

# wwPDB X-ray Structure Validation Summary Report (i)

#### Feb 1, 2024 – 12:08 PM JST

PDB ID : 8HBB

Title : Crystal structure of Caenorhabditis elegans NMAD-1 in complex with ligand

III

Authors: Shang, G.; Chen, Z.

Deposited on : 2022-10-27

Resolution : 3.09 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 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:

 $\begin{array}{ccc} \text{MolProbity} & : & 4.02\text{b-}467 \\ \text{Xtriage (Phenix)} & : & 1.13 \end{array}$ 

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)

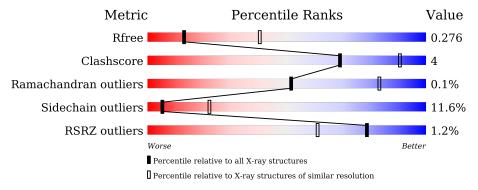
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 3.09 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	286	73% 15%		11%
1	В	286	73% 14%		11%
1	С	286	72% 16%		11%
1	D	286	76% 12	%	11%



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7693 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 DNA N6-methyl adenine demethylase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	255	Total	С	N	О	S	0	0	0
1	A	255	1973	1240	341	376	16	0	U	U
1	В	255	Total	С	N	О	S	0	0	0
1			1957	1228	338	375	16	U	U	U
1	С	254	Total	С	N	О	S	0	0	0
1		204	1882	1182	324	363	13	0	U	U
1	D	255	Total	С	N	О	S	0	0	0
	200	1863	1167	323	358	15	0	U	U	

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	HIS	-	expression tag	UNP Q8MNT9
A	7	HIS	-	expression tag	UNP Q8MNT9
A	8	HIS	-	expression tag	UNP Q8MNT9
A	9	HIS	-	expression tag	UNP Q8MNT9
A	10	HIS	-	expression tag	UNP Q8MNT9
A	11	HIS	-	expression tag	UNP Q8MNT9
A	12	GLU	-	expression tag	UNP Q8MNT9
A	13	ASN	-	expression tag	UNP Q8MNT9
A	14	LEU	-	expression tag	UNP Q8MNT9
A	15	TYR	-	expression tag	UNP Q8MNT9
A	16	PHE	-	expression tag	UNP Q8MNT9
A	17	GLN	ı	expression tag	UNP Q8MNT9
A	18	GLY	-	expression tag	UNP Q8MNT9
A	19	SER	ı	expression tag	UNP Q8MNT9
A	20	MET	ı	expression tag	UNP Q8MNT9
A	109	LYS	GLU	engineered mutation	UNP Q8MNT9
A	112	LYS	GLN	engineered mutation	UNP Q8MNT9
A	114	LYS	GLN	engineered mutation	UNP Q8MNT9
В	6	HIS	=	expression tag	UNP Q8MNT9
В	7	HIS	-	expression tag	UNP Q8MNT9
В	8	HIS	-	expression tag	UNP Q8MNT9



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Chain	Residue	Modelled	Actual	Comment	Reference
В	9	HIS	-	expression tag	UNP Q8MNT9
В	10	HIS	-	expression tag	UNP Q8MNT9
В	11	HIS	-	expression tag	UNP Q8MNT9
В	12	GLU	-	expression tag	UNP Q8MNT9
В	13	ASN	-	expression tag	UNP Q8MNT9
В	14	LEU	-	expression tag	UNP Q8MNT9
В	15	TYR	-	expression tag	UNP Q8MNT9
В	16	PHE	-	expression tag	UNP Q8MNT9
В	17	GLN	_	expression tag	UNP Q8MNT9
В	18	GLY	_	expression tag	UNP Q8MNT9
В	19	SER	_	expression tag	UNP Q8MNT9
В	20	MET	-	expression tag	UNP Q8MNT9
В	109	LYS	GLU	engineered mutation	UNP Q8MNT9
В	112	LYS	GLN	engineered mutation	UNP Q8MNT9
В	114	LYS	GLN	engineered mutation	UNP Q8MNT9
С	6	HIS	_	expression tag	UNP Q8MNT9
С	7	HIS	-	expression tag	UNP Q8MNT9
С	8	HIS	-	expression tag	UNP Q8MNT9
С	9	HIS	-	expression tag	UNP Q8MNT9
С	10	HIS	-	expression tag	UNP Q8MNT9
С	11	HIS	-	expression tag	UNP Q8MNT9
С	12	GLU	-	expression tag	UNP Q8MNT9
С	13	ASN	-	expression tag	UNP Q8MNT9
С	14	LEU	-	expression tag	UNP Q8MNT9
С	15	TYR	-	expression tag	UNP Q8MNT9
С	16	PHE	-	expression tag	UNP Q8MNT9
С	17	GLN	-	expression tag	UNP Q8MNT9
С	18	GLY	-	expression tag	UNP Q8MNT9
С	19	SER	-	expression tag	UNP Q8MNT9
С	20	MET	_	expression tag	UNP Q8MNT9
С	109	LYS	GLU	engineered mutation	UNP Q8MNT9
С	112	LYS	GLN	engineered mutation	UNP Q8MNT9
С	114	LYS	GLN	engineered mutation	UNP Q8MNT9
D	6	HIS	-	expression tag	UNP Q8MNT9
D	7	HIS	-	expression tag	UNP Q8MNT9
D	8	HIS	-	expression tag	UNP Q8MNT9
D	9	HIS	-	expression tag	UNP Q8MNT9
D	10	HIS	-	expression tag	UNP Q8MNT9
D	11	HIS	-	expression tag	UNP Q8MNT9
D	12	GLU	-	expression tag	UNP Q8MNT9
D	13	ASN	-	expression tag	UNP Q8MNT9
D	14	LEU	-	expression tag	UNP Q8MNT9



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Chain	Residue	Modelled	Actual	Comment	Reference
D	15	TYR	-	expression tag	UNP Q8MNT9
D	16	PHE	-	expression tag	UNP Q8MNT9
D	17	GLN	-	expression tag	UNP Q8MNT9
D	18	GLY	-	expression tag	UNP Q8MNT9
D	19	SER	-	expression tag	UNP Q8MNT9
D	20	MET	-	expression tag	UNP Q8MNT9
D	109	LYS	GLU	engineered mutation	UNP Q8MNT9
D	112	LYS	GLN	engineered mutation	UNP Q8MNT9
D	114	LYS	GLN	engineered mutation	UNP Q8MNT9

• Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	В	2	Total Mn 2 2	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0
3	В	1	Total Cl 1 1	0	0
3	С	1	Total Cl 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	С	2	Total O 2 2	0	0



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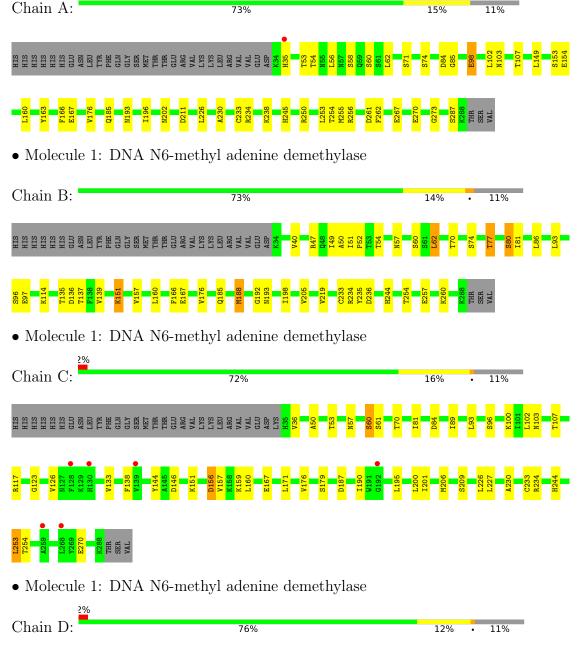
M	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1	D	4	Total O 4 4	0	0



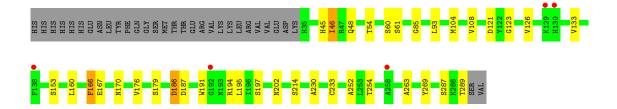
# 3 Residue-property plots (i)

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: DNA N6-methyl adenine demethylase









# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	183.18Å 75.33Å 118.18Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 113.19° 90.00°	Depositor
Resolution (Å)	47.18 - 3.09	Depositor
Resolution (A)	47.18 - 3.09	EDS
% Data completeness	67.8 (47.18-3.09)	Depositor
(in resolution range)	81.1 (47.18-3.09)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	8.63 (at 3.06Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
D D.	0.260 , 0.282	Depositor
$R, R_{free}$	0.267 , $0.276$	DCC
$R_{free}$ test set	1125 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.8	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.35, 34.2	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.45, < L^2> = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	7693	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.54% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: CL, MN

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	Moi Chain		# Z  > 5	RMSZ	# Z  > 5
1	A	0.57	0/2013	0.75	0/2727
1	В	0.57	0/1996	0.75	0/2705
1	С	0.58	0/1917	0.73	0/2606
1	D	0.58	0/1901	0.73	0/2592
All	All	0.58	0/7827	0.74	0/10630

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	1973	0	1851	12	2
1	В	1957	0	1814	15	1
1	С	1882	0	1714	17	0
1	D	1863	0	1640	12	1
2	A	1	0	0	0	0
2	В	2	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0



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COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	1	0	0	0	0
3	С	1	0	0	0	0
4	A	3	0	0	0	0
4	С	2	0	0	0	0
4	D	4	0	0	0	0
All	All	7693	0	7019	55	2

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 4.

The worst 5 of 55 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:D:123:GLY:HA3	1:D:167:GLU:HG2	1.69	0.74
1:C:123:GLY:HA3	1:C:167:GLU:HG3	1.83	0.60
1:A:103:ASN:O	1:A:107:THR:HG23	2.02	0.58
1:C:156:ASP:HB3	1:C:159:LYS:HB2	1.86	0.58
1:B:188:MET:HB3	1:B:235:TYR:HE1	1.68	0.57

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:A:270:GLU:OE1	1:B:236:ASP:OD2[1_565]	1.69	0.51
1:A:154:GLU:OE1	1:D:45:HIS:NE2[4_545]	2.15	0.05

#### 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	Percentiles
1	A	253/286 (88%)	250 (99%)	3 (1%)	0	100 100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	В	253/286 (88%)	249 (98%)	4 (2%)	0	100	100
1	С	252/286 (88%)	246 (98%)	5 (2%)	1 (0%)	34	69
1	D	253/286 (88%)	246 (97%)	7 (3%)	0	100	100
All	All	1011/1144 (88%)	991 (98%)	19 (2%)	1 (0%)	51	83

#### All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	201	ILE

#### 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	Perce	entiles
1	A	$207/260\ (80\%)$	186 (90%)	21 (10%)	7	28
1	В	$202/260\ (78\%)$	175 (87%)	27 (13%)	4	16
1	$\mathbf{C}$	187/260~(72%)	164 (88%)	23 (12%)	4	19
1	D	$180/260\ (69\%)$	161 (89%)	19 (11%)	6	26
All	All	$776/1040 \ (75\%)$	686 (88%)	90 (12%)	5	22

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	144	TYR
1	D	46	ILE
1	С	156	ASP
1	С	209	SER
1	D	61	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:



Mol	Chain	Res	Type
1	С	199	ASN
1	D	185	GLN
1	D	202	ASN
1	D	199	ASN
1	В	244	HIS

#### 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)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 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></rsrz>	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	255/286 (89%)	-0.12	1 (0%) 92 84	37, 41, 48, 55	0
1	В	255/286 (89%)	0.00	0 100 100	40, 45, 51, 61	0
1	С	254/286 (88%)	0.20	6 (2%) 59 37	47, 55, 68, 73	0
1	D	255/286 (89%)	0.15	5 (1%) 65 44	43, 55, 71, 75	0
All	All	1019/1144 (89%)	0.06	12 (1%) 79 61	37, 48, 67, 75	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	130	HIS	4.7
1	С	259	ALA	3.0
1	D	192	GLY	3.0
1	D	258	ALA	2.7
1	С	268	LEU	2.7

#### 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)

There are no monosaccharides in this entry.

#### 6.4 Ligands (i)

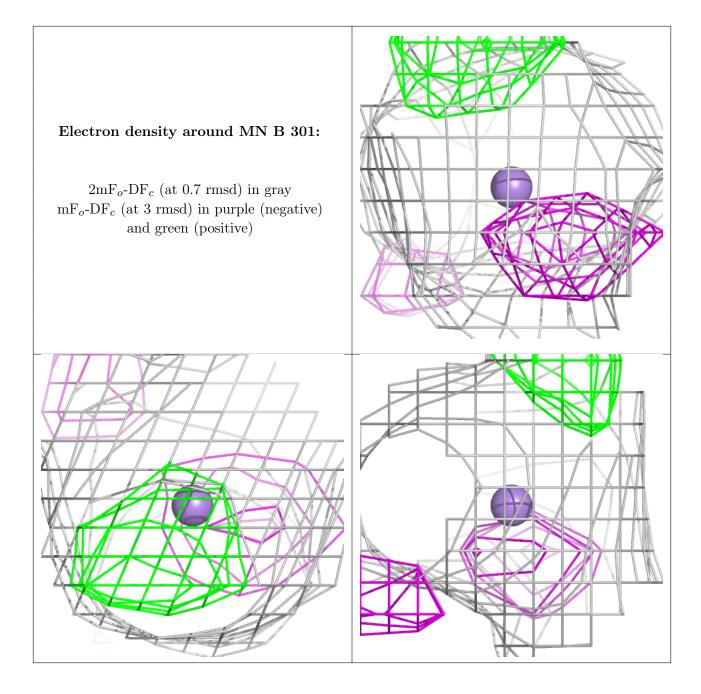
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	MN	В	301	1/1	0.85	0.12	51,51,51,51	0
2	MN	В	303	1/1	0.92	0.12	49,49,49,49	0
2	MN	D	301	1/1	0.92	0.12	57,57,57,57	0
2	MN	С	301	1/1	0.94	0.16	56,56,56,56	0
3	CL	В	302	1/1	0.94	0.10	42,42,42,42	0
3	CL	A	302	1/1	0.95	0.21	37,37,37,37	0
3	$\operatorname{CL}$	A	303	1/1	0.96	0.15	37,37,37,37	0
3	CL	С	302	1/1	0.96	0.19	47,47,47,47	0
2	MN	A	301	1/1	0.98	0.19	38,38,38,38	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.

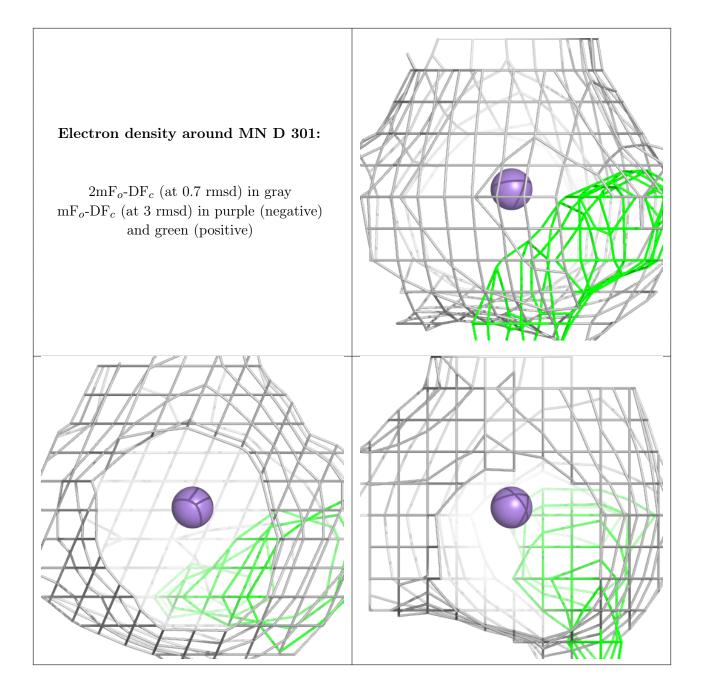




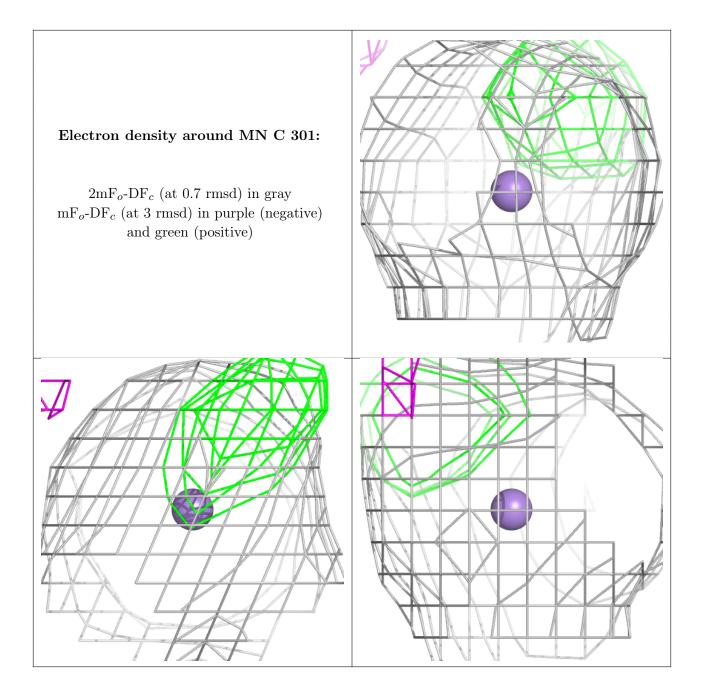


# 





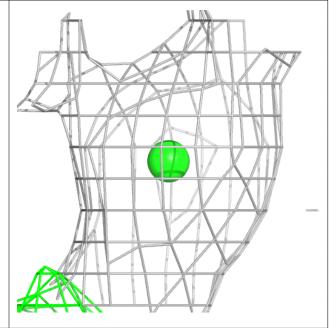


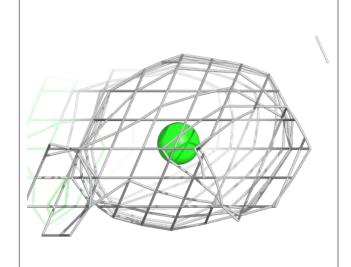


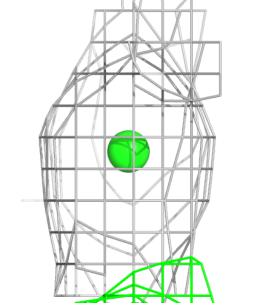


#### Electron density around CL B 302:

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

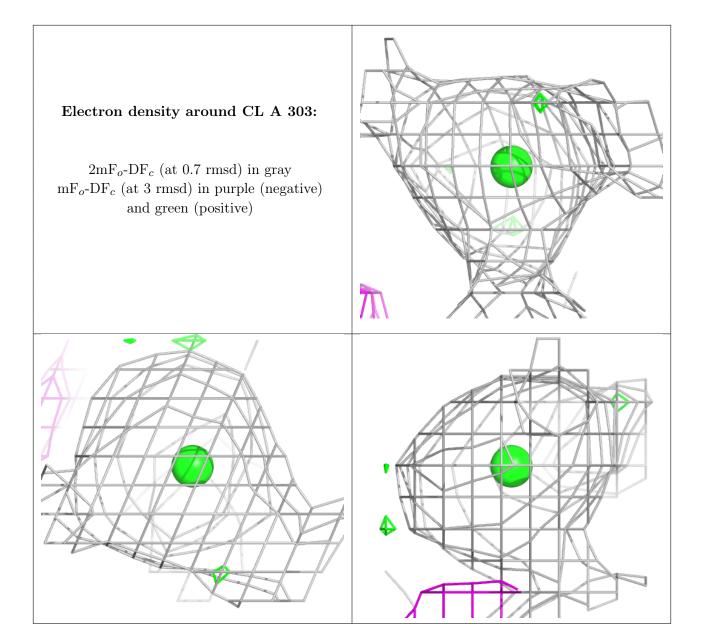




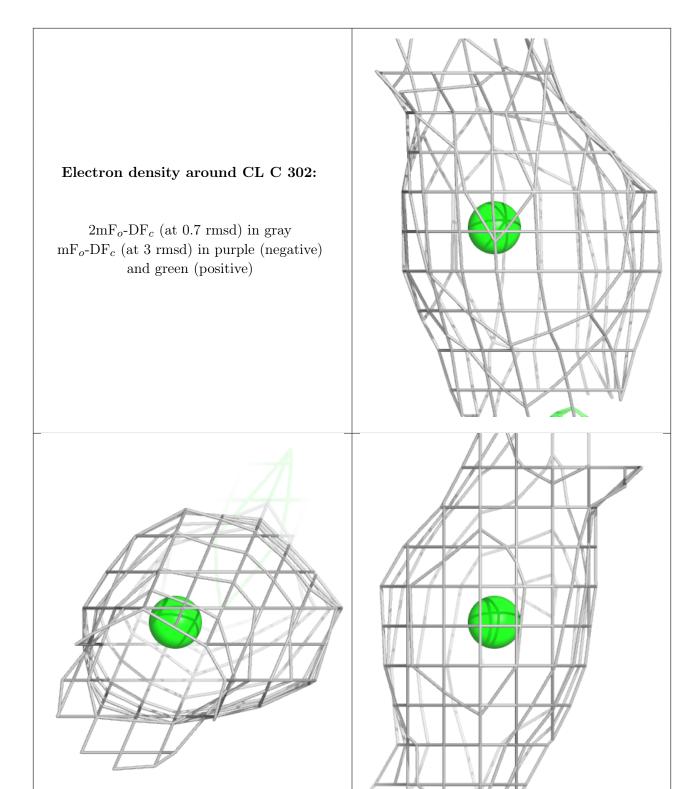


# Electron density around CL A 302: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

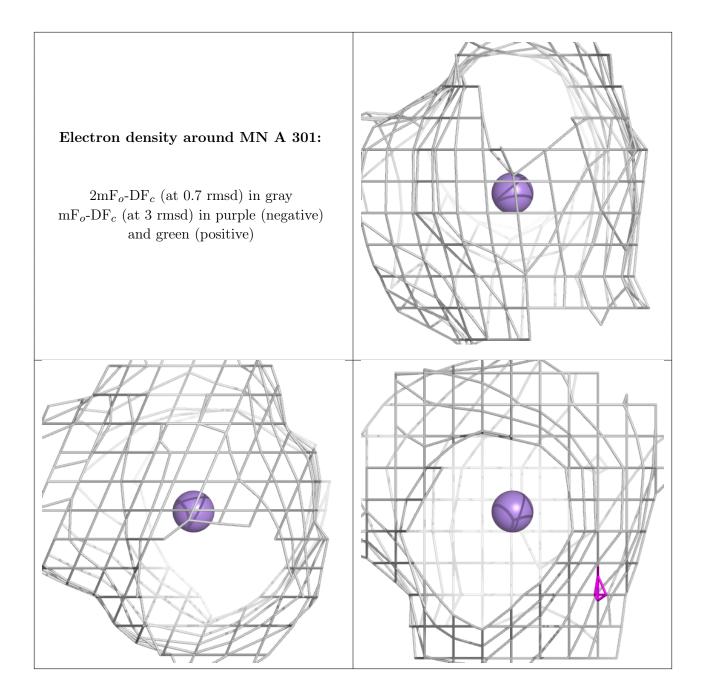












# 6.5 Other polymers (i)

There are no such residues in this entry.

