



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:00 AM UTC

PDB ID : 6LL7 / pdb_00006ll7
Title : Type II inorganic pyrophosphatase (PPase) from the psychrophilic bacterium
Shewanella sp. AS-11, Mn-activated form
Authors : Horitani, M.; Kusubayashi, K.; Oshima, K.; Yato, A.; Sugimoto, H.; Watanabe, K.
Deposited on : 2019-12-21
Resolution : 2.20 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

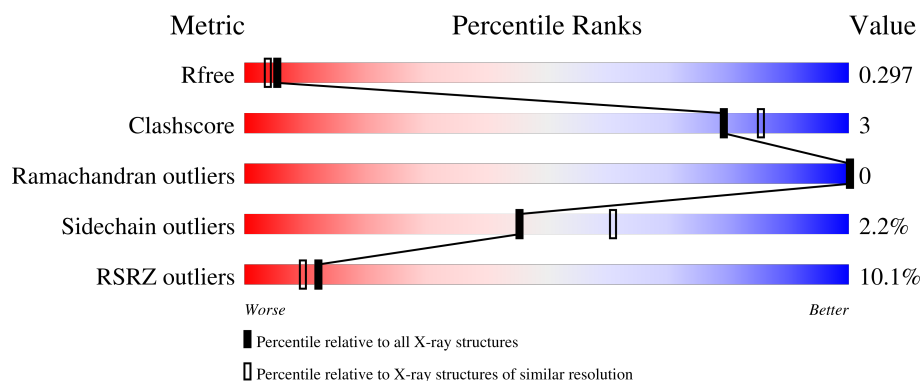
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	309	11% 93% 6%
1	B	309	10% 92% 7%
1	C	309	9% 92% 7%
1	D	309	10% 92% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9646 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 Inorganic pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2340	1488	380	455	17			
1	B	306	Total	C	N	O	S	0	0	0
			2340	1488	380	455	17			
1	C	306	Total	C	N	O	S	0	0	0
			2340	1488	380	455	17			
1	D	306	Total	C	N	O	S	0	0	0
			2340	1488	380	455	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	cloning artifact	UNP L8AXY8
A	1	GLY	-	cloning artifact	UNP L8AXY8
A	116	SER	ARG	conflict	UNP L8AXY8
B	0	MET	-	cloning artifact	UNP L8AXY8
B	1	GLY	-	cloning artifact	UNP L8AXY8
B	116	SER	ARG	conflict	UNP L8AXY8
C	0	MET	-	cloning artifact	UNP L8AXY8
C	1	GLY	-	cloning artifact	UNP L8AXY8
C	116	SER	ARG	conflict	UNP L8AXY8
D	0	MET	-	cloning artifact	UNP L8AXY8
D	1	GLY	-	cloning artifact	UNP L8AXY8
D	116	SER	ARG	conflict	UNP L8AXY8

- 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		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Mn 2	0	0
2	C	2	Total 2	Mn 2	0	0
2	D	2	Total 2	Mn 2	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0

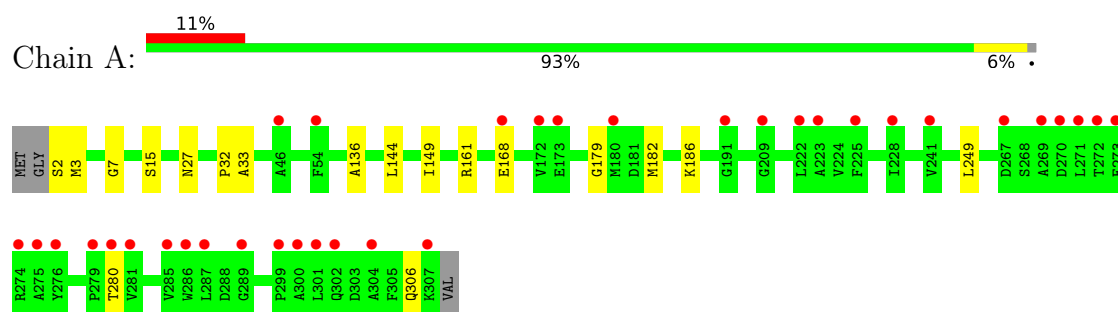
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total 63	O 63	0	0
4	B	78	Total 78	O 78	0	0
4	C	72	Total 72	O 72	0	0
4	D	63	Total 63	O 63	0	0

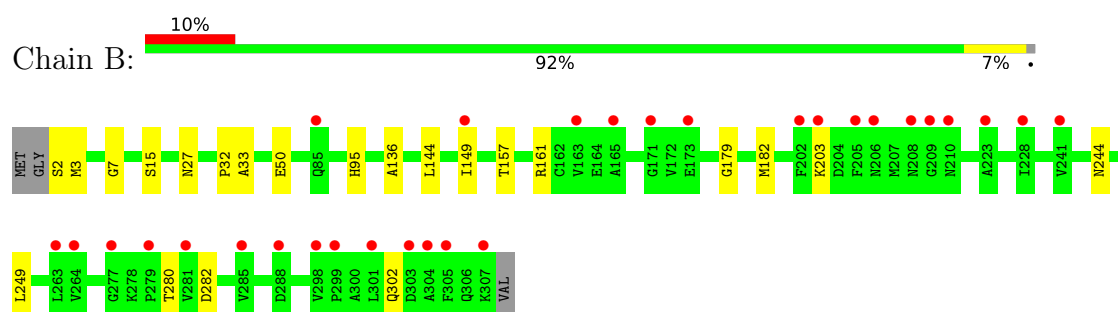
3 Residue-property plots [i](#)

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.

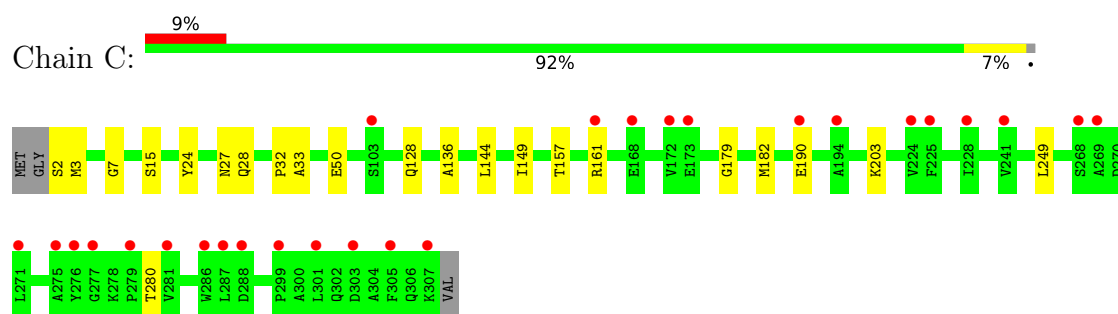
- Molecule 1: Inorganic pyrophosphatase



- Molecule 1: Inorganic pyrophosphatase

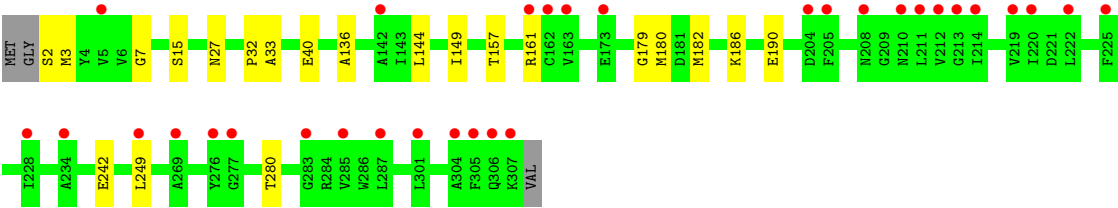


- Molecule 1: Inorganic pyrophosphatase



- Molecule 1: Inorganic pyrophosphatase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.53Å 75.57Å 85.67Å 107.40° 90.06° 92.17°	Depositor
Resolution (Å)	47.51 – 2.20 47.51 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.0 (47.51-2.20) 95.0 (47.51-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.256 , 0.297 0.259 , 0.297	Depositor DCC
R_{free} test set	2985 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.106 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9646	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.12% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	1.06	0/2379	1.44	2/3223 (0.1%)
1	B	1.07	0/2379	1.46	3/3223 (0.1%)
1	C	1.07	0/2379	1.46	2/3223 (0.1%)
1	D	1.06	0/2379	1.45	2/3223 (0.1%)
All	All	1.06	0/9516	1.45	9/12892 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	ALA	CA-C-N	5.46	126.01	119.94
1	C	136	ALA	C-N-CA	5.46	126.01	119.94
1	A	136	ALA	CA-C-N	5.39	125.93	119.94
1	A	136	ALA	C-N-CA	5.39	125.93	119.94
1	B	244	ASN	CB-CA-C	5.34	121.05	110.42
1	D	136	ALA	CA-C-N	5.23	125.74	119.94
1	D	136	ALA	C-N-CA	5.23	125.74	119.94
1	B	136	ALA	CA-C-N	5.17	125.68	119.94
1	B	136	ALA	C-N-CA	5.17	125.68	119.94

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	2340	0	2353	10	0
1	B	2340	0	2353	14	0
1	C	2340	0	2353	13	0
1	D	2340	0	2353	14	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	63	0	0	3	0
4	B	78	0	0	4	0
4	C	72	0	0	4	0
4	D	63	0	0	5	0
All	All	9646	0	9412	50	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 3.

All (50) 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:A:179:GLY:HA2	1:A:182:MET:HE3	1.49	0.93
1:C:179:GLY:HA2	1:C:182:MET:HE3	1.46	0.93
1:B:179:GLY:HA2	1:B:182:MET:HE3	1.49	0.92
1:B:282:ASP:OD1	1:D:242:GLU:HA	1.73	0.89
1:D:179:GLY:HA2	1:D:182:MET:HE3	1.52	0.89
1:C:27:ASN:HD21	1:C:33:ALA:H	1.48	0.62
1:D:161:ARG:HD2	4:D:526:HOH:O	2.00	0.61
1:D:27:ASN:HD21	1:D:33:ALA:H	1.49	0.59
1:B:7:GLY:HA3	1:B:15:SER:HB3	1.85	0.58
1:B:27:ASN:HD21	1:B:33:ALA:H	1.51	0.58
1:A:27:ASN:HD21	1:A:33:ALA:H	1.50	0.58
1:A:144:LEU:HB2	1:A:182:MET:HE1	1.86	0.58
1:C:179:GLY:HA2	1:C:182:MET:CE	2.28	0.57
1:D:179:GLY:HA2	1:D:182:MET:CE	2.30	0.57
1:B:179:GLY:HA2	1:B:182:MET:CE	2.28	0.56
1:C:203:LYS:NZ	4:C:503:HOH:O	2.37	0.56
1:A:7:GLY:HA3	1:A:15:SER:HB3	1.87	0.56
1:A:179:GLY:HA2	1:A:182:MET:CE	2.30	0.56
1:D:7:GLY:HA3	1:D:15:SER:HB3	1.87	0.55
1:C:144:LEU:HB2	1:C:182:MET:HE1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:HB2	1:B:182:MET:HE1	1.89	0.54
1:C:7:GLY:HA3	1:C:15:SER:HB3	1.89	0.53
1:C:203:LYS:HD3	4:C:569:HOH:O	2.08	0.53
1:A:161:ARG:HD2	4:A:538:HOH:O	2.08	0.53
1:D:161:ARG:CD	4:D:526:HOH:O	2.55	0.53
1:A:27:ASN:ND2	1:A:32:PRO:HA	2.25	0.52
1:D:144:LEU:HB2	1:D:182:MET:HE1	1.92	0.51
1:B:27:ASN:ND2	1:B:32:PRO:HA	2.26	0.51
1:D:186:LYS:HE3	4:D:548:HOH:O	2.11	0.51
1:A:186:LYS:HE2	4:A:556:HOH:O	2.10	0.51
1:C:27:ASN:ND2	1:C:32:PRO:HA	2.27	0.50
1:D:27:ASN:ND2	1:D:32:PRO:HA	2.27	0.49
1:C:157:THR:HG22	1:C:161:ARG:NH1	2.28	0.49
1:B:157:THR:HG22	1:B:161:ARG:HH11	1.78	0.47
1:C:161:ARG:HD2	4:C:555:HOH:O	2.15	0.46
1:B:157:THR:HG22	1:B:161:ARG:HD3	1.97	0.46
1:D:157:THR:HG22	1:D:161:ARG:NH1	2.31	0.46
1:B:95:HIS:HE1	4:B:515:HOH:O	2.00	0.45
1:D:3:MET:O	1:D:33:ALA:HA	2.18	0.44
1:B:3:MET:O	1:B:33:ALA:HA	2.18	0.44
1:B:95:HIS:CE1	4:B:515:HOH:O	2.69	0.44
1:D:40:GLU:OE1	4:D:501:HOH:O	2.21	0.44
1:C:3:MET:O	1:C:33:ALA:HA	2.18	0.43
1:A:3:MET:O	1:A:33:ALA:HA	2.19	0.42
1:D:180:MET:HE1	4:D:524:HOH:O	2.20	0.42
1:C:24:TYR:CE1	1:C:28:GLN:HG3	2.55	0.42
1:B:161:ARG:NE	4:B:503:HOH:O	2.34	0.41
1:C:128:GLN:HG2	4:C:527:HOH:O	2.19	0.41
1:B:203:LYS:HD3	4:B:532:HOH:O	2.19	0.41
1:A:161:ARG:CD	4:A:538:HOH:O	2.67	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	304/309 (98%)	297 (98%)	7 (2%)	0	100	100
1	B	304/309 (98%)	296 (97%)	8 (3%)	0	100	100
1	C	304/309 (98%)	295 (97%)	9 (3%)	0	100	100
1	D	304/309 (98%)	298 (98%)	6 (2%)	0	100	100
All	All	1216/1236 (98%)	1186 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	256/258 (99%)	250 (98%)	6 (2%)	44	59
1	B	256/258 (99%)	250 (98%)	6 (2%)	44	59
1	C	256/258 (99%)	250 (98%)	6 (2%)	44	59
1	D	256/258 (99%)	251 (98%)	5 (2%)	48	64
All	All	1024/1032 (99%)	1001 (98%)	23 (2%)	45	61

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	149	ILE
1	A	168	GLU
1	A	249	LEU
1	A	280	THR
1	A	306	GLN
1	B	2	SER
1	B	50	GLU
1	B	149	ILE
1	B	249	LEU

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Mol	Chain	Res	Type
1	B	280	THR
1	B	302	GLN
1	C	2	SER
1	C	50	GLU
1	C	149	ILE
1	C	190	GLU
1	C	249	LEU
1	C	280	THR
1	D	2	SER
1	D	149	ILE
1	D	190	GLU
1	D	249	LEU
1	D	280	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	78	GLN
1	A	206	ASN
1	A	306	GLN
1	B	27	ASN
1	B	78	GLN
1	B	206	ASN
1	B	244	ASN
1	C	27	ASN
1	C	78	GLN
1	C	206	ASN
1	C	302	GLN
1	D	27	ASN
1	D	78	GLN
1	D	206	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 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

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	306/309 (99%)	1.04	35 (11%)	10 7	23, 39, 86, 105	0
1	B	306/309 (99%)	0.96	30 (9%)	13 10	23, 36, 67, 100	0
1	C	306/309 (99%)	0.94	27 (8%)	15 13	24, 36, 73, 85	0
1	D	306/309 (99%)	0.95	32 (10%)	11 9	24, 39, 70, 103	0
All	All	1224/1236 (99%)	0.97	124 (10%)	12 10	23, 38, 73, 105	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	ILE	4.6
1	B	298	VAL	4.4
1	B	228	ILE	4.1
1	B	203	LYS	3.9
1	A	271	LEU	3.8
1	B	303	ASP	3.8
1	A	173	GLU	3.7
1	B	301	LEU	3.7
1	A	269	ALA	3.7
1	D	213	GLY	3.6
1	D	307	LYS	3.5
1	C	228	ILE	3.5
1	C	307	LYS	3.5
1	B	307	LYS	3.4
1	D	287	LEU	3.3
1	B	285	VAL	3.3
1	A	272	THR	3.3
1	A	286	TRP	3.3
1	A	54	PHE	3.3
1	C	305	PHE	3.2
1	A	287	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	191	GLY	3.1
1	D	305	PHE	3.1
1	A	223	ALA	3.1
1	D	220	ILE	3.0
1	C	303	ASP	3.0
1	D	277	GLY	3.0
1	A	274	ARG	3.0
1	A	285	VAL	3.0
1	C	286	TRP	3.0
1	A	168	GLU	3.0
1	C	299	PRO	2.9
1	D	142	ALA	2.9
1	A	307	LYS	2.9
1	A	299	PRO	2.8
1	C	271	LEU	2.8
1	A	275	ALA	2.8
1	A	273	GLU	2.8
1	B	209	GLY	2.8
1	A	304	ALA	2.8
1	D	161	ARG	2.8
1	C	288	ASP	2.7
1	D	276	TYR	2.7
1	D	228	ILE	2.7
1	B	163	VAL	2.6
1	A	279	PRO	2.6
1	D	211	LEU	2.6
1	D	249	LEU	2.6
1	A	225	PHE	2.6
1	D	212	VAL	2.6
1	B	279	PRO	2.5
1	A	301	LEU	2.5
1	C	279	PRO	2.5
1	C	281	VAL	2.5
1	D	173	GLU	2.5
1	B	205	PHE	2.5
1	B	304	ALA	2.5
1	A	281	VAL	2.4
1	B	210	ASN	2.4
1	D	234	ALA	2.4
1	D	214	ILE	2.4
1	C	301	LEU	2.4
1	B	173	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	224	VAL	2.3
1	D	219	VAL	2.3
1	C	269	ALA	2.3
1	A	241	VAL	2.3
1	B	202	PHE	2.3
1	B	206	ASN	2.3
1	B	277	GLY	2.3
1	B	165	ALA	2.3
1	C	103	SER	2.3
1	C	173	GLU	2.3
1	B	281	VAL	2.3
1	D	301	LEU	2.2
1	C	161	ARG	2.2
1	C	194	ALA	2.2
1	C	275	ALA	2.2
1	A	267	ASP	2.2
1	D	204	ASP	2.2
1	D	162	CYS	2.2
1	B	171	GLY	2.2
1	A	276	TYR	2.2
1	C	287	LEU	2.2
1	B	241	VAL	2.2
1	D	5	VAL	2.2
1	D	208	ASN	2.2
1	A	280	THR	2.2
1	C	268	SER	2.2
1	C	276	TYR	2.2
1	B	149	ILE	2.2
1	C	277	GLY	2.2
1	B	223	ALA	2.2
1	A	180	MET	2.1
1	B	208	ASN	2.1
1	B	264	VAL	2.1
1	D	285	VAL	2.1
1	B	305	PHE	2.1
1	A	302	GLN	2.1
1	B	85	GLN	2.1
1	D	306	GLN	2.1
1	A	289	GLY	2.1
1	D	283	GLY	2.1
1	A	46	ALA	2.1
1	D	304	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	222	LEU	2.1
1	B	288	ASP	2.1
1	B	299	PRO	2.1
1	A	209	GLY	2.1
1	C	225	PHE	2.1
1	D	205	PHE	2.1
1	D	225	PHE	2.1
1	A	300	ALA	2.1
1	A	270	ASP	2.1
1	D	210	ASN	2.1
1	C	172	VAL	2.1
1	D	163	VAL	2.1
1	D	269	ALA	2.0
1	A	222	LEU	2.0
1	B	263	LEU	2.0
1	A	172	VAL	2.0
1	C	241	VAL	2.0
1	C	168	GLU	2.0
1	C	190	GLU	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	C	401	1/1	0.97	0.04	29,29,29,29	0
2	MN	B	402	1/1	0.98	0.03	24,24,24,24	0
2	MN	B	401	1/1	0.98	0.02	27,27,27,27	0
2	MN	D	402	1/1	0.98	0.03	31,31,31,31	0

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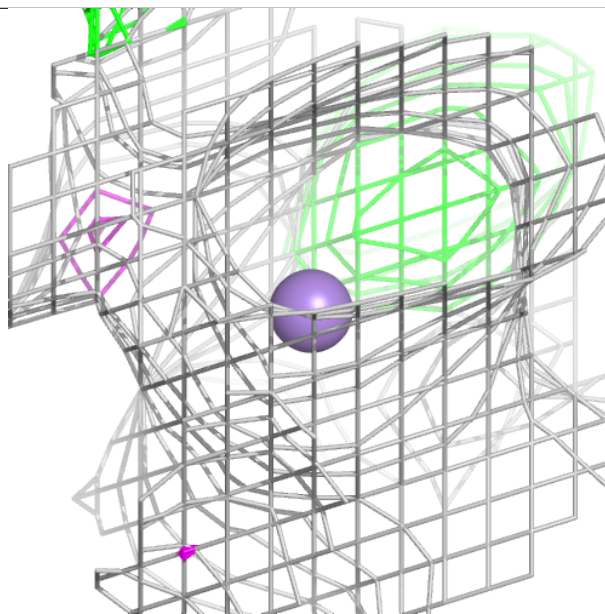
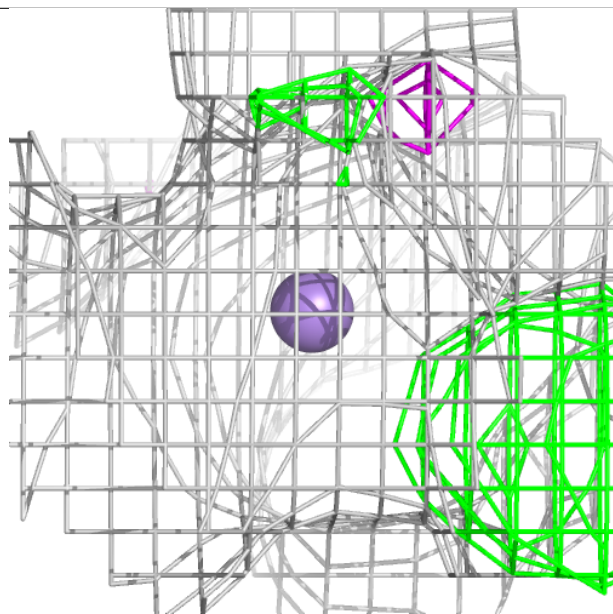
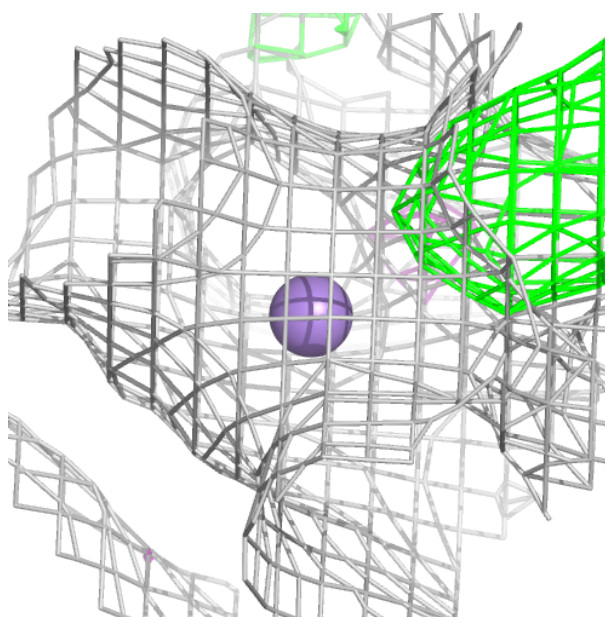
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	403	1/1	0.98	0.03	33,33,33,33	0
3	CA	C	403	1/1	0.98	0.04	30,30,30,30	0
2	MN	D	401	1/1	0.99	0.04	32,32,32,32	0
2	MN	A	402	1/1	0.99	0.02	27,27,27,27	0
2	MN	A	401	1/1	0.99	0.03	31,31,31,31	0
2	MN	C	402	1/1	0.99	0.04	27,27,27,27	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.

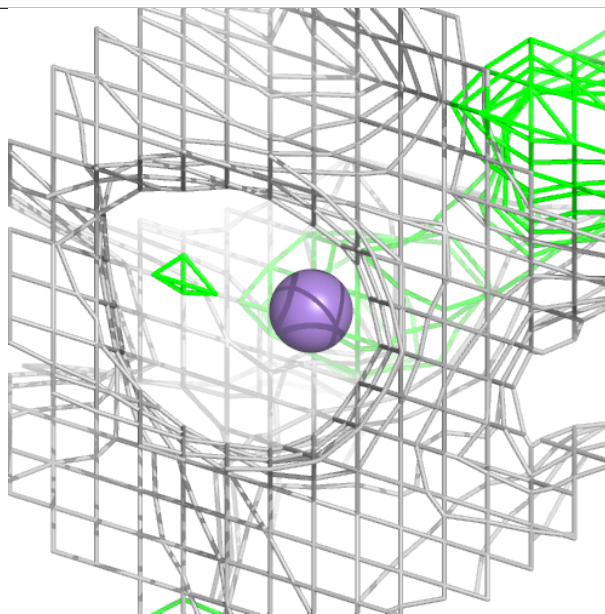
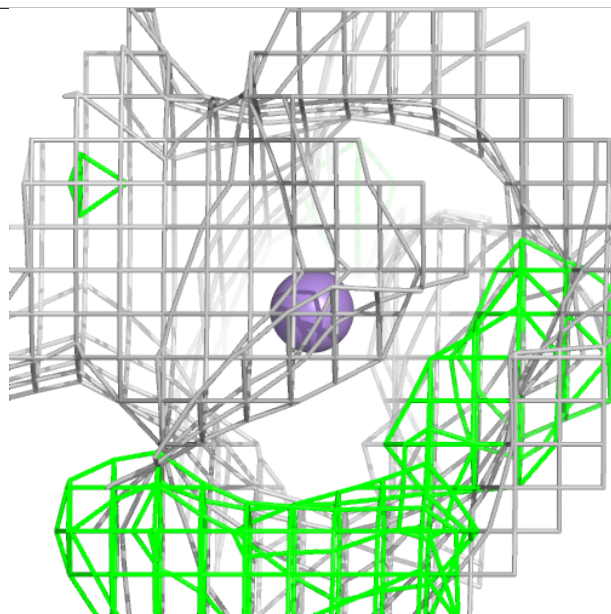
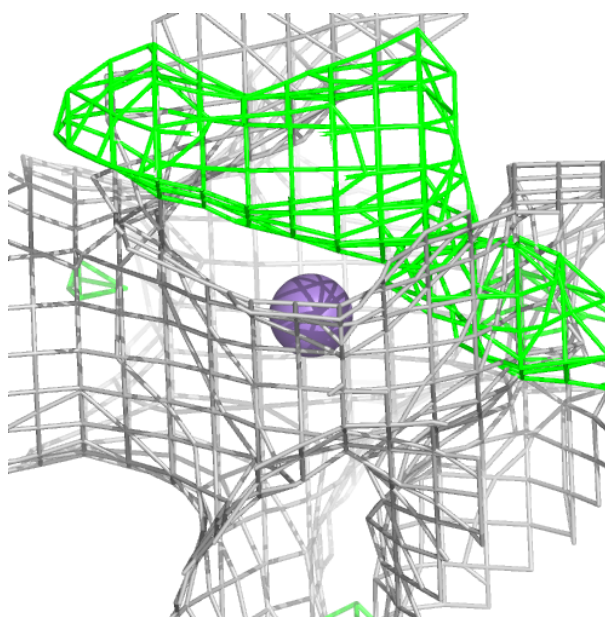
Electron density around MN C 401:

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



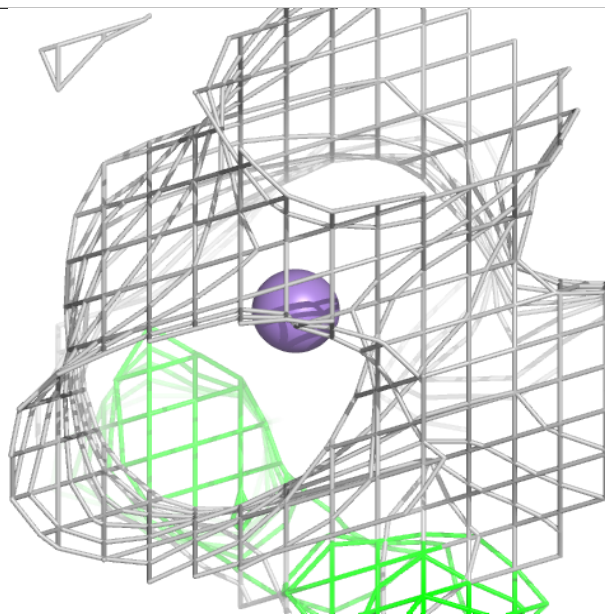
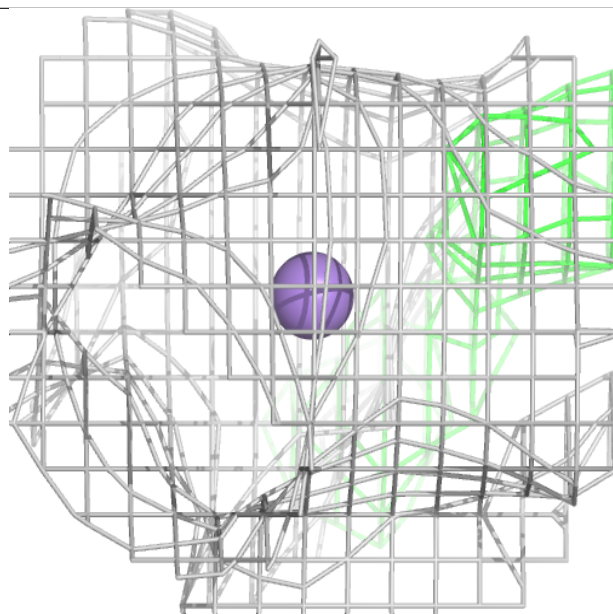
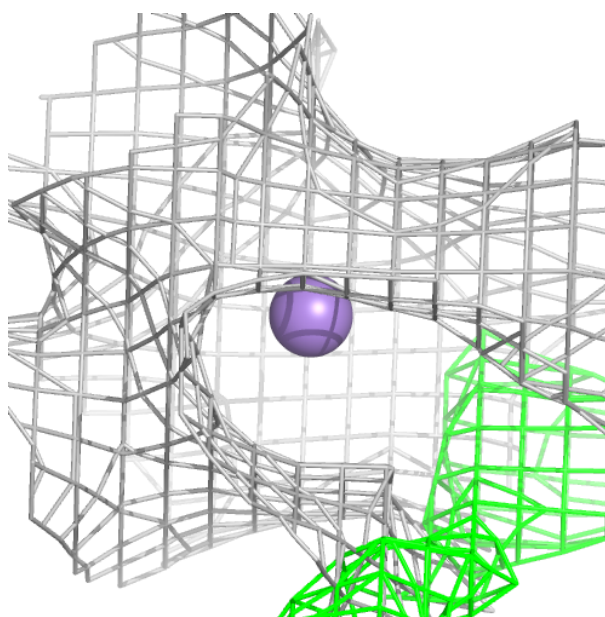
Electron density around MN B 402:

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



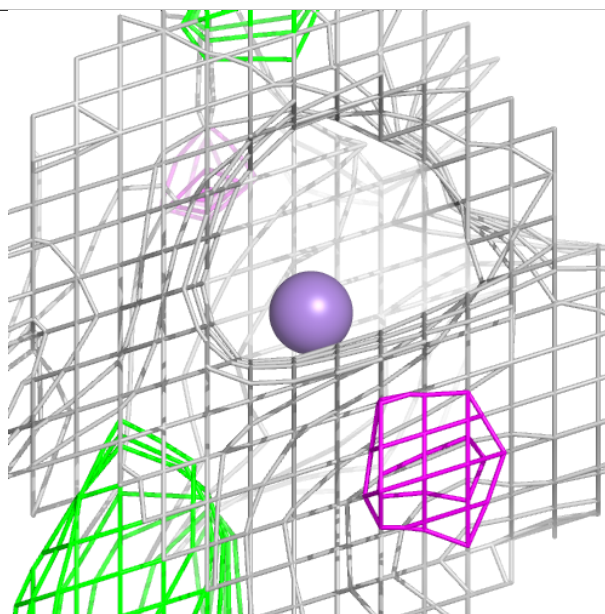
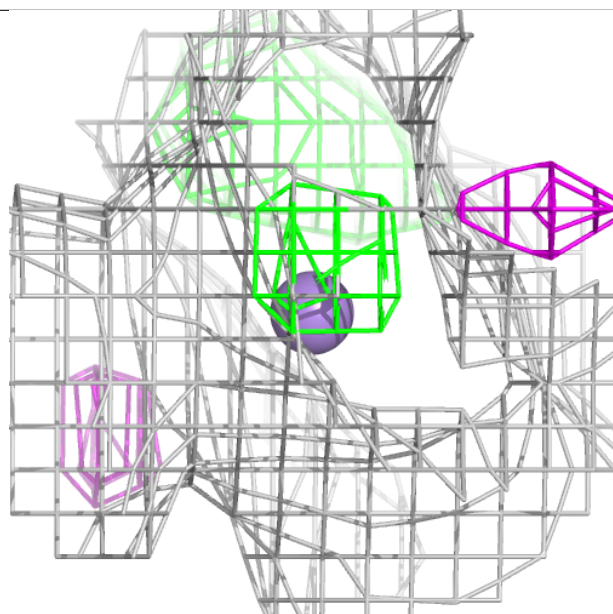
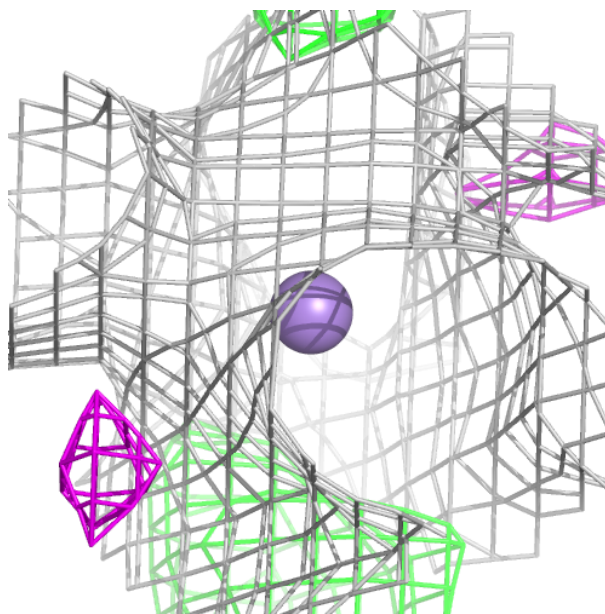
Electron density around MN B 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



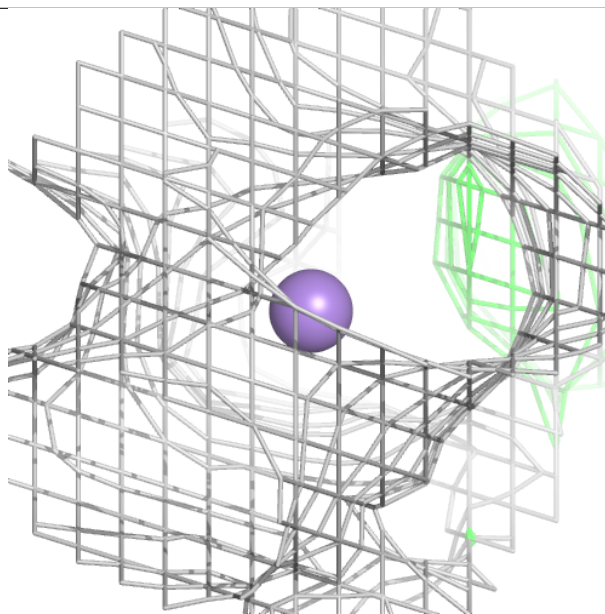
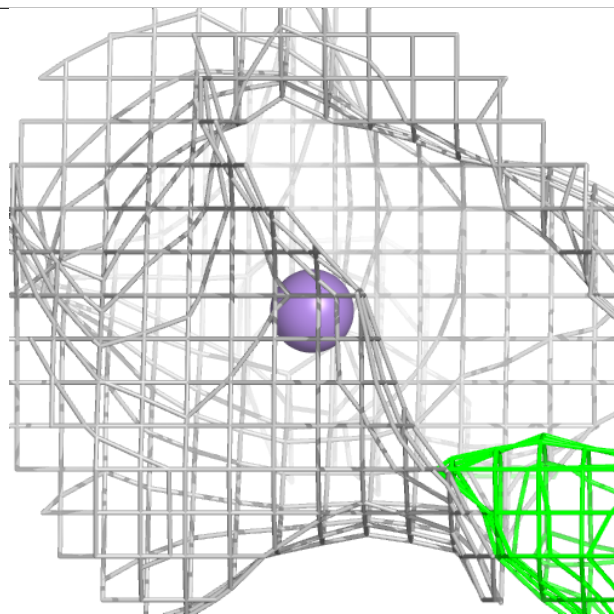
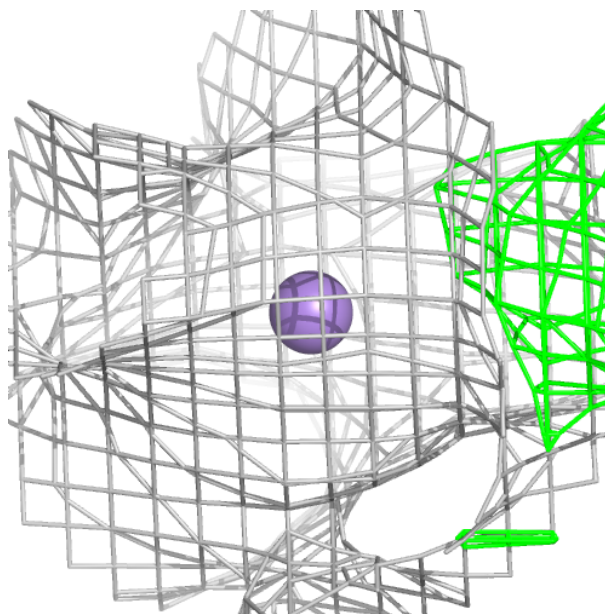
Electron density around MN D 402:

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and green (positive)



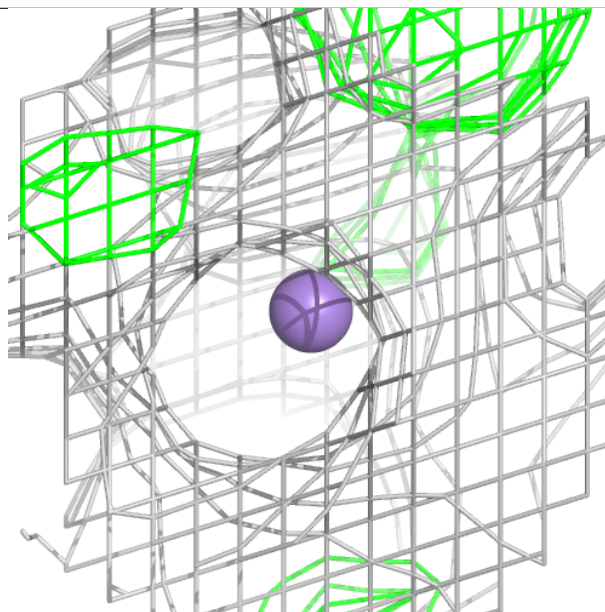
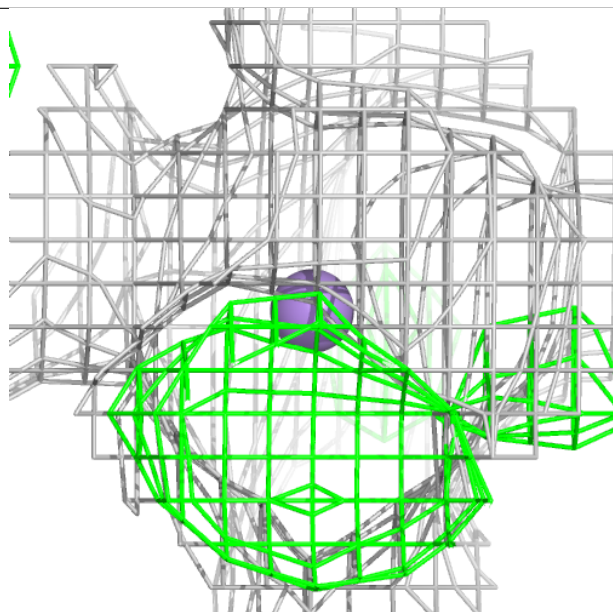
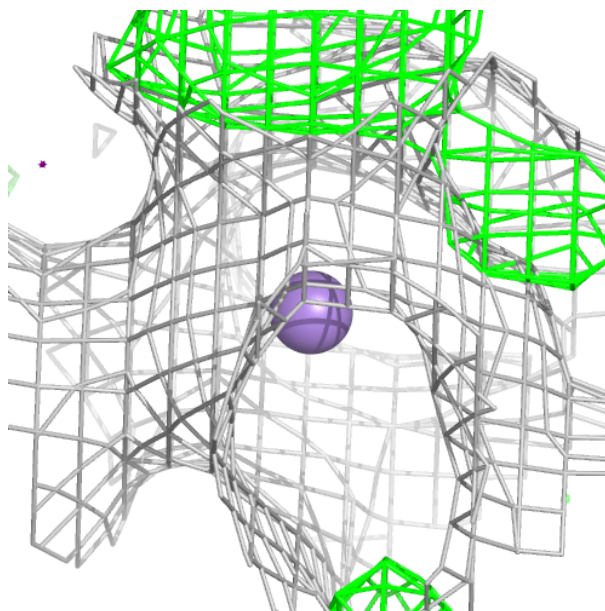
Electron density around MN D 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



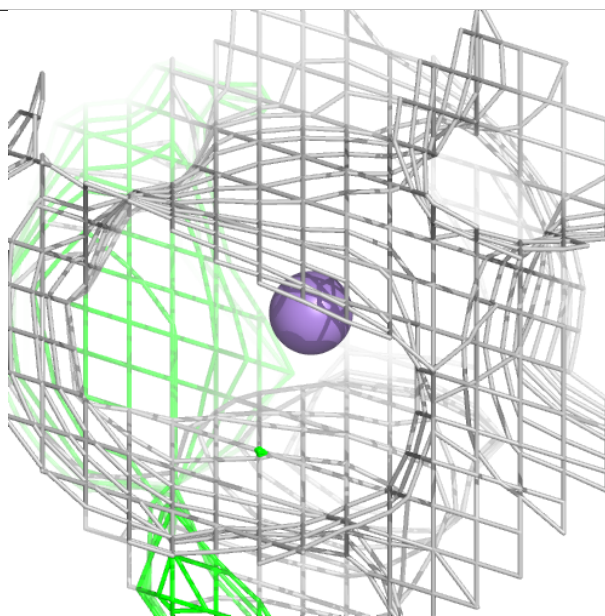
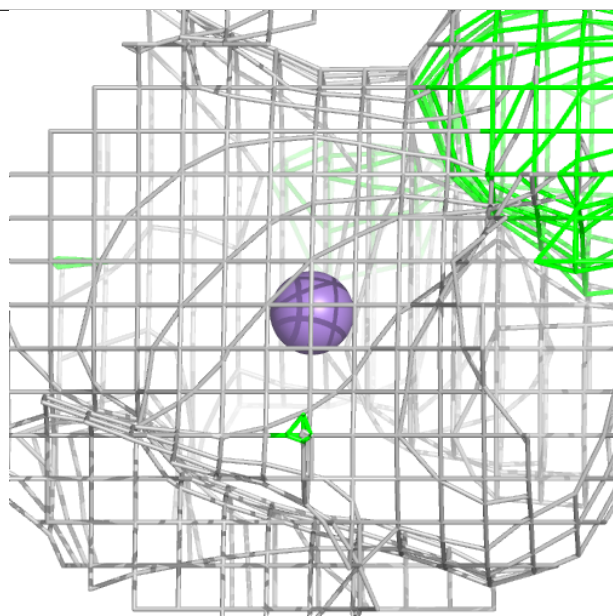
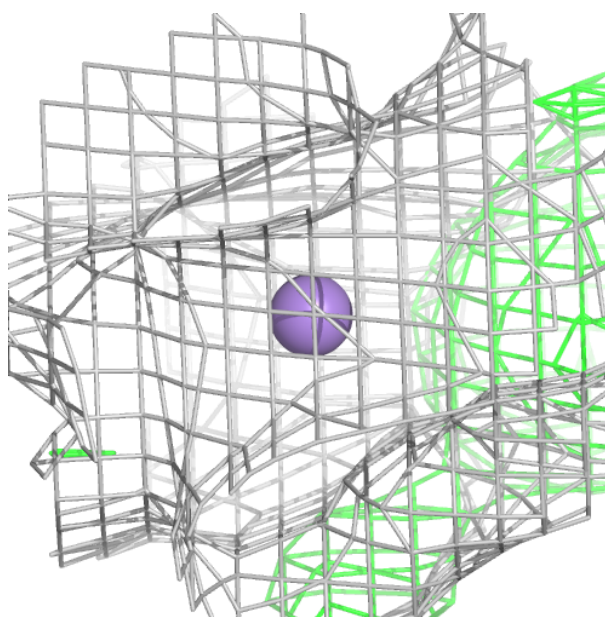
Electron density around MN A 402:

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



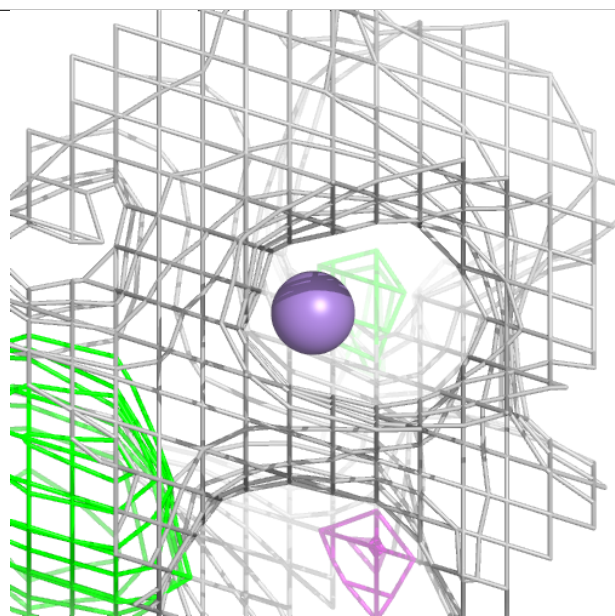
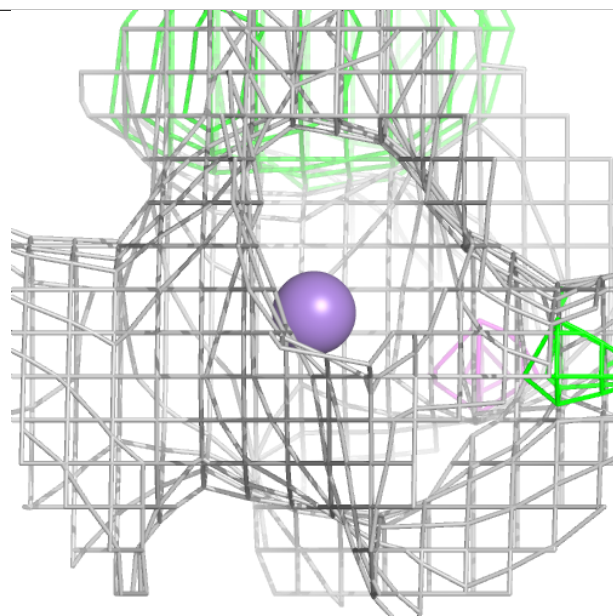
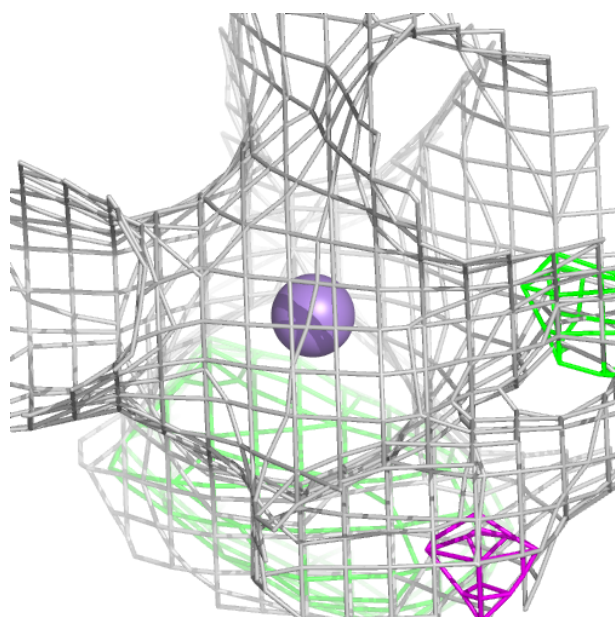
Electron density around MN A 401:

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



Electron density around MN C 402:

$2mF_o-DF_c$ (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.