

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

Dec 27, 2023 – 12:10 AM JST

PDB ID : 8X6Z

Title : 1-naphthylamine GS from Pseudomonas sp. JS3066

Authors: Zhou, N.Y.; Zhang, S.T.

Deposited on : 2023-11-22

Resolution : 2.95 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 : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

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

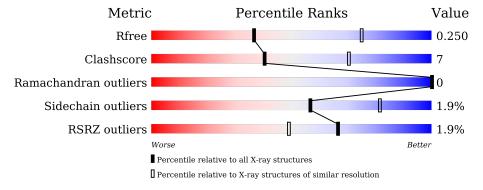
 $\begin{tabular}{lll} Validation Pipeline (wwPDB-VP) & : & 2.36 \end{tabular}$ 

### 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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	510	78%	16%	5%
1	11	010	2 <u>%</u>	1070	J 70
1	В	510	84%	12%	5%
1	С	510	77%	18%	5%
1	D	510	74%	20%	• 5%
1	Е	510	73%	21%	• 5%
1	F	510	79%	16%	5%



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23407 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 Glutamine synthetase.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	1 A 48	482	Total	С	N	О	S	0	0	0
1	Λ	402	3771	2403	634	716	18	U	0	U
1	В	487	Total	С	N	О	S	0	0	0
1	Ъ	401	3801	2421	640	722	18	U	0	
1	С	484	Total C N O S 0	0	0					
1		404	3782	2412	637	715	18	U	U	
1	D	482	Total	С	N	Ο	S	0	0	0
1	D	402	3767	2403	635	711	18	U	U	
1	Е	483	Total	С	N	O	S	0	0	0
1	ш	400	3761	2397	635	711	18	U	0	
1	1 F	485	Total	С	N	О	S	0	0	0
1	I.	400	3786	2413	637	718	18	U	U	

• 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	2	Total Mn 2 2	0	0
2	В	2	Total Mn 2 2	0	0
2	С	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	Ε	2	Total Mn 2 2	0	0
2	F	2	Total Mn 2 2	0	0

• Molecule 3 is water.



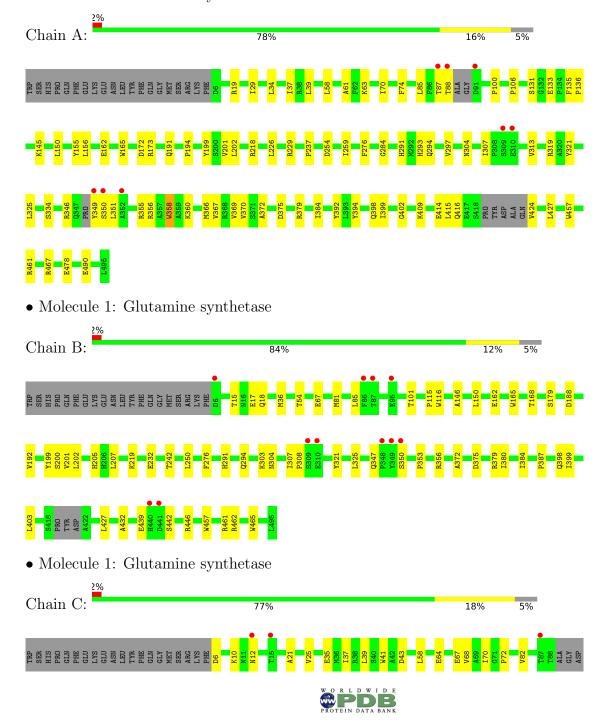
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	143	Total O 143 143	0	0
3	В	113	Total O 113 113	0	0
3	С	129	Total O 129 129	0	0
3	D	126	Total O 126 126	0	0
3	Е	112	Total O 112 112	0	0
3	F	106	Total O 106 106	0	0

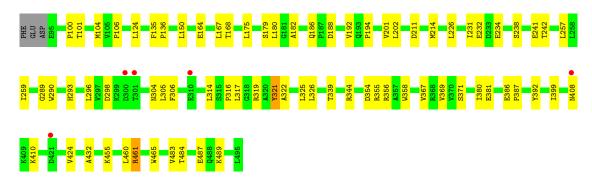


## 3 Residue-property plots (i)

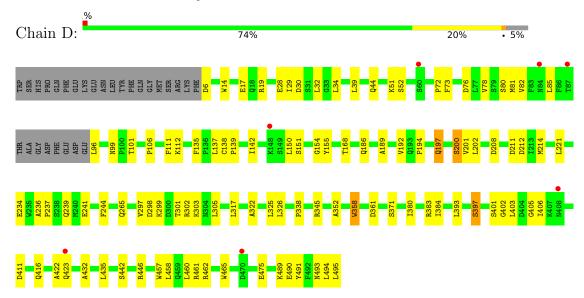
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glutamine synthetase

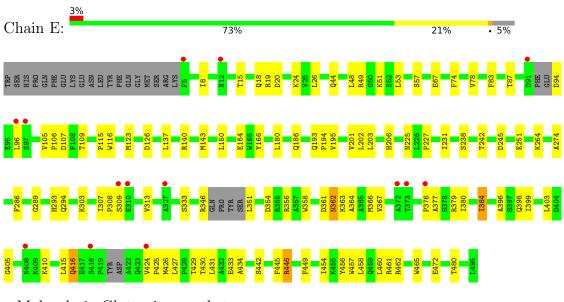




• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase

Chain F: 79% 16% 5%







### 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	121.64Å 140.14Å 218.78Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 - 2.95	Depositor
Resolution (A)	19.98 - 2.95	EDS
% Data completeness	99.8 (19.98-2.95)	Depositor
(in resolution range)	99.9 (19.98-2.95)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.48 (at 2.93Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
D D	0.224 , 0.247	Depositor
$R, R_{free}$	0.227 , $0.250$	DCC
$R_{free}$ test set	3911 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.872	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32, 55.5	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.44, < L^2> = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23407	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 37.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0331e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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: 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	Bo	ond angles
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.50	0/3859	0.66	0/5229
1	В	0.50	0/3892	0.69	1/5278~(0.0%)
1	С	0.50	0/3874	0.70	0/5257
1	D	0.50	0/3859	0.66	0/5235
1	Е	0.46	0/3849	0.67	0/5217
1	F	0.49	0/3877	0.67	0/5258
All	All	0.49	0/23210	0.67	1/31474~(0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	В	199	TYR	CB-CA-C	5.69	121.78	110.40

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	3771	0	3704	53	0
1	В	3801	0	3734	40	0
1	С	3782	0	3723	60	0
1	D	3767	0	3710	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Е	3761	0	3700	63	0
1	F	3786	0	3718	61	0
2	A	2	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
2	Ε	2	0	0	0	0
2	F	2	0	0	0	0
3	A	143	0	0	4	0
3	В	113	0	0	2	0
3	С	129	0	0	0	0
3	D	126	0	0	3	0
3	Е	112	0	0	1	0
3	F	106	0	0	2	0
All	All	23407	0	22289	323	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 7.

The worst 5 of 323 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:B:15:THR:HG22	1:B:17:GLU:H	1.30	0.94
1:A:321:TYR:O	1:A:325:LEU:HD13	1.77	0.84
1:C:164:GLU:HG2	1:C:241:GLU:HG3	1.63	0.78
1:A:201:VAL:HG22	1:A:202:LEU:HG	1.66	0.77
1:C:408:ASN:OD1	1:C:408:ASN:O	2.04	0.75

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	Percentil	es
1	A	474/510~(93%)	458 (97%)	16 (3%)	0	100 10	0
1	В	$483/510 \ (95\%)$	459 (95%)	24 (5%)	0	100 10	0
1	С	480/510 (94%)	463 (96%)	17 (4%)	0	100 10	0
1	D	478/510 (94%)	459 (96%)	19 (4%)	0	100 10	0
1	E	475/510~(93%)	461 (97%)	14 (3%)	0	100 10	0
1	F	481/510 (94%)	466 (97%)	15 (3%)	0	100 10	0
All	All	$2871/3060 \ (94\%)$	2766 (96%)	105 (4%)	0	100 10	0

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	403/427 (94%)	397 (98%)	6 (2%)	65 85
1	В	$405/427 \ (95\%)$	401 (99%)	4 (1%)	76 90
1	С	404/427 (95%)	398 (98%)	6 (2%)	65 85
1	D	402/427 (94%)	385 (96%)	17 (4%)	30 63
1	E	400/427 (94%)	387 (97%)	13 (3%)	38 70
1	F	403/427 (94%)	402 (100%)	1 (0%)	93 98
All	All	2417/2562 (94%)	2370 (98%)	47 (2%)	57 81

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	384	ILE
1	Е	87	THR
1	D	397	SER
1	D	475	GLU
1	Е	96	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:



Mol	Chain	Res	Type
1	Е	362	ASN
1	F	191	GLN
1	С	191	GLN
1	С	408	ASN
1	D	205	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 10 ligands modelled in this entry, 10 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>	# RSRZ > 2	$OWAB(Å^2)$	Q < 0.9
1	A	482/510 (94%)	-0.23	8 (1%) 70 53	19, 36, 66, 87	0
1	В	487/510 (95%)	-0.15	11 (2%) 60 43	22, 37, 72, 102	0
1	С	484/510 (94%)	-0.11	8 (1%) 70 53	23, 39, 67, 90	0
1	D	482/510 (94%)	-0.11	7 (1%) 73 57	23, 40, 62, 77	0
1	E	483/510 (94%)	-0.02	14 (2%) 51 35	22, 43, 69, 96	0
1	F	485/510 (95%)	-0.09	7 (1%) 75 59	21, 40, 65, 87	0
All	All	2903/3060 (94%)	-0.12	55 (1%) 66 49	19, 39, 67, 102	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	349	TYR	4.7
1	Ε	91	ASP	4.6
1	Е	5	PHE	4.1
1	В	348	PRO	4.0
1	D	423	GLN	3.9

#### 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.



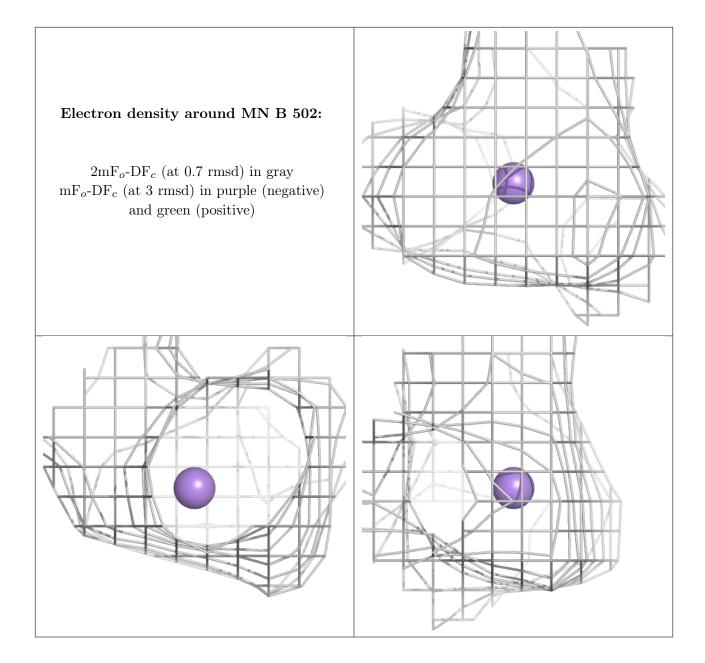
#### 6.4 Ligands (i)

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	502	1/1	0.53	0.16	95,95,95,95	0
2	MN	A	501	1/1	0.67	0.16	90,90,90,90	0
2	MN	С	501	1/1	0.71	0.12	104,104,104,104	0
2	MN	D	501	1/1	0.75	0.18	113,113,113,113	0
2	MN	Е	501	1/1	0.81	0.12	85,85,85,85	0
2	MN	Ε	502	1/1	0.83	0.13	107,107,107,107	0
2	MN	В	501	1/1	0.91	0.08	64,64,64,64	0
2	MN	F	502	1/1	0.91	0.10	73,73,73,73	0
2	MN	A	502	1/1	0.94	0.06	74,74,74,74	0
2	MN	F	501	1/1	0.96	0.11	79,79,79,79	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.

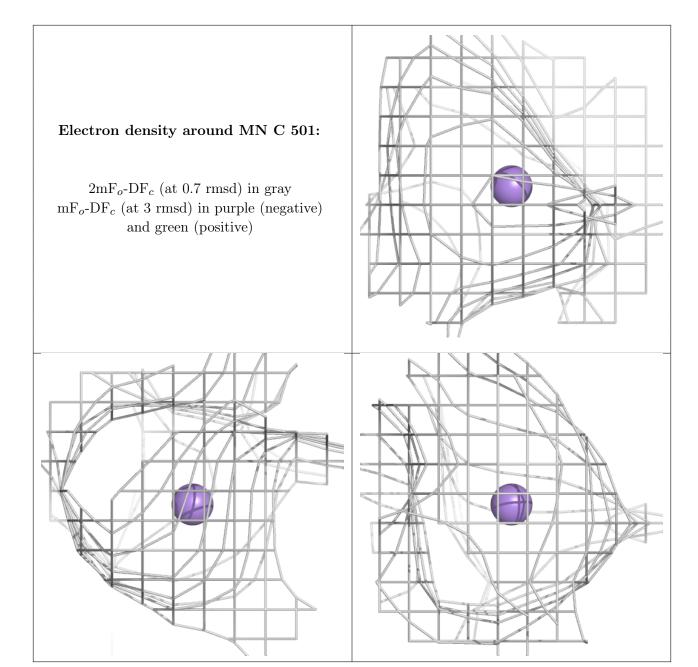




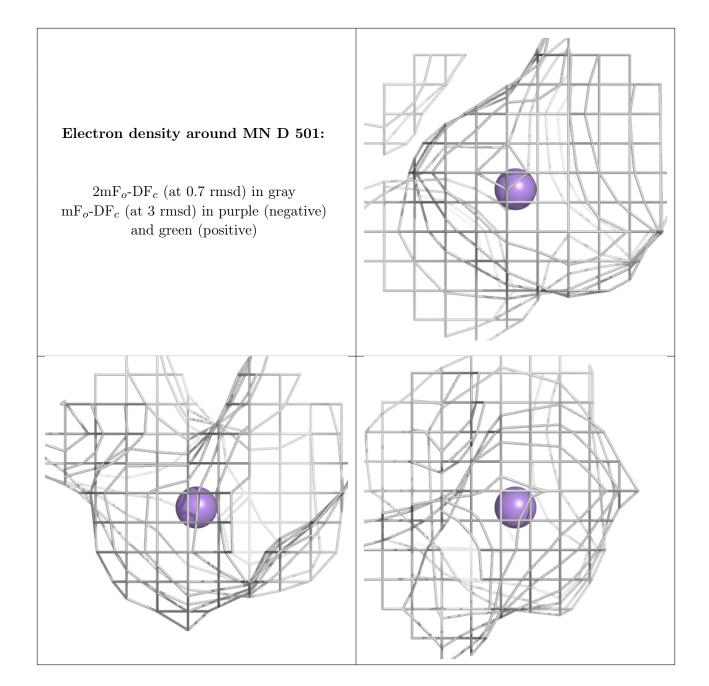


## Electron density around MN A 501: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











# Electron density around MN E 501: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

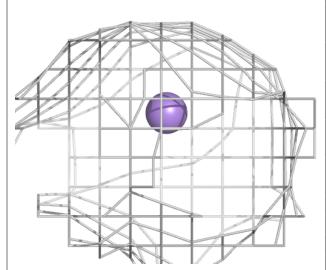


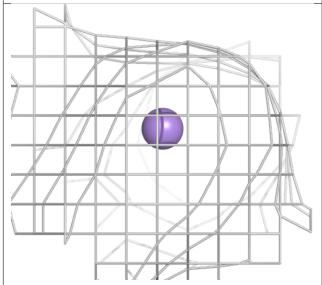
## 

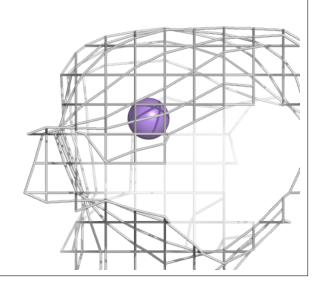


#### Electron density around MN B 501:

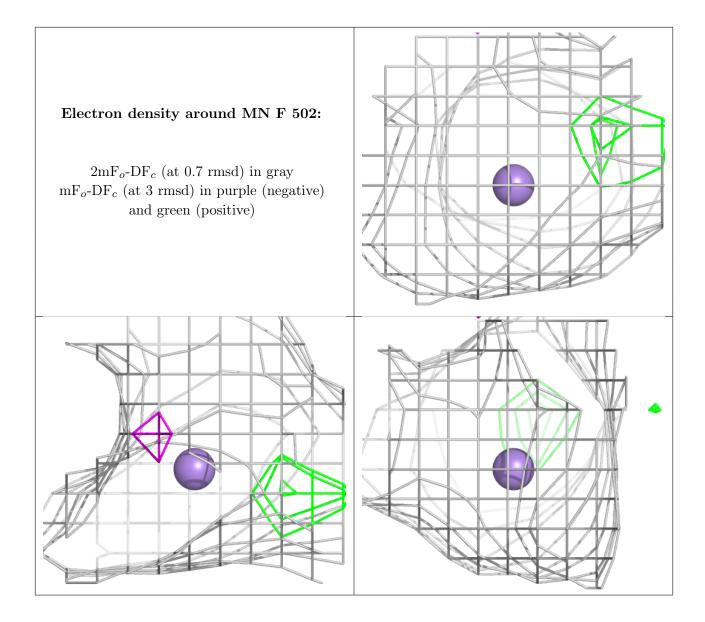
 $2 {
m mF}_o {
m -DF}_c$  (at 0.7 rmsd) in gray  ${
m mF}_o {
m -DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)







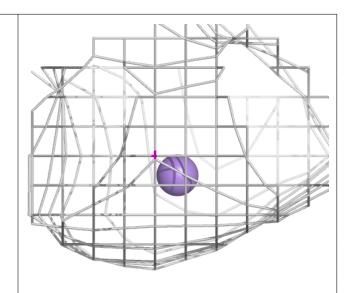


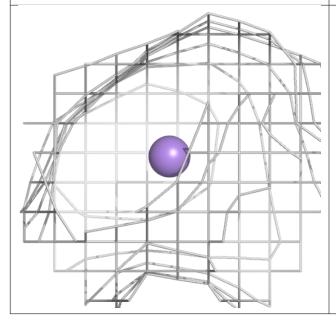


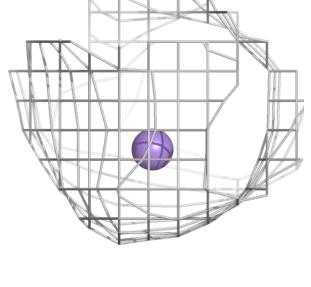


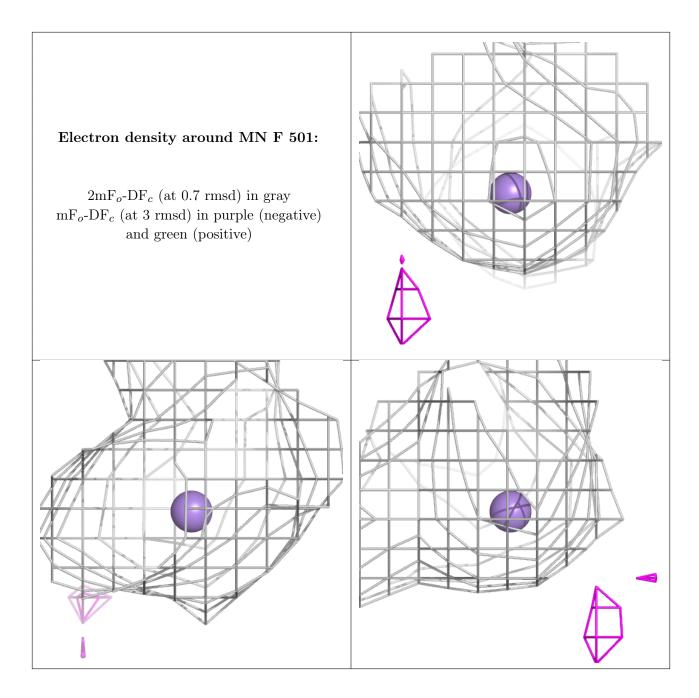
#### Electron density around MN A 502:

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









## 6.5 Other polymers (i)

There are no such residues in this entry.

