



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:14 PM UTC

PDB ID : 7DBT / pdb_00007dbt
Title : Crystal structure of catalytic domain of Anhydrobiosis-related Mn-dependent Peroxidase (AMNP) from *Ramazzottius varieornatus* (Mn²⁺-bound form)
Authors : Yoshida, Y.; Satoh, T.; Ota, C.; Tanaka, S.; Horikawa, D.D.; Tomita, M.; Kato, K.; Arakawa, K.
Deposited on : 2020-10-21
Resolution : 2.30 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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

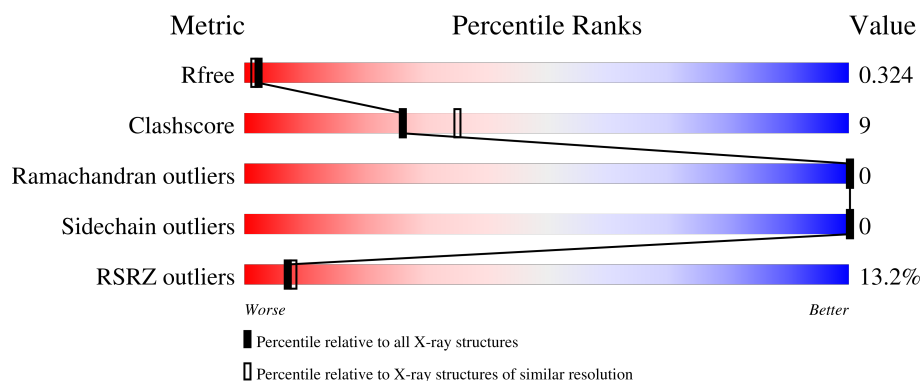
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	173	12% 76% 14% 10%
1	B	173	12% 73% 17% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2468 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 AMNP/g12777.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1182	735	209	230	8			
1	B	155	Total	C	N	O	S	0	0	0
			1182	735	209	230	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	GLY	-	expression tag	UNP A0A1D1VPD8
A	60	SER	-	expression tag	UNP A0A1D1VPD8
A	61	HIS	-	expression tag	UNP A0A1D1VPD8
A	62	MET	-	expression tag	UNP A0A1D1VPD8
B	59	GLY	-	expression tag	UNP A0A1D1VPD8
B	60	SER	-	expression tag	UNP A0A1D1VPD8
B	61	HIS	-	expression tag	UNP A0A1D1VPD8
B	62	MET	-	expression tag	UNP A0A1D1VPD8

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

- Molecule 3 is water.

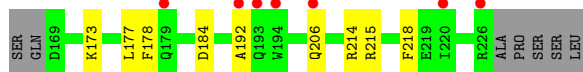
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total	O	0	0
			48	48		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	52	Total	O	0	0
			52	52		

- Molecule 1: AMNP/g12777



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.40Å 41.16Å 79.77Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.30 19.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.93-2.30) 97.3 (19.93-2.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.30Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.262 , 0.325 0.261 , 0.324	Depositor DCC
R_{free} test set	691 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	1.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2468	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 54.21 % 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 3.7716e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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.

5 Model quality

5.1 Standard geometry

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		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/1203	0.72	0/1628
1	B	0.36	0/1203	0.65	0/1628
All	All	0.38	0/2406	0.68	0/3256

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

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	1182	0	1148	19	0
1	B	1182	0	1148	25	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	48	0	0	2	0
3	B	52	0	0	2	0
All	All	2468	0	2296	44	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 9.

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ARG:NH2	3:B:401:HOH:O	1.57	0.85
1:A:161:ASP:OD2	3:A:1101:HOH:O	2.02	0.78
1:A:120:ALA:HA	1:A:123:TRP:CE2	2.28	0.69
1:A:179:GLN:HE21	1:A:183:ARG:HH21	1.46	0.64
1:A:179:GLN:HE21	1:A:183:ARG:NH2	1.99	0.61
1:B:145:MET:HA	1:B:145:MET:HE2	1.83	0.60
1:A:109:SER:OG	1:A:117:SER:N	2.36	0.58
1:B:143:ARG:HB2	1:B:143:ARG:HH21	1.68	0.58
1:B:107:LEU:CD2	1:B:145:MET:HE3	2.34	0.58
1:B:90:LYS:HB2	1:B:93:PHE:CE2	2.40	0.56
1:B:120:ALA:HA	1:B:123:TRP:CE2	2.41	0.56
1:B:136:THR:HG23	3:B:416:HOH:O	2.08	0.54
1:B:105:LEU:HB3	1:B:143:ARG:HH21	1.73	0.54
1:B:109:SER:OG	1:B:117:SER:N	2.42	0.52
1:B:192:ALA:HB2	1:B:218:PHE:HB3	1.91	0.52
1:B:102:THR:HG22	1:B:125:THR:HA	1.92	0.51
1:B:107:LEU:HD21	1:B:145:MET:HE3	1.93	0.51
1:A:206:GLN:H	1:A:206:GLN:CD	2.20	0.50
1:A:107:LEU:HD13	1:A:145:MET:HE3	1.95	0.49
1:A:120:ALA:HA	1:A:123:TRP:CD2	2.48	0.49
1:A:145:MET:HA	1:A:145:MET:HE2	1.94	0.48
1:A:102:THR:HG22	1:A:125:THR:HA	1.95	0.48
1:B:107:LEU:O	1:B:107:LEU:HD23	2.14	0.48
1:B:206:GLN:H	1:B:206:GLN:CD	2.22	0.48
1:B:143:ARG:NH2	1:B:143:ARG:HB2	2.30	0.47
1:A:184:ASP:OD1	1:A:215:ARG:NH2	2.49	0.46
1:B:123:TRP:CH2	1:B:156:ARG:HB3	2.50	0.46
1:A:85:LEU:HB3	3:A:1103:HOH:O	2.14	0.46
1:B:105:LEU:O	1:B:143:ARG:HD2	2.16	0.45
1:B:114:TRP:CE2	1:B:173:LYS:HB3	2.52	0.45
1:A:79:ASP:OD1	1:A:81:PRO:HD3	2.16	0.45
1:A:75:ILE:H	1:A:75:ILE:HD12	1.82	0.45
1:B:90:LYS:HB2	1:B:93:PHE:CD2	2.51	0.45
1:B:177:LEU:HD13	1:B:178:PHE:N	2.32	0.45
1:B:96:ALA:HB3	1:B:131:ASP:HA	2.00	0.44
1:B:74:GLU:OE2	1:B:214:ARG:NH2	2.47	0.43
1:A:183:ARG:HH11	1:A:183:ARG:HD2	1.69	0.42
1:A:87:ASN:OD1	1:A:87:ASN:C	2.62	0.42
1:A:75:ILE:HG13	1:A:155:LEU:HD21	2.02	0.42
1:A:174:PHE:HA	1:A:201:THR:O	2.21	0.41
1:A:177:LEU:HD13	1:A:178:PHE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLU:OE2	1:B:214:ARG:NE	2.50	0.41
1:B:137:ILE:HG22	1:B:139:ARG:HG2	2.03	0.40
1:B:184:ASP:OD1	1:B:215:ARG:NH2	2.55	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	Percentiles	
1	A	151/173 (87%)	149 (99%)	2 (1%)	0	100	100
1	B	151/173 (87%)	147 (97%)	4 (3%)	0	100	100
All	All	302/346 (87%)	296 (98%)	6 (2%)	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	128/143 (90%)	128 (100%)	0	100	100
1	B	128/143 (90%)	128 (100%)	0	100	100
All	All	256/286 (90%)	256 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	GLN
1	B	160	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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

6.1 Protein, DNA and RNA chains

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	155/173 (89%)	1.12	21 (13%) 7 8	20, 27, 42, 67	0
1	B	155/173 (89%)	1.12	20 (12%) 7 8	21, 28, 42, 58	0
All	All	310/346 (89%)	1.12	41 (13%) 7 8	20, 28, 42, 67	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	GLY	4.8
1	A	150	ALA	4.8
1	A	146	CYS	4.0
1	B	150	ALA	3.7
1	B	143	ARG	3.0
1	A	147	GLY	3.0
1	A	193	GLN	2.7
1	B	136	THR	2.7
1	B	192	ALA	2.7
1	A	220	ILE	2.7
1	B	116	GLY	2.6
1	A	84	ILE	2.6
1	B	117	SER	2.6
1	B	194	TRP	2.5
1	B	75	ILE	2.5
1	A	148	GLY	2.5
1	A	176	CYS	2.4
1	A	120	ALA	2.4
1	B	93	PHE	2.4
1	A	217	ALA	2.4
1	A	179	GLN	2.4
1	B	114	TRP	2.3
1	B	109	SER	2.3
1	A	185	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	194	TRP	2.3
1	A	66	ALA	2.2
1	A	171	ILE	2.2
1	B	179	GLN	2.2
1	B	96	ALA	2.2
1	A	117	SER	2.2
1	A	175	SER	2.2
1	B	226	ARG	2.2
1	B	162	ALA	2.2
1	A	183	ARG	2.1
1	B	141	VAL	2.1
1	B	206	GLN	2.1
1	A	224	SER	2.0
1	B	97	CYS	2.0
1	B	193	GLN	2.0
1	B	220	ILE	2.0
1	A	200	CYS	2.0

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 oligosaccharides 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, 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.

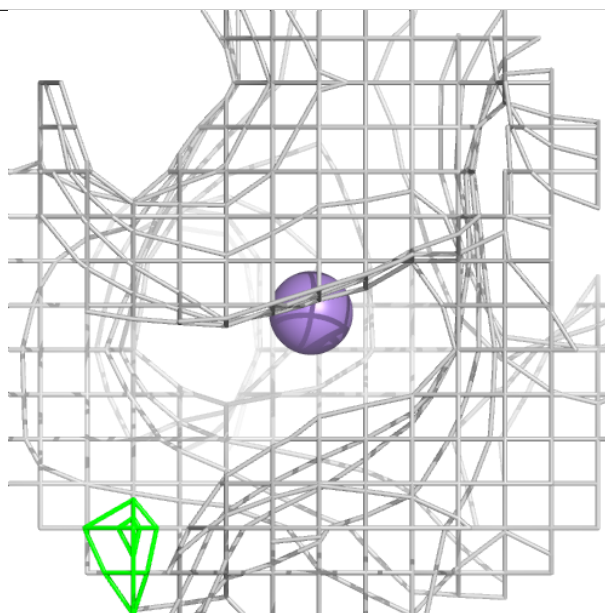
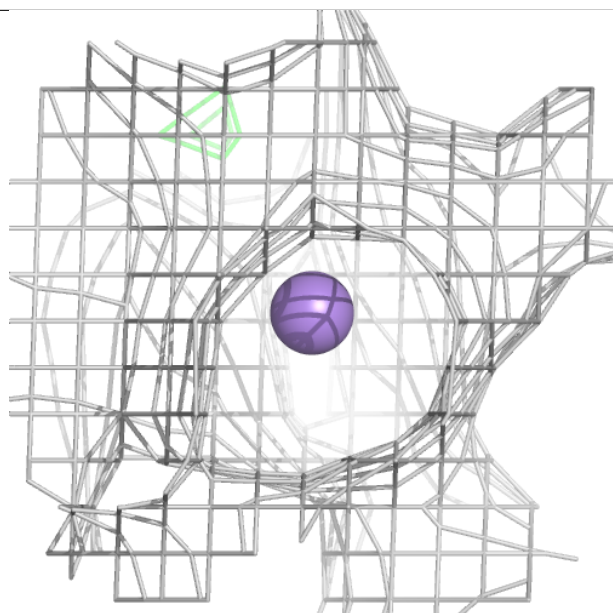
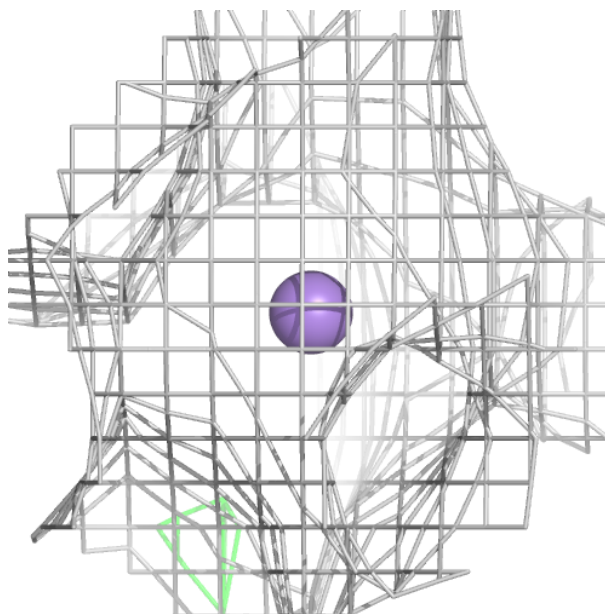
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	B	301	1/1	0.92	0.05	49,49,49,49	0
2	MN	A	1001	1/1	0.93	0.05	44,44,44,44	0
2	MN	A	1002	1/1	0.98	0.05	22,22,22,22	0
2	MN	B	302	1/1	0.98	0.04	21,21,21,21	0

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.

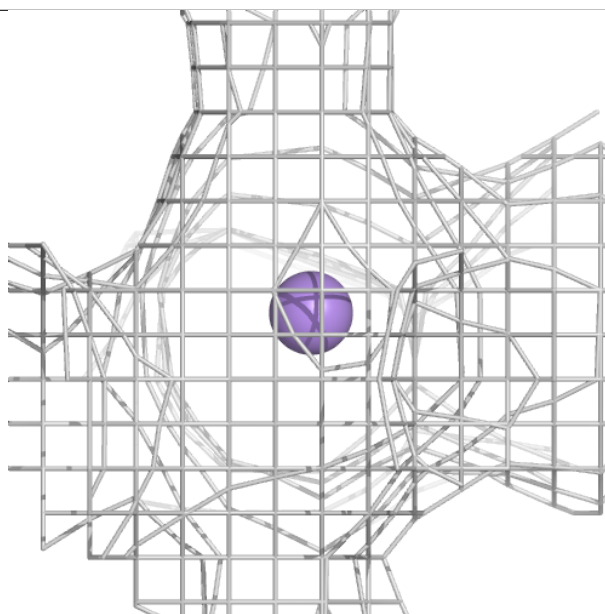
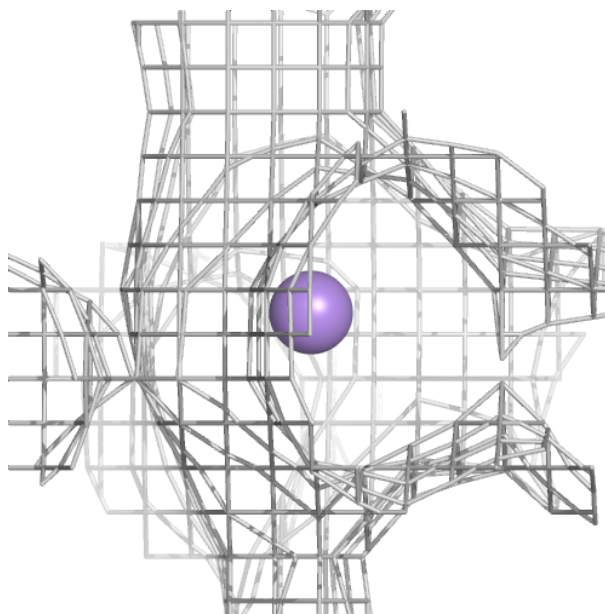
Electron density around MN B 301:

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



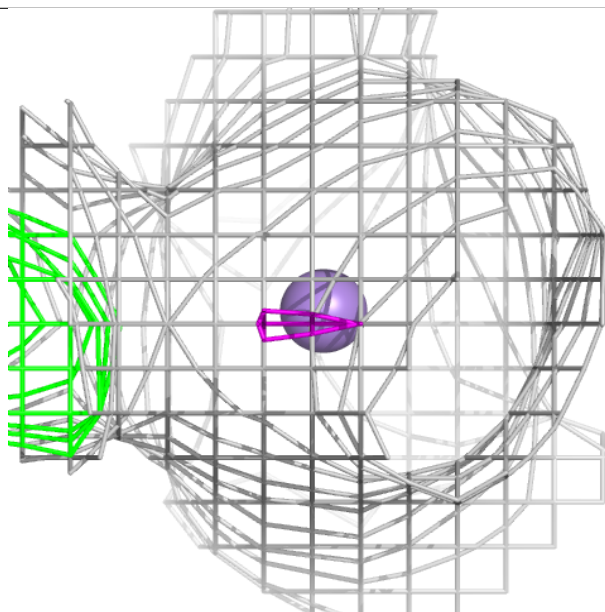
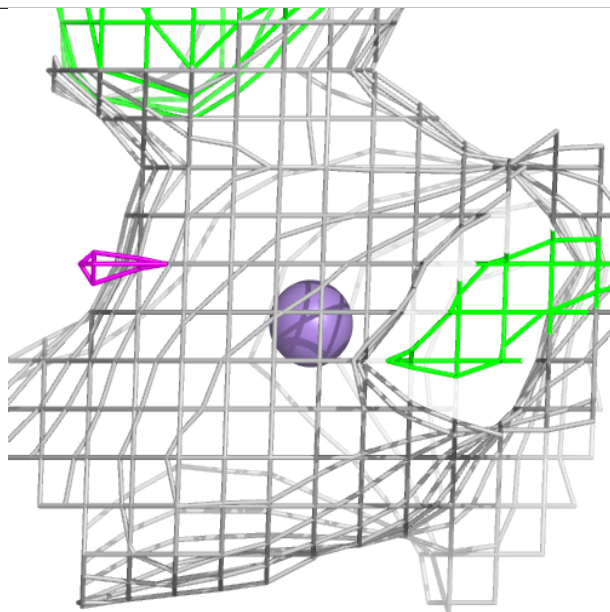
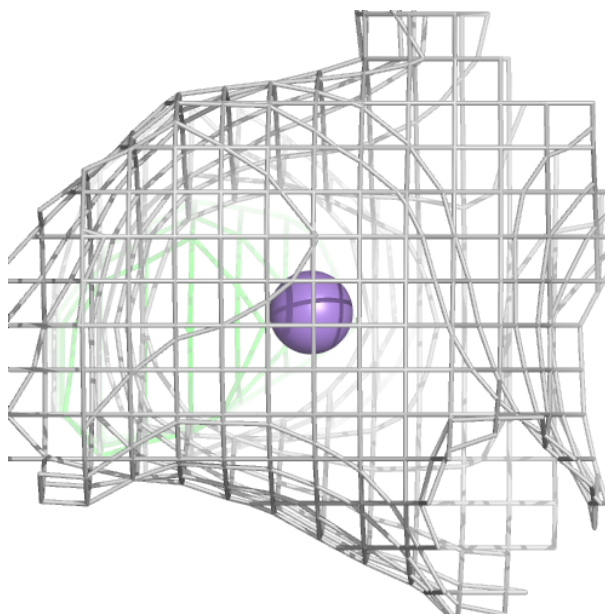
Electron density around MN A 1001:

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



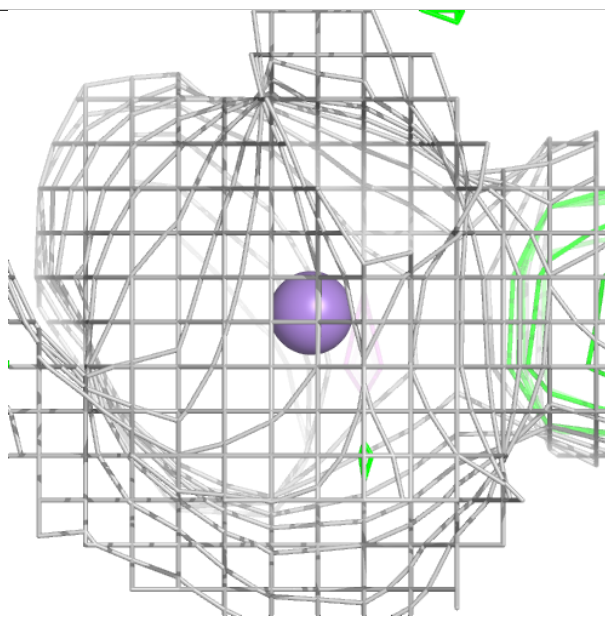
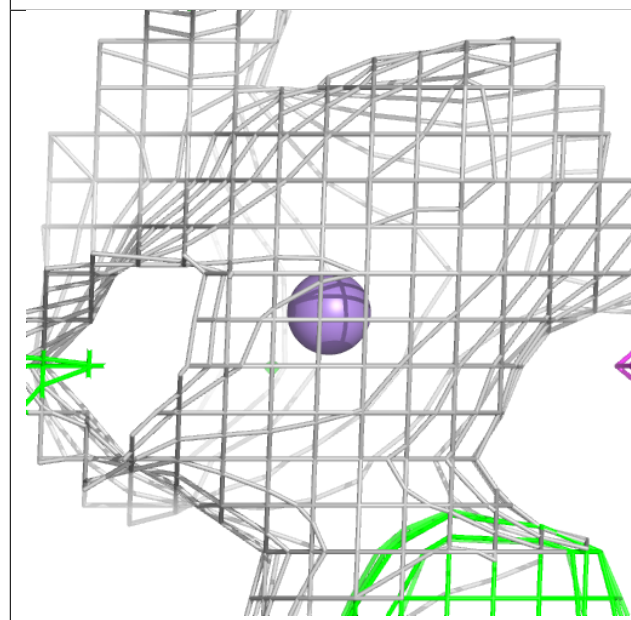
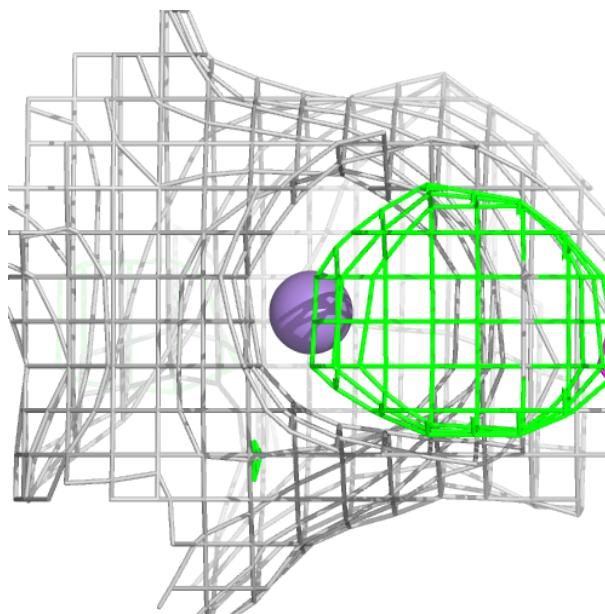
Electron density around MN A 1002:

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



Electron density around MN B 302:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.