



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:41 PM UTC

PDB ID : 7K3U / pdb_00007k3u
Title : X-ray crystallographic structure model of Lactococcus lactis prolidase mutant R293S
Authors : Xu, S.; Grochulski, P.; Tanaka, T.
Deposited on : 2020-09-13
Resolution : 2.70 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

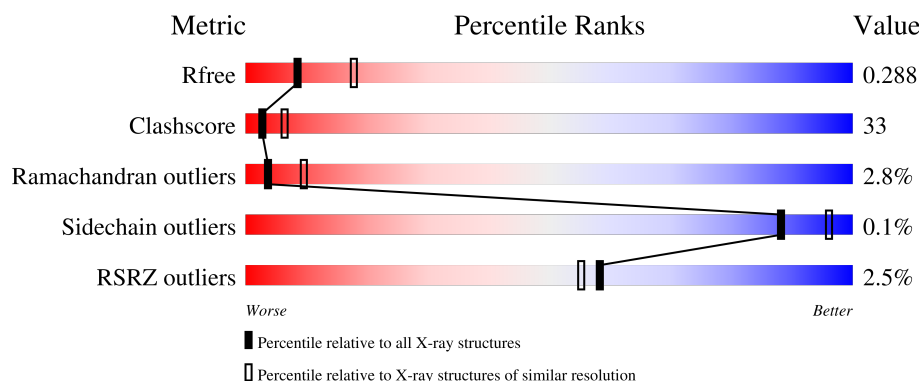
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	362	0.1% 59% 39% 0.1%
1	B	362	0.1% 73% 25% 0.1%
1	C	362	2% 60% 38% 0.1%
1	D	362	0.1% 51% 48% 0.1%
1	E	362	2% 47% 52% 0.1%

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Mol	Chain	Length	Quality of chain
1	F	362	 4% 51% 46% .
1	G	362	 2% 55% 42% .
1	H	362	 2% 48% 49% .
1	I	362	 5% 33% 62% .
1	J	362	 6% 40% 57% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28480 atoms, of which 40 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 Aminopeptidase P family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	B	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	C	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	D	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	E	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	F	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	G	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	H	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	I	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			
1	J	362	Total	C	N	O	S	0	0	0
			2801	1774	463	547	17			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	293	SER	ARG	engineered mutation	UNP A8WBX8
B	293	SER	ARG	engineered mutation	UNP A8WBX8
C	293	SER	ARG	engineered mutation	UNP A8WBX8
D	293	SER	ARG	engineered mutation	UNP A8WBX8
E	293	SER	ARG	engineered mutation	UNP A8WBX8
F	293	SER	ARG	engineered mutation	UNP A8WBX8
G	293	SER	ARG	engineered mutation	UNP A8WBX8
H	293	SER	ARG	engineered mutation	UNP A8WBX8
I	293	SER	ARG	engineered mutation	UNP A8WBX8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	293	SER	ARG	engineered mutation	UNP A8WBX8

- 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 2 2	0	0
2	B	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0
2	E	2	Total Mn 2 2	0	0
2	F	2	Total Mn 2 2	0	0
2	G	2	Total Mn 2 2	0	0
2	H	2	Total Mn 2 2	0	0
2	I	2	Total Mn 2 2	0	0
2	J	2	Total Mn 2 2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	G	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	B	88	Total	O	0	0
			88	88		
4	C	77	Total	O	0	0
			77	77		
4	D	38	Total	O	0	0
			38	38		
4	E	16	Total	O	0	0
			16	16		
4	F	35	Total	O	0	0
			35	35		
4	G	33	Total	O	0	0
			33	33		

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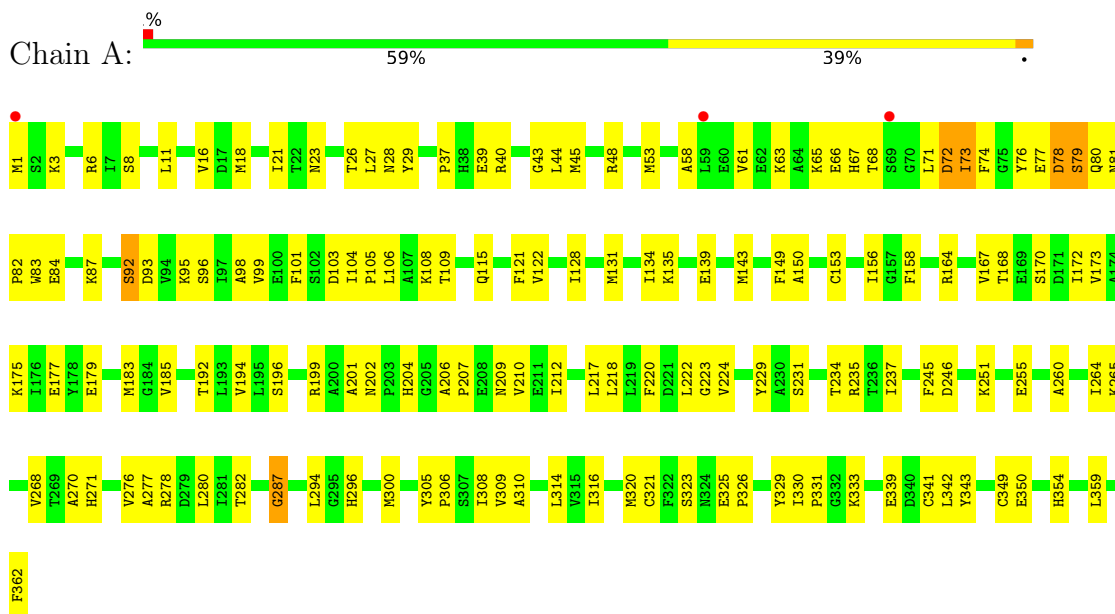
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	14	Total 14	O 14	0	0
4	I	15	Total 15	O 15	0	0
4	J	26	Total 26	O 26	0	0

3 Residue-property plots

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: Aminopeptidase P family protein

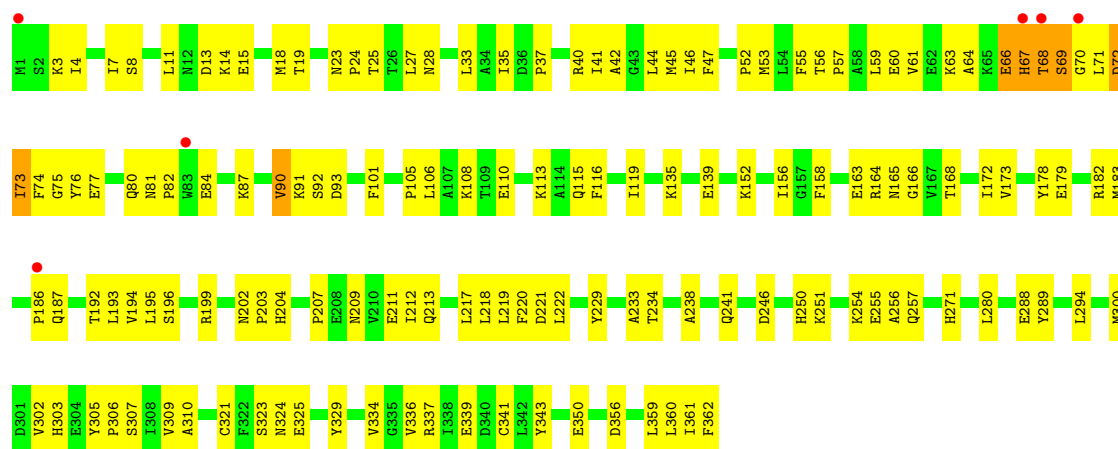


• Molecule 1: Aminopeptidase P family protein

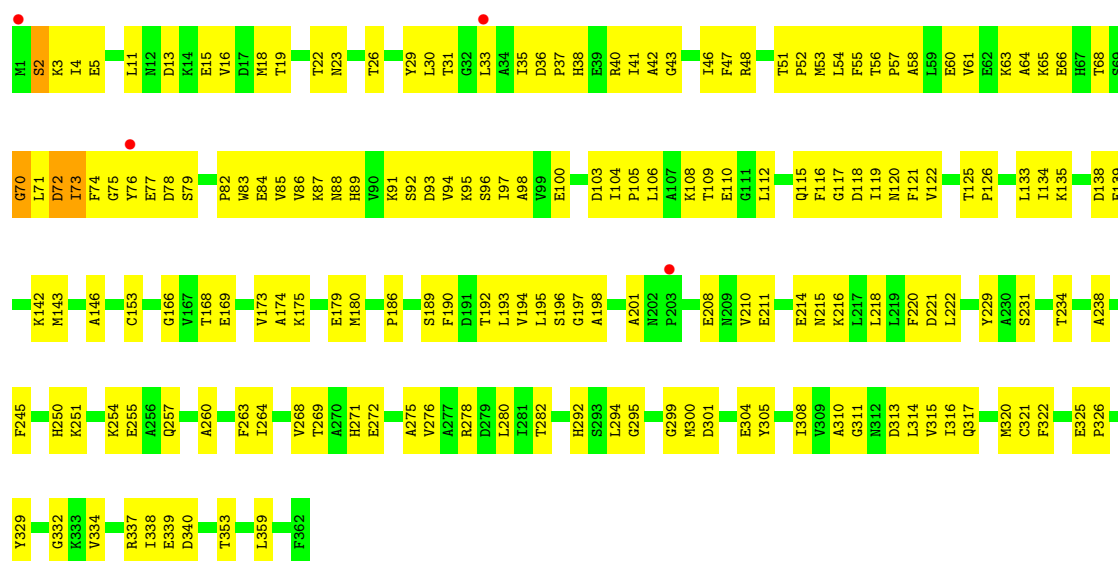


• Molecule 1: Aminopeptidase P family protein

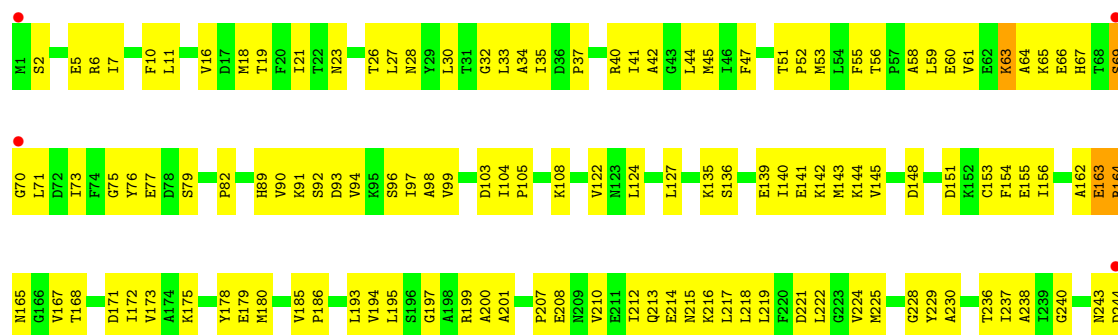


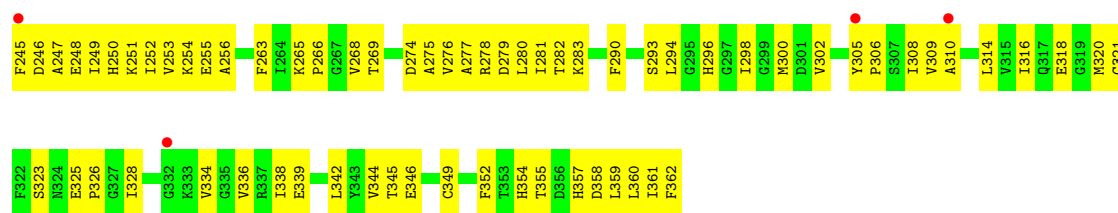


• Molecule 1: Aminopeptidase P family protein

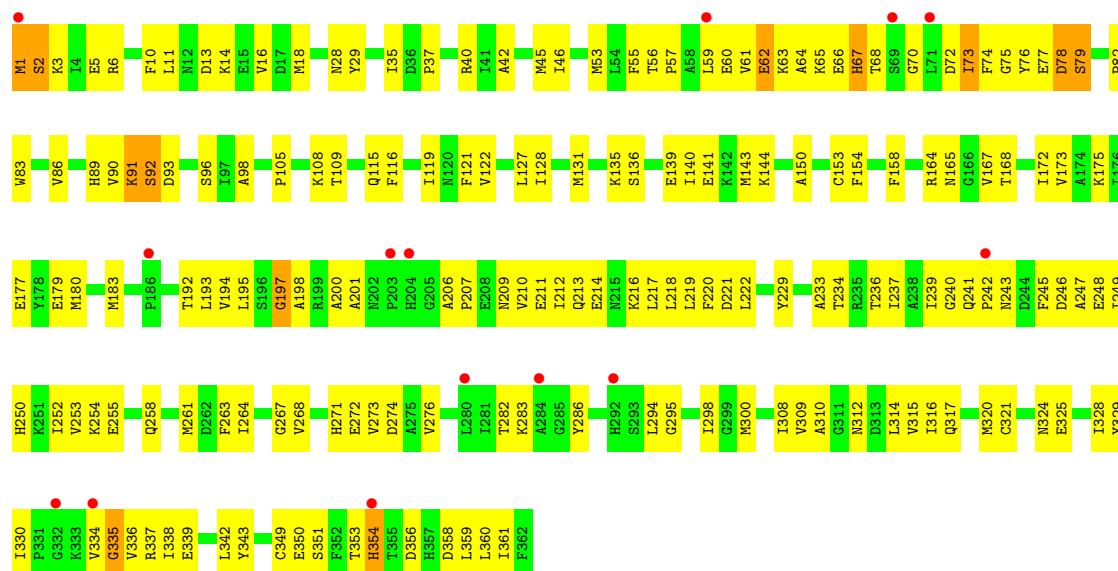


• Molecule 1: Aminopeptidase P family protein

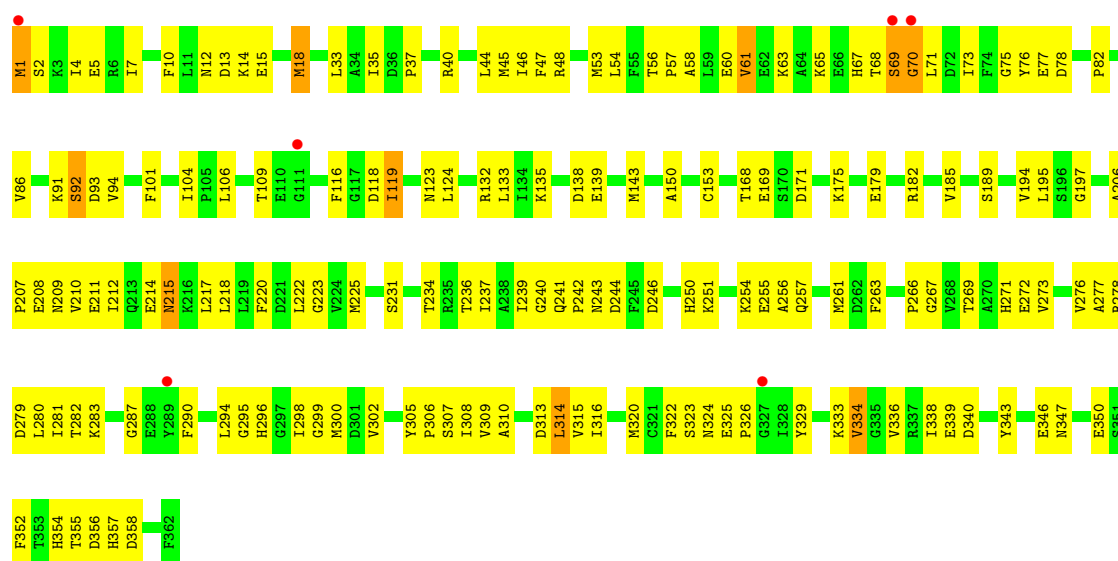




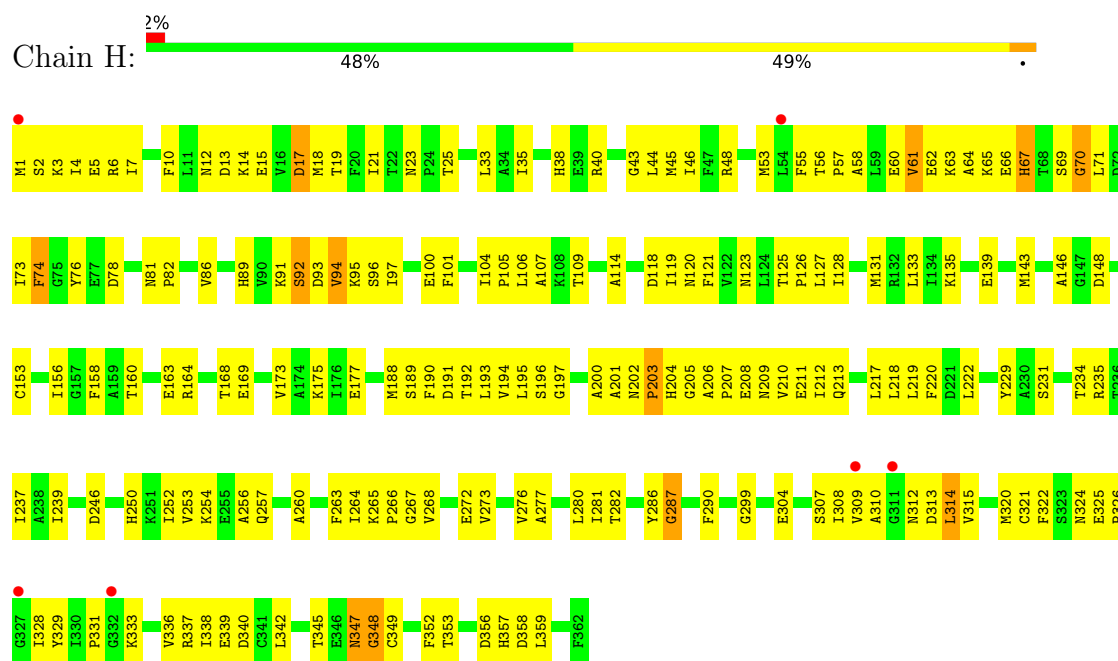
• Molecule 1: Aminopeptidase P family protein



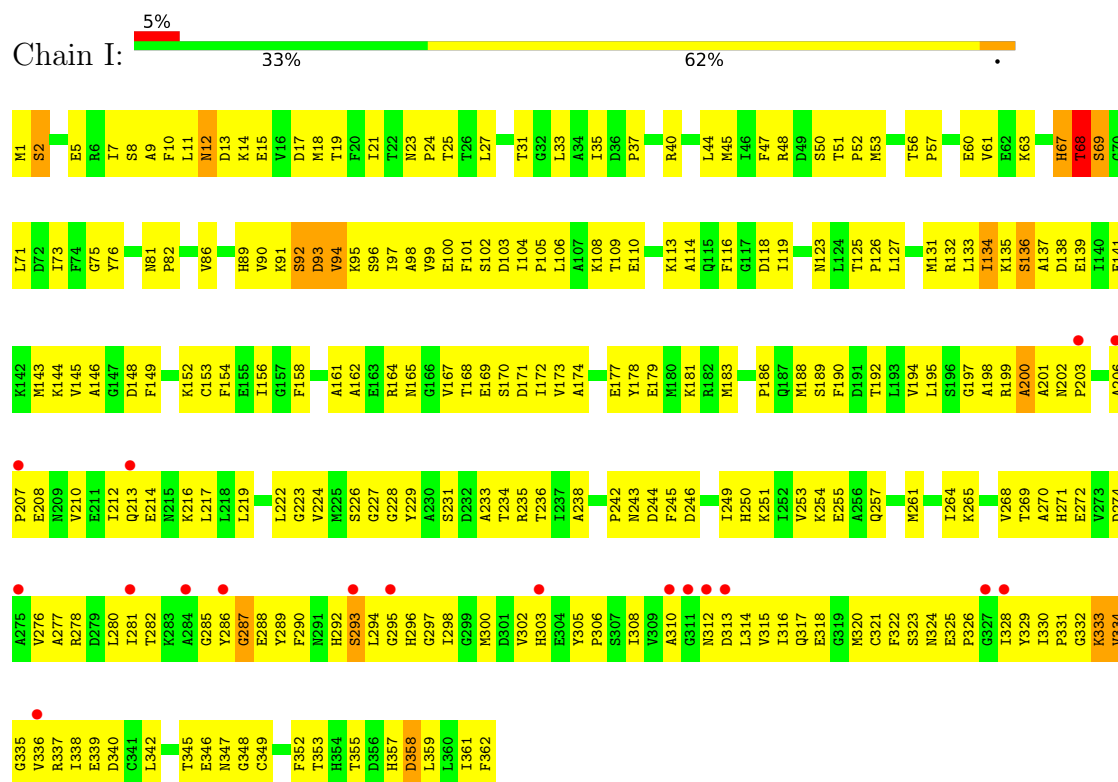
• Molecule 1: Aminopeptidase P family protein



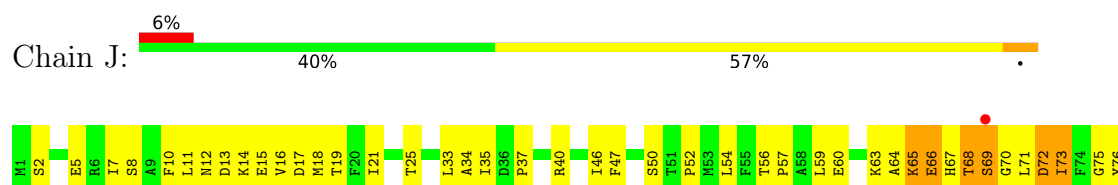
• Molecule 1: Aminopeptidase P family protein



• Molecule 1: Aminopeptidase P family protein



• Molecule 1: Aminopeptidase P family protein



E77	D78	P82	V86	V90	K91	V94	K95	S96	I97	A98	V99	E100	F101	I104	P105	K108	T109	F116	I119	N120	F121	V122	N123	L124	L127	M131	E132	L133	I134	K135	S136	E139	A146	F149	K152	I156	T160	A161	A162	E163	R164	N165	G166													
V167	T168	E169	S170	D171	I172	V173	A174	K175	Y178	E179	M180	K181	M182	P186	Q187	M188	L193	V194	L195	S196	G197	R199	A200	A201	N202	P203	H204	G205	P207	E208	N209	V210	E211	I212	L217	L218	L219	F220	D221	L222	G223	V224	N225	G227	G228	Y229	A230	S231	D232	A233	T234					
E235	T236	I237	A238	Q241	P242	N243	D244	F245	D246	A247	E248	I249	H250	K251	L252	V253	K254	E255	A256	Q257	Q258	A259	A260	F263	P266	G267	V268	T269	A270	H271	E272	V273	D274	A275	V276	A277	R278	D279	L280	T281	T282	K283	A284	G285	Y286	G287	E288	Y289	F290	N291	H292	S293	L294	G295	H296	G297
I298	G299	M300	D301	V302	H303	E304	Y305	P306	V309	A310	G311	N312	D313	L314	V315	I316	G319	M320	C321	F322	S323	N324	E325	P326	G327	I328	Y329	I330	P331	G332	K333	V334	G335	V336	R337	I338	E339	D340	C341	V344	T345	E346	N347	G348	C349	E350	T353	H357	D358	L359	L360	I361	F362			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	146.30Å 80.00Å 187.15Å 90.00° 102.03° 90.00°	Depositor
Resolution (Å)	49.19 – 2.70 49.19 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.19-2.70) 94.7 (49.19-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.198 , 0.288 0.203 , 0.288	Depositor DCC
R_{free} test set	5831 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28480	wwPDB-VP
Average B, all atoms (Å ²)	65.0	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 48.35 % 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 8.7153e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, GOL

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	0.39	0/2856	0.60	0/3864
1	B	0.51	0/2856	0.73	2/3864 (0.1%)
1	C	0.46	0/2856	0.67	0/3864
1	D	0.35	0/2856	0.58	0/3864
1	E	0.33	0/2856	0.56	0/3864
1	F	0.41	0/2856	0.70	7/3864 (0.2%)
1	G	0.41	0/2856	0.66	2/3864 (0.1%)
1	H	0.34	0/2856	0.58	0/3864
1	I	0.36	0/2856	0.60	6/3864 (0.2%)
1	J	0.41	1/2856 (0.0%)	0.62	0/3864
All	All	0.40	1/28560 (0.0%)	0.63	17/38640 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	E	0	2
1	G	0	1
1	J	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	91	LYS	CB-CG	5.00	1.67	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1	MET	CB-CG-SD	-7.80	89.29	112.70
1	I	69	SER	N-CA-C	-7.38	95.09	110.80
1	F	70	GLY	CA-C-N	-6.61	109.77	121.87
1	F	70	GLY	C-N-CA	-6.61	109.77	121.87
1	I	68	THR	O-C-N	6.40	128.69	122.03

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	311	GLY	Peptide
1	B	93	ASP	Peptide
1	E	63	LYS	Peptide
1	E	65	LYS	Peptide
1	G	1	MET	Peptide

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	2801	0	2748	128	0
1	B	2801	0	2748	79	0
1	C	2801	0	2748	143	0
1	D	2801	0	2748	174	0
1	E	2801	0	2748	190	0
1	F	2801	0	2748	224	0
1	G	2801	0	2748	172	0
1	H	2801	0	2748	199	1
1	I	2801	0	2748	288	1
1	J	2801	0	2748	267	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
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	2	0	0	0	0
2	J	2	0	0	0	0
3	A	6	8	8	0	0
3	B	6	8	8	0	0
3	C	6	8	7	0	0
3	D	6	8	8	0	0
3	G	6	8	8	1	0
4	A	38	0	0	6	1
4	B	88	0	0	0	0
4	C	77	0	0	5	0
4	D	38	0	0	5	0
4	E	16	0	0	4	1
4	F	35	0	0	1	0
4	G	33	0	0	3	0
4	H	14	0	0	2	0
4	I	15	0	0	8	0
4	J	26	0	0	5	0
All	All	28440	40	27519	1842	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 33.

The worst 5 of 1842 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:E:70:GLY:O	1:E:71:LEU:HD22	1.12	1.24
1:H:196:SER:HB2	1:H:218:LEU:CD1	1.71	1.19
1:I:282:THR:HG23	1:I:287:GLY:N	1.61	1.15
1:H:53:MET:HE1	1:H:89:HIS:HB3	1.28	1.13
1:J:16:VAL:HG13	1:J:96:SER:HB3	1.27	1.13

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	Interatomic distance (Å)	Clash overlap (Å)
4:A:536:HOH:O	4:E:511:HOH:O[2_455]	0.49	1.71
1:H:358:ASP:OD1	1:I:68:THR:OG1[2_355]	2.02	0.18

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	360/362 (99%)	338 (94%)	16 (4%)	6 (2%)	7	19
1	B	360/362 (99%)	337 (94%)	15 (4%)	8 (2%)	5	14
1	C	360/362 (99%)	323 (90%)	29 (8%)	8 (2%)	5	14
1	D	360/362 (99%)	321 (89%)	32 (9%)	7 (2%)	6	17
1	E	360/362 (99%)	318 (88%)	38 (11%)	4 (1%)	11	29
1	F	360/362 (99%)	306 (85%)	43 (12%)	11 (3%)	3	8
1	G	360/362 (99%)	317 (88%)	33 (9%)	10 (3%)	4	9
1	H	360/362 (99%)	300 (83%)	47 (13%)	13 (4%)	2	6
1	I	360/362 (99%)	304 (84%)	38 (11%)	18 (5%)	1	3
1	J	360/362 (99%)	307 (85%)	36 (10%)	17 (5%)	2	3
All	All	3600/3620 (99%)	3171 (88%)	327 (9%)	102 (3%)	4	9

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ASP
1	B	66	GLU
1	B	68	THR
1	B	72	ASP
1	B	93	ASP

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	303/303 (100%)	303 (100%)	0	100	100
1	B	303/303 (100%)	303 (100%)	0	100	100
1	C	303/303 (100%)	303 (100%)	0	100	100
1	D	303/303 (100%)	303 (100%)	0	100	100
1	E	303/303 (100%)	303 (100%)	0	100	100
1	F	303/303 (100%)	303 (100%)	0	100	100
1	G	303/303 (100%)	303 (100%)	0	100	100
1	H	303/303 (100%)	302 (100%)	1 (0%)	86	94
1	I	303/303 (100%)	301 (99%)	2 (1%)	76	90
1	J	303/303 (100%)	303 (100%)	0	100	100
All	All	3030/3030 (100%)	3027 (100%)	3 (0%)	88	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	148	ASP
1	I	67	HIS
1	I	68	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	347	ASN
1	H	291	ASN
1	H	202	ASN
1	H	292	HIS
1	D	80	GLN

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 25 ligands modelled in this entry, 20 are monoatomic - leaving 5 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	$\# Z > 2$
3	GOL	D	403	-	5,5,5	0.91	0	5,5,5	0.72	0
3	GOL	B	403	-	5,5,5	1.00	0	5,5,5	1.41	1 (20%)
3	GOL	G	403	-	5,5,5	0.98	0	5,5,5	0.94	0
3	GOL	C	403	-	5,5,5	1.72	2 (40%)	5,5,5	2.14	1 (20%)
3	GOL	A	403	-	5,5,5	1.25	0	5,5,5	1.10	1 (20%)

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	GOL	D	403	-	-	0/4/4/4	-
3	GOL	B	403	-	-	0/4/4/4	-
3	GOL	G	403	-	-	0/4/4/4	-
3	GOL	C	403	-	-	0/4/4/4	-
3	GOL	A	403	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	GOL	O2-C2	-2.59	1.35	1.43
3	C	403	GOL	C1-C2	2.32	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	GOL	C3-C2-C1	-4.30	96.04	111.80
3	B	403	GOL	C3-C2-C1	-2.67	102.01	111.80
3	A	403	GOL	C3-C2-C1	-2.22	103.65	111.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	GOL	O1-C1-C2-O2
3	A	403	GOL	O1-C1-C2-C3
3	A	403	GOL	C1-C2-C3-O3
3	A	403	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	403	GOL	1	0

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	362/362 (100%)	-0.21	3 (0%) 82 81	41, 58, 93, 137	0
1	B	362/362 (100%)	-0.57	5 (1%) 73 72	27, 35, 68, 115	0
1	C	362/362 (100%)	-0.40	6 (1%) 69 67	28, 45, 90, 180	0
1	D	362/362 (100%)	-0.09	4 (1%) 78 76	38, 60, 111, 158	0
1	E	362/362 (100%)	0.12	8 (2%) 62 59	43, 73, 108, 145	0
1	F	362/362 (100%)	0.09	14 (3%) 43 39	34, 65, 115, 160	0
1	G	362/362 (100%)	-0.23	6 (1%) 69 67	34, 56, 91, 169	0
1	H	362/362 (100%)	0.09	6 (1%) 69 67	49, 72, 104, 143	0
1	I	362/362 (100%)	0.35	18 (4%) 34 30	52, 85, 123, 157	0
1	J	362/362 (100%)	0.18	22 (6%) 27 24	38, 68, 119, 159	0
All	All	3620/3620 (100%)	-0.07	92 (2%) 58 55	27, 63, 109, 180	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	71	LEU	6.3
1	J	311	GLY	5.0
1	J	335	GLY	4.5
1	J	203	PRO	4.2
1	B	69	SER	4.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

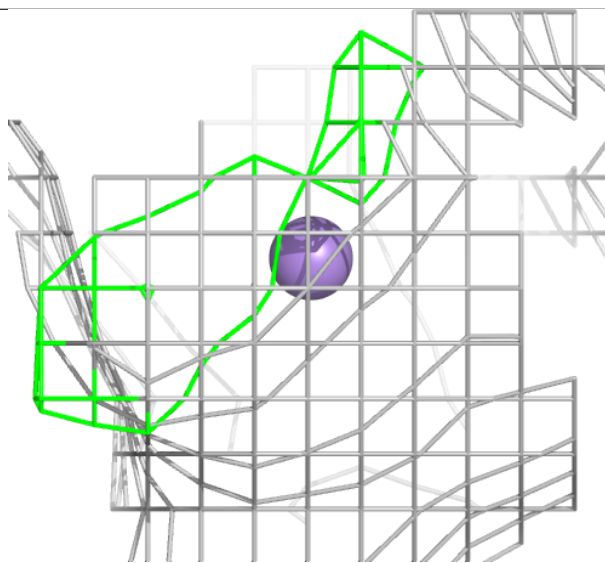
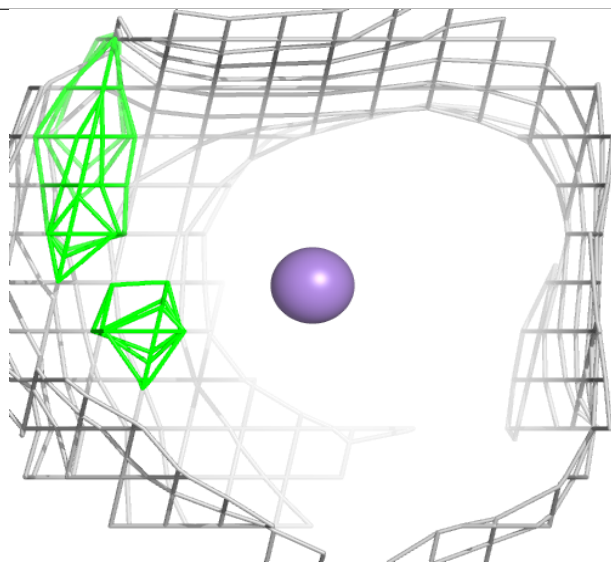
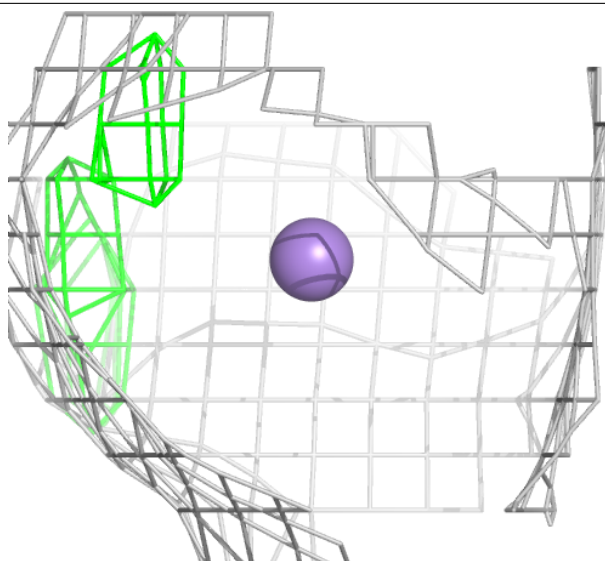
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	D	403	6/6	0.86	0.10	56,74,89,89	0
3	GOL	G	403	6/6	0.88	0.12	91,109,123,124	0
3	GOL	C	403	6/6	0.89	0.10	49,66,87,105	0
3	GOL	A	403	6/6	0.92	0.09	45,68,87,87	0
3	GOL	B	403	6/6	0.95	0.10	44,57,80,96	0
2	MN	E	401	1/1	0.96	0.05	69,69,69,69	0
2	MN	D	401	1/1	0.96	0.08	59,59,59,59	0
2	MN	G	402	1/1	0.97	0.06	44,44,44,44	0
2	MN	A	402	1/1	0.97	0.11	58,58,58,58	0
2	MN	J	402	1/1	0.98	0.05	64,64,64,64	0
2	MN	D	402	1/1	0.98	0.03	34,34,34,34	0
2	MN	C	401	1/1	0.98	0.04	42,42,42,42	0
2	MN	E	402	1/1	0.98	0.05	67,67,67,67	0
2	MN	G	401	1/1	0.98	0.04	40,40,40,40	0
2	MN	A	401	1/1	0.98	0.06	53,53,53,53	0
2	MN	H	402	1/1	0.99	0.08	72,72,72,72	0
2	MN	I	401	1/1	0.99	0.02	79,79,79,79	0
2	MN	I	402	1/1	0.99	0.03	78,78,78,78	0
2	MN	J	401	1/1	0.99	0.03	63,63,63,63	0
2	MN	B	402	1/1	0.99	0.02	33,33,33,33	0
2	MN	F	401	1/1	0.99	0.04	69,69,69,69	0
2	MN	F	402	1/1	0.99	0.07	62,62,62,62	0
2	MN	B	401	1/1	0.99	0.03	30,30,30,30	0
2	MN	C	402	1/1	0.99	0.05	35,35,35,35	0
2	MN	H	401	1/1	0.99	0.10	71,71,71,71	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.

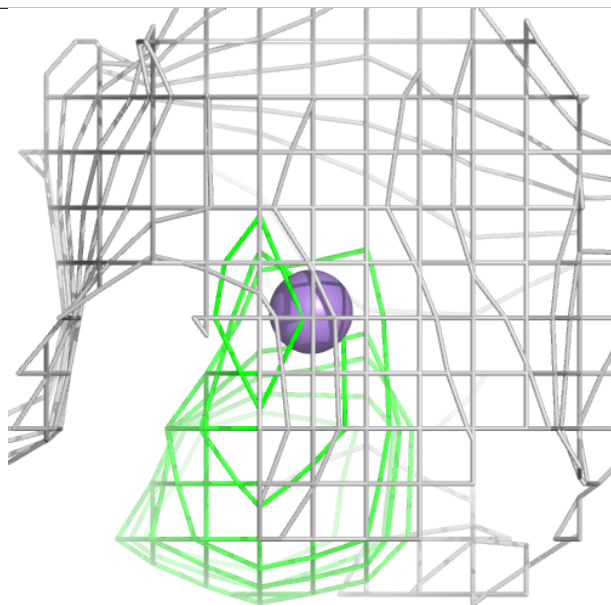
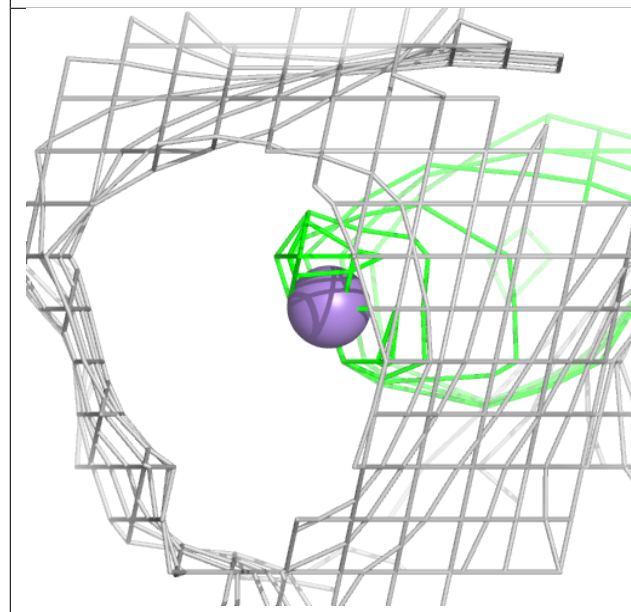
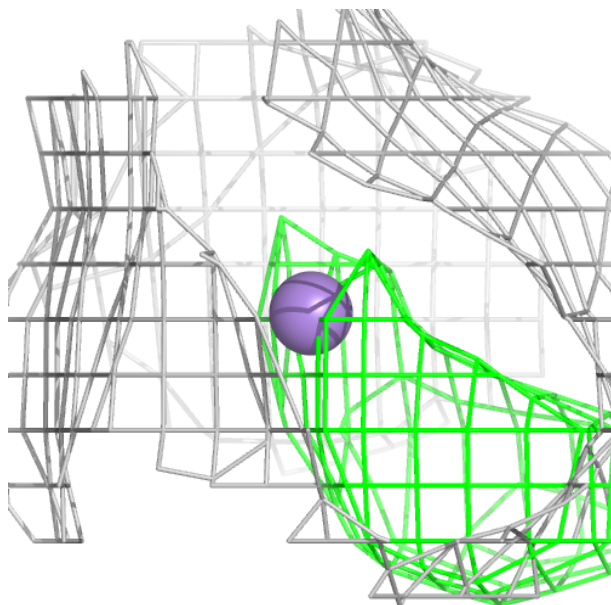
Electron density around MN E 401:

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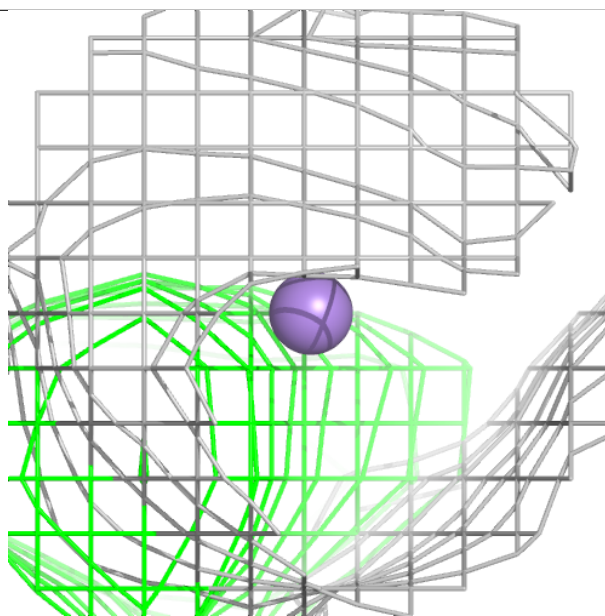
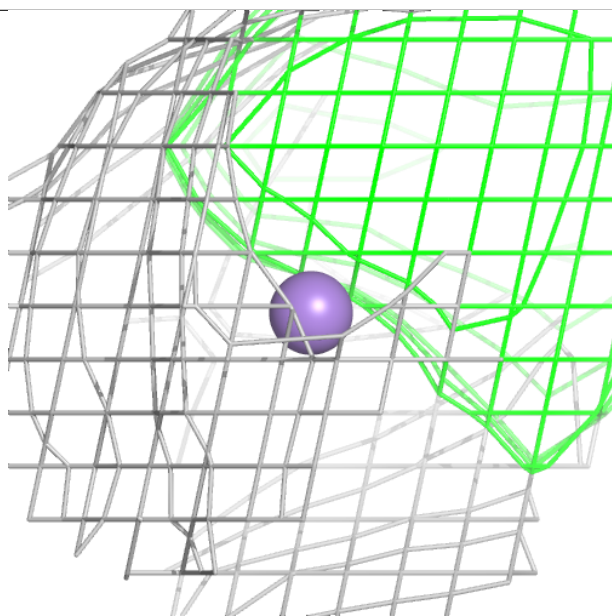
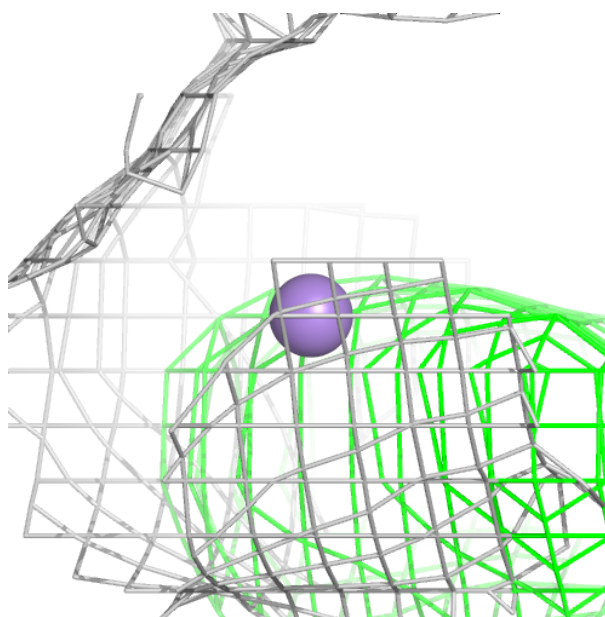
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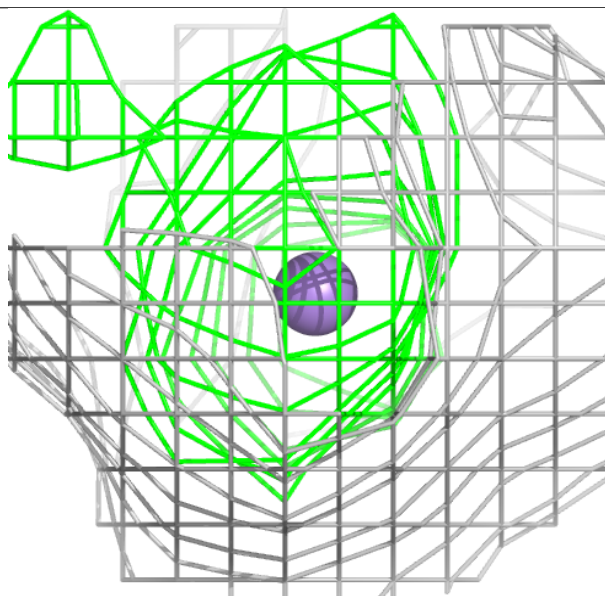
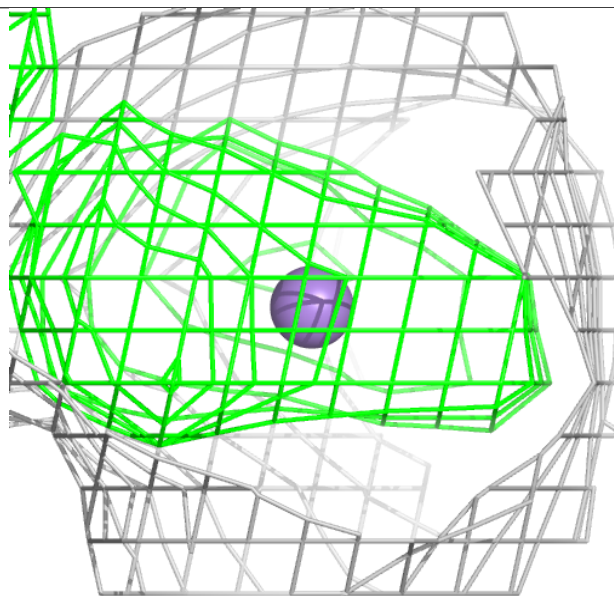
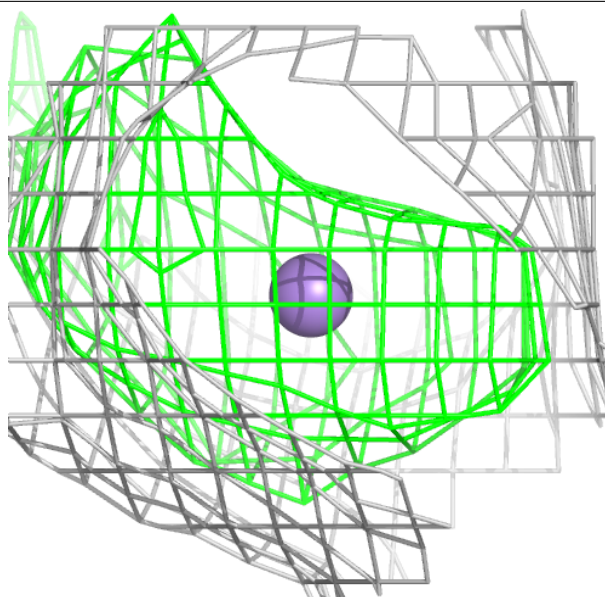
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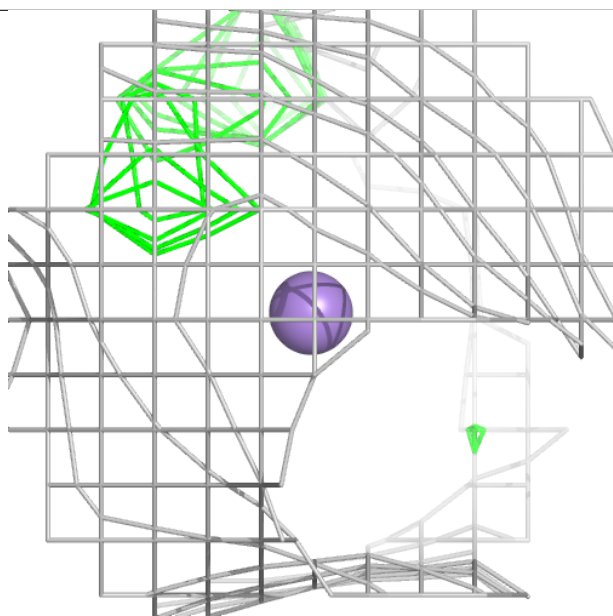
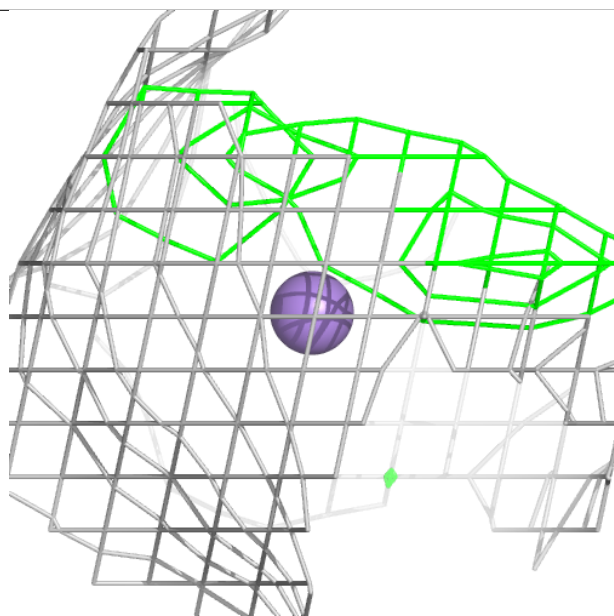
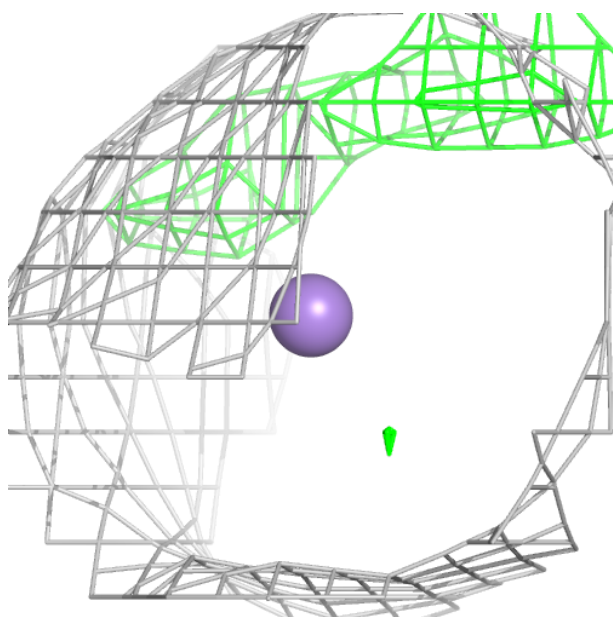
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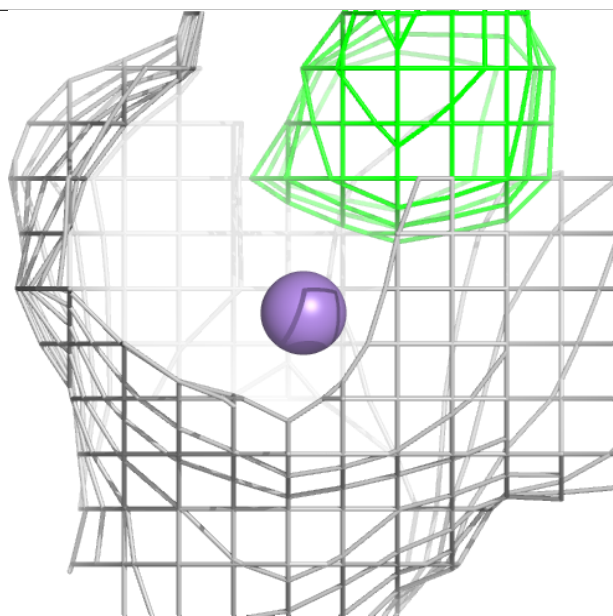
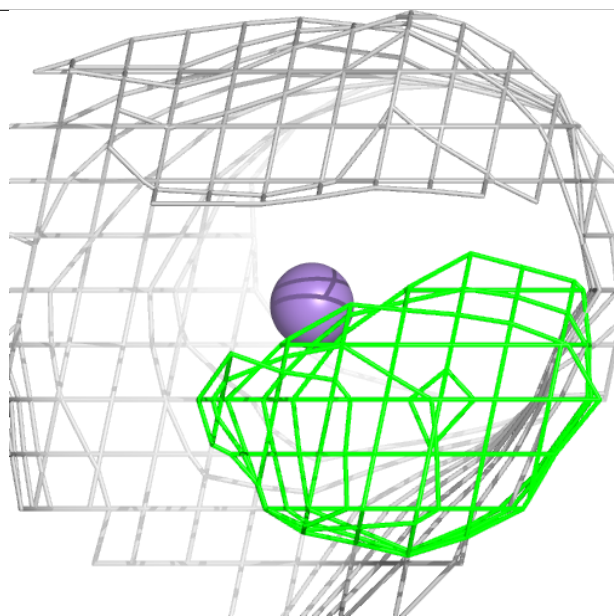
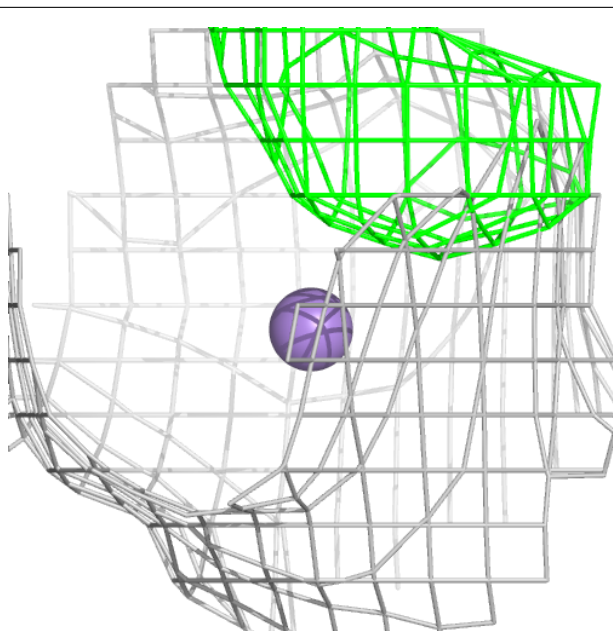
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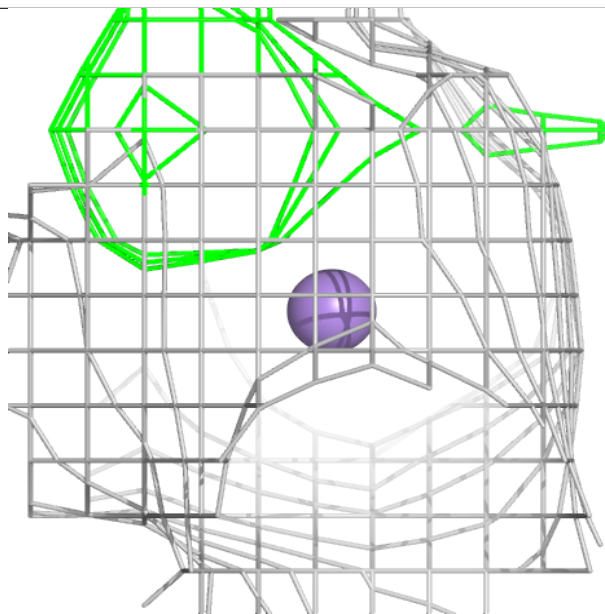
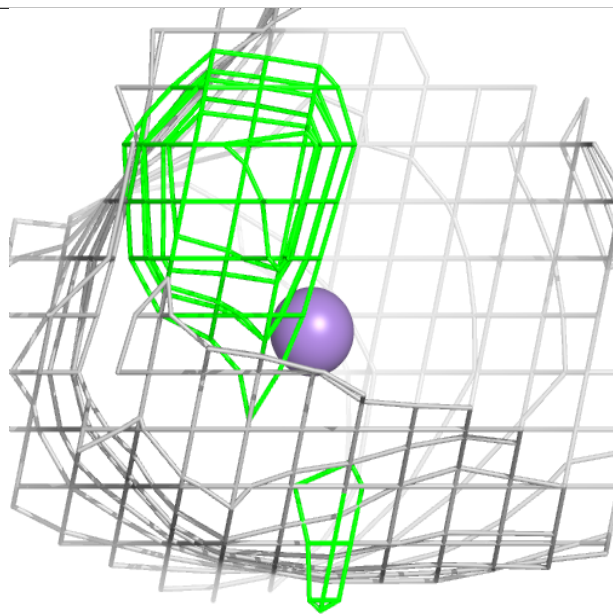
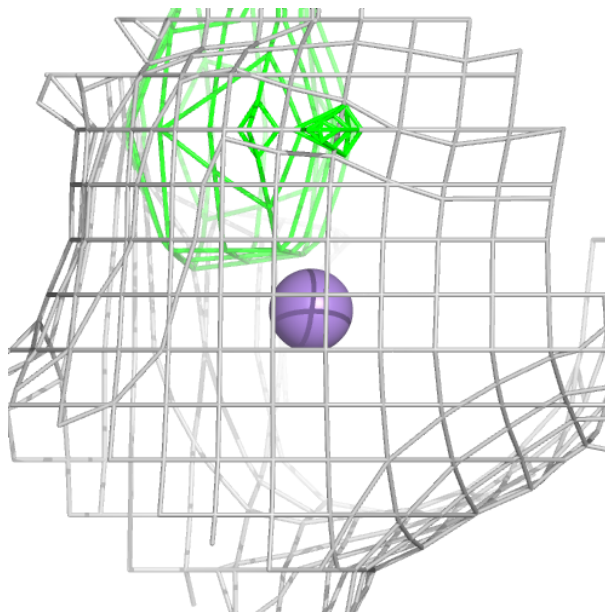
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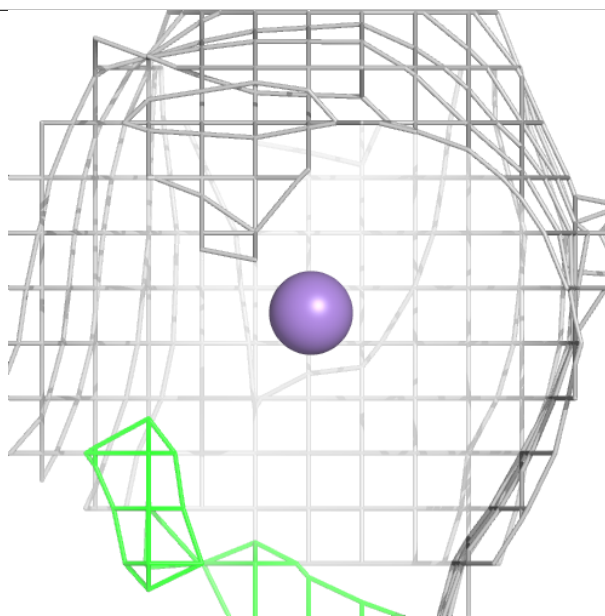
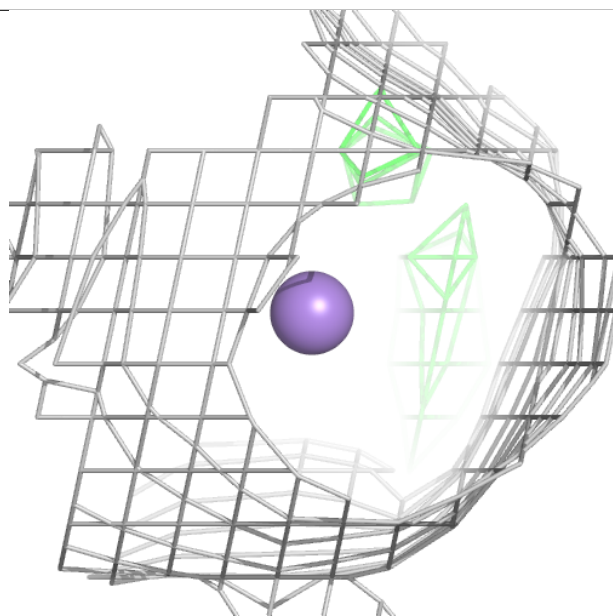
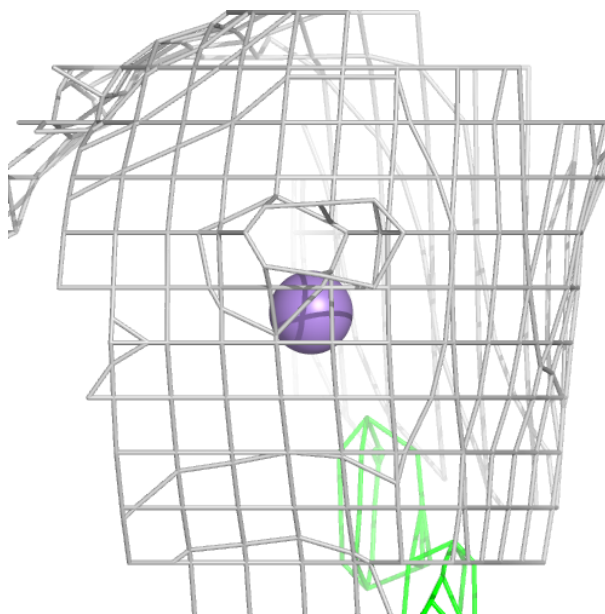
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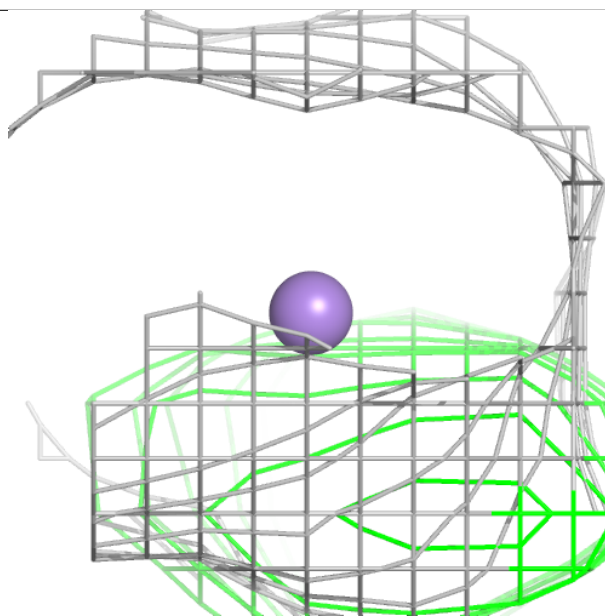
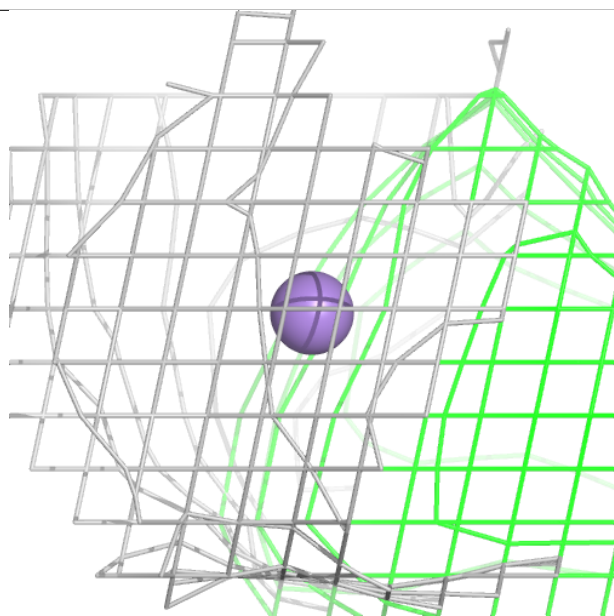
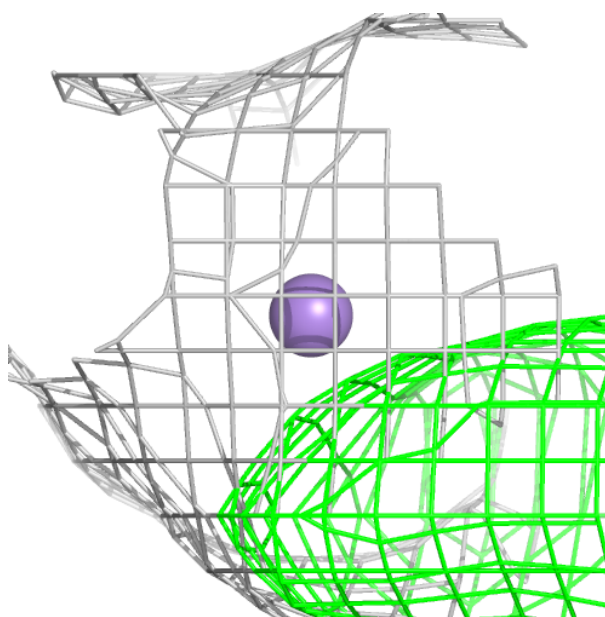
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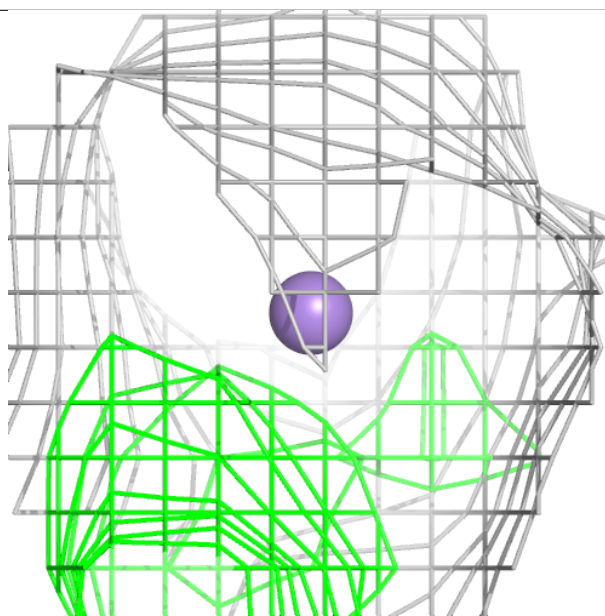
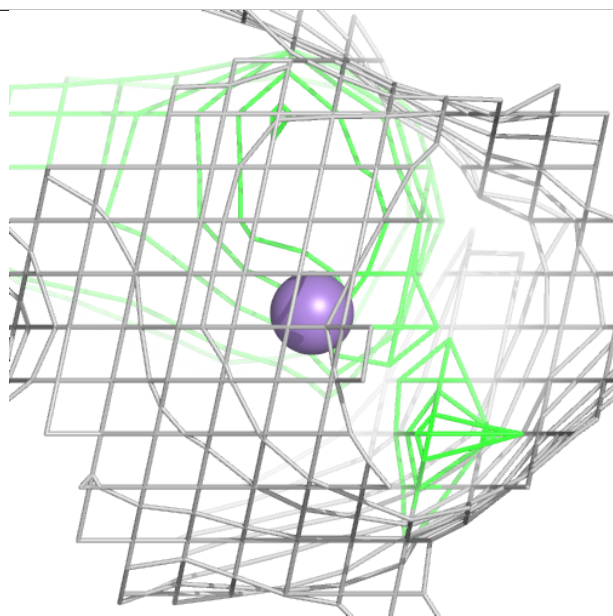
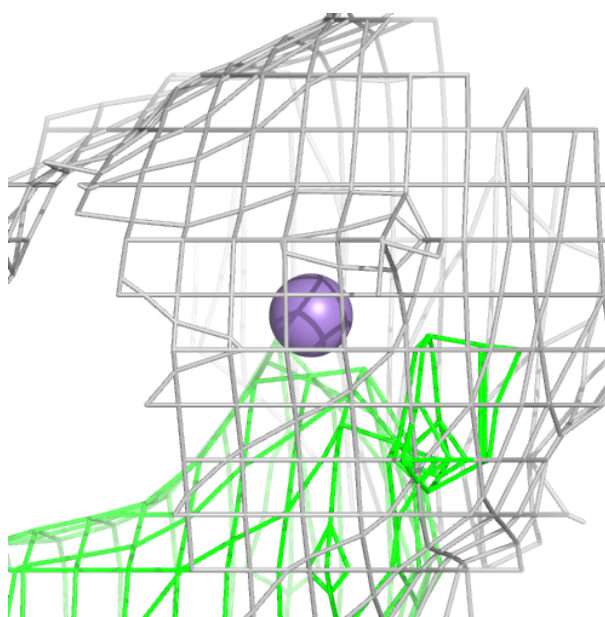
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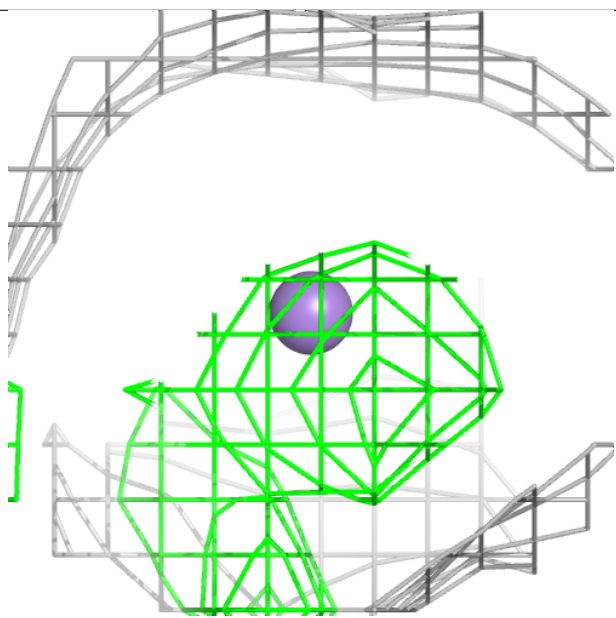
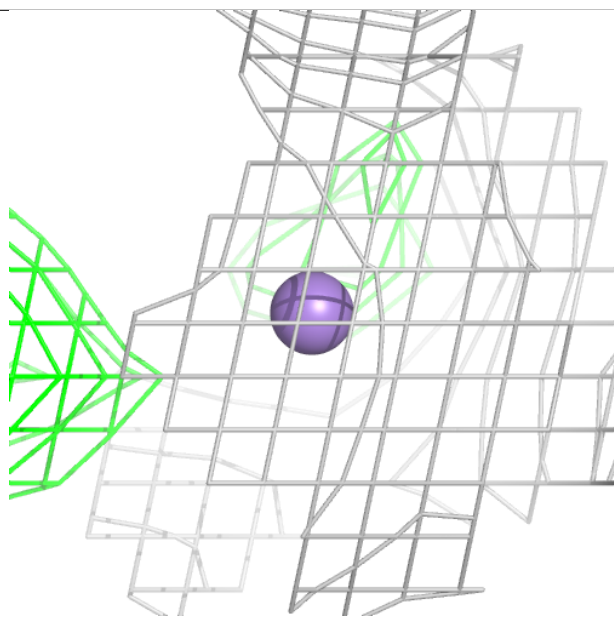
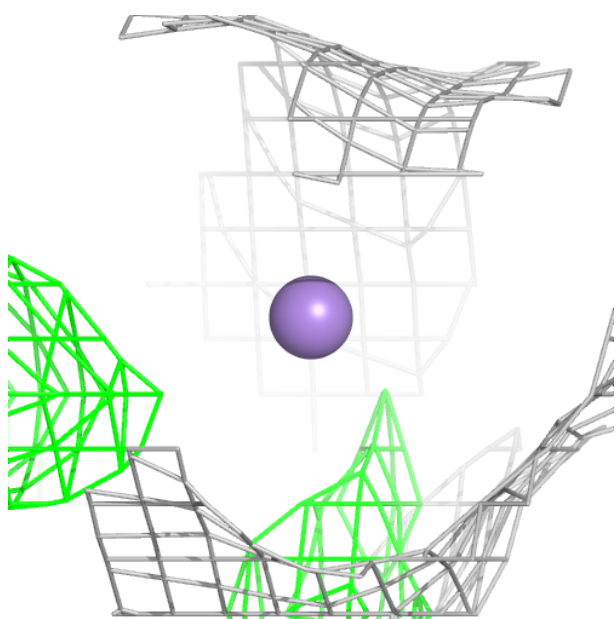
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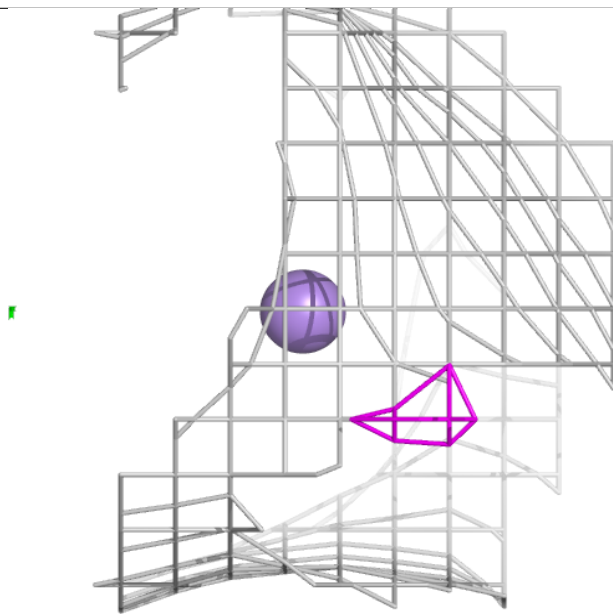
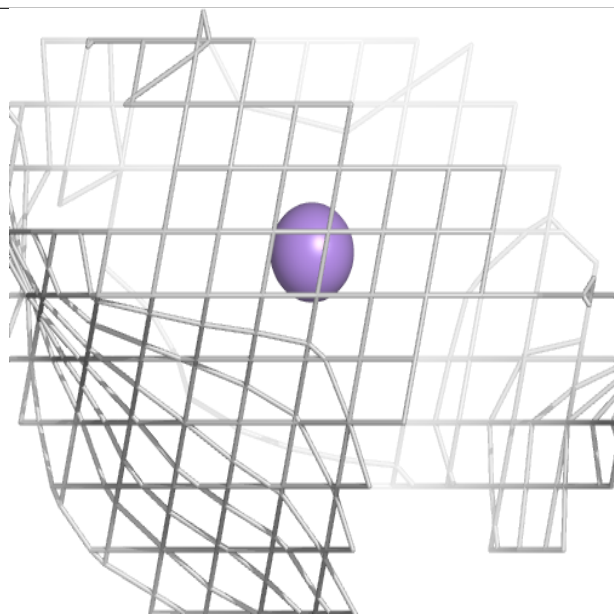
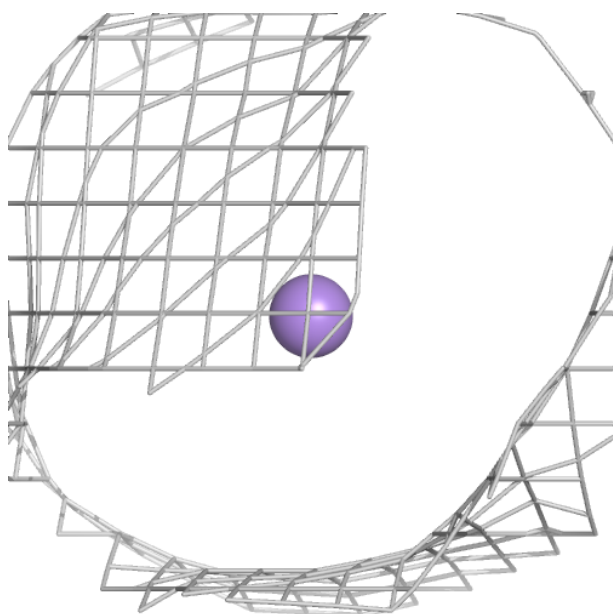
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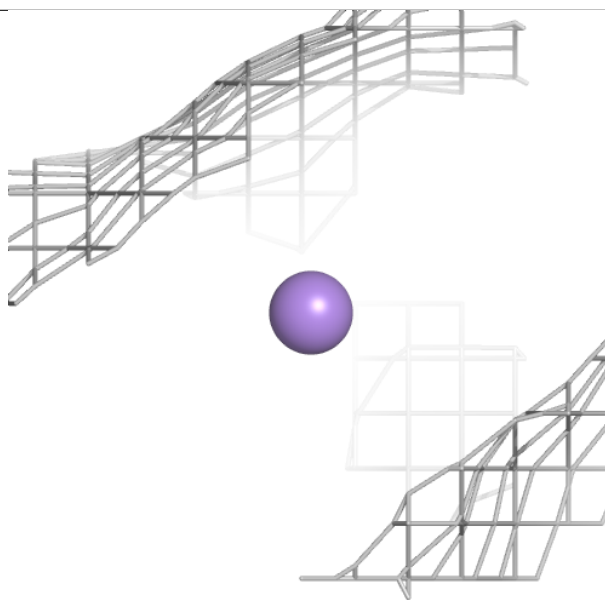
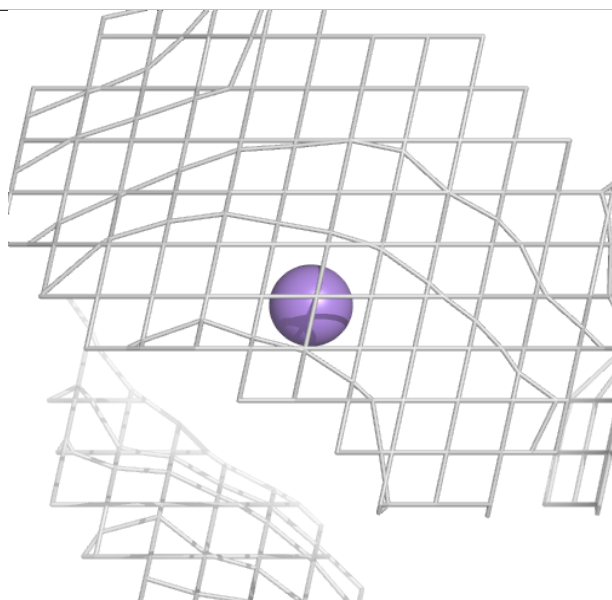
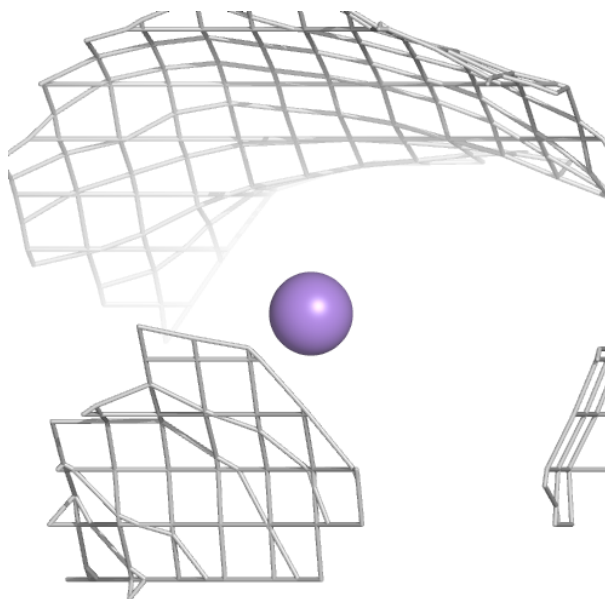
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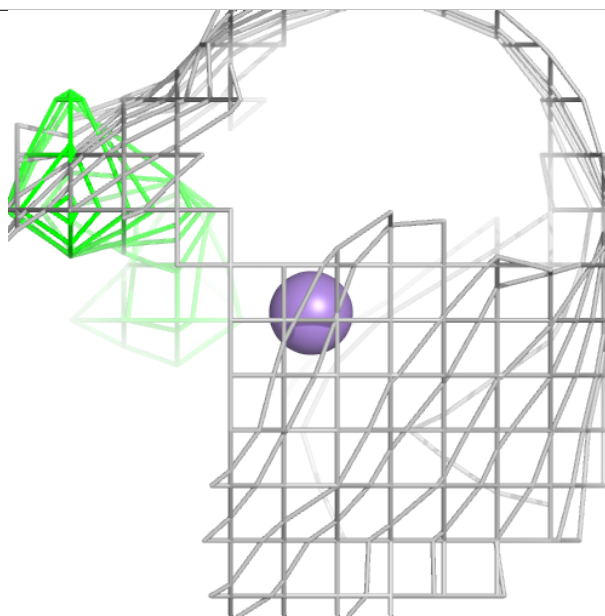
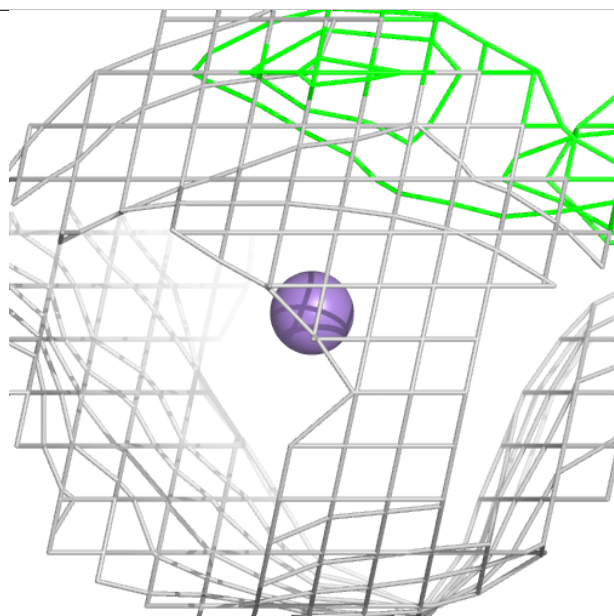
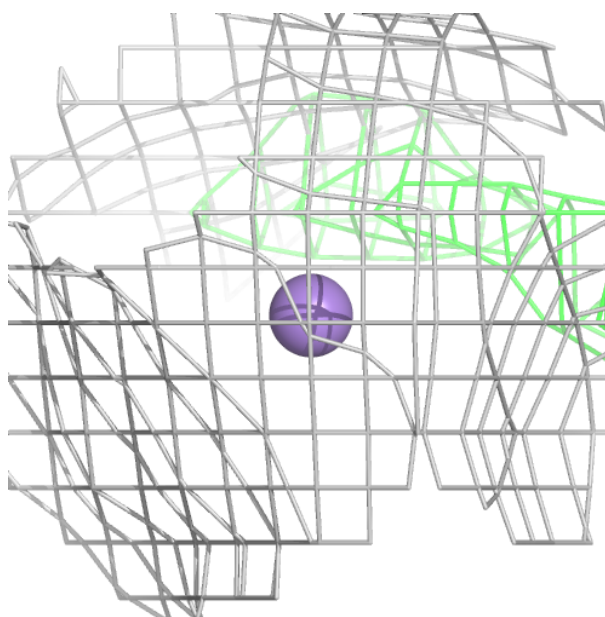
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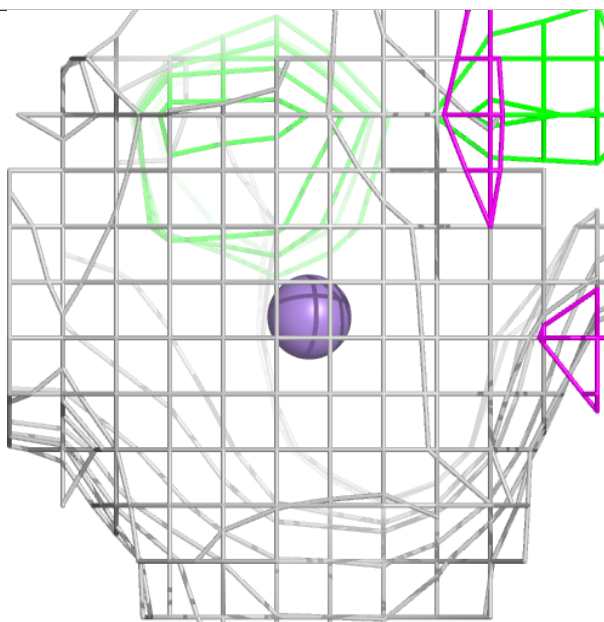
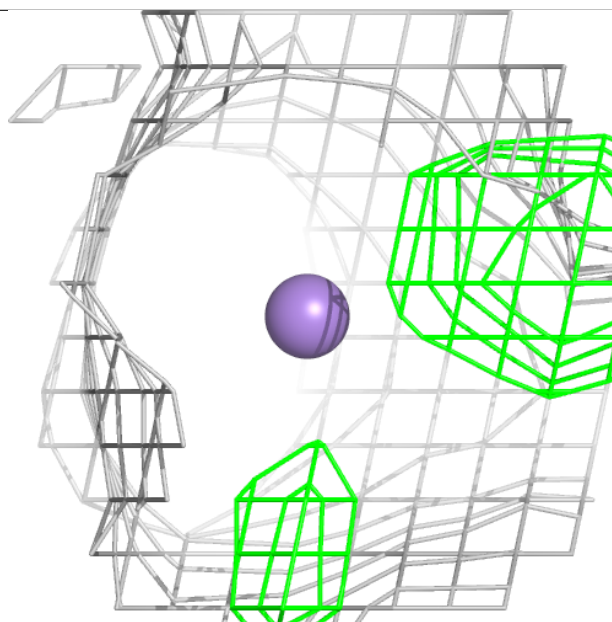
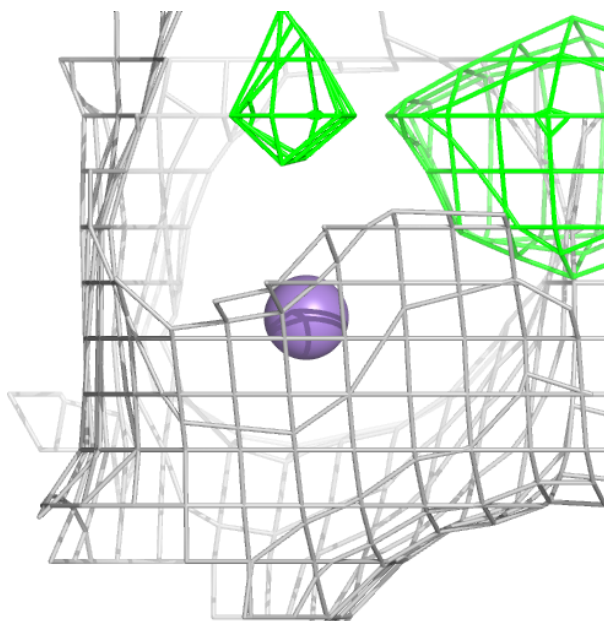
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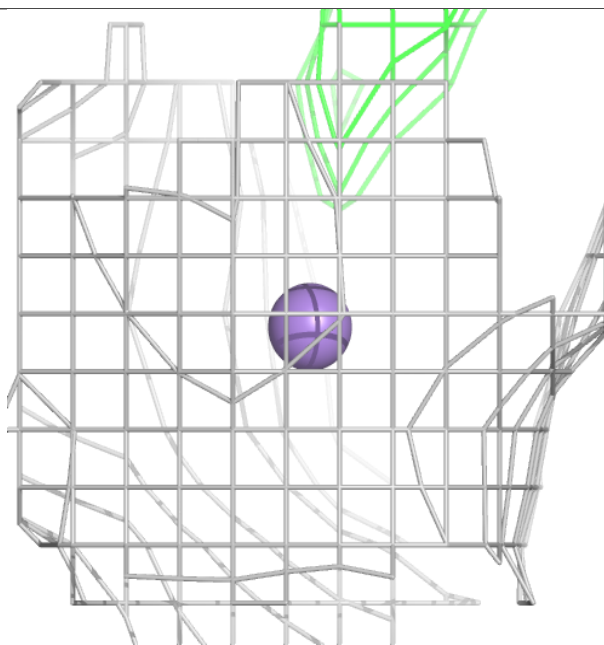
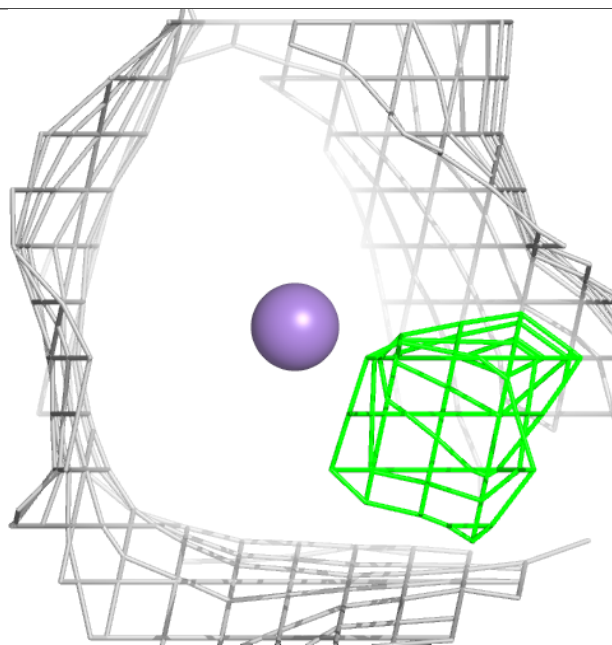
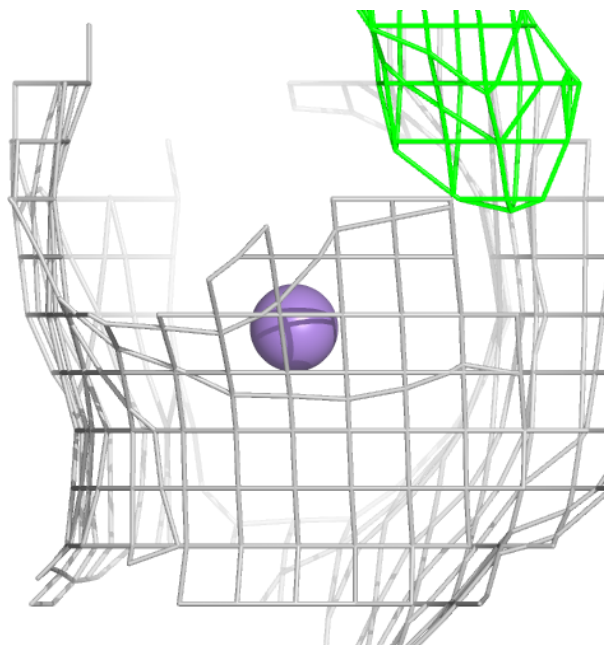
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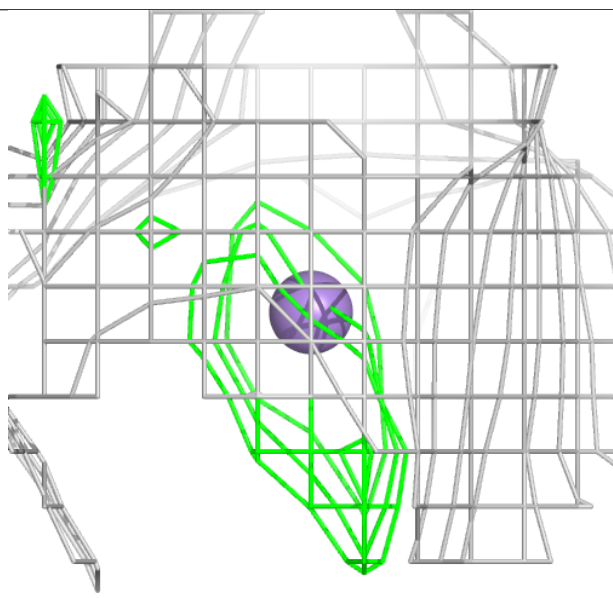
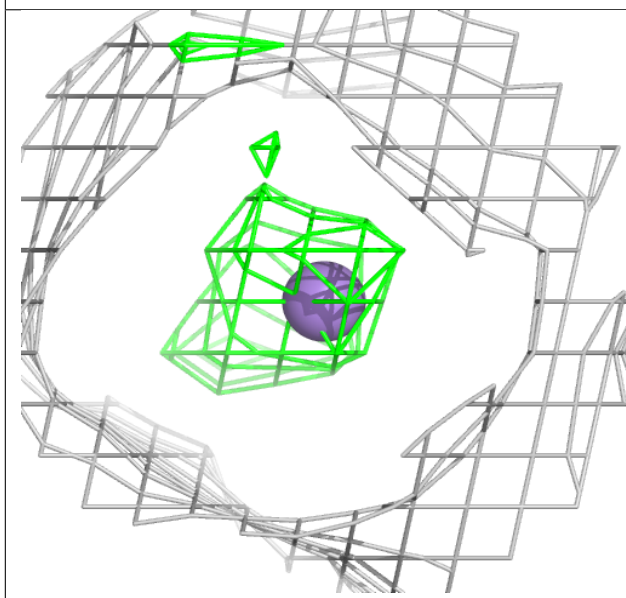
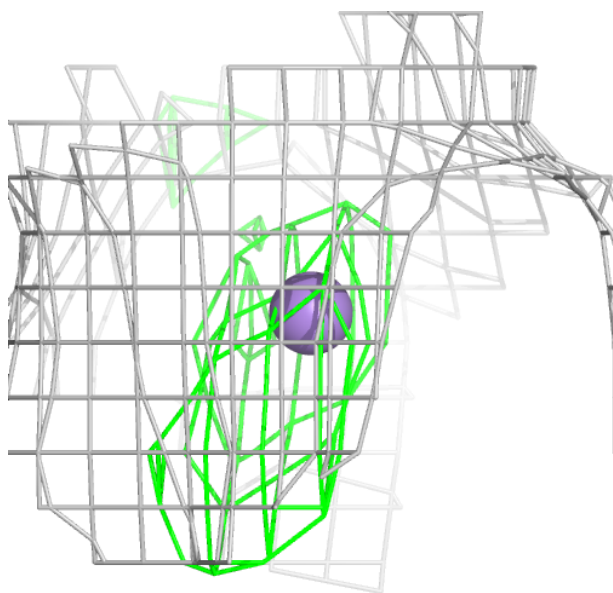
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and green (positive)



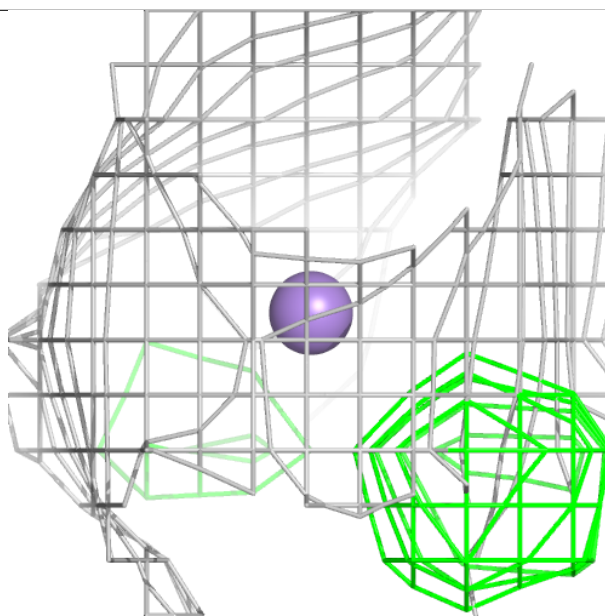
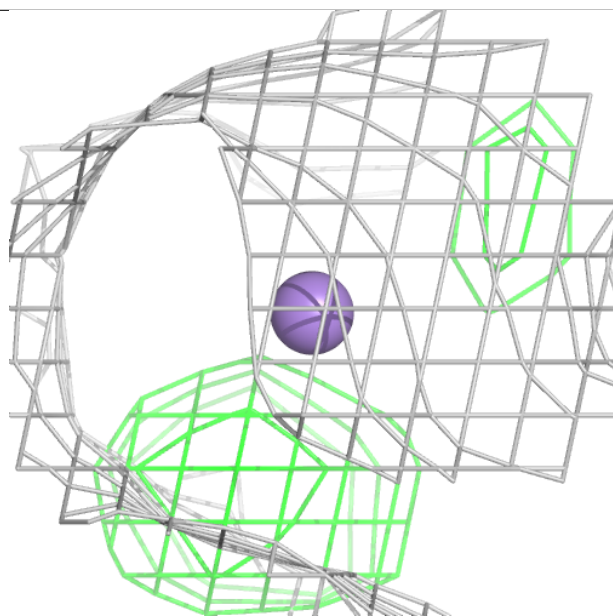
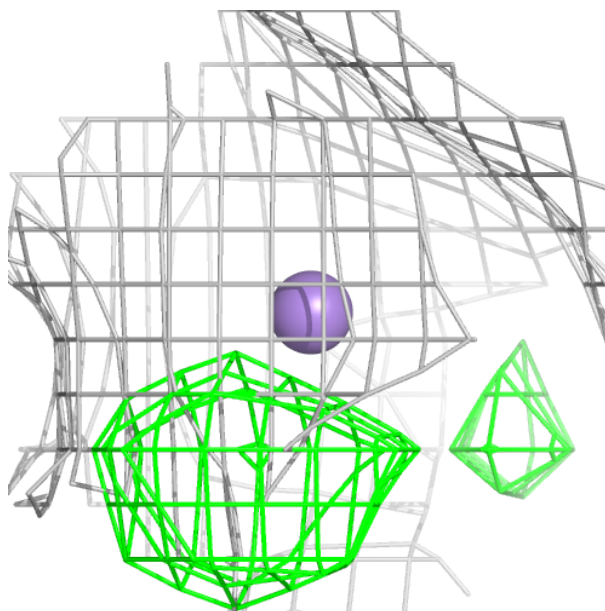
Electron density around MN F 402:

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



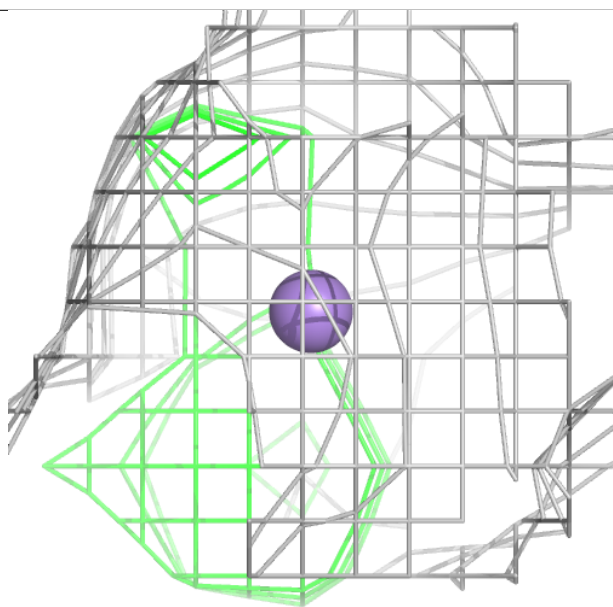
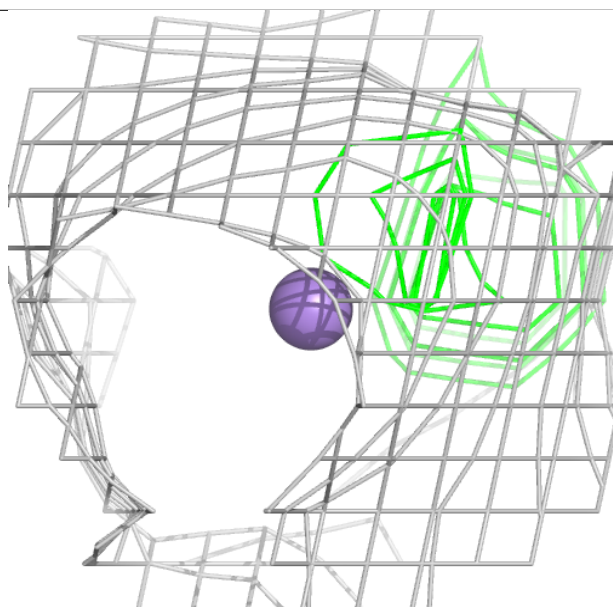
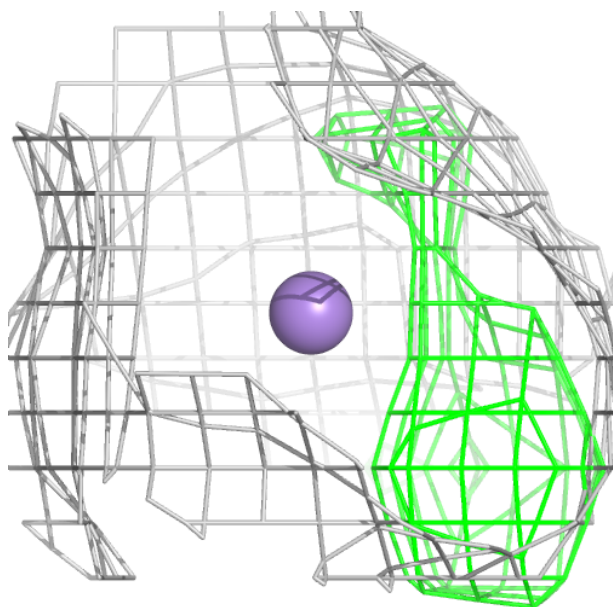
Electron density around MN B 401:

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



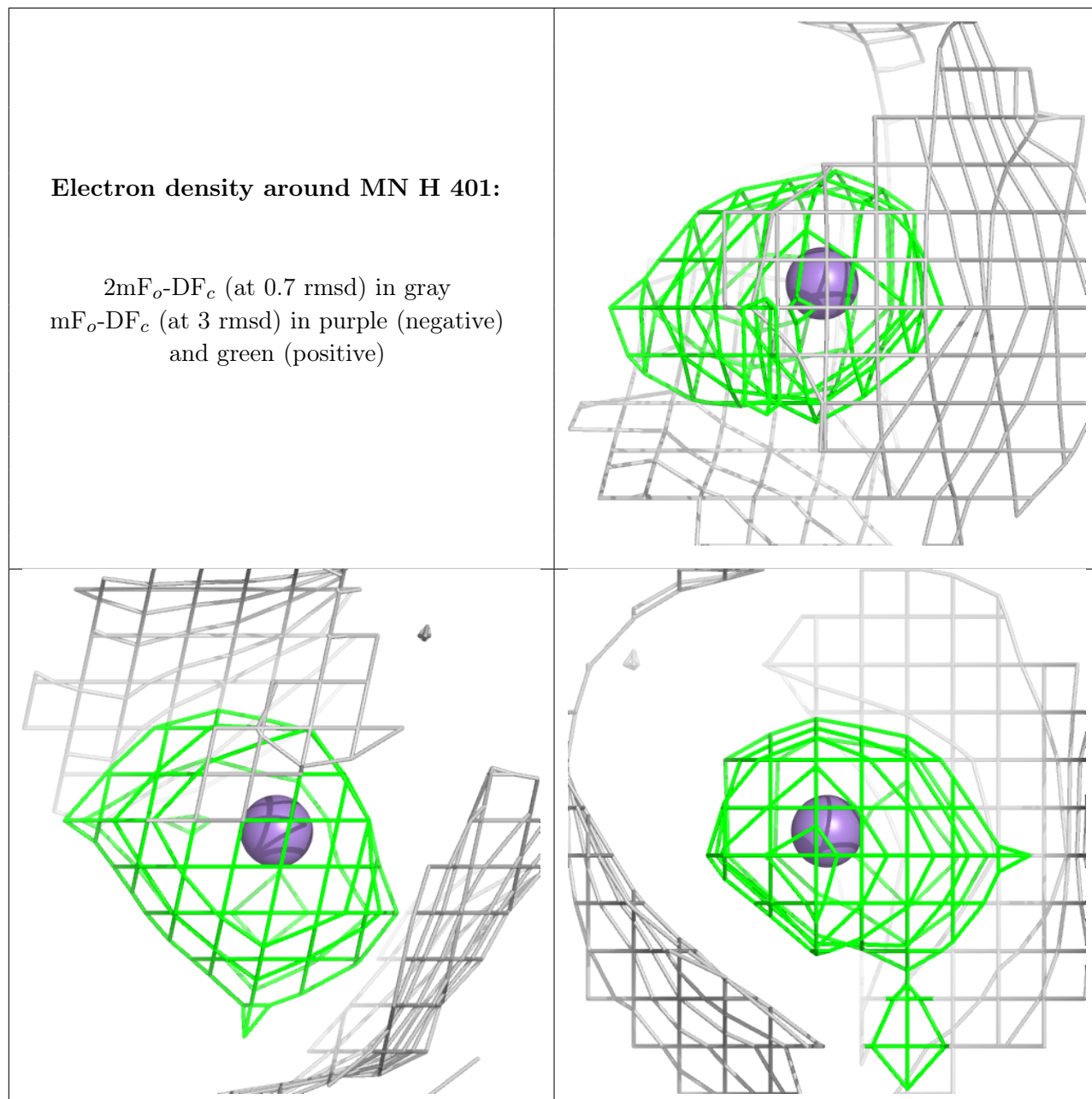
Electron density around MN C 402:

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



Electron density around MN H 401:

$2mF_o-DF_c$ (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.