3 (2%)	55	51
1	C	148/149 (99%)	145 (98%)	3 (2%)	55	51
1	D	148/149 (99%)	145 (98%)	3 (2%)	55	51
All	All	593/596 (100%)	582 (98%)	11 (2%)	57	53

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	97	ASP
1	B	12	LYS
1	B	16	ASP
1	B	25	ASN
1	C	11	PHE
1	C	25	ASN
1	C	82	SER
1	D	11	PHE
1	D	25	ASN
1	D	85	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	B	25	ASN
1	B	27	GLN
1	B	83	ASN
1	B	89	GLN
1	B	148	GLN
1	C	25	ASN
1	D	25	ASN

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Mol	Chain	Res	Type
1	D	148	GLN

### 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	BGC	E	1	2	12,12,12	2.25	4 (33%)	17,17,17	2.48	9 (52%)
2	GAL	E	2	2	11,11,12	1.63	3 (27%)	15,15,17	1.47	2 (13%)
2	NAG	E	3	2	14,14,15	1.74	3 (21%)	17,19,21	1.23	1 (5%)
2	GAL	E	4	2	11,11,12	2.90	4 (36%)	15,15,17	2.01	4 (26%)
2	FUC	E	5	2	10,10,11	1.88	3 (30%)	14,14,16	1.24	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	E	1	2	-	2/2/22/22	0/1/1/1
2	GAL	E	2	2	-	1/2/19/22	0/1/1/1
2	NAG	E	3	2	-	0/6/23/26	0/1/1/1
2	GAL	E	4	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUC	E	5	2	-	-	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	GAL	O4-C4	7.46	1.60	1.43
2	E	1	BGC	O2-C2	-4.60	1.32	1.43
2	E	1	BGC	O5-C1	4.15	1.53	1.42
2	E	5	FUC	C4-C5	4.01	1.61	1.52
2	E	4	GAL	O5-C5	3.93	1.51	1.43
2	E	3	NAG	C3-C2	3.80	1.60	1.52
2	E	2	GAL	O3-C3	-3.69	1.34	1.43
2	E	3	NAG	O5-C1	-3.38	1.38	1.43
2	E	1	BGC	C4-C5	2.97	1.59	1.53
2	E	4	GAL	O5-C1	2.94	1.48	1.43
2	E	3	NAG	C2-N2	2.59	1.50	1.46
2	E	5	FUC	O2-C2	-2.57	1.37	1.43
2	E	4	GAL	C4-C5	2.54	1.58	1.53
2	E	5	FUC	C2-C3	-2.47	1.48	1.52
2	E	2	GAL	C2-C3	2.38	1.56	1.52
2	E	2	GAL	O5-C5	-2.29	1.38	1.43
2	E	1	BGC	C3-C2	-2.15	1.46	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	BGC	C1-O5-C5	-4.69	104.82	113.66
2	E	3	NAG	O5-C5-C6	-4.31	100.44	107.20
2	E	1	BGC	C4-C3-C2	-4.26	103.38	110.82
2	E	1	BGC	O3-C3-C4	4.02	119.64	110.35
2	E	4	GAL	C1-O5-C5	3.93	117.52	112.19
2	E	2	GAL	C1-O5-C5	-3.88	106.94	112.19
2	E	4	GAL	O4-C4-C5	3.72	118.54	109.30
2	E	1	BGC	O3-C3-C2	-3.12	103.14	110.35
2	E	1	BGC	O4-C4-C3	2.91	117.08	110.35
2	E	4	GAL	O5-C5-C6	-2.78	102.85	107.20
2	E	5	FUC	O5-C5-C4	2.54	114.08	109.52
2	E	1	BGC	O2-C2-C3	-2.50	104.56	110.35
2	E	1	BGC	O1-C1-O5	2.45	117.74	110.38
2	E	1	BGC	O5-C1-C2	2.44	114.64	110.28
2	E	4	GAL	C3-C4-C5	-2.37	106.01	110.24
2	E	5	FUC	C1-O5-C5	2.23	117.83	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	GAL	O5-C5-C6	-2.19	103.78	107.20
2	E	1	BGC	O5-C5-C6	2.06	111.56	106.44

There are no chirality outliers.

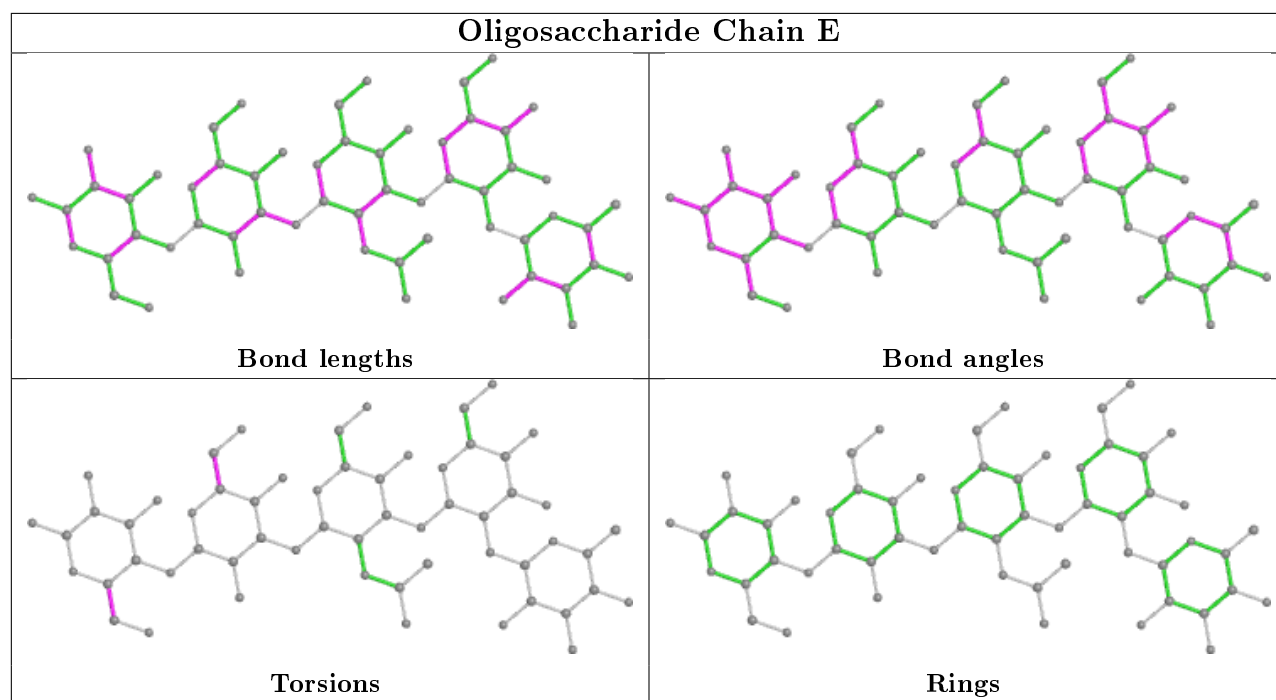
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	BGC	O5-C5-C6-O6
2	E	1	BGC	C4-C5-C6-O6
2	E	2	GAL	O5-C5-C6-O6

There are no ring outliers.

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.



## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	159/159 (100%)	-0.25	0 100 100	13, 19, 31, 42	0
1	B	158/159 (99%)	-0.23	0 100 100	14, 19, 32, 38	0
1	C	158/159 (99%)	-0.23	0 100 100	14, 20, 36, 47	0
1	D	158/159 (99%)	-0.23	0 100 100	16, 22, 33, 40	0
All	All	633/636 (99%)	-0.24	0 100 100	13, 20, 33, 47	0

There are no RSRZ outliers to report.

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

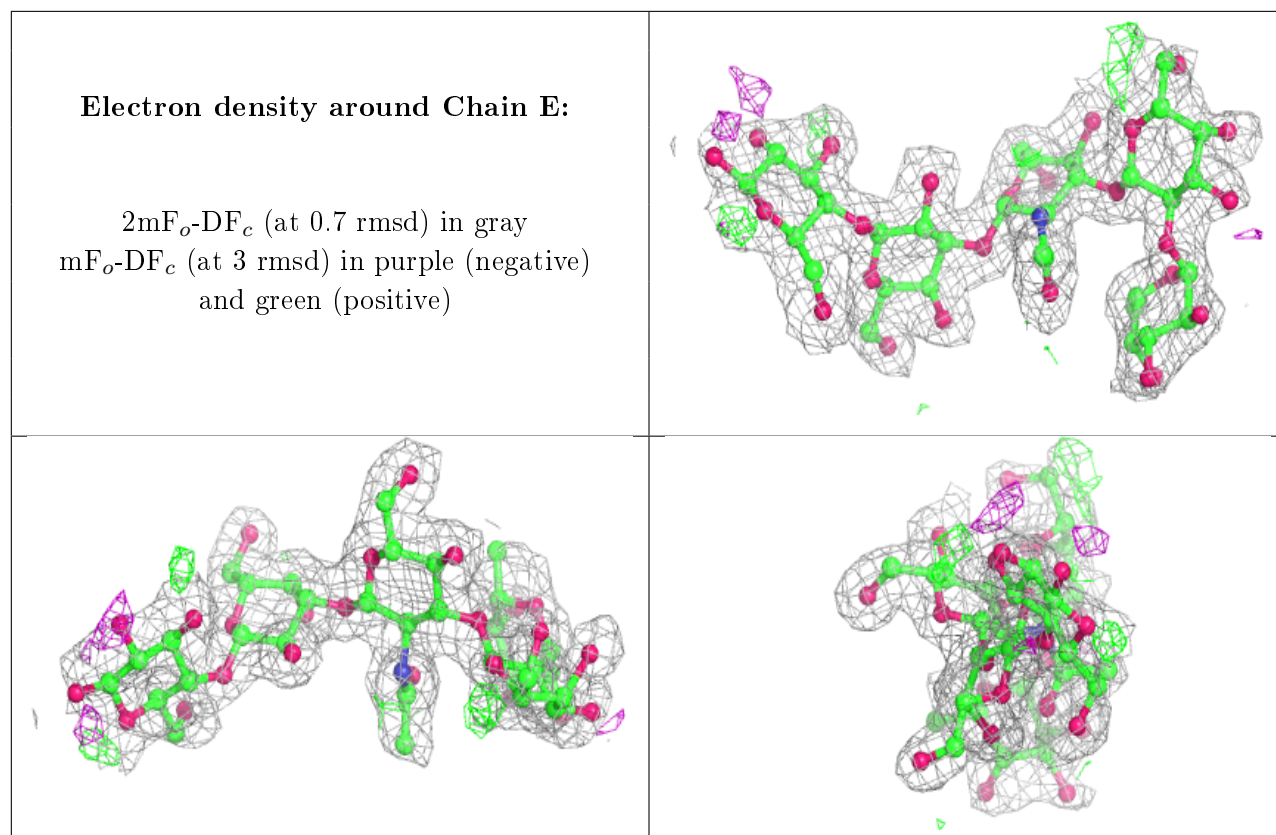
There are no non-standard protein/DNA/RNA residues in this entry.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	BGC	E	1	12/12	0.82	0.18	30,40,50,50	0
2	GAL	E	4	11/12	0.85	0.19	34,41,45,48	0
2	FUC	E	5	10/11	0.92	0.14	36,41,49,50	0
2	GAL	E	2	11/12	0.95	0.08	19,23,29,30	0
2	NAG	E	3	14/15	0.96	0.08	19,23,27,27	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.