



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:19 PM UTC

PDB ID : 6VSS / pdb_00006vss
Title : Arginase from *Medicago truncatula*
Authors : Sekula, B.
Deposited on : 2020-02-11
Resolution : 1.93 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

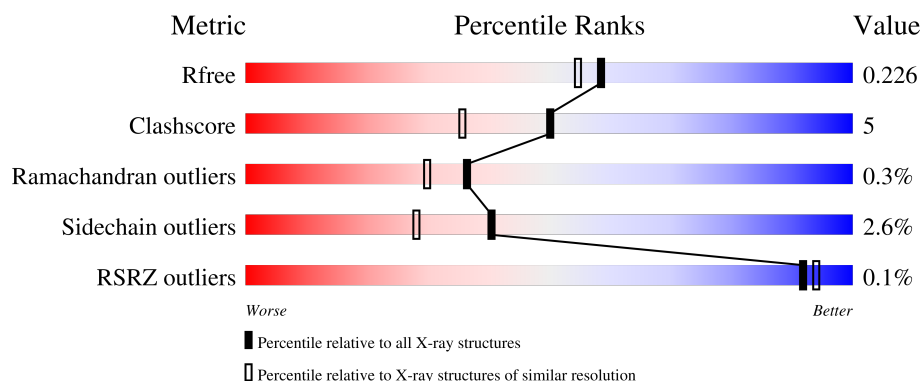
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	341	74% 17% • 7%
1	B	341	83% 10% • 6%
1	C	341	79% 13% • 7%
1	D	341	77% 15% • 7%
1	E	341	75% 16% • 7%

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Mol	Chain	Length	Quality of chain
1	F	341	79% 13% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15295 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 Arginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2441	1531	439	464	7			
1	B	319	Total	C	N	O	S	0	1	0
			2470	1547	445	471	7			
1	C	318	Total	C	N	O	S	0	0	0
			2455	1537	441	470	7			
1	D	318	Total	C	N	O	S	0	1	0
			2463	1542	444	470	7			
1	E	316	Total	C	N	O	S	0	1	0
			2449	1535	442	465	7			
1	F	318	Total	C	N	O	S	0	0	0
			2455	1537	441	470	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP G7JFU5
A	-1	ASN	-	expression tag	UNP G7JFU5
A	0	ALA	-	expression tag	UNP G7JFU5
B	-2	SER	-	expression tag	UNP G7JFU5
B	-1	ASN	-	expression tag	UNP G7JFU5
B	0	ALA	-	expression tag	UNP G7JFU5
C	-2	SER	-	expression tag	UNP G7JFU5
C	-1	ASN	-	expression tag	UNP G7JFU5
C	0	ALA	-	expression tag	UNP G7JFU5
D	-2	SER	-	expression tag	UNP G7JFU5
D	-1	ASN	-	expression tag	UNP G7JFU5
D	0	ALA	-	expression tag	UNP G7JFU5
E	-2	SER	-	expression tag	UNP G7JFU5
E	-1	ASN	-	expression tag	UNP G7JFU5
E	0	ALA	-	expression tag	UNP G7JFU5
F	-2	SER	-	expression tag	UNP G7JFU5
F	-1	ASN	-	expression tag	UNP G7JFU5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP G7JFU5

- 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

- Molecule 3 is water.

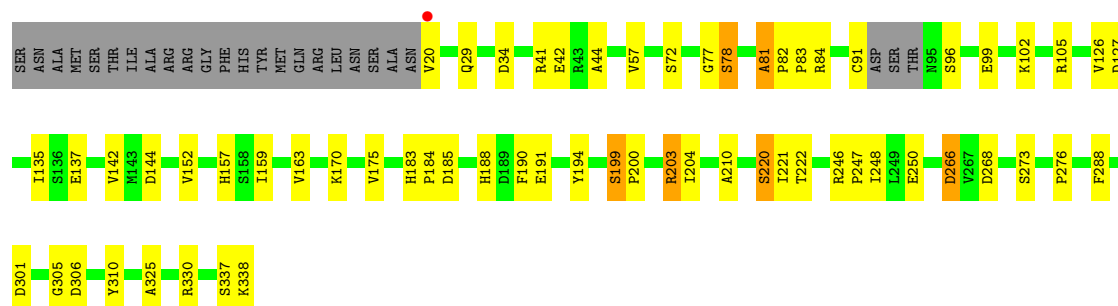
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	104	Total O 105 105	0	1
3	B	91	Total O 92 92	0	1
3	C	78	Total O 78 78	0	0
3	D	78	Total O 78 78	0	0
3	E	95	Total O 96 96	0	1
3	F	101	Total O 101 101	0	0

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.

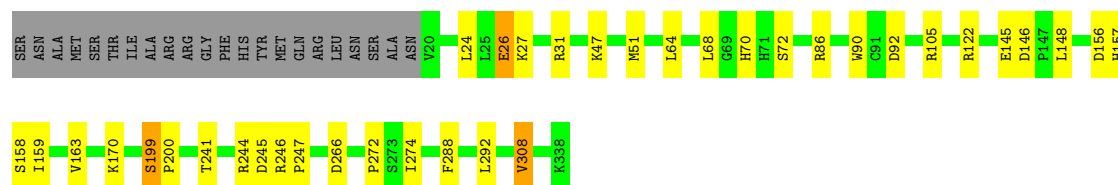
• Molecule 1: Arginase

Chain A: 



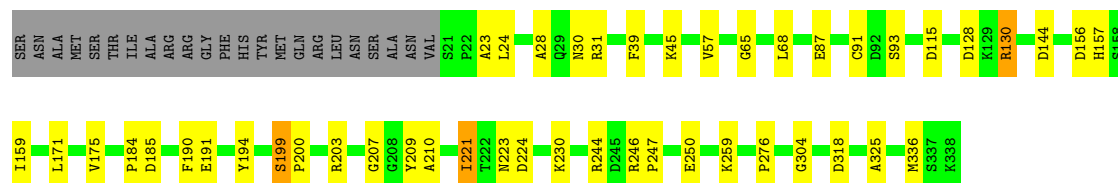
• Molecule 1: Arginase

Chain B: 



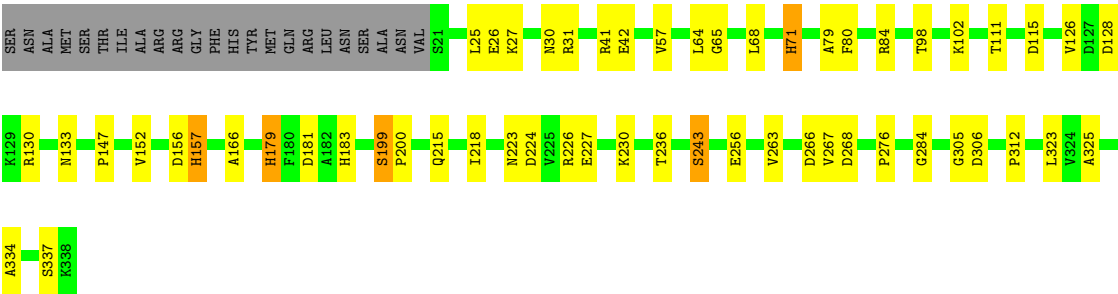
• Molecule 1: Arginase

Chain C: 

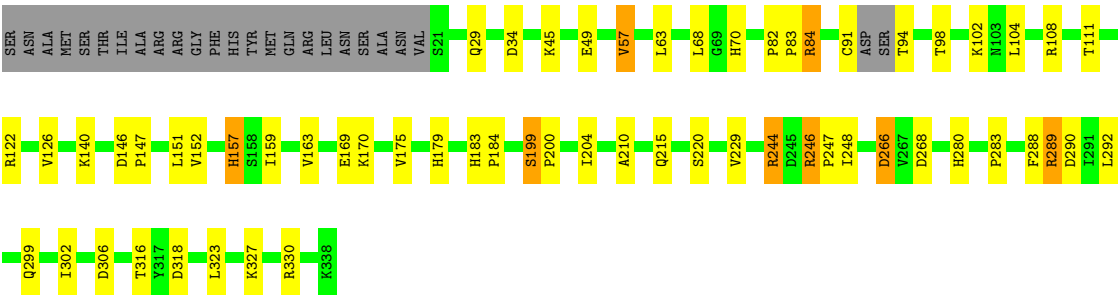


• Molecule 1: Arginase

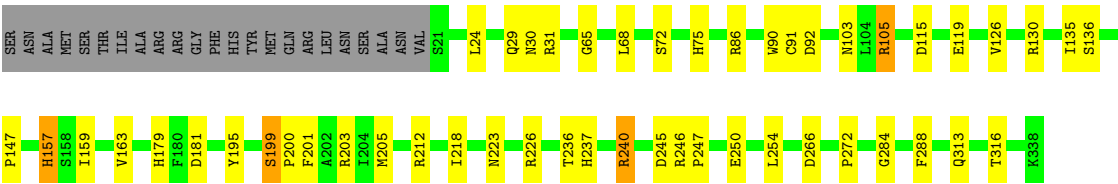
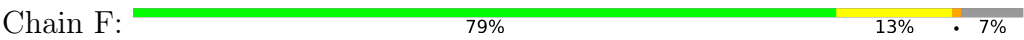
Chain D: 



• Molecule 1: Arginase



• Molecule 1: Arginase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.33Å 142.91Å 90.05Å 90.00° 115.90° 90.00°	Depositor
Resolution (Å)	44.55 – 1.93 44.55 – 1.93	Depositor EDS
% Data completeness (in resolution range)	95.9 (44.55-1.93) 95.1 (44.55-1.93)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.182 , 0.218 0.191 , 0.226	Depositor DCC
R_{free} test set	1040 reflections (0.80%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.240 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15295	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.25	10/2485 (0.4%)	1.49	16/3362 (0.5%)
1	B	1.21	2/2518 (0.1%)	1.43	4/3408 (0.1%)
1	C	1.25	3/2500 (0.1%)	1.48	6/3384 (0.2%)
1	D	1.26	8/2511 (0.3%)	1.49	9/3398 (0.3%)
1	E	1.25	6/2496 (0.2%)	1.47	7/3376 (0.2%)
1	F	1.26	6/2500 (0.2%)	1.49	10/3384 (0.3%)
All	All	1.25	35/15010 (0.2%)	1.48	52/20312 (0.3%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	HIS	CE1-NE2	10.39	1.43	1.32
1	E	183	HIS	CE1-NE2	7.48	1.40	1.32
1	B	272	PRO	C-O	-7.04	1.14	1.24
1	E	280	HIS	CE1-NE2	6.97	1.39	1.32
1	A	183	HIS	CG-ND1	6.87	1.45	1.38
1	F	136	SER	C-O	6.84	1.31	1.24
1	E	152	VAL	C-O	6.82	1.32	1.24
1	D	276	PRO	C-O	-6.52	1.15	1.24
1	E	157	HIS	CG-ND1	-6.24	1.31	1.38
1	E	289	ARG	C-O	6.19	1.31	1.24
1	D	325	ALA	C-O	-5.97	1.17	1.24
1	A	305	GLY	C-O	5.75	1.29	1.23
1	F	135	ILE	C-O	5.73	1.30	1.24
1	A	204	ILE	C-O	5.73	1.30	1.24
1	E	283	PRO	C-O	-5.67	1.17	1.23
1	A	135	ILE	C-O	-5.61	1.17	1.24
1	F	237	HIS	CE1-NE2	5.56	1.38	1.32
1	D	64	LEU	C-O	5.49	1.30	1.24
1	D	79	ALA	C-O	-5.46	1.17	1.24
1	D	179	HIS	C-O	5.41	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	ALA	C-O	5.39	1.30	1.24
1	D	323	LEU	C-O	-5.32	1.17	1.24
1	C	325	ALA	C-O	5.25	1.30	1.24
1	B	158	SER	C-O	5.25	1.30	1.24
1	C	39	PHE	C-O	5.23	1.30	1.24
1	A	44	ALA	C-O	5.19	1.30	1.24
1	A	83	PRO	C-O	-5.19	1.17	1.24
1	D	166	ALA	C-O	5.17	1.30	1.24
1	F	179	HIS	C-O	-5.15	1.18	1.24
1	F	288	PHE	C-O	-5.13	1.18	1.24
1	A	220	SER	C-O	5.13	1.29	1.23
1	C	276	PRO	C-O	-5.08	1.18	1.24
1	D	183	HIS	CE1-NE2	5.06	1.37	1.32
1	F	181	ASP	C-O	-5.04	1.17	1.23
1	A	276	PRO	C-O	-5.02	1.18	1.24

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ASP	CA-CB-CG	7.83	120.42	112.60
1	A	266	ASP	CA-CB-CG	6.81	119.41	112.60
1	E	266	ASP	CA-CB-CG	6.72	119.32	112.60
1	E	268	ASP	CA-CB-CG	6.70	119.30	112.60
1	A	77	GLY	CA-C-N	6.14	128.79	120.38
1	A	77	GLY	C-N-CA	6.14	128.79	120.38
1	D	111	THR	CA-CB-OG1	-6.08	100.47	109.60
1	A	288	PHE	CA-C-N	6.00	128.32	120.28
1	A	288	PHE	C-N-CA	6.00	128.32	120.28
1	A	34	ASP	CA-CB-CG	-5.94	106.66	112.60
1	E	34	ASP	CA-CB-CG	-5.90	106.70	112.60
1	A	81	ALA	O-C-N	-5.83	115.78	120.38
1	F	284	GLY	CA-C-N	-5.80	117.27	122.43
1	F	284	GLY	C-N-CA	-5.80	117.27	122.43
1	F	316	THR	CA-CB-OG1	-5.70	101.05	109.60
1	E	306	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	90	TRP	CB-CA-C	5.63	119.78	111.06
1	D	181	ASP	CA-CB-CG	5.57	118.17	112.60
1	E	290	ASP	N-CA-C	-5.53	105.15	111.07
1	D	268	ASP	CA-CB-CG	5.49	118.09	112.60
1	D	256	GLU	CB-CG-CD	5.49	121.93	112.60
1	C	250	GLU	CB-CG-CD	5.43	121.83	112.60
1	F	272	PRO	CA-C-N	5.41	127.53	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	272	PRO	C-N-CA	5.41	127.53	120.28
1	A	142	VAL	CA-C-N	5.40	127.78	120.38
1	A	142	VAL	C-N-CA	5.40	127.78	120.38
1	F	195	TYR	CA-C-N	5.39	128.36	120.71
1	F	195	TYR	C-N-CA	5.39	128.36	120.71
1	C	250	GLU	CB-CA-C	5.39	119.96	110.37
1	B	64	LEU	CA-C-N	5.38	126.13	120.43
1	B	64	LEU	C-N-CA	5.38	126.13	120.43
1	D	71	HIS	N-CA-C	-5.37	106.32	112.92
1	B	308	VAL	O-C-N	5.35	128.69	122.97
1	A	188	HIS	CA-CB-CG	-5.35	108.45	113.80
1	F	250	GLU	CB-CG-CD	5.32	121.64	112.60
1	C	128	ASP	CA-CB-CG	-5.28	107.32	112.60
1	A	188	HIS	N-CA-C	-5.25	105.45	111.07
1	C	157	HIS	CA-CB-CG	-5.25	108.55	113.80
1	D	133	ASN	CA-CB-CG	-5.20	107.40	112.60
1	C	223	ASN	CB-CA-C	5.19	119.67	110.85
1	A	127	ASP	CA-CB-CG	5.18	117.78	112.60
1	D	27	LYS	CA-C-N	5.17	127.16	120.44
1	D	27	LYS	C-N-CA	5.17	127.16	120.44
1	F	237	HIS	CA-C-N	5.16	129.95	121.39
1	F	237	HIS	C-N-CA	5.16	129.95	121.39
1	C	28	ALA	O-C-N	5.14	127.44	122.09
1	E	229	VAL	N-CA-C	-5.11	105.52	110.42
1	D	267	VAL	CA-C-O	-5.10	115.11	120.57
1	A	222	THR	CA-C-N	5.10	127.53	120.29
1	A	222	THR	C-N-CA	5.10	127.53	120.29
1	E	204	ILE	CA-C-O	-5.09	115.77	121.17
1	A	137	GLU	CA-C-O	-5.03	115.22	120.55

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	2441	0	2443	31	0
1	B	2470	0	2473	24	0
1	C	2455	0	2451	20	0
1	D	2463	0	2464	27	0
1	E	2449	0	2454	34	0
1	F	2455	0	2451	27	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
3	A	105	0	0	5	0
3	B	92	0	0	2	0
3	C	78	0	0	1	0
3	D	78	0	0	3	0
3	E	96	0	0	5	0
3	F	101	0	0	5	0
All	All	15295	0	14736	157	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 5.

All (157) 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:F:240:ARG:HG3	1:F:240:ARG:HH11	1.27	0.99
1:E:299:GLN:HG3	3:E:590:HOH:O	1.65	0.94
1:B:26:GLU:HG2	1:B:27:LYS:N	1.91	0.84
1:C:190:PHE:CE2	1:C:191:GLU:OE2	2.38	0.76
1:F:240:ARG:HH11	1:F:240:ARG:CG	1.98	0.74
1:B:27:LYS:O	1:B:31:ARG:HG3	1.89	0.72
1:A:247:PRO:HD2	3:A:552:HOH:O	1.89	0.71
1:E:84[A]:ARG:HD2	3:E:501:HOH:O	1.92	0.68
1:E:288:PHE:HZ	1:E:327:LYS:HG2	1.59	0.68
1:C:30:ASN:OD1	1:C:130:ARG:NH2	2.27	0.66
1:B:24:LEU:HD11	1:E:49:GLU:HB3	1.77	0.65
1:A:246:ARG:O	1:A:250:GLU:HG3	2.00	0.62
1:D:65:GLY:HA3	1:D:115:ASP:OD1	2.01	0.60
1:D:30:ASN:OD1	1:D:130:ARG:NH2	2.35	0.60
1:E:289:ARG:HB2	3:E:569:HOH:O	2.00	0.60
1:F:199:SER:N	1:F:200:PRO:CD	2.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84[A]:ARG:NH1	1:E:84[A]:ARG:HG3	2.17	0.59
1:A:81:ALA:HB2	1:A:310:TYR:O	2.03	0.58
1:D:84[B]:ARG:NE	3:D:501:HOH:O	2.26	0.57
1:F:90:TRP:HD1	3:F:595:HOH:O	1.87	0.56
1:E:70:HIS:CE1	1:E:122:ARG:HD3	2.40	0.56
1:C:199:SER:N	1:C:200:PRO:CD	2.69	0.55
1:D:152:VAL:O	1:D:306:ASP:HA	2.07	0.55
1:E:84[A]:ARG:CG	1:E:84[A]:ARG:HH11	2.19	0.55
1:B:70:HIS:CE1	1:B:122:ARG:HD2	2.42	0.54
1:D:41:ARG:NH1	1:D:42:GLU:OE2	2.32	0.54
1:E:288:PHE:CZ	1:E:327:LYS:HG2	2.41	0.54
1:B:159:ILE:O	1:B:163:VAL:HG23	2.07	0.54
1:E:94:THR:HG21	1:E:323:LEU:HD11	1.89	0.54
1:A:96:SER:HB3	1:A:105:ARG:CZ	2.39	0.53
1:D:243:SER:HB2	3:D:513:HOH:O	2.07	0.53
1:F:86:ARG:NH1	3:F:503:HOH:O	2.42	0.53
1:C:207:GLY:HA3	1:C:209:TYR:CE2	2.45	0.52
1:A:29:GLN:HG2	1:A:126:VAL:HG23	1.92	0.52
1:C:194:TYR:CZ	1:C:203:ARG:HD3	2.45	0.52
1:E:244:ARG:HD3	3:E:592:HOH:O	2.09	0.52
1:B:156:ASP:OD1	1:B:156:ASP:C	2.53	0.51
1:A:96:SER:HB3	1:A:105:ARG:NH2	2.25	0.51
1:C:175:VAL:O	1:C:210:ALA:HA	2.09	0.51
1:B:86:ARG:NH1	3:B:502:HOH:O	2.41	0.51
1:E:82:PRO:HB2	1:E:83:PRO:HD3	1.92	0.51
1:A:20:VAL:HG13	1:A:20:VAL:O	2.11	0.51
1:E:316:THR:OG1	1:E:318:ASP:OD1	2.27	0.50
1:E:199:SER:N	1:E:200:PRO:CD	2.74	0.50
1:A:248:ILE:HG13	3:A:552:HOH:O	2.10	0.50
1:A:301:ASP:OD1	1:A:338:LYS:NZ	2.41	0.50
1:B:68:LEU:C	1:B:68:LEU:HD23	2.37	0.50
1:B:199:SER:N	1:B:200:PRO:CD	2.74	0.50
1:C:65:GLY:HA3	1:C:115:ASP:OD1	2.12	0.50
1:D:68:LEU:C	1:D:68:LEU:HD23	2.37	0.50
1:B:72:SER:HB3	3:B:552:HOH:O	2.13	0.49
1:F:199:SER:N	1:F:200:PRO:HD2	2.26	0.49
1:D:284:GLY:HA2	3:F:563:HOH:O	2.13	0.49
1:D:199:SER:N	1:D:200:PRO:CD	2.75	0.49
1:F:218:ILE:HG13	1:F:236:THR:HG23	1.95	0.49
1:D:224:ASP:O	1:D:227:GLU:HB2	2.12	0.48
1:E:84[A]:ARG:NH1	1:E:84[A]:ARG:CG	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:LEU:O	1:D:26:GLU:C	2.55	0.48
1:C:23:ALA:O	1:C:24:LEU:C	2.56	0.48
1:C:184:PRO:HG2	1:C:221:ILE:HD12	1.95	0.48
1:A:199:SER:N	1:A:200:PRO:CD	2.77	0.48
1:F:75:HIS:HE1	1:F:313:GLN:OE1	1.96	0.48
1:D:98:THR:HG21	1:D:334:ALA:HB2	1.94	0.48
1:F:91:CYS:SG	1:F:92:ASP:N	2.88	0.47
1:D:157:HIS:CE1	1:D:266:ASP:HB2	2.50	0.47
1:A:273:SER:HB3	1:B:274:ILE:HD13	1.97	0.47
1:B:145:GLU:O	1:B:148:LEU:HG	2.14	0.47
1:C:68:LEU:C	1:C:68:LEU:HD23	2.39	0.47
1:E:179:HIS:O	1:E:215:GLN:HA	2.15	0.47
1:F:159:ILE:O	1:F:163:VAL:HG23	2.15	0.46
1:B:199:SER:N	1:B:200:PRO:HD2	2.30	0.46
1:B:105:ARG:HG2	1:B:105:ARG:HH11	1.80	0.46
1:E:84[A]:ARG:HG3	1:E:84[A]:ARG:HH11	1.79	0.46
1:F:212:ARG:NH1	1:F:254:LEU:HD23	2.31	0.46
1:F:201:PHE:O	1:F:205:MET:HG2	2.15	0.46
1:D:80:PHE:HB2	1:D:312:PRO:HG2	1.97	0.46
1:A:190:PHE:CE1	1:A:191:GLU:HG3	2.50	0.46
1:A:221:ILE:O	1:A:221:ILE:HG23	2.16	0.46
1:D:218:ILE:HG13	1:D:236:THR:HG23	1.98	0.46
1:E:63:LEU:HA	1:E:151:LEU:O	2.16	0.46
1:C:199:SER:N	1:C:200:PRO:HD2	2.31	0.45
1:A:194:TYR:CZ	1:A:203:ARG:HD2	2.51	0.45
1:C:156:ASP:O	1:C:159:ILE:HG12	2.16	0.45
1:D:126:VAL:HG13	1:D:130:ARG:HG2	1.98	0.45
1:F:72:SER:HB3	3:F:561:HOH:O	2.15	0.45
1:F:240:ARG:HG3	1:F:240:ARG:NH1	2.07	0.45
1:E:104:LEU:HD11	1:E:330:ARG:NE	2.31	0.45
1:F:24:LEU:O	1:F:24:LEU:HD12	2.16	0.45
1:A:157:HIS:CE1	1:A:266:ASP:HB2	2.52	0.45
1:A:42:GLU:CD	1:D:31:ARG:HH21	2.25	0.45
1:F:119:GLU:HG3	3:F:585:HOH:O	2.16	0.45
1:B:246:ARG:N	1:B:247:PRO:CD	2.79	0.45
1:D:199:SER:N	1:D:200:PRO:HD2	2.31	0.45
1:F:68:LEU:HD23	1:F:68:LEU:C	2.42	0.45
1:A:84:ARG:NH1	1:D:84[B]:ARG:NH2	2.65	0.44
1:E:244:ARG:CD	3:E:592:HOH:O	2.66	0.44
1:A:78:SER:HB2	3:A:536:HOH:O	2.16	0.44
1:E:199:SER:H	1:E:200:PRO:CD	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:SER:O	1:B:200:PRO:C	2.58	0.44
1:D:84[B]:ARG:NH2	3:D:501:HOH:O	2.48	0.44
1:E:98:THR:OG1	1:E:102:LYS:HB2	2.18	0.44
1:A:175:VAL:O	1:A:210:ALA:HA	2.18	0.44
1:F:157:HIS:CE1	1:F:266:ASP:HB2	2.53	0.43
1:A:102:LYS:NZ	1:A:337:SER:O	2.51	0.43
1:C:318:ASP:OD1	1:C:318:ASP:N	2.46	0.43
1:E:140:LYS:NZ	1:E:169:GLU:OE1	2.44	0.43
1:F:65:GLY:HA3	1:F:115:ASP:OD1	2.18	0.43
1:E:175:VAL:O	1:E:210:ALA:HA	2.17	0.43
1:E:184:PRO:HD3	1:E:220:SER:O	2.18	0.43
1:C:185:ASP:HB3	1:C:200:PRO:HD2	2.00	0.43
1:C:246:ARG:HB2	1:C:247:PRO:HD3	2.01	0.43
1:A:246:ARG:N	1:A:247:PRO:CD	2.82	0.43
1:F:246:ARG:N	1:F:247:PRO:CD	2.82	0.43
1:A:96:SER:CB	1:A:105:ARG:NH1	2.82	0.43
1:A:184:PRO:HD3	1:A:220:SER:O	2.19	0.43
1:A:273:SER:CB	1:B:274:ILE:HD13	2.49	0.43
1:C:244:ARG:HD2	3:C:576:HOH:O	2.18	0.43
1:D:71:HIS:HE1	1:D:128:ASP:OD2	2.02	0.43
1:B:47:LYS:O	1:B:51:MET:HG2	2.19	0.42
1:B:244:ARG:HG3	1:B:245:ASP:N	2.34	0.42
1:F:223:ASN:HA	1:F:226:ARG:HG3	2.01	0.42
1:C:199:SER:H	1:C:200:PRO:CD	2.33	0.42
1:D:156:ASP:C	1:D:156:ASP:OD1	2.62	0.42
1:E:29:GLN:HG2	1:E:126:VAL:HG23	2.01	0.42
1:B:157:HIS:CE1	1:B:266:ASP:HB2	2.53	0.42
1:F:240:ARG:CG	1:F:240:ARG:NH1	2.66	0.42
1:E:288:PHE:HZ	1:E:327:LYS:CG	2.28	0.42
1:B:157:HIS:CG	1:B:308:VAL:HG21	2.55	0.42
1:D:263:VAL:O	1:D:305:GLY:HA2	2.20	0.42
1:A:91:CYS:SG	1:A:91:CYS:O	2.78	0.42
1:A:159:ILE:O	1:A:163:VAL:HG23	2.20	0.42
1:C:45:LYS:HE3	1:F:31:ARG:NH1	2.35	0.42
1:E:246:ARG:CB	1:E:247:PRO:HD3	2.50	0.42
1:B:241:THR:O	1:B:244:ARG:HG2	2.20	0.41
1:A:330:ARG:NH1	3:A:501:HOH:O	2.52	0.41
1:A:185:ASP:HB3	1:A:200:PRO:HD2	2.02	0.41
1:E:68:LEU:C	1:E:68:LEU:HD23	2.45	0.41
1:A:72:SER:HB3	3:A:569:HOH:O	2.20	0.41
1:E:57:VAL:HG11	1:E:108:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:HIS:CE1	1:E:266:ASP:HB2	2.55	0.41
1:F:30:ASN:OD1	1:F:130:ARG:NH2	2.53	0.41
1:B:157:HIS:CD2	1:B:308:VAL:HG21	2.55	0.41
1:D:25:LEU:HD23	1:D:25:LEU:HA	1.93	0.41
1:F:29:GLN:HG2	1:F:126:VAL:HG22	2.03	0.41
1:C:171:LEU:O	1:C:259:LYS:HE3	2.21	0.41
1:A:152:VAL:O	1:A:306:ASP:HA	2.20	0.41
1:C:304:GLY:HA2	1:C:336:MET:SD	2.60	0.41
1:F:245:ASP:O	1:F:246:ARG:C	2.63	0.41
1:A:81:ALA:O	1:A:82:PRO:C	2.62	0.40
1:E:170:LYS:HB2	1:E:170:LYS:HE2	1.87	0.40
1:F:103:ASN:HD21	1:F:105:ARG:HB2	1.86	0.40
1:B:288:PHE:HE2	1:B:292:LEU:HD11	1.86	0.40
1:D:102:LYS:NZ	1:D:337:SER:O	2.54	0.40
1:D:223:ASN:O	1:D:226:ARG:HB2	2.22	0.40
1:E:146:ASP:HA	1:E:147:PRO:HA	1.88	0.40
1:D:179:HIS:O	1:D:215:GLN:HA	2.21	0.40
1:E:159:ILE:O	1:E:163:VAL:HG23	2.21	0.40

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	312/341 (92%)	302 (97%)	9 (3%)	1 (0%)	36	30
1	B	318/341 (93%)	301 (95%)	16 (5%)	1 (0%)	36	30
1	C	316/341 (93%)	298 (94%)	17 (5%)	1 (0%)	36	30
1	D	317/341 (93%)	304 (96%)	12 (4%)	1 (0%)	36	30
1	E	313/341 (92%)	305 (97%)	7 (2%)	1 (0%)	36	30
1	F	316/341 (93%)	302 (96%)	13 (4%)	1 (0%)	36	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1892/2046 (92%)	1812 (96%)	74 (4%)	6 (0%)	36 30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	199	SER
1	E	199	SER
1	A	199	SER
1	D	199	SER
1	B	199	SER
1	F	199	SER

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	265/286 (93%)	258 (97%)	7 (3%)	40 28
1	B	269/286 (94%)	265 (98%)	4 (2%)	57 49
1	C	267/286 (93%)	257 (96%)	10 (4%)	30 16
1	D	268/286 (94%)	263 (98%)	5 (2%)	50 40
1	E	266/286 (93%)	255 (96%)	11 (4%)	27 14
1	F	267/286 (93%)	262 (98%)	5 (2%)	50 40
All	All	1602/1716 (93%)	1560 (97%)	42 (3%)	40 28

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	57	VAL
1	A	78	SER
1	A	99	GLU
1	A	144	ASP
1	A	170	LYS

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Mol	Chain	Res	Type
1	A	203	ARG
1	B	26	GLU
1	B	92	ASP
1	B	146	ASP
1	B	170	LYS
1	C	31	ARG
1	C	57	VAL
1	C	87	GLU
1	C	91	CYS
1	C	93	SER
1	C	130	ARG
1	C	144	ASP
1	C	221	ILE
1	C	224	ASP
1	C	230	LYS
1	D	57	VAL
1	D	147	PRO
1	D	157	HIS
1	D	230	LYS
1	D	243	SER
1	E	45	LYS
1	E	57	VAL
1	E	84[A]	ARG
1	E	84[B]	ARG
1	E	91	CYS
1	E	111	THR
1	E	244	ARG
1	E	246	ARG
1	E	248	ILE
1	E	292	LEU
1	E	302	ILE
1	F	105	ARG
1	F	147	PRO
1	F	157	HIS
1	F	203	ARG
1	F	240	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	228	GLN

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Mol	Chain	Res	Type
1	B	188	HIS
1	B	215	GLN
1	B	223	ASN
1	C	215	GLN
1	D	215	GLN
1	E	70	HIS
1	E	103	ASN
1	E	215	GLN
1	F	112	ASN
1	F	215	GLN

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 12 ligands modelled in this entry, 12 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 ⓘ

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, 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	316/341 (92%)	-1.24	1 (0%) 90 93	21, 33, 58, 99	0
1	B	319/341 (93%)	-1.22	0 100 100	16, 35, 54, 71	1 (0%)
1	C	318/341 (93%)	-1.21	0 100 100	21, 33, 67, 87	0
1	D	318/341 (93%)	-1.21	0 100 100	14, 34, 58, 79	1 (0%)
1	E	316/341 (92%)	-1.25	0 100 100	16, 34, 56, 81	1 (0%)
1	F	318/341 (93%)	-1.17	0 100 100	21, 32, 68, 88	0
All	All	1905/2046 (93%)	-1.22	1 (0%) 92 94	14, 34, 62, 99	3 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	VAL	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](#)

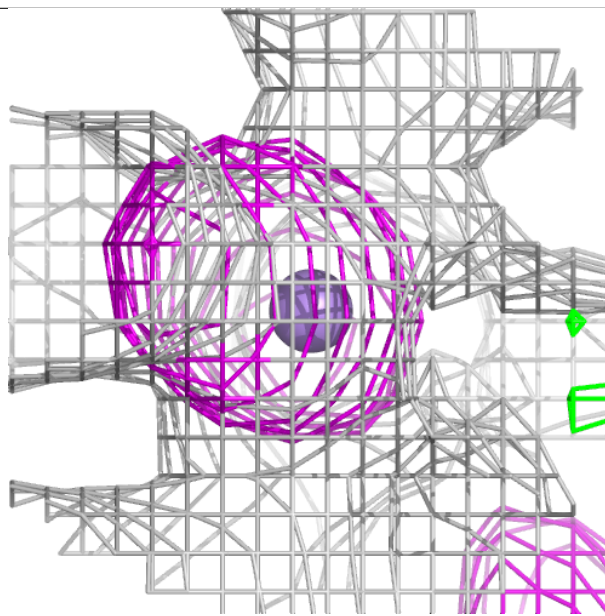
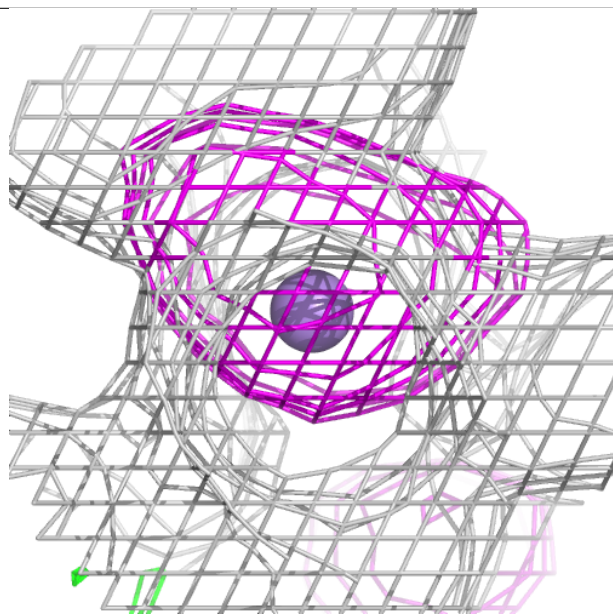
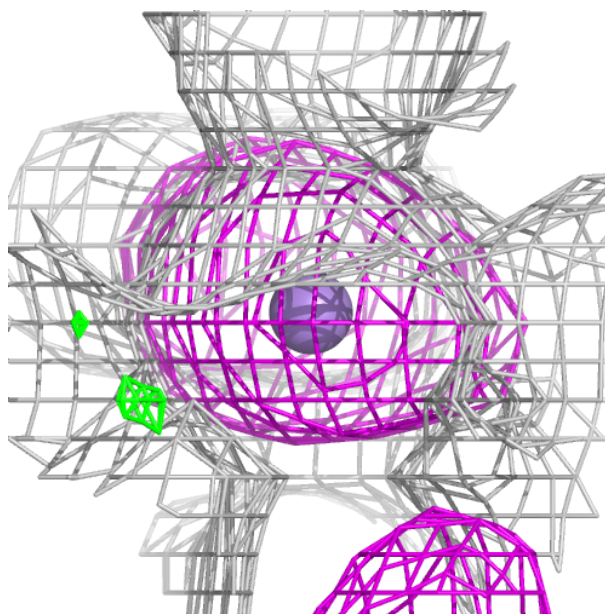
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	A	401	1/1	1.00	0.05	27,27,27,27	0
2	MN	A	402	1/1	1.00	0.04	29,29,29,29	0
2	MN	B	401	1/1	1.00	0.03	29,29,29,29	0
2	MN	B	402	1/1	1.00	0.02	34,34,34,34	0
2	MN	C	401	1/1	1.00	0.03	33,33,33,33	0
2	MN	C	402	1/1	1.00	0.04	37,37,37,37	0
2	MN	D	401	1/1	1.00	0.04	29,29,29,29	0
2	MN	D	402	1/1	1.00	0.04	36,36,36,36	0
2	MN	E	401	1/1	1.00	0.05	25,25,25,25	0
2	MN	E	402	1/1	1.00	0.02	27,27,27,27	0
2	MN	F	401	1/1	1.00	0.04	33,33,33,33	0
2	MN	F	402	1/1	1.00	0.08	43,43,43,43	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

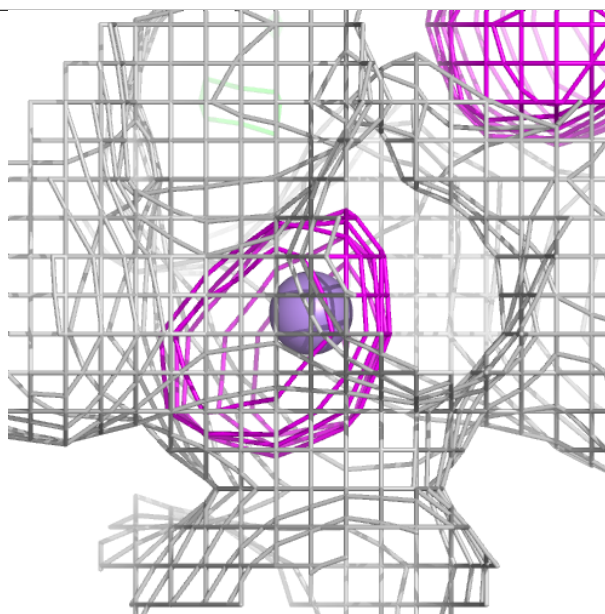
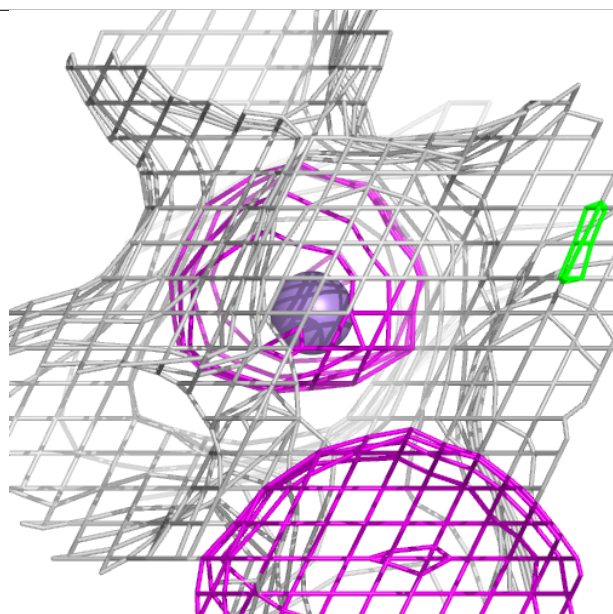
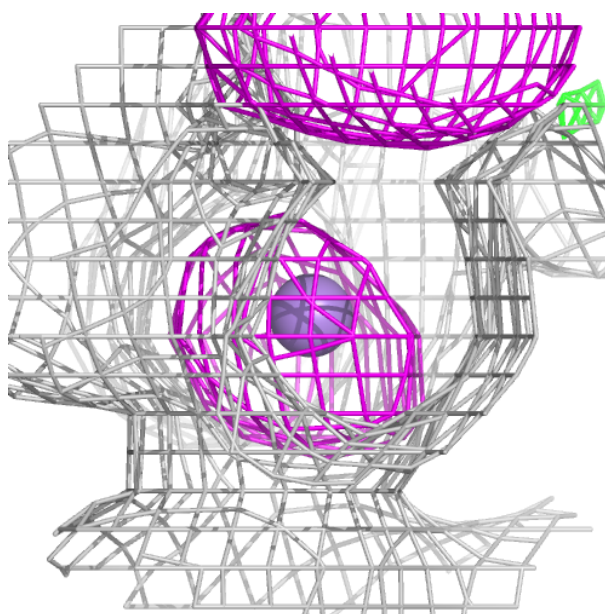
Electron density around MN A 401:

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



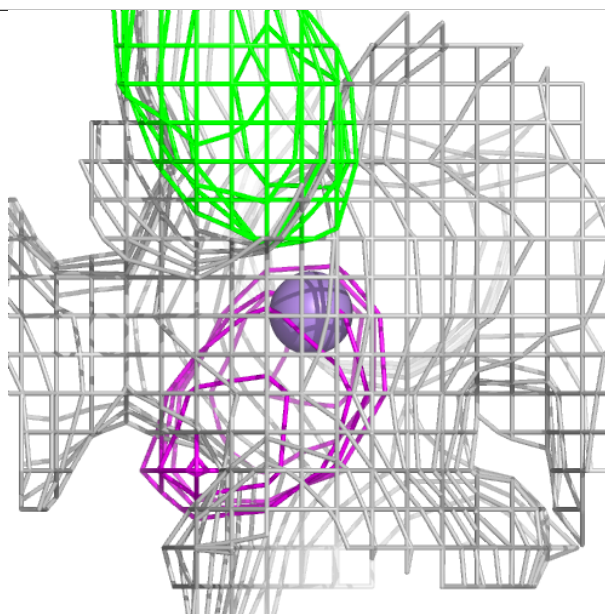
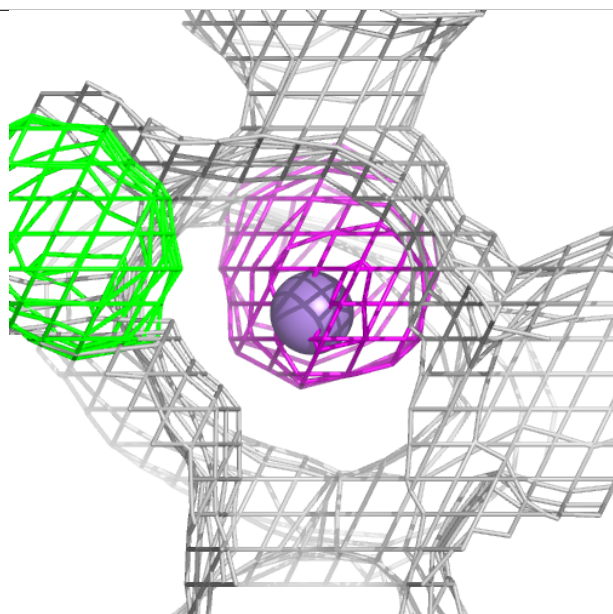
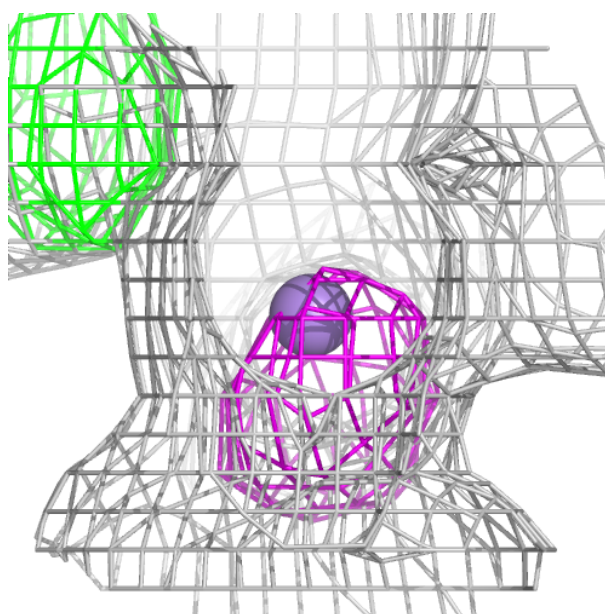
Electron density around MN A 402:

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



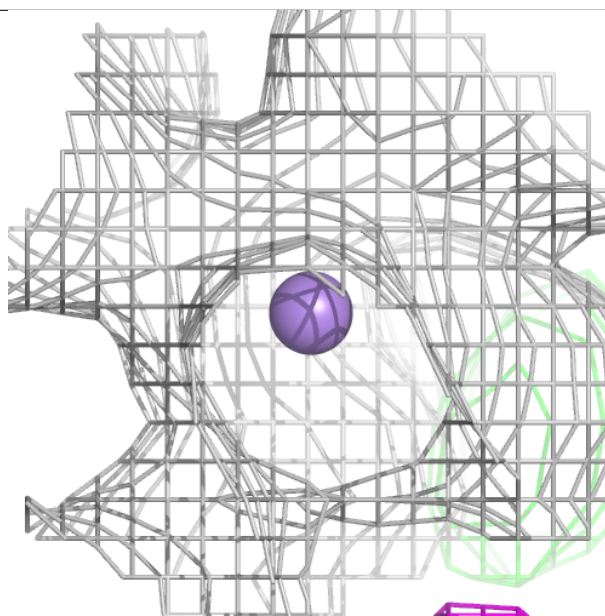
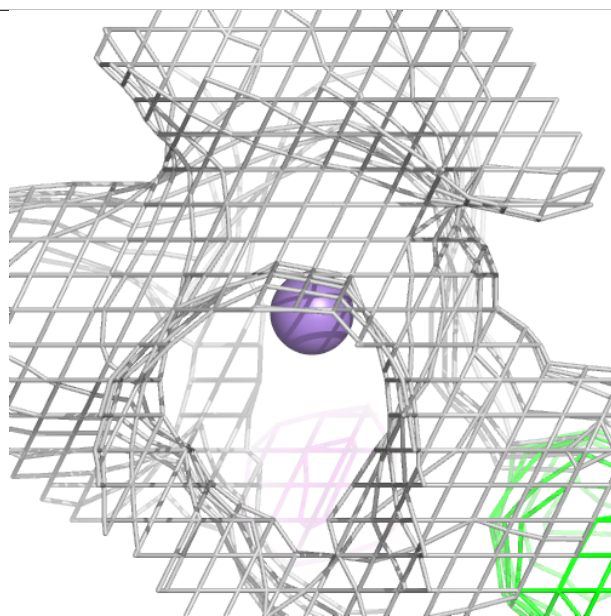
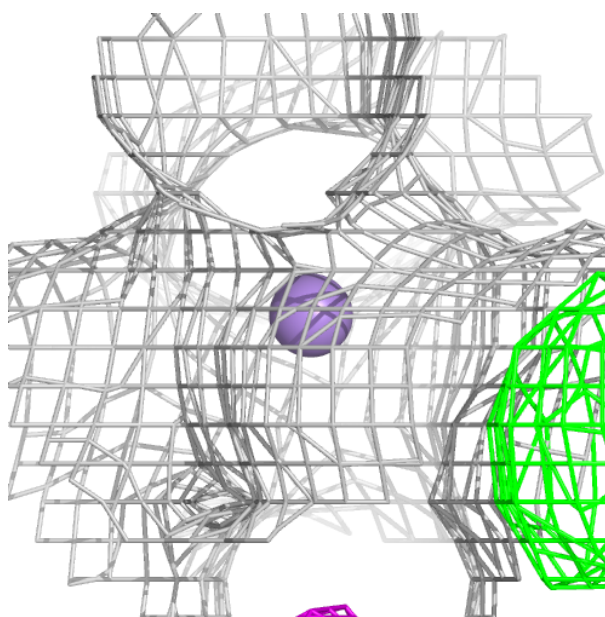
Electron density around MN B 401:

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



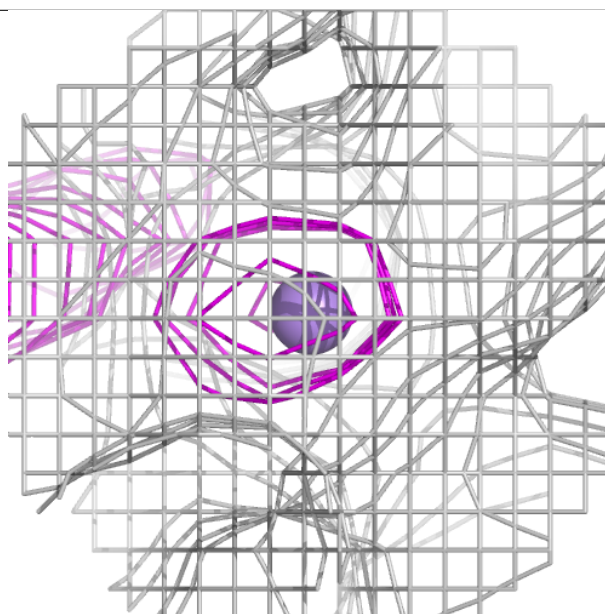
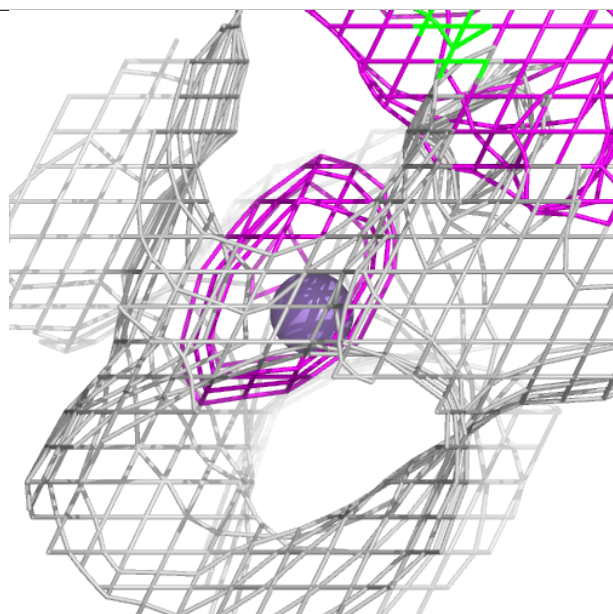
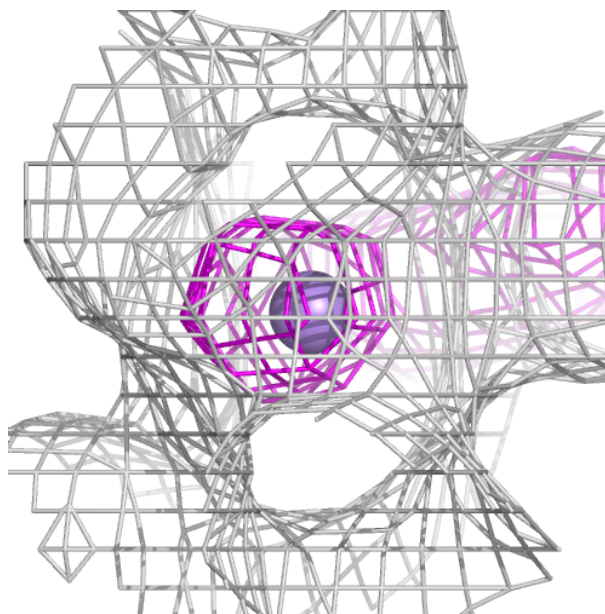
Electron density around MN B 402:

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



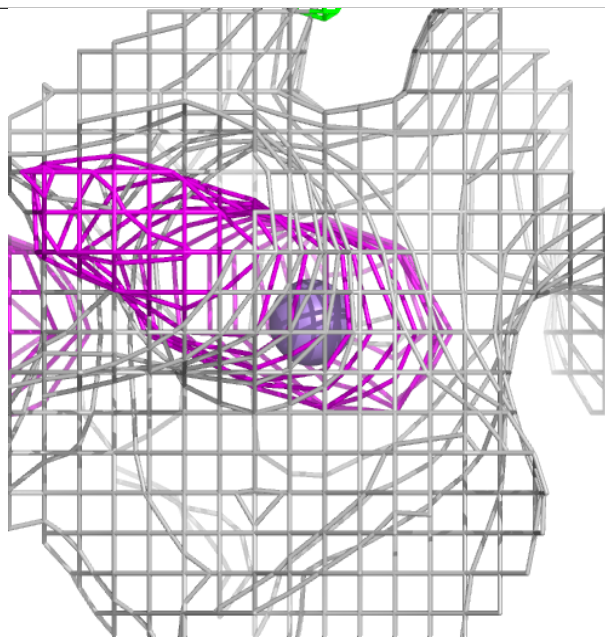
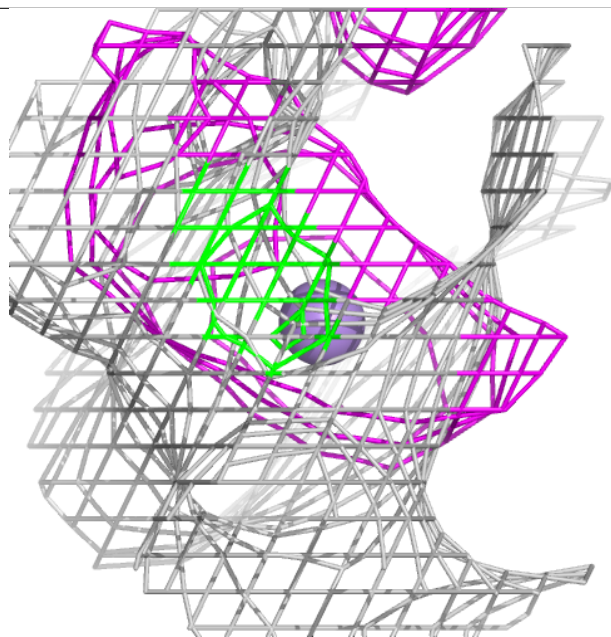
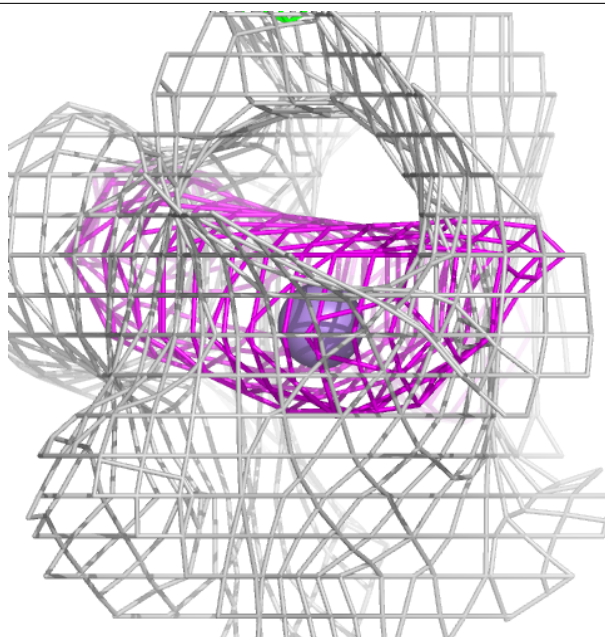
Electron density around MN C 401:

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



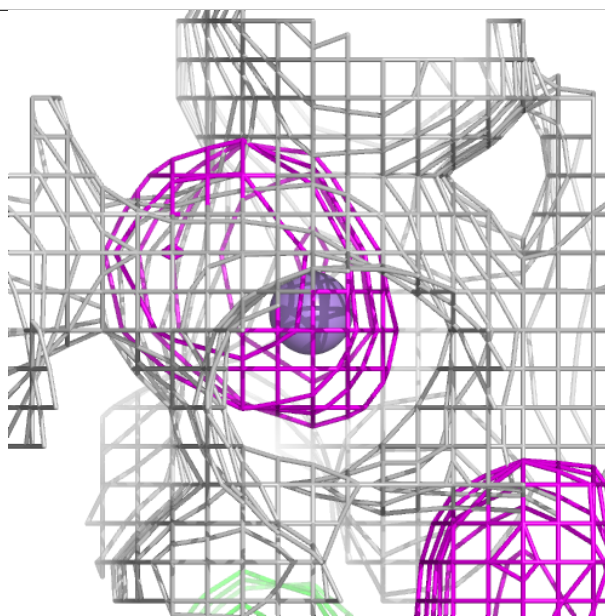
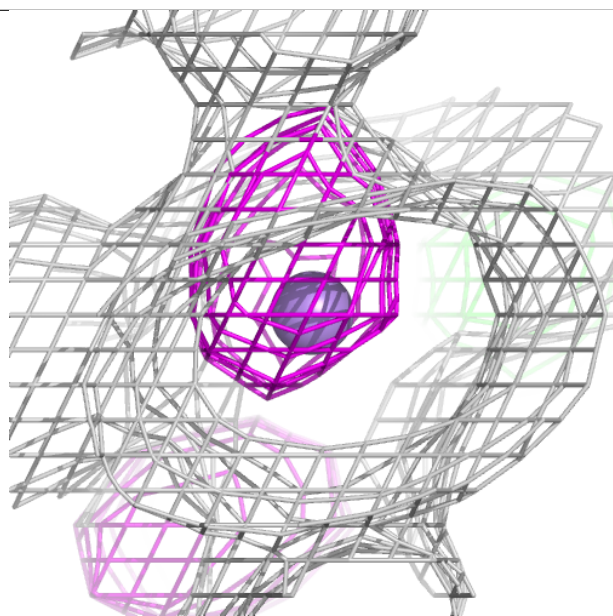
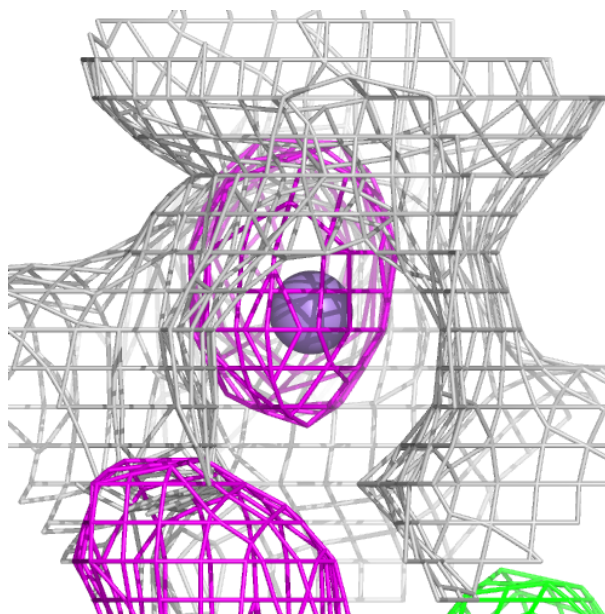
Electron density around MN C 402:

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



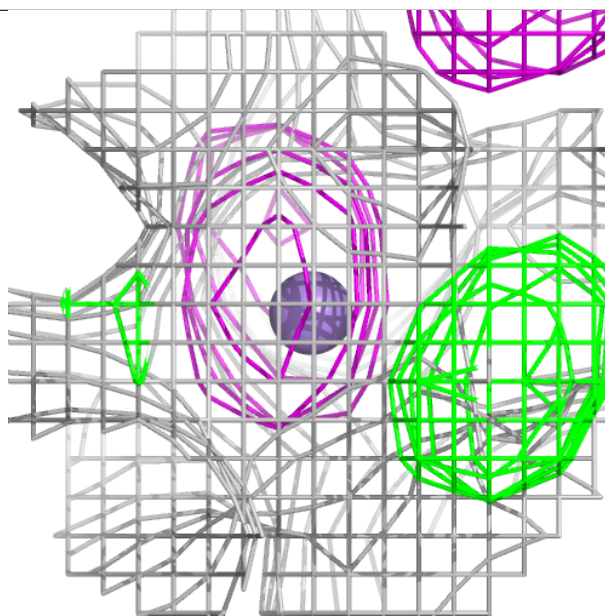
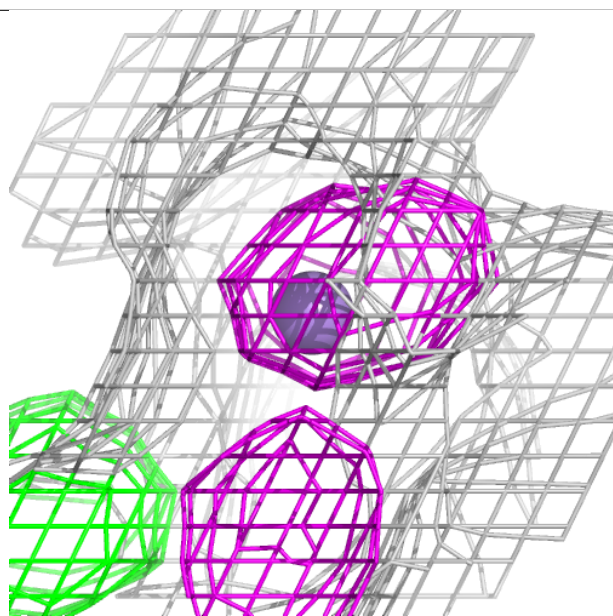
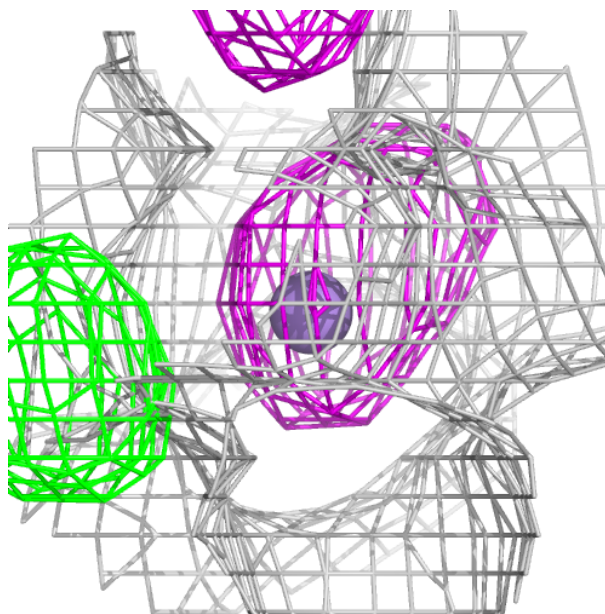
Electron density around MN D 401:

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



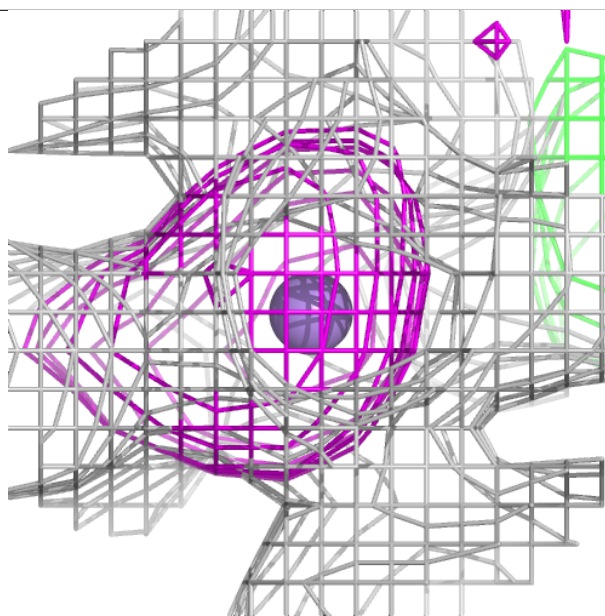
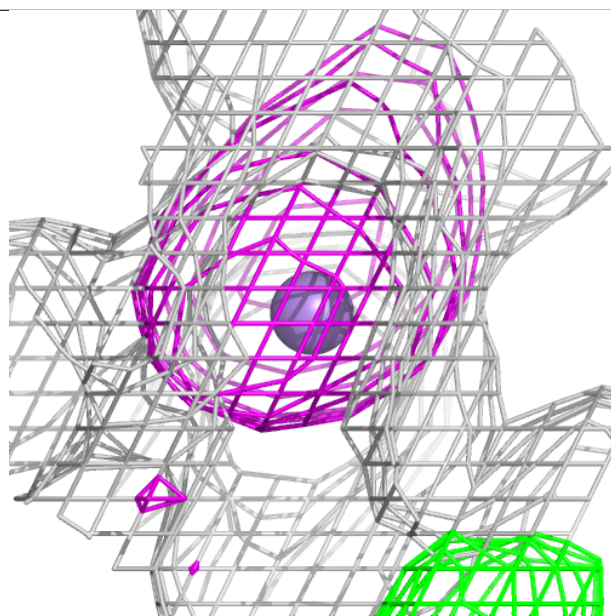
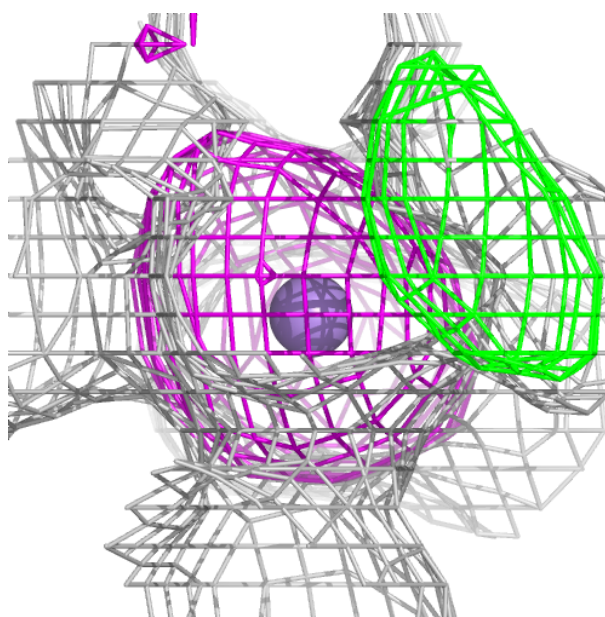
Electron density around MN D 402:

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



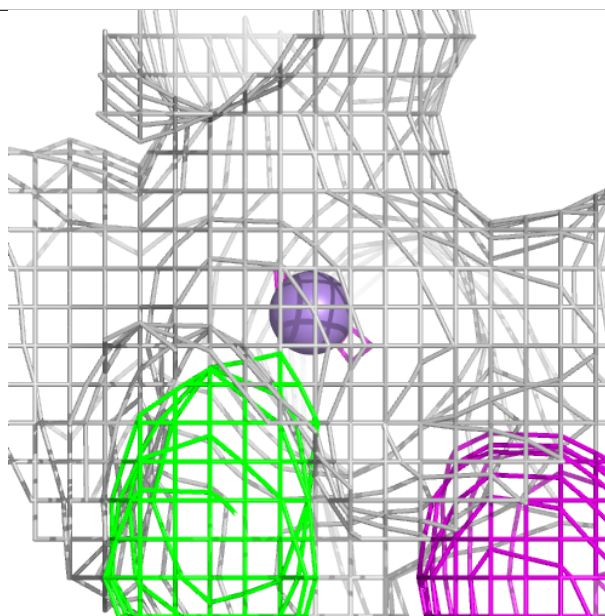
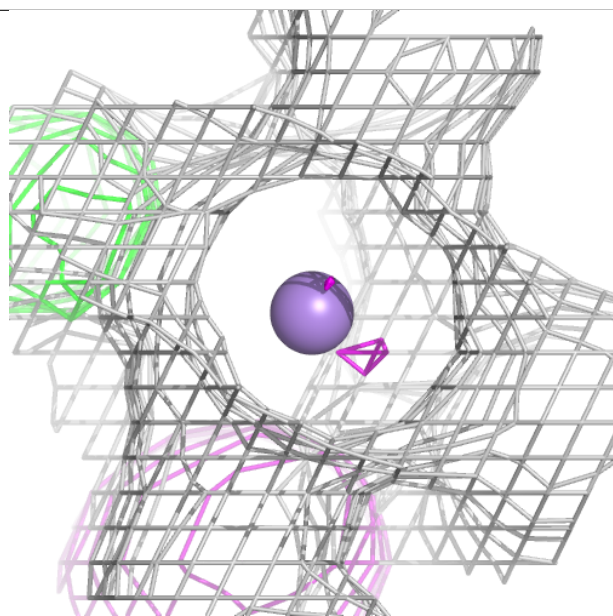
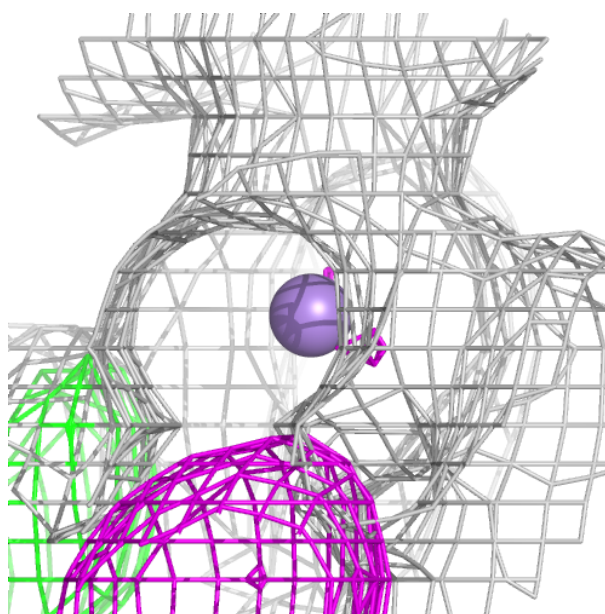
Electron density around MN E 401:

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



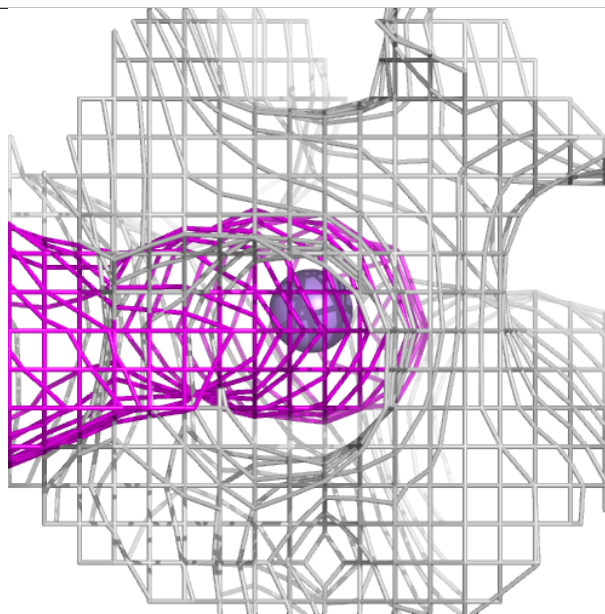
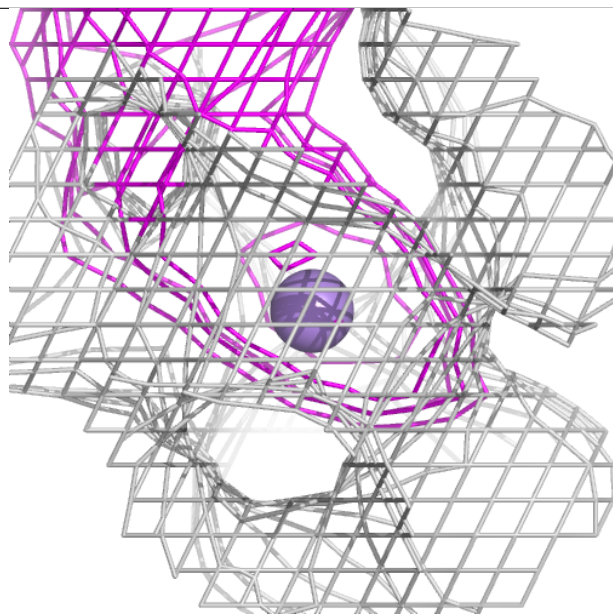
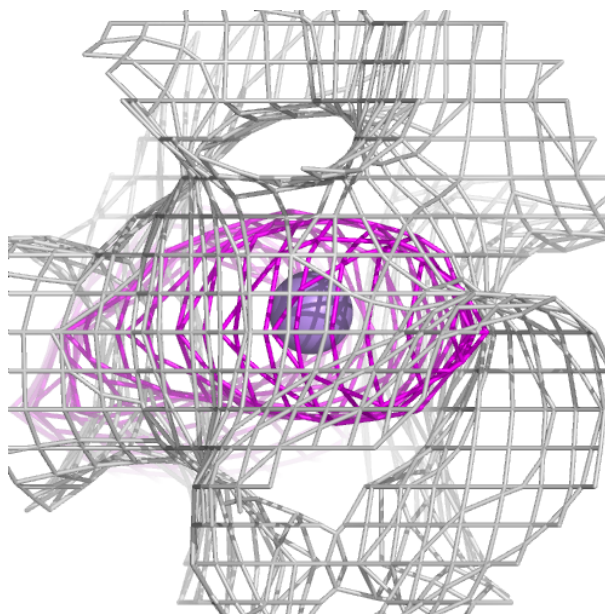
Electron density around MN E 402:

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



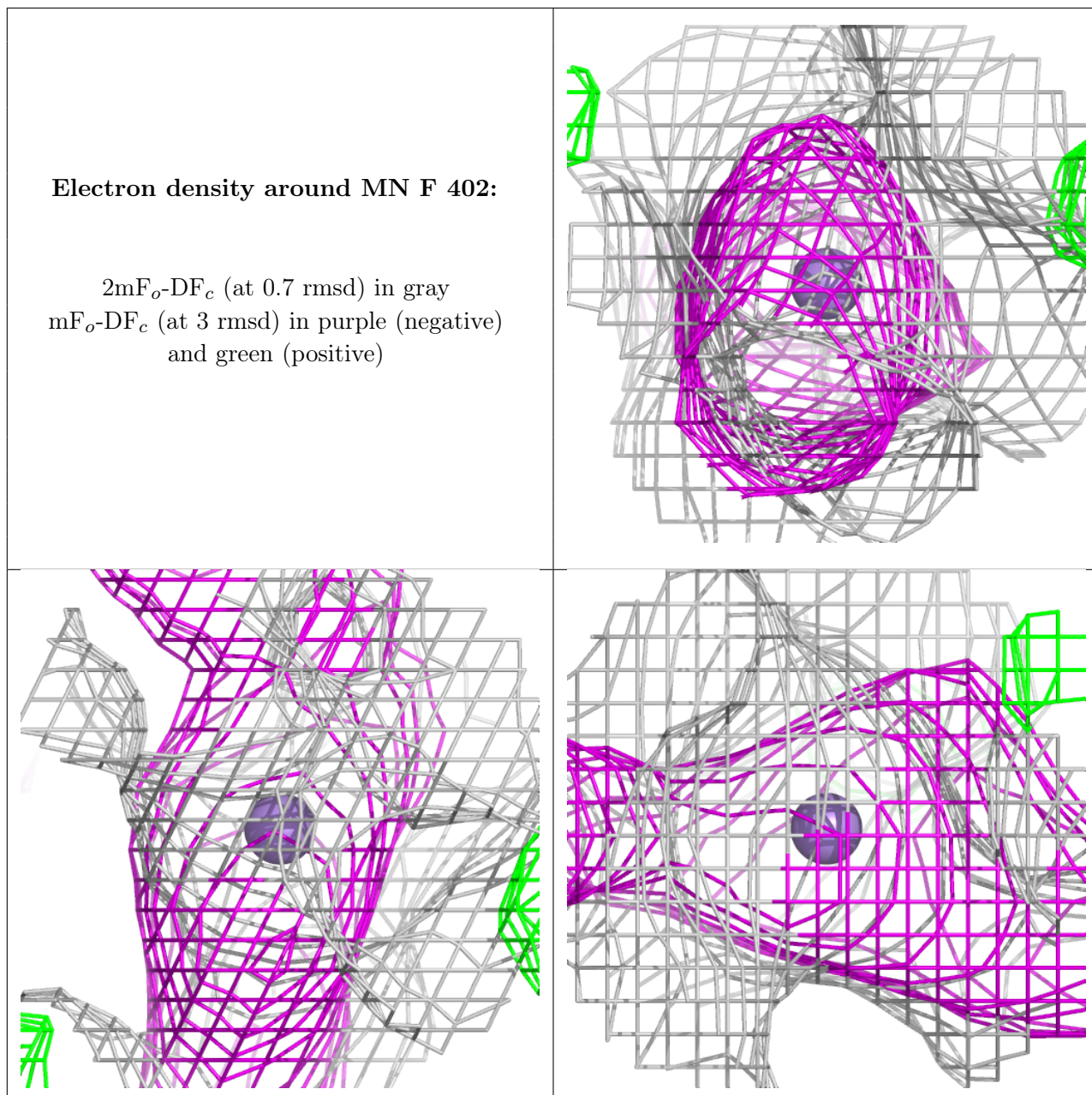
Electron density around MN F 401:

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



Electron density around MN 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.