

Full wwPDB X-ray Structure Validation Report (i)

Apr 10, 2024 – 02:04 PM EDT

PDB ID : 8TM2

Title : Preclinical Characterization of Pan-NKG2D Ligand-Binding NKG2D Receptor

Decoys

Authors: Rupert, P.B.; Strong, R.

Deposited on : 2023-07-27

Resolution : 2.85 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 (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 : 2.36.1

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)

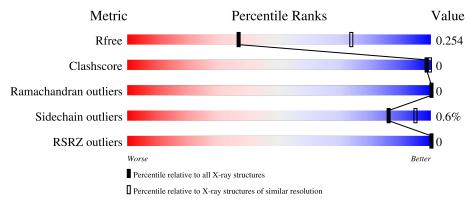
Validation Pipeline (wwPDB-VP) : 2.36.1

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 2.85 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	264	95%		•		
2	С	188	85%		• 12%		
3	В	2	50%	50%			
3	D	2	100%				



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3472 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 NKG2-D type II integral membrane protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	253	Total	С	N	О	S	0	0	0
1	A	200	2016	1280	324	388	24	U	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P26718
A	2	SER	-	expression tag	UNP P26718

• Molecule 2 is a protein called MHC class I polypeptide-related sequence A.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	С	165	Total 1316	C 823	N 236	O 248	S 9	0	1	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	68	ALA	GLY	conflict	UNP Q29983
С	69	TRP	ASN	conflict	UNP Q29983
С	125	LEU	LYS	conflict	UNP Q29983
С	152	GLN	LYS	conflict	UNP Q29983
С	154	ASP	LYS	conflict	UNP Q29983
С	158	ARG	HIS	conflict	UNP Q29983
С	166	PHE	GLN	conflict	UNP Q29983
С	183	HIS	-	expression tag	UNP Q29983
С	184	HIS	ı	expression tag	UNP Q29983
С	185	HIS	-	expression tag	UNP Q29983
С	186	HIS	-	expression tag	UNP Q29983
С	187	HIS	-	expression tag	UNP Q29983
С	188	HIS	-	expression tag	UNP Q29983

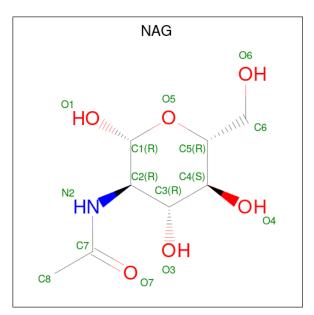


• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	2	Total C N O 28 16 2 10	0	0	0
3	В	2	Total C N O 28 16 2 10	0	0	0

• 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	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	С	1	Total C N O 14 8 1 5	0	0

• Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	1	Total C O 6 3 3	0	0

• Molecule 6 is water.

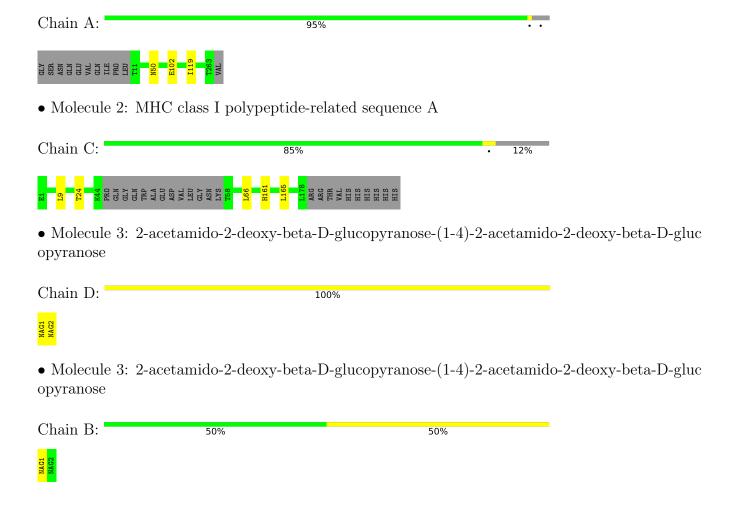
\mathbf{Mol}	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
6	A	15	Total O 15 15	0	0
6	C	7	Total O 7 7	0	0



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.







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	56.57Å 69.78Å 145.37Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.69 - 2.85	Depositor
rtesolution (A)	44.64 - 2.85	EDS
% Data completeness	83.0 (72.69-2.85)	Depositor
(in resolution range)	83.0 (44.64-2.85)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.68 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
D D.	0.214 , 0.253	Depositor
R, R_{free}	0.215 , 0.254	DCC
R_{free} test set	609 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 39.2	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3472	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.12% 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: GOL, NAG

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		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.36	0/2074	0.53	0/2819	
2	С	0.35	0/1348	0.55	0/1826	
All	All	0.36	0/3422	0.54	0/4645	

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	A	2016	0	1853	1	0
2	С	1316	0	1223	2	0
3	В	28	0	25	0	0
3	D	28	0	25	0	0
4	A	42	0	39	0	0
4	С	14	0	13	0	0
5	С	6	0	8	0	0
6	A	15	0	0	0	0
6	С	7	0	0	0	0
All	All	3472	0	3186	3	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 0.

All (3) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{c} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	Clash overlap (Å)
2:C:24:THR:HG21	2:C:66:LEU:HD22	1.94	0.48
2:C:161:HIS:CE1	2:C:165:LEU:HD11	2.51	0.46
1:A:102:GLU:HA	1:A:119:ILE:HD12	2.03	0.40

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	Perce	ntiles
1	A	251/264~(95%)	235 (94%)	16 (6%)	0	100	100
2	\mathbf{C}	162/188 (86%)	155 (96%)	7 (4%)	0	100	100
All	All	413/452 (91%)	390 (94%)	23 (6%)	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	A	224/243 (92%)	223 (100%)	1 (0%)	91 96		
2	С	139/170 (82%)	138 (99%)	1 (1%)	84 94		

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Mol	Chain	Analysed	Analysed Rotameric		Percentiles	
All	All	363/413 (88%)	361 (99%)	2 (1%)	86 95	

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
2	С	9	LEU

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	136	GLN
1	A	150	ASN
1	A	172	GLN
1	A	261	GLN

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	Trms	Chain	Dag	es Link Bond lengths		Bond angles				
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	NAG	В	1	3,1	14,14,15	0.64	0	17,19,21	0.98	1 (5%)
3	NAG	В	2	3	14,14,15	0.34	0	17,19,21	0.85	0



Mol	Trus	Chain	Res Link		Link Bond lengths			Bond angles		
IVIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	1	3,2	14,14,15	0.41	0	17,19,21	1.04	2 (11%)
3	NAG	D	2	3	14,14,15	0.30	0	17,19,21	1.02	2 (11%)

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	NAG	В	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	В	2	3	-	1/6/23/26	0/1/1/1
3	NAG	D	1	3,2	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
3	В	1	NAG	C4-C3-C2	2.27	114.35	111.02
3	D	2	NAG	C1-O5-C5	2.24	115.22	112.19
3	D	1	NAG	C4-C3-C2	2.22	114.28	111.02
3	D	1	NAG	C1-O5-C5	2.18	115.15	112.19
3	D	2	NAG	O5-C1-C2	-2.04	108.07	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

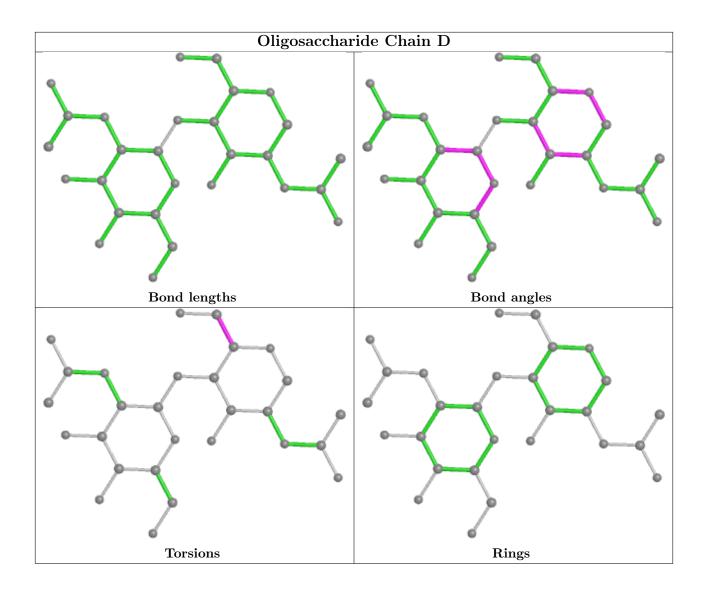
Mol	Chain	Res	Type	Atoms
3	В	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	В	1	NAG	C1-C2-N2-C7
3	В	1	NAG	C3-C2-N2-C7

There are no ring outliers.

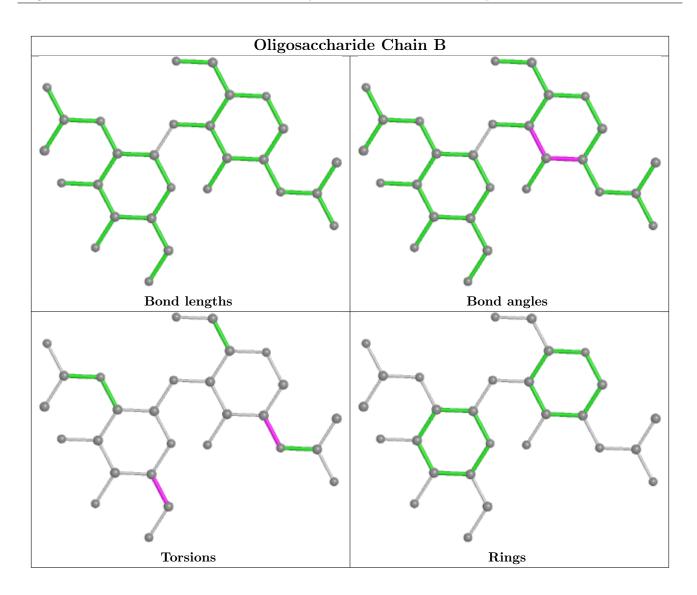
No monomer is involved in short contacts.

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)

5 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	Trunc	Chain	Res	Link	Bo	ond leng	${ m ths}$	Bond angles		
MIOI	Type	Chain		Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	NAG	С	201	2	14,14,15	0.30	0	17,19,21	0.95	1 (5%)
4	NAG	A	301	1	14,14,15	0.60	0	17,19,21	2.03	5 (29%)
4	NAG	A	303	1	14,14,15	0.45	0	17,19,21	1.29	2 (11%)



Mol	Type Chain Re		Res	Link	Bo	ond leng	$ ag{ths}$	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	NAG	A	302	1	14,14,15	0.29	0	17,19,21	1.28	2 (11%)
5	GOL	С	202	-	5,5,5	0.32	0	5,5,5	0.15	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
4	NAG	С	201	2	-	2/6/23/26	0/1/1/1
4	NAG	A	301	1	-	3/6/23/26	0/1/1/1
4	NAG	A	303	1	-	1/6/23/26	0/1/1/1
4	NAG	A	302	1	-	2/6/23/26	0/1/1/1
5	GOL	С	202	-	-	2/4/4/4	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
4	A	301	NAG	C2-N2-C7	5.24	130.37	122.90
4	A	301	NAG	C8-C7-N2	3.73	122.42	116.10
4	A	303	NAG	C1-O5-C5	3.13	116.44	112.19
4	A	302	NAG	C2-N2-C7	2.59	126.59	122.90
4	A	302	NAG	C8-C7-N2	2.48	120.29	116.10
4	A	301	NAG	O5-C1-C2	-2.47	107.39	111.29
4	A	303	NAG	C2-N2-C7	2.32	126.21	122.90
4	A	301	NAG	C1-C2-N2	2.18	114.21	110.49
4	С	201	NAG	O5-C5-C6	2.06	110.44	107.20
4	A	301	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	С	201	NAG	O5-C5-C6-O6
4	С	201	NAG	C4-C5-C6-O6
4	A	301	NAG	C8-C7-N2-C2
4	A	301	NAG	O7-C7-N2-C2
4	A	302	NAG	C8-C7-N2-C2
4	A	302	NAG	O7-C7-N2-C2

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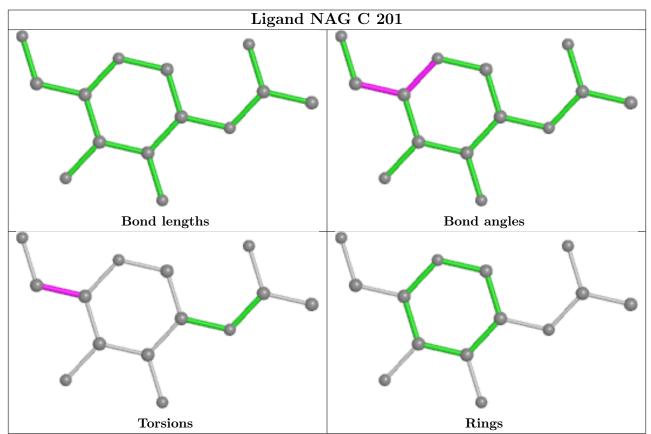
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Mol	Chain	Res	Type	Atoms
5	С	202	GOL	O1-C1-C2-C3
5	С	202	GOL	O1-C1-C2-O2
4	A	301	NAG	C3-C2-N2-C7
4	A	303	NAG	C3-C2-N2-C7

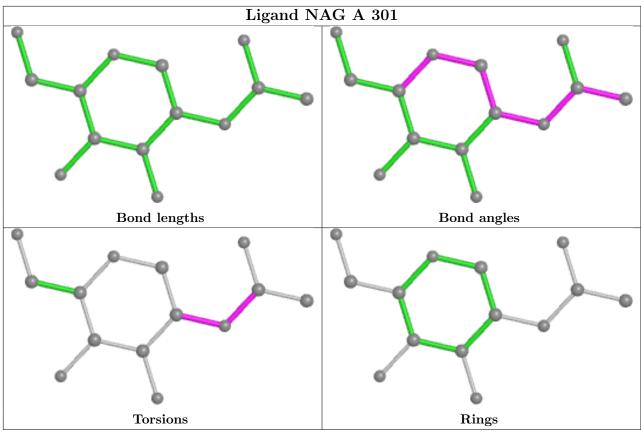
There are no ring outliers.

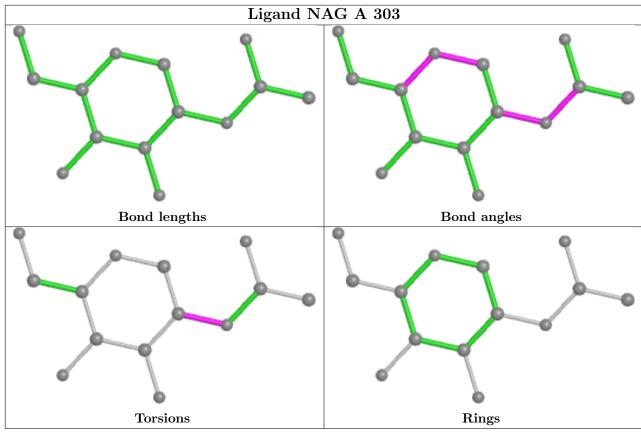
No monomer is involved in short contacts.

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 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.

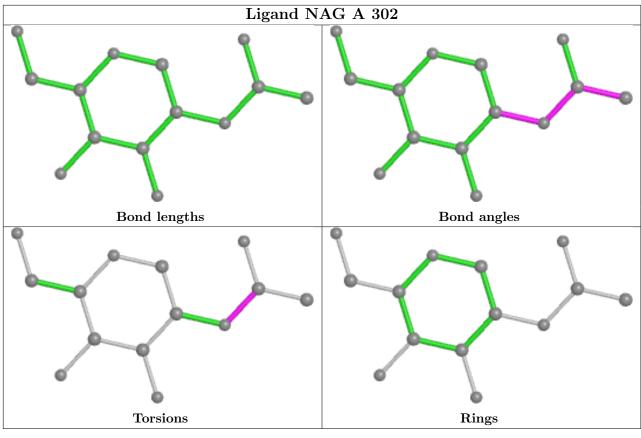


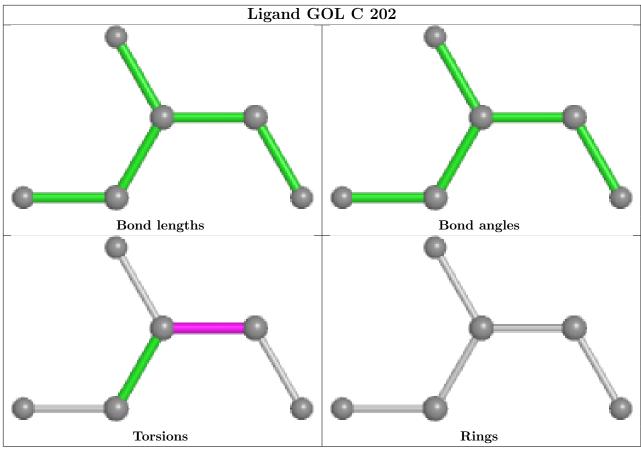














5.7 Other polymers (i)

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 $>$	#	₽RSF	RZ>2	$OWAB(A^2)$	Q<0.9
1	A	253/264~(95%)	-0.05	0	100	100	37, 54, 82, 110	0
2	С	165/188 (87%)	-0.11	0	100	100	40, 55, 80, 90	0
All	All	418/452 (92%)	-0.08	0	100	100	37, 55, 82, 110	0

There are no RSRZ outliers to report.

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

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

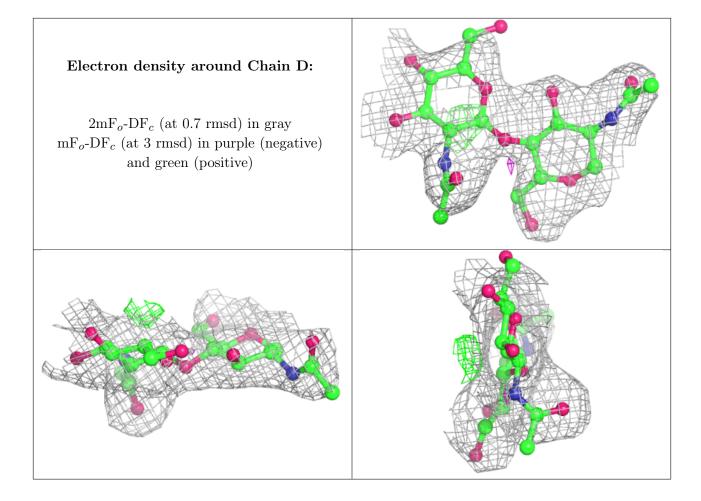
6.3 Carbohydrates (i)

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.

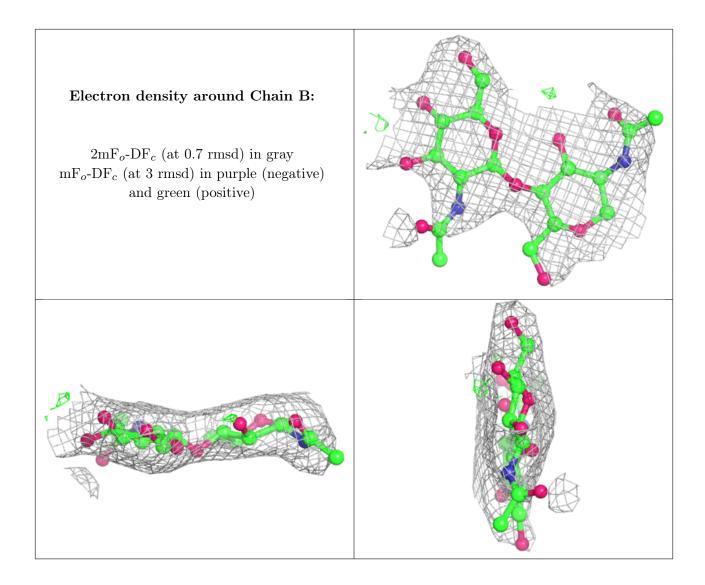
Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f A}^2)$	Q<0.9
3	NAG	D	2	14/15	0.81	0.26	77,83,86,86	0
3	NAG	В	1	14/15	0.85	0.35	81,85,87,92	0
3	NAG	В	2	14/15	0.87	0.36	93,95,101,102	0
3	NAG	D	1	14/15	0.93	0.18	60,63,68,75	0

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)

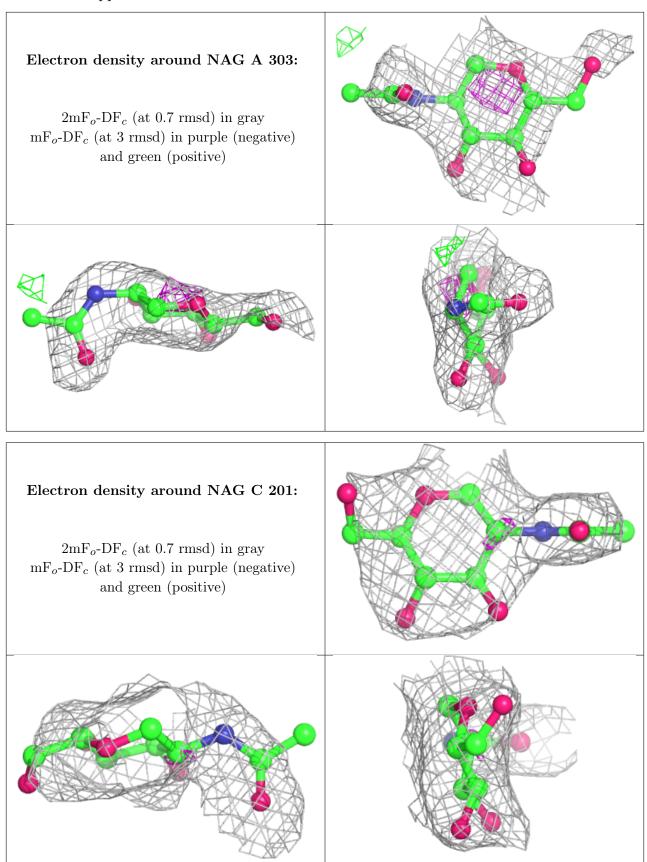
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	NAG	A	303	14/15	0.81	0.48	83,89,90,91	0
4	NAG	С	201	14/15	0.85	0.32	79,84,88,88	0
4	NAG	A	301	14/15	0.88	0.18	74,78,80,83	0
5	GOL	С	202	6/6	0.90	0.34	74,74,75,75	0
4	NAG	A	302	14/15	0.95	0.20	54,56,58,58	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



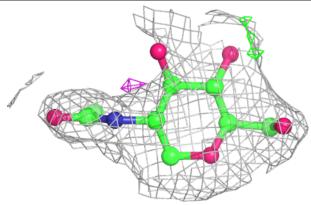
orientation to approximate a three-dimensional view.

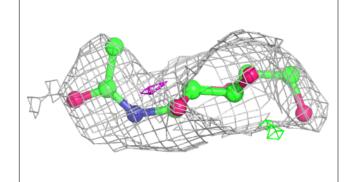


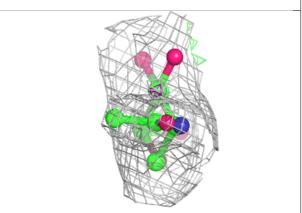


Electron density around NAG A 301:

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

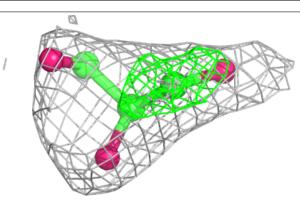


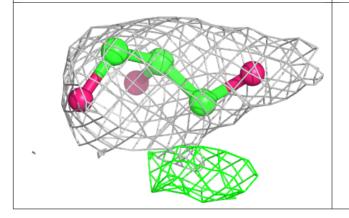


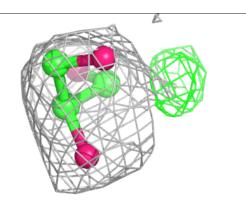


Electron density around GOL C 202:

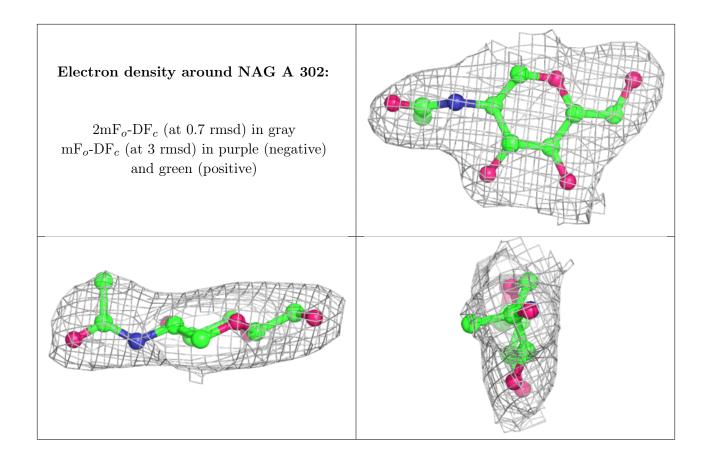
 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

