



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2024 – 11:34 am 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

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:

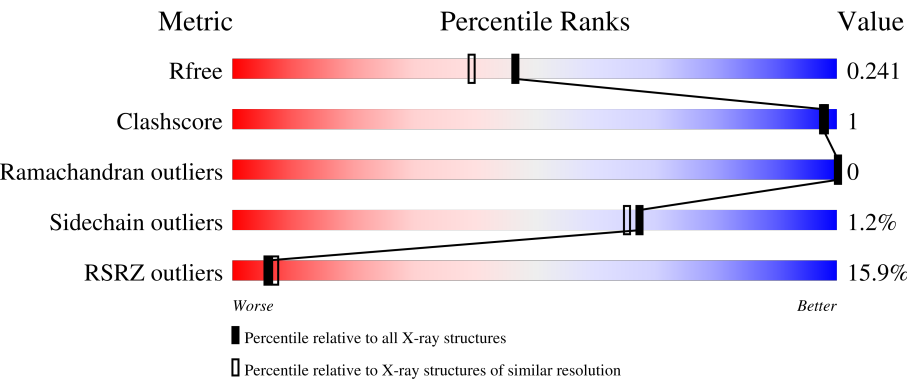
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 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}	164625	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (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 ≥ 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	<div><div>12%</div><div>81%</div><div>16%</div></div>
1	BBB	312	<div><div>15%</div><div>85%</div><div>14%</div></div>
1	CCC	312	<div><div>11%</div><div>90%</div><div>8%</div></div>
1	DDD	312	<div><div>17%</div><div>86%</div><div>13%</div></div>
2	BaB	2	<div><div>100%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	CcC	2	 100%

2 Entry composition

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

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

Continued on next page...

Continued from previous page...

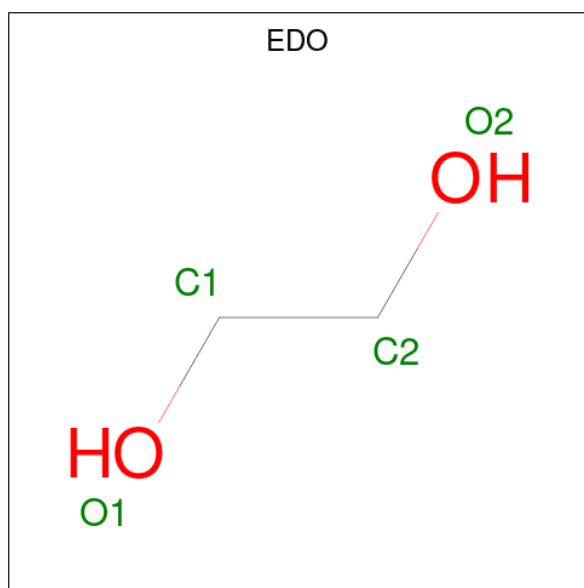
Chain	Residue	Modelled	Actual	Comment	Reference
DDD	339	TYR	-	expression tag	UNP Q9LX29
DDD	340	PHE	-	expression tag	UNP Q9LX29
DDD	341	GLN	-	expression tag	UNP Q9LX29

- 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
2	BaB	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	CcC	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



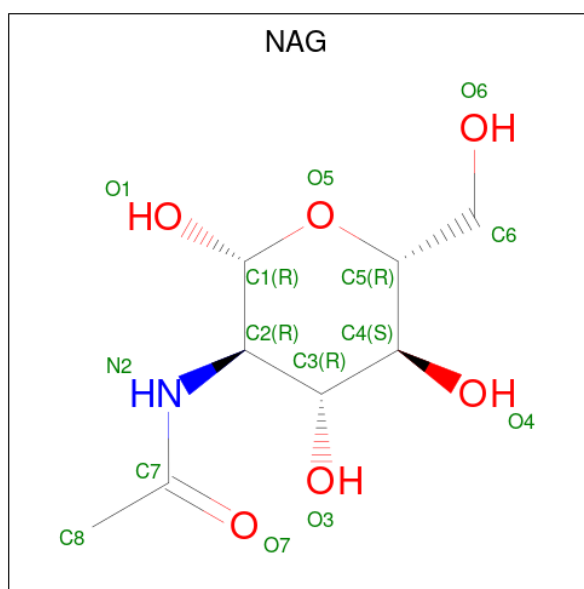
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	CCC	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

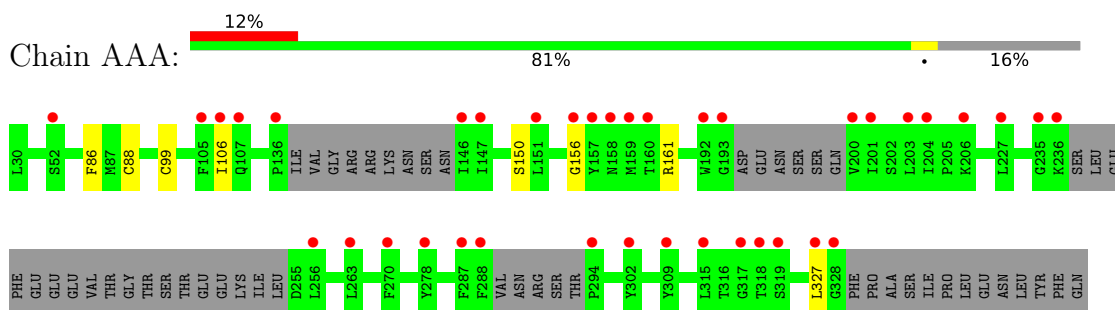
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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

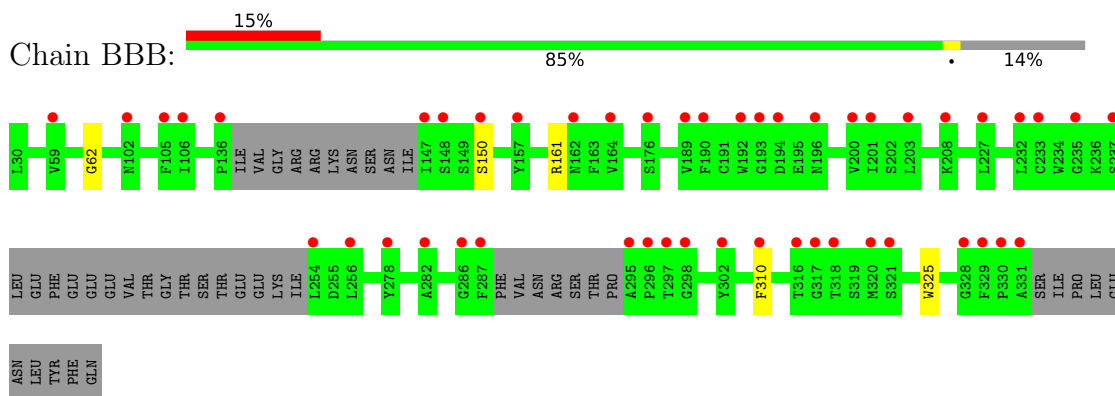
3 Residue-property plots [i](#)

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.

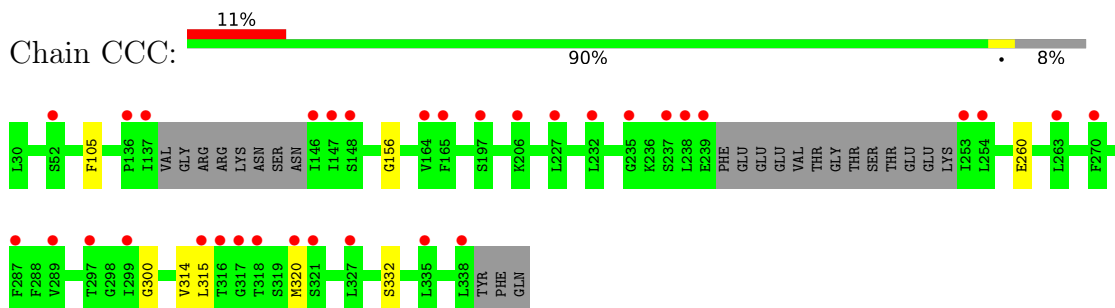
- Molecule 1: Serine/threonine-protein kinase-like protein ACR4



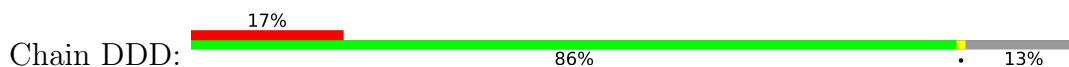
- Molecule 1: Serine/threonine-protein kinase-like protein ACR4

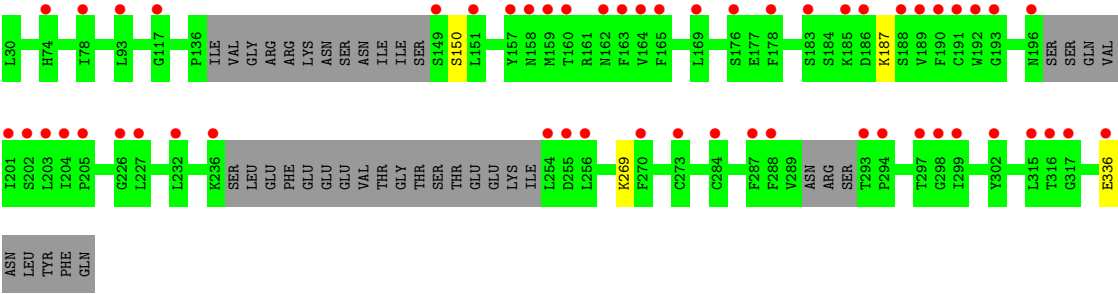


- Molecule 1: Serine/threonine-protein kinase-like protein ACR4



- Molecule 1: Serine/threonine-protein kinase-like protein ACR4





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

Chain BaB: 100%



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

Chain CcC: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.99Å 87.95Å 88.62Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	48.05 – 1.95 48.05 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.05-1.95) 99.9 (48.05-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.220 , 0.239 0.223 , 0.241	Depositor DCC
R_{free} test set	4038 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: EDO, 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	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

Continued on next page...

Continued from previous page...

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 ⓘ

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	AAA	254/312 (81%)	247 (97%)	7 (3%)	0	100 100

Continued on next page...

Continued from previous page...

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 ⓘ

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%)	73	72
1	BBB	198/256 (77%)	195 (98%)	3 (2%)	60	57
1	CCC	225/256 (88%)	223 (99%)	2 (1%)	75	75
1	DDD	199/256 (78%)	195 (98%)	4 (2%)	50	44
All	All	819/1024 (80%)	808 (99%)	11 (1%)	67	62

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 ⓘ

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 ⓘ

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(°)	Ideal(°)
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

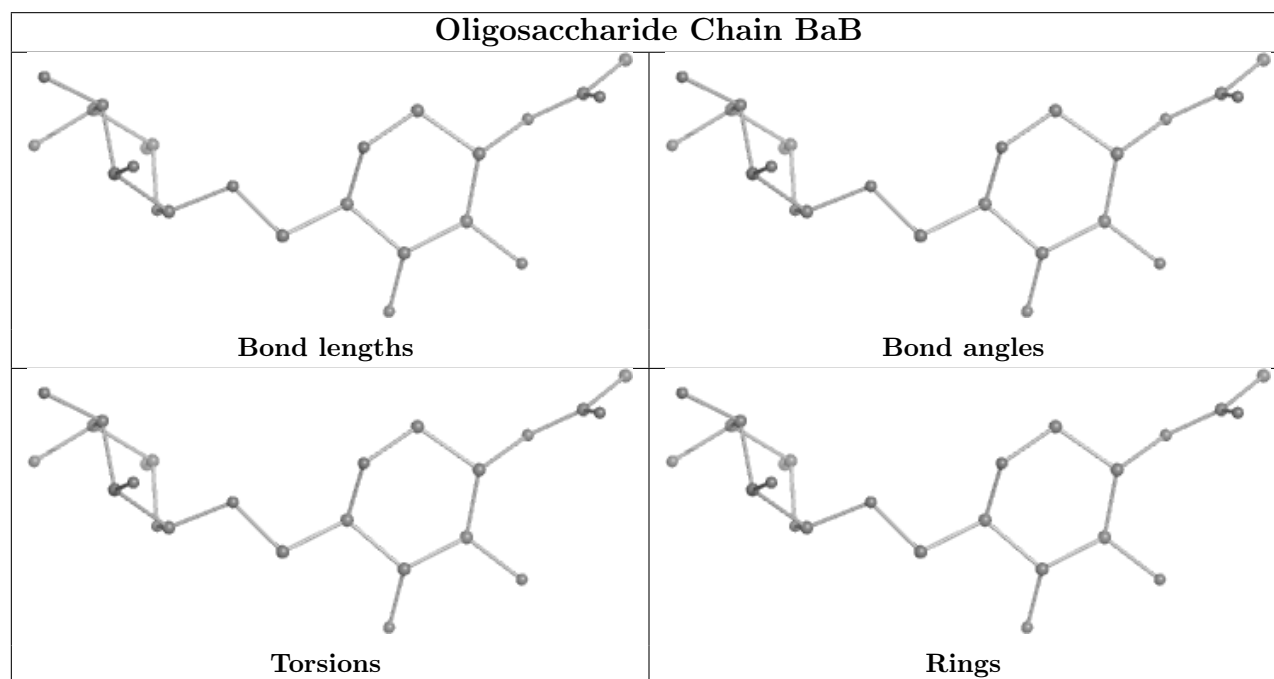
There are no chirality outliers.

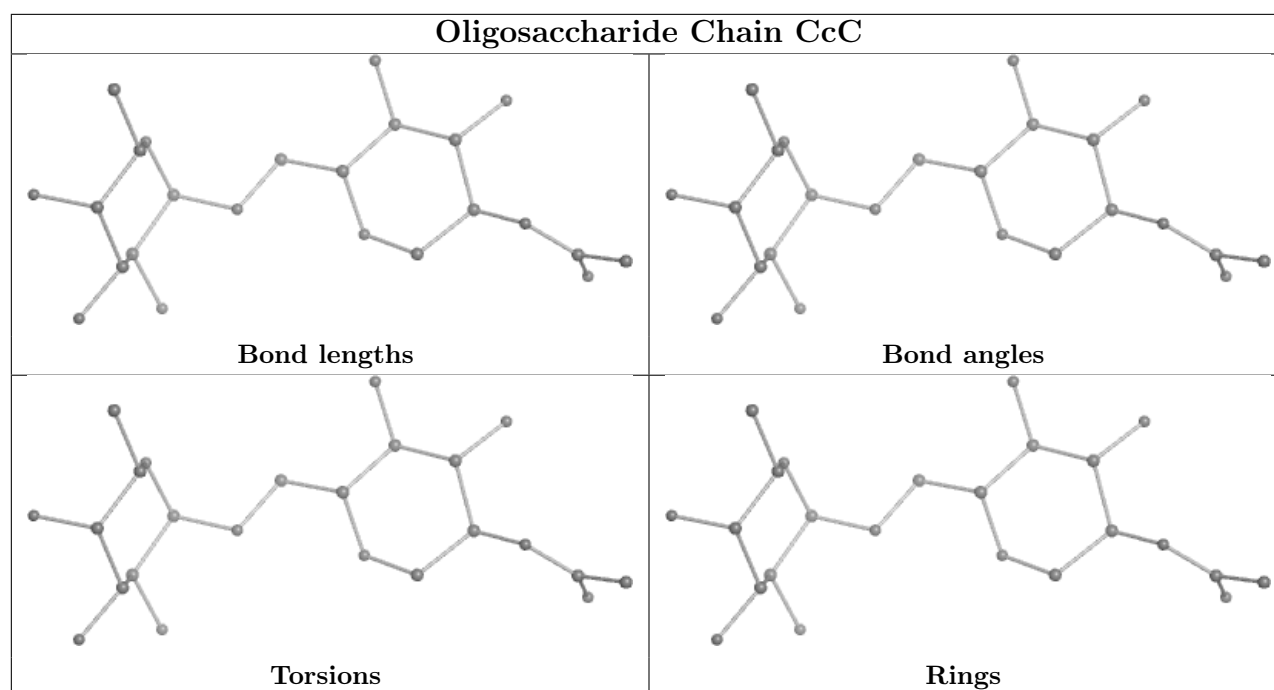
There are no torsion outliers.

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 [i](#)

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	CCC	406	-	3,3,3	0.06	0	2,2,2	0.20	0
3	EDO	CCC	405	-	3,3,3	0.06	0	2,2,2	0.22	0
3	EDO	CCC	402	-	3,3,3	0.06	0	2,2,2	0.16	0
3	EDO	DDD	402	-	3,3,3	0.06	0	2,2,2	0.34	0
3	EDO	CCC	403	-	3,3,3	0.04	0	2,2,2	0.14	0
3	EDO	CCC	401	-	3,3,3	0.06	0	2,2,2	0.14	0
4	NAG	DDD	401	1	14,14,15	0.28	0	17,19,21	0.74	0
3	EDO	CCC	407	-	3,3,3	0.07	0	2,2,2	0.19	0
3	EDO	CCC	408	-	3,3,3	0.05	0	2,2,2	0.16	0
3	EDO	AAA	401	-	3,3,3	0.07	0	2,2,2	0.22	0
3	EDO	CCC	404	-	3,3,3	0.06	0	2,2,2	0.18	0
3	EDO	AAA	402	-	3,3,3	0.06	0	2,2,2	0.22	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	CCC	406	-	-	1/1/1/1	-
3	EDO	CCC	405	-	-	0/1/1/1	-
3	EDO	CCC	402	-	-	0/1/1/1	-
3	EDO	DDD	402	-	-	1/1/1/1	-
3	EDO	CCC	403	-	-	1/1/1/1	-
3	EDO	CCC	401	-	-	0/1/1/1	-
4	NAG	DDD	401	1	-	0/6/23/26	0/1/1/1
3	EDO	CCC	407	-	-	1/1/1/1	-
3	EDO	CCC	408	-	-	1/1/1/1	-
3	EDO	AAA	401	-	-	0/1/1/1	-
3	EDO	CCC	404	-	-	0/1/1/1	-
3	EDO	AAA	402	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

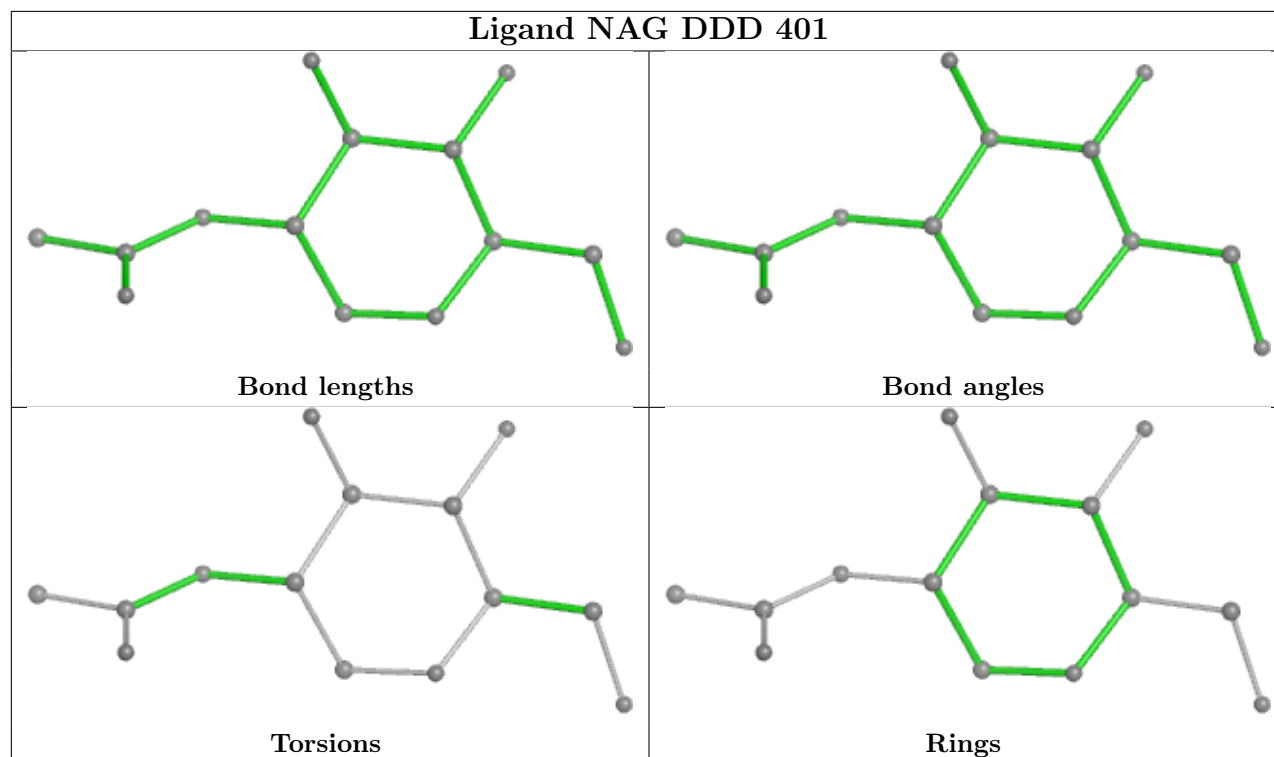
Mol	Chain	Res	Type	Atoms
3	CCC	403	EDO	O1-C1-C2-O2
3	CCC	407	EDO	O1-C1-C2-O2
3	DDD	402	EDO	O1-C1-C2-O2
3	CCC	406	EDO	O1-C1-C2-O2
3	AAA	402	EDO	O1-C1-C2-O2
3	CCC	408	EDO	O1-C1-C2-O2

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 ⓘ

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	AAA	261/312 (83%)	0.88	38 (14%) 7 8	20, 49, 74, 94	3 (1%)
1	BBB	269/312 (86%)	1.00	48 (17%) 4 5	23, 55, 88, 100	2 (0%)
1	CCC	288/312 (92%)	0.76	33 (11%) 11 13	20, 47, 73, 94	5 (1%)
1	DDD	271/312 (86%)	1.04	54 (19%) 3 4	20, 52, 97, 121	3 (1%)
All	All	1089/1248 (87%)	0.92	173 (15%) 6 7	20, 51, 83, 121	13 (1%)

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	146	ILE	6.4
1	DDD	316	THR	5.6
1	AAA	294	PRO	5.5
1	AAA	146	ILE	5.4
1	AAA	319	SER	5.4
1	DDD	201	ILE	5.1
1	AAA	193	GLY	4.9
1	AAA	288	PHE	4.8
1	DDD	203	LEU	4.4
1	BBB	296	PRO	4.4
1	AAA	327	LEU	4.4
1	DDD	151	LEU	4.3
1	BBB	147	ILE	4.2
1	CCC	315[A]	LEU	4.2
1	DDD	287	PHE	4.2
1	DDD	202	SER	4.1
1	DDD	232	LEU	4.1
1	CCC	253	ILE	4.1
1	DDD	302	TYR	4.1
1	BBB	237	SER	4.0
1	DDD	288	PHE	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	DDD	191	CYS	3.9
1	BBB	320	MET	3.9
1	DDD	299	ILE	3.9
1	DDD	317	GLY	3.8
1	CCC	338	LEU	3.8
1	BBB	190	PHE	3.7
1	DDD	297	THR	3.7
1	AAA	157	TYR	3.7
1	AAA	317	GLY	3.7
1	AAA	160	THR	3.7
1	BBB	329	PHE	3.6
1	AAA	200	VAL	3.5
1	BBB	331	ALA	3.5
1	AAA	278	TYR	3.4
1	BBB	295	ALA	3.4
1	CCC	238	LEU	3.4
1	DDD	157	TYR	3.4
1	CCC	137	ILE	3.4
1	AAA	318	THR	3.3
1	BBB	162	ASN	3.3
1	BBB	302	TYR	3.3
1	DDD	190	PHE	3.3
1	BBB	254	LEU	3.3
1	CCC	254	LEU	3.3
1	AAA	203	LEU	3.2
1	BBB	203	LEU	3.2
1	DDD	254	LEU	3.2
1	DDD	192	TRP	3.2
1	AAA	287	PHE	3.2
1	AAA	158	ASN	3.1
1	AAA	328	GLY	3.1
1	DDD	336	GLU	3.1
1	CCC	320	MET	3.1
1	CCC	318	THR	3.1
1	BBB	193	GLY	3.1
1	CCC	317	GLY	3.1
1	CCC	147	ILE	3.0
1	BBB	287	PHE	3.0
1	AAA	106	ILE	3.0
1	DDD	149	SER	3.0
1	AAA	302	TYR	3.0
1	DDD	293	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	CCC	52	SER	2.9
1	CCC	164	VAL	2.9
1	DDD	204	ILE	2.9
1	BBB	200	VAL	2.8
1	DDD	236	LYS	2.8
1	BBB	102[A]	ASN	2.8
1	BBB	196	ASN	2.8
1	BBB	278	TYR	2.8
1	BBB	330	PRO	2.8
1	BBB	233	CYS	2.8
1	CCC	316	THR	2.8
1	BBB	192	TRP	2.8
1	BBB	201	ILE	2.8
1	AAA	107[A]	GLN	2.7
1	DDD	159	MET	2.7
1	AAA	105	PHE	2.7
1	DDD	164	VAL	2.7
1	BBB	282	ALA	2.7
1	BBB	297	THR	2.7
1	DDD	74	HIS	2.7
1	AAA	256	LEU	2.6
1	CCC	263	LEU	2.6
1	AAA	309	TYR	2.6
1	CCC	232	LEU	2.6
1	CCC	299	ILE	2.6
1	DDD	188	SER	2.5
1	DDD	315	LEU	2.5
1	BBB	105	PHE	2.5
1	BBB	310	PHE	2.5
1	CCC	239	GLU	2.5
1	AAA	147	ILE	2.5
1	DDD	93	LEU	2.5
1	BBB	235	GLY	2.5
1	BBB	157	TYR	2.5
1	AAA	159	MET	2.5
1	CCC	327	LEU	2.5
1	CCC	237	SER	2.4
1	DDD	183	SER	2.4
1	DDD	193	GLY	2.4
1	AAA	201	ILE	2.4
1	BBB	227	LEU	2.4
1	DDD	169	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	DDD	162	ASN	2.4
1	CCC	165	PHE	2.4
1	BBB	194	ASP	2.4
1	AAA	263	LEU	2.4
1	DDD	163	PHE	2.4
1	DDD	78	ILE	2.4
1	DDD	255	ASP	2.4
1	CCC	136	PRO	2.4
1	BBB	317	GLY	2.4
1	BBB	106	ILE	2.3
1	AAA	192	TRP	2.3
1	DDD	298	GLY	2.3
1	DDD	189	VAL	2.3
1	DDD	165	PHE	2.3
1	DDD	178	PHE	2.3
1	DDD	158	ASN	2.3
1	BBB	232	LEU	2.3
1	CCC	227	LEU	2.3
1	AAA	136	PRO	2.3
1	BBB	136	PRO	2.3
1	BBB	59	VAL	2.3
1	CCC	270	PHE	2.3
1	CCC	287	PHE	2.3
1	BBB	328	GLY	2.2
1	CCC	297	THR	2.2
1	DDD	160	THR	2.2
1	BBB	256	LEU	2.2
1	BBB	148	SER	2.2
1	DDD	176	SER	2.2
1	AAA	151	LEU	2.2
1	BBB	176	SER	2.2
1	CCC	148	SER	2.2
1	CCC	321	SER	2.2
1	AAA	206	LYS	2.2
1	BBB	208	LYS	2.2
1	AAA	235	GLY	2.2
1	DDD	226	GLY	2.2
1	CCC	335	LEU	2.2
1	DDD	294	PRO	2.2
1	BBB	316	THR	2.1
1	AAA	236	LYS	2.1
1	CCC	289	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BBB	286	GLY	2.1
1	DDD	273	CYS	2.1
1	DDD	270	PHE	2.1
1	AAA	315	LEU	2.1
1	BBB	298	GLY	2.1
1	BBB	189	VAL	2.1
1	DDD	284	CYS	2.1
1	DDD	227	LEU	2.1
1	DDD	186	ASP	2.1
1	DDD	185	LYS	2.1
1	DDD	196	ASN	2.1
1	CCC	235	GLY	2.1
1	AAA	227	LEU	2.1
1	BBB	150	SER	2.1
1	BBB	321	SER	2.1
1	CCC	197	SER	2.1
1	CCC	206	LYS	2.1
1	AAA	156	GLY	2.1
1	BBB	164	VAL	2.0
1	DDD	256	LEU	2.0
1	AAA	52	SER	2.0
1	AAA	204	ILE	2.0
1	BBB	318	THR	2.0
1	DDD	117	GLY	2.0
1	DDD	205	PRO	2.0
1	AAA	270	PHE	2.0

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](#)

SUGAR-RSR INFOmissingINFO

6.4 Ligands [i](#)

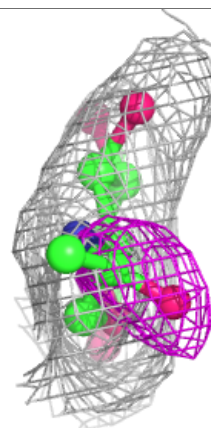
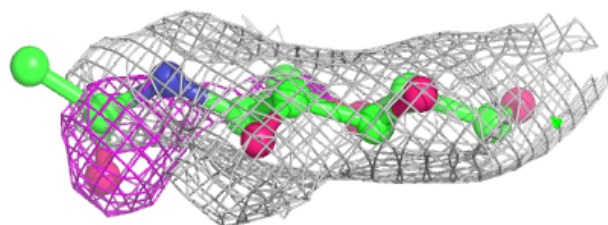
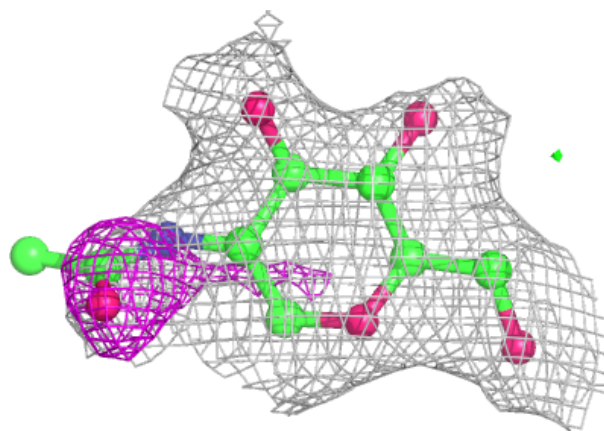
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	DDD	401	14/15	0.57	0.16	58,63,65,67	0
3	EDO	CCC	407	4/4	0.71	0.27	69,70,70,70	0
3	EDO	CCC	401	4/4	0.75	0.20	55,56,57,58	0
3	EDO	CCC	402	4/4	0.80	0.15	55,55,56,58	0
3	EDO	CCC	405	4/4	0.80	0.20	49,49,49,49	0
3	EDO	CCC	406	4/4	0.81	0.17	77,78,78,78	0
3	EDO	AAA	401	4/4	0.82	0.19	55,56,57,58	0
3	EDO	CCC	404	4/4	0.83	0.19	60,60,60,60	0
3	EDO	CCC	403	4/4	0.84	0.16	63,64,64,65	0
3	EDO	DDD	402	4/4	0.89	0.14	40,40,40,40	0
3	EDO	AAA	402	4/4	0.90	0.13	60,60,60,61	0
3	EDO	CCC	408	4/4	0.92	0.14	57,58,58,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAG DDD 401:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.