



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:15 AM BST

PDB ID : 1I3H  
Title : CONCANAVALIN A-DIMANNOSE STRUCTURE  
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Deposited on : 2001-02-15  
Resolution : 1.20 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](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

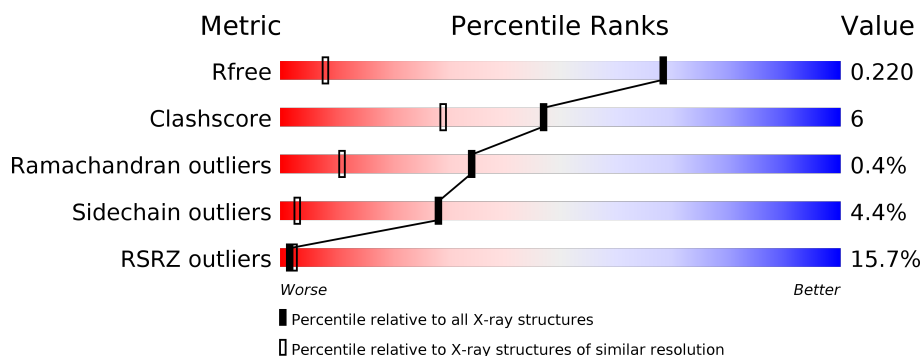
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.20 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	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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	237	<div> <div>16%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>...</div> </div> </div>
2	B	2	<div> <div>100%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2174 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 Concanavalin-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	25	11	0
			1896	1193	321	379	3			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

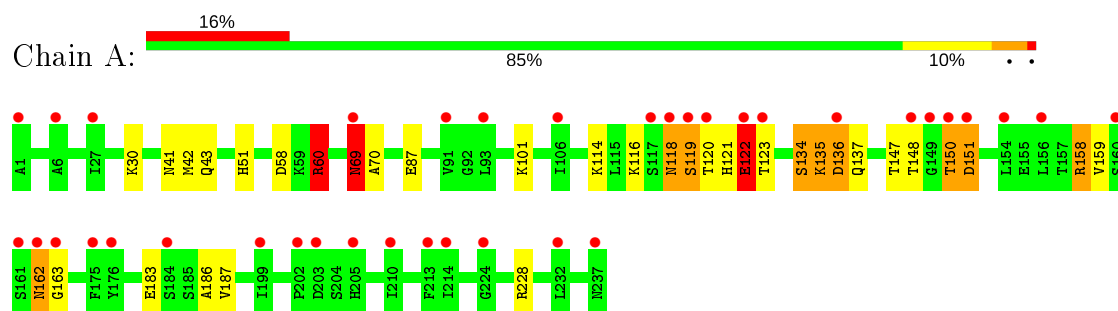
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	253	Total	O	0	0
			253	253		

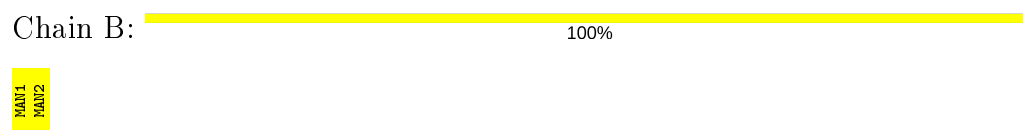
### 3 Residue-property plots

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: Concanavalin-A



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.90 Å   86.41 Å   65.42 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	40.00 – 1.20 19.51 – 1.20	Depositor EDS
% Data completeness (in resolution range)	95.1 (40.00-1.20) 95.3 (19.51-1.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 1.20 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.167   ,   0.190 0.203   ,   0.220	Depositor DCC
$R_{free}$ test set	7754 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2174	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MN, 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		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.87	6/1939 (0.3%)	1.46	19/2639 (0.7%)

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	A	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60[A]	ARG	CZ-NH2	50.34	1.98	1.33
1	A	60[B]	ARG	CZ-NH2	50.34	1.98	1.33
1	A	30	LYS	CE-NZ	14.09	1.84	1.49
1	A	69	ASN	CB-CG	10.52	1.75	1.51
1	A	42	MET	SD-CE	-8.20	1.31	1.77
1	A	114	LYS	CE-NZ	7.96	1.69	1.49

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60[A]	ARG	NH1-CZ-NH2	-29.72	86.70	119.40
1	A	60[B]	ARG	NH1-CZ-NH2	-29.72	86.70	119.40
1	A	120	THR	O-C-N	16.56	149.19	122.70
1	A	69	ASN	CB-CG-ND2	-14.99	80.72	116.70
1	A	60[A]	ARG	NE-CZ-NH1	13.76	127.18	120.30
1	A	60[B]	ARG	NE-CZ-NH1	13.76	127.18	120.30
1	A	120	THR	C-N-CA	13.37	155.12	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	THR	CA-C-N	-12.14	90.49	117.20
1	A	69	ASN	CB-CG-OD1	9.43	140.45	121.60
1	A	30	LYS	CD-CE-NZ	-8.40	92.37	111.70
1	A	121	HIS	C-N-CA	6.35	137.56	121.70
1	A	69	ASN	CB-CA-C	5.87	122.14	110.40
1	A	69	ASN	N-CA-CB	-5.70	100.33	110.60
1	A	151	ASP	CA-CB-CG	5.67	125.88	113.40
1	A	158	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	134	SER	C-N-CA	-5.52	107.89	121.70
1	A	158	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	87	GLU	N-CA-CB	-5.12	101.39	110.60
1	A	136	ASP	CB-CG-OD2	5.10	122.89	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60[A]	ARG	Sidechain
1	A	69	ASN	Sidechain

## 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	1896	0	1837	23	2
2	B	23	0	21	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	253	0	0	9	3
All	All	2174	0	1858	23	5

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 (23) 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:183:GLU:HG2	1:A:186:ALA:HB2	1.65	0.78
1:A:150:THR:HG22	5:A:283:HOH:O	1.84	0.77
1:A:41:ASN:HB3	5:A:456:HOH:O	1.99	0.63
1:A:162:ASN:C	1:A:162:ASN:HD22	2.05	0.59
1:A:150:THR:HG21	5:A:402:HOH:O	2.02	0.58
1:A:118:ASN:C	1:A:118:ASN:HD22	2.07	0.58
1:A:159:VAL:CG1	1:A:163:GLY:HA2	2.35	0.57
1:A:116:LYS:HD3	1:A:123:THR:HB	1.92	0.52
1:A:135:LYS:NZ	1:A:147:THR:HA	2.26	0.51
1:A:116:LYS:CD	1:A:123:THR:HB	2.41	0.50
1:A:150:THR:CG2	5:A:283:HOH:O	2.53	0.50
1:A:150:THR:CG2	5:A:402:HOH:O	2.59	0.50
1:A:70:ALA:HB1	5:A:449:HOH:O	2.15	0.47
1:A:162:ASN:C	1:A:162:ASN:ND2	2.69	0.46
1:A:51[A]:HIS:ND1	5:A:277:HOH:O	2.35	0.46
1:A:119:SER:HB2	1:A:122:GLU:OE2	2.16	0.46
1:A:136:ASP:CG	1:A:136:ASP:O	2.55	0.45
1:A:134:SER:H	1:A:137:GLN:HE21	1.65	0.44
1:A:135:LYS:HZ1	1:A:147:THR:HA	1.82	0.44
1:A:118:ASN:HB3	1:A:187:VAL:CG2	2.48	0.44
1:A:135:LYS:NZ	1:A:148:THR:H	2.17	0.43
1:A:135:LYS:NZ	5:A:398:HOH:O	2.51	0.43
1:A:43:GLN:NE2	5:A:334:HOH:O	2.54	0.40

All (5) 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)
5:A:477:HOH:O	5:A:477:HOH:O[4_565]	1.59	0.61
5:A:291:HOH:O	5:A:479:HOH:O[2_665]	1.72	0.48
1:A:58:ASP:OD1	1:A:60[A]:ARG:NH1[4_565]	1.76	0.44
5:A:332:HOH:O	5:A:454:HOH:O[6_554]	1.80	0.40
1:A:69:ASN:O	1:A:228[A]:ARG:NH1[6_554]	2.00	0.20

## 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	246/237 (104%)	239 (97%)	6 (2%)	1 (0%)	34 11

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLU

### 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	214/203 (105%)	205 (96%)	9 (4%)	30 3

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	118	ASN
1	A	119	SER
1	A	122	GLU
1	A	135	LYS
1	A	150	THR
1	A	151	ASP
1	A	158	ARG
1	A	162	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	104	ASN
1	A	118	ASN
1	A	127	HIS

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Mol	Chain	Res	Type
1	A	132	GLN
1	A	137	GLN
1	A	162	ASN
1	A	166	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 ⓘ

2 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	MAN	B	1	2	12,12,12	0.66	0	17,17,17	1.65	4 (23%)
2	MAN	B	2	2	11,11,12	0.69	0	15,15,17	1.18	1 (6%)

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	MAN	B	1	2	-	0/2/22/22	0/1/1/1
2	MAN	B	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	MAN	O5-C1-C2	3.80	117.07	110.28
2	B	2	MAN	C1-O5-C5	3.56	117.02	112.19
2	B	1	MAN	C1-C2-C3	-3.36	103.34	110.31
2	B	1	MAN	C1-O5-C5	-2.82	108.35	113.66
2	B	1	MAN	O1-C1-C2	2.25	115.38	109.03

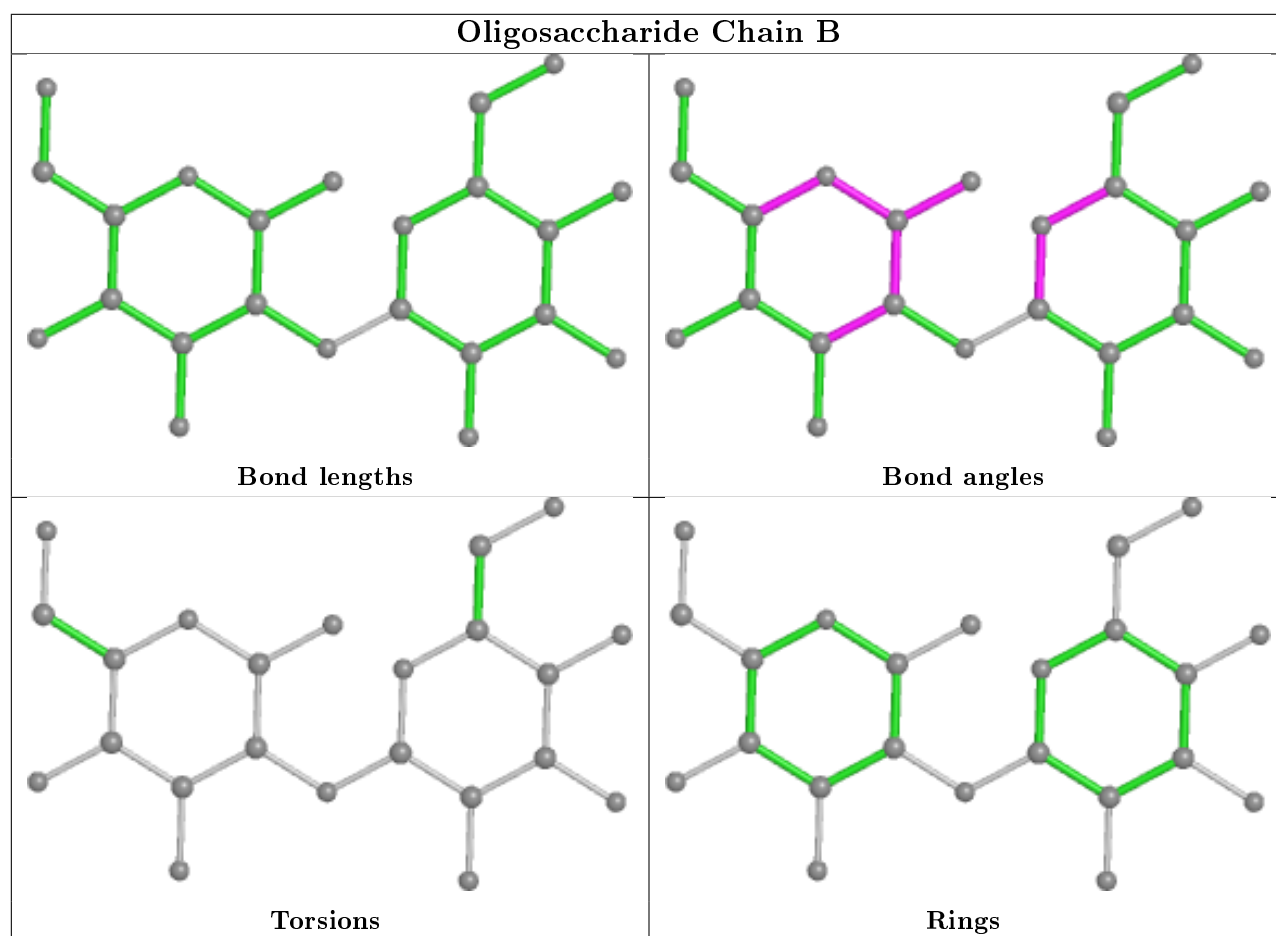
There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

Of 2 ligands modelled in this entry, 2 are 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 [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 ⓘ

### 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	236/237 (99%)	1.04	37 (15%) 2 2	18, 20, 28, 39	7 (2%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	SER	7.4
1	A	150	THR	7.3
1	A	120	THR	6.8
1	A	119	SER	5.7
1	A	162	ASN	5.2
1	A	149	GLY	5.0
1	A	136	ASP	4.5
1	A	122	GLU	4.5
1	A	118	ASN	4.5
1	A	163	GLY	4.4
1	A	160	SER	4.4
1	A	117[A]	SER	4.3
1	A	151	ASP	3.5
1	A	156	LEU	3.5
1	A	27[A]	ILE	3.4
1	A	202	PRO	3.2
1	A	232	LEU	3.1
1	A	1	ALA	3.1
1	A	210	ILE	3.1
1	A	214	ILE	3.0
1	A	184	SER	3.0
1	A	154	LEU	2.9
1	A	91	VAL	2.7
1	A	106	ILE	2.6
1	A	203	ASP	2.5
1	A	205	HIS	2.5
1	A	123	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	93	LEU	2.5
1	A	176	TYR	2.4
1	A	213	PHE	2.4
1	A	6	ALA	2.4
1	A	69	ASN	2.3
1	A	148	THR	2.2
1	A	224	GLY	2.2
1	A	237	ASN	2.2
1	A	199	ILE	2.2
1	A	175	PHE	2.1

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

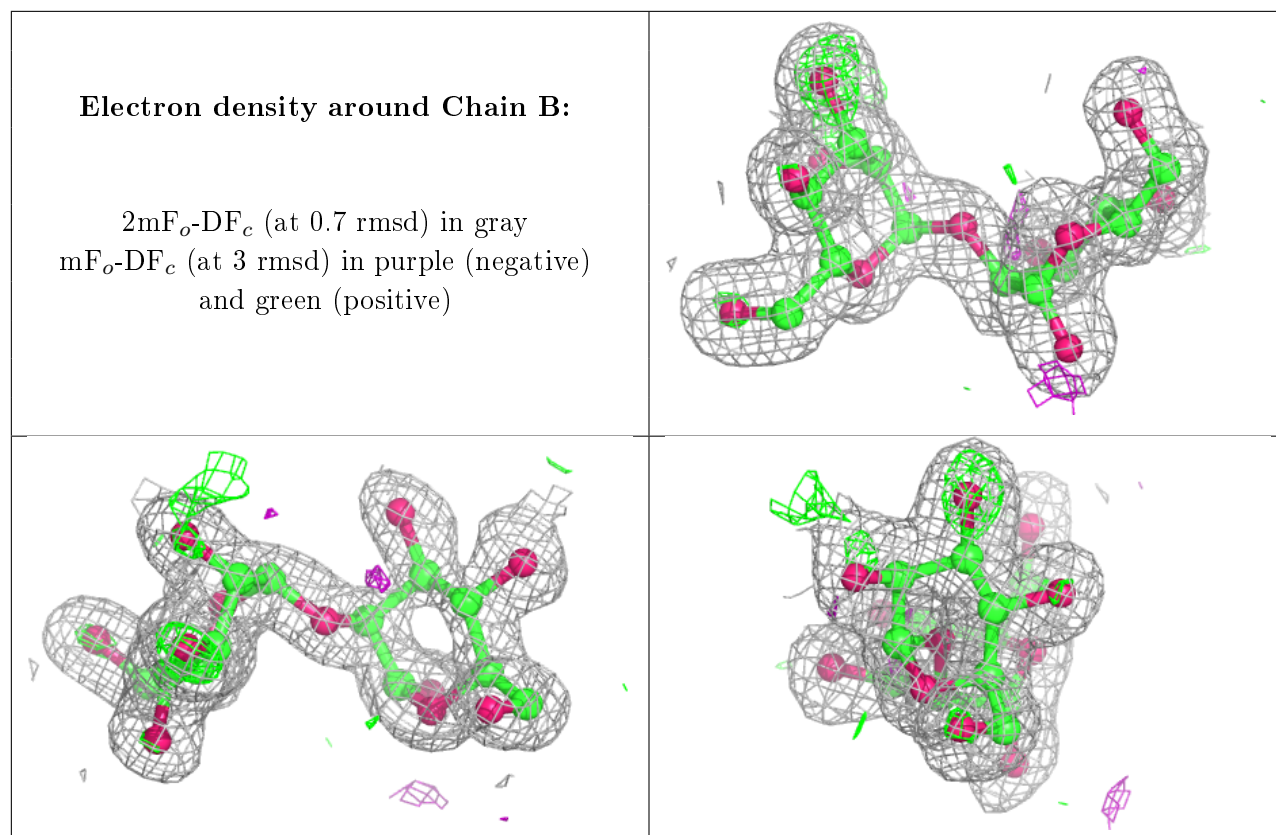
There are no non-standard protein/DNA/RNA residues in this entry.

## 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<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	MAN	B	1	12/12	0.80	0.12	27,29,30,33	0
2	MAN	B	2	11/12	0.90	0.15	24,25,27,27	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](#)

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( $\text{\AA}^2$ )	Q<0.9
3	MN	A	240	1/1	0.99	0.16	23,23,23,23	0
4	CA	A	241	1/1	0.99	0.19	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.