

wwPDB X-ray Structure Validation Summary Report (i)

Mar 24, 2022 – 03:48 pm GMT

PDB ID : 6THB

Title: Receptor binding domain of the Cedar Virus attachment glycoprotein (G)

Authors: Pryce, R.; Rissanen, I.; Harlos, K.; Bowden, T.

Deposited on : 2019-11-19

Resolution : 2.78 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.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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.27

buster-report : 1.1.7 (2018)

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

 $Refmac \quad : \quad 5.8.0267$

CCP4 : 7.1.010 (Gargrove)

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

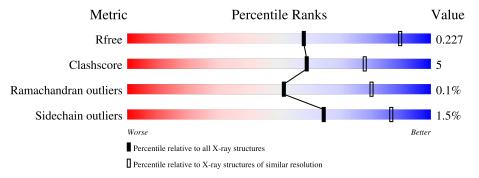
Validation Pipeline (wwPDB-VP) : 2.27

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 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)

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%

Mol	Chain	Length	Quality of chain		
1	A	426	85%	12%	
1	В	426	84%	14%	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6889 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 Attachment glycoprotein.

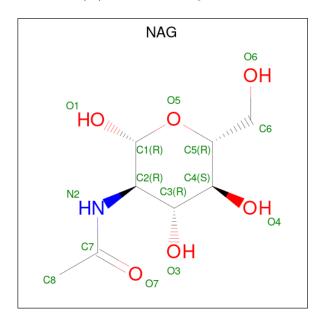
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	417	Total 3347	C 2125	N 553	O 645	S 24	0	0	0
1	В	418	Total 3351	C 2127	N 554	O 646	S 24	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	GLU	-	expression tag	UNP A0A185KRV2
A	207	THR	-	expression tag	UNP A0A185KRV2
A	208	GLY	-	expression tag	UNP A0A185KRV2
A	623	GLY	-	expression tag	UNP A0A185KRV2
A	624	THR	-	expression tag	UNP A0A185KRV2
A	625	LYS	-	expression tag	UNP A0A185KRV2
A	626	HIS	-	expression tag	UNP A0A185KRV2
A	627	HIS	-	expression tag	UNP A0A185KRV2
A	628	HIS	-	expression tag	UNP A0A185KRV2
A	629	HIS	-	expression tag	UNP A0A185KRV2
A	630	HIS	-	expression tag	UNP A0A185KRV2
A	631	HIS	-	expression tag	UNP A0A185KRV2
В	206	GLU	-	expression tag	UNP A0A185KRV2
В	207	THR	-	expression tag	UNP A0A185KRV2
В	208	GLY	-	expression tag	UNP A0A185KRV2
В	623	GLY	-	expression tag	UNP A0A185KRV2
В	624	THR	-	expression tag	UNP A0A185KRV2
В	625	LYS	-	expression tag	UNP A0A185KRV2
В	626	HIS	-	expression tag	UNP A0A185KRV2
В	627	HIS	-	expression tag	UNP A0A185KRV2
В	628	HIS	-	expression tag	UNP A0A185KRV2
В	629	HIS	-	expression tag	UNP A0A185KRV2
В	630	HIS	-	expression tag	UNP A0A185KRV2
В	631	HIS	-	expression tag	UNP A0A185KRV2



• Molecule 2 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
2	A	1	Total C N	Ō	0	0
			14 8 1	5		
2	A	1	Total C N	O	0	0
			14 8 1	5		_
2	A	1	Total C N	O	0	0
		-	14 8 1	5		
2	A	1	Total C N	О	0	0
	11	1	14 8 1	5	0	O .
2	A	1	Total C N	O	0	0
	11	1	14 8 1	5	O	U
2	A	1	Total C N	О	0	0
2	Λ	1	14 8 1	5	U	0
2	A	1	Total C N	О	0	0
2	А	1	14 8 1	5	U	U
9	D	1	Total C N	О	0	0
2	В	1	14 8 1	5	0	0
0	D	1	Total C N	О	0	0
2	В	1	14 8 1	5	0	0
0	D	1	Total C N	О	0	0
2	В	1	14 8 1	5	0	0
2	В	1	Total C N	О	0	0
	Б	1	14 8 1	5	U	U
2	В	1	Total C N	О	0	0
2	Б	1	14 8 1	5	U	U

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Mol	Chain	Residues	Ato	ns		ZeroOcc	AltConf
2	В	1	Total C 14 8	N 1	O 5	0	0

• Molecule 3 is water.

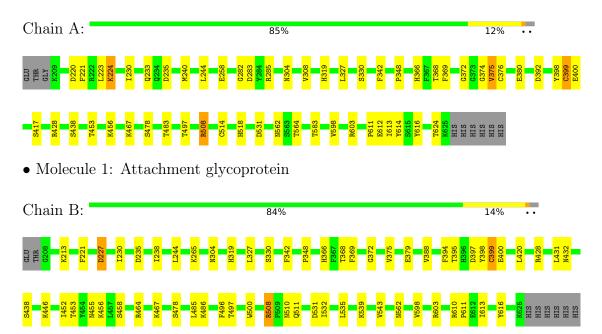
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	В	5	Total O 5 5	0	0



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. 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. 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: Attachment glycoprotein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants	201.46Å 201.46Å 112.89Å	Danagitan
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.24 - 2.78	Depositor
Resolution (A)	49.24 - 2.78	EDS
% Data completeness	99.9 (49.24-2.78)	Depositor
(in resolution range)	99.9 (49.24-2.78)	EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.66 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.14_3228	Depositor
D.D.	0.201 , 0.227	Depositor
R, R_{free}	0.201 , 0.227	DCC
R_{free} test set	3272 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6889	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.62% 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: 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		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.26	0/3430	0.46	0/4652	
1	В	0.25	0/3434	0.44	0/4657	
All	All	0.25	0/6864	0.45	0/9309	

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	3347	0	3229	31	0
1	В	3351	0	3233	35	0
2	A	98	0	91	0	0
2	В	84	0	78	1	0
3	A	4	0	0	0	0
3	В	5	0	0	0	0
All	All	6889	0	6631	63	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 5.

The worst 5 of 63 close contacts within the same asymmetric unit are listed below, sorted by their



clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:330:SER:O	1:A:428:ARG:NH2	2.26	0.68
1:A:453:THR:HB	1:A:497:THR:HG22	1.75	0.66
1:A:399:CYS:SG	1:A:400:GLU:N	2.69	0.64
1:B:438:SER:HB3	1:B:446:LYS:HB2	1.80	0.64
1:B:227:ASP:OD1	1:B:610:ARG:NH2	2.31	0.63

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	hain Analysed Favoured Allowed		Outliers	Perce	ntiles	
1	A	415/426 (97%)	390 (94%)	25 (6%)	0	100	100
1	В	416/426 (98%)	390 (94%)	25 (6%)	1 (0%)	47	76
All	All	831/852 (98%)	780 (94%)	50 (6%)	1 (0%)	51	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	562	ASN

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	Percen	tiles
1	A	390/398 (98%)	384 (98%)	6 (2%)	65	87
1	В	390/398 (98%)	384 (98%)	6 (2%)	65	87
All	All	780/796 (98%)	768 (98%)	12 (2%)	65	87

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	366	HIS
1	В	399	CYS
1	В	603	ARG
1	В	420	LEU
1	A	376	CYS

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

13 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	Вс	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	703	1	14,14,15	0.34	0	17,19,21	0.39	0
2	NAG	A	705	1	14,14,15	0.25	0	17,19,21	0.40	0
2	NAG	A	707	1	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	A	706	1	14,14,15	0.35	0	17,19,21	0.42	0
2	NAG	В	702	1	14,14,15	0.37	0	17,19,21	0.59	0
2	NAG	A	701	1	14,14,15	0.25	0	17,19,21	0.71	1 (5%)
2	NAG	В	703	1	14,14,15	0.28	0	17,19,21	0.64	1 (5%)
2	NAG	В	706	1	14,14,15	0.41	0	17,19,21	0.56	0
2	NAG	В	701	1	14,14,15	0.31	0	17,19,21	0.50	0
2	NAG	A	704	1	14,14,15	0.27	0	17,19,21	0.38	0
2	NAG	В	704	1	14,14,15	0.39	0	17,19,21	0.51	0
2	NAG	В	705	1	14,14,15	0.30	0	17,19,21	0.49	0
2	NAG	A	702	1	14,14,15	0.29	0	17,19,21	0.52	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	A	703	1	-	0/6/23/26	0/1/1/1
2	NAG	A	705	1	-	0/6/23/26	0/1/1/1
2	NAG	A	707	1	-	0/6/23/26	0/1/1/1
2	NAG	A	706	1	-	1/6/23/26	0/1/1/1
2	NAG	В	702	1	-	1/6/23/26	0/1/1/1
2	NAG	A	701	1	-	0/6/23/26	0/1/1/1
2	NAG	В	703	1	-	1/6/23/26	0/1/1/1
2	NAG	В	706	1	-	3/6/23/26	0/1/1/1
2	NAG	В	701	1	-	0/6/23/26	0/1/1/1
2	NAG	A	704	1	-	2/6/23/26	0/1/1/1
2	NAG	В	704	1	-	2/6/23/26	0/1/1/1
2	NAG	В	705	1	-	3/6/23/26	0/1/1/1
2	NAG	A	702	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

	Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
	2	В	703	NAG	C1-O5-C5	2.25	115.24	112.19
ĺ	2	A	701	NAG	C1-O5-C5	2.18	115.15	112.19



There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	704	NAG	C4-C5-C6-O6
2	A	704	NAG	O5-C5-C6-O6
2	В	705	NAG	O5-C5-C6-O6
2	В	703	NAG	O5-C5-C6-O6
2	В	705	NAG	C4-C5-C6-O6

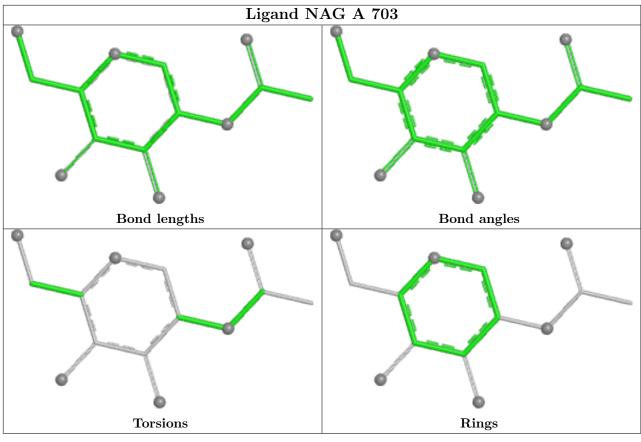
There are no ring outliers.

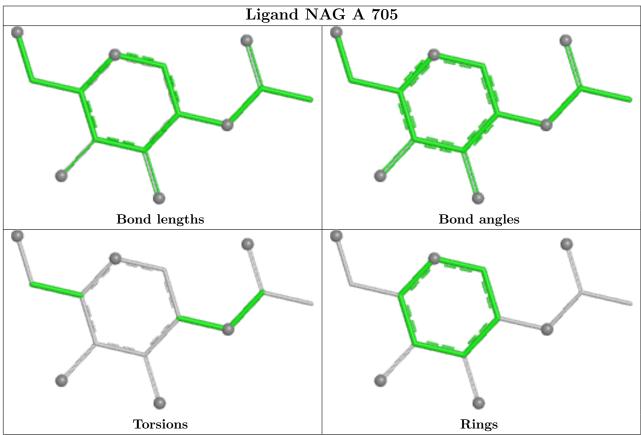
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	701	NAG	1	0

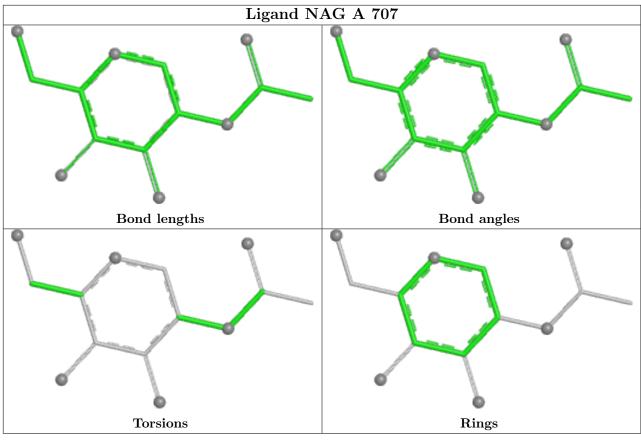
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

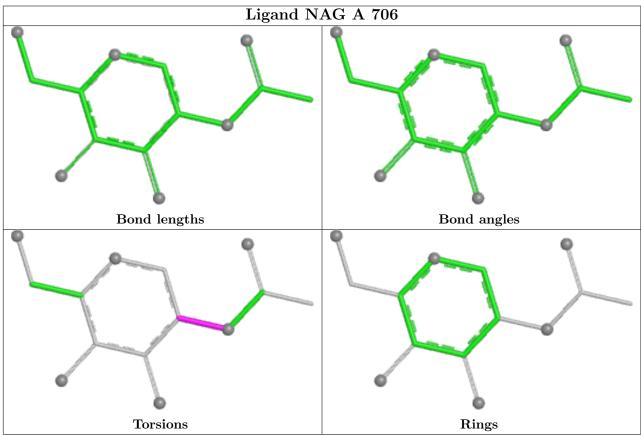




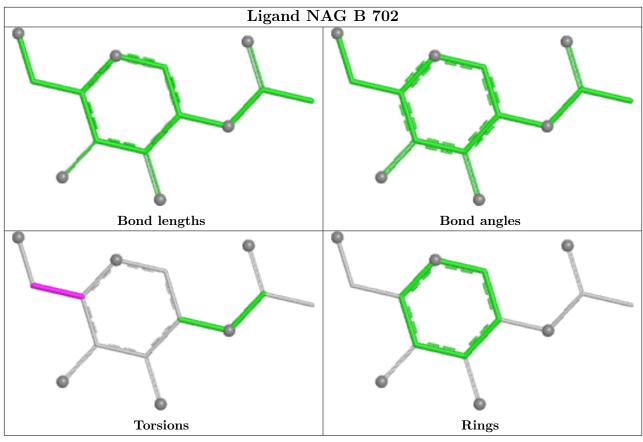


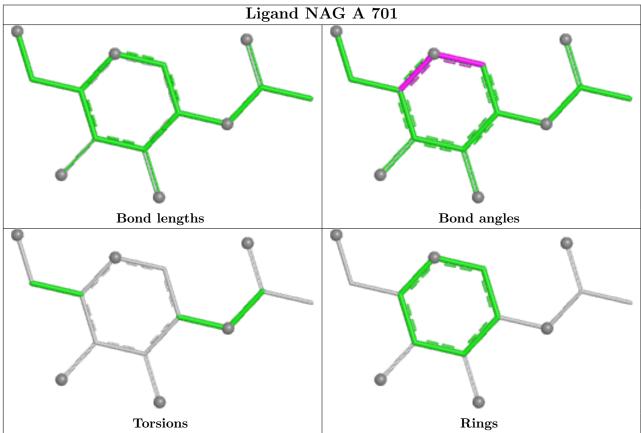




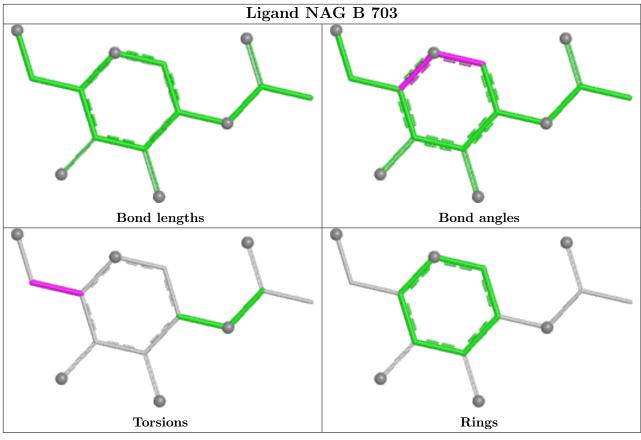


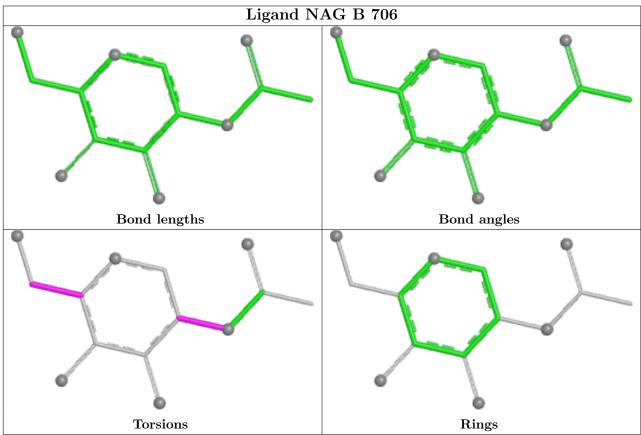




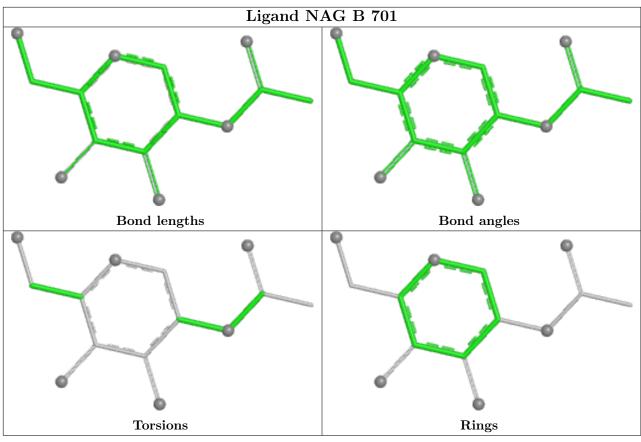


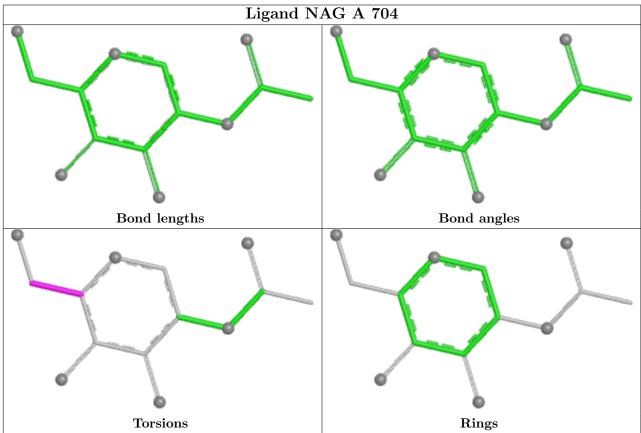




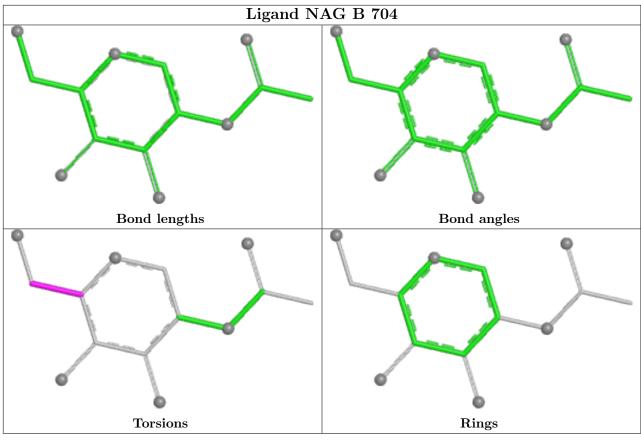


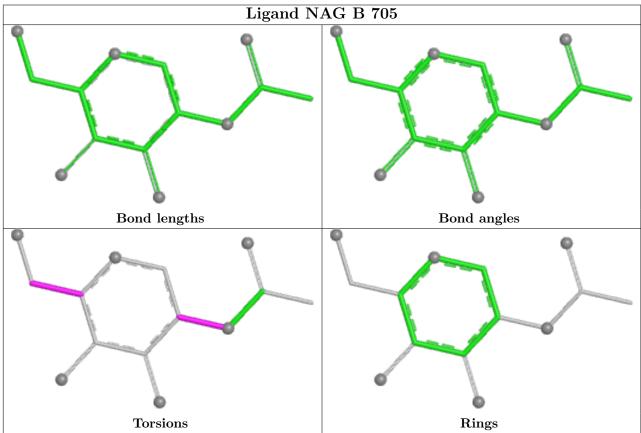




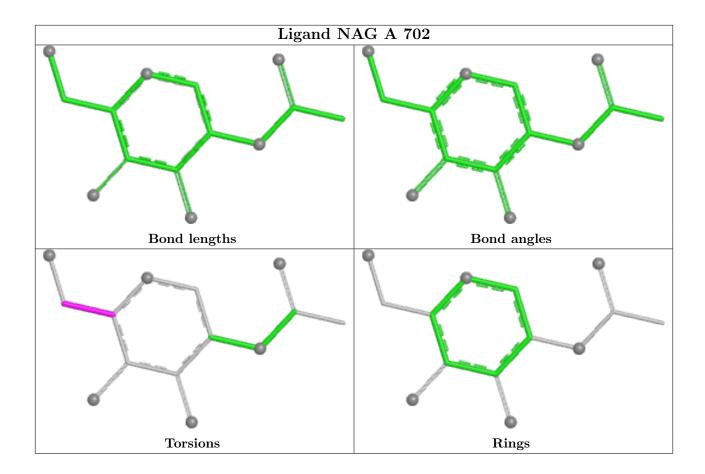












5.7 Other polymers (i)

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

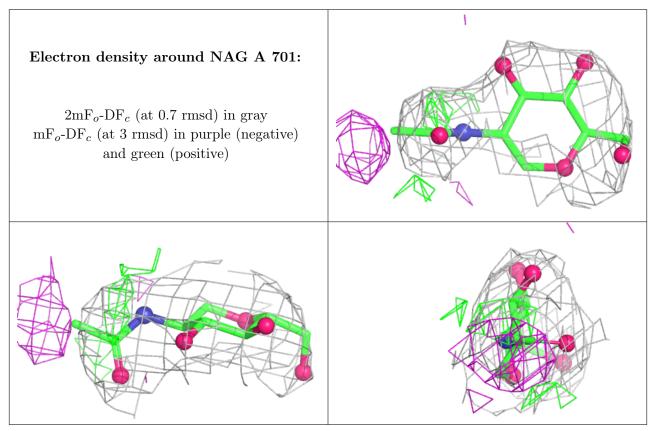
6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

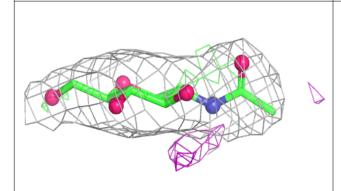
Unable to reproduce the depositors R factor - this section is therefore empty.

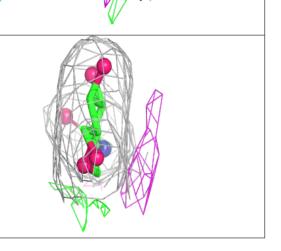
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





Electron density around NAG A 702: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) V Electron density around NAG A 703: $2mF_o$ -DF_c (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

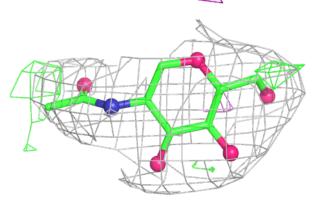


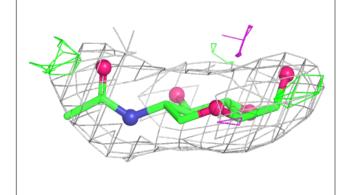


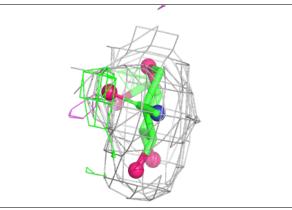


Electron density around NAG A 704:

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

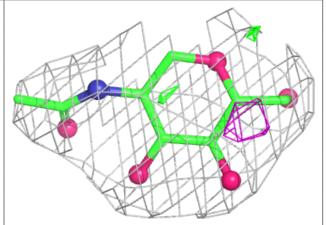


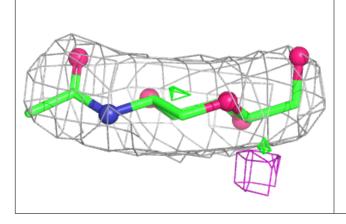


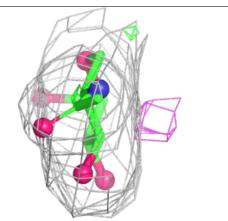


Electron density around NAG A 705:

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









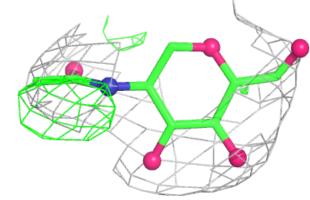
Electron density around NAG A 706: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

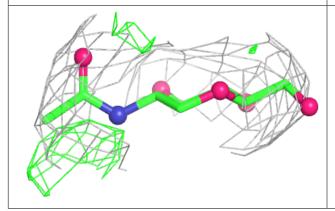
Electron density around NAG A 707: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

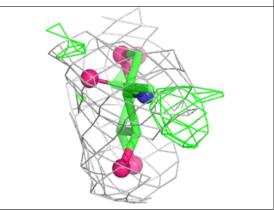


Electron density around NAG B 701:

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

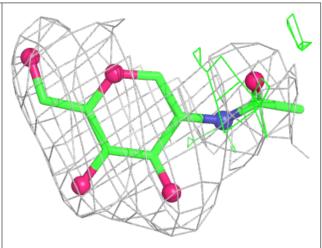


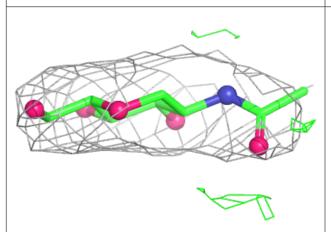


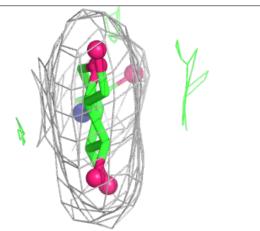


Electron density around NAG B 702:

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



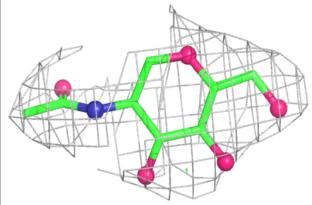


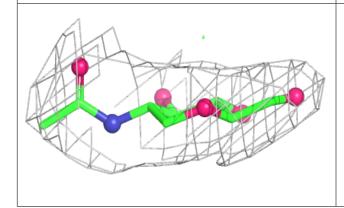


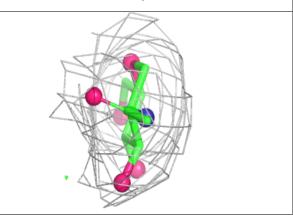


Electron density around NAG B 703:

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

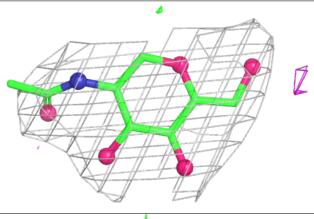


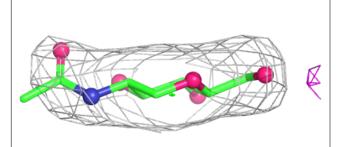


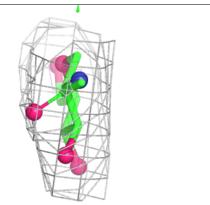


Electron density around NAG B 704:

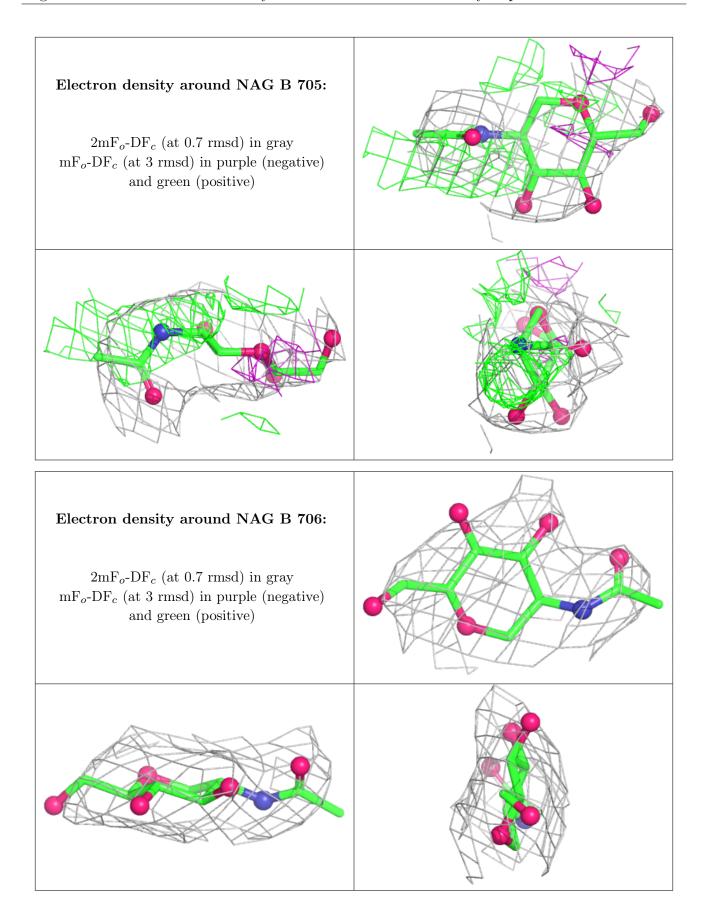
 $2 \mathrm{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)













6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

