



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2021 – 01:07 pm BST

PDB ID : 7A0J  
Title : Crystal structure of the CRINKLY WD40 ectodomain from the Arabidopsis thaliana receptor kinase ACR4  
Authors : Hothorn, M.; Okuda, S.  
Deposited on : 2020-08-09  
Resolution : 1.95 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 : 2.23.1  
buster-report : 1.1.7 (2018)  
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) : 2.23.1

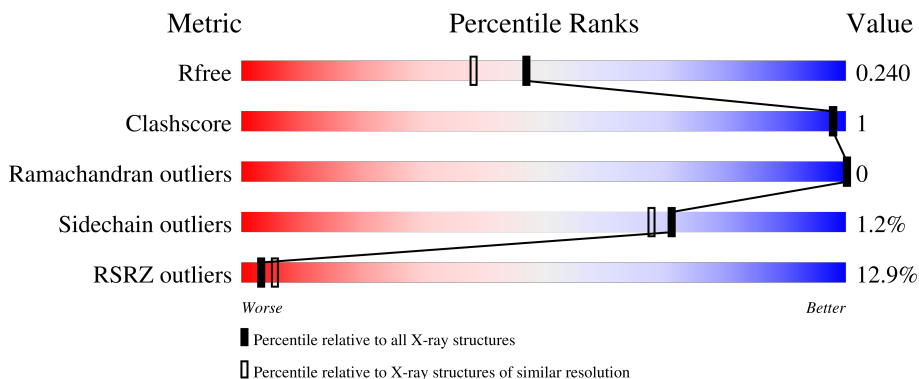
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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  $\geq 3$ , 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	AAA	312	
1	BBB	312	
1	CCC	312	
1	DDD	312	
2	BaB	2	

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Mol	Chain	Length	Quality of chain
2	CcC	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUC	BaB	2	-	-	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 8356 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 Serine/threonine-protein kinase-like protein ACR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	261	Total 1913	C 1226	N 316	O 349	S 22	0	3	0
1	BBB	269	Total 1949	C 1242	N 324	O 362	S 21	0	2	0
1	CCC	288	Total 2144	C 1374	N 349	O 399	S 22	0	5	0
1	DDD	271	Total 1974	C 1270	N 323	O 360	S 21	0	3	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	336	GLU	-	expression tag	UNP Q9LX29
AAA	337	ASN	-	expression tag	UNP Q9LX29
AAA	338	LEU	-	expression tag	UNP Q9LX29
AAA	339	TYR	-	expression tag	UNP Q9LX29
AAA	340	PHE	-	expression tag	UNP Q9LX29
AAA	341	GLN	-	expression tag	UNP Q9LX29
BBB	336	GLU	-	expression tag	UNP Q9LX29
BBB	337	ASN	-	expression tag	UNP Q9LX29
BBB	338	LEU	-	expression tag	UNP Q9LX29
BBB	339	TYR	-	expression tag	UNP Q9LX29
BBB	340	PHE	-	expression tag	UNP Q9LX29
BBB	341	GLN	-	expression tag	UNP Q9LX29
CCC	336	GLU	-	expression tag	UNP Q9LX29
CCC	337	ASN	-	expression tag	UNP Q9LX29
CCC	338	LEU	-	expression tag	UNP Q9LX29
CCC	339	TYR	-	expression tag	UNP Q9LX29
CCC	340	PHE	-	expression tag	UNP Q9LX29
CCC	341	GLN	-	expression tag	UNP Q9LX29
DDD	336	GLU	-	expression tag	UNP Q9LX29
DDD	337	ASN	-	expression tag	UNP Q9LX29
DDD	338	LEU	-	expression tag	UNP Q9LX29

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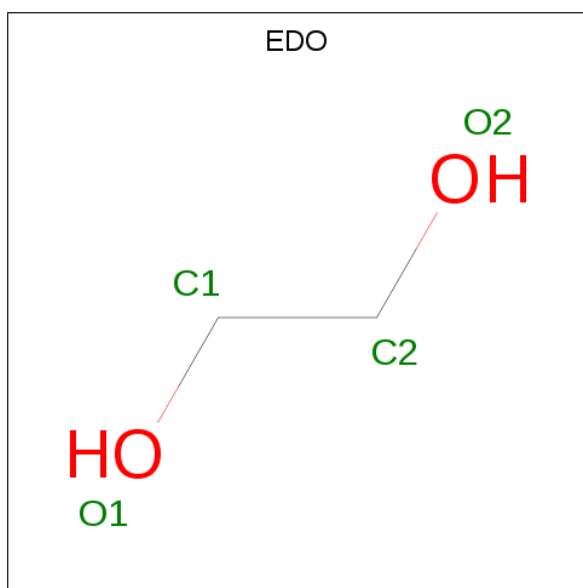
Chain	Residue	Modelled	Actual	Comment	Reference
DDD	339	TYR	-	expression tag	UNP Q9LX29
DDD	340	PHE	-	expression tag	UNP Q9LX29
DDD	341	GLN	-	expression tag	UNP Q9LX29

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
2	BaB	2	24	14	1	9	0	0	0
2	CcC	2	24	14	1	9	0	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



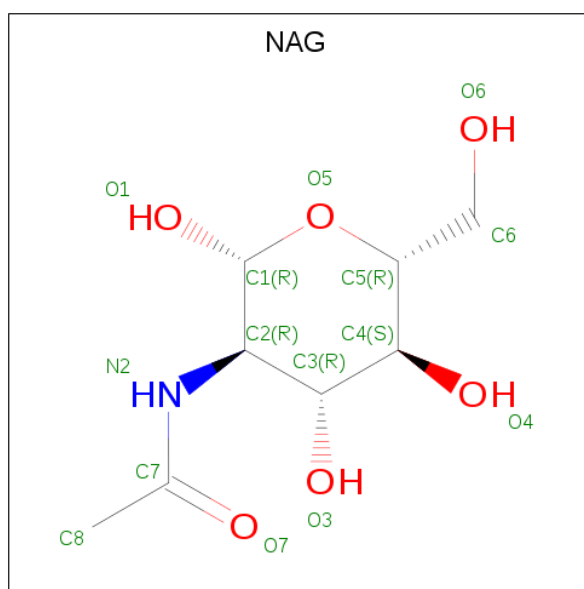
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	AAA	1	4	2	2	0	0
3	AAA	1	4	2	2	0	0
3	CCC	1	4	2	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	DDD	1	Total C O 4 2 2	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



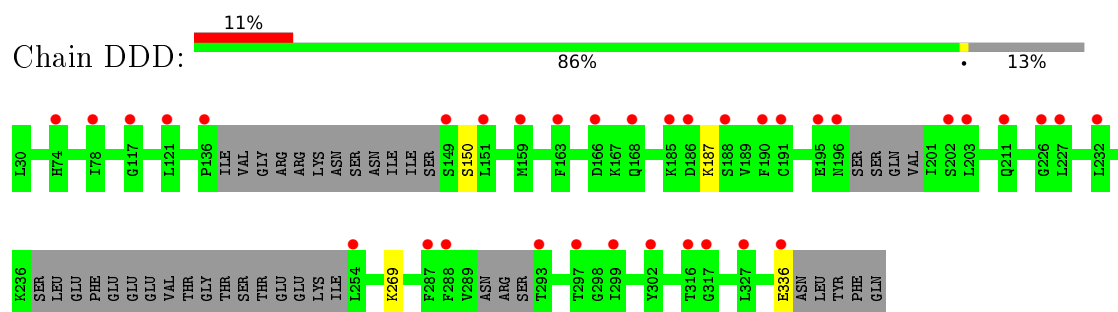
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	DDD	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	AAA	76	Total 76	O 76	0	0
5	BBB	41	Total 41	O 41	0	0
5	CCC	87	Total 87	O 87	0	0
5	DDD	66	Total 66	O 66	0	0







- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BaB: 100%

MAG1  
FUC2

- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CcC: 100%

MAG1  
FUC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.99Å 87.95Å 88.62Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	48.05 – 1.95 48.01 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.05-1.95) 99.9 (48.01-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.220 , 0.239 0.223 , 0.240	Depositor DCC
$R_{free}$ test set	4029 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.7	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.001 for -h,l,k 0.022 for -h,-l,-k 0.027 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8356	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: NAG, FUC, EDO

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	AAA	0.66	0/1970	0.71	0/2662
1	BBB	0.67	0/2004	0.71	0/2715
1	CCC	0.66	0/2210	0.70	0/2998
1	DDD	0.66	0/2037	0.71	0/2764
All	All	0.67	0/8221	0.71	0/11139

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	AAA	1913	0	1805	5	0
1	BBB	1949	0	1804	2	0
1	CCC	2144	0	2011	6	0
1	DDD	1974	0	1827	0	0
2	BaB	24	0	22	0	0
2	CcC	24	0	22	0	0
3	AAA	8	0	12	0	0
3	CCC	32	0	48	0	0
3	DDD	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	DDD	14	0	13	0	0
5	AAA	76	0	0	0	0
5	BBB	41	0	0	0	0
5	CCC	87	0	0	0	0
5	DDD	66	0	0	0	0
All	All	8356	0	7570	11	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 1.

All (11) 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:CCC:300:GLY:O	1:CCC:315[A]:LEU:HD22	2.04	0.57
1:AAA:327:LEU:N	1:AAA:327:LEU:HD23	2.23	0.53
1:AAA:86:PHE:CG	1:AAA:106:ILE:HD11	2.46	0.50
1:AAA:106:ILE:HG22	1:AAA:156:GLY:HA2	1.97	0.47
1:BBB:62:GLY:O	1:CCC:332:SER:HA	2.13	0.47
1:BBB:325:TRP:HB3	1:CCC:320:MET:SD	2.56	0.45
1:AAA:88[B]:CYS:SG	1:AAA:99:CYS:SG	3.12	0.45
1:CCC:315[A]:LEU:HD12	1:CCC:320:MET:HG3	2.00	0.44
1:CCC:105:PHE:O	1:CCC:156:GLY:HA2	2.20	0.41
1:CCC:314:VAL:C	1:CCC:315[A]:LEU:HD23	2.40	0.41
1:AAA:327:LEU:O	1:AAA:327:LEU:HG	2.21	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	AAA	254/312 (81%)	247 (97%)	7 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	263/312 (84%)	256 (97%)	7 (3%)	0	100	100
1	CCC	287/312 (92%)	276 (96%)	11 (4%)	0	100	100
1	DDD	264/312 (85%)	255 (97%)	9 (3%)	0	100	100
All	All	1068/1248 (86%)	1034 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	AAA	197/256 (77%)	195 (99%)	2 (1%)	76	74
1	BBB	198/256 (77%)	195 (98%)	3 (2%)	65	60
1	CCC	225/256 (88%)	223 (99%)	2 (1%)	78	77
1	DDD	199/256 (78%)	195 (98%)	4 (2%)	55	48
All	All	819/1024 (80%)	808 (99%)	11 (1%)	71	65

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

Mol	Chain	Res	Type
1	AAA	150	SER
1	AAA	161	ARG
1	BBB	150	SER
1	BBB	161	ARG
1	BBB	310	PHE
1	CCC	260[A]	GLU
1	CCC	260[B]	GLU
1	DDD	150	SER
1	DDD	187	LYS
1	DDD	269	LYS
1	DDD	336	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

4 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	BaB	1	1,2	14,14,15	0.30	0	17,19,21	0.97	1 (5%)
2	FUC	BaB	2	2	10,10,11	0.31	0	14,14,16	0.81	1 (7%)
2	NAG	CcC	1	1,2	14,14,15	0.31	0	17,19,21	0.71	0
2	FUC	CcC	2	2	10,10,11	0.28	0	14,14,16	0.54	0

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	BaB	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	BaB	2	2	-	-	0/1/1/1
2	NAG	CcC	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	CcC	2	2	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	BaB	1	NAG	O5-C5-C6	2.85	111.67	107.20
2	BaB	2	FUC	C1-C2-C3	2.34	112.54	109.67

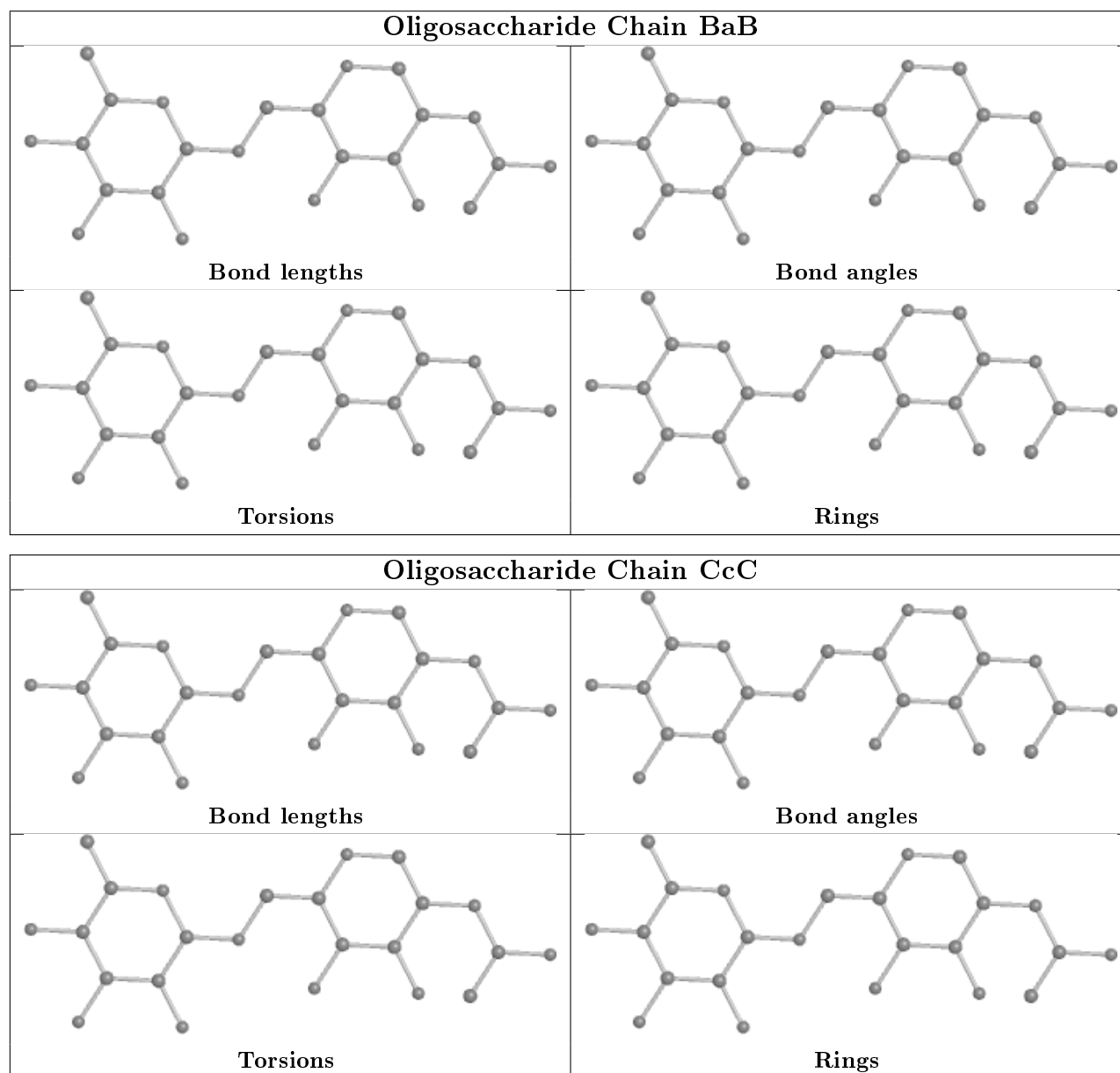
There are no chirality outliers.

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

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	AAA	401	-	3,3,3	0.07	0	2,2,2	0.22	0
3	EDO	DDD	402	-	3,3,3	0.06	0	2,2,2	0.34	0
3	EDO	CCC	401	-	3,3,3	0.06	0	2,2,2	0.14	0
3	EDO	CCC	403	-	3,3,3	0.04	0	2,2,2	0.14	0
3	EDO	CCC	406	-	3,3,3	0.06	0	2,2,2	0.20	0
3	EDO	CCC	408	-	3,3,3	0.05	0	2,2,2	0.16	0
3	EDO	CCC	405	-	3,3,3	0.06	0	2,2,2	0.22	0
4	NAG	DDD	401	1	14,14,15	0.28	0	17,19,21	0.74	0
3	EDO	AAA	402	-	3,3,3	0.06	0	2,2,2	0.22	0
3	EDO	CCC	407	-	3,3,3	0.07	0	2,2,2	0.19	0
3	EDO	CCC	402	-	3,3,3	0.06	0	2,2,2	0.16	0
3	EDO	CCC	404	-	3,3,3	0.06	0	2,2,2	0.18	0

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
3	EDO	AAA	401	-	-	0/1/1/1	-
3	EDO	DDD	402	-	-	1/1/1/1	-
3	EDO	CCC	401	-	-	0/1/1/1	-
3	EDO	CCC	403	-	-	1/1/1/1	-
3	EDO	CCC	406	-	-	1/1/1/1	-
3	EDO	CCC	408	-	-	1/1/1/1	-
3	EDO	CCC	405	-	-	0/1/1/1	-
4	NAG	DDD	401	1	-	0/6/23/26	0/1/1/1
3	EDO	AAA	402	-	-	1/1/1/1	-
3	EDO	CCC	407	-	-	1/1/1/1	-
3	EDO	CCC	402	-	-	0/1/1/1	-
3	EDO	CCC	404	-	-	0/1/1/1	-



There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

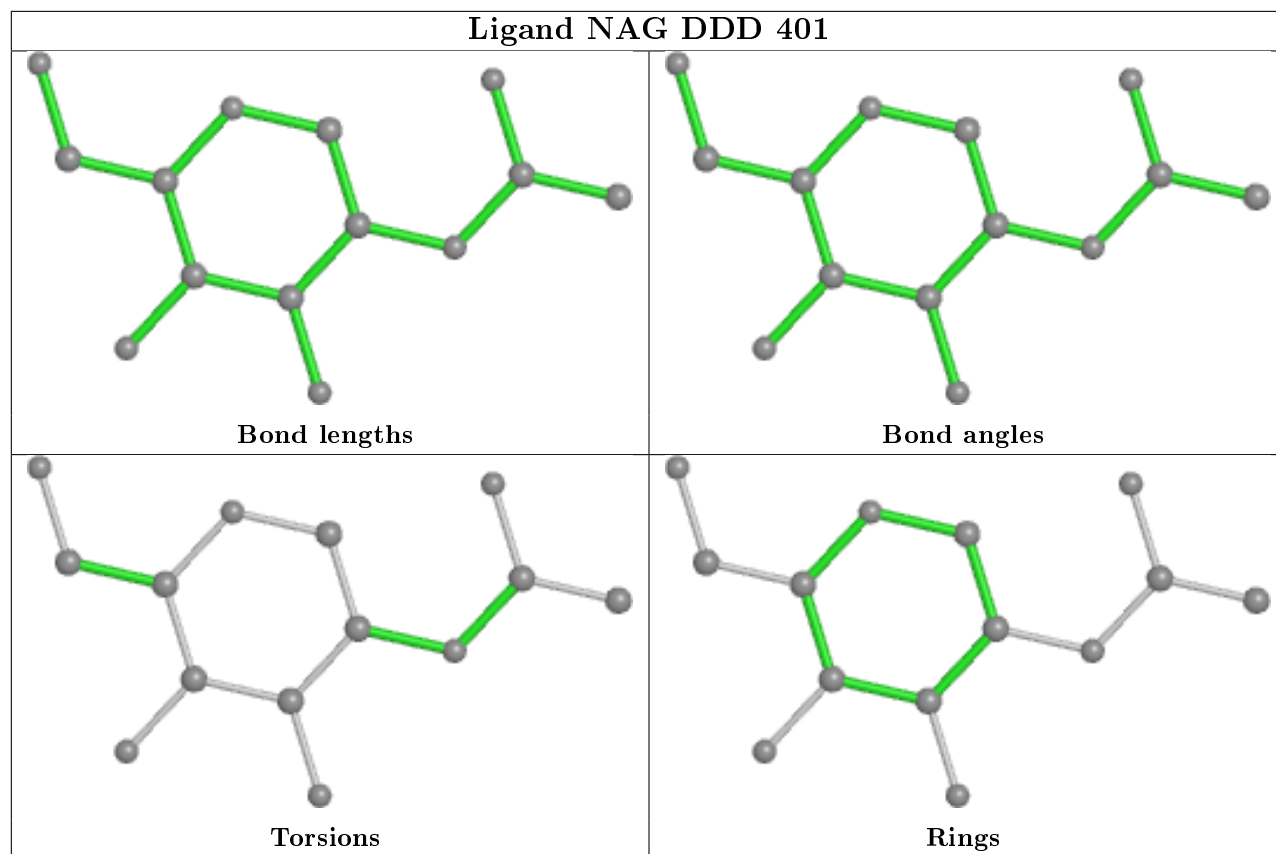
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	CCC	403	EDO	O1-C1-C2-O2
3	CCC	407	EDO	O1-C1-C2-O2
3	DDD	402	EDO	O1-C1-C2-O2
3	CCC	406	EDO	O1-C1-C2-O2
3	AAA	402	EDO	O1-C1-C2-O2
3	CCC	408	EDO	O1-C1-C2-O2

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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	AAA	261/312 (83%)	0.88	22 (8%) <b>11</b> <b>17</b>	30, 49, 74, 94	0
1	BBB	269/312 (86%)	1.20	54 (20%) <b>1</b> <b>1</b>	34, 55, 88, 100	0
1	CCC	288/312 (92%)	0.97	30 (10%) <b>6</b> <b>10</b>	28, 47, 73, 94	0
1	DDD	271/312 (86%)	0.96	35 (12%) <b>3</b> <b>5</b>	31, 52, 97, 121	0
All	All	1089/1248 (87%)	1.00	141 (12%) <b>3</b> <b>5</b>	28, 51, 83, 121	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	146	ILE	7.6
1	BBB	147	ILE	7.5
1	AAA	146	ILE	7.3
1	BBB	295	ALA	6.5
1	BBB	232	LEU	5.8
1	AAA	158	ASN	5.3
1	AAA	147	ILE	5.1
1	CCC	147	ILE	4.9
1	CCC	315[A]	LEU	4.8
1	BBB	201	ILE	4.8
1	DDD	316	THR	4.8
1	DDD	185	LYS	4.7
1	DDD	302	TYR	4.7
1	AAA	256	LEU	4.5
1	CCC	137	ILE	4.3
1	DDD	149	SER	4.3
1	BBB	331	ALA	4.3
1	DDD	232	LEU	4.2
1	BBB	168	GLN	4.1
1	BBB	296	PRO	4.1
1	AAA	157	TYR	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	BBB	254	LEU	4.1
1	AAA	200	VAL	4.0
1	AAA	201	ILE	4.0
1	DDD	226	GLY	3.9
1	AAA	327	LEU	3.9
1	DDD	203	LEU	3.9
1	BBB	226	GLY	3.8
1	AAA	317	GLY	3.8
1	CCC	253	ILE	3.7
1	BBB	162	ASN	3.7
1	BBB	302	TYR	3.7
1	BBB	297	THR	3.6
1	CCC	238	LEU	3.6
1	DDD	293	THR	3.6
1	BBB	329	PHE	3.5
1	AAA	318	THR	3.5
1	BBB	207	GLU	3.5
1	BBB	148	SER	3.5
1	AAA	227	LEU	3.5
1	BBB	151	LEU	3.5
1	BBB	197	SER	3.4
1	DDD	168	GLN	3.4
1	BBB	205	PRO	3.3
1	CCC	254	LEU	3.3
1	CCC	317	GLY	3.3
1	DDD	297	THR	3.2
1	BBB	203	LEU	3.2
1	BBB	224	LEU	3.2
1	BBB	263	LEU	3.2
1	BBB	185	LYS	3.2
1	BBB	208	LYS	3.2
1	DDD	136	PRO	3.1
1	BBB	278	TYR	3.1
1	CCC	207	GLU	3.1
1	DDD	254	LEU	3.1
1	AAA	302	TYR	3.0
1	AAA	294	PRO	3.0
1	BBB	189	VAL	3.0
1	AAA	151	LEU	2.9
1	CCC	136	PRO	2.9
1	CCC	318	THR	2.9
1	BBB	228	GLU	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	CCC	327	LEU	2.9
1	DDD	299	ILE	2.9
1	AAA	263	LEU	2.8
1	DDD	227	LEU	2.8
1	AAA	159	MET	2.8
1	BBB	164	VAL	2.8
1	BBB	187	LYS	2.8
1	BBB	206	LYS	2.8
1	DDD	202	SER	2.8
1	BBB	234	TRP	2.8
1	DDD	190	PHE	2.7
1	CCC	151	LEU	2.7
1	AAA	136	PRO	2.7
1	AAA	278	TYR	2.7
1	BBB	227	LEU	2.7
1	BBB	184	SER	2.7
1	CCC	287	PHE	2.7
1	DDD	166	ASP	2.7
1	BBB	170	HIS	2.7
1	BBB	310	PHE	2.6
1	AAA	319	SER	2.6
1	CCC	190	PHE	2.6
1	DDD	288	PHE	2.6
1	DDD	117	GLY	2.6
1	BBB	59	VAL	2.5
1	BBB	287	PHE	2.5
1	BBB	190	PHE	2.5
1	DDD	317	GLY	2.5
1	CCC	275	ILE	2.5
1	DDD	186	ASP	2.5
1	DDD	151	LEU	2.5
1	DDD	196	ASN	2.5
1	BBB	102[A]	ASN	2.4
1	DDD	159	MET	2.4
1	BBB	213	ILE	2.4
1	BBB	183	SER	2.4
1	BBB	136	PRO	2.4
1	DDD	74	HIS	2.4
1	DDD	191	CYS	2.4
1	DDD	78	ILE	2.4
1	CCC	335	LEU	2.3
1	DDD	163	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	CCC	167	LYS	2.3
1	CCC	264	ALA	2.3
1	AAA	297	THR	2.3
1	CCC	323	VAL	2.3
1	BBB	211	GLN	2.3
1	AAA	160	THR	2.3
1	CCC	205	PRO	2.3
1	DDD	195	GLU	2.2
1	DDD	211	GLN	2.2
1	BBB	157	TYR	2.2
1	CCC	237	SER	2.2
1	CCC	206	LYS	2.2
1	BBB	299	ILE	2.2
1	BBB	286	GLY	2.2
1	BBB	233	CYS	2.1
1	CCC	201	ILE	2.1
1	BBB	257	PRO	2.1
1	DDD	287	PHE	2.1
1	BBB	328	GLY	2.1
1	CCC	232	LEU	2.1
1	DDD	121	LEU	2.1
1	AAA	287	PHE	2.1
1	BBB	277	ARG	2.1
1	BBB	223	ILE	2.1
1	BBB	194	ASP	2.1
1	CCC	164	VAL	2.1
1	DDD	188	SER	2.1
1	CCC	168	GLN	2.0
1	CCC	196	ASN	2.0
1	CCC	73	GLY	2.0
1	CCC	227	LEU	2.0
1	BBB	318	THR	2.0
1	DDD	336	GLU	2.0
1	DDD	327	LEU	2.0
1	BBB	237	SER	2.0
1	BBB	316	THR	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 [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	FUC	BaB	2	10/11	0.67	0.43	74,77,78,78	0
2	NAG	BaB	1	14/15	0.85	0.19	56,59,65,69	0
2	FUC	CcC	2	10/11	0.87	0.29	62,65,67,67	0
2	NAG	CcC	1	14/15	0.91	0.14	49,53,56,59	0

### 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(Å <sup>2</sup> )	Q<0.9
3	EDO	CCC	407	4/4	0.63	0.36	69,70,70,70	0
3	EDO	CCC	406	4/4	0.78	0.15	77,78,78,78	0
4	NAG	DDD	401	14/15	0.78	0.35	58,63,65,67	0
3	EDO	CCC	402	4/4	0.82	0.24	55,55,56,58	0
3	EDO	CCC	405	4/4	0.83	0.21	49,49,49,49	0
3	EDO	DDD	402	4/4	0.83	0.16	40,40,40,40	0
3	EDO	CCC	401	4/4	0.83	0.32	55,56,57,58	0
3	EDO	CCC	403	4/4	0.88	0.15	63,64,64,65	0
3	EDO	CCC	408	4/4	0.90	0.18	57,58,58,59	0
3	EDO	AAA	401	4/4	0.92	0.26	55,56,57,58	0
3	EDO	CCC	404	4/4	0.92	0.21	60,60,60,60	0
3	EDO	AAA	402	4/4	0.95	0.15	60,60,60,61	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.