



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:57 AM UTC

PDB ID : 8FFD / pdb\_00008ffd  
Title : Crystal structure of manganese bound Dps protein (PA0962) from *Pseudomonas aeruginosa* (cubic form)  
Authors : Lovell, S.; Seibold, S.; Battaile, K.P.; Rivera, M.  
Deposited on : 2022-12-08  
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](mailto: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>.

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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

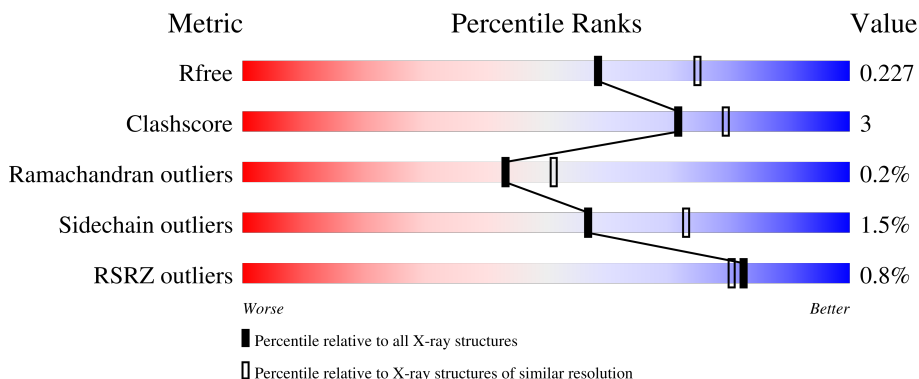
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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  $\geq 3$ , 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	156	
1	B	156	
1	C	156	
1	D	156	
1	E	156	

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Mol	Chain	Length	Quality of chain
1	F	156	<p>2% 89% 10% ..</p>
1	G	156	<p>2% 90% 10%</p>
1	H	156	<p>% 92% 8% .</p>
1	I	156	<p>93% 6% ..</p>
1	J	156	<p>89% 10% .</p>
1	K	156	<p>% 94% 5% ..</p>
1	L	156	<p>2% 89% 9% ..</p>
1	M	156	<p>92% 7% .</p>
1	N	156	<p>% 91% 8% .</p>
1	O	156	<p>% 92% 6% ..</p>
1	P	156	<p>% 88% 11% .</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21641 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.

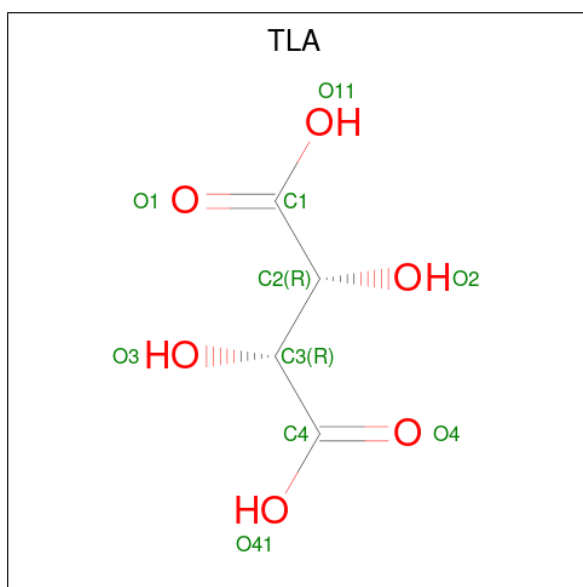
- Molecule 1 is a protein called Probable dna-binding stress protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	155	1216	773	211	226	6	0	2	0
1	B	156	1235	783	213	233	6	0	2	0
1	C	155	1217	774	210	227	6	0	2	0
1	D	155	1217	775	212	224	6	0	2	0
1	E	155	1216	773	211	226	6	0	2	0
1	F	155	1216	773	210	227	6	0	2	0
1	G	156	1223	776	211	230	6	0	2	0
1	H	156	1227	779	213	229	6	0	2	0
1	I	155	1223	777	212	228	6	0	2	0
1	J	155	1208	769	210	223	6	0	2	0
1	K	155	1217	772	211	228	6	0	2	0
1	L	155	1206	767	210	223	6	0	2	0
1	M	155	1223	777	212	228	6	0	2	0
1	N	155	1213	772	210	225	6	0	2	0
1	O	155	1224	778	212	228	6	0	2	0
1	P	156	1223	776	211	230	6	0	2	0

- 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	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0
2	G	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0
2	I	1	Total Mn 1 1	0	0
2	J	1	Total Mn 1 1	0	0
2	K	1	Total Mn 1 1	0	0
2	L	1	Total Mn 1 1	0	0
2	M	1	Total Mn 1 1	0	0
2	N	1	Total Mn 1 1	0	0
2	O	1	Total Mn 1 1	0	0
2	P	1	Total Mn 1 1	0	0

- Molecule 3 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 10 4 6	0	0
3	K	1	Total C O 10 4 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	123	Total O 123 123	0	0
4	B	171	Total O 171 171	0	0
4	C	114	Total O 114 114	0	0
4	D	143	Total O 143 143	0	0
4	E	133	Total O 133 133	0	0
4	F	101	Total O 101 101	0	0
4	G	114	Total O 114 114	0	0
4	H	171	Total O 171 171	0	0
4	I	162	Total O 162 162	0	0
4	J	113	Total O 113 113	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	K	130	Total 130	O 130	0	0
4	L	126	Total 126	O 126	0	0
4	M	164	Total 164	O 164	0	0
4	N	116	Total 116	O 116	0	0
4	O	114	Total 114	O 114	0	0
4	P	106	Total 106	O 106	0	0

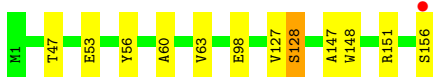
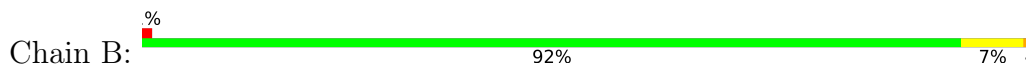
### 3 Residue-property plots [i](#)

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.

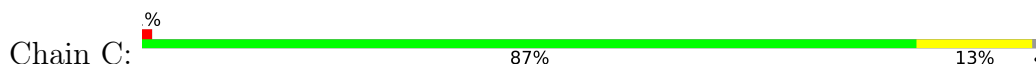
- Molecule 1: Probable dna-binding stress protein



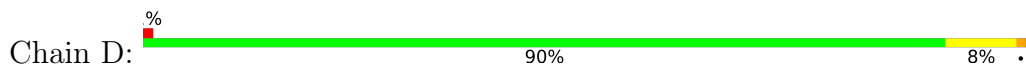
- Molecule 1: Probable dna-binding stress protein



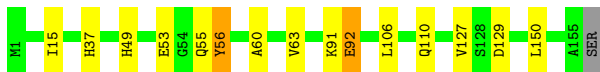
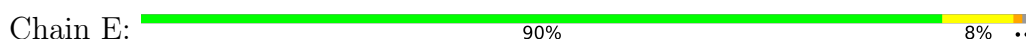
- Molecule 1: Probable dna-binding stress protein



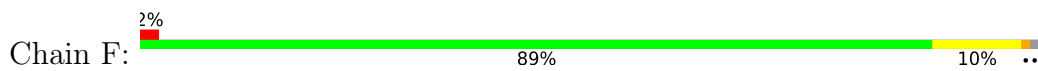
- Molecule 1: Probable dna-binding stress protein



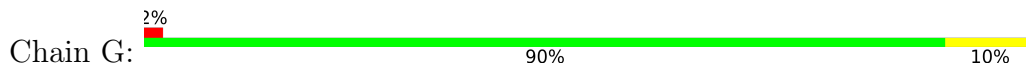
- Molecule 1: Probable dna-binding stress protein



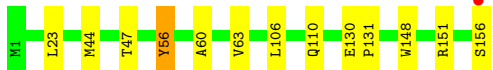
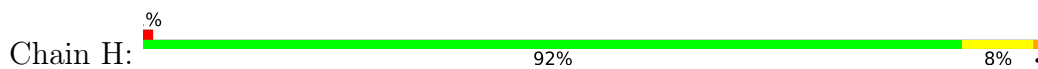
- Molecule 1: Probable dna-binding stress protein



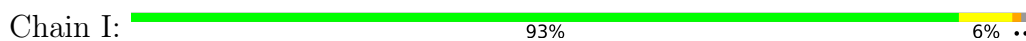
- Molecule 1: Probable dna-binding stress protein



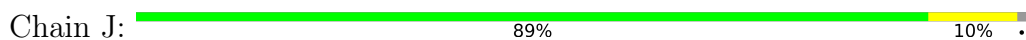
- Molecule 1: Probable dna-binding stress protein



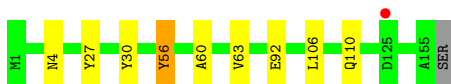
- Molecule 1: Probable dna-binding stress protein



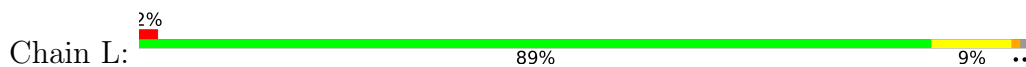
- Molecule 1: Probable dna-binding stress protein



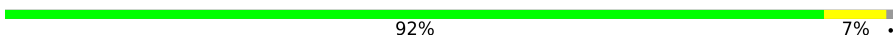
- Molecule 1: Probable dna-binding stress protein



- Molecule 1: Probable dna-binding stress protein

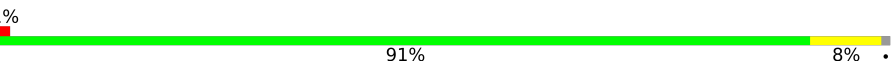


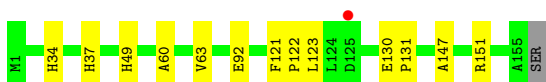
- Molecule 1: Probable dna-binding stress protein

Chain M:  92% 7%

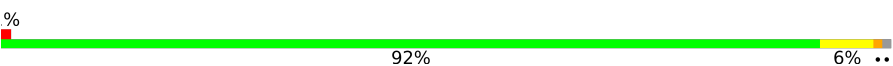


- Molecule 1: Probable dna-binding stress protein

Chain N:  91% 8%




- Molecule 1: Probable dna-binding stress protein

Chain O:  92% 6%



- Molecule 1: Probable dna-binding stress protein

Chain P:  88% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.91Å 223.91Å 223.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.86 – 2.20 48.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.86-2.20) 100.0 (48.86-2.20)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.170 , 0.224 0.176 , 0.227	Depositor DCC
$R_{free}$ test set	9437 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.023 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21641	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TLA, 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	0.39	0/1245	0.54	0/1692
1	B	0.46	0/1264	0.61	0/1714
1	C	0.40	0/1246	0.56	0/1693
1	D	0.43	0/1246	0.53	0/1692
1	E	0.43	0/1245	0.56	0/1692
1	F	0.40	0/1245	0.57	0/1692
1	G	0.42	0/1252	0.57	0/1700
1	H	0.45	0/1256	0.58	0/1704
1	I	0.45	0/1252	0.61	0/1700
1	J	0.39	0/1237	0.53	0/1682
1	K	0.44	0/1246	0.60	0/1693
1	L	0.43	0/1235	0.58	0/1679
1	M	0.42	0/1252	0.58	0/1700
1	N	0.42	0/1242	0.58	0/1688
1	O	0.43	0/1253	0.52	0/1701
1	P	0.38	0/1252	0.54	0/1700
All	All	0.42	0/19968	0.57	0/27122

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	1216	0	1208	7	0
1	B	1235	0	1232	7	0
1	C	1217	0	1208	14	0
1	D	1217	0	1217	7	0
1	E	1216	0	1208	10	0
1	F	1216	0	1206	10	0
1	G	1223	0	1211	9	0
1	H	1227	0	1224	7	0
1	I	1223	0	1221	5	0
1	J	1208	0	1198	9	0
1	K	1217	0	1203	6	0
1	L	1206	0	1191	10	0
1	M	1223	0	1221	6	0
1	N	1213	0	1204	9	0
1	O	1224	0	1223	7	0
1	P	1223	0	1211	8	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	D	10	0	4	0	0
3	K	10	0	4	1	0
4	A	123	0	0	0	0
4	B	171	0	0	2	0
4	C	114	0	0	2	0
4	D	143	0	0	2	0
4	E	133	0	0	2	0
4	F	101	0	0	1	0
4	G	114	0	0	1	0
4	H	171	0	0	2	0
4	I	162	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	113	0	0	1	0
4	K	130	0	0	1	0
4	L	126	0	0	0	0
4	M	164	0	0	1	0
4	N	116	0	0	2	0
4	O	114	0	0	1	0
4	P	106	0	0	0	0
All	All	21641	0	19394	129	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 (129) 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:C:118:ARG:NH2	4:C:302:HOH:O	2.28	0.67
1:E:92:GLU:HB2	4:E:364:HOH:O	1.99	0.63
1:P:103:ILE:O	1:P:107:VAL:HG23	2.00	0.62
1:I:60:ALA:O	1:I:63[A]:VAL:HG22	2.00	0.62
1:C:7:ILE:HG23	1:C:127:VAL:HG11	1.84	0.58
1:A:60:ALA:O	1:A:63[A]:VAL:HG22	2.03	0.58
1:O:106:LEU:O	1:O:110:GLN:HG2	2.03	0.58
1:D:37:HIS:CE1	1:D:49:HIS:CE1	2.94	0.56
1:H:60:ALA:O	1:H:63[A]:VAL:HG22	2.05	0.56
1:J:60:ALA:O	1:J:63[A]:VAL:HG22	2.06	0.56
1:O:60:ALA:O	1:O:63[A]:VAL:HG22	2.07	0.55
1:D:60:ALA:O	1:D:63[A]:VAL:HG22	2.06	0.55
1:K:106:LEU:O	1:K:110:GLN:HG2	2.07	0.55
1:L:60:ALA:O	1:L:63[A]:VAL:HG22	2.08	0.54
1:C:111:GLU:OE2	1:C:151[B]:ARG:NH2	2.41	0.54
1:P:106:LEU:O	1:P:110:GLN:HG2	2.08	0.53
1:H:106:LEU:O	1:H:110:GLN:HG2	2.08	0.53
1:J:106:LEU:O	1:J:110:GLN:HG2	2.10	0.52
1:L:147:ALA:O	1:L:151[B]:ARG:HG2	2.09	0.52
1:K:4:ASN:ND2	3:K:202:TLA:O3	2.41	0.51
1:E:15:ILE:HD11	1:E:127:VAL:HG21	1.91	0.50
1:A:37:HIS:CE1	1:A:49:HIS:CE1	3.00	0.50
1:N:123:LEU:HD12	1:N:123:LEU:O	2.12	0.50
1:G:121:PHE:O	1:G:122:PRO:C	2.55	0.49
1:M:151[B]:ARG:NH2	4:M:302:HOH:O	2.44	0.49
1:B:60:ALA:O	1:B:63[A]:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:HIS:CE1	1:G:49:HIS:CE1	3.00	0.49
1:N:60:ALA:O	1:N:63[A]:VAL:HG22	2.11	0.49
1:N:147:ALA:O	1:N:151[B]:ARG:HG2	2.12	0.49
1:P:29:LEU:HD13	1:P:109:GLY:HA3	1.94	0.49
1:O:23:LEU:HD11	1:O:63[B]:VAL:HG13	1.95	0.49
1:I:37:HIS:CE1	1:I:49:HIS:CE1	3.00	0.49
1:O:83:ALA:O	1:O:87:LEU:HD12	2.13	0.48
1:G:123:LEU:HD12	1:G:123:LEU:O	2.12	0.48
1:L:97:PRO:O	1:L:102:MET:HE3	2.13	0.48
1:C:92:GLU:HB2	4:C:367:HOH:O	2.13	0.48
1:G:92:GLU:HB2	4:G:378:HOH:O	2.12	0.48
1:M:60:ALA:O	1:M:63[A]:VAL:HG22	2.14	0.48
1:C:37:HIS:CE1	1:C:49:HIS:CE1	3.02	0.47
1:L:123:LEU:HD12	1:L:123:LEU:O	2.15	0.47
1:E:106:LEU:O	1:E:110:GLN:HG2	2.14	0.47
1:C:123:LEU:HD12	1:C:123:LEU:O	2.15	0.46
1:C:7:ILE:HG23	1:C:127:VAL:CG1	2.46	0.46
1:L:124:LEU:HD22	1:L:129:ASP:HB3	1.97	0.46
1:J:35:ASN:C	1:J:35:ASN:OD1	2.58	0.45
1:F:37:HIS:CE1	1:F:49:HIS:CE1	3.05	0.45
1:F:120:ILE:HG22	1:F:120:ILE:O	2.16	0.45
1:K:27:TYR:O	1:K:30:TYR:HB3	2.16	0.45
1:H:44:MET:O	1:H:47:THR:HG22	2.16	0.45
1:C:106:LEU:O	1:C:110:GLN:HG2	2.17	0.45
1:B:127:VAL:O	1:B:128:SER:CB	2.64	0.45
1:H:130:GLU:N	1:H:131:PRO:CD	2.80	0.45
1:L:56:TYR:C	1:L:56:TYR:CD1	2.95	0.45
1:L:106:LEU:O	1:L:110:GLN:HG2	2.17	0.45
1:F:2:GLU:CB	4:F:381:HOH:O	2.64	0.45
1:F:147:ALA:O	1:F:151[B]:ARG:HG2	2.16	0.45
1:A:56:TYR:C	1:A:56:TYR:CD1	2.95	0.44
1:I:130:GLU:N	1:I:131:PRO:CD	2.80	0.44
1:A:121:PHE:N	1:A:122:PRO:CD	2.80	0.44
1:C:60:ALA:O	1:C:63[A]:VAL:HG22	2.17	0.44
1:F:56:TYR:C	1:F:56:TYR:CD1	2.96	0.44
1:B:127:VAL:O	1:B:128:SER:HB3	2.17	0.44
1:K:60:ALA:O	1:K:63[A]:VAL:HG22	2.18	0.44
1:B:47:THR:CG2	4:B:419:HOH:O	2.65	0.44
1:O:37:HIS:CE1	1:O:49:HIS:CE1	3.06	0.44
1:D:79:GLY:HA2	1:D:84:TYR:CZ	2.52	0.44
1:E:56:TYR:C	1:E:56:TYR:CD1	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:LYS:CB	4:E:396:HOH:O	2.65	0.43
1:F:100:GLU:HG3	1:F:154:LEU:CD2	2.48	0.43
1:G:79:GLY:HA2	1:G:84:TYR:CZ	2.52	0.43
4:N:358:HOH:O	1:P:141:GLN:HG3	2.17	0.43
1:A:129:ASP:OD2	1:A:132:THR:OG1	2.28	0.43
1:E:37:HIS:CE1	1:E:49:HIS:CE1	3.06	0.43
1:E:53:GLU:HA	1:E:56:TYR:CD2	2.54	0.43
1:I:127:VAL:O	1:I:128:SER:CB	2.66	0.43
1:L:44:MET:O	1:L:45:PHE:C	2.61	0.43
1:N:151[A]:ARG:NH2	4:N:305:HOH:O	2.37	0.43
1:F:53:GLU:HA	1:F:56:TYR:CD2	2.52	0.43
1:K:92:GLU:HB2	4:K:372:HOH:O	2.16	0.43
1:P:60:ALA:O	1:P:63[A]:VAL:HG22	2.18	0.43
1:F:106:LEU:O	1:F:110:GLN:HG2	2.19	0.43
1:J:53:GLU:HA	1:J:56:TYR:CD2	2.53	0.43
1:N:130:GLU:N	1:N:131:PRO:CD	2.82	0.43
1:O:101:GLU:OE1	4:O:301:HOH:O	2.21	0.43
1:E:60:ALA:O	1:E:63[B]:VAL:HG22	2.19	0.43
1:N:121:PHE:O	1:N:122:PRO:C	2.59	0.43
1:B:53:GLU:HA	1:B:56:TYR:CD2	2.54	0.42
1:B:98:GLU:HB3	4:B:384:HOH:O	2.19	0.42
1:D:115:ARG:NH2	4:D:305:HOH:O	2.33	0.42
1:M:130:GLU:N	1:M:131:PRO:CD	2.82	0.42
1:G:35:ASN:OD1	1:G:35:ASN:C	2.62	0.42
1:J:7:ILE:HG22	1:J:12:ARG:HG3	2.01	0.42
1:M:37:HIS:CE1	1:M:49:HIS:CE1	3.07	0.42
1:N:37:HIS:CE1	1:N:49:HIS:CE1	3.07	0.42
1:H:23:LEU:HD11	1:H:63[B]:VAL:HG13	2.00	0.42
1:C:121:PHE:O	1:C:122:PRO:C	2.60	0.42
1:C:46:ASN:OD1	1:G:51:MET:HE3	2.19	0.42
1:C:149:MET:HE1	4:H:457:HOH:O	2.18	0.42
1:E:129:ASP:OD1	1:E:129:ASP:C	2.62	0.42
1:H:56:TYR:C	1:H:56:TYR:CD1	2.97	0.42
1:J:53:GLU:HA	1:J:56:TYR:CE2	2.55	0.42
1:O:56:TYR:CD1	1:O:56:TYR:C	2.98	0.42
1:C:79:GLY:HA2	1:C:84:TYR:CZ	2.55	0.42
1:J:56:TYR:C	1:J:56:TYR:CD1	2.97	0.42
1:C:56:TYR:CD1	1:C:56:TYR:C	2.97	0.42
1:E:55:GLN:HE22	1:E:150:LEU:HD21	1.85	0.42
1:I:25:ASP:OD1	1:I:89:SER:N	2.42	0.42
1:M:56:TYR:CD1	1:M:56:TYR:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:LEU:O	1:D:110:GLN:HG2	2.20	0.41
1:H:151[A]:ARG:NE	4:H:311:HOH:O	2.51	0.41
1:N:34:HIS:O	1:N:37:HIS:HB3	2.20	0.41
1:P:121:PHE:N	1:P:122:PRO:CD	2.83	0.41
1:A:53:GLU:HA	1:A:56:TYR:CE2	2.55	0.41
1:D:129:ASP:OD2	1:D:132:THR:OG1	2.29	0.41
4:D:311:HOH:O	1:L:151[A]:ARG:HD2	2.20	0.41
1:A:42:GLY:O	1:D:153:LEU:HA	2.21	0.41
1:P:13:ALA:HB2	1:P:75:PHE:CZ	2.55	0.41
1:F:127:VAL:O	1:F:127:VAL:HG12	2.20	0.41
1:K:56:TYR:CD1	1:K:56:TYR:C	2.98	0.41
1:M:106:LEU:O	1:M:110:GLN:HG2	2.21	0.41
1:F:120:ILE:O	1:F:120:ILE:CG2	2.69	0.41
1:J:80:THR:HG22	4:J:301:HOH:O	2.21	0.41
1:P:127:VAL:O	1:P:128:SER:CB	2.68	0.41
1:J:97:PRO:HB3	1:J:101:GLU:HG2	2.03	0.41
1:L:138:GLN:OE1	1:L:138:GLN:HA	2.20	0.41
1:N:147:ALA:O	1:N:151[A]:ARG:HG2	2.21	0.41
1:B:147:ALA:O	1:B:151[B]:ARG:HG2	2.21	0.40
1:G:23:LEU:HD23	1:G:78:PRO:HG2	2.03	0.40
1:G:60:ALA:O	1:G:63[A]:VAL:HG22	2.22	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	155/156 (99%)	153 (99%)	2 (1%)	0	100 100
1	B	156/156 (100%)	152 (97%)	3 (2%)	1 (1%)	21 23
1	C	155/156 (99%)	151 (97%)	4 (3%)	0	100 100
1	D	155/156 (99%)	152 (98%)	2 (1%)	1 (1%)	21 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	155/156 (99%)	151 (97%)	4 (3%)	0	100	100
1	F	155/156 (99%)	149 (96%)	5 (3%)	1 (1%)	21	23
1	G	156/156 (100%)	152 (97%)	4 (3%)	0	100	100
1	H	156/156 (100%)	151 (97%)	5 (3%)	0	100	100
1	I	155/156 (99%)	148 (96%)	6 (4%)	1 (1%)	21	23
1	J	155/156 (99%)	151 (97%)	4 (3%)	0	100	100
1	K	155/156 (99%)	150 (97%)	5 (3%)	0	100	100
1	L	155/156 (99%)	150 (97%)	5 (3%)	0	100	100
1	M	155/156 (99%)	148 (96%)	7 (4%)	0	100	100
1	N	155/156 (99%)	153 (99%)	2 (1%)	0	100	100
1	O	155/156 (99%)	152 (98%)	3 (2%)	0	100	100
1	P	156/156 (100%)	153 (98%)	2 (1%)	1 (1%)	21	23
All	All	2484/2496 (100%)	2416 (97%)	63 (2%)	5 (0%)	43	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	128	SER
1	P	128	SER
1	F	128	SER
1	I	128	SER
1	D	79	GLY

### 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	125/129 (97%)	124 (99%)	1 (1%)	73	85
1	B	129/129 (100%)	127 (98%)	2 (2%)	55	71
1	C	125/129 (97%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	125/129 (97%)	123 (98%)	2 (2%)	55	71
1	E	125/129 (97%)	123 (98%)	2 (2%)	55	71
1	F	125/129 (97%)	122 (98%)	3 (2%)	43	58
1	G	126/129 (98%)	124 (98%)	2 (2%)	55	71
1	H	127/129 (98%)	124 (98%)	3 (2%)	43	58
1	I	127/129 (98%)	127 (100%)	0	100	100
1	J	123/129 (95%)	119 (97%)	4 (3%)	33	45
1	K	125/129 (97%)	124 (99%)	1 (1%)	73	85
1	L	122/129 (95%)	119 (98%)	3 (2%)	42	56
1	M	127/129 (98%)	126 (99%)	1 (1%)	73	85
1	N	124/129 (96%)	123 (99%)	1 (1%)	73	85
1	O	127/129 (98%)	126 (99%)	1 (1%)	73	85
1	P	126/129 (98%)	123 (98%)	3 (2%)	43	58
All	All	2008/2064 (97%)	1979 (99%)	29 (1%)	57	75

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	B	148	TRP
1	B	156	SER
1	D	47	THR
1	D	119	SER
1	E	56	TYR
1	E	92	GLU
1	F	34	HIS
1	F	47	THR
1	F	56	TYR
1	G	34	HIS
1	G	90	ILE
1	H	56	TYR
1	H	148	TRP
1	H	156	SER
1	J	34	HIS
1	J	47	THR
1	J	127	VAL
1	J	128	SER

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Mol	Chain	Res	Type
1	K	56	TYR
1	L	34	HIS
1	L	56	TYR
1	L	123	LEU
1	M	115	ARG
1	N	92	GLU
1	O	56	TYR
1	P	47	THR
1	P	56	TYR
1	P	156	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	E	49	HIS
1	E	55	GLN
1	E	110	GLN
1	G	55	GLN
1	I	49	HIS
1	K	4	ASN
1	M	49	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 16 are monoatomic - leaving 2 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	TLA	K	202	-	9,9,9	1.48	1 (11%)	12,12,12	1.16	1 (8%)
3	TLA	D	202	-	9,9,9	1.57	2 (22%)	12,12,12	1.02	1 (8%)

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	TLA	K	202	-	-	7/12/12/12	-
3	TLA	D	202	-	-	4/12/12/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	202	TLA	C2-C1	2.79	1.56	1.52
3	K	202	TLA	C3-C4	2.68	1.56	1.52
3	D	202	TLA	C3-C4	2.39	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	202	TLA	O1-C1-C2	-2.37	115.30	121.62
3	D	202	TLA	O4-C4-C3	-2.08	116.08	121.62

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	202	TLA	C2-C3-C4-O41
3	K	202	TLA	C2-C3-C4-O4
3	K	202	TLA	O1-C1-C2-O2
3	K	202	TLA	O11-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	K	202	TLA	O1-C1-C2-C3
3	K	202	TLA	O11-C1-C2-C3
3	D	202	TLA	O3-C3-C4-O41
3	D	202	TLA	C2-C3-C4-O41
3	D	202	TLA	C2-C3-C4-O4
3	D	202	TLA	O3-C3-C4-O4
3	K	202	TLA	O3-C3-C4-O41

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	202	TLA	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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	155/156 (99%)	-0.32	2 (1%) 75 73	15, 31, 51, 62	2 (1%)
1	B	156/156 (100%)	-0.58	1 (0%) 85 83	14, 25, 41, 69	2 (1%)
1	C	155/156 (99%)	-0.09	2 (1%) 75 73	18, 35, 54, 69	2 (1%)
1	D	155/156 (99%)	-0.14	1 (0%) 85 83	17, 32, 47, 75	2 (1%)
1	E	155/156 (99%)	-0.43	0 100 100	15, 29, 43, 53	2 (1%)
1	F	155/156 (99%)	0.02	3 (1%) 66 63	20, 36, 57, 78	2 (1%)
1	G	156/156 (100%)	-0.13	3 (1%) 66 63	19, 33, 55, 73	2 (1%)
1	H	156/156 (100%)	-0.55	1 (0%) 85 83	14, 25, 41, 81	2 (1%)
1	I	155/156 (99%)	-0.51	0 100 100	16, 27, 42, 57	2 (1%)
1	J	155/156 (99%)	0.11	0 100 100	21, 36, 51, 67	2 (1%)
1	K	155/156 (99%)	-0.45	1 (0%) 85 83	15, 28, 49, 66	2 (1%)
1	L	155/156 (99%)	-0.31	3 (1%) 66 63	15, 30, 47, 67	2 (1%)
1	M	155/156 (99%)	-0.57	0 100 100	14, 26, 41, 53	2 (1%)
1	N	155/156 (99%)	-0.24	1 (0%) 85 83	17, 31, 50, 66	2 (1%)
1	O	155/156 (99%)	-0.18	2 (1%) 75 73	17, 33, 48, 75	2 (1%)
1	P	156/156 (100%)	-0.22	1 (0%) 85 83	19, 33, 50, 85	2 (1%)
All	All	2484/2496 (99%)	-0.29	21 (0%) 82 80	14, 31, 50, 85	32 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	156	SER	3.5
1	F	125	ASP	3.1
1	O	125	ASP	3.1
1	B	156	SER	2.8
1	G	123	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	121	PHE	2.8
1	P	125	ASP	2.8
1	L	125	ASP	2.7
1	C	123	LEU	2.5
1	K	125	ASP	2.5
1	F	124	LEU	2.4
1	G	125	ASP	2.4
1	O	127	VAL	2.3
1	C	125	ASP	2.2
1	A	155	ALA	2.1
1	G	156	SER	2.1
1	A	125	ASP	2.1
1	L	127	VAL	2.1
1	L	124	LEU	2.0
1	D	125	ASP	2.0
1	N	125	ASP	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	TLA	K	202	10/10	0.83	0.12	58,65,72,76	0
3	TLA	D	202	10/10	0.88	0.10	54,65,70,73	0
2	MN	G	201	1/1	0.98	0.08	48,48,48,48	0
2	MN	J	201	1/1	0.98	0.06	51,51,51,51	0
2	MN	N	201	1/1	0.98	0.07	42,42,42,42	0
2	MN	B	201	1/1	0.98	0.08	41,41,41,41	0
2	MN	D	201	1/1	0.98	0.08	44,44,44,44	0

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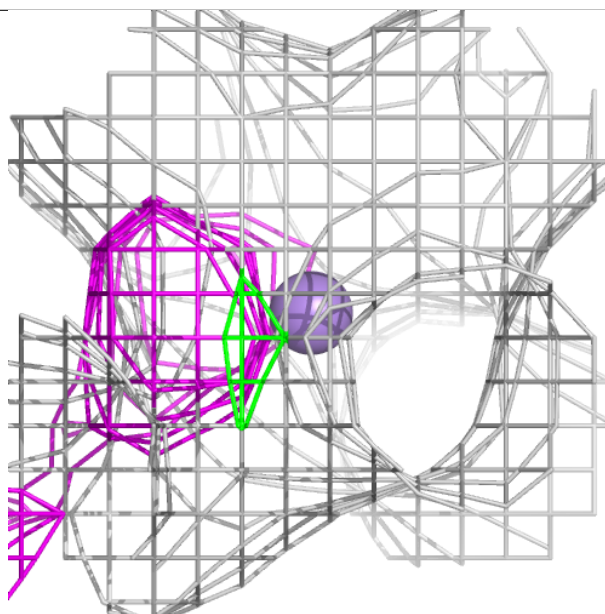
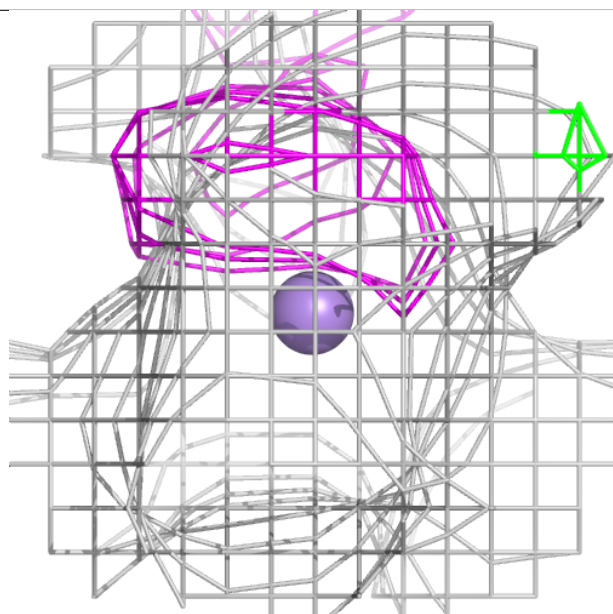
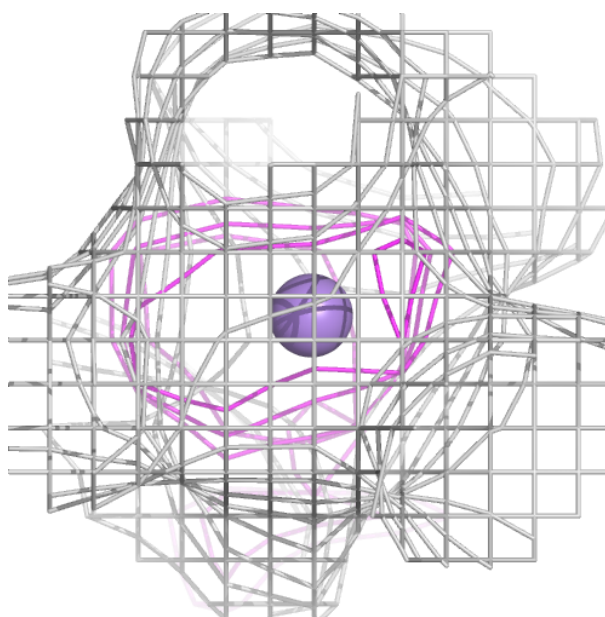
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	I	201	1/1	0.99	0.09	42,42,42,42	0
2	MN	E	201	1/1	0.99	0.06	41,41,41,41	0
2	MN	L	201	1/1	0.99	0.10	37,37,37,37	0
2	MN	M	201	1/1	0.99	0.07	43,43,43,43	0
2	MN	F	201	1/1	0.99	0.09	49,49,49,49	0
2	MN	O	201	1/1	0.99	0.07	42,42,42,42	0
2	MN	P	201	1/1	0.99	0.08	44,44,44,44	0
2	MN	A	201	1/1	0.99	0.06	42,42,42,42	0
2	MN	H	201	1/1	0.99	0.07	41,41,41,41	0
2	MN	K	201	1/1	1.00	0.07	40,40,40,40	0
2	MN	C	201	1/1	1.00	0.08	46,46,46,46	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.

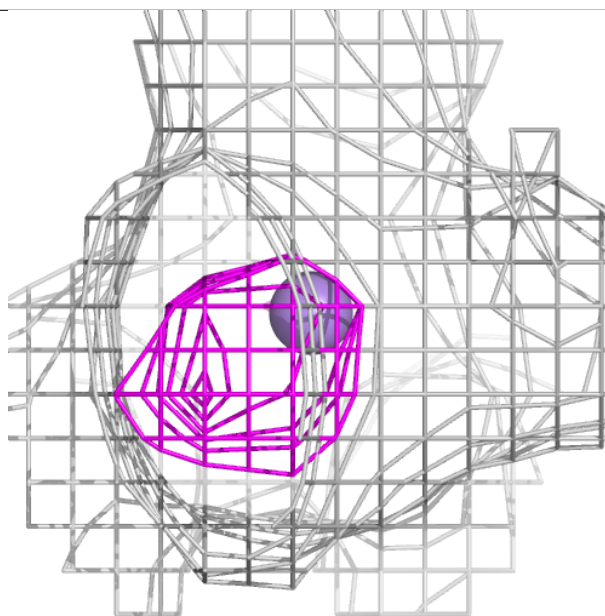
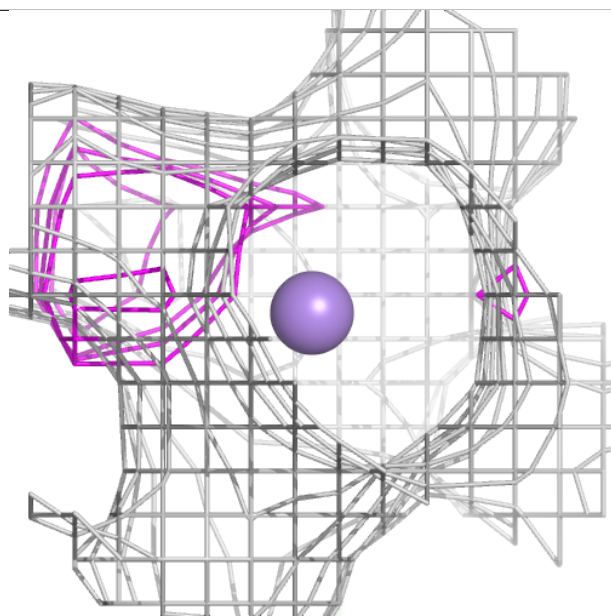
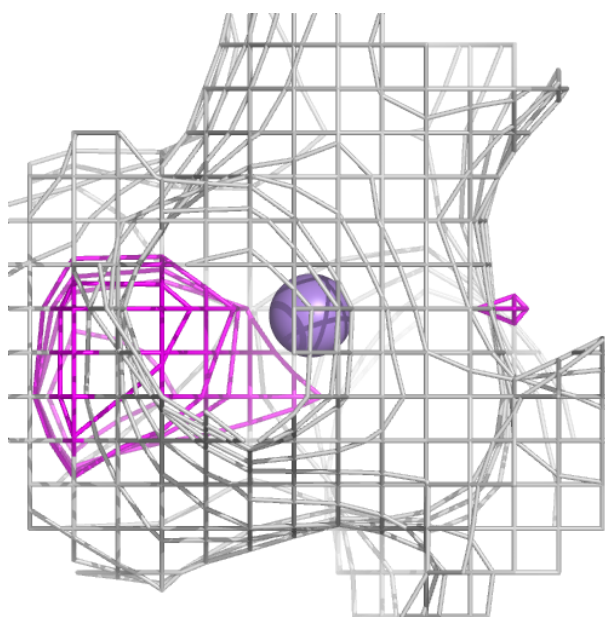
**Electron density around MN G 201:**

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



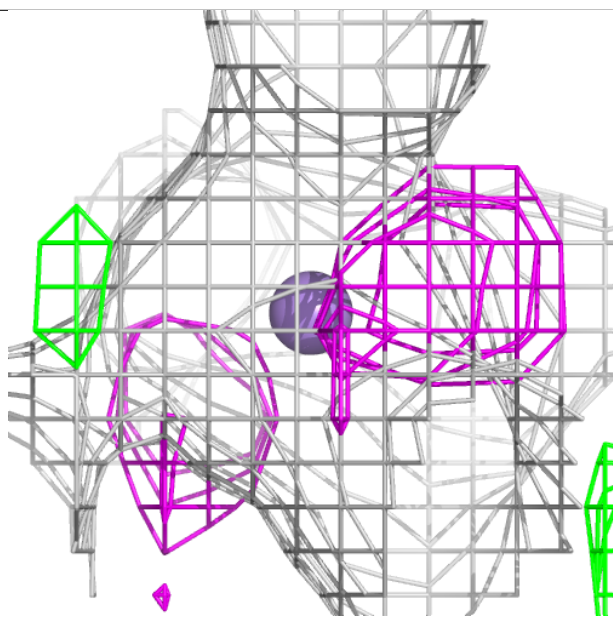
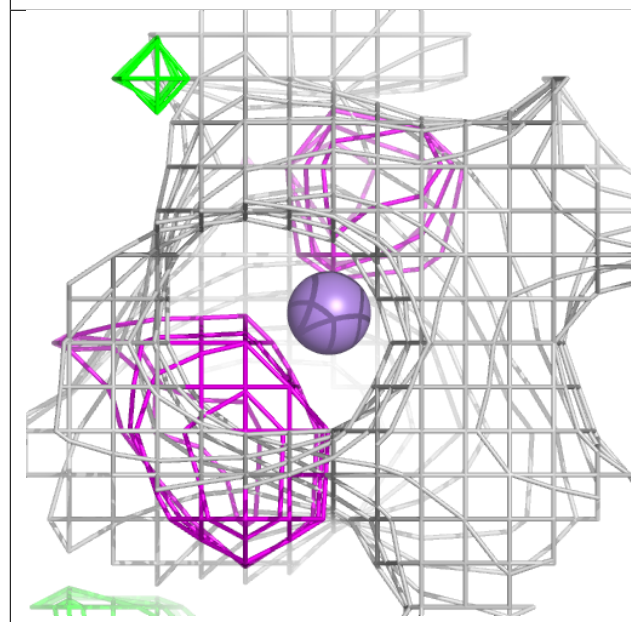
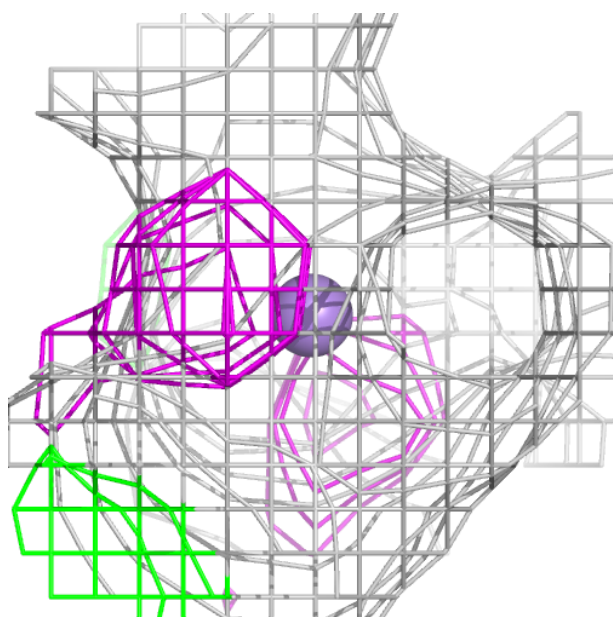
**Electron density around MN J 201:**

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



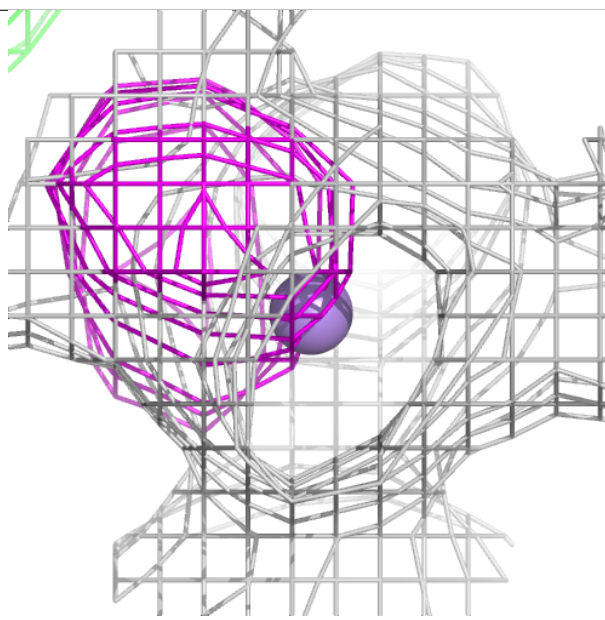
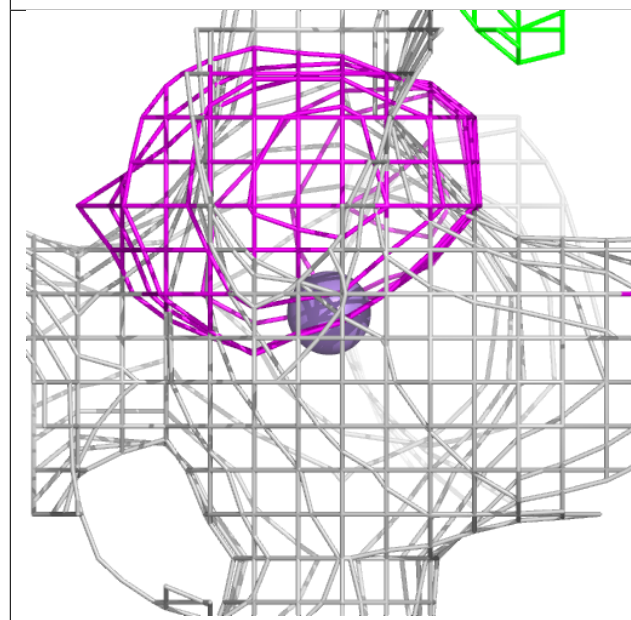
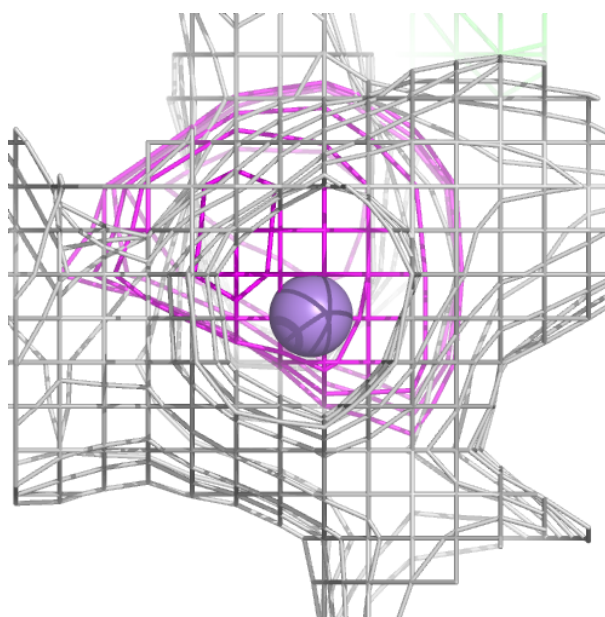
**Electron density around MN N 201:**

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



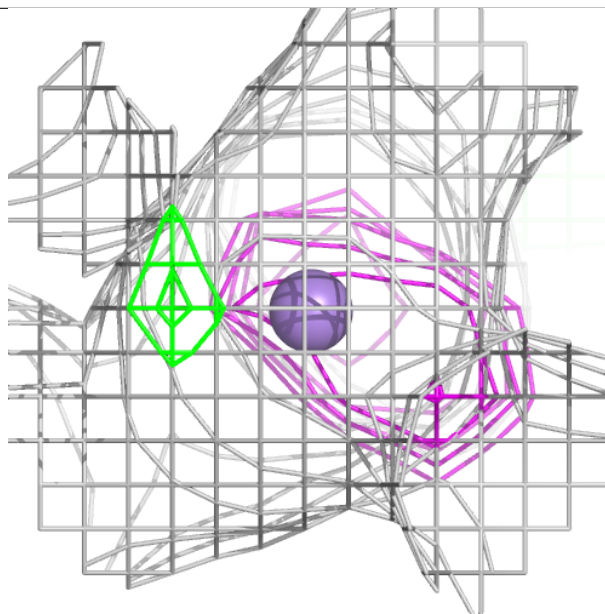
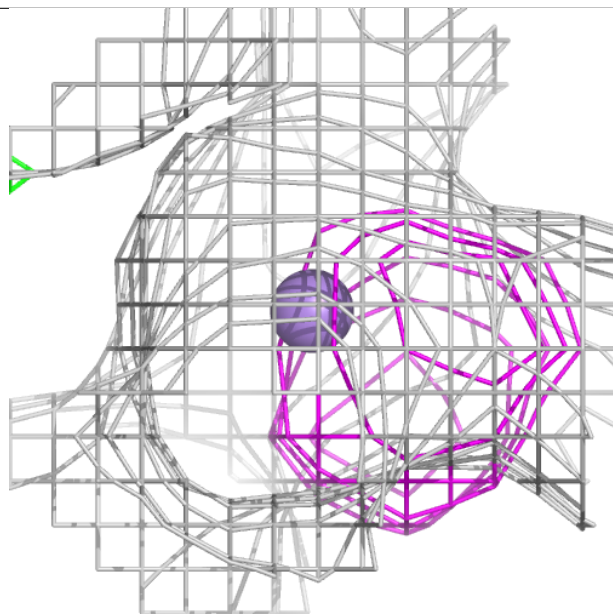
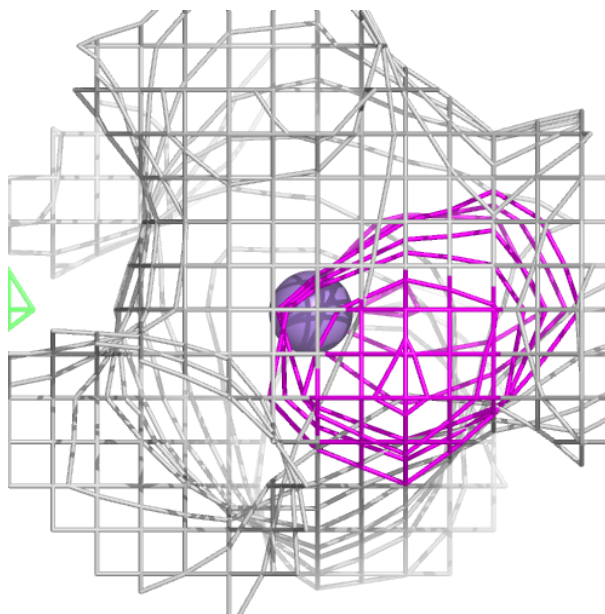
**Electron density around MN B 201:**

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



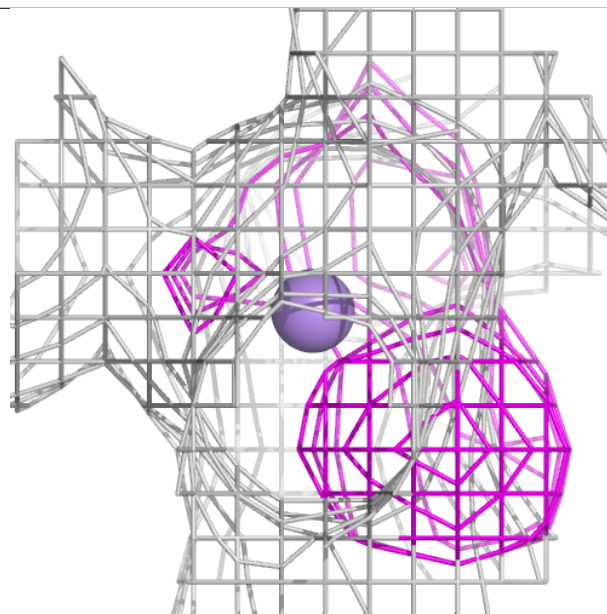
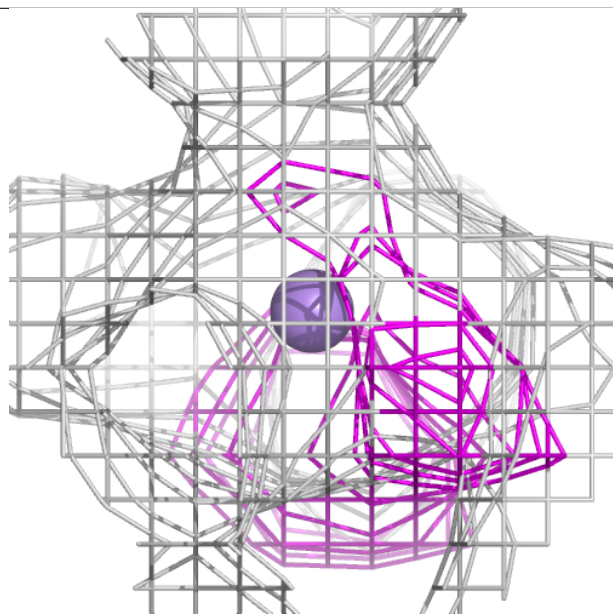
**Electron density around MN D 201:**

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



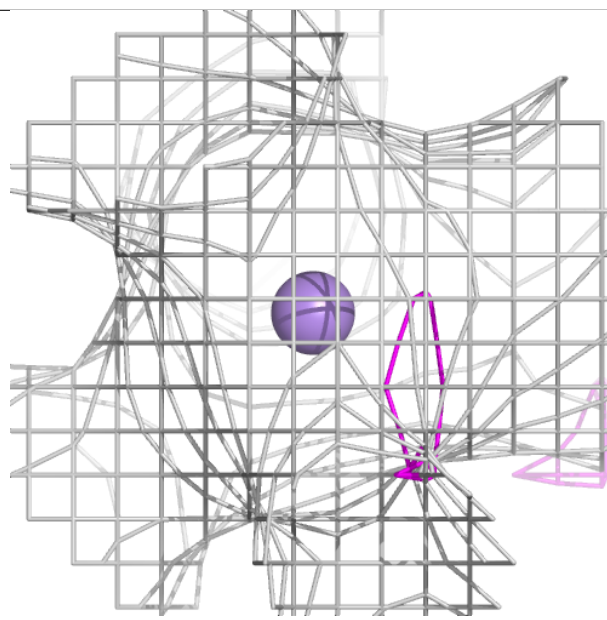
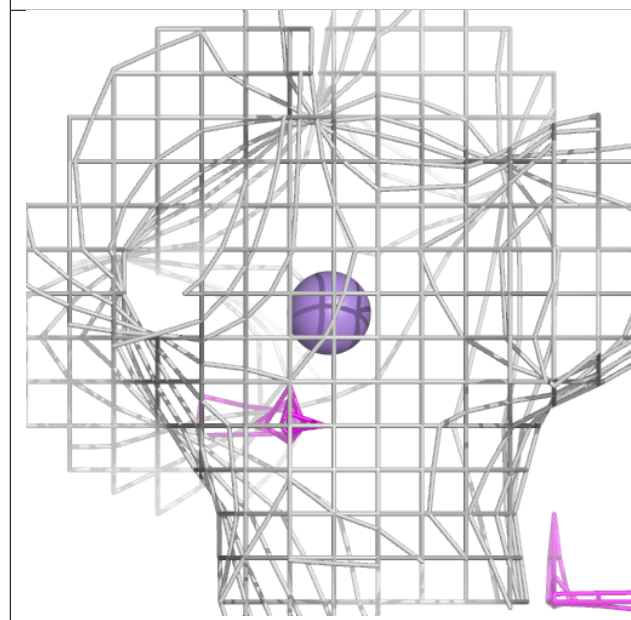
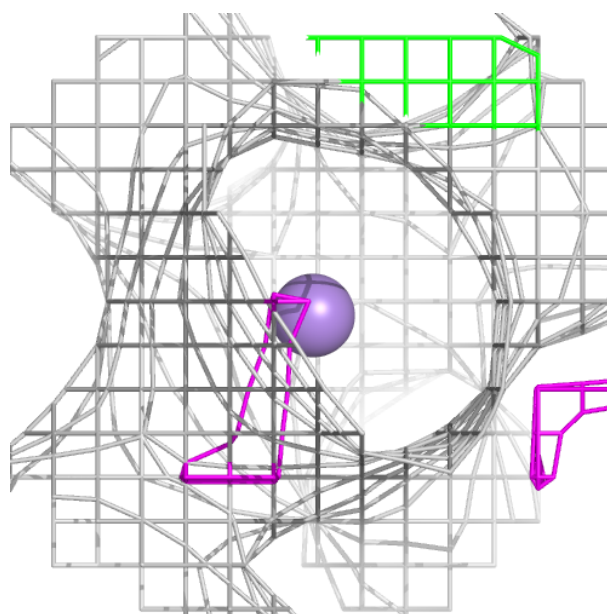
**Electron density around MN I 201:**

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



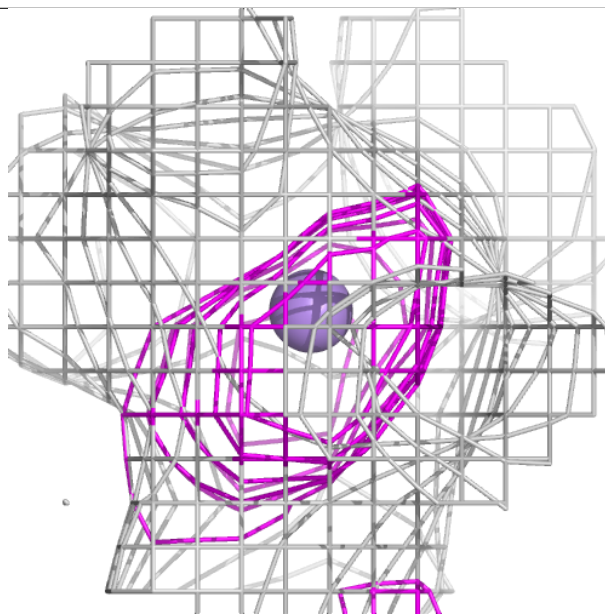
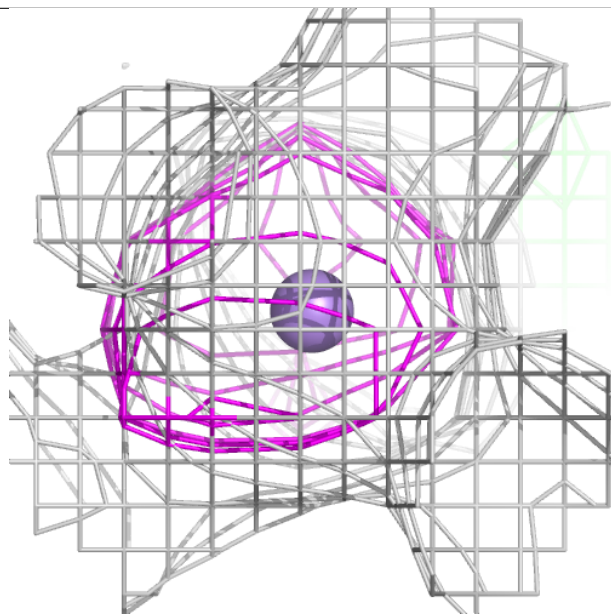
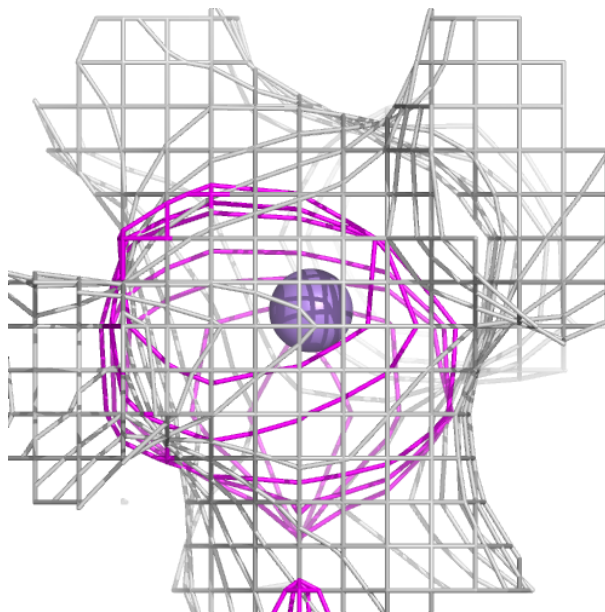
**Electron density around MN E 201:**

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



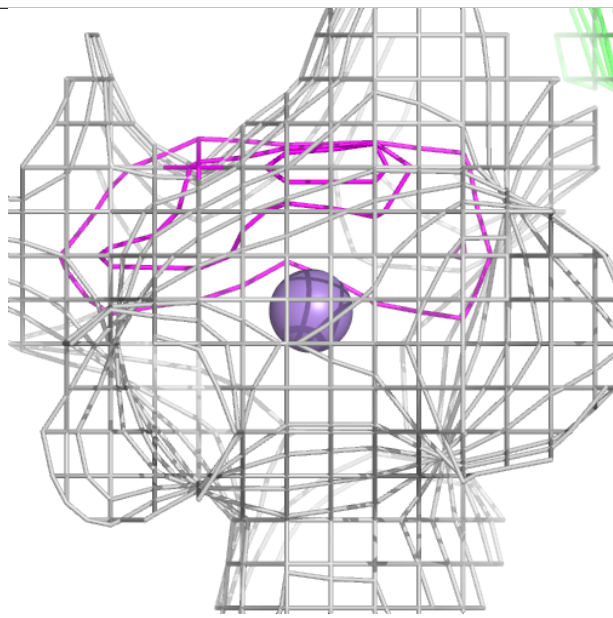
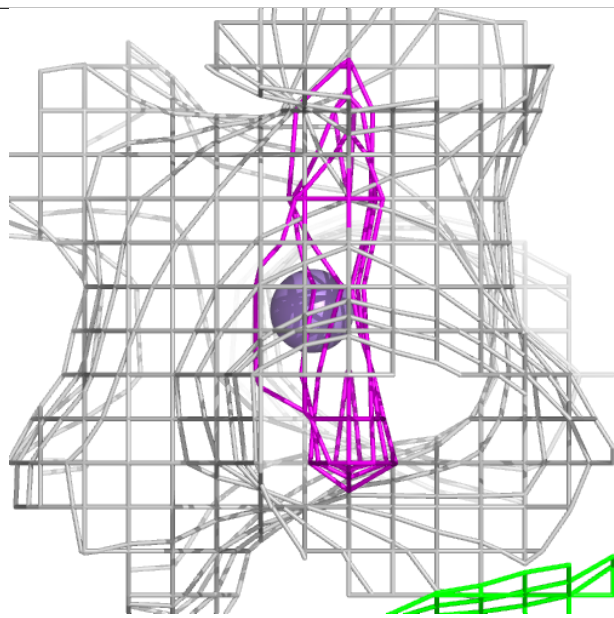
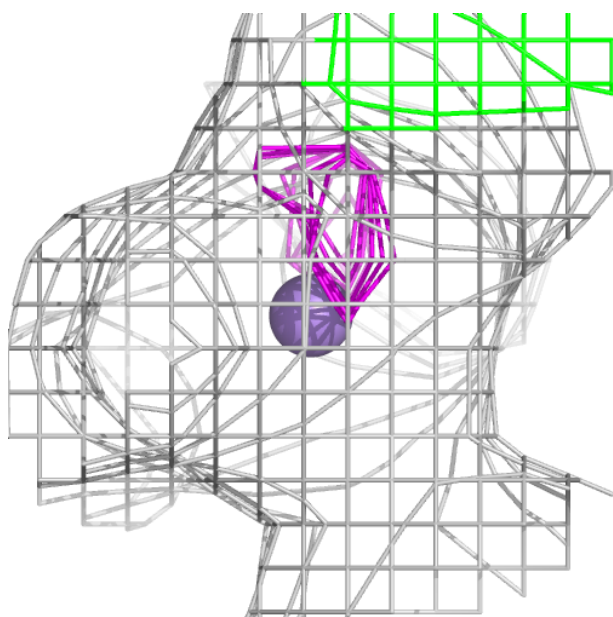
**Electron density around MN L 201:**

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



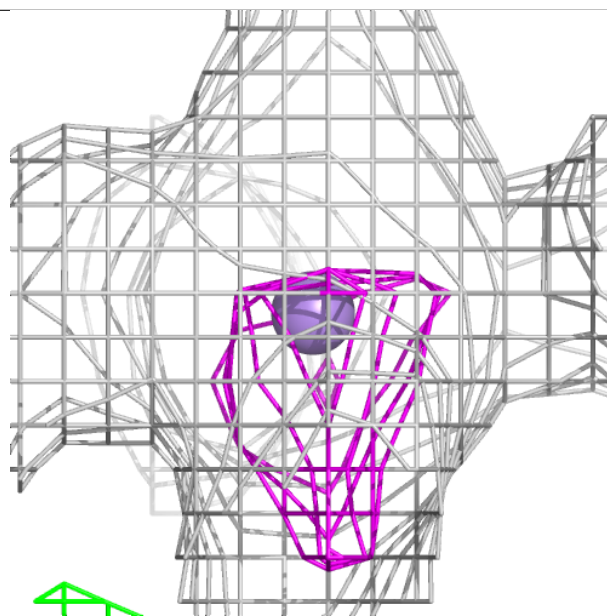
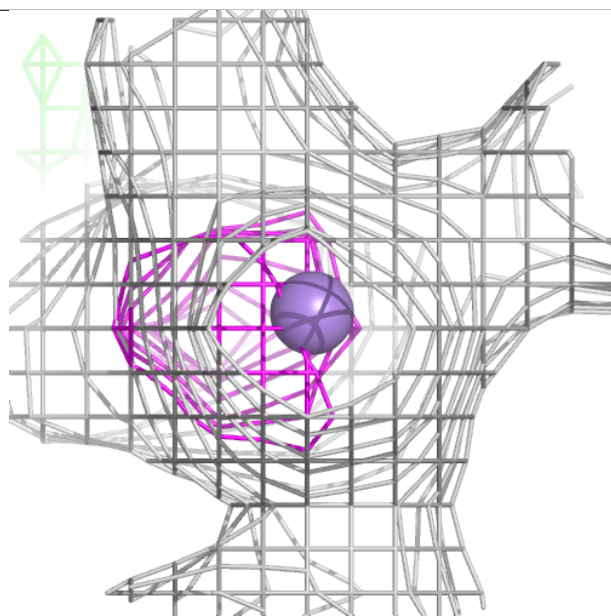
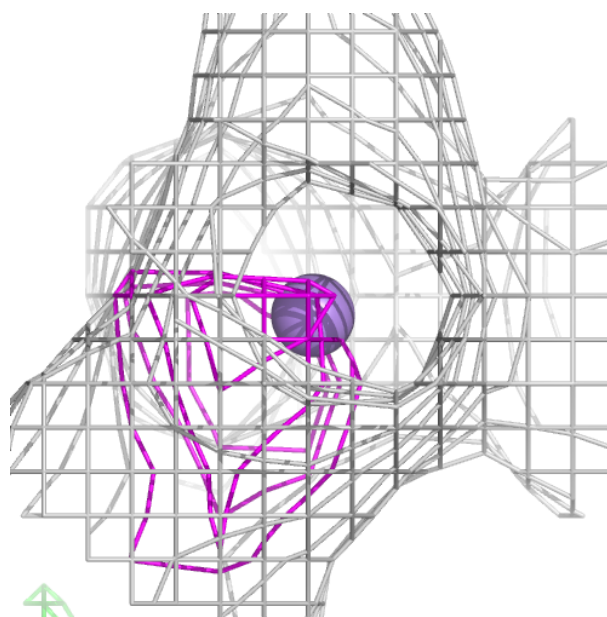
**Electron density around MN M 201:**

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



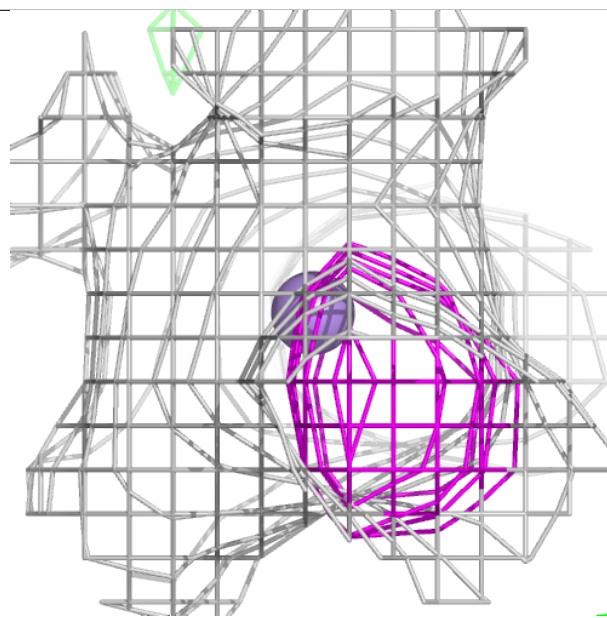
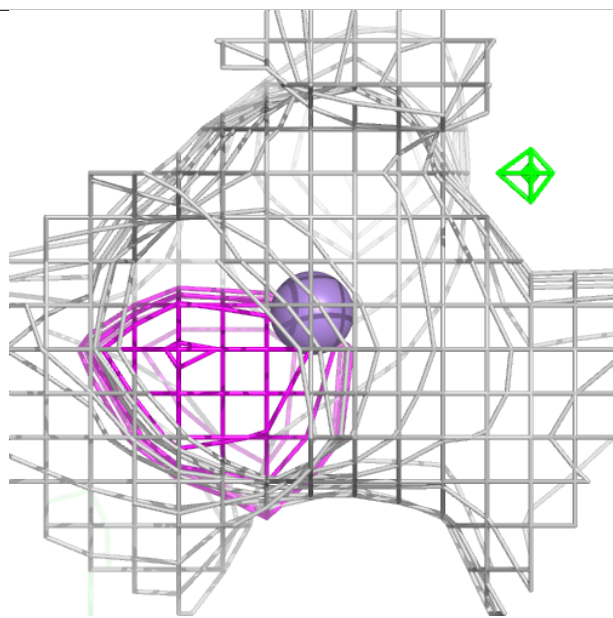
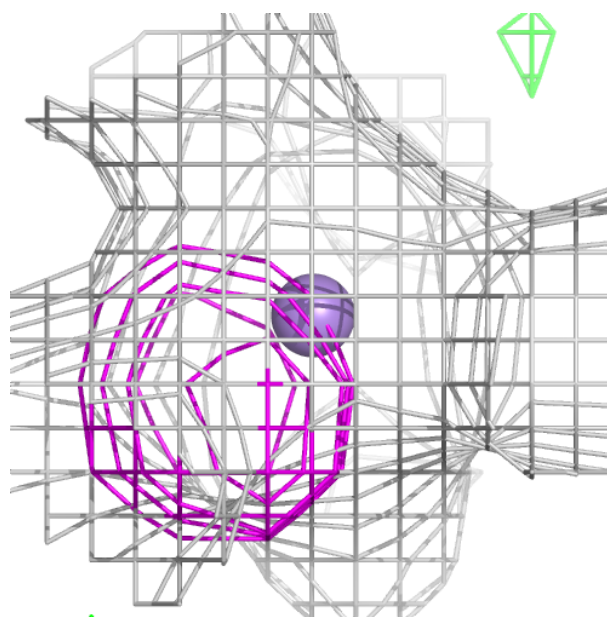
**Electron density around MN F 201:**

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



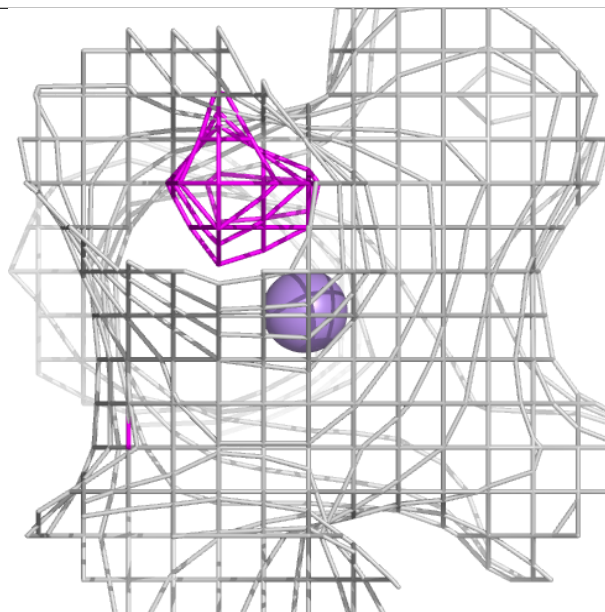
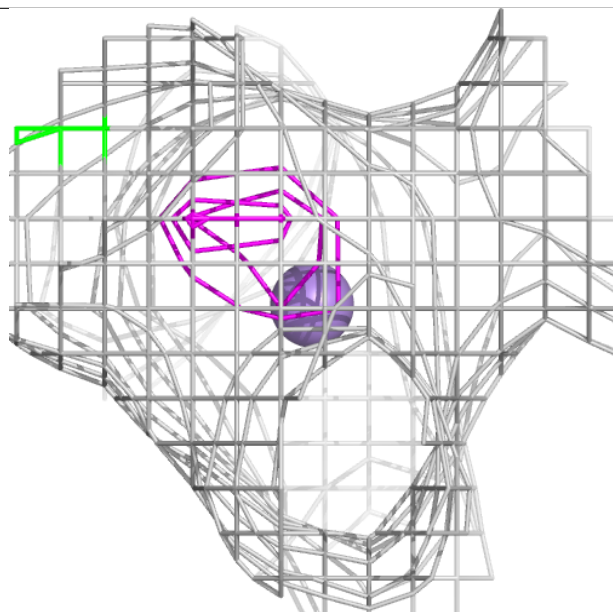
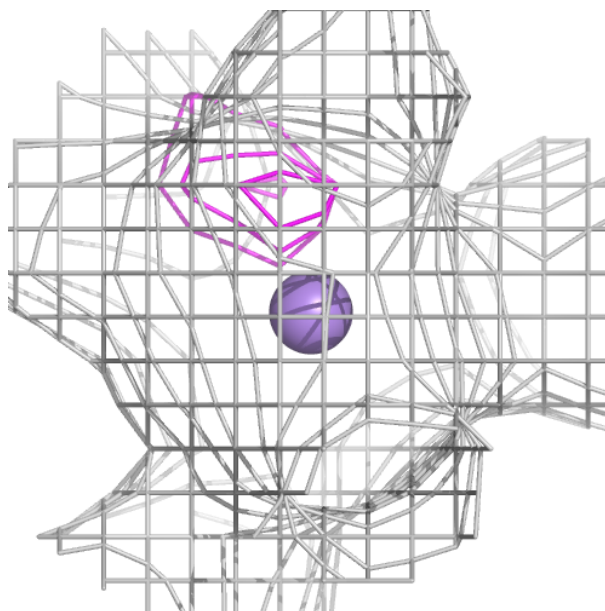
**Electron density around MN O 201:**

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



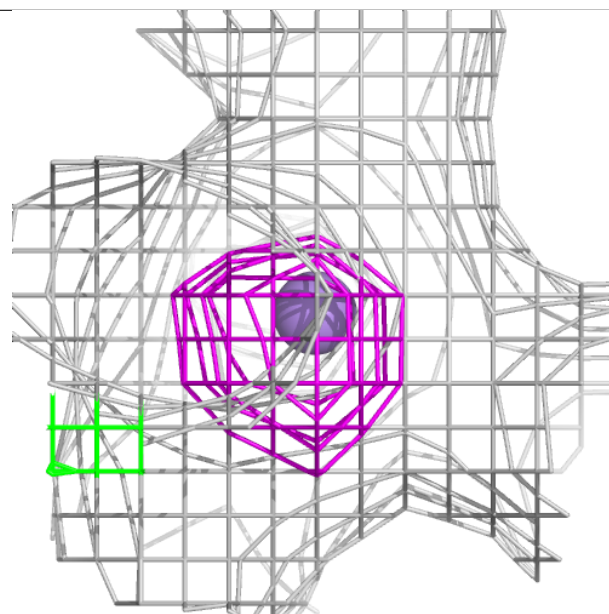
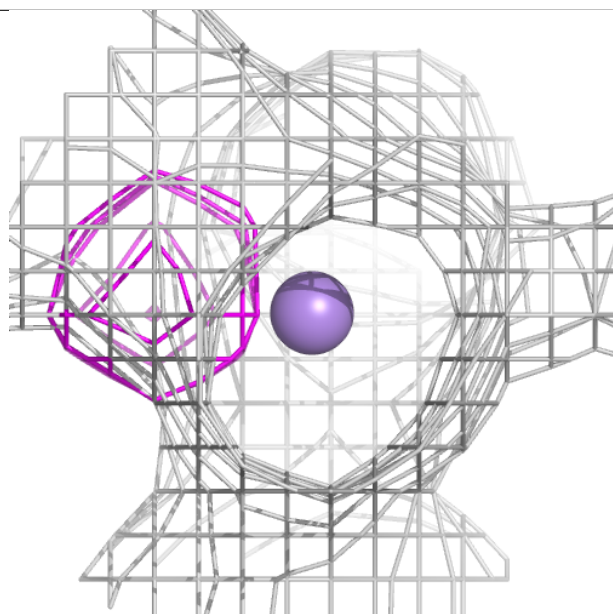
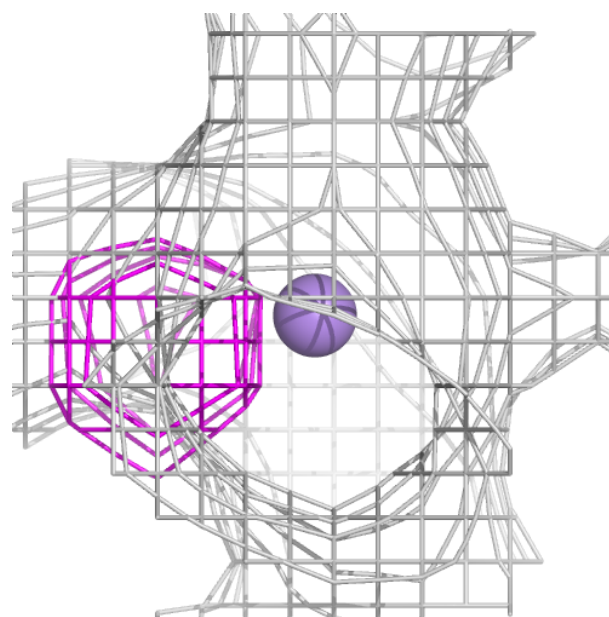
**Electron density around MN P 201:**

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



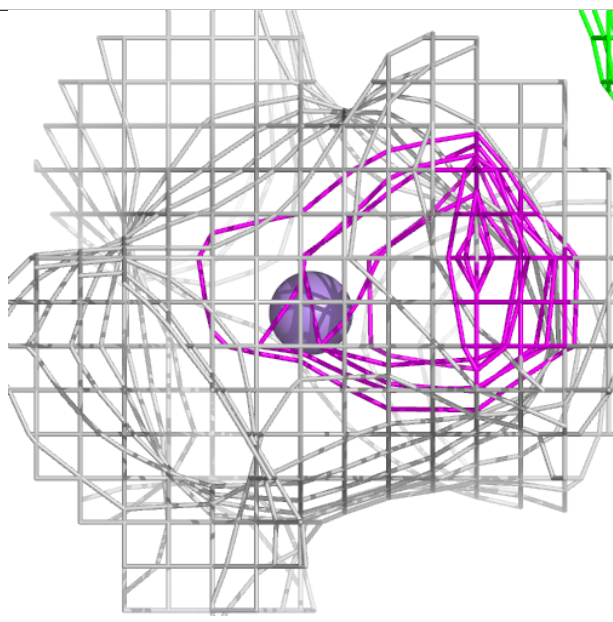
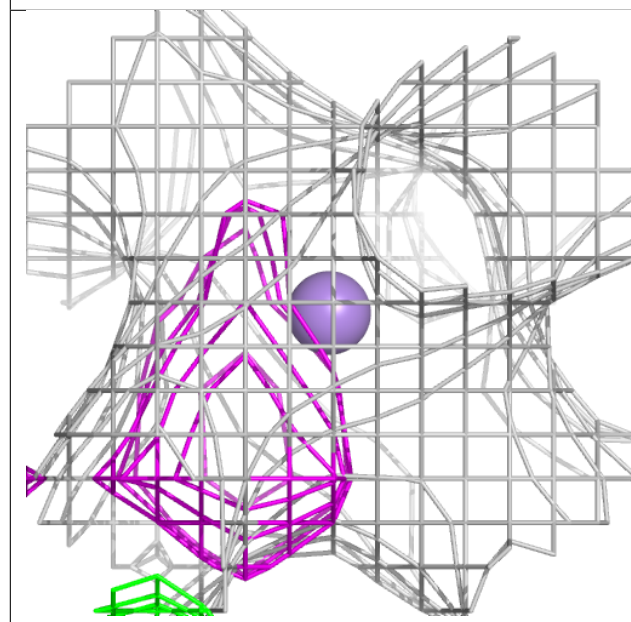
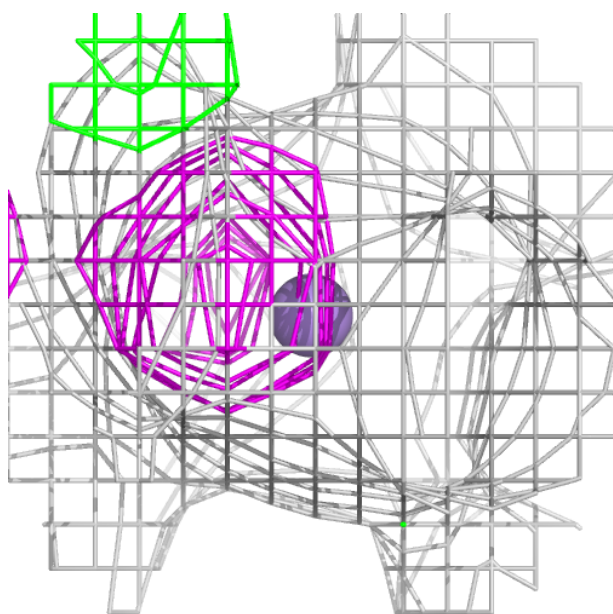
**Electron density around MN A 201:**

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



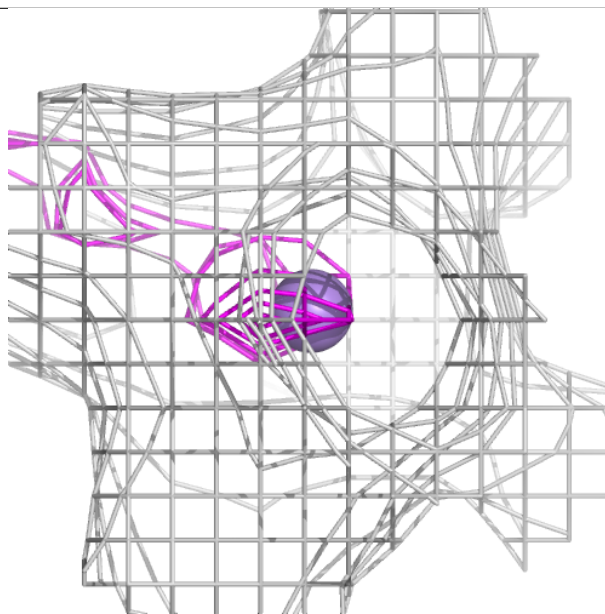
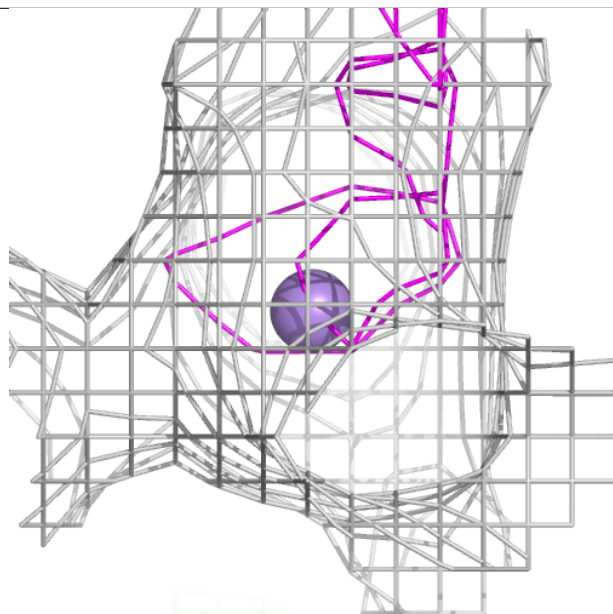
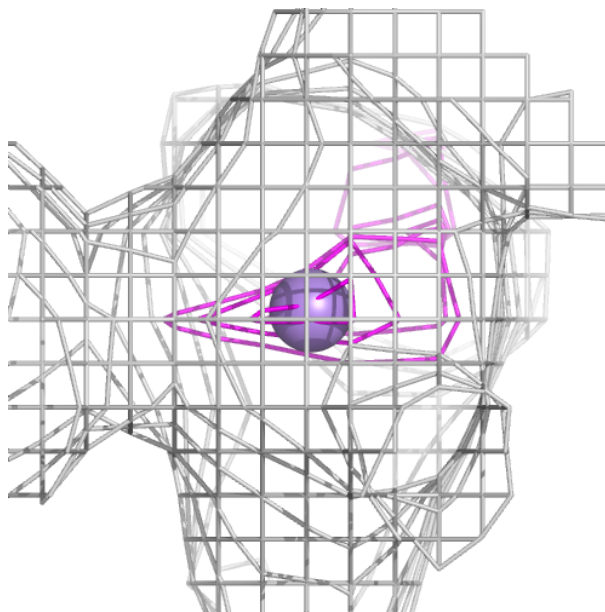
**Electron density around MN H 201:**

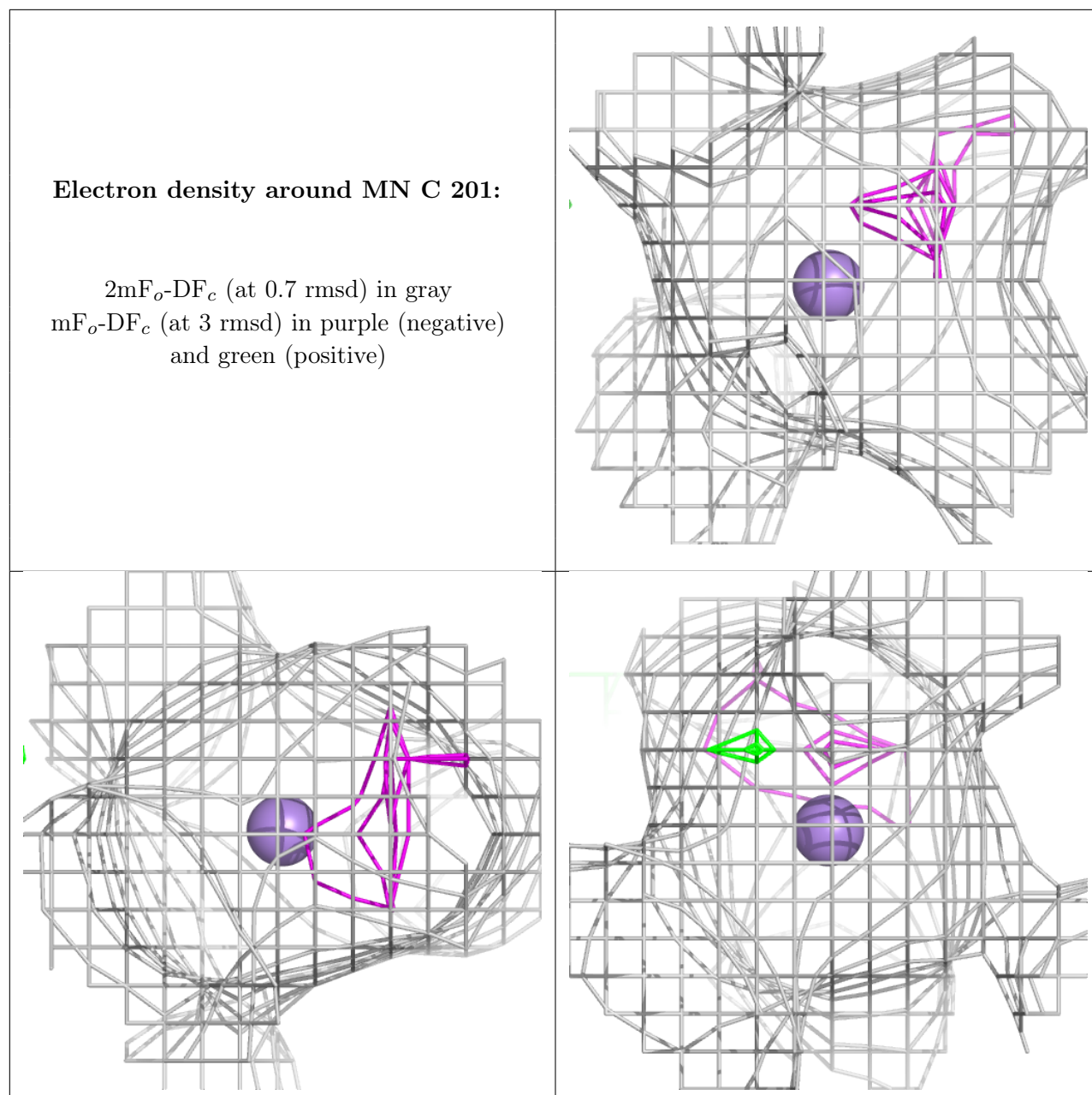
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MN K 201:**

$2mF_o-DF_c$  (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.