



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 2, 2026 – 12:29 PM JST

PDB ID : 9XPL / pdb_00009xpl
Title : Crystal structure of the pufferfish taste receptor Tas1r1-Tas1r3 ligand binding domains in complex with D-phenylalanine
Authors : Mizoguchi, R.; Matsuura, H.; Hirata, K.; Yamashita, A.
Deposited on : 2025-11-16
Resolution : 2.90 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 ⓘ 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

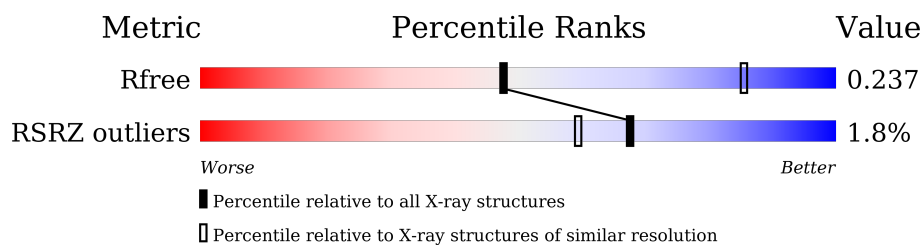
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7253 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 Taste receptor, type 1, member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3506	2253	577	661	15			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	SER	CYS	engineered mutation	UNP Q2MHK1
A	502	GLY	-	expression tag	UNP Q2MHK1
A	503	VAL	-	expression tag	UNP Q2MHK1
A	504	ALA	-	expression tag	UNP Q2MHK1
A	505	MET	-	expression tag	UNP Q2MHK1
A	506	PRO	-	expression tag	UNP Q2MHK1
A	507	GLY	-	expression tag	UNP Q2MHK1
A	508	ALA	-	expression tag	UNP Q2MHK1
A	509	GLU	-	expression tag	UNP Q2MHK1
A	510	ASP	-	expression tag	UNP Q2MHK1
A	511	ASP	-	expression tag	UNP Q2MHK1
A	512	VAL	-	expression tag	UNP Q2MHK1
A	513	VAL	-	expression tag	UNP Q2MHK1

- Molecule 2 is a protein called Taste receptor type 1 member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	457	Total	C	N	O	S	0	0	0
			3596	2311	589	681	15			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	238	SER	CYS	engineered mutation	UNP H2UNJ5
B	497	ASP	-	expression tag	UNP H2UNJ5
B	498	TYR	-	expression tag	UNP H2UNJ5

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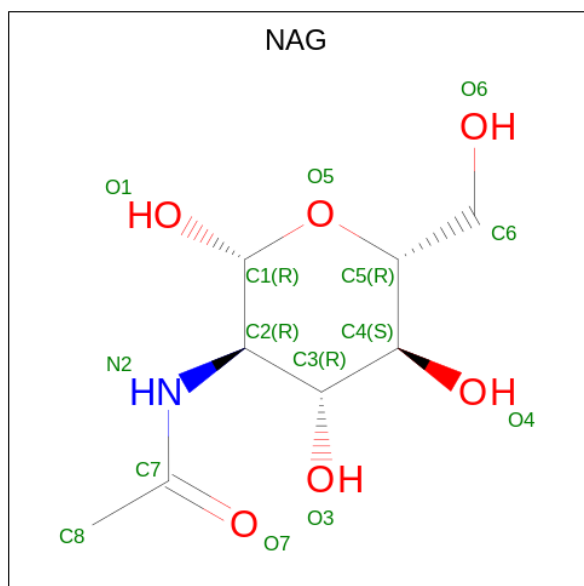
Chain	Residue	Modelled	Actual	Comment	Reference
B	499	LYS	-	expression tag	UNP H2UNJ5
B	500	ASP	-	expression tag	UNP H2UNJ5
B	501	ASP	-	expression tag	UNP H2UNJ5
B	502	ASP	-	expression tag	UNP H2UNJ5
B	503	ASP	-	expression tag	UNP H2UNJ5
B	504	LYS	-	expression tag	UNP H2UNJ5

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



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



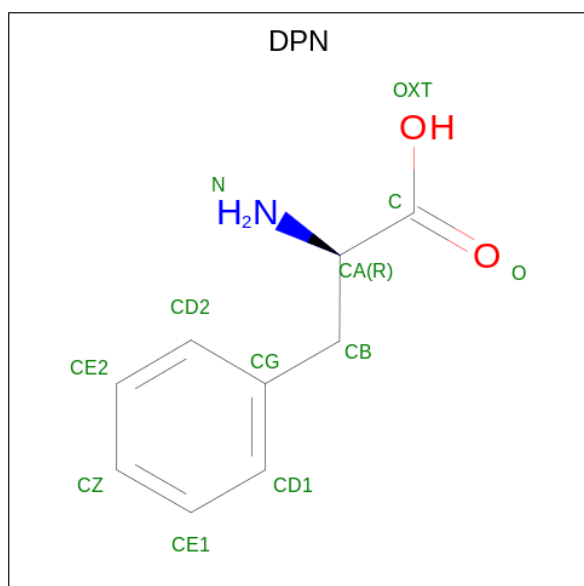
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is D-PHENYLALANINE (CCD ID: DPN) (formula: $C_9H_{11}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			12	9	1	2		
5	B	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 1	Cl 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	19	Total 19	O 19	0	0
8	B	8	Total 8	O 8	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	99.46Å 106.90Å 101.67Å 90.00° 91.91° 90.00°	Depositor
Resolution (Å)	45.25 – 2.90 45.25 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.25-2.90) 99.6 (45.25-2.90)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.21_5207:	Depositor
R, R_{free}	0.215 , 0.237 0.215 , 0.237	Depositor DCC
R_{free} test set	1204 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7253	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

2 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
3	NAG	C	1	2,3	14,14,15	0.59	0	17,19,21	0.75	1 (5%)
3	NAG	C	2	3	14,14,15	0.58	0	17,19,21	0.62	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	NAG	C	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	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	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	2.24	115.22	112.19

There are no chirality outliers.

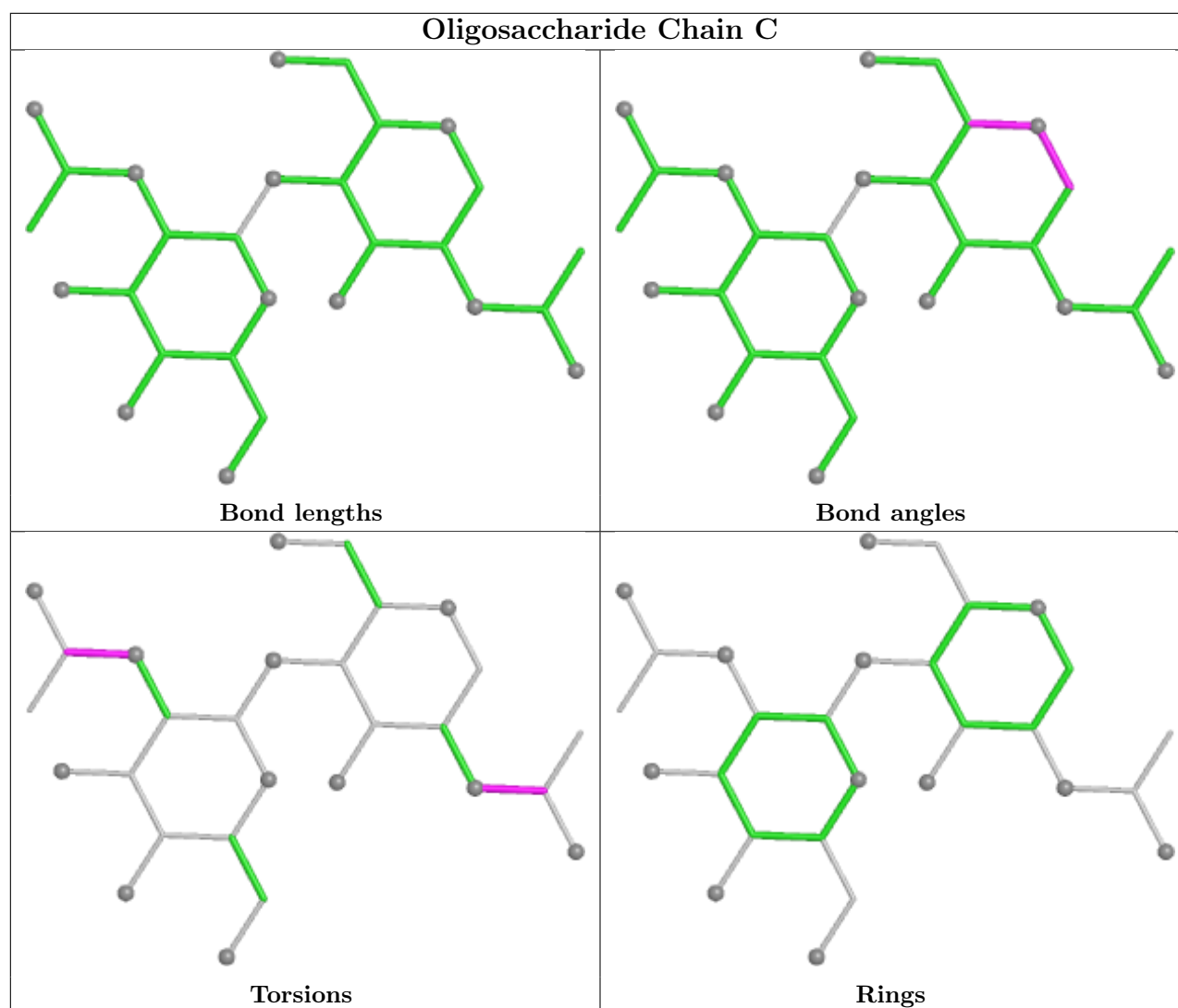
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2

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.



4.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	901	2	14,14,15	0.59	0	17,19,21	0.76	1 (5%)
5	DPN	A	904	-	11,12,12	0.73	1 (9%)	14,15,15	0.97	2 (14%)
4	NAG	B	902	2	14,14,15	0.57	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	902	1	14,14,15	0.53	0	17,19,21	0.80	0
4	NAG	A	903	1	14,14,15	0.52	0	17,19,21	0.90	1 (5%)
5	DPN	B	903	-	11,12,12	0.70	1 (9%)	14,15,15	0.96	2 (14%)
4	NAG	A	901	1	14,14,15	0.60	0	17,19,21	0.72	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	B	901	2	-	3/6/23/26	0/1/1/1
5	DPN	A	904	-	-	0/8/8/8	0/1/1/1
4	NAG	B	902	2	-	2/6/23/26	0/1/1/1
4	NAG	A	902	1	-	2/6/23/26	0/1/1/1
4	NAG	A	903	1	-	2/6/23/26	0/1/1/1
5	DPN	B	903	-	-	0/8/8/8	0/1/1/1
4	NAG	A	901	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	904	DPN	OXT-C	-2.19	1.23	1.30
5	B	903	DPN	OXT-C	-2.18	1.23	1.30

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	904	DPN	OXT-C-O	-2.73	117.89	124.09
4	A	903	NAG	C1-O5-C5	2.72	115.88	112.19
5	B	903	DPN	OXT-C-O	-2.71	117.94	124.09
4	B	901	NAG	C1-O5-C5	2.31	115.32	112.19
5	A	904	DPN	OXT-C-CA	2.31	121.24	113.38

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	NAG	C8-C7-N2-C2
4	A	901	NAG	O7-C7-N2-C2

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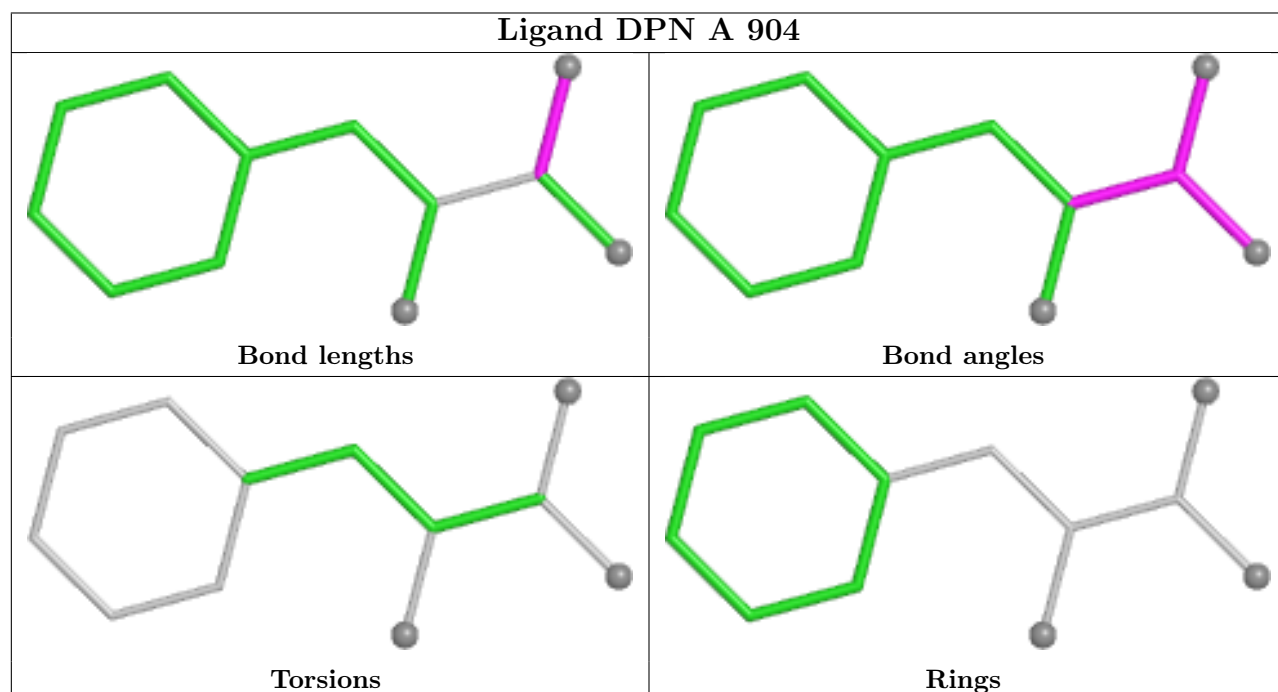
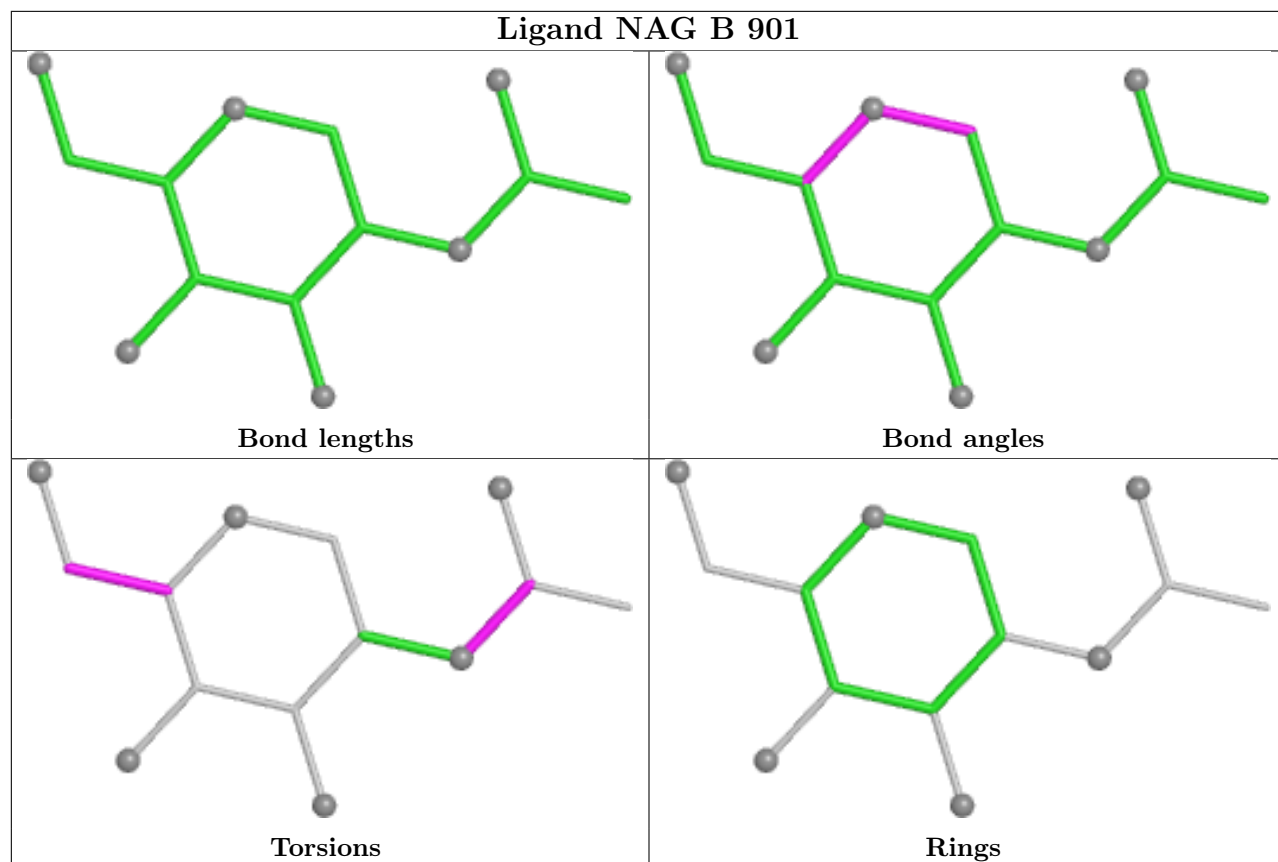
Mol	Chain	Res	Type	Atoms
4	A	902	NAG	C8-C7-N2-C2
4	A	902	NAG	O7-C7-N2-C2
4	A	903	NAG	C8-C7-N2-C2

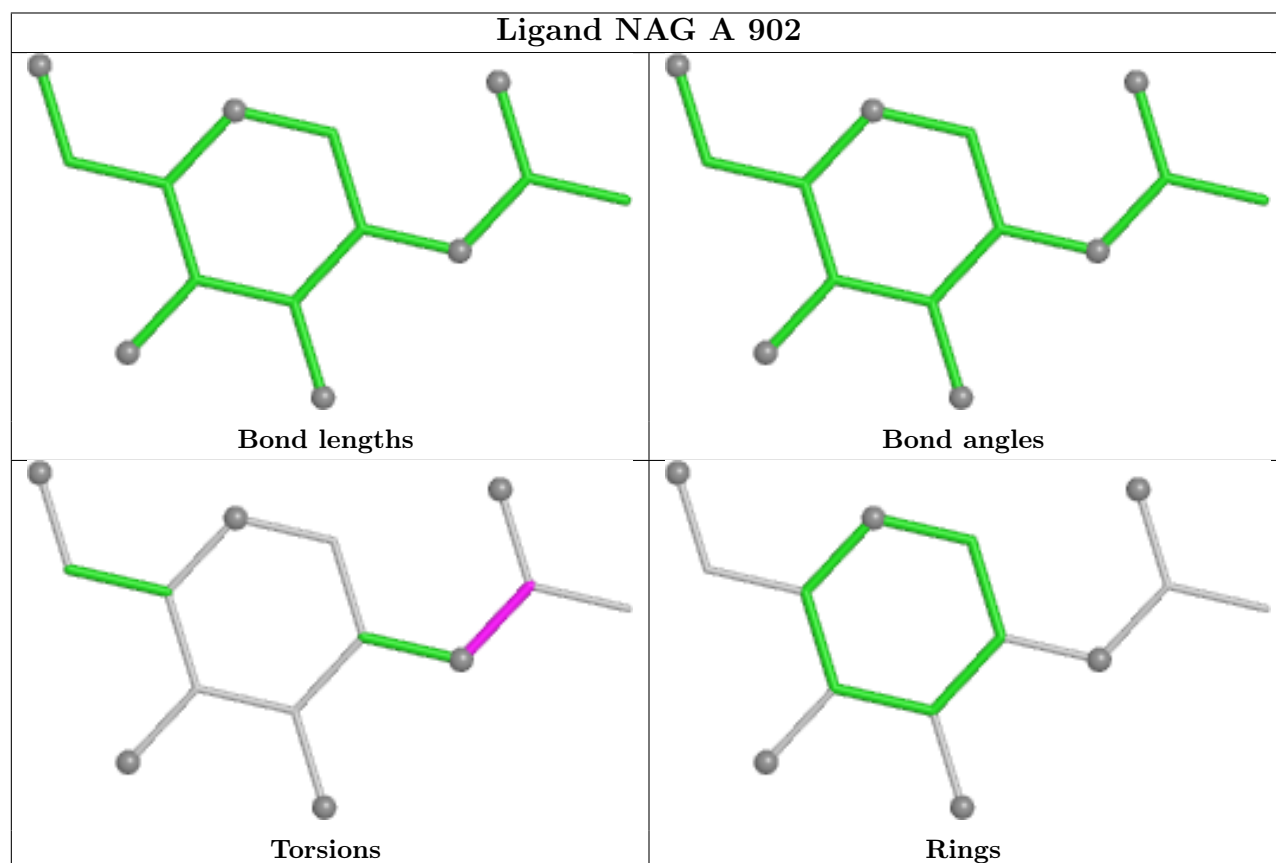
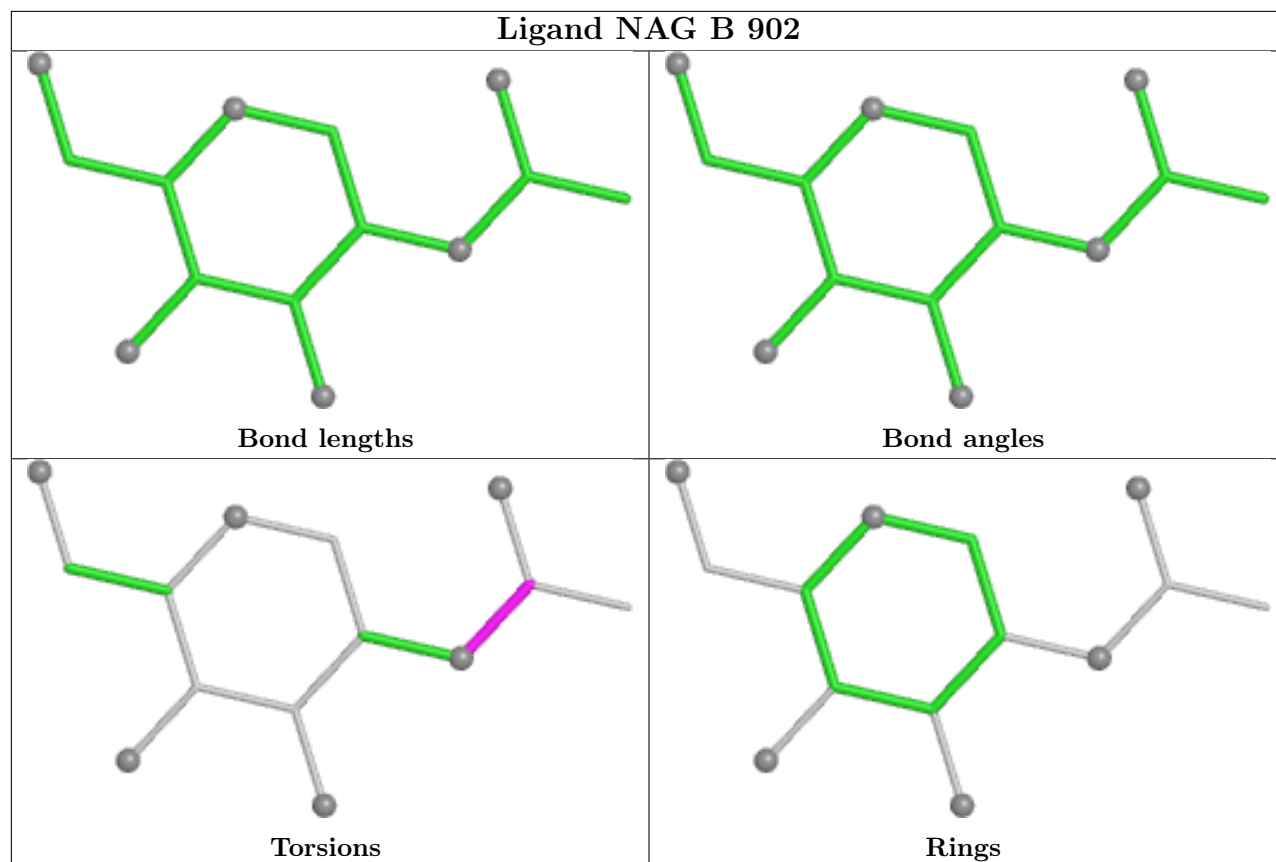
There are no ring outliers.

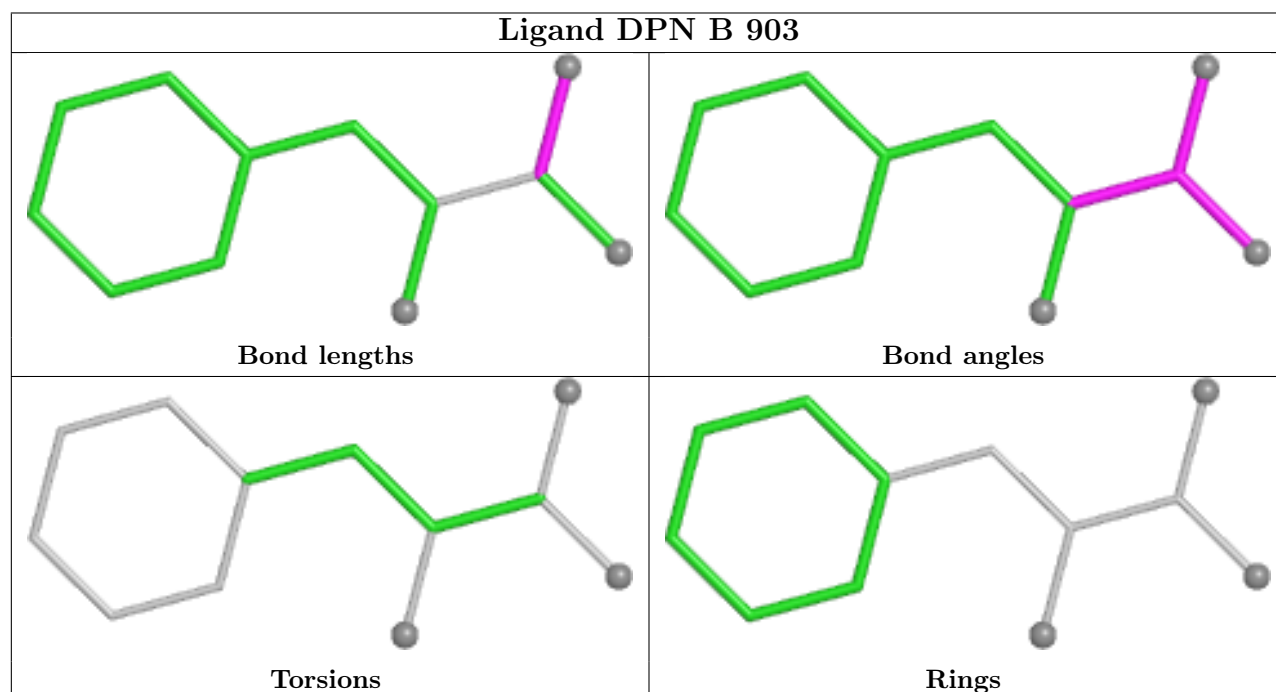
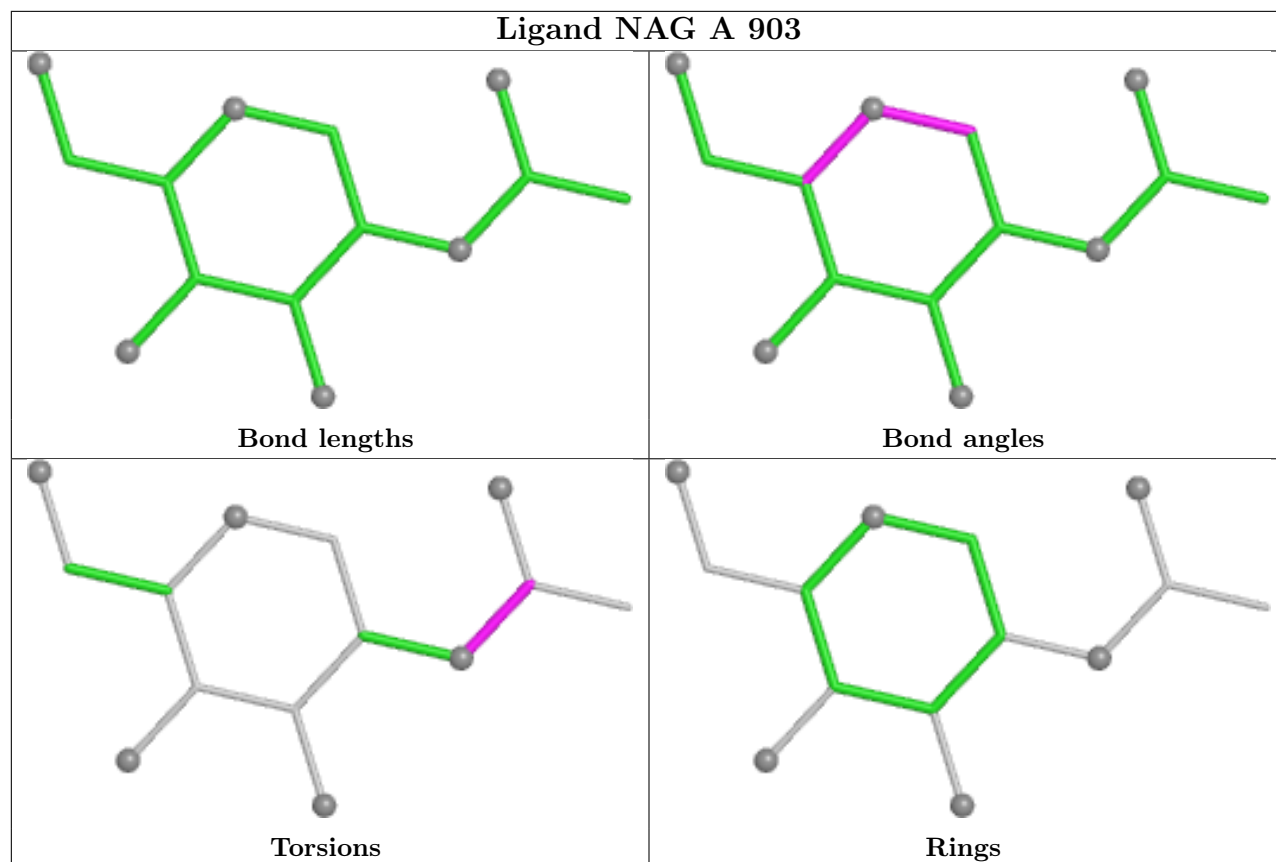
1 monomer is involved in 1 short contact:

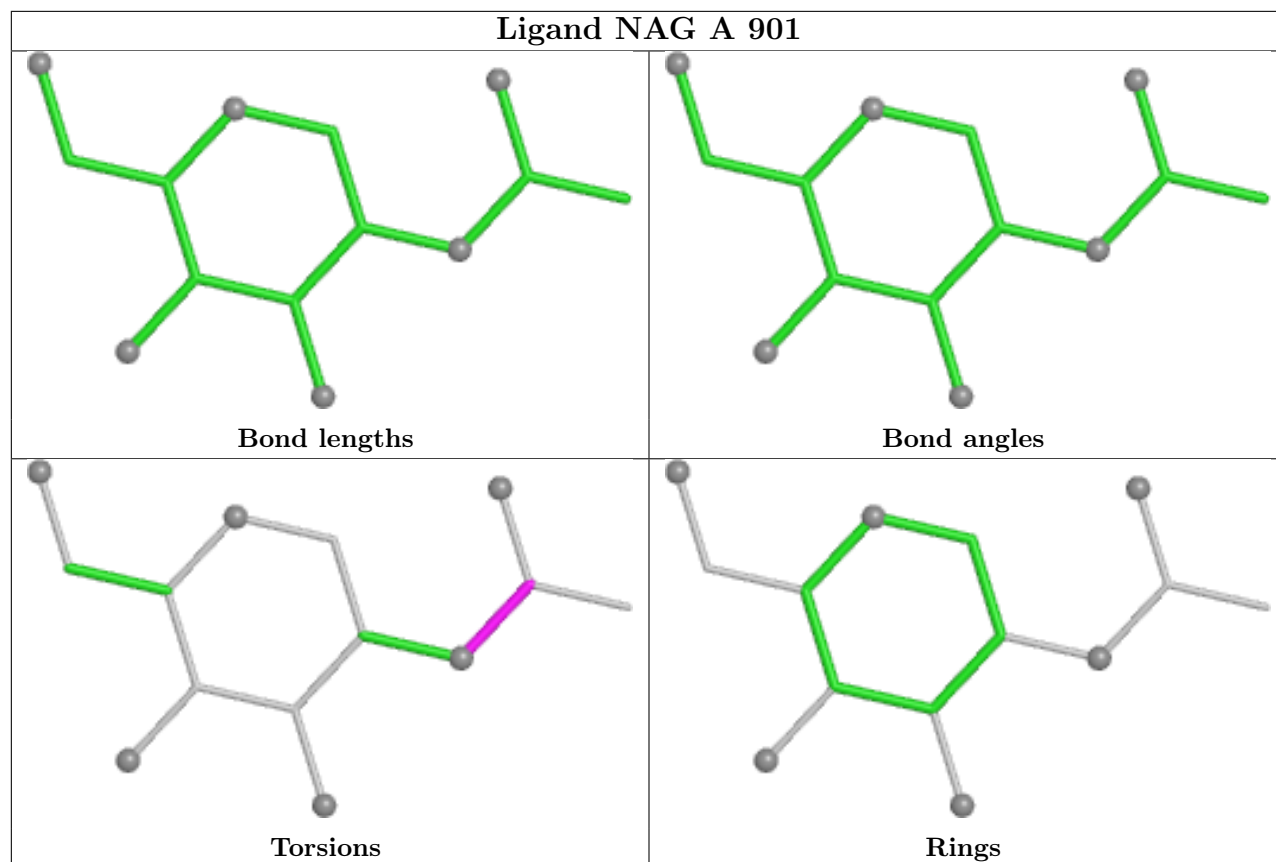
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	903	NAG	0	1

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.









4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

5.1 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, 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	A	449/513 (87%)	0.02	4 (0%) 81 75	32, 53, 84, 103	0
2	B	457/504 (90%)	0.49	12 (2%) 57 48	37, 84, 115, 131	0
All	All	906/1017 (89%)	0.26	16 (1%) 67 59	32, 64, 110, 131	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	VAL	4.3
2	B	126	THR	3.4
2	B	418	VAL	3.3
2	B	124	ASP	3.1
2	B	301	TRP	2.9

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

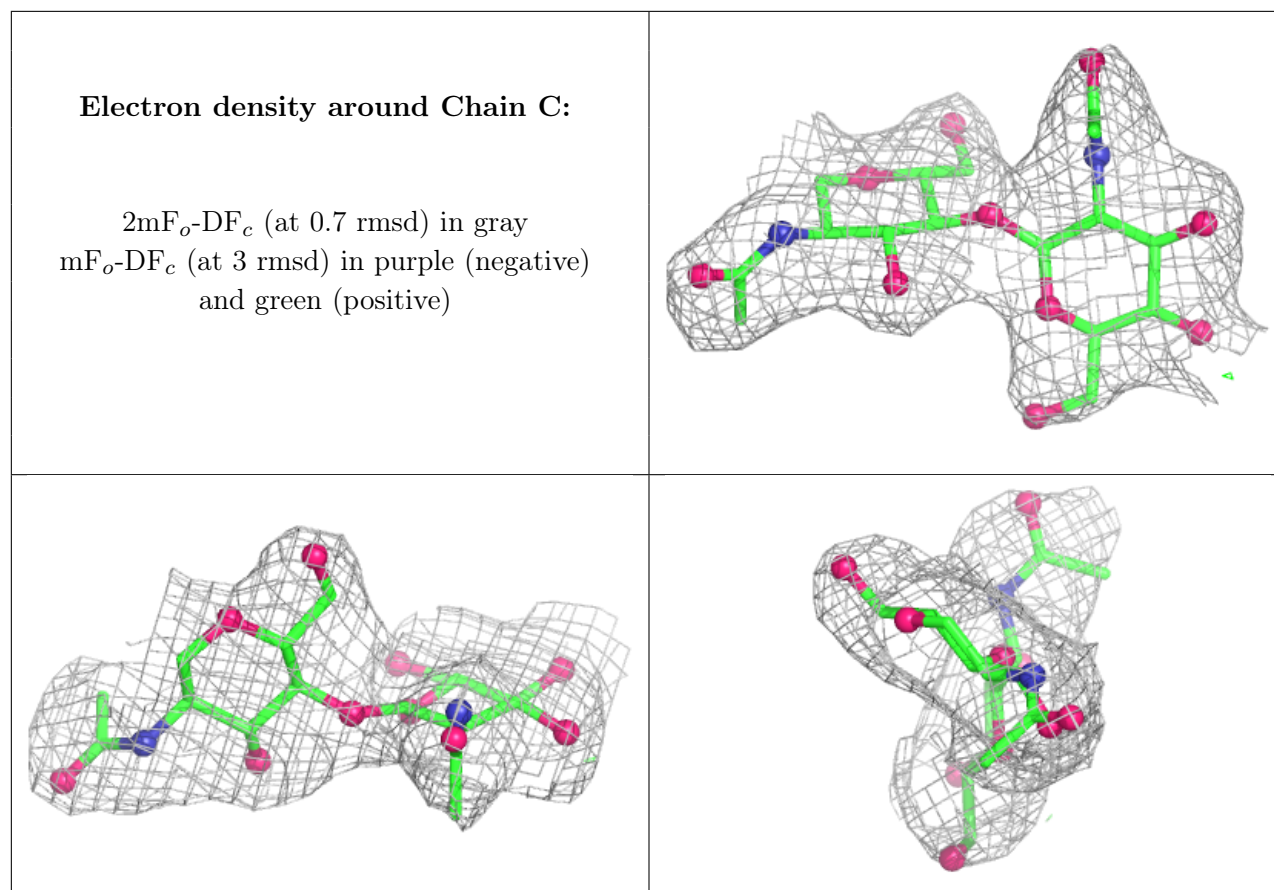
There are no non-standard protein/DNA/RNA residues in this entry.

5.3 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, 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(Å ²)	Q<0.9
3	NAG	C	2	14/15	0.78	0.13	64,84,91,98	0
3	NAG	C	1	14/15	0.88	0.10	47,56,67,71	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.



5.4 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.

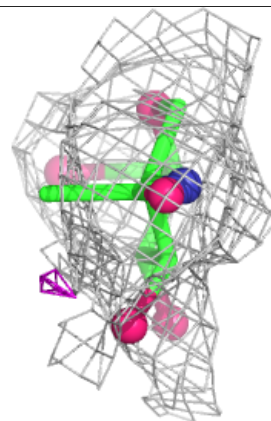
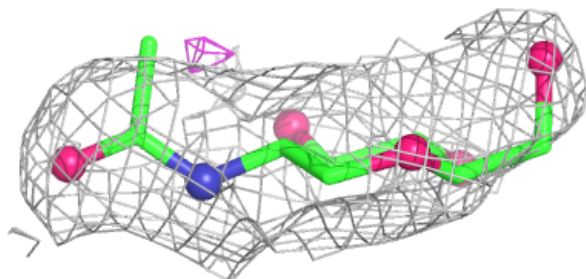
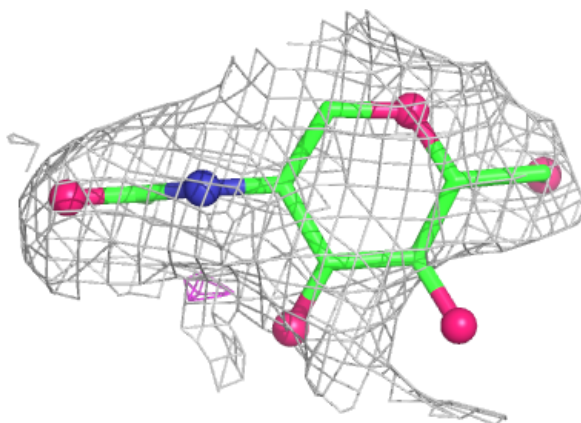
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	903	14/15	0.75	0.14	79,101,108,113	0
4	NAG	B	901	14/15	0.78	0.10	73,80,90,102	0
4	NAG	A	902	14/15	0.79	0.13	89,96,101,101	0
4	NAG	B	902	14/15	0.80	0.12	78,94,100,101	0
5	DPN	B	903	12/12	0.87	0.14	68,78,81,86	0
4	NAG	A	901	14/15	0.88	0.10	43,54,63,67	0
6	NA	A	905	1/1	0.90	0.06	58,58,58,58	0
7	CL	B	904	1/1	0.93	0.08	52,52,52,52	0
5	DPN	A	904	12/12	0.95	0.10	40,46,52,53	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.

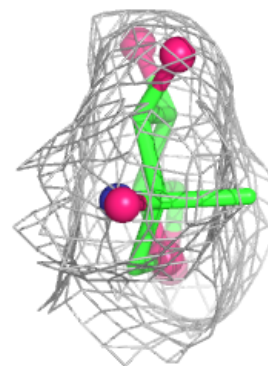
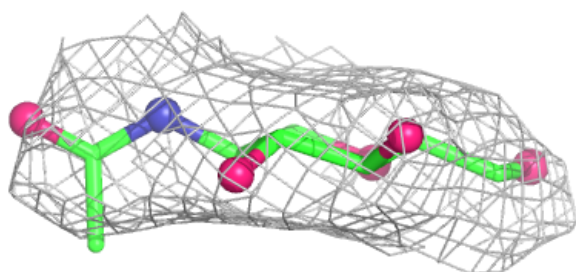
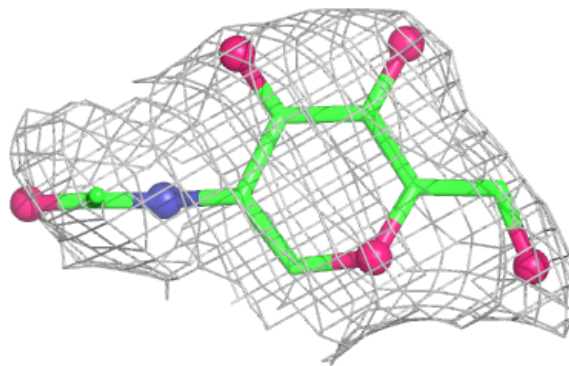
Electron density around NAG A 903:

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

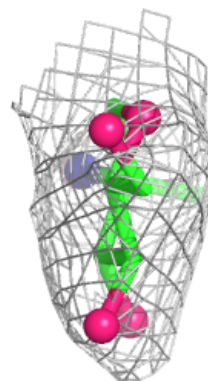
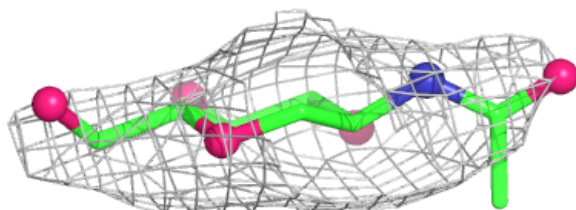
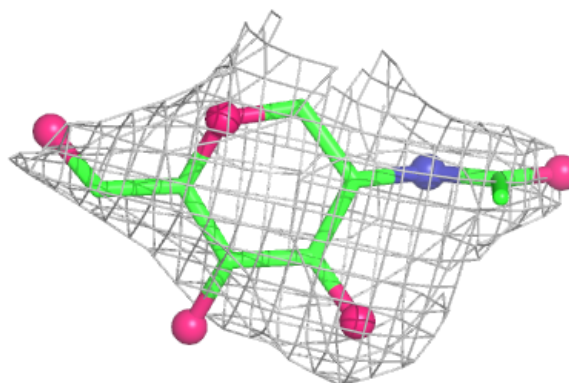


Electron density around NAG B 901:

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

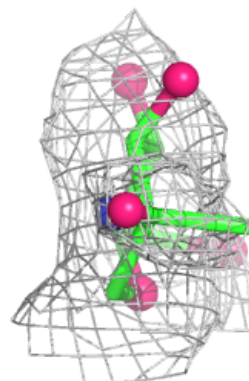
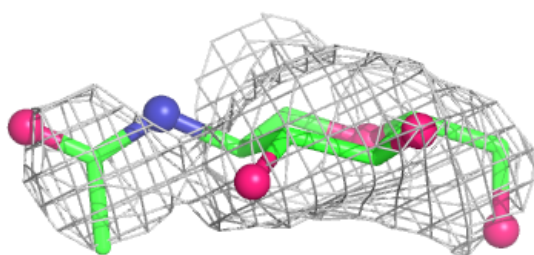
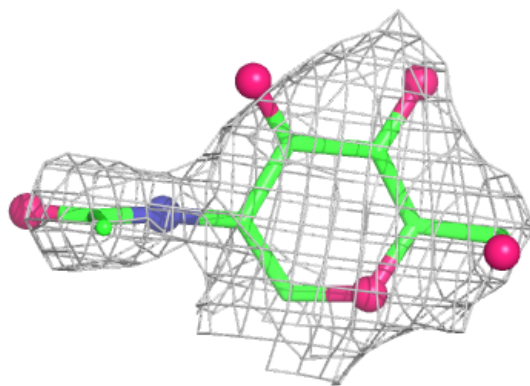
**Electron density around NAG A 902:**

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

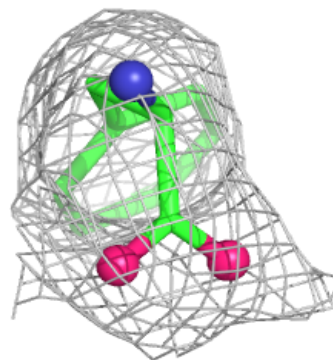
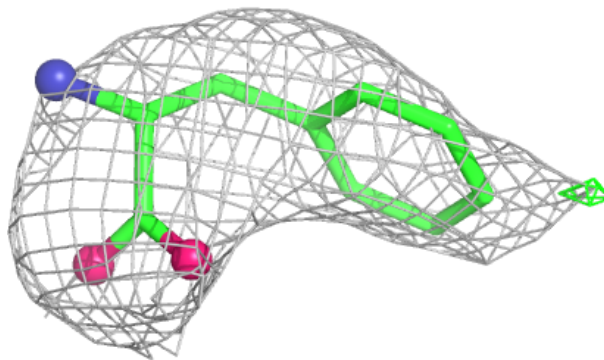


Electron density around NAG B 902:

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

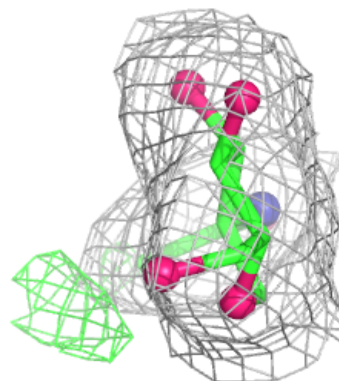
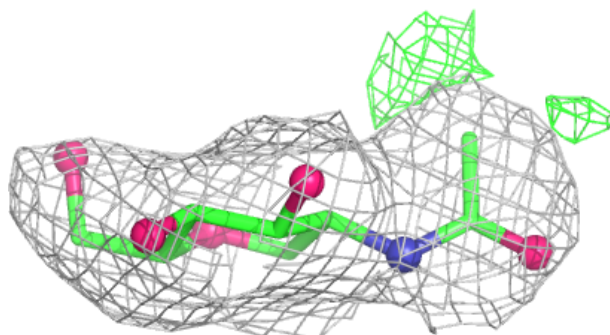
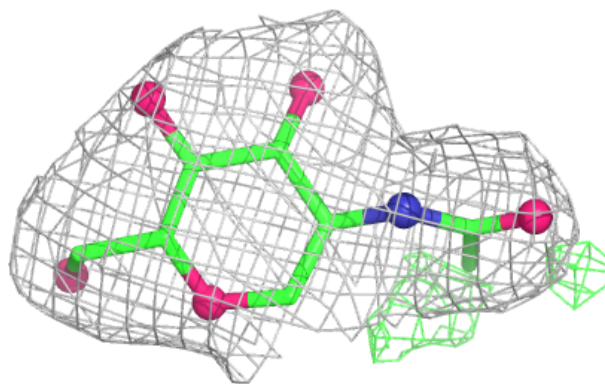
**Electron density around DPN B 903:**

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



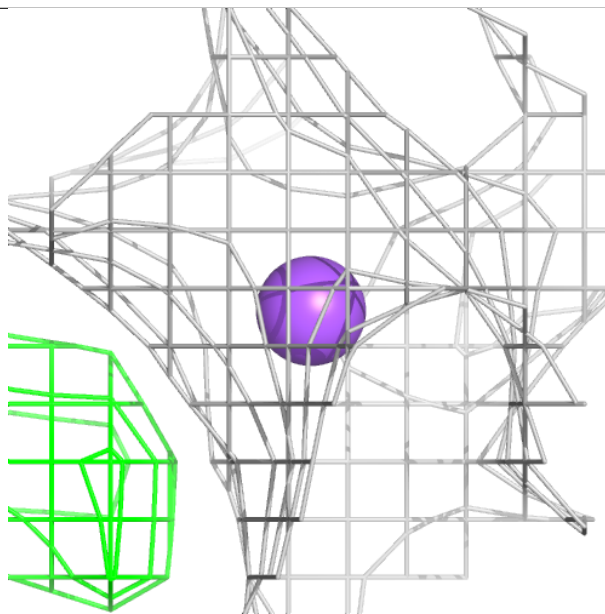
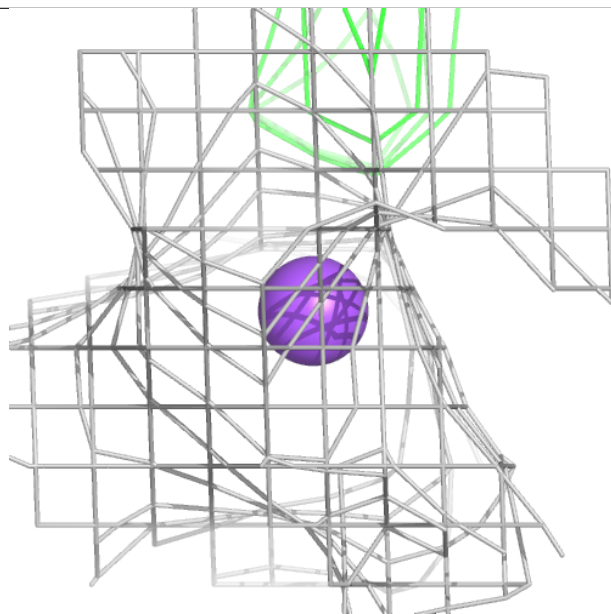
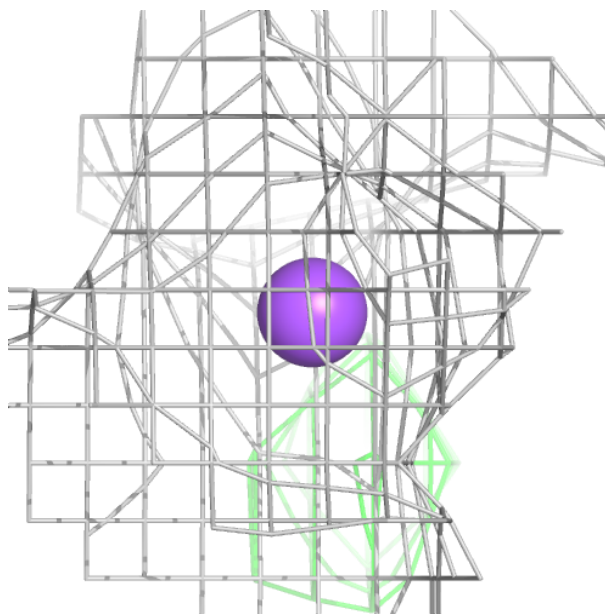
Electron density around NAG A 901:

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



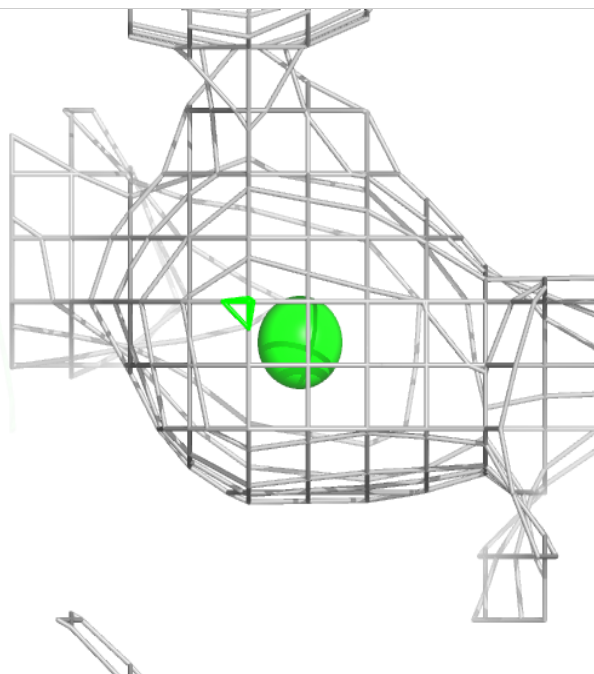
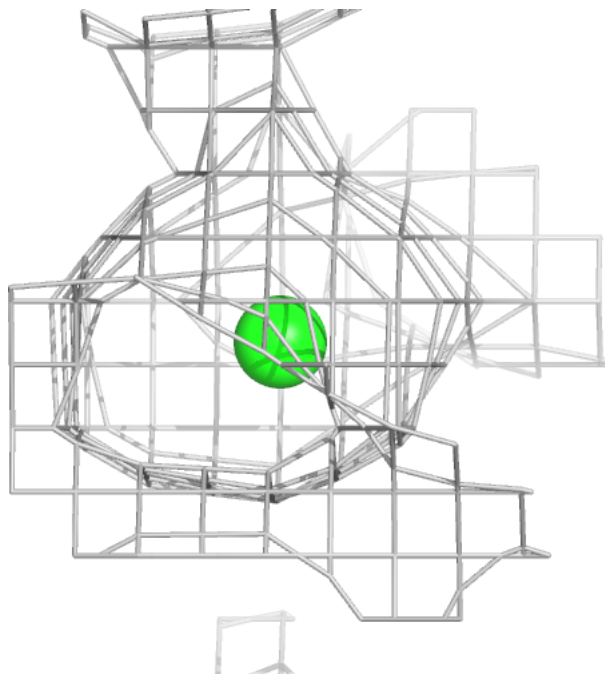
Electron density around NA A 905:

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



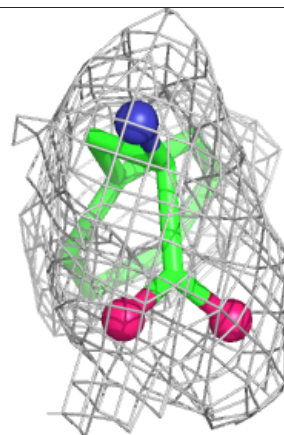
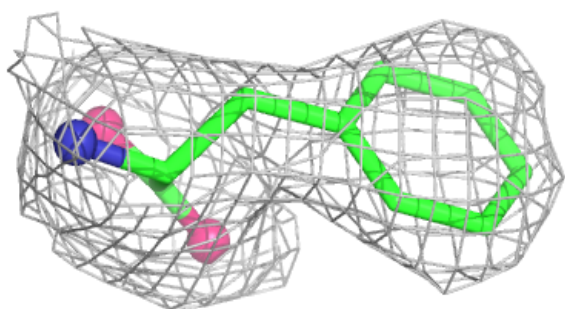
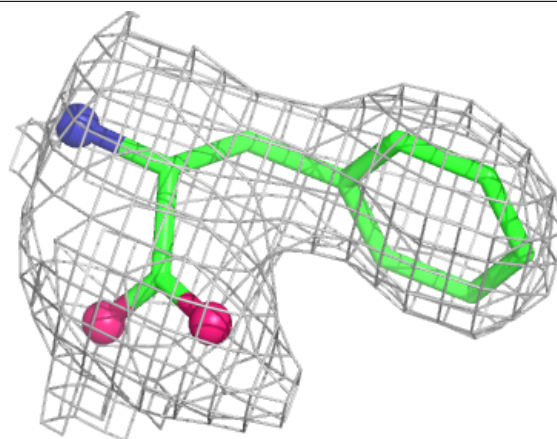
Electron density around CL B 904:

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



Electron density around DPN A 904:

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



5.5 Other polymers [i](#)

There are no such residues in this entry.