

wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 10:31 PM EDT

PDB ID : 8D3Z

Title : Crystal structure of GalS1 in complex with Manganese from Populus tri-

chocarpas

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Deposited on : 2022-06-01

Resolution : 2.56 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.orgA user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) 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 : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

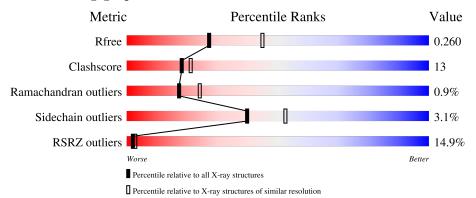
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.56 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	Similar resolution	
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$	
R_{free}	130704	1279 (2.58-2.54)	
Clashscore	141614	1327 (2.58-2.54)	
Ramachandran outliers	138981	1312 (2.58-2.54)	
Sidechain outliers	138945	1312 (2.58-2.54)	
RSRZ outliers	127900	1269 (2.58-2.54)	

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain						
1	A	424	70%	22% •• 6%					
1	В	424	23%	33% • 6%					
2	С	2	50%	50%					
2	Е	2	50%	50%					
3	D	7	14%	6%					



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Mol	Chain	Length		Quality of chain					
3	F	7	14%	71%	14%				

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	NAG	Е	2	-	-	=	X
3	NAG	F	2	-	-	=	X
5	NAG	A	505	-	-	=	X
5	NAG	В	502	-	-	=	X
5	NAG	В	504	-	-	=	X
5	NAG	В	505	-	-	=	X



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6928 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 Galactan synthase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	399	Total C N O S		S	0	0	0		
1	1 A	399	3278	2105	562	598	13	0	0	
1	D	399	Total	С	N	N O S	0	0		
1	Б	399	3278	2105	562	598	13	U		U

There are 2 discrepancies between the modelled and reference sequences:

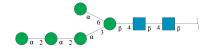
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A2K2AMS7
В	1	GLY	-	expression tag	UNP A0A2K2AMS7

• Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
2	С	2	Total 28			0	0	0
2	Е	2	Total 27			0	0	0

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



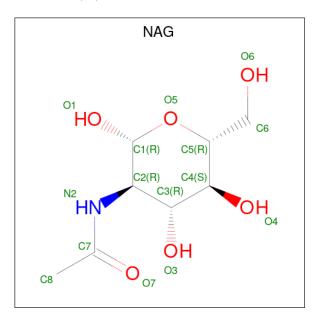


Mo	l Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
3	D	7	Total 83	C N 46 2		0	0	0
3	F	7	Total 83	C N 46 2		0	0	0

• Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mn 1 1	0	0
4	В	1	Total Mn 1 1	0	0

• Molecule 5 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
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	В	1	Total C N O 14 8 1 5	0	0



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

• Molecule 6 is water.

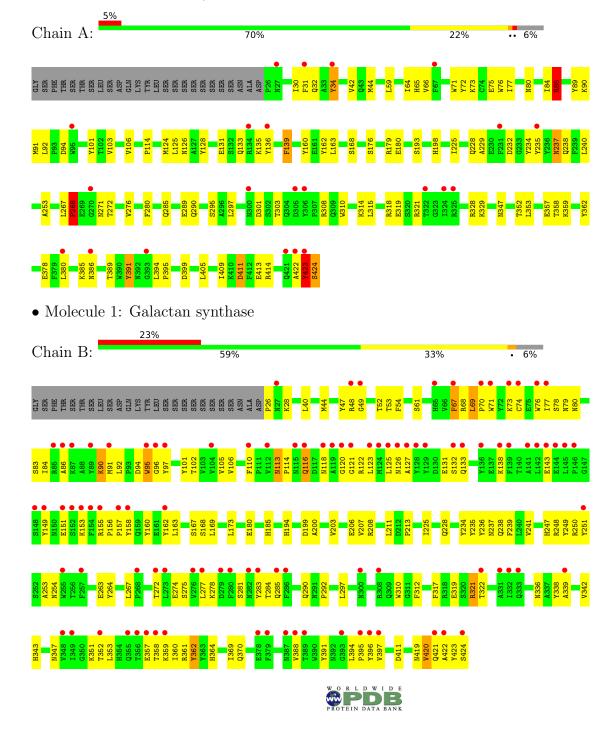
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	32	Total O 32 32	0	0
6	В	5	Total O 5 5	0	0



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: Galactan synthase



• Molecule :	2: 2-acetamido-2-deo:	xy-beta-D-glucopyranose	e-(1-4)-2-acetamid	lo-2-deoxy-beta-D-gluo
Chain C:	50%		50%	
NAG1 NAG2				
• Molecule :	2: 2-acetamido-2-deo:	xy-beta-D-glucopyranose	e-(1-4)-2-acetamid	o-2-deoxy-beta-D-gluo
Chain E:	50%		50%	
NAG1 NAG2				
ose-(1-3)-[al]	pha-D-mannopyranos	ranose-(1-2)-alpha-D-man se-(1-6)]beta-D-mannopy do-2-deoxy-beta-D-glucop	vanose-(1-4)-2-ac	
Chain D:	14%	86%		
NAG2 BMA3 BMA3 MAN4 MAN5 MAN6 MAN7				
ose-(1-3)-[al]	pha-D-mannopyranos	ranose-(1-2)-alpha-D-man se-(1-6)]beta-D-mannopy do-2-deoxy-beta-D-glucop	vanose-(1-4)-2-ac	
Chain F:	14%	71%	14%	
NAG1 NAG2 BMA3 MAN4 MAN5 MAN6				



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	169.98Å 169.98Å 73.96Å	Domositon
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.07 - 2.56	Depositor
Resolution (A)	49.07 - 2.56	EDS
% Data completeness	100.0 (49.07-2.56)	Depositor
(in resolution range)	$100.0 \ (49.07 - 2.56)$	EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.01 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D.D.	0.230 , 0.264	Depositor
R, R_{free}	0.227 , 0.260	DCC
R_{free} test set	2005 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31 , 64.1	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6928	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: MN, MAN, NAG, BMA

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	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.42	0/3381	0.66	$2/4591 \ (0.0\%)$
1	В	0.37	0/3381	0.63	2/4591 (0.0%)
All	All	0.40	0/6762	0.65	4/9182 (0.0%)

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	В	0	3
All	All	0	6

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	85	ARG	CG-CD-NE	6.90	126.29	111.80
1	A	423	TYR	CA-CB-CG	6.03	124.86	113.40
1	В	69	LEU	CA-CB-CG	5.46	127.86	115.30
1	В	90	LYS	CD-CE-NZ	-5.02	100.15	111.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	PRO	Peptide
1	A	422	ALA	Peptide



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Mol	Chain	Res	Type	Group
1	A	85	ARG	Sidechain
1	В	116	GLN	Peptide
1	В	361	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3278	0	3092	75	0
1	В	3278	0	3093	105	0
2	С	28	0	25	0	0
2	Е	27	0	24	2	0
3	D	83	0	70	0	0
3	F	83	0	70	4	0
4	A	1	0	0	0	0
4	В	1	0	0	0	0
5	A	56	0	52	1	0
5	В	56	0	52	1	0
6	A	32	0	0	4	0
6	В	5	0	0	0	0
All	All	6928	0	6478	179	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 13.

The worst 5 of 179 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:B:284:THR:HG21	1:B:336:ASN:HD22	1.28	0.95
1:A:77:ILE:HD12	1:A:124:MET:HG3	1.50	0.93
1:B:362:TYR:HE1	1:B:364:HIS:HB2	1.38	0.88
1:A:94:ASP:OD2	6:A:601:HOH:O	1.93	0.86
1:A:90:LYS:HE2	1:A:92:LEU:HD21	1.59	0.84

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	Perc	entiles
1	A	397/424 (94%)	374 (94%)	20 (5%)	3 (1%)	19	27
1	В	397/424 (94%)	360 (91%)	33 (8%)	4 (1%)	15	21
All	All	794/848 (94%)	734 (92%)	53 (7%)	7 (1%)	17	24

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	TYR
1	В	95	TRP
1	A	65	HIS
1	В	423	TYR
1	В	322	THR

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	A	342/365 (94%)	331 (97%)	11 (3%)	39 51
1	В	342/365 (94%)	332 (97%)	10 (3%)	42 55
All	All	684/730 (94%)	663 (97%)	21 (3%)	40 52

5 of 21 residues with a non-rotameric sidechain are listed below:

\mathbf{Mol}	Chain	Res	\mathbf{Type}
1	В	162	TYR



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Mol	Chain	Res	Type
1	В	321	ARG
1	В	411	ASP
1	В	338	TYR
1	В	235	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	ASN
1	A	386	ASN
1	В	238	GLN
1	В	336	ASN

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)

18 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	Bo	Bond lengths			Bond angles		
MIOI					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	NAG	С	1	2,1	14,14,15	1.35	1 (7%)	17,19,21	0.89	1 (5%)	
2	NAG	С	2	2	14,14,15	0.39	0	17,19,21	0.39	0	
3	NAG	D	1	1,3	14,14,15	0.53	0	17,19,21	0.48	0	
3	NAG	D	2	3	14,14,15	0.61	1 (7%)	17,19,21	0.58	0	
3	BMA	D	3	3	11,11,12	0.90	1 (9%)	15,15,17	1.10	1 (6%)	



Mal	Trino	Chain	Dag	Link	Вс	ond leng	ths	В	ond ang	eles
Mol	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	D	4	3	11,11,12	0.69	0	15,15,17	1.27	2 (13%)
3	MAN	D	5	3	11,11,12	0.85	1 (9%)	15,15,17	1.20	2 (13%)
3	MAN	D	6	3	11,11,12	0.96	0	15,15,17	1.14	1 (6%)
3	MAN	D	7	3	11,11,12	1.01	1 (9%)	15,15,17	1.15	2 (13%)
2	NAG	Е	1	2	12,12,15	0.21	0	15,15,21	0.60	0
2	NAG	Е	2	2	14,14,15	0.32	0	17,19,21	0.36	0
3	NAG	F	1	1,3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	F	2	3	14,14,15	0.22	0	17,19,21	0.53	0
3	BMA	F	3	3	11,11,12	1.03	2 (18%)	15,15,17	0.98	0
3	MAN	F	4	3	11,11,12	0.77	0	15,15,17	1.17	2 (13%)
3	MAN	F	5	3	11,11,12	1.00	1 (9%)	15,15,17	0.96	0
3	MAN	F	6	3	11,11,12	0.84	1 (9%)	15,15,17	1.35	2 (13%)
3	MAN	F	7	3	11,11,12	0.79	0	15,15,17	0.99	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	NAG	С	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	С	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
3	MAN	D	6	3	-	1/2/19/22	0/1/1/1
3	MAN	D	7	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	2	-	9/15/15/26	-
2	NAG	Ε	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
3	MAN	F	6	3	-	2/2/19/22	0/1/1/1
3	MAN	F	7	3	-	0/2/19/22	0/1/1/1



The worst	5	of	9	bond	length	outliers	are	listed	below:
THE WOLDS	\circ	$O_{\mathbf{I}}$	J	DOM	10115 011	Outilities	COL C	mouca	DCIOW.

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	Ideal(Å)
2	С	1	NAG	O5-C1	-4.69	1.36	1.43
3	D	7	MAN	O5-C5	3.00	1.49	1.43
3	F	6	MAN	C1-C2	2.39	1.57	1.52
3	D	3	BMA	C1-C2	2.36	1.57	1.52
3	D	5	MAN	O5-C1	-2.29	1.40	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	D	4	MAN	O2-C2-C3	-3.46	103.20	110.14
3	F	6	MAN	C1-O5-C5	3.34	116.72	112.19
3	D	6	MAN	C1-O5-C5	3.13	116.43	112.19
3	D	5	MAN	O2-C2-C3	-2.97	104.18	110.14
3	F	4	MAN	O2-C2-C3	-2.96	104.20	110.14

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Е	1	NAG	N2-C2-C3-C4
2	Е	1	NAG	N2-C2-C3-O3
3	F	1	NAG	O5-C5-C6-O6
3	D	7	MAN	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6

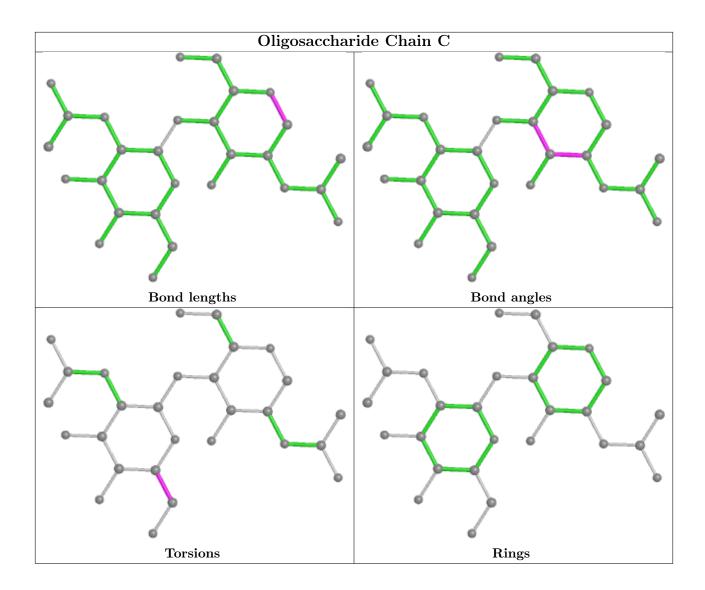
There are no ring outliers.

3 monomers are involved in 6 short contacts:

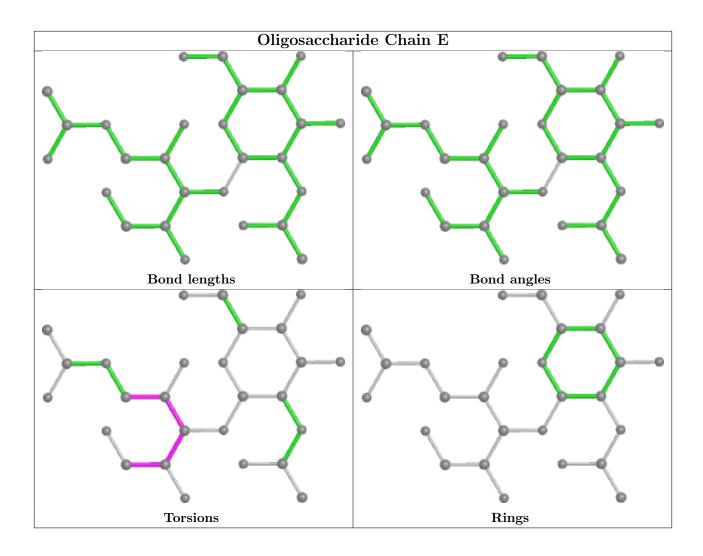
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Е	1	NAG	2	0
3	F	4	MAN	1	0
3	F	1	NAG	3	0

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

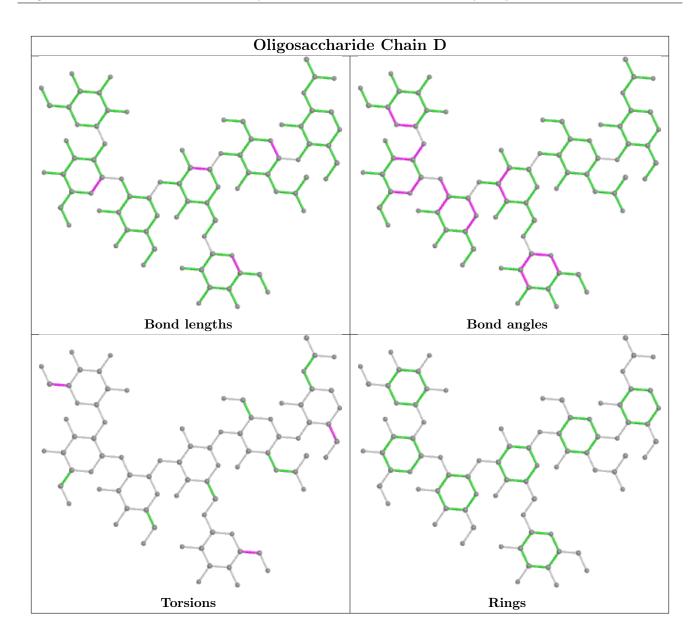




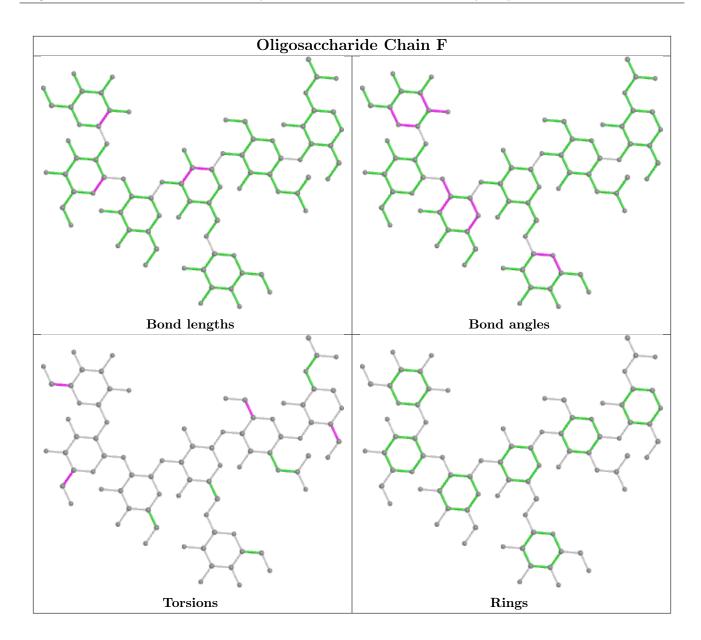












5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	l Type	Chain	Res	Link	Bond lengths			Bond angles		
IVIOI					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	В	504	1	14,14,15	0.36	0	17,19,21	0.47	0



Mol	Tuno	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	В	502	-	14,14,15	0.24	0	17,19,21	0.38	0
5	NAG	В	503	1	14,14,15	0.26	0	17,19,21	0.46	0
5	NAG	A	504	1	14,14,15	0.47	0	17,19,21	0.83	1 (5%)
5	NAG	В	505	1	14,14,15	0.39	0	17,19,21	0.52	0
5	NAG	A	502	-	14,14,15	0.52	0	17,19,21	0.43	0
5	NAG	A	505	1	14,14,15	0.43	0	17,19,21	0.55	0
5	NAG	A	503	1	14,14,15	0.23	0	17,19,21	0.53	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
5	NAG	В	504	1	-	0/6/23/26	0/1/1/1
5	NAG	В	502	-	-	2/6/23/26	0/1/1/1
5	NAG	В	503	1	-	2/6/23/26	0/1/1/1
5	NAG	A	504	1	-	0/6/23/26	0/1/1/1
5	NAG	В	505	1	-	3/6/23/26	0/1/1/1
5	NAG	A	502	-	-	2/6/23/26	0/1/1/1
5	NAG	A	505	1	_	4/6/23/26	0/1/1/1
5	NAG	A	503	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
5	A	504	NAG	C1-O5-C5	3.05	116.33	112.19

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	502	NAG	O5-C5-C6-O6
5	A	505	NAG	O5-C5-C6-O6
5	В	505	NAG	O5-C5-C6-O6
5	В	503	NAG	O5-C5-C6-O6
5	В	502	NAG	C4-C5-C6-O6

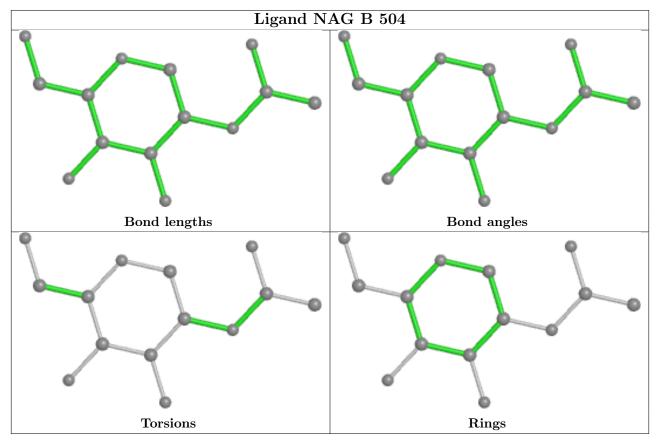
There are no ring outliers.



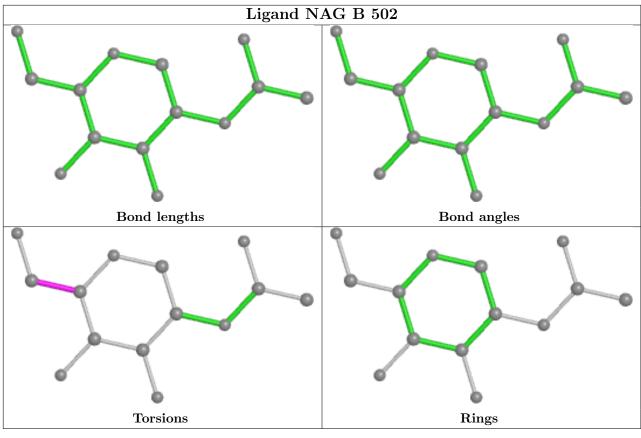
2 monomers are involved in 2 short contacts:

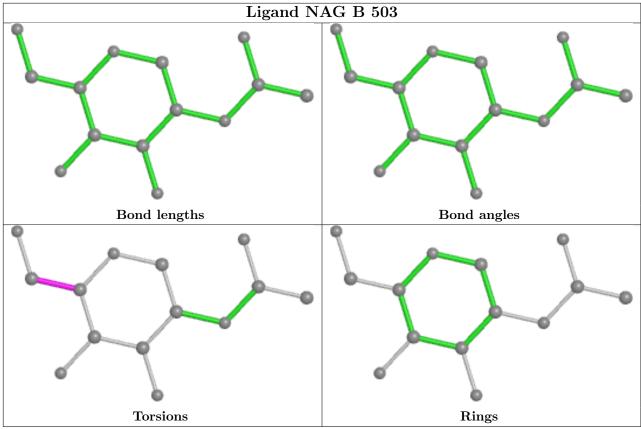
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	В	502	NAG	1	0
5	A	502	NAG	1	0

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 then 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.

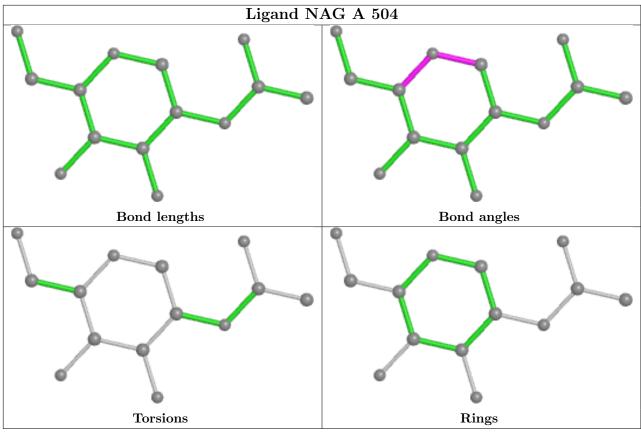


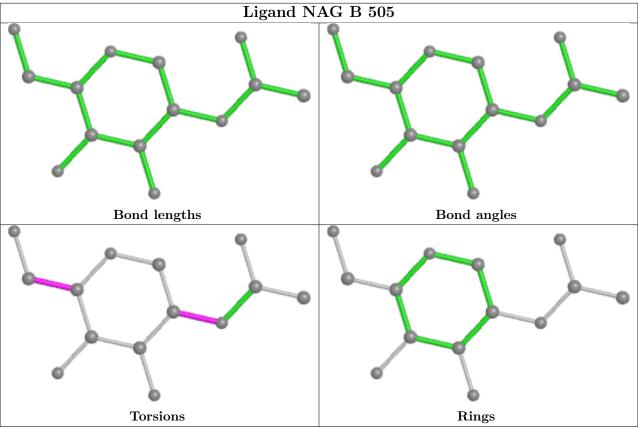




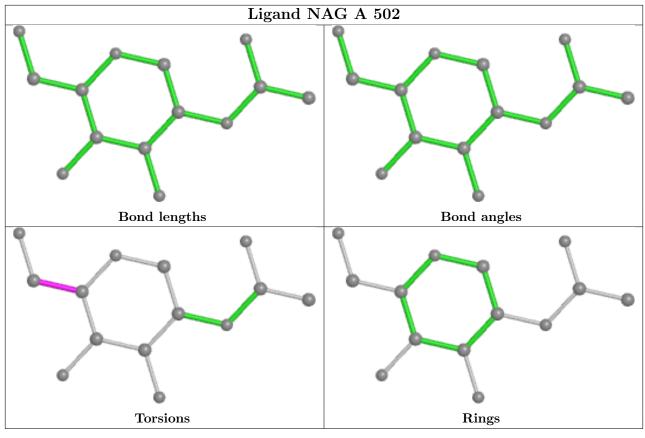


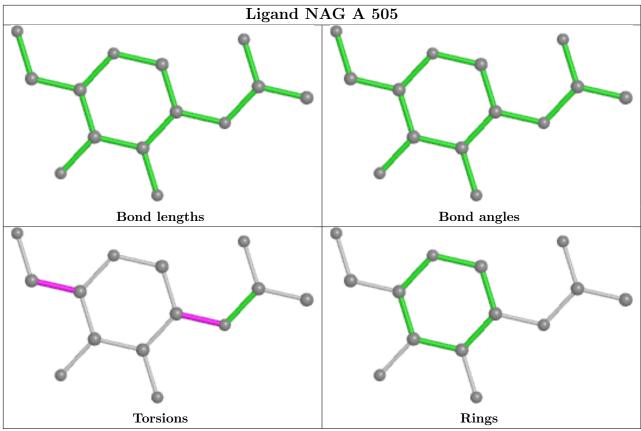




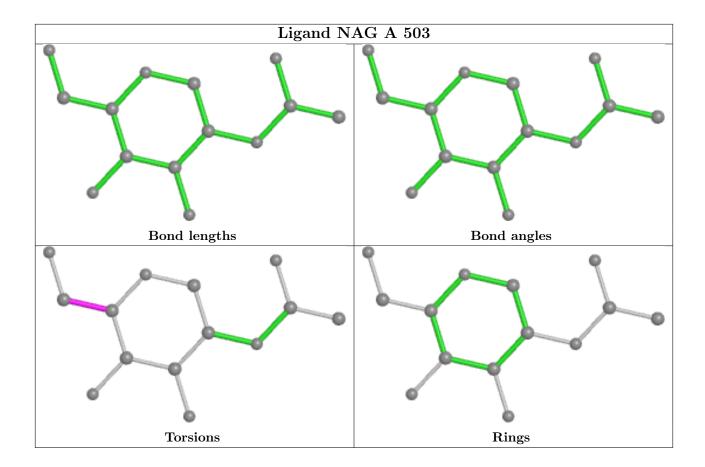












5.7 Other polymers (i)

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^{th} 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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	399/424 (94%)	0.44	22 (5%) 25 32	50, 78, 132, 179	0
1	В	399/424 (94%)	1.33	97 (24%) 0 0	71, 124, 187, 214	0
All	All	798/848 (94%)	0.88	119 (14%) 2 3	50, 99, 177, 214	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	125	LEU	8.7
1	В	349	ILE	8.5
1	В	142	LEU	8.4
1	В	422	ALA	8.4
1	В	76	TRP	7.7

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^{th} 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.

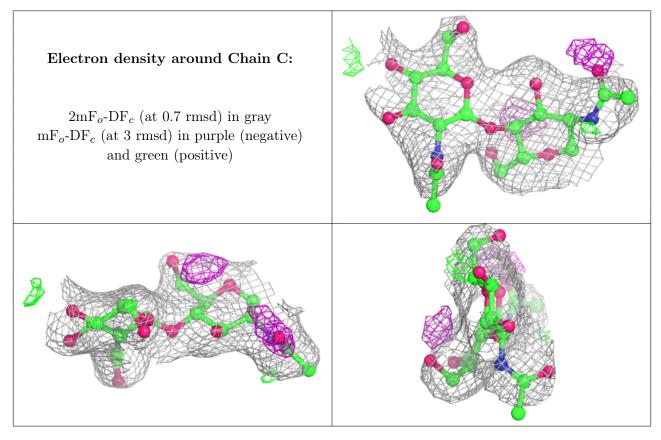
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
3	NAG	F	2	14/15	0.52	0.45	164,179,184,184	0
3	MAN	F	7	11/12	0.52	0.35	156,170,176,178	0
3	BMA	F	3	11/12	0.66	0.16	163,168,173,174	0
2	NAG	Е	2	14/15	0.67	0.66	167,188,197,199	0
3	NAG	F	1	14/15	0.69	0.23	156,174,179,181	0



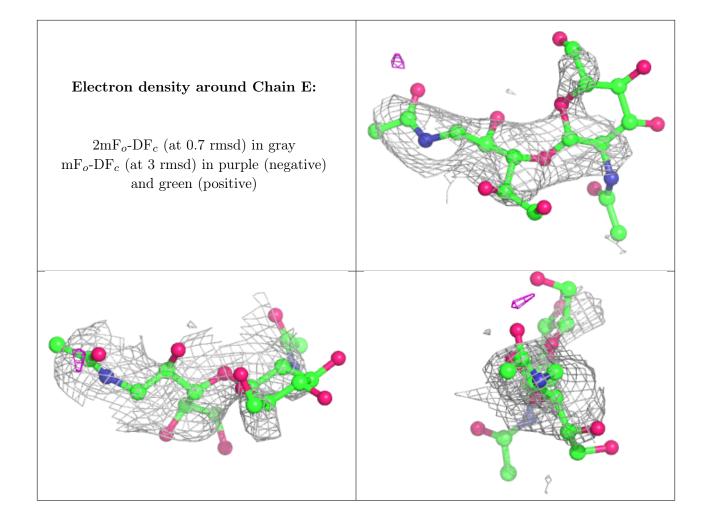
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
3	MAN	F	4	11/12	0.71	0.21	164,173,177,178	0
3	MAN	F	6	11/12	0.76	0.33	147,155,161,161	0
2	NAG	Е	1	13/15	0.76	0.38	150,160,174,183	0
3	MAN	F	5	11/12	0.80	0.25	153,171,173,176	0
3	MAN	D	7	11/12	0.84	0.16	87,102,112,119	0
2	NAG	С	2	14/15	0.87	0.25	96,106,118,118	0
3	MAN	D	6	11/12	0.92	0.20	95,98,109,110	0
2	NAG	С	1	14/15	0.93	0.17	63,78,94,99	0
3	NAG	D	2	14/15	0.94	0.16	65,73,84,95	0
3	NAG	D	1	14/15	0.96	0.18	58,64,73,77	0
3	BMA	D	3	11/12	0.96	0.14	56,68,78,91	0
3	MAN	D	5	11/12	0.96	0.16	83,89,99,99	0
3	MAN	D	4	11/12	0.97	0.15	68,70,77,80	0

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



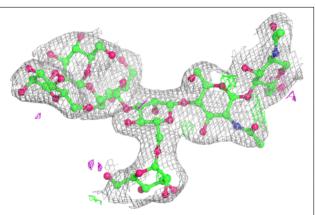


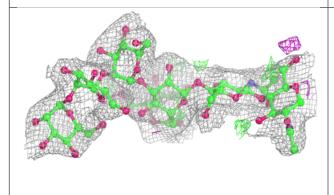


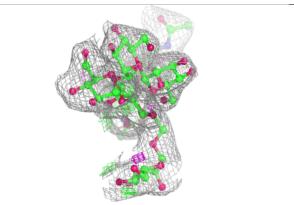


Electron density around Chain D:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

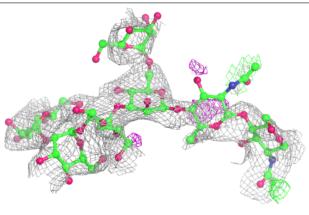


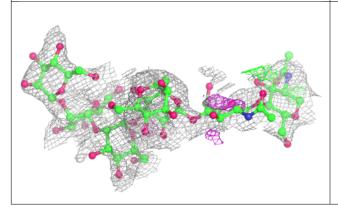


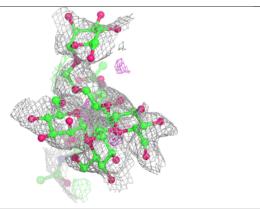


Electron density around Chain F:

 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)







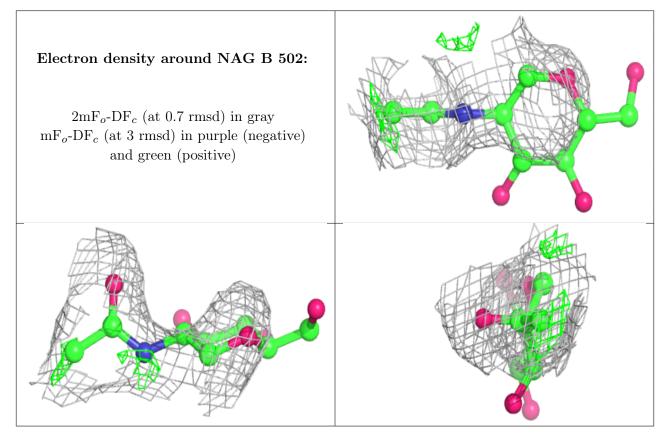


6.4 Ligands (i)

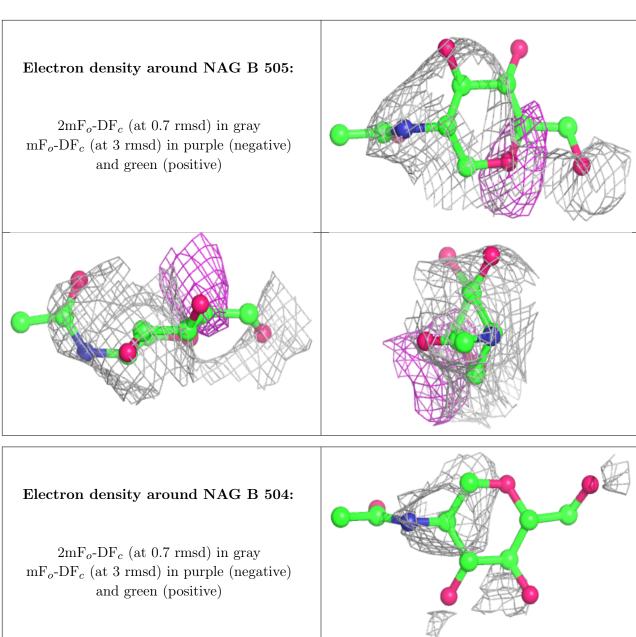
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

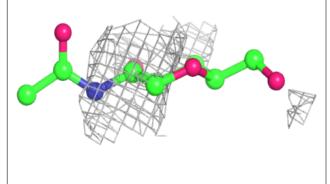
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
5	NAG	В	502	14/15	0.47	0.56	160,179,187,188	0
5	NAG	В	505	14/15	0.56	0.45	145,161,174,176	0
5	NAG	В	504	14/15	0.64	0.51	171,186,195,197	0
5	NAG	В	503	14/15	0.70	0.31	122,148,154,154	0
4	MN	A	501	1/1	0.73	0.39	108,108,108,108	0
5	NAG	A	505	14/15	0.79	0.52	141,158,164,170	0
5	NAG	A	502	14/15	0.82	0.15	63,92,98,100	0
5	NAG	A	504	14/15	0.83	0.19	92,111,118,118	0
4	MN	В	501	1/1	0.83	0.30	111,111,111,111	0
5	NAG	A	503	14/15	0.90	0.28	118,131,139,139	0

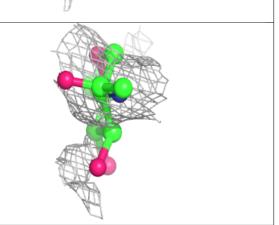
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



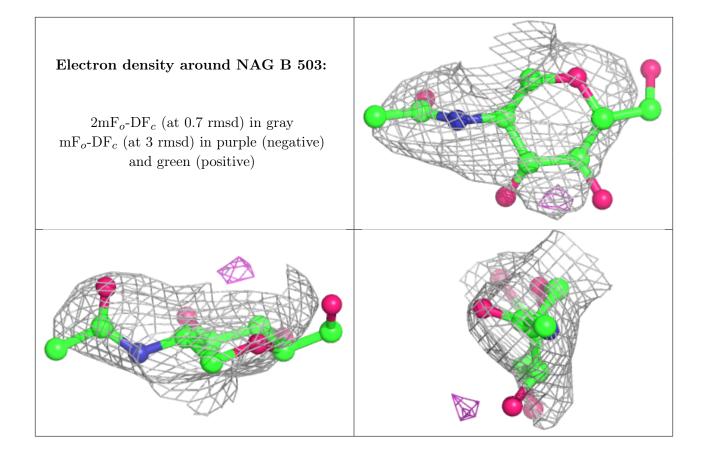




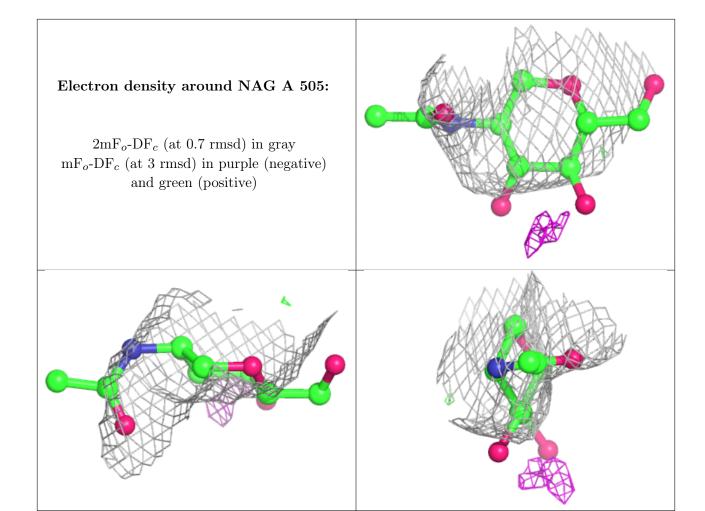








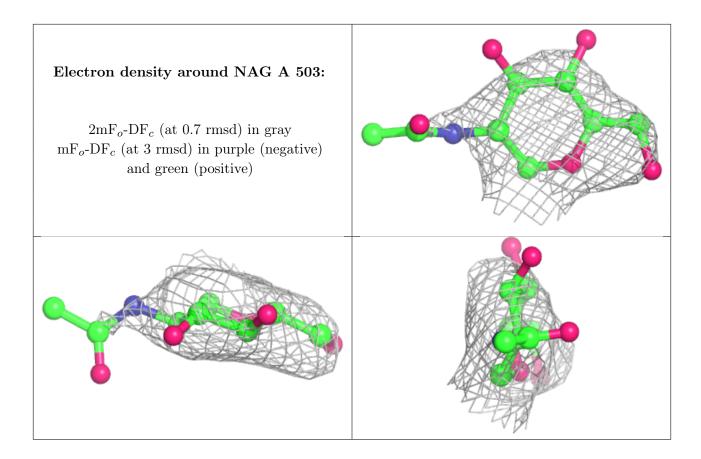






Electron density around NAG A 502: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around NAG A 504: $2mF_o$ -DF_c (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.

