



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:07 PM UTC

PDB ID : 6VSU / pdb_00006vsu
Title : Arginase from Arabidopsis thaliana in Complex with Ornithine
Authors : Sekula, B.
Deposited on : 2020-02-11
Resolution : 2.25 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

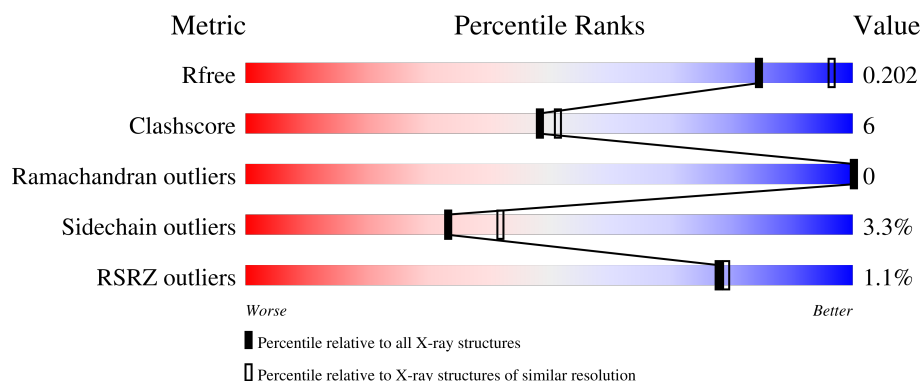
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	321	2% 81%16%..
1	B	321	87%12%.
1	C	321	4% 61%32%..
1	D	321	86%11%..
1	E	321	% 89%9%..

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Mol	Chain	Length	Quality of chain
1	F	321	 90% 8% .
1	G	321	 87% 12% .
1	H	321	 88% 11% .
1	I	321	 89% 8% ..
1	J	321	 86% 12% ..
1	K	321	 86% 12% ..
1	L	321	 85% 12% ..
1	M	321	 4% 71% 23% . .
1	N	321	 85% 13% ..
1	O	321	 3% 77% 19% . .
1	P	321	 88% 10% ..
1	Q	321	 88% 10% .
1	R	321	 88% 9% ..
1	S	321	 85% 12% ..
1	T	321	 85% 12% ..
1	U	321	 85% 12% ..
1	V	321	 4% 69% 26% . .
1	W	321	 2% 82% 16% ..
1	X	321	 85% 13% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 63508 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 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	1	0
			2426	1517	432	465	12			
1	B	317	Total	C	N	O	S	0	0	0
			2426	1516	433	466	11			
1	C	316	Total	C	N	O	S	0	2	0
			2431	1521	432	465	13			
1	D	316	Total	C	N	O	S	0	0	0
			2421	1513	432	465	11			
1	E	318	Total	C	N	O	S	0	0	0
			2431	1519	434	467	11			
1	F	316	Total	C	N	O	S	0	1	0
			2426	1516	433	466	11			
1	G	316	Total	C	N	O	S	0	1	0
			2427	1517	432	467	11			
1	H	317	Total	C	N	O	S	0	0	0
			2426	1516	433	466	11			
1	I	316	Total	C	N	O	S	0	0	0
			2421	1513	432	465	11			
1	J	317	Total	C	N	O	S	0	0	0
			2426	1516	433	466	11			
1	K	316	Total	C	N	O	S	0	0	0
			2421	1513	432	465	11			
1	L	317	Total	C	N	O	S	0	0	0
			2426	1516	433	466	11			
1	M	316	Total	C	N	O	S	0	0	0
			2421	1513	432	465	11			
1	N	316	Total	C	N	O	S	0	0	0
			2421	1513	432	465	11			
1	O	316	Total	C	N	O	S	0	0	0
			2421	1513	432	465	11			
1	P	316	Total	C	N	O	S	0	0	0
			2421	1513	432	465	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	316	Total	C	N	O	S	0	0	0
			2421	1513	432	465	11			
1	R	316	Total	C	N	O	S	0	1	0
			2429	1518	435	465	11			
1	S	316	Total	C	N	O	S	0	0	0
			2421	1513	432	465	11			
1	T	318	Total	C	N	O	S	0	0	0
			2432	1519	434	468	11			
1	U	316	Total	C	N	O	S	0	1	0
			2426	1518	432	465	11			
1	V	316	Total	C	N	O	S	0	0	0
			2421	1513	432	465	11			
1	W	317	Total	C	N	O	S	0	0	0
			2426	1516	433	466	11			
1	X	316	Total	C	N	O	S	0	0	0
			2421	1513	432	465	11			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	-	expression tag	UNP P46637
A	23	ASN	-	expression tag	UNP P46637
A	24	ALA	-	expression tag	UNP P46637
B	22	SER	-	expression tag	UNP P46637
B	23	ASN	-	expression tag	UNP P46637
B	24	ALA	-	expression tag	UNP P46637
C	22	SER	-	expression tag	UNP P46637
C	23	ASN	-	expression tag	UNP P46637
C	24	ALA	-	expression tag	UNP P46637
D	22	SER	-	expression tag	UNP P46637
D	23	ASN	-	expression tag	UNP P46637
D	24	ALA	-	expression tag	UNP P46637
E	22	SER	-	expression tag	UNP P46637
E	23	ASN	-	expression tag	UNP P46637
E	24	ALA	-	expression tag	UNP P46637
F	22	SER	-	expression tag	UNP P46637
F	23	ASN	-	expression tag	UNP P46637
F	24	ALA	-	expression tag	UNP P46637
G	22	SER	-	expression tag	UNP P46637
G	23	ASN	-	expression tag	UNP P46637
G	24	ALA	-	expression tag	UNP P46637
H	22	SER	-	expression tag	UNP P46637
H	23	ASN	-	expression tag	UNP P46637

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Chain	Residue	Modelled	Actual	Comment	Reference
H	24	ALA	-	expression tag	UNP P46637
I	22	SER	-	expression tag	UNP P46637
I	23	ASN	-	expression tag	UNP P46637
I	24	ALA	-	expression tag	UNP P46637
J	22	SER	-	expression tag	UNP P46637
J	23	ASN	-	expression tag	UNP P46637
J	24	ALA	-	expression tag	UNP P46637
K	22	SER	-	expression tag	UNP P46637
K	23	ASN	-	expression tag	UNP P46637
K	24	ALA	-	expression tag	UNP P46637
L	22	SER	-	expression tag	UNP P46637
L	23	ASN	-	expression tag	UNP P46637
L	24	ALA	-	expression tag	UNP P46637
M	22	SER	-	expression tag	UNP P46637
M	23	ASN	-	expression tag	UNP P46637
M	24	ALA	-	expression tag	UNP P46637
N	22	SER	-	expression tag	UNP P46637
N	23	ASN	-	expression tag	UNP P46637
N	24	ALA	-	expression tag	UNP P46637
O	22	SER	-	expression tag	UNP P46637
O	23	ASN	-	expression tag	UNP P46637
O	24	ALA	-	expression tag	UNP P46637
P	22	SER	-	expression tag	UNP P46637
P	23	ASN	-	expression tag	UNP P46637
P	24	ALA	-	expression tag	UNP P46637
Q	22	SER	-	expression tag	UNP P46637
Q	23	ASN	-	expression tag	UNP P46637
Q	24	ALA	-	expression tag	UNP P46637
R	22	SER	-	expression tag	UNP P46637
R	23	ASN	-	expression tag	UNP P46637
R	24	ALA	-	expression tag	UNP P46637
S	22	SER	-	expression tag	UNP P46637
S	23	ASN	-	expression tag	UNP P46637
S	24	ALA	-	expression tag	UNP P46637
T	22	SER	-	expression tag	UNP P46637
T	23	ASN	-	expression tag	UNP P46637
T	24	ALA	-	expression tag	UNP P46637
U	22	SER	-	expression tag	UNP P46637
U	23	ASN	-	expression tag	UNP P46637
U	24	ALA	-	expression tag	UNP P46637
V	22	SER	-	expression tag	UNP P46637
V	23	ASN	-	expression tag	UNP P46637

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Chain	Residue	Modelled	Actual	Comment	Reference
V	24	ALA	-	expression tag	UNP P46637
W	22	SER	-	expression tag	UNP P46637
W	23	ASN	-	expression tag	UNP P46637
W	24	ALA	-	expression tag	UNP P46637
X	22	SER	-	expression tag	UNP P46637
X	23	ASN	-	expression tag	UNP P46637
X	24	ALA	-	expression tag	UNP P46637

- 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
2	K	2	Total Mn 2 2	0	0
2	L	2	Total Mn 2 2	0	0
2	M	2	Total Mn 2 2	0	0
2	N	2	Total Mn 2 2	0	0
2	O	2	Total Mn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	2	Total 2	Mn 2	0	0
2	Q	2	Total 2	Mn 2	0	0
2	R	2	Total 2	Mn 2	0	0
2	S	2	Total 2	Mn 2	0	0
2	T	2	Total 2	Mn 2	0	0
2	U	2	Total 2	Mn 2	0	0
2	V	2	Total 2	Mn 2	0	0
2	W	2	Total 2	Mn 2	0	0
2	X	2	Total 2	Mn 2	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

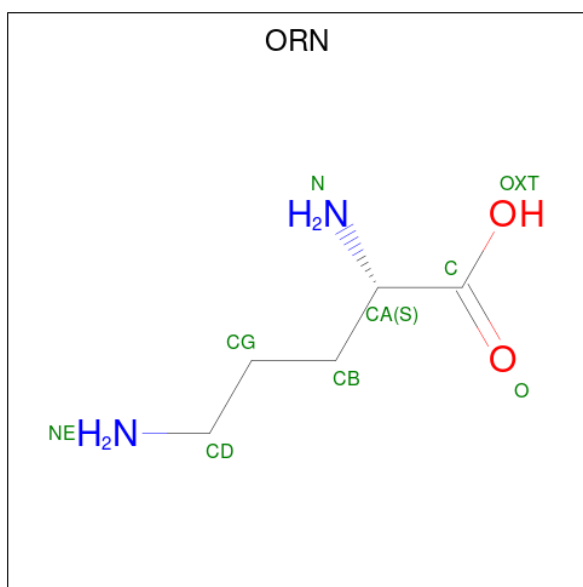
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	B	1	Total 1	Na 1	0	0
3	C	1	Total 1	Na 1	0	0
3	D	1	Total 1	Na 1	0	0
3	E	1	Total 1	Na 1	0	0
3	F	1	Total 1	Na 1	0	0
3	G	1	Total 1	Na 1	0	0
3	H	1	Total 1	Na 1	0	0
3	I	1	Total 1	Na 1	0	0
3	J	1	Total 1	Na 1	0	0

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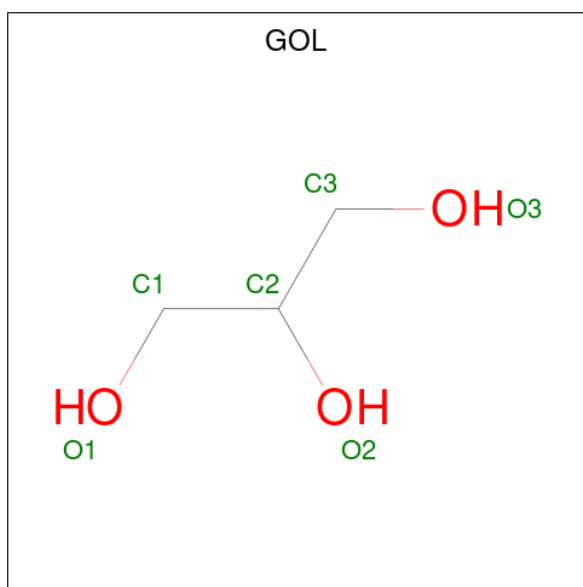
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	1	Total	Na	0	0
			1	1		
3	L	1	Total	Na	0	0
			1	1		
3	M	1	Total	Na	0	0
			1	1		
3	N	1	Total	Na	0	0
			1	1		
3	O	1	Total	Na	0	0
			1	1		
3	P	1	Total	Na	0	0
			1	1		
3	Q	1	Total	Na	0	0
			1	1		
3	R	1	Total	Na	0	0
			1	1		
3	S	1	Total	Na	0	0
			1	1		
3	T	1	Total	Na	0	0
			1	1		
3	U	1	Total	Na	0	0
			1	1		
3	V	1	Total	Na	0	0
			1	1		
3	W	1	Total	Na	0	0
			1	1		
3	X	1	Total	Na	0	0
			1	1		

- Molecule 4 is L-ornithine (CCD ID: ORN) (formula: $C_5H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	5	2	2		
4	C	1	Total	C	N	O	0	0
			9	5	2	2		
4	E	1	Total	C	N	O	0	0
			9	5	2	2		
4	F	1	Total	C	N	O	0	0
			9	5	2	2		
4	G	1	Total	C	N	O	0	0
			9	5	2	2		
4	K	1	Total	C	N	O	0	0
			9	5	2	2		
4	P	1	Total	C	N	O	0	0
			9	5	2	2		
4	U	1	Total	C	N	O	0	0
			9	5	2	2		
4	V	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



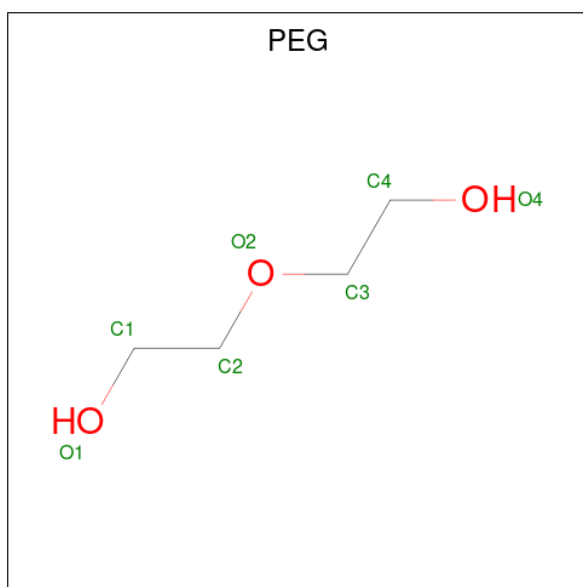
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	J	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	N	1	Total	C	O	0	0
			6	3	3		
5	P	1	Total	C	O	0	0
			6	3	3		
5	Q	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	S	1	Total	C	O	0	0
			6	3	3		
5	S	1	Total	C	O	0	0
			6	3	3		
5	T	1	Total	C	O	0	0
			6	3	3		
5	U	1	Total	C	O	0	0
			6	3	3		
5	W	1	Total	C	O	0	0
			6	3	3		
5	W	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			7	4	3		
6	G	1	Total	C	O	0	0
			7	4	3		
6	L	1	Total	C	O	0	0
			7	4	3		
6	L	1	Total	C	O	0	0
			7	4	3		
6	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	126	Total	O	0	0
			126	126		
7	B	240	Total	O	0	0
			240	240		
7	C	138	Total	O	0	0
			138	138		
7	D	265	Total	O	0	0
			265	265		
7	E	345	Total	O	0	0
			345	345		
7	F	268	Total	O	0	0
			268	268		
7	G	340	Total	O	0	0
			340	340		

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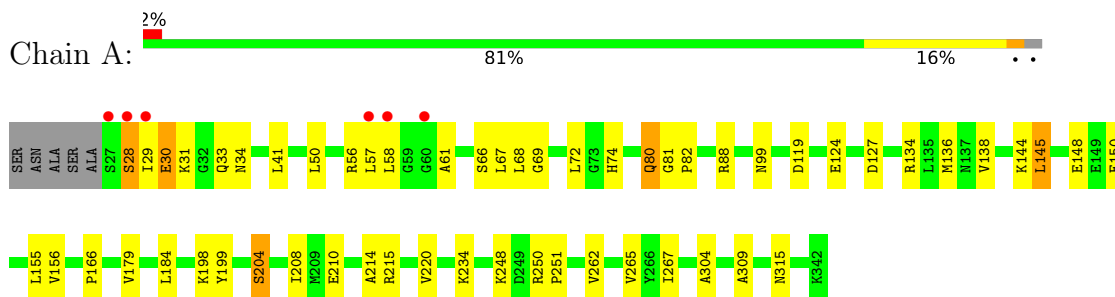
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	260	Total 260	O 260	0	0
7	I	265	Total 265	O 265	0	0
7	J	336	Total 336	O 336	0	0
7	K	276	Total 276	O 276	0	0
7	L	231	Total 231	O 231	0	0
7	M	61	Total 61	O 61	0	0
7	N	182	Total 182	O 182	0	0
7	O	79	Total 79	O 79	0	0
7	P	192	Total 192	O 192	0	0
7	Q	203	Total 203	O 203	0	0
7	R	184	Total 184	O 184	0	0
7	S	178	Total 178	O 178	0	0
7	T	196	Total 196	O 196	0	0
7	U	191	Total 191	O 191	0	0
7	V	136	Total 136	O 136	0	0
7	W	107	Total 107	O 107	0	0
7	X	152	Total 152	O 152	0	0

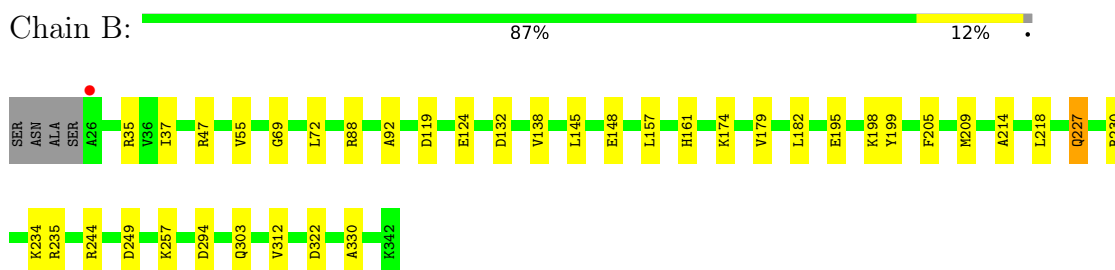
3 Residue-property plots [i](#)

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.

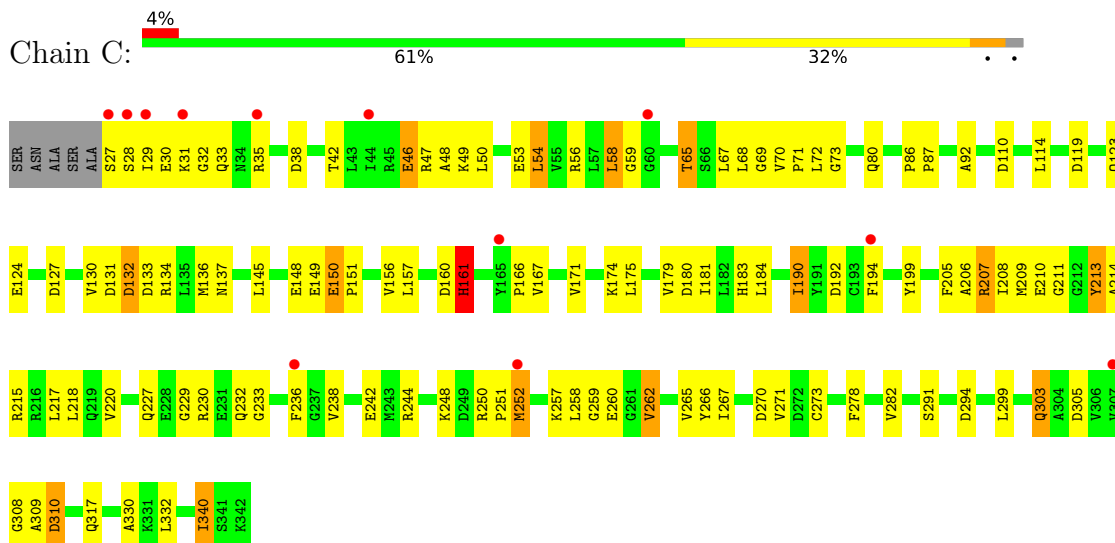
- Molecule 1: Arginase 1, mitochondrial



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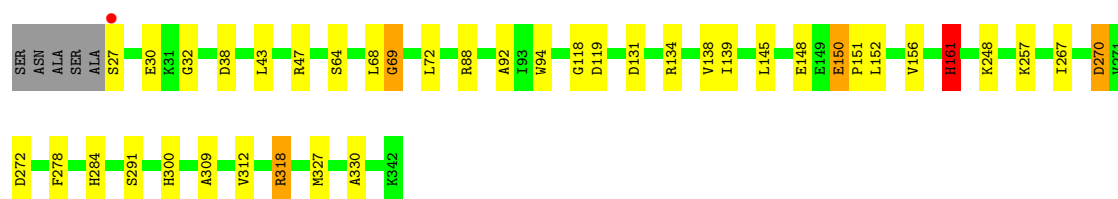


- Molecule 1: Arginase 1, mitochondrial



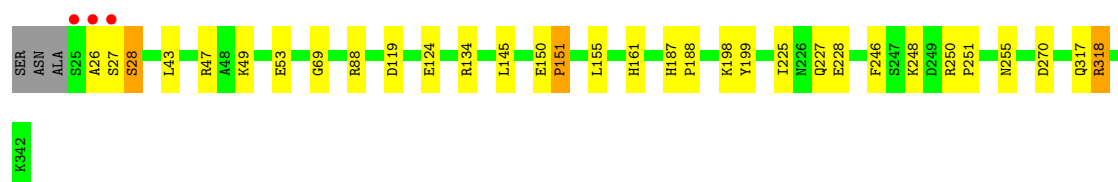
- Molecule 1: Arginase 1, mitochondrial

Chain D:  86% 11% ..



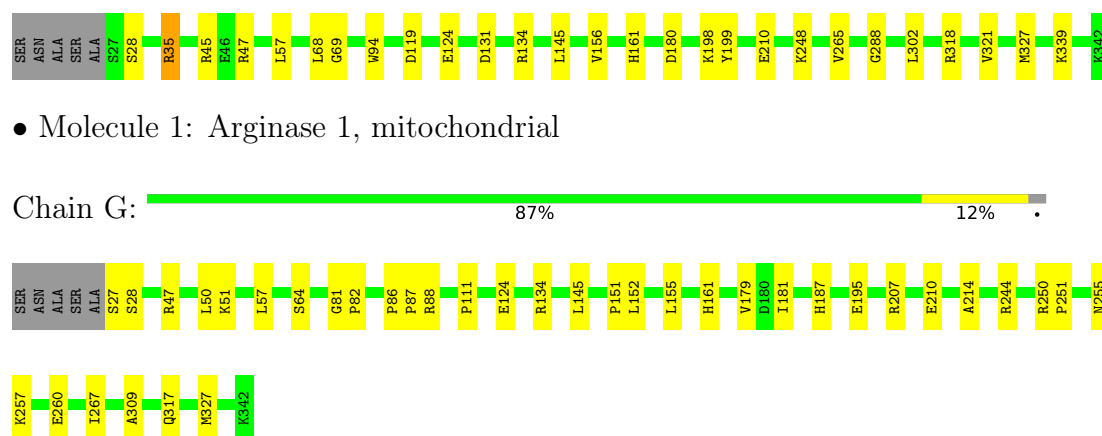
- Molecule 1: Arginase 1, mitochondrial

Chain E:  89% 9% ..



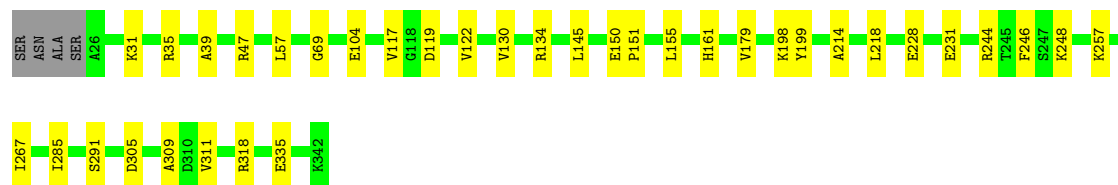
- Molecule 1: Arginase 1, mitochondrial

Chain F:  90% 8% .



- Molecule 1: Arginase 1, mitochondrial

Chain H:  88% 11% .



- Molecule 1: Arginase 1, mitochondrial

Chain I:  89% 8% ..



• Molecule 1: Arginase 1, mitochondrial

Chain J:  86% 12% ..



• Molecule 1: Arginase 1, mitochondrial

Chain K:  86% 12% ..



• Molecule 1: Arginase 1, mitochondrial

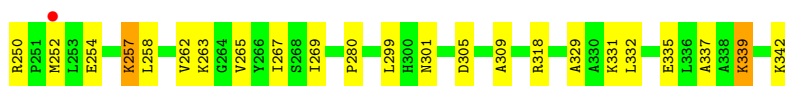
Chain L:  85% 12% ..



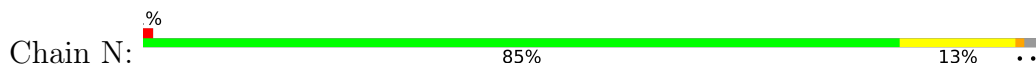
• Molecule 1: Arginase 1, mitochondrial

Chain M:  71% 23% ..

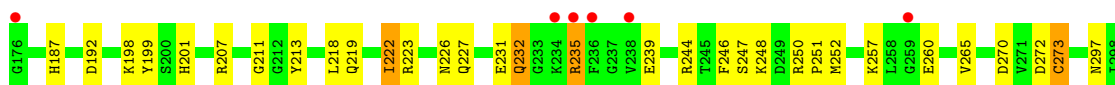
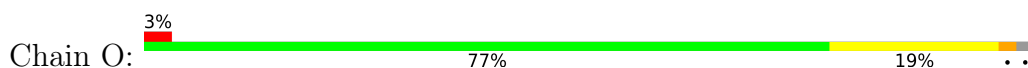




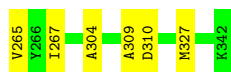
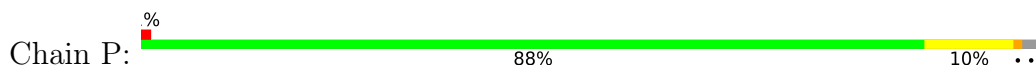
- Molecule 1: Arginase 1, mitochondrial



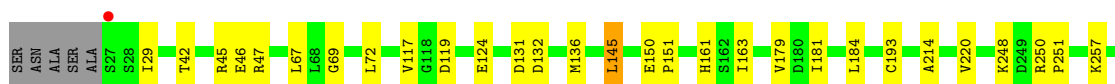
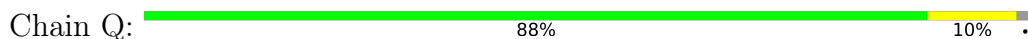
- Molecule 1: Arginase 1, mitochondrial



- Molecule 1: Arginase 1, mitochondrial

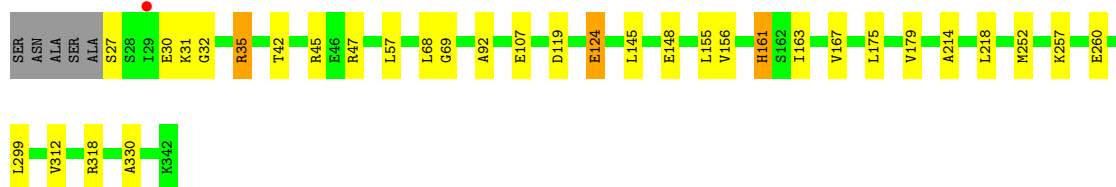


- Molecule 1: Arginase 1, mitochondrial



- Molecule 1: Arginase 1, mitochondrial

Chain R:  88% 9% ..



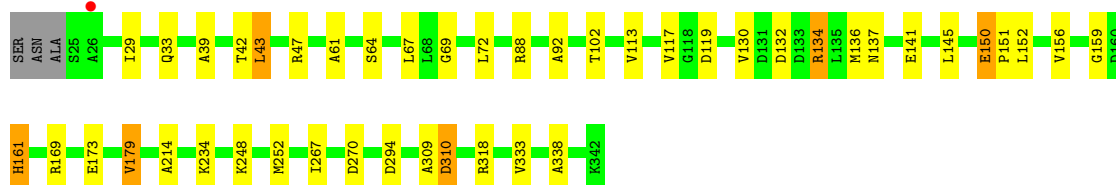
- Molecule 1: Arginase 1, mitochondrial

Chain S:  85% 12% ..



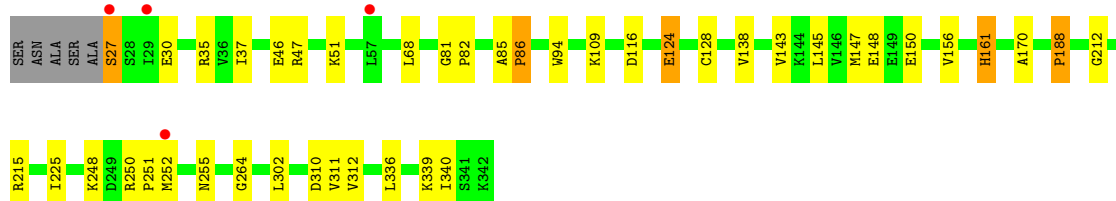
- Molecule 1: Arginase 1, mitochondrial

Chain T:  85% 12% ..



- Molecule 1: Arginase 1, mitochondrial

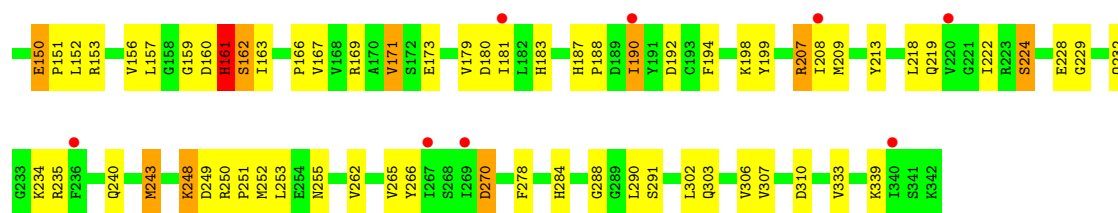
Chain U:  85% 12% ..



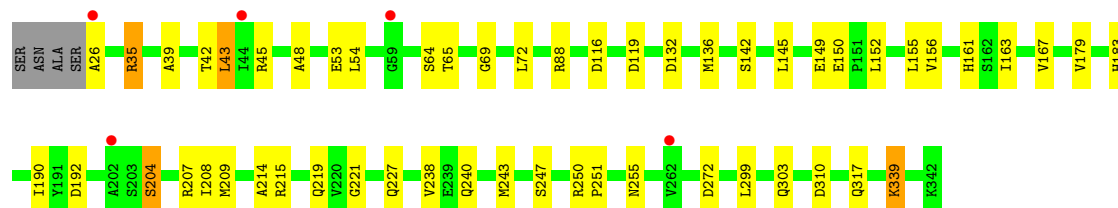
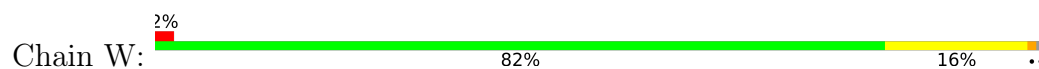
- Molecule 1: Arginase 1, mitochondrial

Chain V:  69% 26% 4% ..

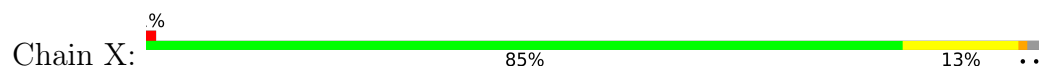




- Molecule 1: Arginase 1, mitochondrial



- Molecule 1: Arginase 1, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	267.32Å 267.32Å 262.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.25 29.97 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.97-2.25) 98.4 (29.97-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.159 , 0.197 0.167 , 0.202	Depositor DCC
R_{free} test set	2263 reflections (0.52%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h 0.014 for -l,-k,-h 0.011 for -h,-l,-k 0.011 for -h,l,k 0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	63508	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ORN, MN, PEG, NA, 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	1.15	4/2468 (0.2%)	1.45	0/3331
1	B	1.24	6/2465 (0.2%)	1.44	2/3328 (0.1%)
1	C	1.28	11/2476 (0.4%)	1.58	10/3341 (0.3%)
1	D	1.18	4/2460 (0.2%)	1.37	6/3321 (0.2%)
1	E	1.20	0/2470	1.35	6/3335 (0.2%)
1	F	1.17	3/2468 (0.1%)	1.34	1/3332 (0.0%)
1	G	1.22	4/2469 (0.2%)	1.36	2/3333 (0.1%)
1	H	1.21	3/2465 (0.1%)	1.36	3/3328 (0.1%)
1	I	1.20	3/2460 (0.1%)	1.40	1/3321 (0.0%)
1	J	1.20	1/2465 (0.0%)	1.43	8/3328 (0.2%)
1	K	1.30	4/2460 (0.2%)	1.45	3/3321 (0.1%)
1	L	1.33	10/2465 (0.4%)	1.42	4/3328 (0.1%)
1	M	1.18	8/2460 (0.3%)	1.46	4/3321 (0.1%)
1	N	1.17	4/2460 (0.2%)	1.41	3/3321 (0.1%)
1	O	1.16	1/2460 (0.0%)	1.47	8/3321 (0.2%)
1	P	1.10	1/2460 (0.0%)	1.38	1/3321 (0.0%)
1	Q	1.17	1/2460 (0.0%)	1.39	0/3321
1	R	1.12	0/2471	1.39	3/3335 (0.1%)
1	S	1.16	3/2460 (0.1%)	1.42	5/3321 (0.2%)
1	T	1.19	2/2471 (0.1%)	1.42	5/3336 (0.1%)
1	U	1.19	4/2468 (0.2%)	1.45	4/3332 (0.1%)
1	V	1.41	11/2460 (0.4%)	1.66	19/3321 (0.6%)
1	W	1.19	1/2465 (0.0%)	1.50	3/3328 (0.1%)
1	X	1.18	5/2460 (0.2%)	1.44	2/3321 (0.1%)
All	All	1.21	94/59146 (0.2%)	1.43	103/79846 (0.1%)

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	183	HIS	CE1-NE2	8.43	1.41	1.32
1	I	183	HIS	CE1-NE2	8.24	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	161	HIS	CE1-NE2	7.78	1.40	1.32
1	D	161	HIS	CE1-NE2	7.60	1.40	1.32
1	M	140	SER	C-O	7.37	1.32	1.24
1	U	311	VAL	C-O	7.27	1.32	1.24
1	L	42	THR	C-O	7.21	1.32	1.24
1	C	217	LEU	C-O	7.12	1.32	1.23
1	H	311	VAL	C-O	6.99	1.31	1.24
1	C	50	LEU	C-O	6.98	1.32	1.24
1	L	289	GLY	C-O	6.93	1.29	1.23
1	V	207	ARG	C-O	6.92	1.32	1.24
1	V	306	VAL	C-O	6.88	1.31	1.24
1	U	46	GLU	C-O	6.79	1.32	1.24
1	B	234	LYS	C-O	6.78	1.32	1.24
1	X	293	ARG	C-O	6.78	1.32	1.24
1	D	300	HIS	CE1-NE2	6.51	1.39	1.32
1	B	249	ASP	C-O	6.41	1.32	1.24
1	L	74	HIS	CE1-NE2	6.39	1.39	1.32
1	A	61	ALA	C-O	6.27	1.31	1.23
1	L	222	ILE	C-O	6.21	1.30	1.24
1	B	157	LEU	C-O	6.20	1.31	1.24
1	V	142	SER	C-O	6.16	1.31	1.24
1	N	201	HIS	CE1-NE2	6.15	1.38	1.32
1	G	181	ILE	C-O	6.14	1.30	1.24
1	M	280	PRO	C-O	-6.11	1.16	1.24
1	G	317	GLN	C-O	-6.08	1.16	1.24
1	V	161	HIS	CG-ND1	6.08	1.45	1.38
1	F	57	LEU	C-O	-6.03	1.17	1.24
1	C	54	LEU	C-O	6.02	1.31	1.24
1	M	108	LEU	C-O	5.99	1.31	1.24
1	U	188	PRO	C-O	-5.98	1.17	1.24
1	K	340	ILE	C-O	5.97	1.30	1.24
1	V	152	LEU	C-O	5.95	1.30	1.23
1	D	284	HIS	CE1-NE2	5.92	1.38	1.32
1	N	87	PRO	C-O	-5.91	1.16	1.24
1	M	49	LYS	C-O	5.89	1.30	1.24
1	C	340	ILE	C-O	5.72	1.30	1.24
1	G	111	PRO	C-O	-5.72	1.17	1.24
1	L	40	SER	C-O	5.69	1.30	1.24
1	F	288	GLY	C-O	-5.66	1.16	1.23
1	X	116	ASP	C-O	5.63	1.30	1.23
1	X	89	ILE	C-O	5.62	1.30	1.24
1	L	37	ILE	C-O	5.59	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	322	ASP	C-O	-5.59	1.16	1.23
1	A	80	GLN	C-O	5.59	1.31	1.23
1	T	92	ALA	C-O	-5.58	1.17	1.24
1	M	44	ILE	C-O	5.58	1.30	1.24
1	I	34	ASN	C-O	5.54	1.30	1.24
1	X	108	LEU	C-O	5.51	1.31	1.24
1	O	144	LYS	C-O	5.50	1.30	1.24
1	Q	317	GLN	C-O	-5.48	1.17	1.24
1	C	183	HIS	CE1-NE2	5.42	1.38	1.32
1	K	273	CYS	C-O	5.42	1.30	1.24
1	X	262	VAL	C-O	5.36	1.30	1.23
1	T	179	VAL	C-O	5.32	1.30	1.23
1	N	95	CYS	C-O	5.31	1.30	1.23
1	J	145	LEU	C-O	5.30	1.30	1.24
1	U	94	TRP	C-O	-5.30	1.16	1.24
1	B	132	ASP	C-O	-5.29	1.17	1.24
1	V	75	ASN	C-O	5.29	1.31	1.24
1	V	243	MET	C-O	5.28	1.30	1.24
1	M	65	THR	C-O	5.27	1.30	1.23
1	H	335	GLU	C-O	5.27	1.30	1.24
1	L	219	GLN	C-O	5.27	1.30	1.24
1	A	210	GLU	C-O	-5.27	1.17	1.24
1	C	332	LEU	C-O	5.26	1.30	1.24
1	C	207	ARG	C-O	5.26	1.30	1.24
1	W	35	ARG	C-O	5.26	1.30	1.24
1	S	115	THR	C-O	-5.22	1.16	1.23
1	C	110	ASP	C-O	5.21	1.30	1.24
1	K	183	HIS	CE1-NE2	5.21	1.37	1.32
1	K	79	LEU	C-O	5.20	1.30	1.23
1	F	94	TRP	C-O	-5.19	1.16	1.24
1	L	312	VAL	C-O	5.19	1.29	1.23
1	V	222	ILE	C-O	5.17	1.29	1.24
1	M	147	MET	C-O	5.17	1.30	1.24
1	A	74	HIS	CE1-NE2	5.16	1.37	1.32
1	L	141	GLU	C-O	5.16	1.30	1.24
1	C	161	HIS	CE1-NE2	-5.15	1.27	1.32
1	S	300	HIS	CE1-NE2	5.15	1.37	1.32
1	C	213	TYR	C-O	5.12	1.30	1.24
1	B	182	LEU	C-O	5.11	1.30	1.24
1	D	94	TRP	C-O	-5.10	1.17	1.24
1	L	132	ASP	C-O	5.10	1.30	1.24
1	N	183	HIS	CE1-NE2	5.07	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	43	LEU	C-O	5.06	1.30	1.24
1	M	47	ARG	C-O	5.03	1.29	1.24
1	V	208	ILE	C-O	5.03	1.29	1.24
1	S	268	SER	CA-CB	-5.03	1.46	1.53
1	H	291	SER	C-O	5.02	1.30	1.23
1	G	187	HIS	CE1-NE2	5.01	1.37	1.32
1	C	65	THR	C-O	5.01	1.29	1.23
1	P	52	GLY	C-O	5.01	1.29	1.23

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	272	ASP	CA-CB-CG	7.45	120.05	112.60
1	N	272	ASP	CA-CB-CG	7.45	120.05	112.60
1	K	127	ASP	CA-CB-CG	-7.24	105.36	112.60
1	V	310	ASP	CA-CB-CG	6.76	119.36	112.60
1	E	228	GLU	CB-CG-CD	6.68	123.96	112.60
1	P	150	GLU	CB-CA-C	6.65	119.09	109.11
1	C	310	ASP	CA-CB-CG	6.63	119.23	112.60
1	C	59	GLY	CA-C-O	-6.47	117.41	122.52
1	S	228	GLU	CB-CG-CD	6.29	123.29	112.60
1	L	161	HIS	CA-CB-CG	-6.25	107.55	113.80
1	V	31	LYS	CA-C-N	6.09	126.58	119.94
1	V	31	LYS	C-N-CA	6.09	126.58	119.94
1	O	38	ASP	CB-CA-C	6.04	120.45	110.90
1	V	179	VAL	CA-C-O	-6.01	115.30	121.67
1	O	110	ASP	CB-CA-C	5.88	116.85	110.08
1	G	260	GLU	CB-CG-CD	5.88	122.59	112.60
1	C	294	ASP	CA-CB-CG	5.87	118.47	112.60
1	J	29	ILE	CA-C-O	-5.84	115.12	120.73
1	V	333	VAL	CA-C-O	-5.83	115.20	121.27
1	R	124	GLU	CB-CG-CD	5.82	122.49	112.60
1	T	310	ASP	CA-CB-CG	5.79	118.39	112.60
1	F	210	GLU	CB-CA-C	-5.77	101.21	110.79
1	C	303	GLN	CB-CA-C	5.73	119.48	110.19
1	K	320	THR	CA-C-O	-5.72	115.47	121.99
1	S	292	PHE	CA-CB-CG	-5.69	108.11	113.80
1	J	160	ASP	CA-CB-CG	5.65	118.25	112.60
1	O	273	CYS	N-CA-C	-5.65	105.13	111.28
1	B	294	ASP	CA-CB-CG	5.63	118.23	112.60
1	U	124	GLU	N-CA-C	-5.62	105.07	111.14
1	O	222	ILE	CB-CA-C	-5.61	102.97	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	86	PRO	N-CA-C	5.61	117.55	110.70
1	E	26	ALA	N-CA-C	5.57	119.27	111.30
1	C	305	ASP	CA-C-O	-5.54	115.17	121.66
1	R	299	LEU	CA-C-O	-5.54	114.99	120.70
1	J	277	ALA	N-CA-C	-5.52	105.27	111.28
1	D	69	GLY	CA-C-O	-5.50	116.34	121.18
1	T	113	VAL	N-CA-C	-5.50	107.08	111.81
1	M	47	ARG	O-C-N	5.50	127.74	122.07
1	E	246	PHE	CA-C-O	-5.46	114.76	120.55
1	L	294	ASP	N-CA-C	-5.46	105.22	111.07
1	T	61	ALA	O-C-N	5.46	129.45	123.01
1	U	170	ALA	CA-C-O	-5.45	115.09	120.70
1	E	227	GLN	CA-C-O	-5.44	115.11	120.82
1	W	116	ASP	CA-CB-CG	5.42	118.02	112.60
1	O	161	HIS	CA-CB-CG	-5.41	108.39	113.80
1	V	270	ASP	N-CA-C	-5.39	100.51	109.46
1	T	294	ASP	CA-CB-CG	5.39	117.99	112.60
1	S	69	GLY	CA-C-O	-5.38	116.69	121.64
1	I	299	LEU	CA-C-O	-5.37	115.19	120.82
1	V	209	MET	CA-C-N	5.35	127.72	120.38
1	V	209	MET	C-N-CA	5.35	127.72	120.38
1	O	297	ASN	N-CA-C	-5.33	105.36	111.07
1	V	171	VAL	CA-C-N	5.33	127.37	120.44
1	V	171	VAL	C-N-CA	5.33	127.37	120.44
1	D	131	ASP	CA-CB-CG	5.31	117.91	112.60
1	H	246	PHE	CA-C-O	-5.31	114.92	120.55
1	T	333	VAL	CA-C-O	-5.29	115.56	121.17
1	C	161	HIS	CA-CB-CG	-5.29	108.51	113.80
1	E	28	SER	N-CA-C	-5.29	105.57	112.23
1	X	38	ASP	CB-CA-C	5.29	119.83	110.85
1	H	122	VAL	CA-C-O	-5.28	115.58	121.17
1	S	124	GLU	CB-CG-CD	5.28	121.57	112.60
1	E	270	ASP	CA-CB-CG	5.27	117.87	112.60
1	O	310	ASP	CA-CB-CG	5.27	117.87	112.60
1	V	262	VAL	CA-C-N	5.26	127.86	120.28
1	V	262	VAL	C-N-CA	5.26	127.86	120.28
1	V	173	GLU	CA-C-O	-5.24	115.29	120.90
1	L	69	GLY	CA-C-O	-5.24	116.82	121.64
1	U	310	ASP	CA-CB-CG	5.24	117.83	112.60
1	V	228	GLU	CB-CG-CD	5.23	121.50	112.60
1	C	273	CYS	N-CA-C	-5.20	105.61	111.28
1	N	38	ASP	CB-CA-C	5.19	119.40	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	36	VAL	CA-C-O	-5.17	115.69	121.17
1	V	160	ASP	CA-CB-CG	5.12	117.72	112.60
1	V	162	SER	CA-C-O	-5.11	114.47	120.20
1	W	26	ALA	CA-C-N	5.11	127.12	120.28
1	W	26	ALA	C-N-CA	5.11	127.12	120.28
1	S	255	ASN	CA-CB-CG	-5.10	107.50	112.60
1	H	228	GLU	CB-CG-CD	5.10	121.27	112.60
1	O	30	GLU	CB-CG-CD	5.10	121.27	112.60
1	G	195	GLU	CB-CG-CD	5.09	121.26	112.60
1	B	55	VAL	CA-C-O	-5.09	115.66	120.95
1	J	121	PRO	CA-C-N	5.08	126.95	120.56
1	J	121	PRO	C-N-CA	5.08	126.95	120.56
1	J	206	ALA	N-CA-C	-5.08	105.83	111.36
1	N	286	GLU	CB-CA-C	5.08	117.26	110.81
1	V	229	GLY	O-C-N	5.07	127.06	122.19
1	X	335	GLU	CB-CA-C	5.07	119.47	110.85
1	C	299	LEU	CA-C-O	-5.07	115.50	120.82
1	D	270	ASP	CA-CB-CG	5.06	117.66	112.60
1	U	86	PRO	N-CA-C	5.05	116.86	110.70
1	V	194	PHE	CA-C-N	5.04	130.00	122.74
1	V	194	PHE	C-N-CA	5.04	130.00	122.74
1	C	194	PHE	CA-C-N	5.03	131.14	121.54
1	C	194	PHE	C-N-CA	5.03	131.14	121.54
1	D	139	ILE	N-CA-C	-5.03	105.81	110.53
1	L	273	CYS	N-CA-C	-5.02	105.93	111.71
1	J	29	ILE	O-C-N	5.01	126.44	121.98
1	M	164	SER	CA-C-N	5.01	125.39	119.83
1	M	164	SER	C-N-CA	5.01	125.39	119.83
1	R	148	GLU	CB-CG-CD	5.01	121.11	112.60
1	D	284	HIS	CA-C-N	5.00	128.69	121.18
1	D	284	HIS	C-N-CA	5.00	128.69	121.18

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	2426	0	2446	35	0
1	B	2426	0	2442	20	0
1	C	2431	0	2455	67	0
1	D	2421	0	2437	24	0
1	E	2431	0	2444	20	0
1	F	2426	0	2443	19	0
1	G	2427	0	2443	23	0
1	H	2426	0	2442	15	0
1	I	2421	0	2437	14	0
1	J	2426	0	2442	24	0
1	K	2421	0	2437	19	0
1	L	2426	0	2442	27	0
1	M	2421	0	2437	81	0
1	N	2421	0	2437	19	0
1	O	2421	0	2437	50	0
1	P	2421	0	2437	24	0
1	Q	2421	0	2437	18	0
1	R	2429	0	2450	24	0
1	S	2421	0	2437	19	0
1	T	2432	0	2447	22	0
1	U	2426	0	2448	24	0
1	V	2421	0	2437	51	0
1	W	2426	0	2442	29	0
1	X	2421	0	2437	28	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
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
2	Q	2	0	0	0	0
2	R	2	0	0	0	0
2	S	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	2	0	0	0	0
2	U	2	0	0	0	0
2	V	2	0	0	0	0
2	W	2	0	0	0	0
2	X	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
4	A	9	0	11	0	0
4	C	9	0	11	1	0
4	E	9	0	11	1	0
4	F	9	0	11	1	0
4	G	9	0	11	1	0
4	K	9	0	11	0	0
4	P	9	0	11	2	0
4	U	9	0	11	3	0
4	V	9	0	11	1	0
5	B	12	0	16	0	0
5	C	6	0	8	3	0
5	D	12	0	16	0	0
5	E	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	6	0	8	0	0
5	G	12	0	16	1	0
5	H	12	0	16	0	0
5	I	12	0	16	1	0
5	J	12	0	16	1	0
5	K	12	0	16	1	0
5	L	12	0	16	0	0
5	N	6	0	8	0	0
5	P	6	0	8	0	0
5	Q	6	0	8	0	0
5	R	6	0	8	1	0
5	S	12	0	16	0	0
5	T	6	0	8	0	0
5	U	6	0	8	0	0
5	W	12	0	16	0	0
6	G	14	0	20	0	0
6	L	21	0	30	4	0
7	A	126	0	0	1	0
7	B	240	0	0	1	0
7	C	138	0	0	3	0
7	D	265	0	0	3	0
7	E	345	0	0	5	0
7	F	268	0	0	5	0
7	G	340	0	0	5	0
7	H	260	0	0	4	0
7	I	265	0	0	3	0
7	J	336	0	0	3	0
7	K	276	0	0	3	0
7	L	231	0	0	5	0
7	M	61	0	0	3	0
7	N	182	0	0	2	0
7	O	79	0	0	6	0
7	P	192	0	0	6	0
7	Q	203	0	0	2	0
7	R	184	0	0	4	0
7	S	178	0	0	1	0
7	T	196	0	0	0	0
7	U	191	0	0	5	0
7	V	136	0	0	8	0
7	W	107	0	0	3	0
7	X	152	0	0	1	0
All	All	63508	0	58982	647	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 6.

All (647) 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:M:175:LEU:CB	1:M:263:LYS:HG2	1.80	1.10
1:M:175:LEU:HB3	1:M:263:LYS:HE3	1.44	0.98
1:O:144:LYS:O	1:O:148:GLU:HG3	1.65	0.96
1:X:34:ASN:HD21	1:X:134:ARG:HH12	1.15	0.94
1:M:175:LEU:HB2	1:M:263:LYS:HG2	1.50	0.93
1:V:161:HIS:CE1	1:V:270:ASP:HB2	2.04	0.93
1:M:95:CYS:HG	1:M:97:SER:HG	1.13	0.92
1:O:265:VAL:HG21	1:O:304:ALA:HB1	1.53	0.90
1:M:175:LEU:HB3	1:M:263:LYS:HG2	1.54	0.88
1:C:47:ARG:CZ	1:F:124:GLU:HG2	2.07	0.85
1:M:95:CYS:SG	1:M:97:SER:OG	2.32	0.84
1:J:80:GLN:HE21	5:J:405:GOL:H32	1.45	0.81
1:M:32:GLY:HA2	1:M:35:ARG:HD3	1.62	0.81
1:O:47:ARG:CZ	1:R:124:GLU:HG2	2.11	0.81
1:C:206:ALA:O	1:C:210:GLU:HG3	1.81	0.80
1:M:47:ARG:CZ	1:P:124:GLU:HG2	2.12	0.80
1:I:124:GLU:HG2	1:L:47:ARG:NH1	1.98	0.79
1:G:124:GLU:HG2	1:J:47:ARG:CZ	2.12	0.79
1:M:175:LEU:HB3	1:M:263:LYS:CE	2.14	0.77
1:G:47:ARG:CZ	1:J:124:GLU:HG2	2.13	0.77
1:P:49:LYS:HD3	7:U:600:HOH:O	1.84	0.76
1:C:257:LYS:HE2	1:C:303:GLN:HB2	1.66	0.76
1:U:47:ARG:CZ	1:X:124:GLU:HG2	2.16	0.76
1:A:124:GLU:HG2	1:D:47:ARG:NH1	2.00	0.76
1:Q:193:CYS:HB3	7:Q:666:HOH:O	1.85	0.75
1:C:136[A]:MET:HE3	1:C:166:PRO:HG3	1.69	0.74
1:M:50:LEU:HD23	1:M:50:LEU:N	2.02	0.74
1:K:216:ARG:HH12	5:K:405:GOL:H2	1.51	0.74
1:M:107:GLU:OE2	1:M:109:LYS:HB2	1.88	0.74
1:M:175:LEU:N	1:M:175:LEU:HD23	2.03	0.74
1:M:169:ARG:O	1:M:173:GLU:HG3	1.87	0.73
1:B:47:ARG:CZ	1:E:124:GLU:HG2	2.18	0.73
1:M:49:LYS:NZ	1:M:50:LEU:HD21	2.05	0.72
1:C:179:VAL:O	1:C:214:ALA:HA	1.89	0.72
1:M:31:LYS:O	1:M:35:ARG:HG3	1.90	0.71
1:C:124:GLU:HG3	1:F:47:ARG:NH2	2.05	0.71
1:M:175:LEU:HB3	1:M:263:LYS:CG	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:33:GLN:O	1:M:37:ILE:HG13	1.91	0.71
1:M:88:ARG:HD2	7:M:557:HOH:O	1.90	0.70
1:A:99:ASN:HB3	4:C:405:ORN:O	1.91	0.70
1:V:71:PRO:O	1:V:123:GLN:NE2	2.24	0.70
1:L:327:MET:HE3	7:L:639:HOH:O	1.90	0.70
1:O:43:LEU:HG	1:O:47:ARG:NH1	2.05	0.70
1:M:47:ARG:NH1	1:P:124:GLU:HG2	2.07	0.69
1:M:107:GLU:OE2	1:M:109:LYS:N	2.25	0.69
1:C:73:GLY:O	1:C:80:GLN:HG2	1.93	0.69
1:E:49:LYS:NZ	1:E:53:GLU:OE1	2.26	0.69
1:B:227:GLN:OE1	1:B:227:GLN:HA	1.92	0.68
1:T:88:ARG:NH2	1:W:88:ARG:HH12	1.93	0.67
1:O:299:LEU:O	1:O:339:LYS:HE2	1.94	0.67
1:M:37:ILE:O	1:M:41:LEU:HD12	1.96	0.66
1:P:327:MET:HE3	7:P:646:HOH:O	1.95	0.66
1:W:303:GLN:HA	7:W:546:HOH:O	1.95	0.66
1:M:178:PRO:O	1:M:262:VAL:HB	1.96	0.66
1:P:35:ARG:NH1	1:X:42:THR:HG21	2.11	0.66
5:C:403:GOL:H2	1:F:321:VAL:HA	1.78	0.65
1:M:31:LYS:HG3	1:M:35:ARG:HH11	1.60	0.65
1:X:34:ASN:ND2	1:X:134:ARG:HH12	1.91	0.65
1:C:124:GLU:HG3	1:F:47:ARG:HH21	1.60	0.65
1:D:69:GLY:HA3	1:D:119:ASP:OD1	1.96	0.65
1:T:69:GLY:HA3	1:T:119:ASP:OD1	1.96	0.65
1:U:212:GLY:HA2	7:U:506:HOH:O	1.97	0.65
1:O:124:GLU:HG2	1:R:47[A]:ARG:CZ	2.27	0.65
1:G:134:ARG:HH11	1:G:134:ARG:HG2	1.61	0.64
1:H:198:LYS:HE3	1:H:199:TYR:CE2	2.32	0.64
1:X:69:GLY:HA3	1:X:119:ASP:OD1	1.96	0.64
1:V:90:ARG:NE	1:V:116:ASP:OD2	2.30	0.64
1:L:43:LEU:HG	1:L:47:ARG:NH1	2.13	0.63
1:M:49:LYS:HZ3	1:M:50:LEU:HD21	1.63	0.63
1:E:317:GLN:HB3	7:E:701:HOH:O	1.98	0.63
4:V:404:ORN:NE	7:V:504:HOH:O	2.30	0.63
1:M:32:GLY:HA3	1:P:50:LEU:HD21	1.81	0.62
1:O:207:ARG:HG3	7:O:503:HOH:O	1.98	0.62
1:A:56:ARG:NH1	1:A:150:GLU:O	2.31	0.62
1:A:215:ARG:HD3	1:A:262:VAL:HG11	1.80	0.62
1:M:49:LYS:HZ3	1:M:50:LEU:CD2	2.11	0.62
1:V:190:ILE:HG23	1:V:232:GLN:HB2	1.82	0.62
1:L:257:LYS:HE3	1:L:303:GLN:HE22	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:250:ARG:HB3	1:J:251:PRO:HD3	1.82	0.62
1:O:211:GLY:HA3	1:O:213:TYR:CE2	2.35	0.62
1:P:265:VAL:HG21	1:P:304:ALA:HB1	1.82	0.62
1:M:246:PHE:HE2	1:M:250:ARG:HH11	1.48	0.62
1:V:243:MET:HE1	1:V:290:LEU:CD2	2.30	0.61
1:C:136[A]:MET:CE	1:C:166:PRO:HG3	2.30	0.61
1:S:124:GLU:HG2	1:V:47:ARG:CZ	2.30	0.61
1:M:49:LYS:HG2	1:M:53:GLU:OE1	2.00	0.61
1:S:34:ASN:HD21	1:S:134:ARG:HH12	1.49	0.61
1:C:250:ARG:HB3	1:C:251:PRO:HD3	1.82	0.61
1:M:175:LEU:CD1	1:M:263:LYS:CG	2.79	0.61
1:J:69:GLY:HA3	1:J:119:ASP:OD1	2.01	0.60
1:M:49:LYS:O	1:M:53:GLU:HG3	2.01	0.60
1:A:265:VAL:HG21	1:A:304:ALA:HB1	1.83	0.60
1:M:32:GLY:HA2	1:M:35:ARG:CD	2.30	0.60
1:R:35:ARG:NH2	7:R:505:HOH:O	2.34	0.60
1:V:161:HIS:HE1	1:V:270:ASP:HB2	1.60	0.60
1:H:69:GLY:HA3	1:H:119:ASP:OD1	2.01	0.60
1:X:34:ASN:HD21	1:X:134:ARG:NH1	1.92	0.60
1:G:27:SER:N	7:G:504:HOH:O	2.35	0.60
1:M:175:LEU:HB3	1:M:263:LYS:CD	2.32	0.59
7:H:695:HOH:O	1:K:49:LYS:HE3	2.02	0.59
1:C:317:GLN:O	5:C:403:GOL:H12	2.03	0.59
1:E:27:SER:HB3	7:E:543:HOH:O	2.03	0.58
1:O:201:HIS:H	1:O:201:HIS:CD2	2.22	0.58
1:V:190:ILE:CG2	1:V:232:GLN:HB2	2.33	0.58
1:C:181:ILE:HA	1:C:266:TYR:O	2.03	0.58
1:M:175:LEU:CD1	1:M:263:LYS:HG2	2.34	0.58
1:C:215:ARG:NH1	1:C:262:VAL:HG22	2.18	0.58
1:G:124:GLU:HG2	1:J:47:ARG:NH1	2.18	0.58
1:M:299:LEU:O	1:M:339:LYS:NZ	2.25	0.58
1:U:124:GLU:HG2	1:X:47:ARG:CZ	2.34	0.58
1:C:47:ARG:NH1	1:F:124:GLU:HG2	2.19	0.57
1:F:47:ARG:HB2	7:F:725:HOH:O	2.04	0.57
1:C:215:ARG:NH1	1:C:260:GLU:O	2.27	0.57
1:S:144:LYS:HE2	7:S:658:HOH:O	2.03	0.57
1:M:107:GLU:OE2	1:M:109:LYS:CB	2.51	0.57
1:B:205:PHE:O	1:B:209:MET:HG2	2.05	0.57
1:A:179:VAL:O	1:A:214:ALA:HA	2.04	0.57
1:M:175:LEU:HD12	1:M:263:LYS:CG	2.35	0.57
1:N:198:LYS:HE2	1:N:199:TYR:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:580:HOH:O	1:X:98:THR:HA	2.03	0.57
1:T:88:ARG:HH22	1:W:88:ARG:HH12	1.50	0.57
1:M:171:VAL:O	1:M:175:LEU:HG	2.05	0.57
1:O:50:LEU:HD21	1:R:32:GLY:HA3	1.86	0.57
1:A:69:GLY:HA3	1:A:119:ASP:OD1	2.04	0.56
1:E:134:ARG:HG2	1:E:134:ARG:HH21	1.70	0.56
1:O:201:HIS:CD2	1:O:201:HIS:N	2.73	0.56
1:M:55:VAL:HG21	1:M:152:LEU:HD21	1.86	0.56
1:O:219:GLN:HB3	1:O:222:ILE:HD11	1.88	0.56
1:U:264:GLY:HA2	7:U:654:HOH:O	2.06	0.56
1:V:250:ARG:N	1:V:251:PRO:CD	2.67	0.56
1:C:161:HIS:CE1	1:C:270:ASP:HB2	2.42	0.55
1:F:327:MET:HE3	7:F:595:HOH:O	2.06	0.55
1:U:124:GLU:HB3	1:X:47:ARG:HD2	1.88	0.55
1:D:43:LEU:HG	1:D:47:ARG:HH11	1.71	0.55
1:K:34:ASN:OD1	1:K:134:ARG:NH1	2.31	0.55
1:K:198:LYS:HE2	1:K:199:TYR:CE2	2.41	0.55
1:I:43:LEU:HD13	1:L:39:ALA:HB3	1.89	0.55
1:L:257:LYS:HE3	1:L:303:GLN:NE2	2.22	0.55
1:O:232:GLN:HE22	1:O:235:ARG:HE	1.53	0.55
1:P:137:ASN:O	1:P:141:GLU:HG2	2.07	0.55
1:M:37:ILE:HG22	1:M:41:LEU:CD1	2.37	0.55
1:O:257:LYS:HB3	1:O:303:GLN:OE1	2.07	0.55
1:E:188:PRO:HG3	1:E:225:ILE:HD12	1.88	0.54
1:Q:69:GLY:HA3	1:Q:119:ASP:OD1	2.06	0.54
1:W:142:SER:HA	1:W:145:LEU:HD12	1.89	0.54
1:A:267:ILE:O	1:A:309:ALA:HA	2.07	0.54
1:M:175:LEU:CD1	1:M:263:LYS:HG3	2.37	0.54
1:O:161:HIS:CE1	1:O:270:ASP:HB2	2.42	0.54
1:N:70:VAL:HG11	1:N:139:ILE:HD13	1.89	0.54
1:M:49:LYS:NZ	1:M:50:LEU:CD2	2.69	0.54
1:E:69:GLY:HA3	1:E:119:ASP:OD1	2.07	0.54
1:G:50:LEU:HD21	1:J:32:GLY:HA3	1.89	0.54
1:N:88:ARG:NE	7:N:502:HOH:O	2.41	0.54
1:N:124:GLU:HG2	1:Q:47:ARG:CZ	2.38	0.54
1:T:130:VAL:HG13	1:T:134:ARG:HB3	1.90	0.54
1:T:161:HIS:CE1	1:T:270:ASP:HB2	2.43	0.54
1:K:69:GLY:HA3	1:K:119:ASP:OD1	2.08	0.54
1:U:27:SER:O	1:U:30:GLU:HG2	2.09	0.54
1:N:51:LYS:HE3	1:N:116:ASP:O	2.09	0.53
1:O:265:VAL:HG21	1:O:304:ALA:CB	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:69:GLY:HA3	1:N:119:ASP:OD1	2.08	0.53
1:V:243:MET:HE1	1:V:290:LEU:HD23	1.89	0.53
1:V:303:GLN:HA	7:V:617:HOH:O	2.08	0.53
1:V:190:ILE:HG23	1:V:232:GLN:CB	2.38	0.53
1:H:47:ARG:HG2	1:H:117:VAL:HA	1.91	0.53
1:X:161:HIS:CD2	1:X:312:VAL:HG21	2.44	0.53
4:G:404:ORN:NE	7:G:503:HOH:O	2.34	0.53
1:T:43:LEU:HD13	1:W:39:ALA:HB3	1.91	0.53
1:V:69:GLY:HA2	1:V:157:LEU:HB2	1.89	0.53
1:C:29:ILE:O	1:C:33:GLN:HG3	2.10	0.52
1:H:231:GLU:HG3	7:H:524:HOH:O	2.09	0.52
1:M:89:ILE:HD13	1:M:329:ALA:HB1	1.89	0.52
1:U:336:LEU:O	1:U:340:ILE:HG13	2.09	0.52
1:O:161:HIS:HE1	1:O:270:ASP:HB2	1.74	0.52
1:U:47:ARG:HD2	1:X:124:GLU:HB3	1.92	0.52
1:V:219:GLN:OE1	1:V:240:GLN:HG2	2.09	0.52
1:W:299:LEU:O	1:W:339:LYS:NZ	2.37	0.52
1:I:124:GLU:HG2	1:L:47:ARG:CZ	2.39	0.52
1:K:179:VAL:O	1:K:214:ALA:HA	2.10	0.52
1:C:180:ASP:O	1:C:265:VAL:HA	2.09	0.52
1:J:106:LYS:NZ	1:J:341:SER:O	2.42	0.52
1:T:67:LEU:O	1:T:117:VAL:HG22	2.09	0.52
1:T:179:VAL:O	1:T:214:ALA:HA	2.10	0.52
1:N:47:ARG:CZ	1:Q:124:GLU:HG2	2.39	0.52
1:O:47:ARG:NH2	1:R:124:GLU:HG2	2.24	0.52
1:D:161:HIS:CE1	1:D:270:ASP:HB2	2.45	0.52
1:C:211:GLY:HA3	1:C:213:TYR:CE2	2.45	0.52
1:V:187:HIS:CD2	1:V:224:SER:HB3	2.45	0.52
1:B:124:GLU:HG2	1:E:47:ARG:CZ	2.40	0.52
1:M:41:LEU:HD21	1:M:141:GLU:HB2	1.90	0.52
1:C:161:HIS:HB2	7:C:569:HOH:O	2.11	0.51
1:G:134:ARG:HG2	1:G:134:ARG:NH1	2.24	0.51
1:V:192:ASP:O	1:V:207:ARG:NH1	2.41	0.51
1:O:46:GLU:CD	1:R:35:ARG:HD3	2.35	0.51
1:A:34:ASN:OD1	1:A:134:ARG:NH1	2.43	0.51
1:D:64:SER:O	1:D:152:LEU:HA	2.09	0.51
1:X:155:LEU:C	1:X:155:LEU:HD23	2.35	0.51
4:E:404:ORN:NE	7:E:507:HOH:O	2.35	0.51
4:F:405:ORN:NE	7:F:501:HOH:O	2.35	0.51
1:M:103:GLU:OE2	1:M:331:LYS:NZ	2.40	0.51
1:O:155:LEU:C	1:O:155:LEU:HD23	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:191:TYR:CE2	7:J:589:HOH:O	2.53	0.51
1:D:318:ARG:HD3	7:D:541:HOH:O	2.10	0.51
1:F:69:GLY:HA3	1:F:119:ASP:OD1	2.09	0.51
1:L:43:LEU:HG	1:L:47:ARG:HH11	1.74	0.51
1:C:46:GLU:HG3	1:F:35:ARG:HB3	1.93	0.51
1:C:205:PHE:HA	1:C:208:ILE:HD12	1.93	0.51
1:V:180:ASP:O	1:V:265:VAL:HA	2.11	0.51
1:H:248:LYS:HE3	7:H:735:HOH:O	2.11	0.51
1:O:47:ARG:NH1	1:R:124:GLU:HG2	2.25	0.51
1:A:88:ARG:NH2	1:D:88:ARG:NH2	2.58	0.51
1:M:55:VAL:HG13	1:M:112:ARG:HG2	1.93	0.51
1:M:175:LEU:HD12	1:M:263:LYS:HG3	1.91	0.51
1:C:86:PRO:HB2	1:C:87:PRO:HD3	1.92	0.50
1:I:327:MET:HE3	7:I:596:HOH:O	2.12	0.50
1:B:198:LYS:HE3	1:B:199:TYR:CE2	2.46	0.50
1:D:92:ALA:HB3	1:D:330:ALA:HB2	1.94	0.50
1:L:263:LYS:NZ	6:L:407:PEG:H42	2.26	0.50
1:A:136[A]:MET:HG3	1:A:199:TYR:CE1	2.46	0.50
1:C:58:LEU:HA	7:C:553:HOH:O	2.10	0.50
1:I:198:LYS:HE3	1:I:199:TYR:CE2	2.46	0.50
1:I:252:MET:HE2	5:I:405:GOL:H12	1.93	0.50
1:K:31:LYS:O	1:K:35:ARG:HG3	2.11	0.50
1:P:35:ARG:HH12	1:X:42:THR:HG21	1.77	0.50
1:W:64:SER:O	1:W:152:LEU:HA	2.12	0.50
1:I:267:ILE:O	1:I:309:ALA:HA	2.10	0.50
1:M:37:ILE:HG22	1:M:41:LEU:HD11	1.94	0.50
1:J:43:LEU:O	1:J:47:ARG:HG3	2.11	0.50
1:W:272:ASP:C	1:W:272:ASP:OD1	2.54	0.50
1:V:243:MET:HG2	1:V:288:GLY:O	2.12	0.49
1:C:48:ALA:HB1	1:C:149:GLU:HG3	1.94	0.49
1:G:86:PRO:HB2	1:G:87:PRO:HD3	1.94	0.49
1:G:327:MET:HE3	7:G:669:HOH:O	2.12	0.49
1:H:305:ASP:OD2	7:H:501:HOH:O	2.20	0.49
1:K:47:ARG:HG2	1:K:117:VAL:HA	1.94	0.49
1:V:255:ASN:HB3	7:V:622:HOH:O	2.10	0.49
1:J:64:SER:O	1:J:152:LEU:HA	2.12	0.49
1:O:250:ARG:HB3	1:O:251:PRO:HD3	1.94	0.49
1:O:124:GLU:HG2	1:R:47[A]:ARG:NH1	2.28	0.49
1:O:306:VAL:HG21	1:O:339:LYS:HD3	1.93	0.49
1:R:252:MET:HG2	7:R:655:HOH:O	2.12	0.49
1:V:218:LEU:HD12	1:V:218:LEU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:184:LEU:HD23	1:L:220:VAL:HB	1.94	0.49
1:V:58:LEU:HA	7:V:555:HOH:O	2.13	0.49
1:V:169:ARG:HG3	1:V:213:TYR:CZ	2.48	0.49
1:C:190:ILE:CD1	1:C:229:GLY:HA2	2.42	0.49
5:G:408:GOL:H11	1:H:104:GLU:O	2.13	0.49
1:Q:250:ARG:HB3	1:Q:251:PRO:HD3	1.95	0.49
1:V:42:THR:O	1:V:46:GLU:HG2	2.13	0.49
1:F:35:ARG:HB3	1:F:35:ARG:HH11	1.78	0.49
4:P:405:ORN:NE	7:P:504:HOH:O	2.34	0.49
1:W:192:ASP:O	1:W:207:ARG:NH2	2.40	0.49
1:W:88:ARG:HG3	1:W:88:ARG:HH11	1.77	0.48
1:P:132:ASP:OD2	7:P:501:HOH:O	2.20	0.48
1:S:72:LEU:O	1:S:159:GLY:HA2	2.14	0.48
1:U:85:ALA:HB3	1:U:86:PRO:HD3	1.95	0.48
1:X:67:LEU:HG	1:X:114:LEU:HD11	1.96	0.48
1:B:88:ARG:NH2	1:E:88:ARG:NH2	2.61	0.48
1:G:250:ARG:HB3	1:G:251:PRO:HD3	1.94	0.48
1:M:143:VAL:HG12	1:M:147:MET:HE2	1.95	0.48
1:L:188:PRO:HG2	7:L:682:HOH:O	2.13	0.48
1:R:27:SER:O	1:R:30:GLU:HB2	2.13	0.48
1:C:56:ARG:NH1	1:C:150:GLU:O	2.46	0.48
1:M:254:GLU:O	1:M:301:ASN:ND2	2.45	0.48
1:H:130:VAL:HG13	1:H:134:ARG:HB3	1.96	0.48
1:U:250:ARG:HB3	1:U:251:PRO:HD3	1.94	0.48
1:H:155:LEU:HD23	1:H:155:LEU:C	2.39	0.48
1:V:190:ILE:HG23	1:V:190:ILE:O	2.13	0.48
1:W:132:ASP:O	1:W:136:MET:HG2	2.13	0.48
1:A:250:ARG:HB3	1:A:251:PRO:HD3	1.95	0.48
1:G:50:LEU:CD2	1:J:32:GLY:HA3	2.44	0.48
1:D:148:GLU:OE2	7:D:501:HOH:O	2.20	0.48
1:M:267:ILE:O	1:M:309:ALA:HA	2.14	0.48
1:X:111:PRO:HA	1:X:114:LEU:O	2.14	0.48
1:L:272:ASP:OD1	1:L:272:ASP:C	2.56	0.48
1:A:72:LEU:HD11	1:A:136[B]:MET:HE1	1.96	0.47
1:D:134:ARG:O	1:D:138:VAL:HG23	2.14	0.47
1:G:50:LEU:HD21	1:J:32:GLY:CA	2.44	0.47
1:M:305:ASP:OD1	1:M:342:LYS:NZ	2.47	0.47
1:O:192:ASP:O	1:O:207:ARG:NH2	2.34	0.47
1:M:37:ILE:CG2	1:M:138:VAL:HG22	2.44	0.47
1:M:103:GLU:HG3	1:M:335:GLU:OE2	2.14	0.47
1:O:67:LEU:HG	1:O:114:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ASP:O	1:C:136[A]:MET:HG2	2.13	0.47
1:E:155:LEU:C	1:E:155:LEU:HD23	2.39	0.47
1:I:127:ASP:HB2	7:I:678:HOH:O	2.13	0.47
1:J:191:TYR:CZ	7:J:589:HOH:O	2.67	0.47
1:L:141:GLU:O	1:L:145:LEU:HD22	2.14	0.47
1:T:39:ALA:HB3	1:W:43:LEU:HD13	1.96	0.47
1:A:136[A]:MET:SD	1:A:166:PRO:HG3	2.55	0.47
1:A:204:SER:O	1:A:208:ILE:HG13	2.14	0.47
1:C:156:VAL:O	1:C:310:ASP:HA	2.14	0.47
1:C:171:VAL:O	1:C:175:LEU:HG	2.15	0.47
1:V:56:ARG:NH1	1:V:150:GLU:O	2.41	0.47
1:A:315:ASN:OD1	1:A:315:ASN:C	2.57	0.47
1:C:32:GLY:HA2	1:C:35:ARG:HD3	1.95	0.47
1:L:263:LYS:HZ3	6:L:407:PEG:H42	1.79	0.47
1:M:179:VAL:O	1:M:214:ALA:HA	2.15	0.47
1:R:218:LEU:N	1:R:218:LEU:HD12	2.29	0.47
1:U:161:HIS:CD2	1:U:312:VAL:HG21	2.49	0.47
1:A:80:GLN:C	1:A:82:PRO:HD2	2.39	0.47
1:R:161:HIS:CD2	1:R:312:VAL:HG21	2.50	0.47
1:A:215:ARG:HD3	1:A:262:VAL:CG1	2.43	0.47
1:C:67:LEU:HD13	1:C:157:LEU:HD11	1.96	0.47
6:L:407:PEG:H11	7:L:707:HOH:O	2.15	0.47
1:O:244:ARG:N	7:O:502:HOH:O	2.34	0.47
1:K:180:ASP:O	1:K:265:VAL:HA	2.15	0.47
1:L:137:ASN:O	1:L:141:GLU:HG2	2.15	0.47
1:N:106:LYS:NZ	7:N:506:HOH:O	2.46	0.47
1:H:179:VAL:O	1:H:214:ALA:HA	2.15	0.47
1:Q:132:ASP:O	1:Q:136:MET:HG2	2.15	0.47
1:Q:327:MET:HE3	7:Q:596:HOH:O	2.15	0.47
5:C:403:GOL:H11	1:F:321:VAL:HB	1.96	0.47
1:M:68:LEU:O	1:M:156:VAL:HA	2.15	0.47
1:R:179:VAL:O	1:R:214:ALA:HA	2.15	0.47
1:T:64:SER:O	1:T:152:LEU:HA	2.15	0.47
1:D:150:GLU:HA	1:D:151:PRO:HA	1.79	0.46
1:M:161:HIS:HB2	7:M:501:HOH:O	2.15	0.46
1:U:51:LYS:HE3	1:U:116:ASP:O	2.15	0.46
1:A:198:LYS:HE3	1:A:199:TYR:CE2	2.50	0.46
1:C:267:ILE:O	1:C:309:ALA:HA	2.15	0.46
1:M:215:ARG:HD2	1:M:262:VAL:CG1	2.45	0.46
1:N:137:ASN:O	1:N:141:GLU:HG2	2.16	0.46
1:W:183:HIS:O	1:W:219:GLN:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:LEU:O	1:F:156:VAL:HA	2.16	0.46
1:I:68:LEU:O	1:I:156:VAL:HA	2.15	0.46
1:W:238:VAL:HG12	1:W:240:GLN:HG3	1.98	0.46
1:I:130:VAL:HG13	1:I:134:ARG:HB2	1.98	0.46
1:O:69:GLY:HA3	1:O:119:ASP:OD1	2.15	0.46
1:O:218:LEU:HA	1:O:239:GLU:O	2.15	0.46
1:Q:42:THR:HA	1:Q:45:ARG:NH1	2.30	0.46
1:R:42:THR:HA	1:R:45:ARG:NH1	2.31	0.46
1:S:198:LYS:HE2	1:S:199:TYR:CE2	2.51	0.46
1:T:47:ARG:HG2	1:T:117:VAL:HA	1.96	0.46
1:V:198:LYS:HE3	1:V:199:TYR:CE2	2.50	0.46
1:C:230:ARG:HH22	1:C:242:GLU:CD	2.24	0.46
1:Q:42:THR:O	1:Q:46:GLU:HG2	2.16	0.46
1:X:72:LEU:C	1:X:72:LEU:HD23	2.41	0.46
1:B:47:ARG:HD2	1:E:124:GLU:HB3	1.98	0.46
1:C:130:VAL:HG13	1:C:134:ARG:HB2	1.97	0.46
1:C:190:ILE:HD13	1:C:232:GLN:HB2	1.96	0.46
1:A:41:LEU:HD21	1:A:138:VAL:HG13	1.98	0.46
1:D:327:MET:HE3	7:D:647:HOH:O	2.16	0.46
1:M:137:ASN:O	1:M:141:GLU:HG2	2.16	0.46
1:U:188:PRO:HG3	1:U:225:ILE:HG13	1.97	0.46
1:C:160:ASP:OD1	1:C:160:ASP:C	2.58	0.46
1:F:302:LEU:HB3	1:F:339:LYS:HE2	1.98	0.46
1:R:68:LEU:O	1:R:156:VAL:HA	2.16	0.46
1:F:45:ARG:HD2	7:F:691:HOH:O	2.16	0.45
1:T:137:ASN:O	1:T:141:GLU:HG2	2.15	0.45
1:W:35:ARG:NH2	7:W:514:HOH:O	2.49	0.45
1:X:145:LEU:HD13	7:X:572:HOH:O	2.16	0.45
1:B:235:ARG:HA	7:B:710:HOH:O	2.15	0.45
1:M:51:LYS:O	1:M:55:VAL:HG23	2.17	0.45
1:N:319:ASP:OD2	1:N:323:GLY:HA2	2.17	0.45
1:U:128:CYS:HB3	7:U:638:HOH:O	2.15	0.45
1:V:136:MET:HG3	1:V:199:TYR:CE1	2.51	0.45
1:A:50:LEU:HD21	1:D:32:GLY:HA3	1.99	0.45
1:C:167:VAL:O	1:C:171:VAL:HG23	2.16	0.45
1:O:92:ALA:HB3	1:O:330:ALA:HB2	1.97	0.45
1:L:155:LEU:C	1:L:155:LEU:HD23	2.41	0.45
1:L:215:ARG:HD3	1:U:215:ARG:HD2	1.99	0.45
1:P:43:LEU:HG	1:P:47:ARG:NH1	2.32	0.45
1:M:49:LYS:HD3	1:U:35:ARG:HH12	1.82	0.45
1:A:88:ARG:HD2	7:A:609:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LEU:C	1:B:72:LEU:HD23	2.42	0.45
1:C:68:LEU:O	1:C:156:VAL:HA	2.17	0.45
1:C:209:MET:HB3	1:C:236:PHE:CD1	2.52	0.45
1:E:43:LEU:O	1:E:47:ARG:HG3	2.16	0.45
1:G:64:SER:O	1:G:152:LEU:HA	2.16	0.45
1:I:64:SER:O	1:I:152:LEU:HA	2.17	0.45
1:O:246:PHE:O	1:O:247:SER:C	2.59	0.45
1:W:72:LEU:C	1:W:72:LEU:HD23	2.42	0.45
1:B:92:ALA:HB3	1:B:330:ALA:HB2	1.99	0.45
1:K:145:LEU:HD13	7:K:501:HOH:O	2.17	0.45
1:P:43:LEU:HD12	1:P:47:ARG:HD3	1.99	0.45
1:P:156:VAL:O	1:P:310:ASP:HA	2.17	0.45
1:B:218:LEU:N	1:B:218:LEU:HD12	2.31	0.45
1:B:227:GLN:OE1	1:B:230:ARG:HD2	2.17	0.45
1:D:68:LEU:O	1:D:156:VAL:HA	2.17	0.45
1:C:67:LEU:HG	1:C:114:LEU:HD11	1.97	0.45
1:D:272:ASP:OD1	1:D:272:ASP:C	2.60	0.45
4:P:405:ORN:NE	7:P:505:HOH:O	2.36	0.45
1:Q:181:ILE:HA	1:Q:266:TYR:O	2.17	0.45
1:S:85:ALA:O	1:S:86:PRO:C	2.60	0.45
1:U:251:PRO:O	1:U:255:ASN:ND2	2.43	0.45
1:X:156:VAL:O	1:X:310:ASP:HA	2.17	0.45
1:A:67:LEU:HA	1:A:155:LEU:O	2.17	0.44
1:D:43:LEU:O	1:D:47:ARG:HD3	2.17	0.44
1:J:183:HIS:O	1:J:219:GLN:HA	2.17	0.44
1:O:223:ARG:NH1	1:O:273:CYS:O	2.48	0.44
1:A:124:GLU:CG	1:D:47:ARG:NH1	2.77	0.44
1:M:35:ARG:HG3	1:M:35:ARG:H	1.58	0.44
1:W:227:GLN:HE21	1:W:227:GLN:HB2	1.50	0.44
1:M:46:GLU:OE1	1:M:46:GLU:HA	2.17	0.44
1:N:156:VAL:O	1:N:310:ASP:HA	2.18	0.44
1:R:175:LEU:HD21	5:R:404:GOL:H11	2.00	0.44
1:W:65:THR:HG23	1:W:155:LEU:HB2	1.99	0.44
1:X:188:PRO:HB2	1:X:190:ILE:HG12	1.98	0.44
1:A:72:LEU:C	1:A:72:LEU:HD23	2.43	0.44
1:A:144:LYS:O	1:A:148:GLU:HG3	2.18	0.44
1:M:140:SER:O	1:M:144:LYS:HG3	2.17	0.44
1:P:265:VAL:CG2	1:P:304:ALA:HB1	2.47	0.44
1:T:29:ILE:O	1:T:33:GLN:HG3	2.18	0.44
1:T:267:ILE:O	1:T:309:ALA:HA	2.17	0.44
1:X:34:ASN:ND2	1:X:134:ARG:HH22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:239:GLU:HB3	6:L:408:PEG:H42	1.99	0.44
1:O:161:HIS:CB	1:O:201:HIS:HB2	2.47	0.44
1:O:192:ASP:HA	7:O:563:HOH:O	2.17	0.44
1:O:248:LYS:HE3	1:O:248:LYS:HA	1.99	0.44
1:S:70:VAL:HG11	1:S:139:ILE:HD13	1.99	0.44
1:E:187:HIS:HB2	7:E:507:HOH:O	2.18	0.44
1:O:265:VAL:HG23	1:O:305:ASP:O	2.18	0.44
1:S:88:ARG:NH2	1:V:88:ARG:NH2	2.66	0.44
1:V:72:LEU:O	1:V:159:GLY:HA2	2.17	0.44
1:V:249:ASP:O	1:V:253:LEU:HG	2.18	0.44
1:X:112:ARG:HE	1:X:112:ARG:HB2	1.68	0.44
1:X:175:LEU:O	1:X:263:LYS:HD3	2.16	0.44
1:B:161:HIS:CD2	1:B:312:VAL:HG21	2.52	0.44
1:T:42:THR:O	1:T:43:LEU:C	2.61	0.44
1:U:81:GLY:N	1:U:82:PRO:CD	2.81	0.44
1:U:248:LYS:NZ	7:U:516:HOH:O	2.51	0.44
1:X:257:LYS:HD3	1:X:303:GLN:HE21	1.83	0.44
1:A:215:ARG:NH2	1:A:262:VAL:HG13	2.32	0.44
1:D:43:LEU:HG	1:D:47:ARG:NH1	2.33	0.44
1:O:160:ASP:OD1	1:O:160:ASP:C	2.61	0.44
1:O:201:HIS:H	1:O:201:HIS:HD2	1.62	0.44
1:Q:184:LEU:HD23	1:Q:220:VAL:HB	2.00	0.44
1:V:302:LEU:HD23	1:V:339:LYS:HE2	1.98	0.44
1:E:134:ARG:HG2	1:E:134:ARG:NH2	2.31	0.43
1:T:156:VAL:O	1:T:310:ASP:HA	2.18	0.43
1:X:267:ILE:O	1:X:309:ALA:HA	2.18	0.43
1:C:184:LEU:HD23	1:C:220:VAL:HB	2.00	0.43
1:D:72:LEU:C	1:D:72:LEU:HD23	2.43	0.43
1:H:150:GLU:HA	1:H:151:PRO:HA	1.84	0.43
1:I:179:VAL:O	1:I:214:ALA:HA	2.18	0.43
1:N:227:GLN:O	1:N:231:GLU:HG2	2.18	0.43
1:S:34:ASN:HD22	1:S:34:ASN:HA	1.67	0.43
1:X:327:MET:HE3	1:X:327:MET:HA	1.99	0.43
1:C:257:LYS:HE2	1:C:303:GLN:CB	2.43	0.43
1:O:198:LYS:O	1:O:207:ARG:NH1	2.51	0.43
1:W:250:ARG:HB3	1:W:251:PRO:HD3	2.00	0.43
1:C:303:GLN:OE1	1:C:303:GLN:HA	2.18	0.43
1:E:250:ARG:HB3	1:E:251:PRO:HD3	2.00	0.43
1:S:179:VAL:O	1:S:214:ALA:HA	2.18	0.43
1:V:75:ASN:CB	1:V:162:SER:HB3	2.48	0.43
1:W:48:ALA:O	1:W:149:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:161:HIS:CD2	1:L:312:VAL:HG21	2.53	0.43
1:N:155:LEU:C	1:N:155:LEU:HD23	2.43	0.43
1:O:137:ASN:O	1:O:141:GLU:HG2	2.18	0.43
1:O:150:GLU:HA	1:O:151:PRO:HA	1.80	0.43
1:G:155:LEU:C	1:G:155:LEU:HD23	2.44	0.43
1:M:33:GLN:O	1:M:37:ILE:CG1	2.61	0.43
1:C:65:THR:OG1	1:C:340:ILE:HB	2.19	0.43
1:C:206:ALA:O	1:C:210:GLU:CG	2.60	0.43
1:K:155:LEU:C	1:K:155:LEU:HD23	2.44	0.43
1:L:230:ARG:HH11	1:L:230:ARG:HG2	1.84	0.43
1:M:257:LYS:O	1:M:258:LEU:HD23	2.18	0.43
1:O:153:ARG:HH11	1:O:307:VAL:HA	1.84	0.43
1:P:267:ILE:O	1:P:309:ALA:HA	2.19	0.43
1:S:267:ILE:O	1:S:309:ALA:HA	2.19	0.43
1:C:233:GLY:HA2	1:C:238:VAL:CG2	2.48	0.43
1:G:207:ARG:HH21	1:G:210:GLU:CD	2.27	0.43
1:M:124:GLU:HG2	1:P:47:ARG:CZ	2.49	0.43
1:T:72:LEU:O	1:T:159:GLY:HA2	2.18	0.43
1:T:169:ARG:O	1:T:173:GLU:HG3	2.19	0.43
1:W:317:GLN:HB3	7:W:581:HOH:O	2.19	0.43
1:X:198:LYS:HE3	1:X:199:TYR:CE2	2.54	0.43
1:Q:131:ASP:OD1	1:Q:131:ASP:C	2.62	0.43
1:V:134:ARG:O	1:V:137:ASN:HB2	2.19	0.43
1:V:181:ILE:HG12	1:V:266:TYR:HB3	1.99	0.43
1:W:163:ILE:O	1:W:167:VAL:HG23	2.18	0.43
1:X:64:SER:O	1:X:152:LEU:HA	2.19	0.43
1:B:257:LYS:HE3	1:B:303:GLN:HE22	1.84	0.43
1:D:161:HIS:CD2	1:D:312:VAL:HG21	2.54	0.43
1:H:285:ILE:HG13	7:I:555:HOH:O	2.19	0.43
1:K:161:HIS:CE1	1:K:270:ASP:HB2	2.54	0.43
1:M:131:ASP:OD1	1:M:134:ARG:HG3	2.19	0.43
1:Q:163:ILE:HD11	1:Q:312:VAL:HG12	2.01	0.43
4:U:405:ORN:O	4:U:405:ORN:HG3	2.18	0.43
1:V:120:VAL:O	1:V:122:VAL:N	2.50	0.43
1:C:150:GLU:HA	1:C:151:PRO:HA	1.76	0.42
1:I:47:ARG:HG3	7:L:648:HOH:O	2.19	0.42
1:D:38:ASP:OD2	1:R:35:ARG:NE	2.51	0.42
1:K:278:PHE:CE2	1:K:291:SER:HA	2.54	0.42
1:O:46:GLU:OE1	1:R:35:ARG:HD3	2.19	0.42
1:Q:72:LEU:HD23	1:Q:72:LEU:C	2.44	0.42
1:U:37:ILE:HG23	1:U:138:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:O	1:A:156:VAL:HA	2.19	0.42
1:C:259:GLY:HA2	1:C:262:VAL:HG23	2.01	0.42
1:C:271:VAL:HG12	1:C:282:VAL:CG1	2.49	0.42
1:G:88:ARG:NH2	1:J:88:ARG:NH2	2.67	0.42
1:L:29:ILE:O	1:L:33:GLN:HG3	2.20	0.42
1:P:155:LEU:C	1:P:155:LEU:HD23	2.44	0.42
1:P:205:PHE:O	1:P:209:MET:HG2	2.20	0.42
1:B:124:GLU:HB3	1:E:47:ARG:CD	2.49	0.42
1:F:131:ASP:OD1	1:F:131:ASP:C	2.62	0.42
1:F:198:LYS:HE2	1:F:199:TYR:CE2	2.54	0.42
1:V:66:SER:HA	1:V:115:THR:O	2.19	0.42
1:V:284:HIS:HD2	7:V:570:HOH:O	2.02	0.42
1:A:28:SER:O	1:A:28:SER:OG	2.32	0.42
1:C:47:ARG:NH2	1:F:124:GLU:HG2	2.34	0.42
1:C:92:ALA:HB3	1:C:330:ALA:HB2	2.00	0.42
1:G:255:ASN:HB3	7:G:524:HOH:O	2.19	0.42
1:L:43:LEU:HD12	1:L:43:LEU:HA	1.89	0.42
1:O:199:TYR:HA	7:O:503:HOH:O	2.20	0.42
1:G:51:LYS:HE2	7:G:711:HOH:O	2.20	0.42
1:G:267:ILE:O	1:G:309:ALA:HA	2.19	0.42
1:R:163:ILE:O	1:R:167:VAL:HG23	2.19	0.42
1:T:248:LYS:HE3	1:T:248:LYS:HB3	1.92	0.42
1:B:37:ILE:HG23	1:B:138:VAL:HG22	2.01	0.42
1:B:179:VAL:O	1:B:214:ALA:HA	2.19	0.42
1:C:70:VAL:O	1:C:72:LEU:N	2.51	0.42
1:M:161:HIS:CE1	1:M:183:HIS:HE2	2.38	0.42
1:O:127:ASP:OD1	7:O:501:HOH:O	2.21	0.42
1:G:179:VAL:O	1:G:214:ALA:HA	2.19	0.42
1:L:69:GLY:HA3	1:L:119:ASP:OD1	2.20	0.42
1:P:90:ARG:NE	1:P:116:ASP:OD2	2.45	0.42
1:R:69:GLY:HA3	1:R:119:ASP:OD1	2.19	0.42
1:U:68:LEU:O	1:U:156:VAL:HA	2.20	0.42
1:V:188:PRO:HG2	7:V:619:HOH:O	2.19	0.42
1:W:204:SER:O	1:W:208:ILE:HG13	2.19	0.42
1:B:69:GLY:HA3	1:B:119:ASP:OD1	2.19	0.42
1:O:226:ASN:O	1:O:227:GLN:C	2.61	0.42
1:Q:179:VAL:O	1:Q:214:ALA:HA	2.20	0.42
1:V:153:ARG:HD3	1:V:307:VAL:HA	2.00	0.42
1:A:145:LEU:HD12	1:A:145:LEU:HA	1.90	0.42
1:C:136[B]:MET:HG3	1:C:199:TYR:CE1	2.55	0.42
1:J:267:ILE:O	1:J:309:ALA:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:107:GLU:OE1	7:R:502:HOH:O	2.22	0.42
1:S:32:GLY:HA3	1:V:50:LEU:HD21	2.02	0.42
1:S:46:GLU:HA	1:S:46:GLU:OE1	2.20	0.42
1:S:99:ASN:HB3	4:U:405:ORN:OXT	2.20	0.42
1:C:71:PRO:O	1:C:123:GLN:NE2	2.52	0.41
1:C:133:ASP:O	1:C:137:ASN:ND2	2.36	0.41
1:E:150:GLU:HA	1:E:151:PRO:HA	1.85	0.41
1:E:318:ARG:HH11	1:E:318:ARG:CG	2.33	0.41
1:F:180:ASP:O	1:F:265:VAL:HA	2.20	0.41
1:K:266:TYR:HA	1:K:308:GLY:O	2.19	0.41
1:M:111:PRO:HA	1:M:114:LEU:O	2.20	0.41
1:M:205:PHE:O	1:M:209:MET:HG2	2.20	0.41
1:U:143:VAL:O	1:U:147:MET:HG3	2.20	0.41
1:C:278:PHE:CE2	1:C:291:SER:HA	2.54	0.41
1:N:72:LEU:O	1:N:159:GLY:HA2	2.20	0.41
1:O:43:LEU:HG	1:O:47:ARG:HH12	1.84	0.41
1:V:278:PHE:CE2	1:V:291:SER:HA	2.55	0.41
1:A:155:LEU:HD23	1:A:155:LEU:C	2.46	0.41
1:K:327:MET:HE3	7:K:570:HOH:O	2.20	0.41
1:M:65:THR:OG1	1:M:337:ALA:HA	2.20	0.41
1:S:161:HIS:CD2	1:S:312:VAL:HG21	2.55	0.41
1:W:156:VAL:O	1:W:310:ASP:HA	2.19	0.41
1:W:221:GLY:HA2	1:W:243:MET:SD	2.60	0.41
1:C:54:LEU:O	1:C:58:LEU:HG	2.20	0.41
1:D:47:ARG:HH21	1:D:118:GLY:HA3	1.85	0.41
1:N:180:ASP:O	1:N:265:VAL:HA	2.20	0.41
1:U:302:LEU:HB3	1:U:339:LYS:HE2	2.02	0.41
1:W:179:VAL:O	1:W:214:ALA:HA	2.20	0.41
1:W:209:MET:SD	1:W:214:ALA:HB3	2.61	0.41
1:A:184:LEU:HD23	1:A:220:VAL:HB	2.01	0.41
1:P:188:PRO:HG2	7:P:662:HOH:O	2.19	0.41
1:S:180:ASP:O	1:S:265:VAL:HA	2.20	0.41
1:V:167:VAL:O	1:V:171:VAL:HG23	2.21	0.41
1:G:81:GLY:N	1:G:82:PRO:CD	2.84	0.41
1:J:179:VAL:O	1:J:214:ALA:HA	2.20	0.41
1:R:155:LEU:HD23	1:R:155:LEU:C	2.45	0.41
1:V:75:ASN:HB3	1:V:162:SER:HB3	2.02	0.41
1:M:180:ASP:O	1:M:265:VAL:HA	2.20	0.41
1:O:223:ARG:NH2	1:O:272:ASP:O	2.54	0.41
1:R:92:ALA:HB3	1:R:330:ALA:HB2	2.03	0.41
1:T:102:THR:HG21	1:T:338:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:TYR:HA	1:C:308:GLY:O	2.20	0.41
1:F:28:SER:HB3	7:F:514:HOH:O	2.21	0.41
1:G:57:LEU:C	1:G:57:LEU:HD23	2.45	0.41
1:J:184:LEU:HD23	1:J:220:VAL:HB	2.03	0.41
1:M:175:LEU:N	1:M:175:LEU:CD2	2.73	0.41
1:O:187:HIS:CE1	7:O:509:HOH:O	2.74	0.41
1:O:272:ASP:OD1	1:O:272:ASP:C	2.64	0.41
1:Q:145:LEU:HD12	1:Q:145:LEU:HA	1.89	0.41
1:T:132:ASP:O	1:T:136:MET:HG2	2.20	0.41
1:T:150:GLU:HA	1:T:151:PRO:HA	1.84	0.41
1:V:44:ILE:HD11	1:V:120:VAL:HA	2.03	0.41
1:V:232:GLN:OE1	1:V:235:ARG:NH1	2.47	0.41
1:V:248:LYS:NZ	1:V:248:LYS:HB3	2.35	0.41
1:A:29:ILE:HG13	1:A:30:GLU:OE1	2.20	0.41
1:C:252:MET:HE1	7:C:609:HOH:O	2.19	0.41
1:C:252:MET:O	1:C:252:MET:SD	2.78	0.41
1:E:318:ARG:HD3	7:E:547:HOH:O	2.21	0.41
1:H:218:LEU:HD12	1:H:218:LEU:N	2.36	0.41
1:I:63:ALA:HB3	1:I:342:LYS:HG2	2.02	0.41
1:J:37:ILE:HG23	1:J:138:VAL:HG22	2.03	0.41
1:J:45:ARG:HD2	7:J:574:HOH:O	2.20	0.41
1:J:49:LYS:NZ	1:J:53:GLU:OE1	2.39	0.41
1:J:184:LEU:HA	1:J:220:VAL:O	2.21	0.41
1:K:194:PHE:CD2	1:K:195:GLU:HG3	2.56	0.41
1:K:248:LYS:NZ	7:K:531:HOH:O	2.54	0.41
1:M:174:LYS:C	1:M:175:LEU:HD23	2.46	0.41
1:N:124:GLU:HB3	1:Q:47:ARG:HD2	2.01	0.41
1:N:205:PHE:O	1:N:209:MET:HG2	2.21	0.41
1:P:66:SER:OG	1:P:117:VAL:HG13	2.21	0.41
1:S:54:LEU:O	1:S:58:LEU:HD23	2.20	0.41
1:V:68:LEU:O	1:V:156:VAL:HA	2.21	0.41
1:V:144:LYS:NZ	7:V:518:HOH:O	2.51	0.41
1:V:302:LEU:O	1:V:339:LYS:NZ	2.48	0.41
1:X:250:ARG:HB3	1:X:251:PRO:HD3	2.03	0.41
1:C:218:LEU:HD22	1:C:258:LEU:HD11	2.03	0.41
1:D:278:PHE:CE2	1:D:291:SER:HA	2.56	0.41
1:M:137:ASN:HB3	7:M:522:HOH:O	2.20	0.41
1:W:42:THR:HA	1:W:45:ARG:NH2	2.36	0.41
1:B:257:LYS:HE3	1:B:303:GLN:NE2	2.36	0.40
1:C:69:GLY:HA3	1:C:119:ASP:OD1	2.20	0.40
1:H:267:ILE:O	1:H:309:ALA:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:198:LYS:HE2	1:K:199:TYR:CZ	2.56	0.40
1:L:64:SER:HB3	7:L:574:HOH:O	2.20	0.40
1:L:163:ILE:HD11	1:L:312:VAL:HG12	2.03	0.40
1:M:31:LYS:HD3	1:U:148:GLU:HB3	2.03	0.40
1:M:147:MET:HE1	1:M:171:VAL:HA	2.03	0.40
1:M:168:VAL:HG11	1:M:181:ILE:HD11	2.03	0.40
1:N:169:ARG:HG3	1:N:213:TYR:CZ	2.56	0.40
1:P:244:ARG:NH2	7:P:521:HOH:O	2.54	0.40
1:R:318:ARG:NE	7:R:501:HOH:O	2.20	0.40
1:S:155:LEU:C	1:S:155:LEU:HD23	2.47	0.40
1:A:81:GLY:N	1:A:82:PRO:CD	2.85	0.40
1:C:38:ASP:O	1:C:42:THR:OG1	2.34	0.40
1:E:198:LYS:HE3	1:E:199:TYR:CE2	2.56	0.40
1:J:27:SER:C	1:J:29:ILE:H	2.28	0.40
1:L:72:LEU:HD23	1:L:72:LEU:C	2.46	0.40
1:M:175:LEU:HD12	1:M:263:LYS:HG2	1.98	0.40
1:M:269:ILE:HG21	1:M:332:LEU:HD13	2.03	0.40
1:S:72:LEU:C	1:S:72:LEU:HD23	2.46	0.40
4:U:405:ORN:O	4:U:405:ORN:CG	2.69	0.40
1:V:150:GLU:HA	1:V:151:PRO:HA	1.90	0.40
1:C:131:ASP:OD1	1:C:133:ASP:HB2	2.21	0.40
1:D:267:ILE:O	1:D:309:ALA:HA	2.20	0.40
1:H:39:ALA:HB3	1:K:43:LEU:HD13	2.03	0.40
1:L:162:SER:HB2	1:L:199:TYR:O	2.21	0.40
1:M:37:ILE:HG23	1:M:138:VAL:CG2	2.51	0.40
1:N:141:GLU:O	1:N:145:LEU:HD22	2.22	0.40
1:Q:67:LEU:O	1:Q:117:VAL:HG22	2.21	0.40
1:W:69:GLY:HA3	1:W:119:ASP:OD1	2.20	0.40
1:A:29:ILE:O	1:A:33:GLN:HG3	2.21	0.40
1:B:148:GLU:OE2	1:B:174:LYS:NZ	2.54	0.40
1:C:49:LYS:O	1:C:53:GLU:HG3	2.21	0.40
1:C:192:ASP:O	1:C:207:ARG:NH2	2.44	0.40
1:G:57:LEU:HD23	1:G:57:LEU:O	2.22	0.40
1:P:32:GLY:O	1:P:35:ARG:HB2	2.21	0.40
1:P:81:GLY:N	1:P:82:PRO:CD	2.85	0.40
1:V:163:ILE:O	1:V:166:PRO:HG2	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	315/321 (98%)	305 (97%)	10 (3%)	0	100	100
1	B	315/321 (98%)	308 (98%)	7 (2%)	0	100	100
1	C	316/321 (98%)	304 (96%)	12 (4%)	0	100	100
1	D	314/321 (98%)	305 (97%)	9 (3%)	0	100	100
1	E	316/321 (98%)	308 (98%)	8 (2%)	0	100	100
1	F	315/321 (98%)	306 (97%)	9 (3%)	0	100	100
1	G	315/321 (98%)	304 (96%)	11 (4%)	0	100	100
1	H	315/321 (98%)	308 (98%)	7 (2%)	0	100	100
1	I	314/321 (98%)	304 (97%)	10 (3%)	0	100	100
1	J	315/321 (98%)	306 (97%)	9 (3%)	0	100	100
1	K	314/321 (98%)	302 (96%)	12 (4%)	0	100	100
1	L	315/321 (98%)	306 (97%)	9 (3%)	0	100	100
1	M	314/321 (98%)	299 (95%)	15 (5%)	0	100	100
1	N	314/321 (98%)	308 (98%)	6 (2%)	0	100	100
1	O	314/321 (98%)	299 (95%)	15 (5%)	0	100	100
1	P	314/321 (98%)	305 (97%)	9 (3%)	0	100	100
1	Q	314/321 (98%)	308 (98%)	6 (2%)	0	100	100
1	R	315/321 (98%)	305 (97%)	10 (3%)	0	100	100
1	S	314/321 (98%)	301 (96%)	13 (4%)	0	100	100
1	T	316/321 (98%)	309 (98%)	7 (2%)	0	100	100
1	U	315/321 (98%)	307 (98%)	8 (2%)	0	100	100
1	V	314/321 (98%)	302 (96%)	12 (4%)	0	100	100
1	W	315/321 (98%)	307 (98%)	8 (2%)	0	100	100
1	X	314/321 (98%)	307 (98%)	7 (2%)	0	100	100
All	All	7552/7704 (98%)	7323 (97%)	229 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/267 (99%)	254 (96%)	11 (4%)	26	31
1	B	264/267 (99%)	259 (98%)	5 (2%)	50	61
1	C	266/267 (100%)	247 (93%)	19 (7%)	13	12
1	D	264/267 (99%)	256 (97%)	8 (3%)	36	45
1	E	264/267 (99%)	257 (97%)	7 (3%)	39	49
1	F	265/267 (99%)	259 (98%)	6 (2%)	44	55
1	G	265/267 (99%)	259 (98%)	6 (2%)	44	55
1	H	264/267 (99%)	256 (97%)	8 (3%)	36	45
1	I	264/267 (99%)	255 (97%)	9 (3%)	32	40
1	J	264/267 (99%)	259 (98%)	5 (2%)	50	61
1	K	264/267 (99%)	258 (98%)	6 (2%)	44	55
1	L	264/267 (99%)	256 (97%)	8 (3%)	36	45
1	M	264/267 (99%)	246 (93%)	18 (7%)	14	14
1	N	264/267 (99%)	255 (97%)	9 (3%)	32	40
1	O	264/267 (99%)	250 (95%)	14 (5%)	20	22
1	P	264/267 (99%)	258 (98%)	6 (2%)	44	55
1	Q	264/267 (99%)	256 (97%)	8 (3%)	36	45
1	R	265/267 (99%)	258 (97%)	7 (3%)	40	50
1	S	264/267 (99%)	255 (97%)	9 (3%)	32	40
1	T	265/267 (99%)	257 (97%)	8 (3%)	36	45
1	U	265/267 (99%)	259 (98%)	6 (2%)	44	55
1	V	264/267 (99%)	252 (96%)	12 (4%)	24	29
1	W	264/267 (99%)	253 (96%)	11 (4%)	26	31
1	X	264/267 (99%)	258 (98%)	6 (2%)	44	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	6344/6408 (99%)	6132 (97%)	212 (3%)	33	42

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	30	GLU
1	A	31	LYS
1	A	57	LEU
1	A	58	LEU
1	A	66	SER
1	A	127	ASP
1	A	145	LEU
1	A	204	SER
1	A	234	LYS
1	A	248	LYS
1	B	35	ARG
1	B	145	LEU
1	B	195	GLU
1	B	227	GLN
1	B	244	ARG
1	C	27	SER
1	C	28	SER
1	C	30	GLU
1	C	31	LYS
1	C	46	GLU
1	C	58	LEU
1	C	127	ASP
1	C	132	ASP
1	C	145	LEU
1	C	148	GLU
1	C	150	GLU
1	C	161	HIS
1	C	174	LYS
1	C	190	ILE
1	C	227	GLN
1	C	244	ARG
1	C	248	LYS
1	C	252	MET
1	C	262	VAL
1	D	27	SER
1	D	30	GLU

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Mol	Chain	Res	Type
1	D	145	LEU
1	D	150	GLU
1	D	161	HIS
1	D	248	LYS
1	D	257	LYS
1	D	318	ARG
1	E	28	SER
1	E	145	LEU
1	E	151	PRO
1	E	161	HIS
1	E	248	LYS
1	E	255	ASN
1	E	318	ARG
1	F	35	ARG
1	F	134	ARG
1	F	145	LEU
1	F	161	HIS
1	F	248	LYS
1	F	318	ARG
1	G	28	SER
1	G	145	LEU
1	G	151	PRO
1	G	161	HIS
1	G	244	ARG
1	G	257	LYS
1	H	31	LYS
1	H	35	ARG
1	H	57	LEU
1	H	145	LEU
1	H	161	HIS
1	H	244	ARG
1	H	257	LYS
1	H	318	ARG
1	I	43	LEU
1	I	130	VAL
1	I	134	ARG
1	I	145	LEU
1	I	150	GLU
1	I	151	PRO
1	I	161	HIS
1	I	248	LYS
1	I	318	ARG

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Mol	Chain	Res	Type
1	J	30	GLU
1	J	145	LEU
1	J	161	HIS
1	J	252	MET
1	J	318	ARG
1	K	145	LEU
1	K	150	GLU
1	K	151	PRO
1	K	161	HIS
1	K	257	LYS
1	K	318	ARG
1	L	43	LEU
1	L	57	LEU
1	L	145	LEU
1	L	161	HIS
1	L	247	SER
1	L	248	LYS
1	L	252	MET
1	L	318	ARG
1	M	29	ILE
1	M	31	LYS
1	M	37	ILE
1	M	49	LYS
1	M	50	LEU
1	M	89	ILE
1	M	104	GLU
1	M	150	GLU
1	M	161	HIS
1	M	175	LEU
1	M	193	CYS
1	M	234	LYS
1	M	247	SER
1	M	248	LYS
1	M	252	MET
1	M	257	LYS
1	M	318	ARG
1	M	339	LYS
1	N	29	ILE
1	N	134	ARG
1	N	145	LEU
1	N	151	PRO
1	N	161	HIS

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Mol	Chain	Res	Type
1	N	190	ILE
1	N	227	GLN
1	N	252	MET
1	N	318	ARG
1	O	28	SER
1	O	43	LEU
1	O	132	ASP
1	O	145	LEU
1	O	149	GLU
1	O	150	GLU
1	O	161	HIS
1	O	231	GLU
1	O	232	GLN
1	O	235	ARG
1	O	252	MET
1	O	260	GLU
1	O	318	ARG
1	O	339	LYS
1	P	29	ILE
1	P	43	LEU
1	P	145	LEU
1	P	161	HIS
1	P	244	ARG
1	P	255	ASN
1	Q	29	ILE
1	Q	145	LEU
1	Q	150	GLU
1	Q	151	PRO
1	Q	161	HIS
1	Q	248	LYS
1	Q	257	LYS
1	Q	318	ARG
1	R	31	LYS
1	R	35	ARG
1	R	57	LEU
1	R	145	LEU
1	R	161	HIS
1	R	257	LYS
1	R	260	GLU
1	S	28	SER
1	S	30	GLU
1	S	31	LYS

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Mol	Chain	Res	Type
1	S	62	LYS
1	S	145	LEU
1	S	151	PRO
1	S	227	GLN
1	S	255	ASN
1	S	318	ARG
1	T	43	LEU
1	T	134	ARG
1	T	145	LEU
1	T	150	GLU
1	T	161	HIS
1	T	234	LYS
1	T	252	MET
1	T	318	ARG
1	U	27	SER
1	U	109	LYS
1	U	145	LEU
1	U	150	GLU
1	U	161	HIS
1	U	252	MET
1	V	29	ILE
1	V	57	LEU
1	V	132	ASP
1	V	136	MET
1	V	145	LEU
1	V	150	GLU
1	V	161	HIS
1	V	190	ILE
1	V	224	SER
1	V	234	LYS
1	V	248	LYS
1	V	252	MET
1	W	43	LEU
1	W	53	GLU
1	W	54	LEU
1	W	150	GLU
1	W	161	HIS
1	W	190	ILE
1	W	204	SER
1	W	215	ARG
1	W	247	SER
1	W	255	ASN

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Mol	Chain	Res	Type
1	W	339	LYS
1	X	30	GLU
1	X	107	GLU
1	X	145	LEU
1	X	161	HIS
1	X	257	LYS
1	X	260	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	GLN
1	A	303	GLN
1	B	240	GLN
1	B	303	GLN
1	B	317	GLN
1	D	301	ASN
1	E	227	GLN
1	E	301	ASN
1	F	80	GLN
1	F	303	GLN
1	F	317	GLN
1	G	137	ASN
1	G	317	GLN
1	H	34	ASN
1	H	240	GLN
1	J	34	ASN
1	J	80	GLN
1	K	301	ASN
1	L	303	GLN
1	N	240	GLN
1	O	232	GLN
1	P	240	GLN
1	P	317	GLN
1	Q	137	ASN
1	Q	255	ASN
1	Q	317	GLN
1	S	34	ASN
1	S	240	GLN
1	S	317	GLN
1	T	240	GLN
1	U	240	GLN

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Mol	Chain	Res	Type
1	V	137	ASN
1	W	227	GLN
1	X	34	ASN
1	X	137	ASN
1	X	240	GLN
1	X	255	ASN
1	X	303	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 116 ligands modelled in this entry, 72 are monoatomic - leaving 44 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	$\# Z > 2$
5	GOL	E	405	-	5,5,5	0.09	0	5,5,5	0.30	0
5	GOL	R	404	-	5,5,5	0.11	0	5,5,5	0.28	0
5	GOL	J	404	-	5,5,5	0.32	0	5,5,5	0.56	0
4	ORN	U	405	-	7,8,8	1.04	1 (14%)	6,9,9	0.28	0
5	GOL	W	403	-	5,5,5	0.17	0	5,5,5	0.32	0
5	GOL	I	404	-	5,5,5	0.17	0	5,5,5	0.44	0
5	GOL	J	405	-	5,5,5	0.15	0	5,5,5	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	S	403	-	5,5,5	0.12	0	5,5,5	0.44	0
5	GOL	K	403	-	5,5,5	0.17	0	5,5,5	0.46	0
5	GOL	B	403	-	5,5,5	0.16	0	5,5,5	0.34	0
5	GOL	N	403	-	5,5,5	0.14	0	5,5,5	0.40	0
4	ORN	P	405	-	7,8,8	0.79	0	6,9,9	1.31	1 (16%)
5	GOL	D	403	-	5,5,5	0.13	0	5,5,5	0.30	0
6	PEG	G	406	-	6,6,6	0.42	0	5,5,5	0.31	0
5	GOL	I	405	-	5,5,5	0.09	0	5,5,5	0.35	0
6	PEG	L	407	-	6,6,6	0.18	0	5,5,5	0.14	0
5	GOL	L	403	-	5,5,5	0.20	0	5,5,5	0.36	0
5	GOL	P	403	-	5,5,5	0.09	0	5,5,5	0.30	0
5	GOL	K	405	-	5,5,5	0.17	0	5,5,5	0.53	0
5	GOL	S	405	-	5,5,5	0.23	0	5,5,5	0.61	0
4	ORN	G	404	-	7,8,8	1.00	1 (14%)	6,9,9	0.54	0
4	ORN	C	405	-	7,8,8	0.80	0	6,9,9	0.51	0
5	GOL	G	408	-	5,5,5	0.16	0	5,5,5	0.50	0
5	GOL	C	403	-	5,5,5	0.27	0	5,5,5	0.94	0
4	ORN	K	406	-	7,8,8	0.64	0	6,9,9	0.90	1 (16%)
5	GOL	E	406	-	5,5,5	0.17	0	5,5,5	0.43	0
5	GOL	D	405	-	5,5,5	0.22	0	5,5,5	0.51	0
4	ORN	E	404	-	7,8,8	0.89	1 (14%)	6,9,9	0.33	0
5	GOL	H	403	-	5,5,5	0.13	0	5,5,5	0.33	0
5	GOL	B	405	-	5,5,5	0.20	0	5,5,5	0.55	0
5	GOL	H	404	-	5,5,5	0.21	0	5,5,5	0.43	0
6	PEG	L	406	-	6,6,6	0.23	0	5,5,5	0.10	0
5	GOL	L	405	-	5,5,5	0.28	0	5,5,5	0.60	0
5	GOL	Q	403	-	5,5,5	0.18	0	5,5,5	0.36	0
5	GOL	W	405	-	5,5,5	0.14	0	5,5,5	0.40	0
5	GOL	G	405	-	5,5,5	0.25	0	5,5,5	0.52	0
4	ORN	F	405	-	7,8,8	0.98	1 (14%)	6,9,9	0.37	0
5	GOL	F	404	-	5,5,5	0.16	0	5,5,5	0.50	0
5	GOL	U	403	-	5,5,5	0.17	0	5,5,5	0.42	0
4	ORN	V	404	-	7,8,8	0.85	1 (14%)	6,9,9	0.41	0
4	ORN	A	404	-	7,8,8	0.78	0	6,9,9	1.18	1 (16%)
5	GOL	T	404	-	5,5,5	0.08	0	5,5,5	0.26	0
6	PEG	G	407	-	6,6,6	0.39	0	5,5,5	0.26	0
6	PEG	L	408	-	6,6,6	0.14	0	5,5,5	0.20	0

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
5	GOL	E	405	-	-	2/4/4/4	-
5	GOL	R	404	-	-	4/4/4/4	-
5	GOL	J	404	-	-	0/4/4/4	-
4	ORN	U	405	-	-	2/8/8/8	-
5	GOL	W	403	-	-	4/4/4/4	-
5	GOL	I	404	-	-	0/4/4/4	-
5	GOL	J	405	-	-	2/4/4/4	-
5	GOL	S	403	-	-	2/4/4/4	-
5	GOL	K	403	-	-	2/4/4/4	-
5	GOL	B	403	-	-	2/4/4/4	-
5	GOL	N	403	-	-	2/4/4/4	-
4	ORN	P	405	-	-	3/8/8/8	-
5	GOL	D	403	-	-	2/4/4/4	-
6	PEG	G	406	-	-	2/4/4/4	-
5	GOL	I	405	-	-	4/4/4/4	-
6	PEG	L	407	-	-	1/4/4/4	-
5	GOL	L	403	-	-	3/4/4/4	-
5	GOL	P	403	-	-	4/4/4/4	-
5	GOL	K	405	-	-	1/4/4/4	-
5	GOL	S	405	-	-	2/4/4/4	-
4	ORN	G	404	-	-	3/8/8/8	-
4	ORN	C	405	-	-	0/8/8/8	-
5	GOL	G	408	-	-	0/4/4/4	-
5	GOL	C	403	-	-	3/4/4/4	-
4	ORN	K	406	-	-	2/8/8/8	-
5	GOL	E	406	-	-	4/4/4/4	-
5	GOL	D	405	-	-	0/4/4/4	-
4	ORN	E	404	-	-	0/8/8/8	-
5	GOL	H	403	-	-	1/4/4/4	-
5	GOL	B	405	-	-	2/4/4/4	-
5	GOL	H	404	-	-	0/4/4/4	-
6	PEG	L	406	-	-	3/4/4/4	-
5	GOL	L	405	-	-	0/4/4/4	-
5	GOL	Q	403	-	-	4/4/4/4	-
5	GOL	W	405	-	-	2/4/4/4	-
5	GOL	G	405	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ORN	F	405	-	-	5/8/8/8	-
5	GOL	F	404	-	-	2/4/4/4	-
5	GOL	U	403	-	-	0/4/4/4	-
4	ORN	V	404	-	-	3/8/8/8	-
4	ORN	A	404	-	-	3/8/8/8	-
5	GOL	T	404	-	-	4/4/4/4	-
6	PEG	G	407	-	-	2/4/4/4	-
6	PEG	L	408	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	405	ORN	OXT-C	-2.72	1.22	1.30
4	G	404	ORN	OXT-C	-2.64	1.22	1.30
4	F	405	ORN	OXT-C	-2.58	1.22	1.30
4	E	404	ORN	OXT-C	-2.31	1.23	1.30
4	V	404	ORN	OXT-C	-2.12	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	405	ORN	OXT-C-O	-2.94	117.41	124.08
4	A	404	ORN	OXT-C-O	-2.78	117.78	124.08
4	K	406	ORN	OXT-C-O	-2.00	119.53	124.08

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	403	GOL	O1-C1-C2-C3
5	D	403	GOL	C1-C2-C3-O3
5	E	405	GOL	O1-C1-C2-C3
5	E	406	GOL	O1-C1-C2-O2
5	E	406	GOL	O1-C1-C2-C3
5	I	405	GOL	C1-C2-C3-O3
5	J	405	GOL	O1-C1-C2-O2
5	J	405	GOL	O1-C1-C2-C3
5	K	403	GOL	O1-C1-C2-C3
5	N	403	GOL	O1-C1-C2-O2
5	N	403	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	P	403	GOL	O1-C1-C2-C3
5	R	404	GOL	O1-C1-C2-O2
5	R	404	GOL	O1-C1-C2-C3
5	R	404	GOL	C1-C2-C3-O3
5	S	403	GOL	O1-C1-C2-C3
5	S	405	GOL	O1-C1-C2-C3
5	T	404	GOL	O1-C1-C2-O2
5	T	404	GOL	O1-C1-C2-C3
5	T	404	GOL	C1-C2-C3-O3
5	W	403	GOL	O1-C1-C2-O2
5	W	403	GOL	C1-C2-C3-O3
5	S	403	GOL	O1-C1-C2-O2
5	S	405	GOL	O1-C1-C2-O2
5	B	403	GOL	O1-C1-C2-C3
5	B	405	GOL	O1-C1-C2-C3
5	E	406	GOL	C1-C2-C3-O3
5	F	404	GOL	C1-C2-C3-O3
5	G	405	GOL	O1-C1-C2-C3
5	I	405	GOL	O1-C1-C2-C3
5	P	403	GOL	C1-C2-C3-O3
5	Q	403	GOL	O1-C1-C2-C3
5	W	403	GOL	O1-C1-C2-C3
5	W	405	GOL	O1-C1-C2-C3
5	C	403	GOL	O1-C1-C2-O2
5	D	403	GOL	O2-C2-C3-O3
5	E	405	GOL	O1-C1-C2-O2
5	G	405	GOL	O1-C1-C2-O2
5	I	405	GOL	O2-C2-C3-O3
5	K	403	GOL	O1-C1-C2-O2
5	P	403	GOL	O1-C1-C2-O2
5	P	403	GOL	O2-C2-C3-O3
5	Q	403	GOL	O1-C1-C2-O2
5	R	404	GOL	O2-C2-C3-O3
5	T	404	GOL	O2-C2-C3-O3
6	L	407	PEG	O2-C3-C4-O4
6	G	407	PEG	O1-C1-C2-O2
6	L	406	PEG	O1-C1-C2-O2
6	L	406	PEG	O2-C3-C4-O4
5	B	405	GOL	O1-C1-C2-O2
5	W	403	GOL	O2-C2-C3-O3
5	H	403	GOL	O2-C2-C3-O3
5	L	403	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	Q	403	GOL	O2-C2-C3-O3
4	V	404	ORN	CA-CB-CG-CD
5	C	403	GOL	O2-C2-C3-O3
4	G	404	ORN	OXT-C-CA-CB
4	P	405	ORN	OXT-C-CA-CB
6	G	406	PEG	C4-C3-O2-C2
5	Q	403	GOL	C1-C2-C3-O3
4	F	405	ORN	OXT-C-CA-CB
4	G	404	ORN	O-C-CA-CB
4	K	406	ORN	O-C-CA-CB
5	W	405	GOL	O1-C1-C2-O2
4	K	406	ORN	OXT-C-CA-CB
6	L	406	PEG	C4-C3-O2-C2
4	A	404	ORN	OXT-C-CA-CB
6	G	406	PEG	C1-C2-O2-C3
5	B	403	GOL	O1-C1-C2-O2
5	E	406	GOL	O2-C2-C3-O3
5	F	404	GOL	O2-C2-C3-O3
5	I	405	GOL	O1-C1-C2-O2
4	P	405	ORN	O-C-CA-CB
4	U	405	ORN	O-C-CA-CB
4	U	405	ORN	OXT-C-CA-CB
4	V	404	ORN	O-C-CA-CB
4	V	404	ORN	OXT-C-CA-CB
4	A	404	ORN	O-C-CA-CB
5	L	403	GOL	C1-C2-C3-O3
4	F	405	ORN	O-C-CA-CB
5	K	405	GOL	O2-C2-C3-O3
5	L	403	GOL	O2-C2-C3-O3
4	G	404	ORN	OXT-C-CA-N
6	G	407	PEG	C1-C2-O2-C3
4	F	405	ORN	OXT-C-CA-N
4	P	405	ORN	OXT-C-CA-N
4	F	405	ORN	N-CA-CB-CG
4	F	405	ORN	O-C-CA-N
4	A	404	ORN	OXT-C-CA-N

There are no ring outliers.

15 monomers are involved in 22 short contacts:

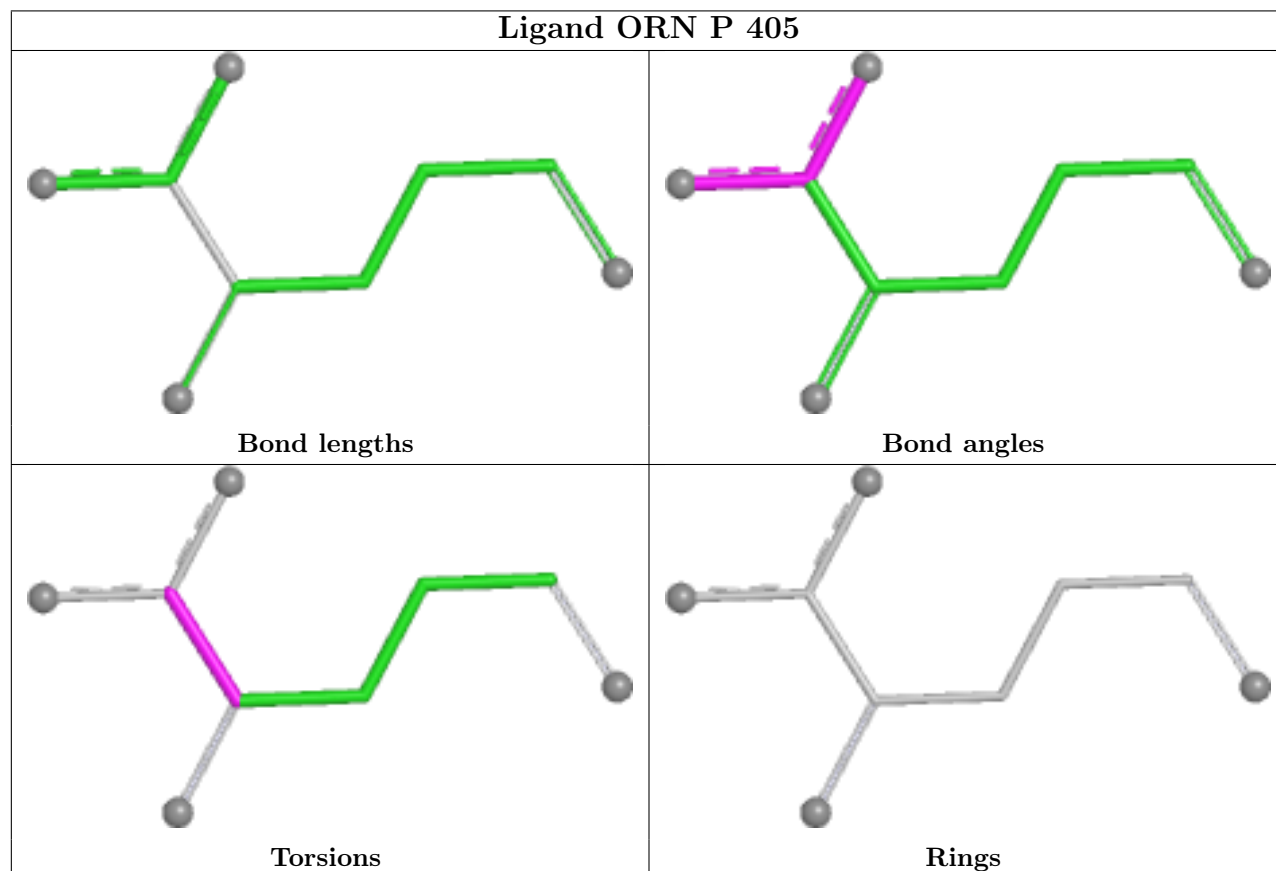
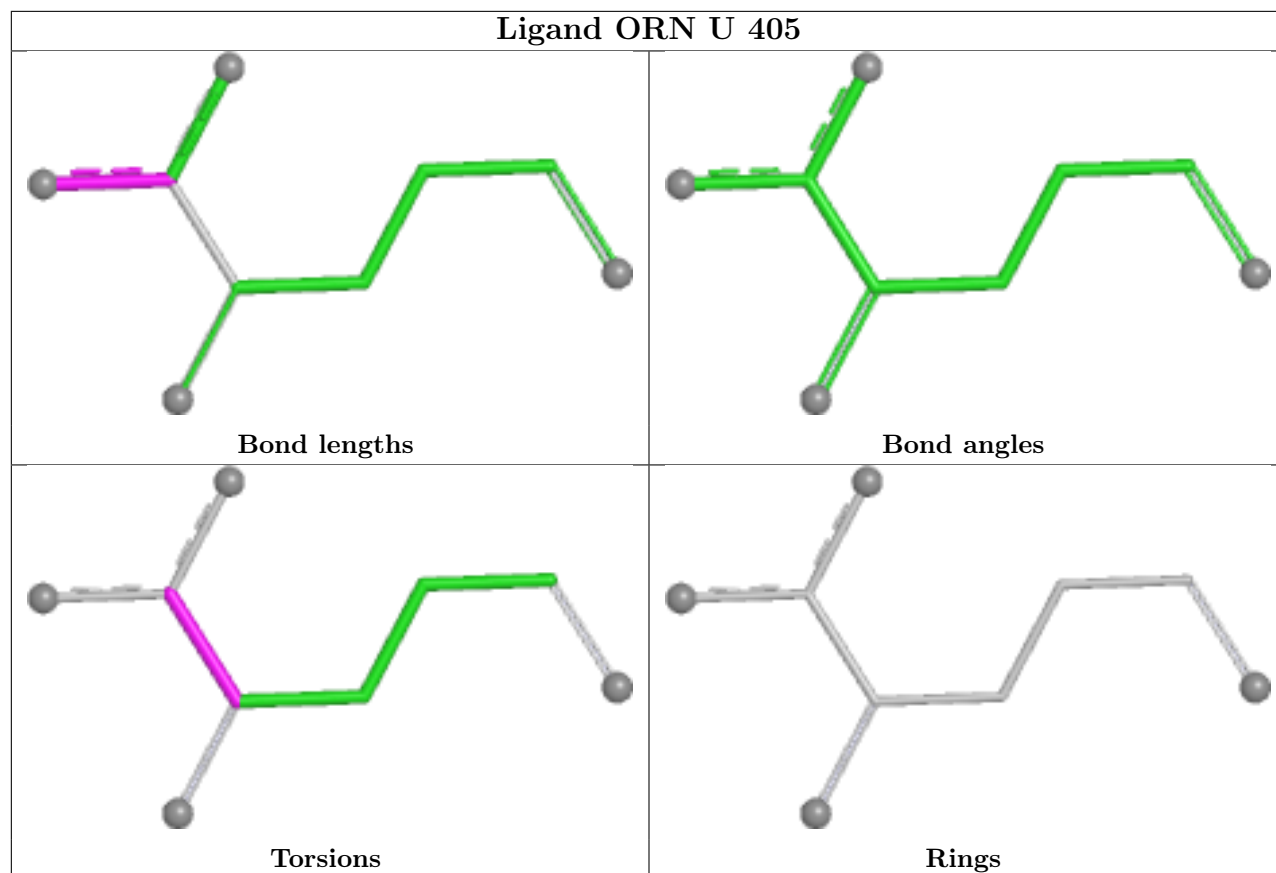
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	404	GOL	1	0

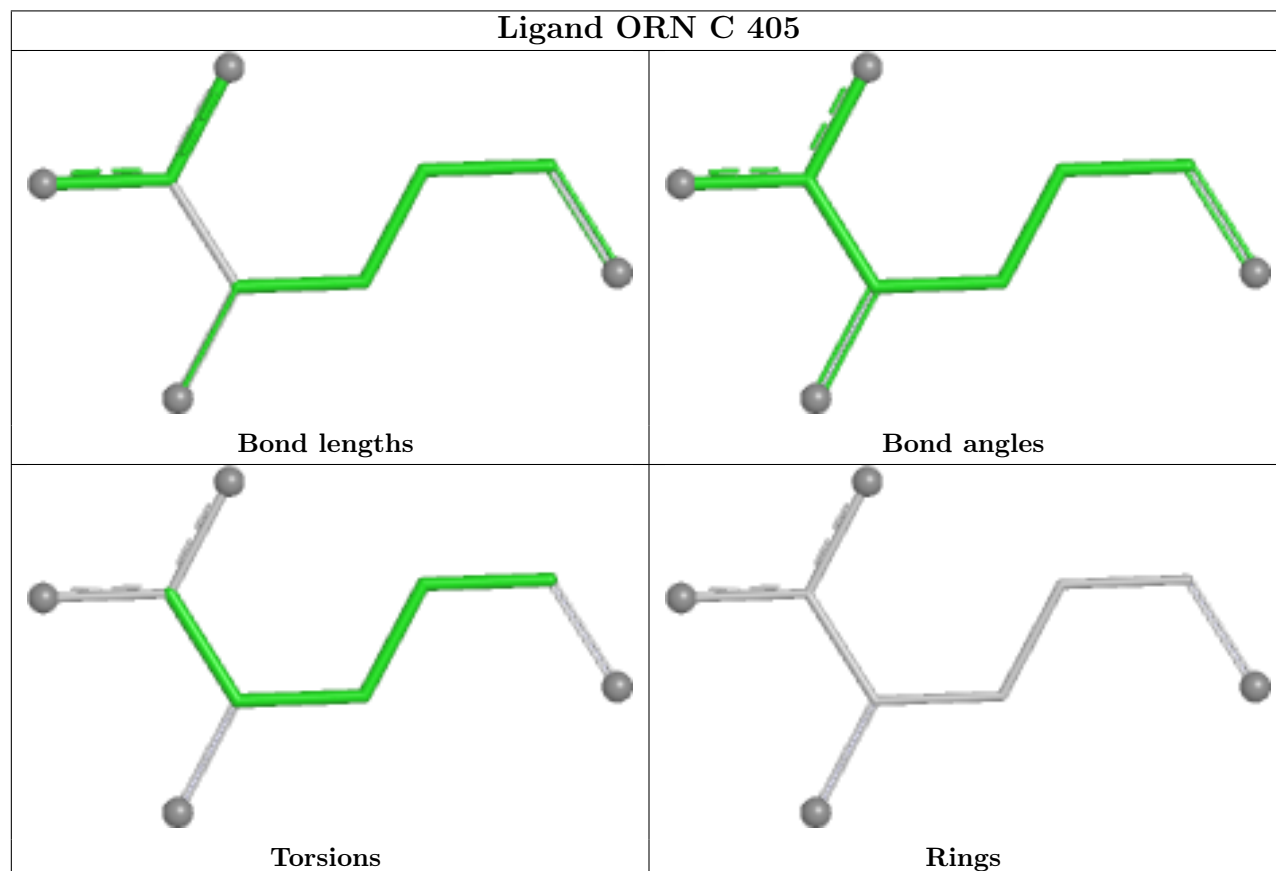
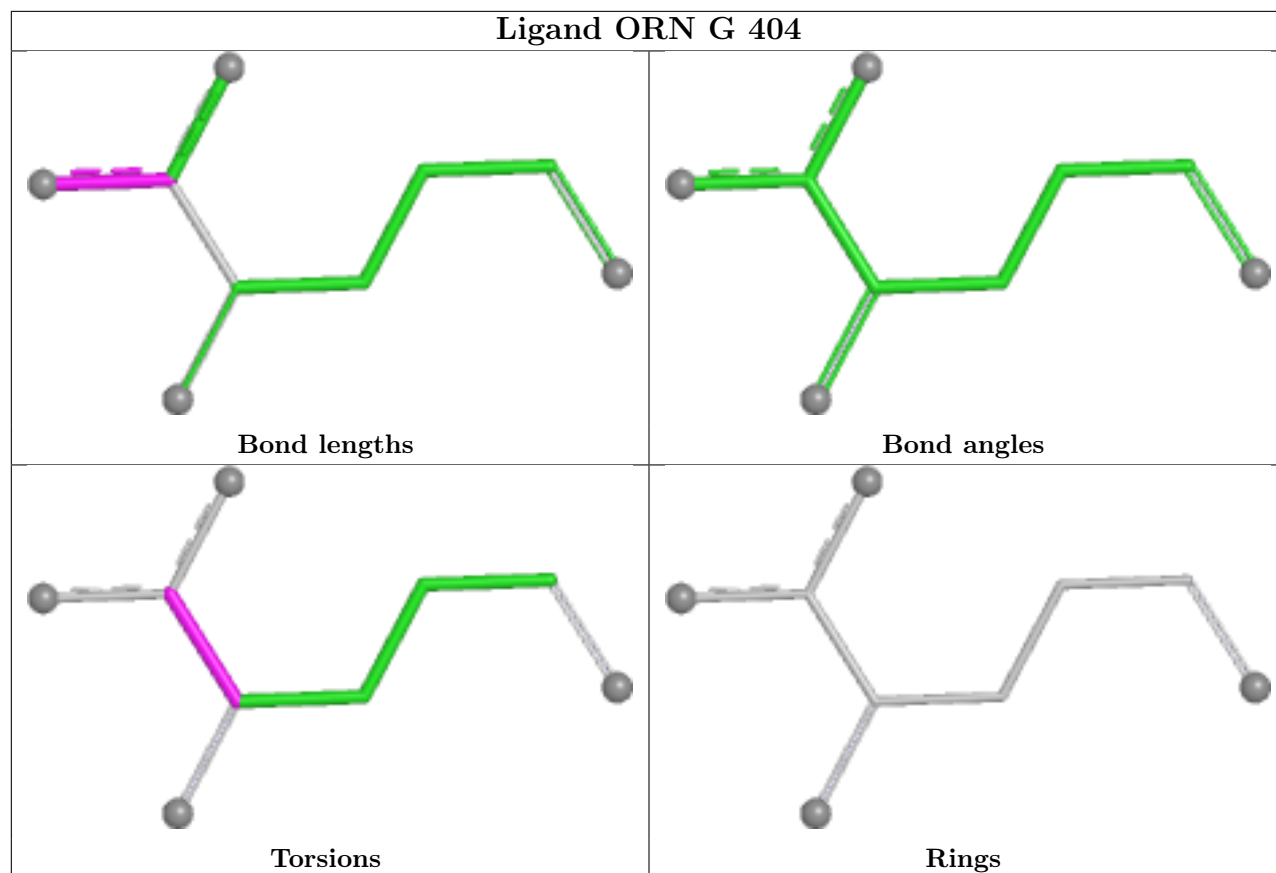
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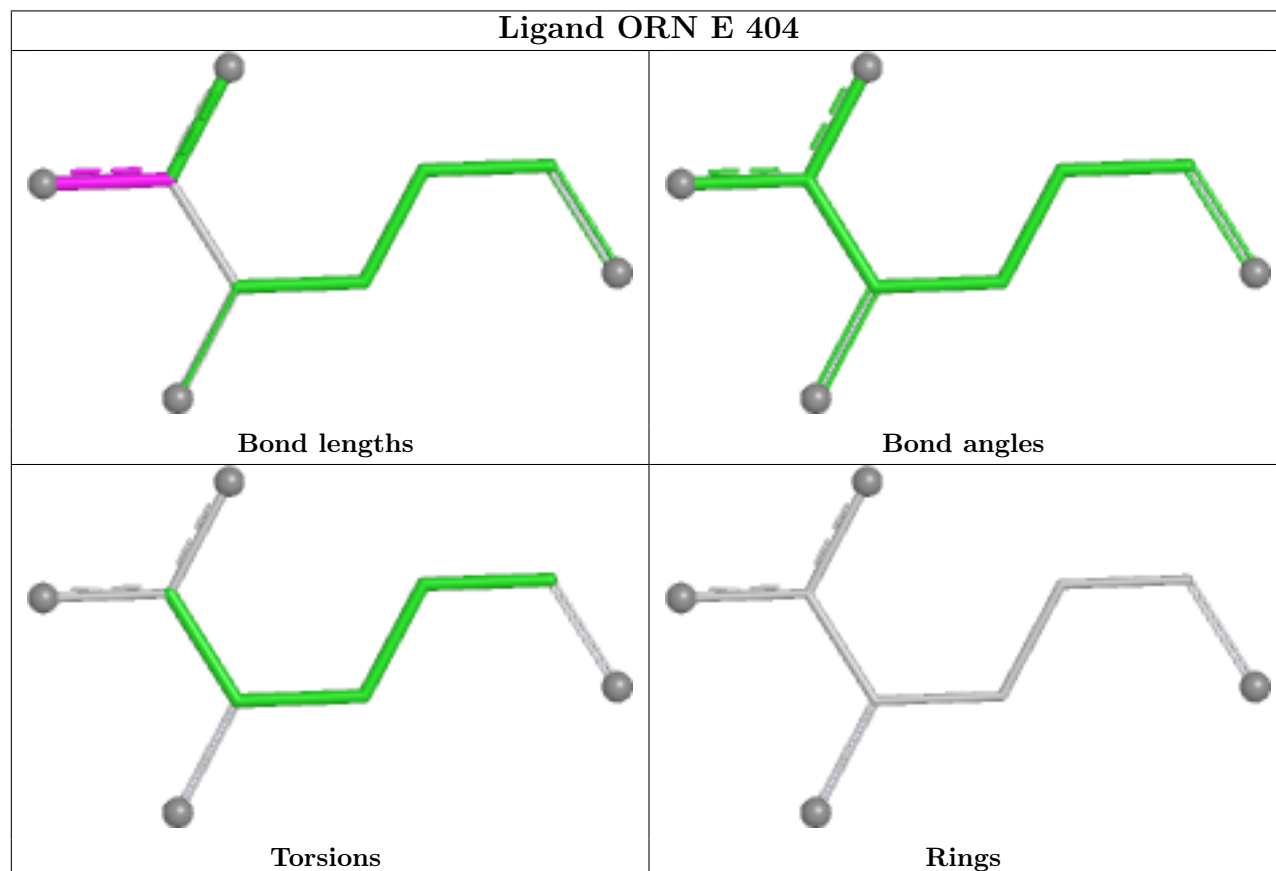
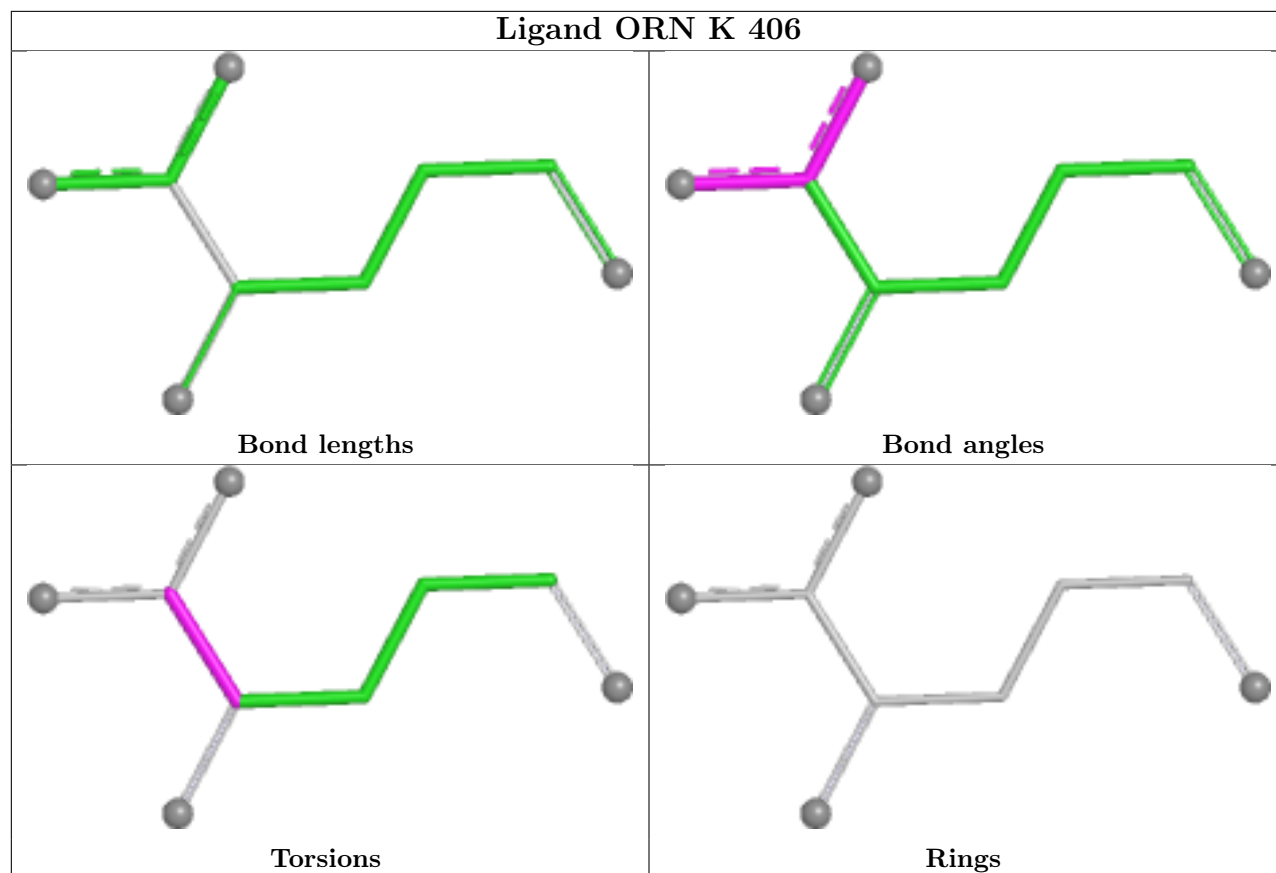
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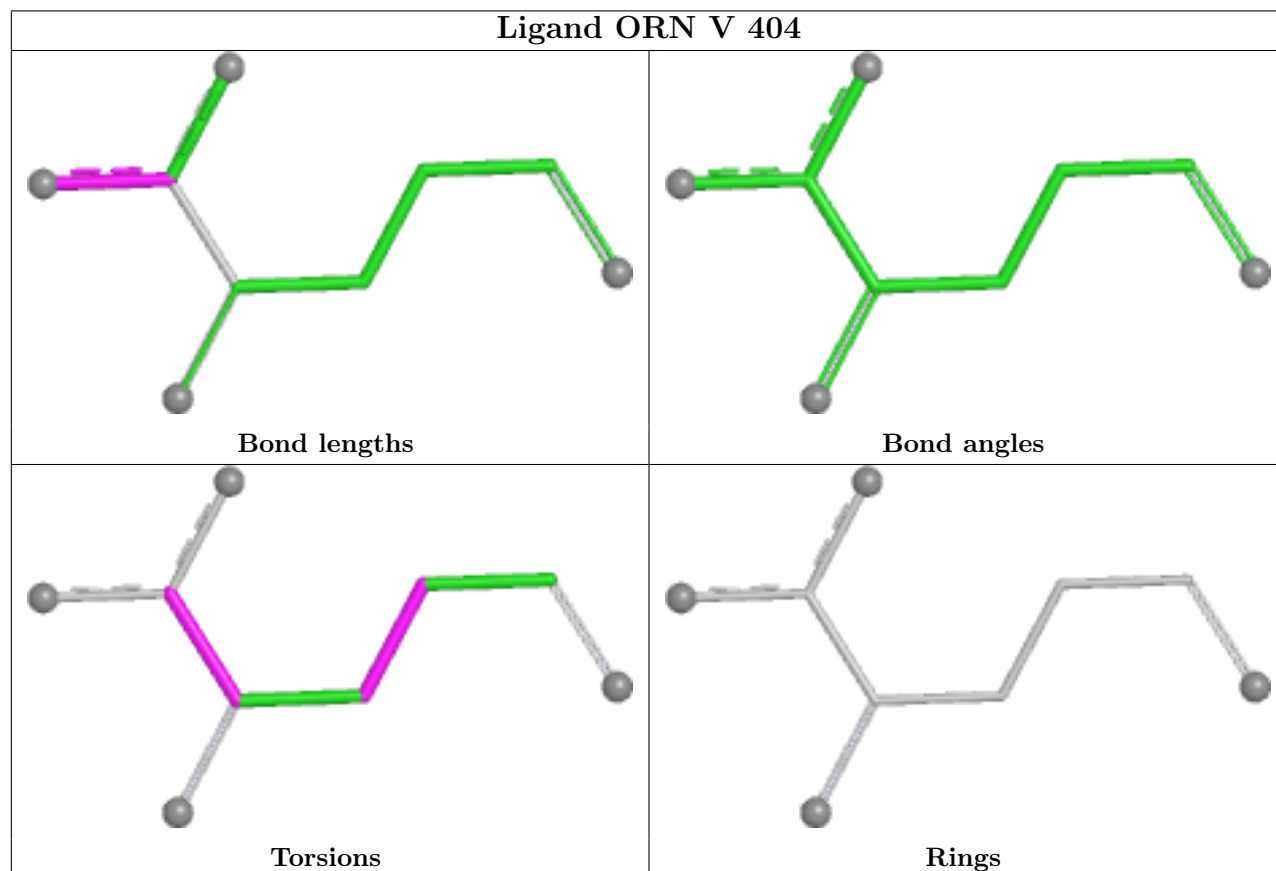
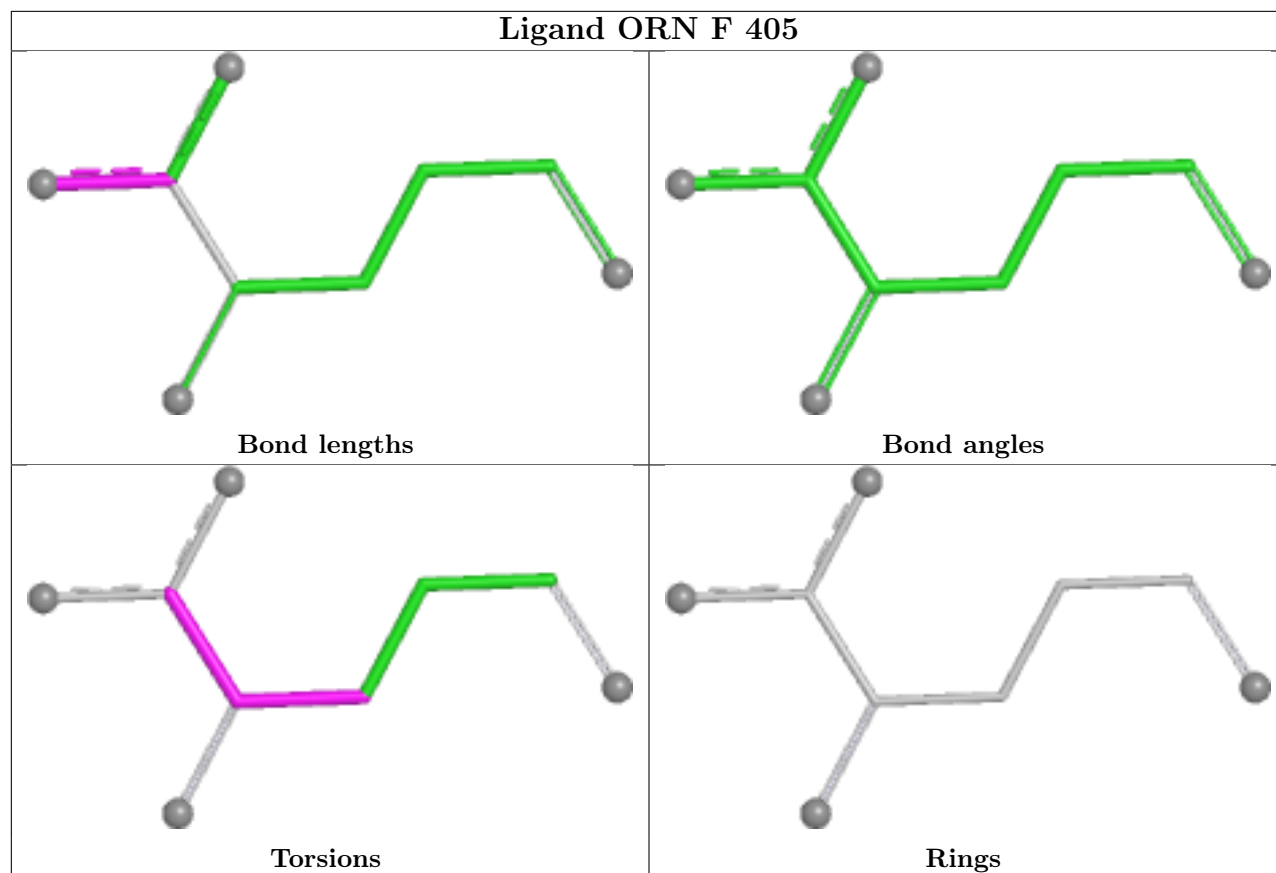
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	U	405	ORN	3	0
5	J	405	GOL	1	0
4	P	405	ORN	2	0
5	I	405	GOL	1	0
6	L	407	PEG	3	0
5	K	405	GOL	1	0
4	G	404	ORN	1	0
4	C	405	ORN	1	0
5	G	408	GOL	1	0
5	C	403	GOL	3	0
4	E	404	ORN	1	0
4	F	405	ORN	1	0
4	V	404	ORN	1	0
6	L	408	PEG	1	0

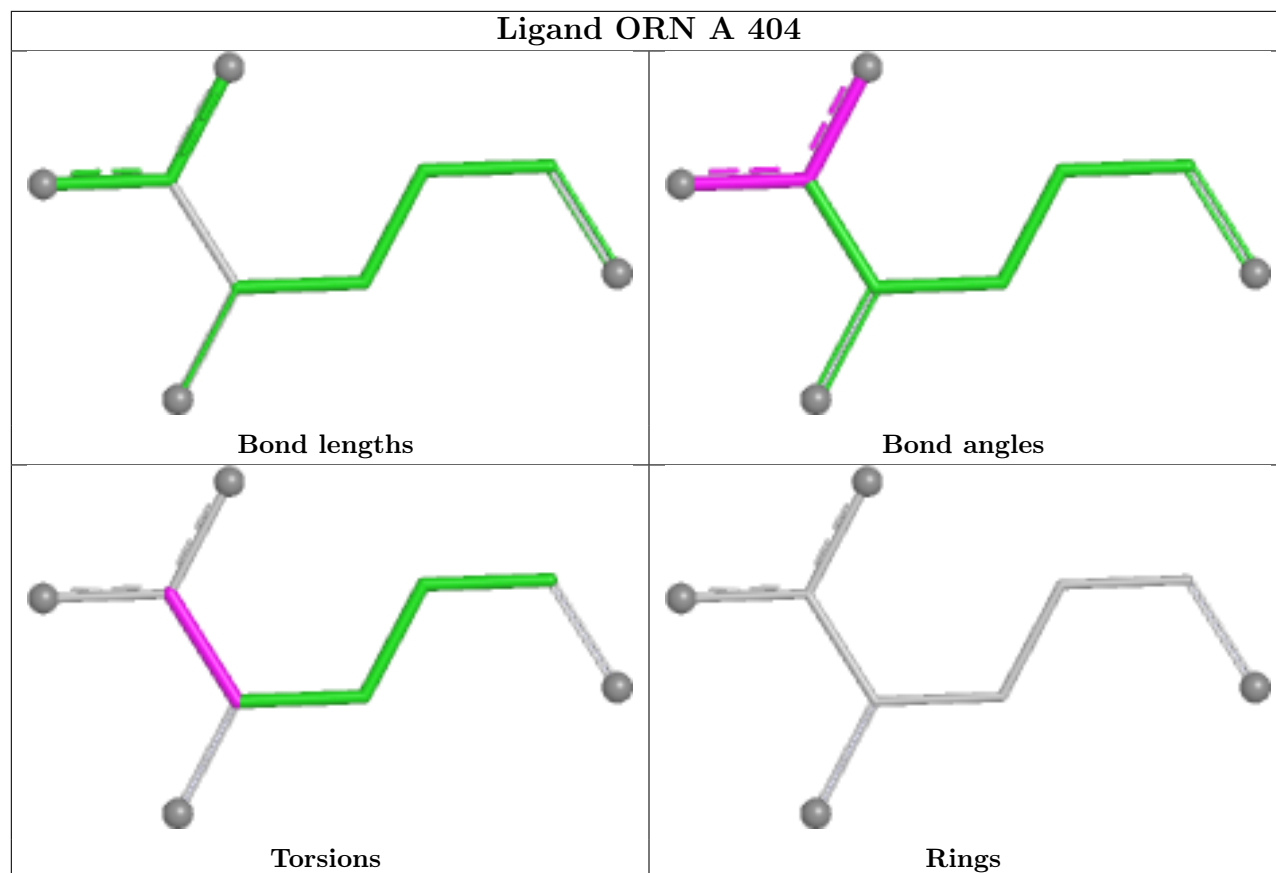
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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	316/321 (98%)	-0.08	6 (1%) 66 67	25, 54, 91, 116	1 (0%)
1	B	317/321 (98%)	-0.63	1 (0%) 90 90	21, 33, 56, 95	0
1	C	316/321 (98%)	0.37	12 (3%) 44 44	26, 59, 84, 125	2 (0%)
1	D	316/321 (98%)	-0.73	1 (0%) 90 90	18, 31, 54, 96	0
1	E	318/321 (99%)	-0.84	3 (0%) 81 82	16, 24, 38, 86	0
1	F	316/321 (98%)	-0.69	0 100 100	18, 31, 53, 80	1 (0%)
1	G	316/321 (98%)	-0.86	0 100 100	15, 25, 40, 58	1 (0%)
1	H	317/321 (98%)	-0.67	0 100 100	17, 31, 54, 69	0
1	I	316/321 (98%)	-0.68	1 (0%) 90 90	17, 32, 53, 78	0
1	J	317/321 (98%)	-0.74	4 (1%) 75 76	17, 25, 40, 93	0
1	K	316/321 (98%)	-0.59	1 (0%) 90 90	20, 33, 51, 82	0
1	L	317/321 (98%)	-0.44	1 (0%) 90 90	20, 36, 57, 74	0
1	M	316/321 (98%)	0.48	12 (3%) 44 44	38, 74, 117, 145	0
1	N	316/321 (98%)	-0.46	2 (0%) 85 86	26, 43, 66, 93	0
1	O	316/321 (98%)	0.36	9 (2%) 55 55	32, 69, 106, 124	0
1	P	316/321 (98%)	-0.45	3 (0%) 81 82	24, 43, 73, 115	0
1	Q	316/321 (98%)	-0.56	1 (0%) 90 90	22, 38, 61, 94	0
1	R	316/321 (98%)	-0.51	1 (0%) 90 90	22, 39, 64, 118	1 (0%)
1	S	316/321 (98%)	-0.39	1 (0%) 90 90	23, 40, 67, 95	0
1	T	318/321 (99%)	-0.50	1 (0%) 90 90	22, 41, 63, 88	0
1	U	316/321 (98%)	-0.26	4 (1%) 75 76	17, 46, 77, 117	1 (0%)
1	V	316/321 (98%)	0.61	12 (3%) 44 44	38, 59, 79, 90	0
1	W	317/321 (98%)	0.28	5 (1%) 70 71	29, 63, 92, 103	0
1	X	316/321 (98%)	-0.32	2 (0%) 85 86	26, 47, 74, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7593/7704 (98%)	-0.35	83 (1%) 78 79	15, 40, 81, 145	7 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	26	ALA	5.7
1	B	26	ALA	5.0
1	C	29	ILE	4.2
1	M	57	LEU	3.9
1	W	26	ALA	3.8
1	M	29	ILE	3.8
1	A	58	LEU	3.8
1	E	26	ALA	3.7
1	M	27	SER	3.7
1	P	27	SER	3.7
1	C	28	SER	3.6
1	J	27	SER	3.4
1	M	61	ALA	3.4
1	A	57	LEU	3.4
1	A	27	SER	3.3
1	K	27	SER	3.2
1	W	202	ALA	3.2
1	X	27	SER	3.2
1	L	26	ALA	3.1
1	D	27	SER	3.0
1	P	29	ILE	2.9
1	O	259	GLY	2.9
1	V	190	ILE	2.9
1	O	60	GLY	2.8
1	R	29	ILE	2.7
1	J	28	SER	2.7
1	W	44	ILE	2.7
1	O	236	PHE	2.6
1	V	36	VAL	2.6
1	I	27	SER	2.6
1	M	58	LEU	2.6
1	V	267	ILE	2.6
1	E	25	SER	2.6
1	N	27	SER	2.6
1	S	27	SER	2.6
1	O	235	ARG	2.5
1	V	220	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	29	ILE	2.5
1	M	252	MET	2.5
1	O	234	LYS	2.5
1	Q	27	SER	2.5
1	C	236	PHE	2.5
1	M	60	GLY	2.5
1	V	236	PHE	2.4
1	X	29	ILE	2.4
1	C	194	PHE	2.4
1	V	269	ILE	2.4
1	V	208	ILE	2.4
1	M	35	ARG	2.4
1	T	26	ALA	2.3
1	V	181	ILE	2.3
1	U	57	LEU	2.3
1	C	307	VAL	2.3
1	C	252	MET	2.2
1	C	27	SER	2.2
1	O	29	ILE	2.2
1	O	176	GLY	2.2
1	N	29	ILE	2.2
1	M	28	SER	2.2
1	U	27	SER	2.2
1	C	165	TYR	2.2
1	M	36	VAL	2.2
1	M	177	GLY	2.2
1	C	35	ARG	2.1
1	V	59	GLY	2.1
1	W	59	GLY	2.1
1	A	28	SER	2.1
1	E	27	SER	2.1
1	O	238	VAL	2.1
1	A	60	GLY	2.1
1	C	60	GLY	2.1
1	M	32	GLY	2.1
1	O	58	LEU	2.0
1	C	44	ILE	2.0
1	J	29	ILE	2.0
1	U	29	ILE	2.0
1	V	340	ILE	2.0
1	W	262	VAL	2.0
1	C	31	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	U	252	MET	2.0
1	V	43	LEU	2.0
1	V	58	LEU	2.0
1	P	31	LYS	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(Å ²)	Q<0.9
5	GOL	W	405	6/6	0.73	0.15	70,72,78,79	0
6	PEG	G	406	7/7	0.75	0.20	62,65,68,69	0
5	GOL	E	406	6/6	0.76	0.18	69,73,74,75	0
4	ORN	V	404	9/9	0.82	0.23	45,56,67,68	9
4	ORN	C	405	9/9	0.82	0.17	56,58,67,68	0
5	GOL	K	405	6/6	0.84	0.15	50,58,64,66	0
5	GOL	Q	403	6/6	0.84	0.15	45,58,62,62	0
5	GOL	C	403	6/6	0.84	0.16	53,57,65,66	0
4	ORN	F	405	9/9	0.84	0.15	45,52,60,61	0
4	ORN	U	405	9/9	0.85	0.15	55,58,70,74	0
6	PEG	L	408	7/7	0.85	0.15	71,73,75,75	0
5	GOL	F	404	6/6	0.86	0.12	54,59,61,70	0
6	PEG	G	407	7/7	0.86	0.16	52,59,63,64	0
4	ORN	P	405	9/9	0.86	0.17	52,57,70,73	0
5	GOL	D	403	6/6	0.87	0.13	46,55,56,61	0
5	GOL	W	403	6/6	0.87	0.16	55,64,68,71	0
4	ORN	K	406	9/9	0.87	0.15	42,49,53,54	0
5	GOL	G	408	6/6	0.88	0.12	53,62,67,68	0
3	NA	O	403	1/1	0.88	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	L	403	6/6	0.88	0.13	40,51,55,55	0
5	GOL	E	405	6/6	0.88	0.12	37,48,51,58	0
6	PEG	L	407	7/7	0.88	0.11	52,55,61,61	0
5	GOL	S	403	6/6	0.88	0.16	54,70,72,73	0
5	GOL	T	404	6/6	0.89	0.10	55,60,62,67	0
4	ORN	E	404	9/9	0.89	0.14	50,55,58,61	0
5	GOL	J	404	6/6	0.89	0.12	33,40,45,48	0
5	GOL	P	403	6/6	0.89	0.16	61,65,67,75	0
5	GOL	J	405	6/6	0.89	0.11	49,51,55,57	0
5	GOL	R	404	6/6	0.89	0.11	59,61,63,66	0
5	GOL	K	403	6/6	0.89	0.15	56,66,67,76	0
4	ORN	G	404	9/9	0.90	0.13	48,53,57,58	0
5	GOL	B	403	6/6	0.90	0.13	50,57,61,64	0
5	GOL	H	403	6/6	0.90	0.14	49,56,59,67	0
5	GOL	H	404	6/6	0.90	0.14	51,57,62,62	0
2	MN	O	401	1/1	0.90	0.08	57,57,57,57	0
4	ORN	A	404	9/9	0.91	0.12	41,48,58,60	0
5	GOL	U	403	6/6	0.91	0.11	47,51,56,56	0
6	PEG	L	406	7/7	0.91	0.11	57,66,78,79	0
5	GOL	L	405	6/6	0.91	0.10	42,49,53,56	0
5	GOL	I	405	6/6	0.91	0.13	55,59,61,62	0
5	GOL	N	403	6/6	0.92	0.13	61,65,73,74	0
5	GOL	I	404	6/6	0.92	0.10	51,53,56,57	0
5	GOL	S	405	6/6	0.92	0.12	54,57,60,61	0
3	NA	M	403	1/1	0.92	0.17	50,50,50,50	0
3	NA	C	404	1/1	0.93	0.19	44,44,44,44	0
2	MN	O	402	1/1	0.93	0.08	63,63,63,63	0
5	GOL	D	405	6/6	0.94	0.07	36,41,46,47	0
2	MN	V	401	1/1	0.95	0.06	42,42,42,42	0
3	NA	U	404	1/1	0.95	0.22	44,44,44,44	0
3	NA	X	403	1/1	0.96	0.06	39,39,39,39	0
2	MN	C	402	1/1	0.96	0.06	48,48,48,48	0
3	NA	Q	404	1/1	0.96	0.08	33,33,33,33	0
3	NA	S	404	1/1	0.96	0.18	42,42,42,42	0
2	MN	C	401	1/1	0.96	0.05	45,45,45,45	0
5	GOL	G	405	6/6	0.96	0.07	34,38,39,41	0
5	GOL	B	405	6/6	0.96	0.07	41,45,46,48	0
3	NA	V	403	1/1	0.96	0.12	38,38,38,38	0
3	NA	H	405	1/1	0.97	0.06	34,34,34,34	0
3	NA	P	404	1/1	0.97	0.07	43,43,43,43	0
3	NA	W	404	1/1	0.97	0.14	47,47,47,47	0
2	MN	V	402	1/1	0.98	0.06	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	T	403	1/1	0.98	0.05	38,38,38,38	0
3	NA	I	403	1/1	0.98	0.05	33,33,33,33	0
3	NA	K	404	1/1	0.98	0.10	34,34,34,34	0
2	MN	W	402	1/1	0.98	0.04	49,49,49,49	0
3	NA	N	404	1/1	0.98	0.15	38,38,38,38	0
2	MN	M	402	1/1	0.98	0.06	54,54,54,54	0
3	NA	D	404	1/1	0.98	0.11	38,38,38,38	0
3	NA	G	403	1/1	0.98	0.14	29,29,29,29	0
3	NA	R	403	1/1	0.98	0.10	33,33,33,33	0
3	NA	L	404	1/1	0.99	0.13	36,36,36,36	0
2	MN	T	401	1/1	0.99	0.02	31,31,31,31	0
2	MN	T	402	1/1	0.99	0.02	36,36,36,36	0
2	MN	L	402	1/1	0.99	0.02	39,39,39,39	0
2	MN	M	401	1/1	0.99	0.02	45,45,45,45	0
2	MN	W	401	1/1	0.99	0.04	48,48,48,48	0
2	MN	B	402	1/1	0.99	0.03	36,36,36,36	0
2	MN	X	402	1/1	0.99	0.02	37,37,37,37	0
3	NA	A	403	1/1	0.99	0.13	34,34,34,34	0
3	NA	B	404	1/1	0.99	0.10	31,31,31,31	0
2	MN	N	401	1/1	0.99	0.02	35,35,35,35	0
2	MN	E	401	1/1	0.99	0.03	21,21,21,21	0
3	NA	E	403	1/1	0.99	0.07	32,32,32,32	0
3	NA	F	403	1/1	0.99	0.06	30,30,30,30	0
2	MN	K	402	1/1	0.99	0.02	32,32,32,32	0
2	MN	P	401	1/1	0.99	0.01	29,29,29,29	0
2	MN	S	401	1/1	0.99	0.02	28,28,28,28	0
3	NA	J	403	1/1	0.99	0.12	29,29,29,29	0
2	MN	S	402	1/1	0.99	0.03	38,38,38,38	0
2	MN	R	402	1/1	1.00	0.02	34,34,34,34	0
2	MN	G	401	1/1	1.00	0.01	21,21,21,21	0
2	MN	G	402	1/1	1.00	0.02	27,27,27,27	0
2	MN	H	401	1/1	1.00	0.01	25,25,25,25	0
2	MN	H	402	1/1	1.00	0.02	31,31,31,31	0
2	MN	U	401	1/1	1.00	0.01	32,32,32,32	0
2	MN	U	402	1/1	1.00	0.03	42,42,42,42	0
2	MN	I	401	1/1	1.00	0.01	22,22,22,22	0
2	MN	I	402	1/1	1.00	0.03	30,30,30,30	0
2	MN	J	401	1/1	1.00	0.01	21,21,21,21	0
2	MN	J	402	1/1	1.00	0.03	27,27,27,27	0
2	MN	X	401	1/1	1.00	0.01	32,32,32,32	0
2	MN	K	401	1/1	1.00	0.02	24,24,24,24	0
2	MN	A	402	1/1	1.00	0.02	41,41,41,41	0

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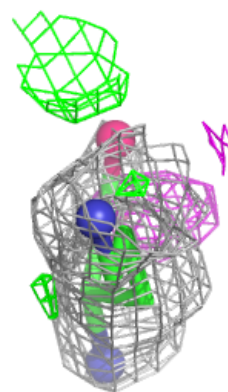
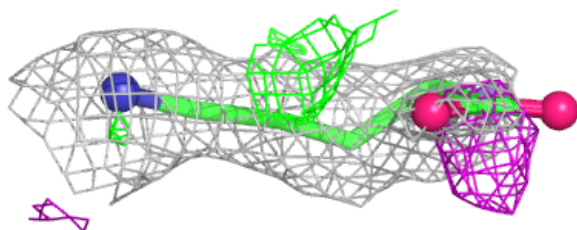
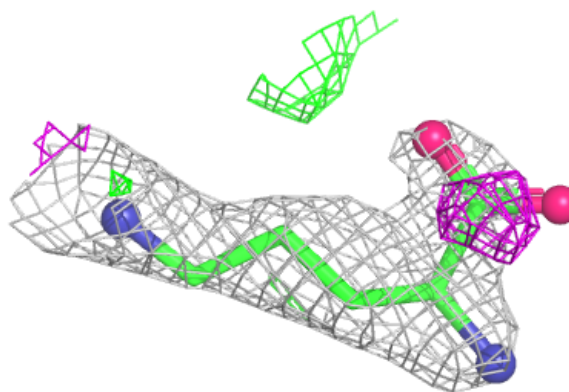
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	L	401	1/1	1.00	0.01	30,30,30,30	0
2	MN	B	401	1/1	1.00	0.02	31,31,31,31	0
2	MN	D	401	1/1	1.00	0.01	26,26,26,26	0
2	MN	D	402	1/1	1.00	0.02	33,33,33,33	0
2	MN	A	401	1/1	1.00	0.01	32,32,32,32	0
2	MN	N	402	1/1	1.00	0.03	41,41,41,41	0
2	MN	E	402	1/1	1.00	0.02	25,25,25,25	0
2	MN	F	401	1/1	1.00	0.01	23,23,23,23	0
2	MN	F	402	1/1	1.00	0.02	31,31,31,31	0
2	MN	P	402	1/1	1.00	0.03	39,39,39,39	0
2	MN	Q	401	1/1	1.00	0.01	29,29,29,29	0
2	MN	Q	402	1/1	1.00	0.02	33,33,33,33	0
2	MN	R	401	1/1	1.00	0.02	27,27,27,27	0

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

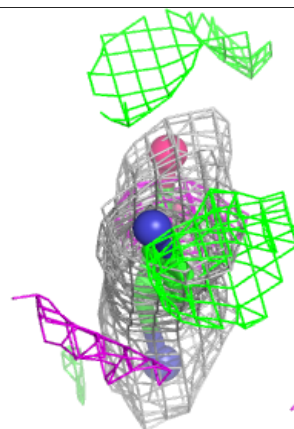
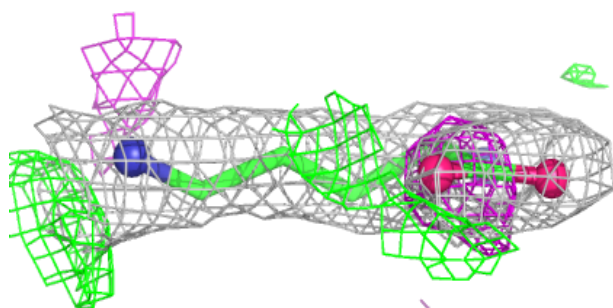
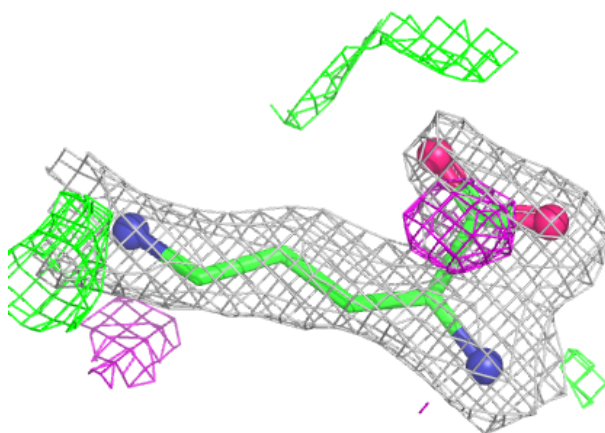
Electron density around ORN V 404:

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

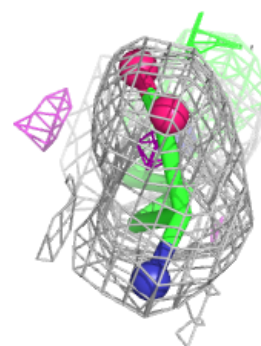
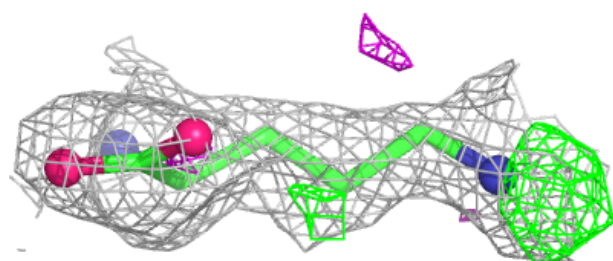
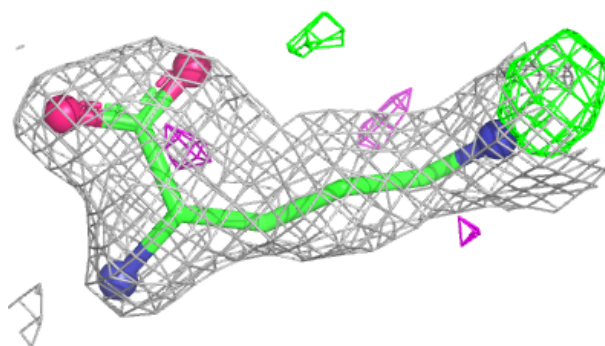


Electron density around ORN C 405:

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

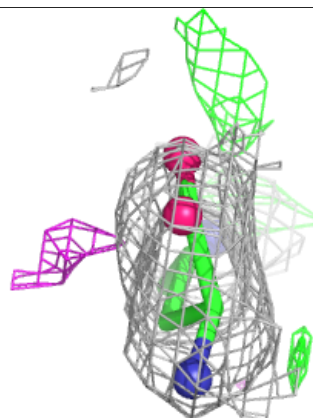
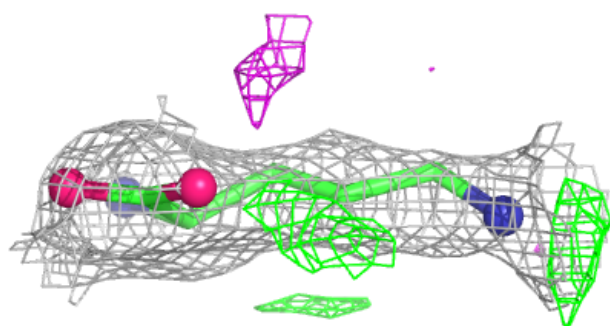
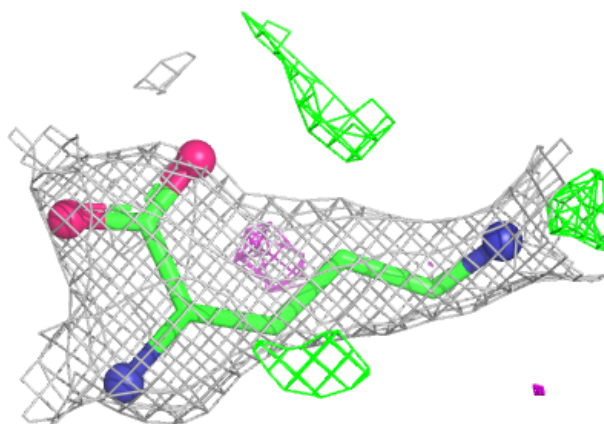
**Electron density around ORN F 405:**

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

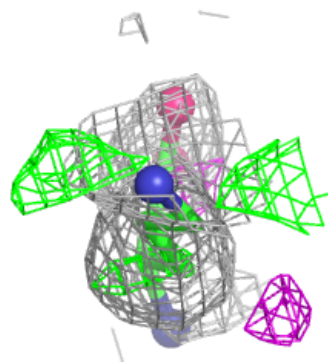
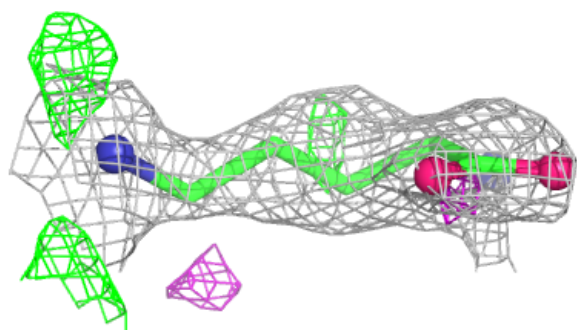
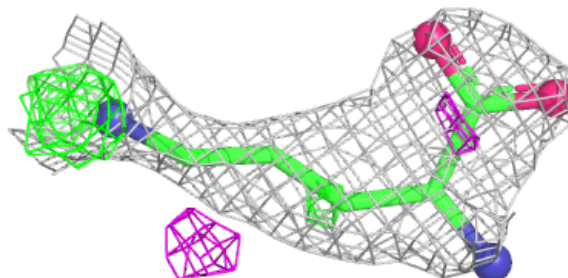


Electron density around ORN U 405:

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

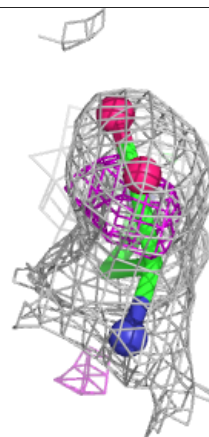
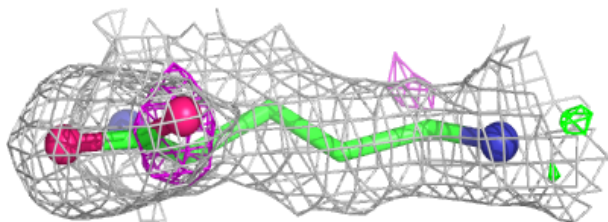
**Electron density around ORN P 405:**

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



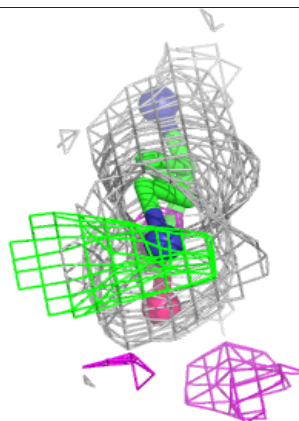
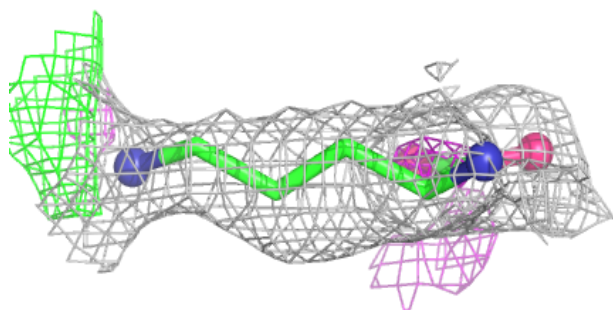
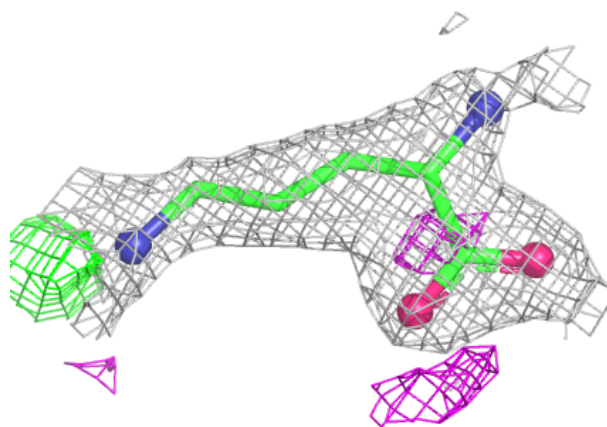
Electron density around ORN K 406:

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



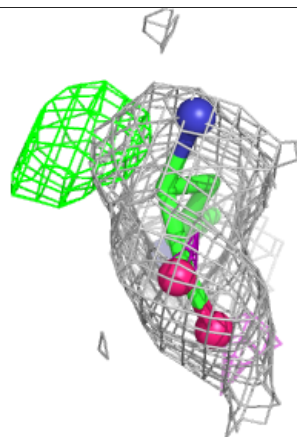
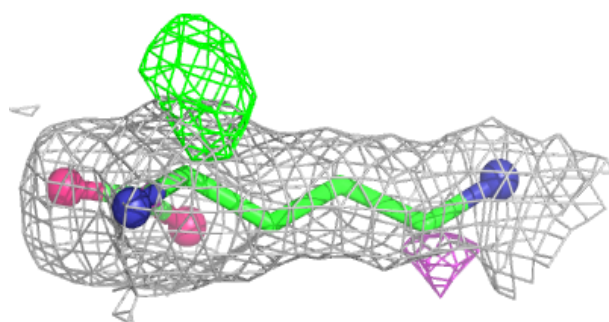
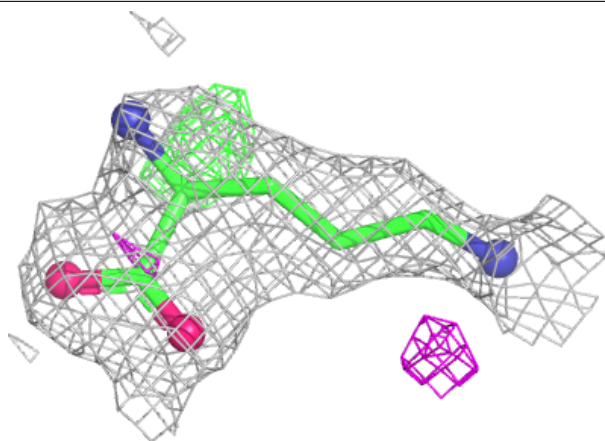
Electron density around ORN E 404:

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



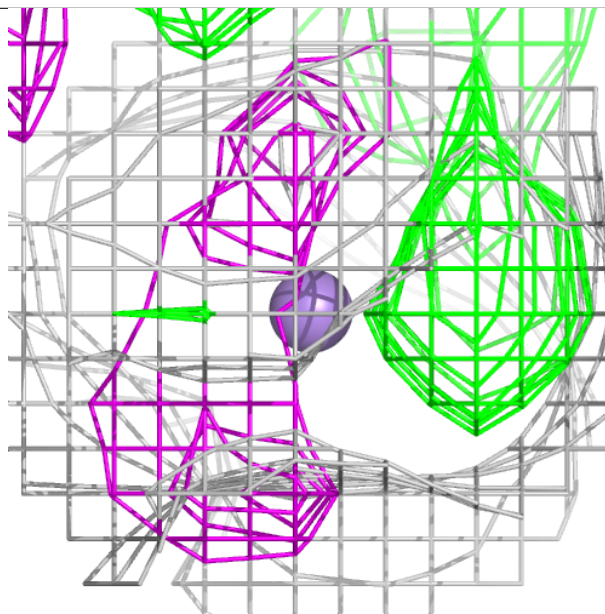
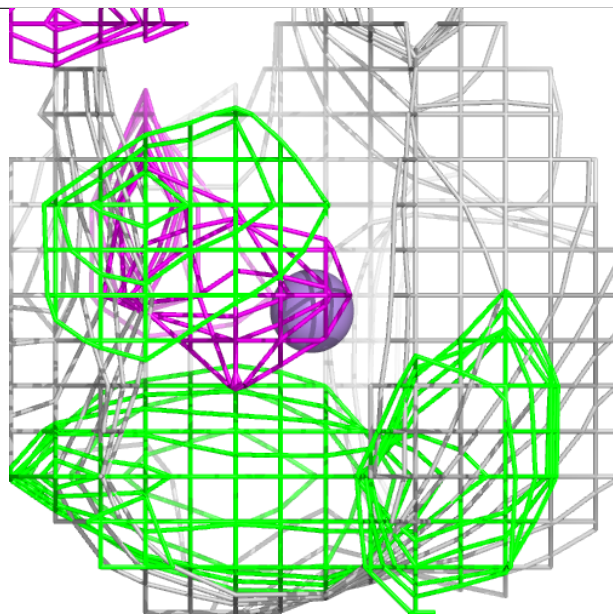
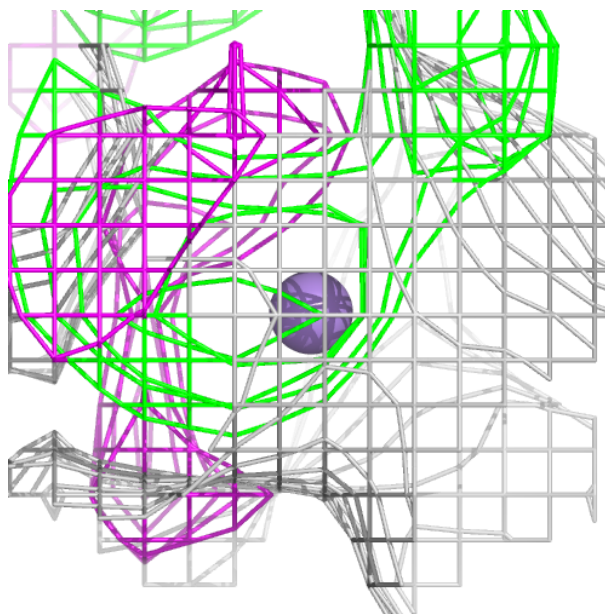
Electron density around ORN G 404:

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and green (positive)



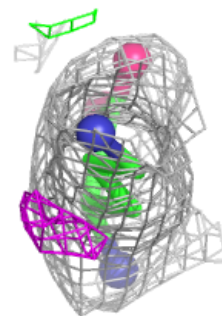
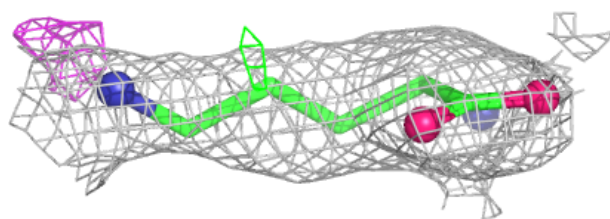
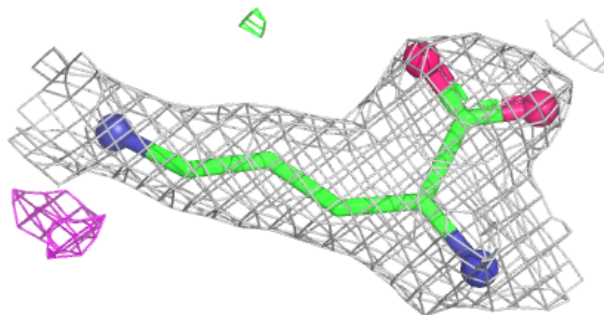
Electron density around MN O 401:

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



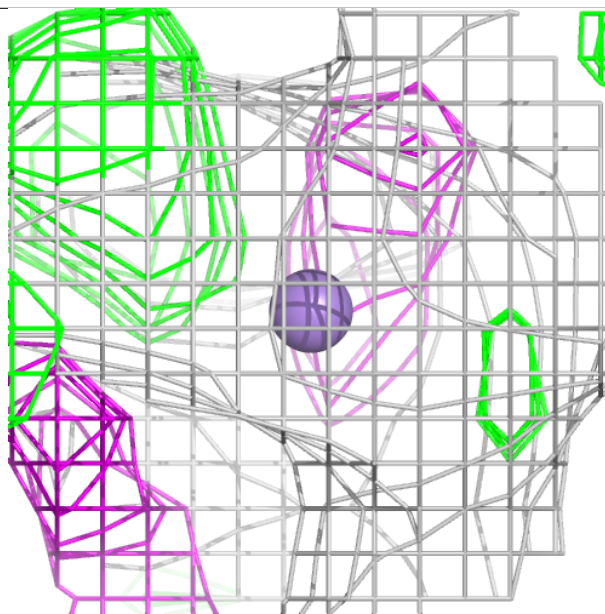
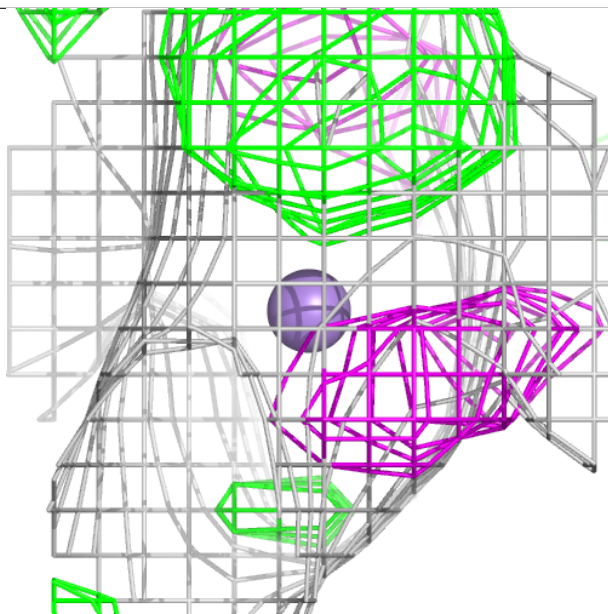
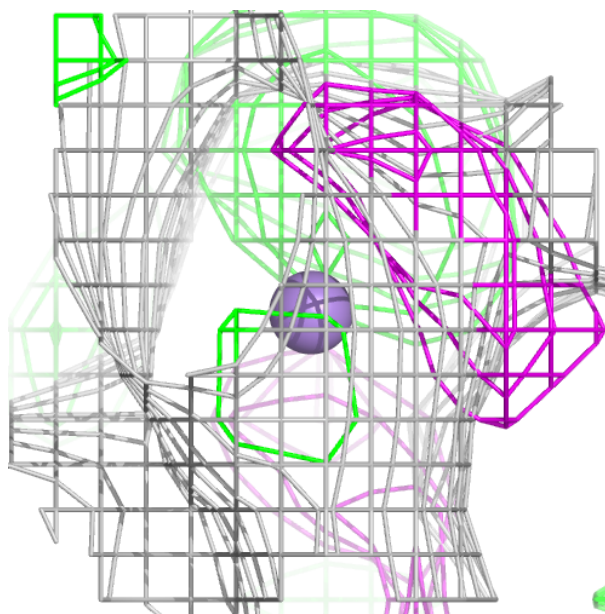
Electron density around ORN A 404:

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



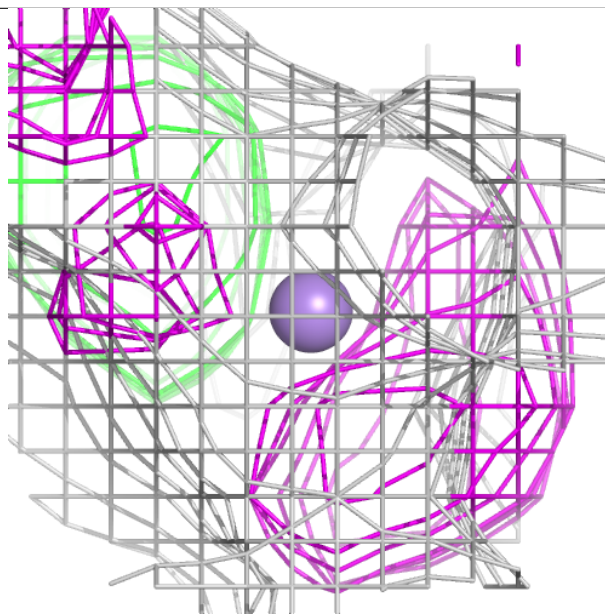
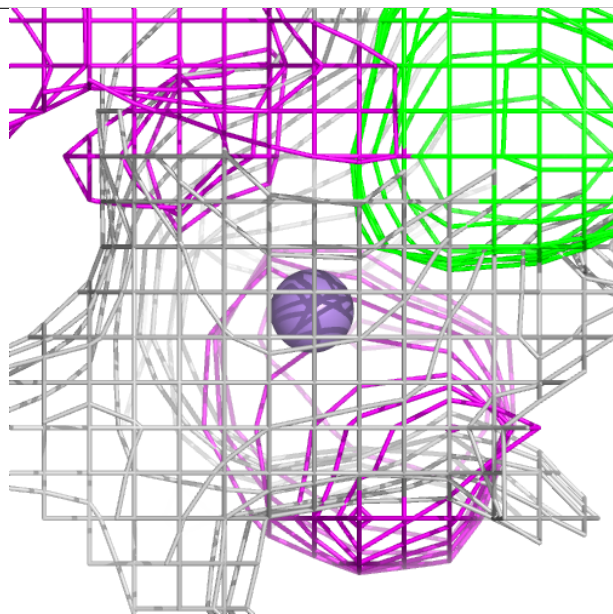
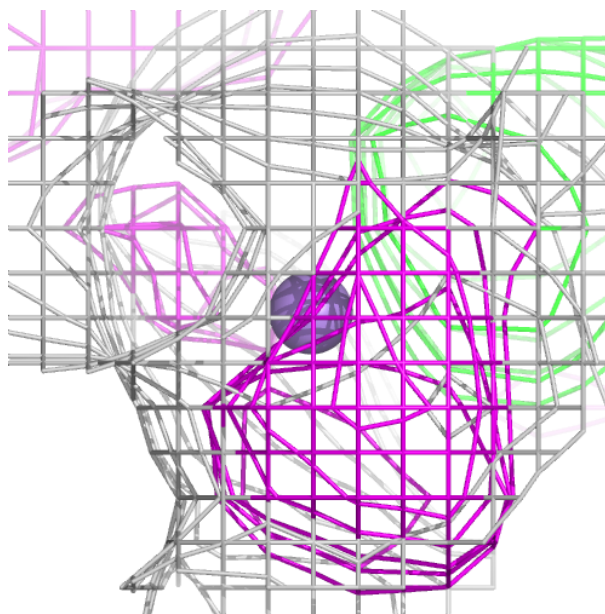
Electron density around MN O 402:

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



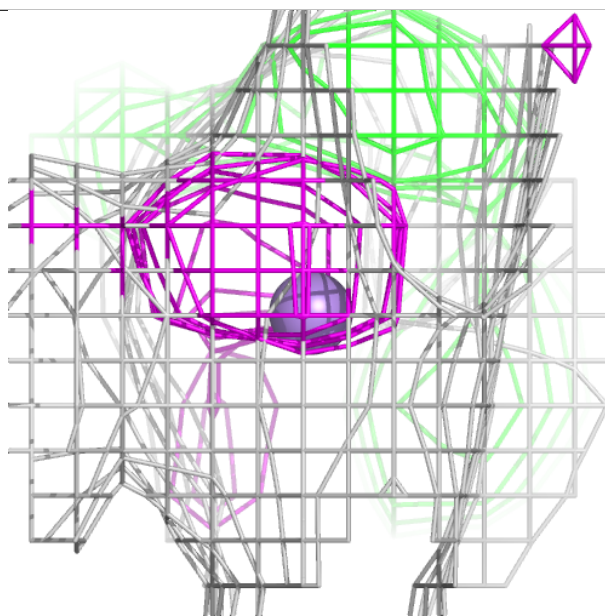
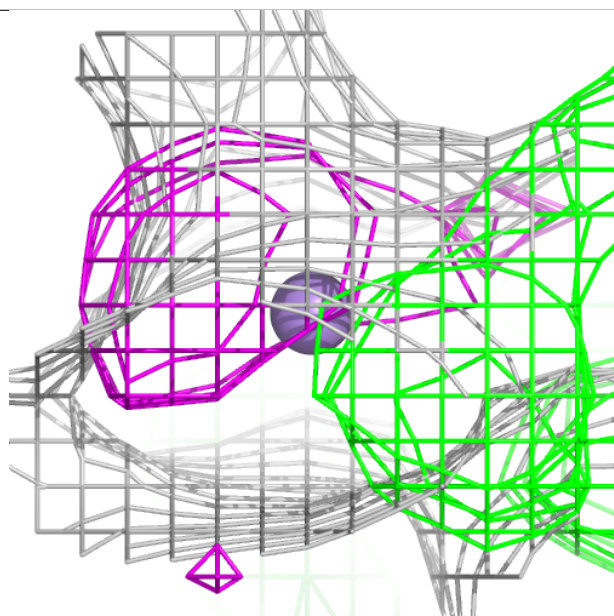
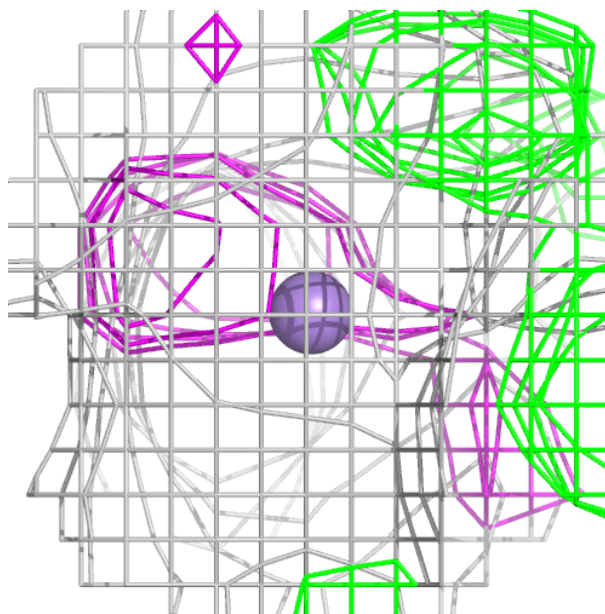
Electron density around MN V 401:

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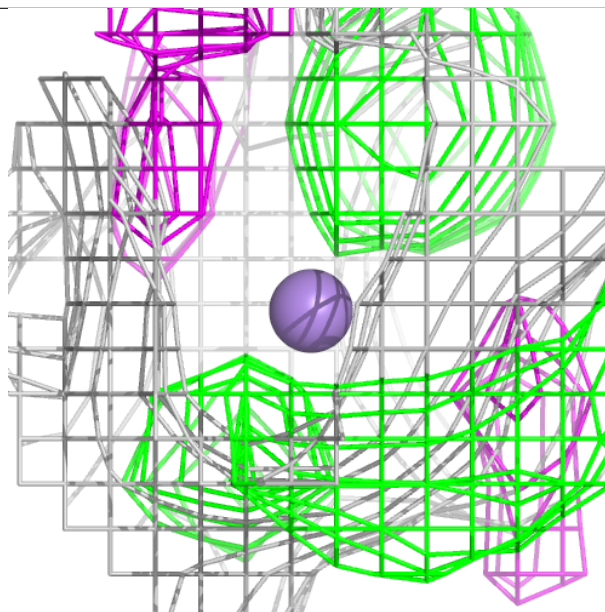
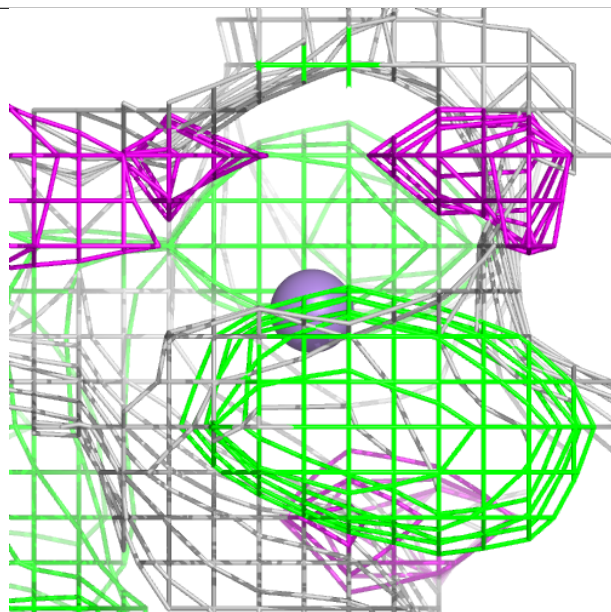
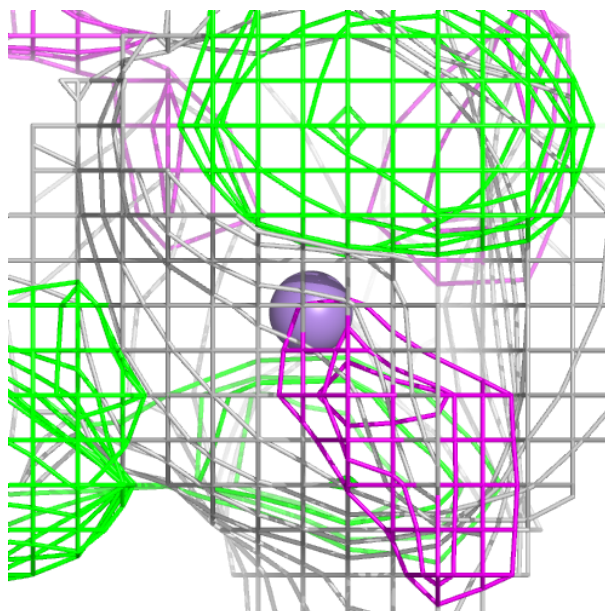
Electron density around MN C 402:

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



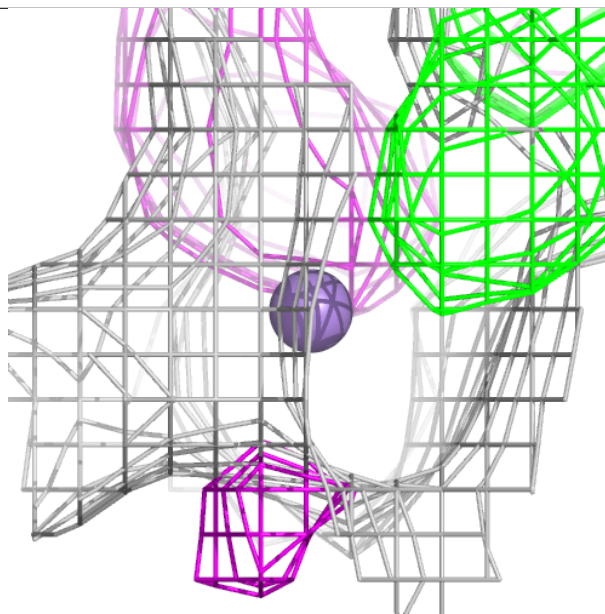
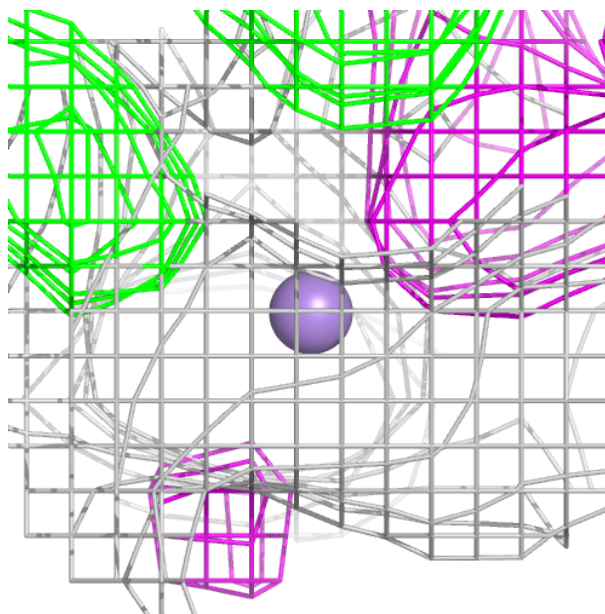
Electron density around MN C 401:

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and green (positive)



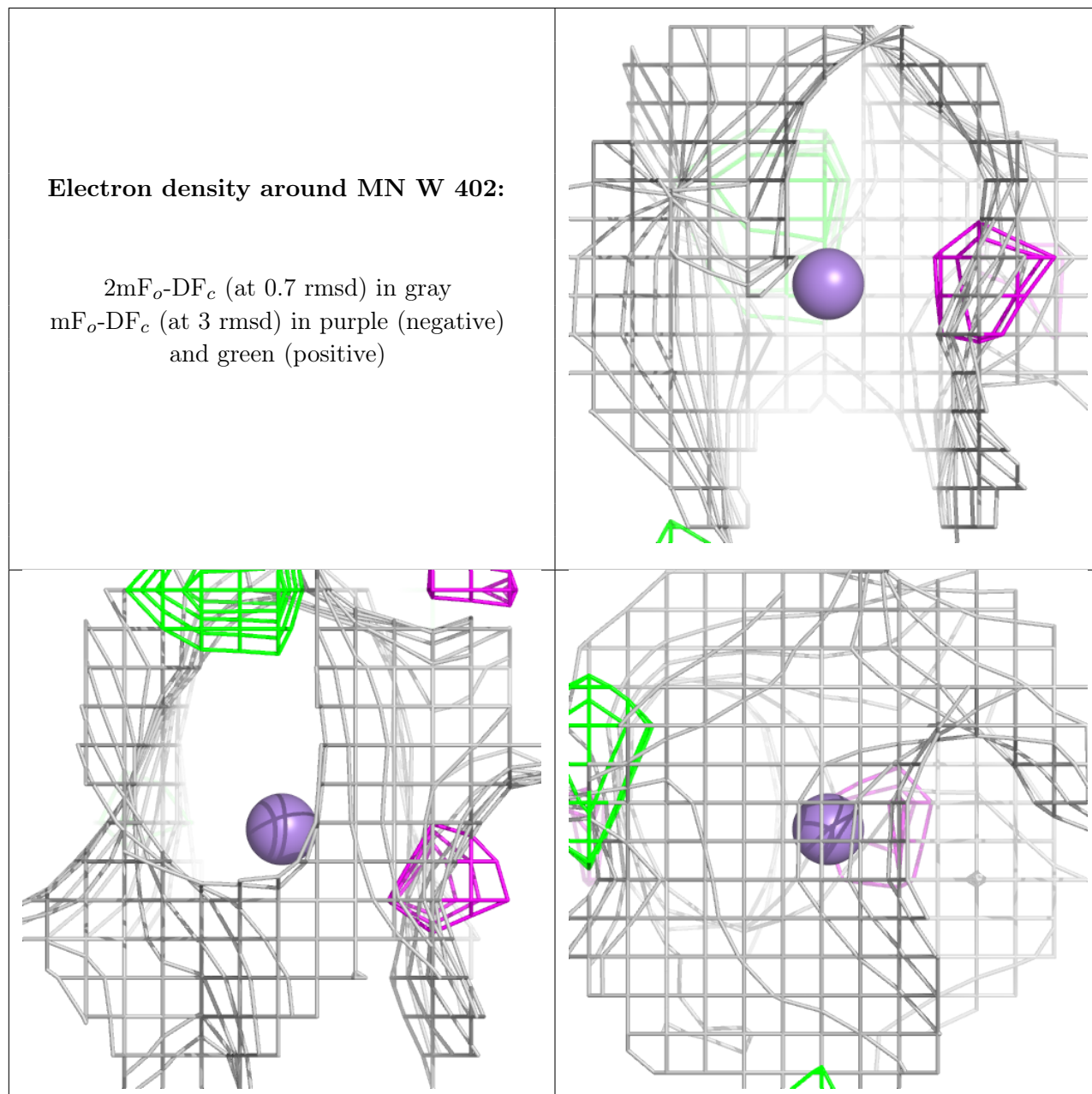
Electron density around MN V 402:

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and green (positive)



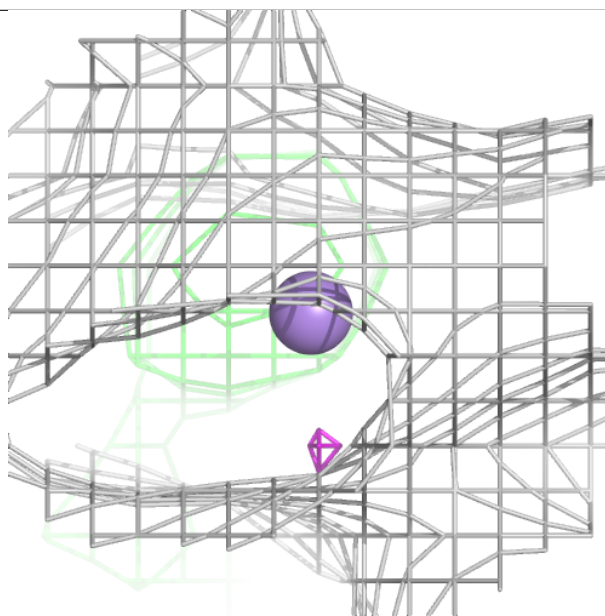
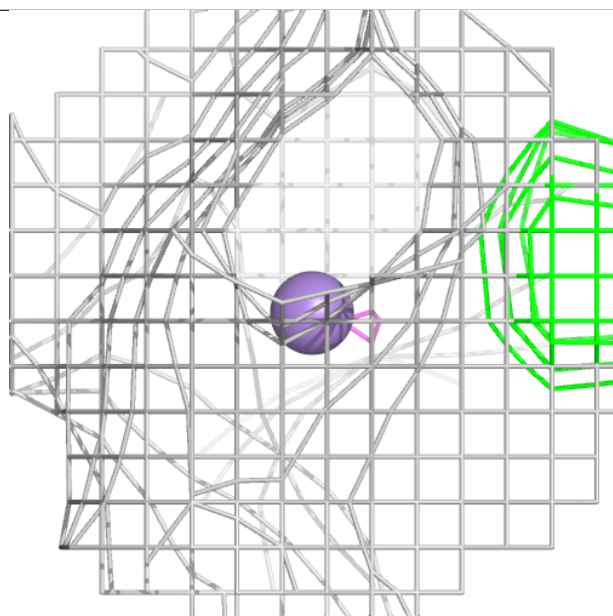
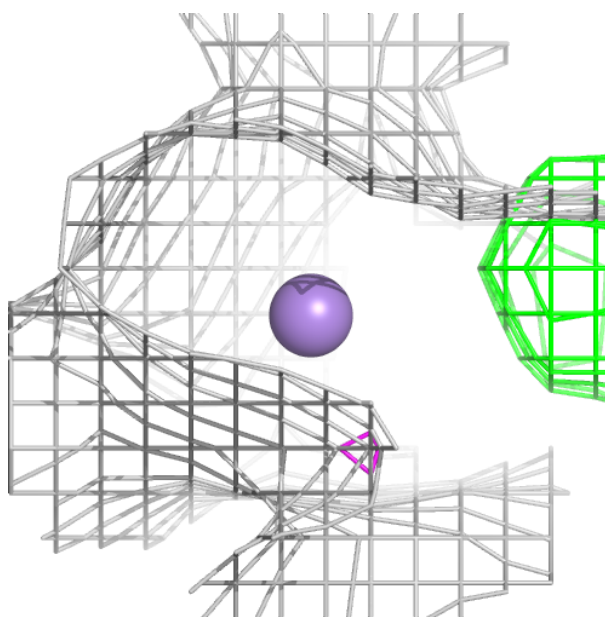
Electron density around MN W 402:

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and green (positive)



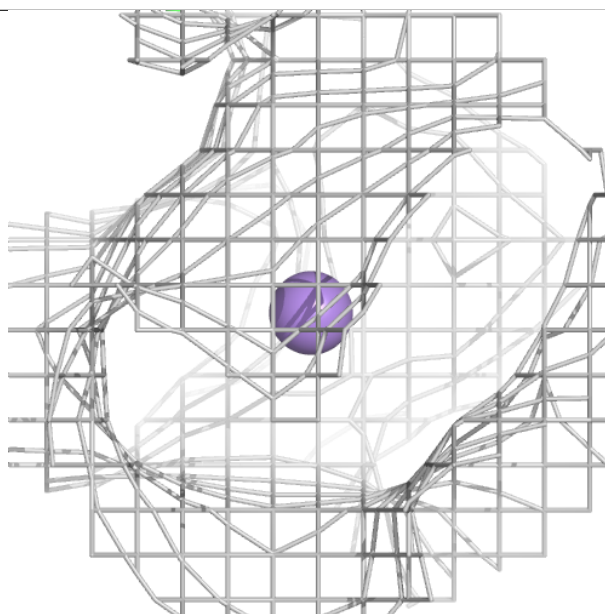
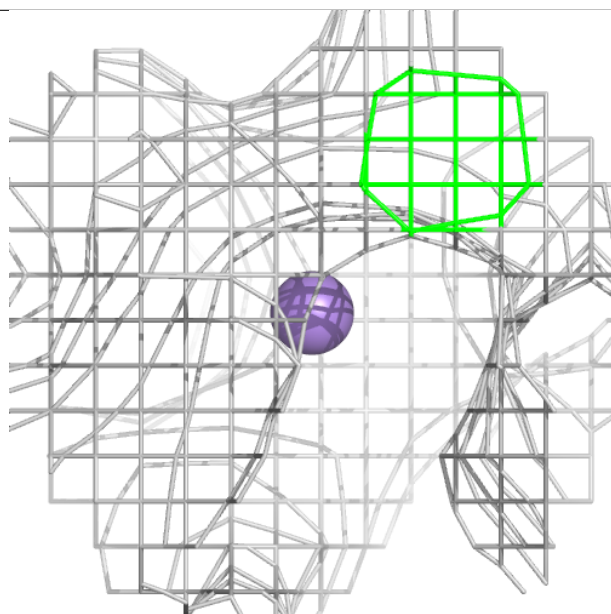
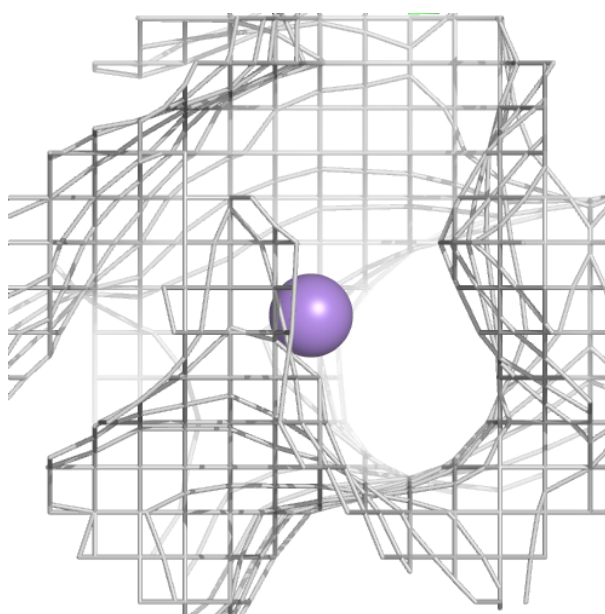
Electron density around MN M 402:

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and green (positive)



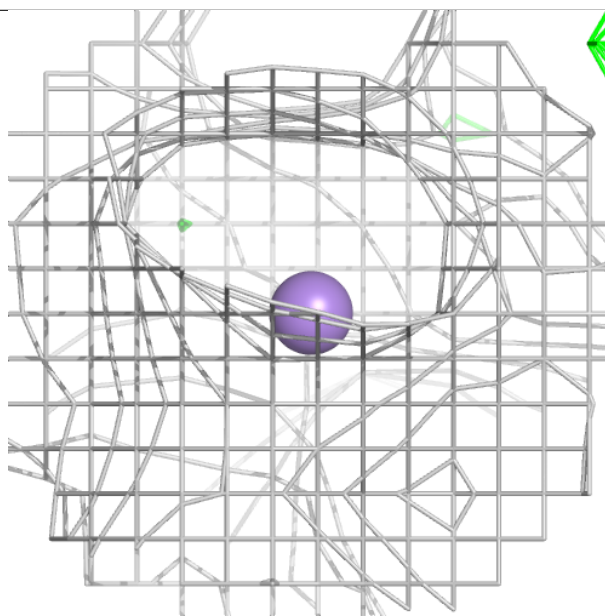
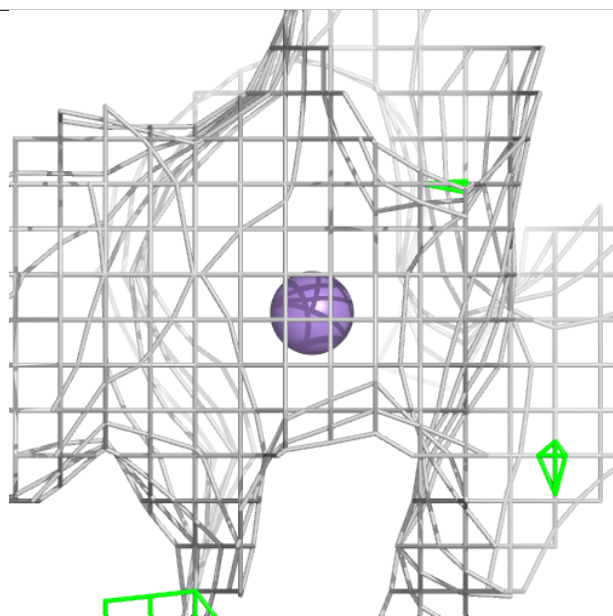
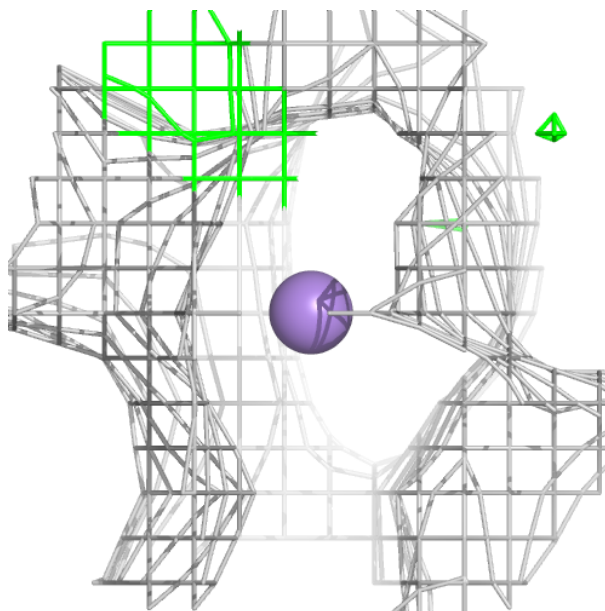
Electron density around MN T 401:

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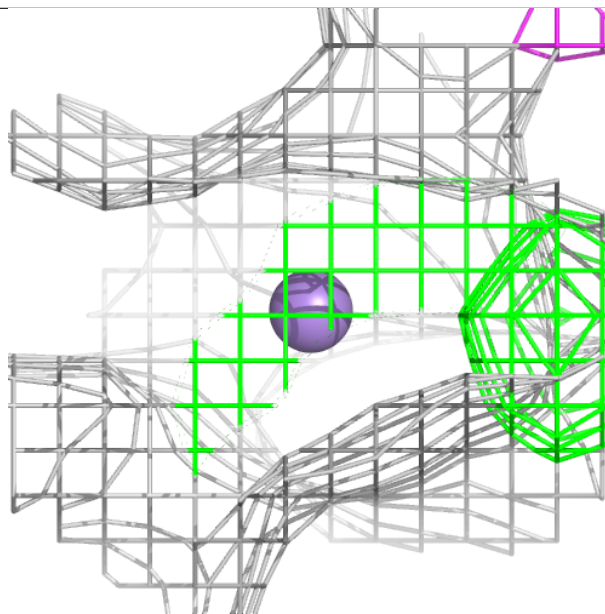
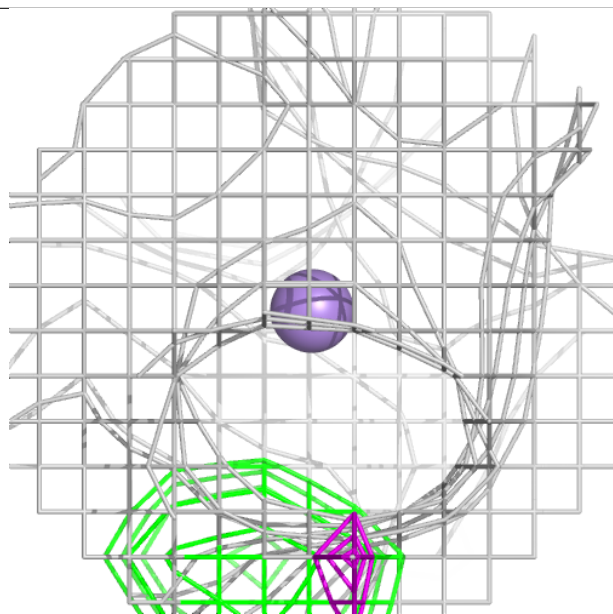
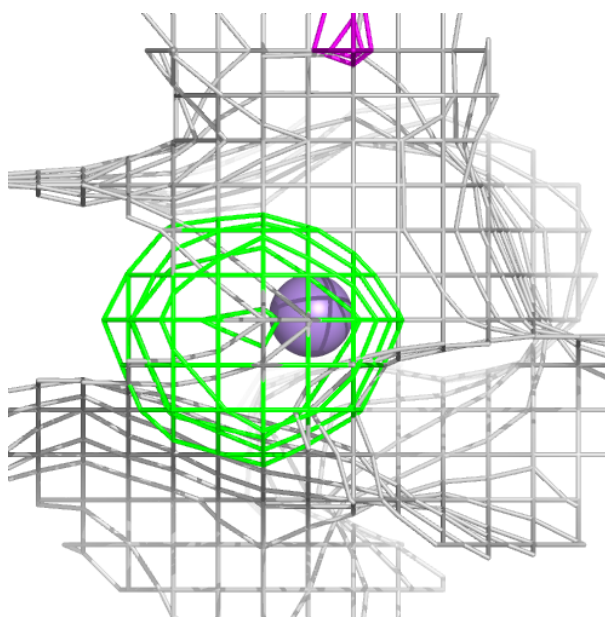
Electron density around MN T 402:

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and green (positive)



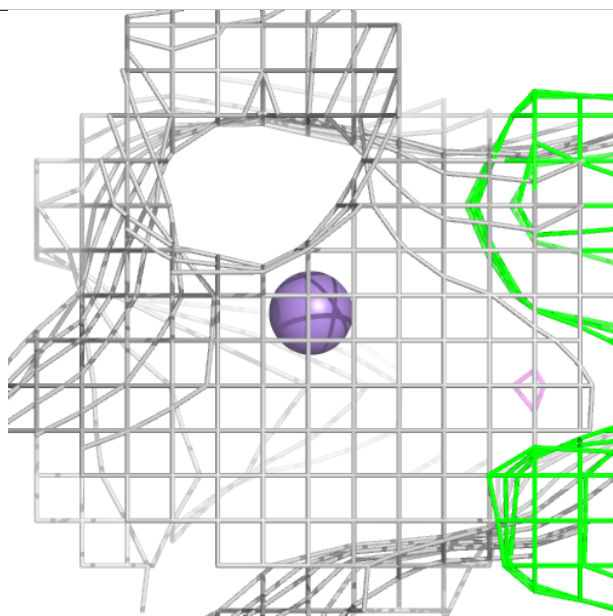
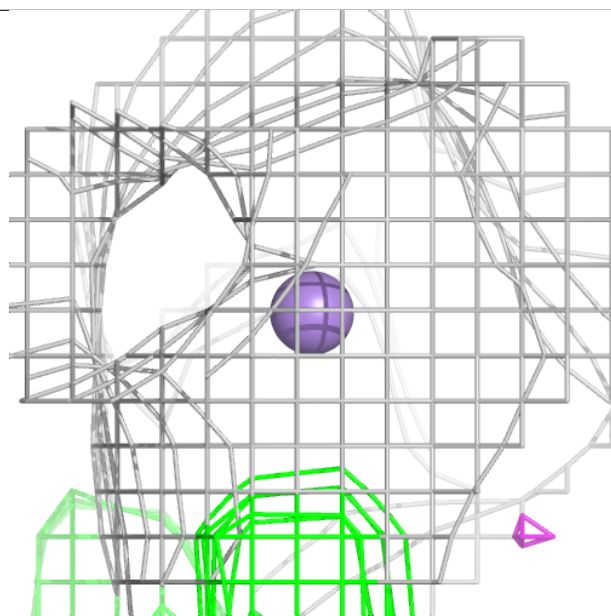
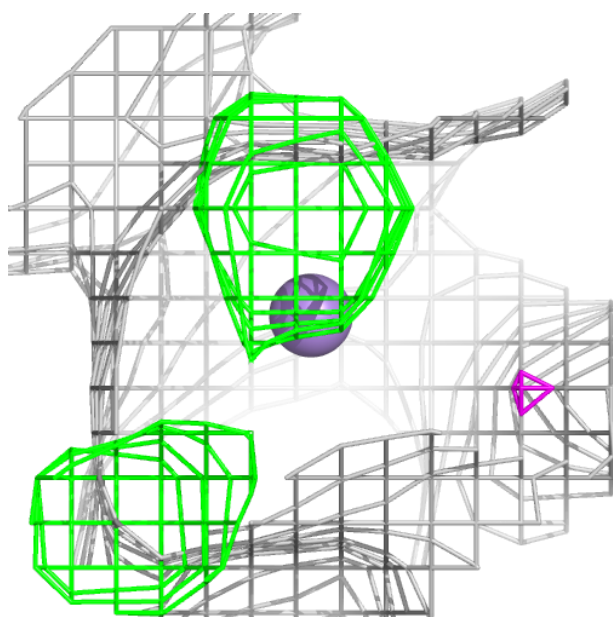
Electron density around MN L 402:

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and green (positive)



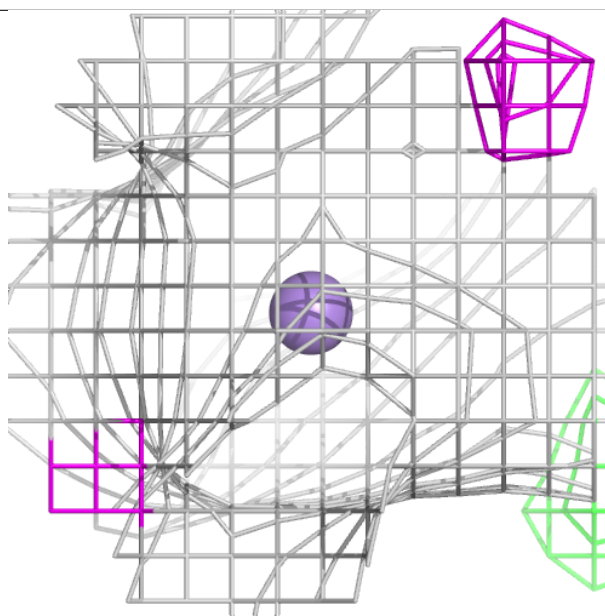
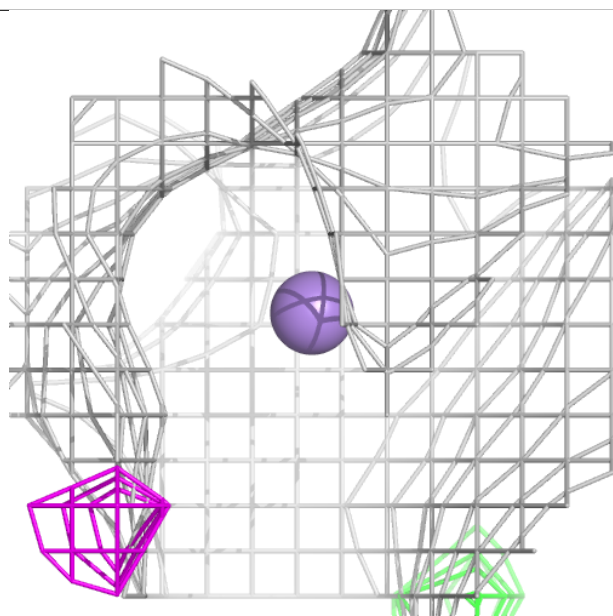
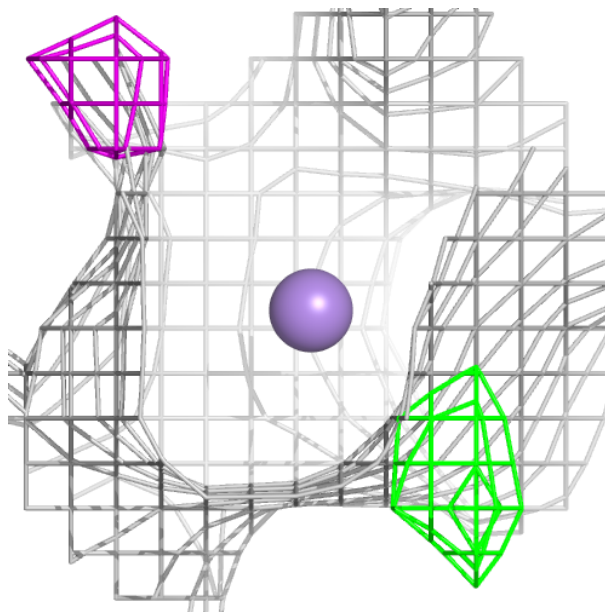
Electron density around MN M 401:

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and green (positive)



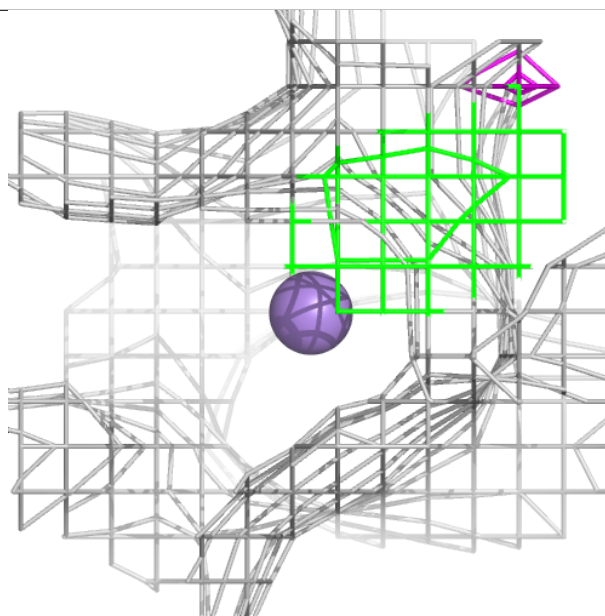
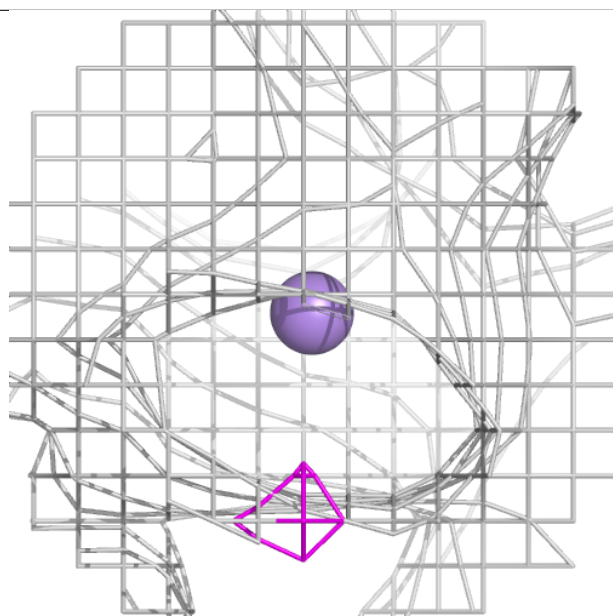
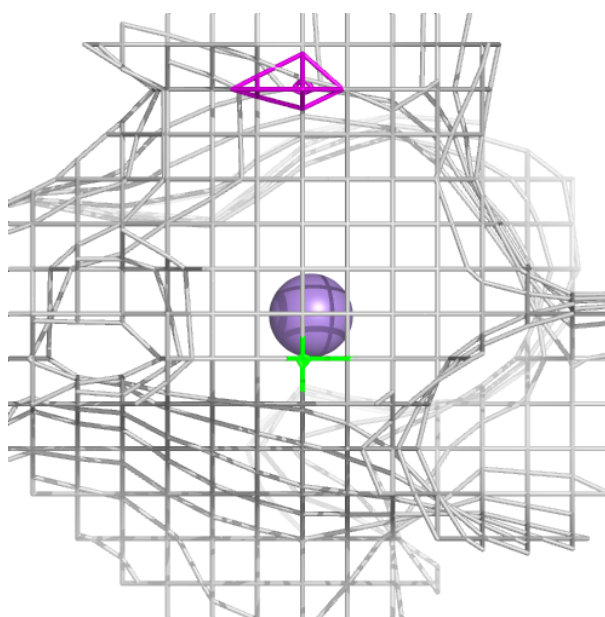
Electron density around MN W 401:

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and green (positive)



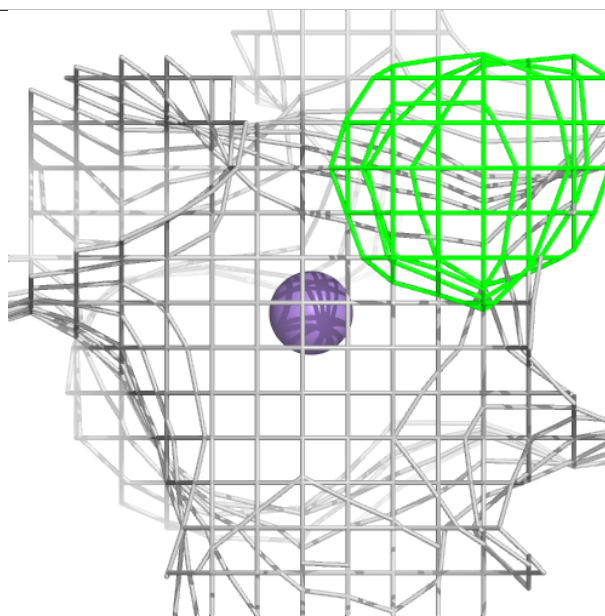
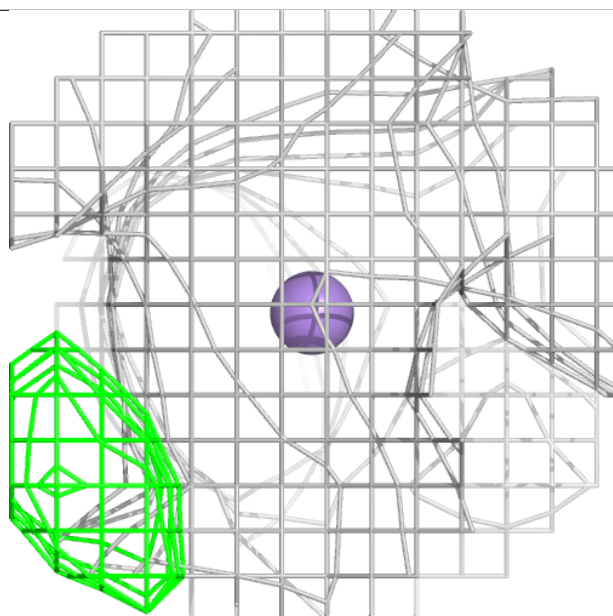
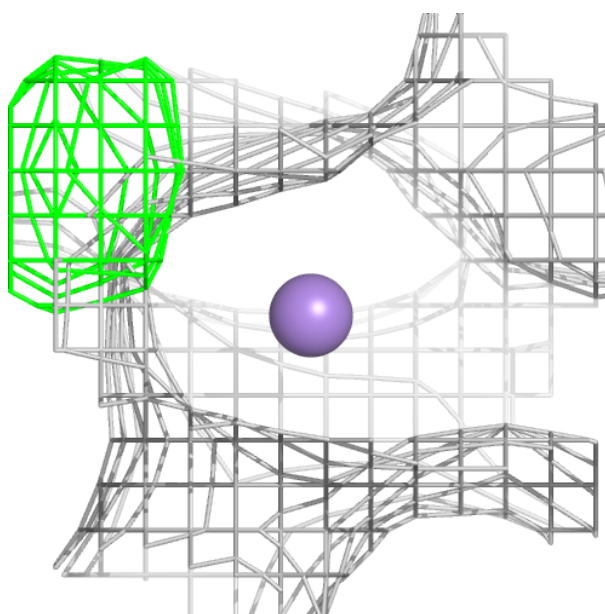
Electron density around MN B 402:

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and green (positive)



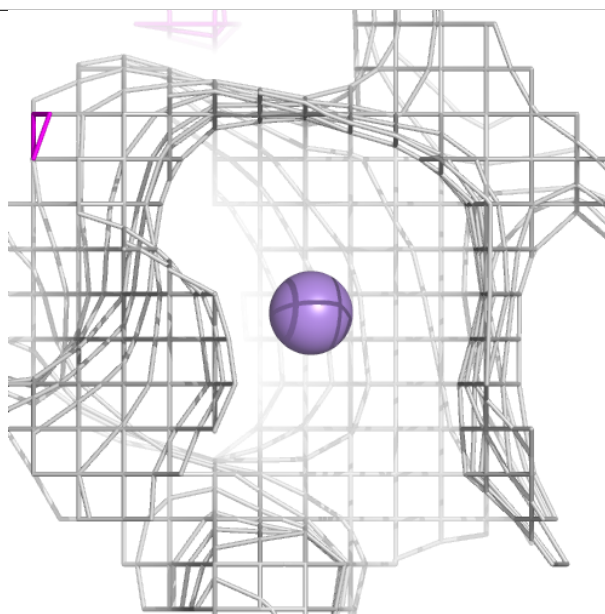
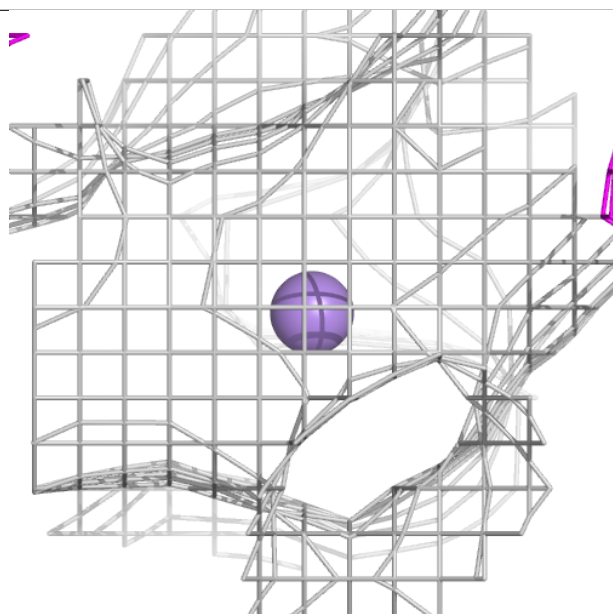
Electron density around MN X 402:

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and green (positive)



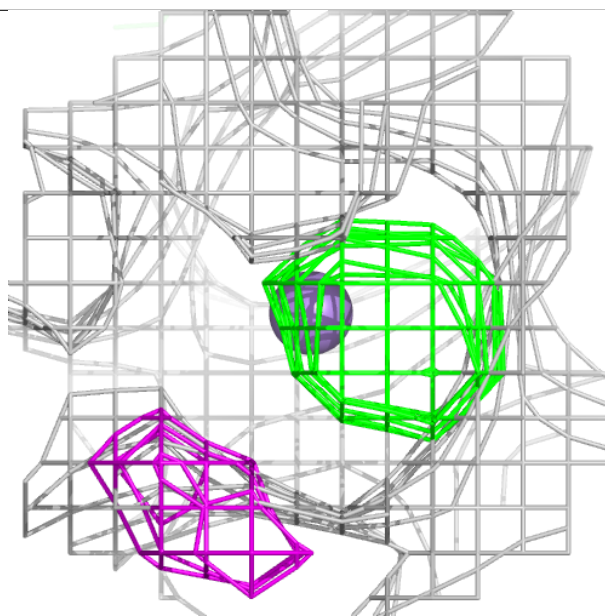
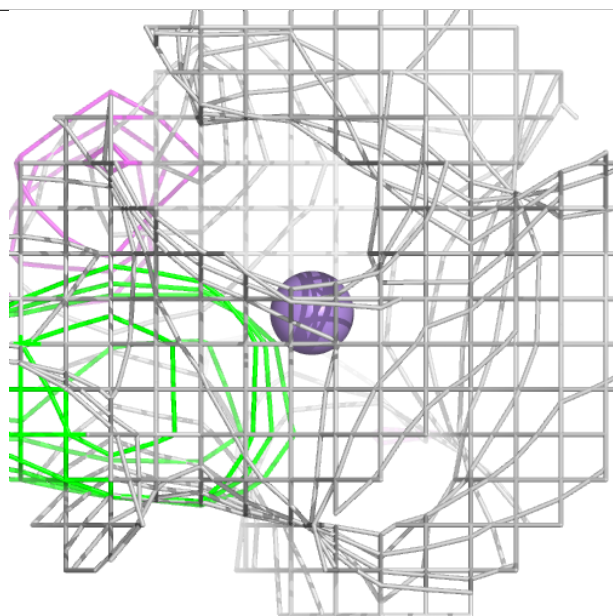
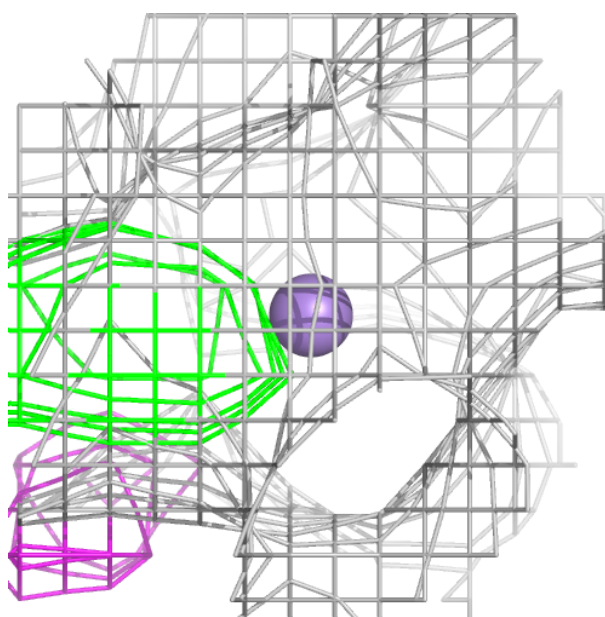
Electron density around MN N 401:

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



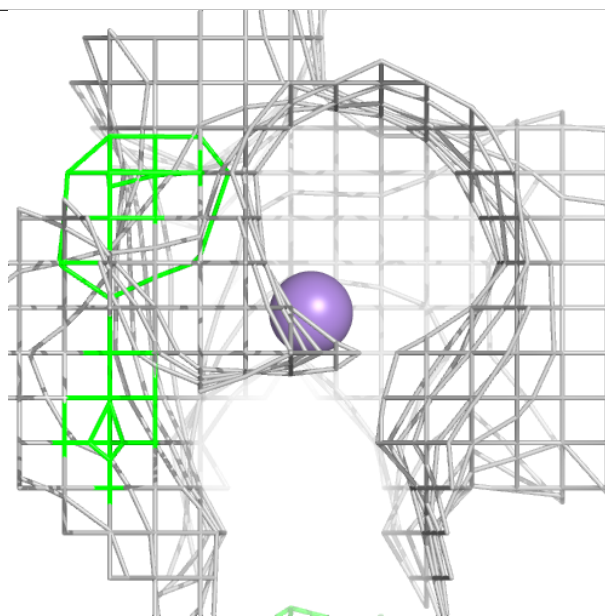
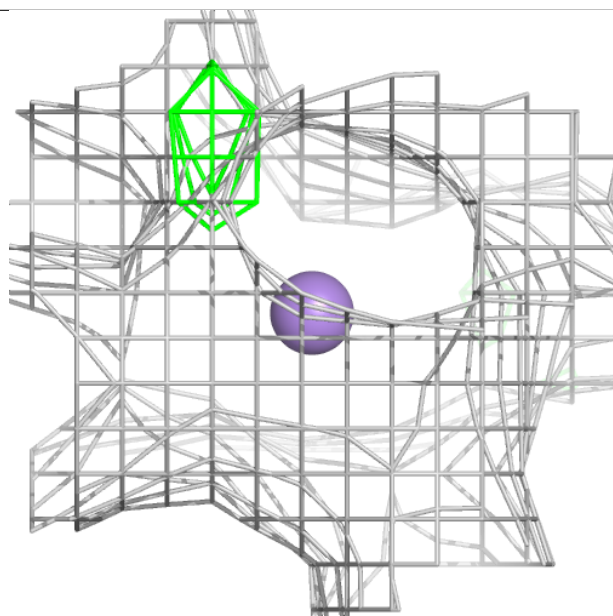
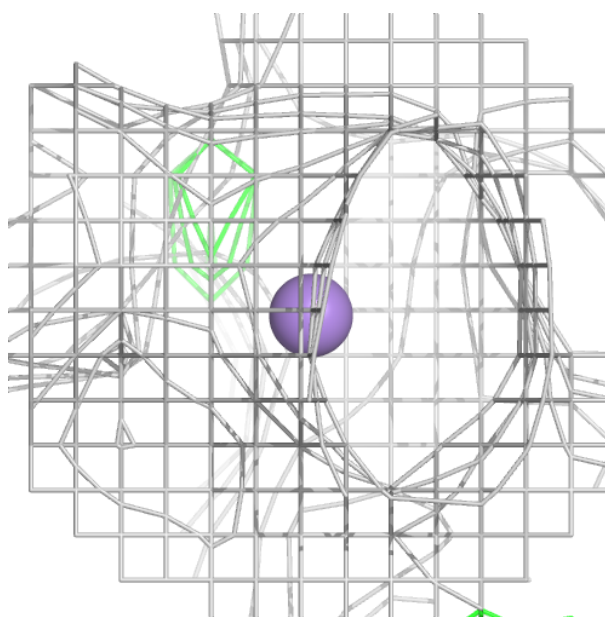
Electron density around MN E 401:

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



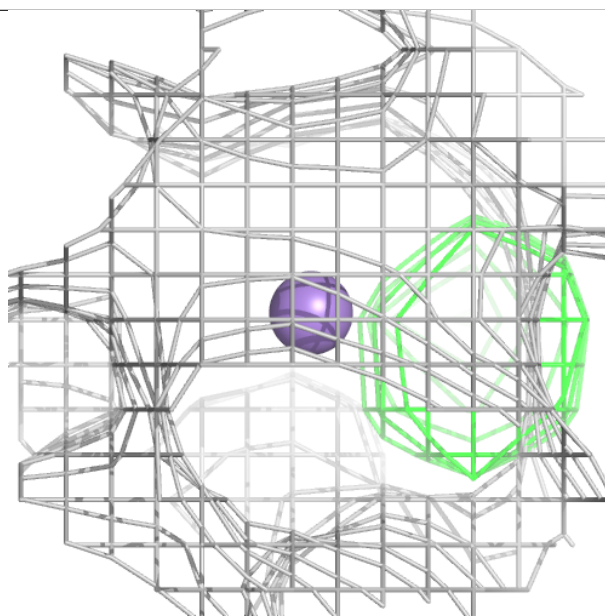
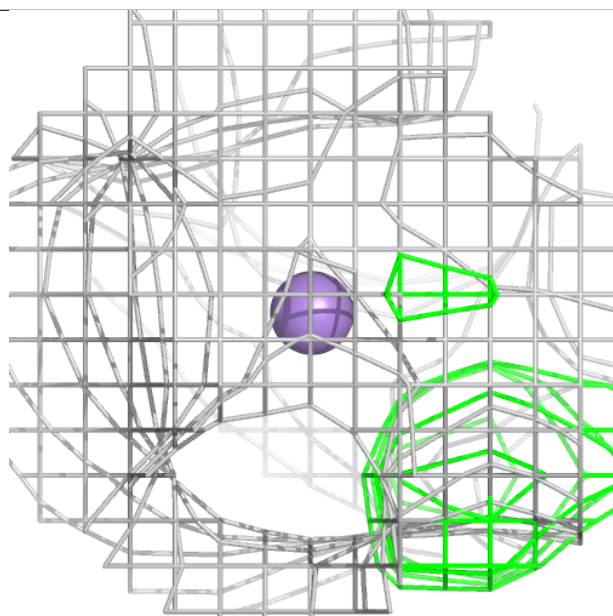
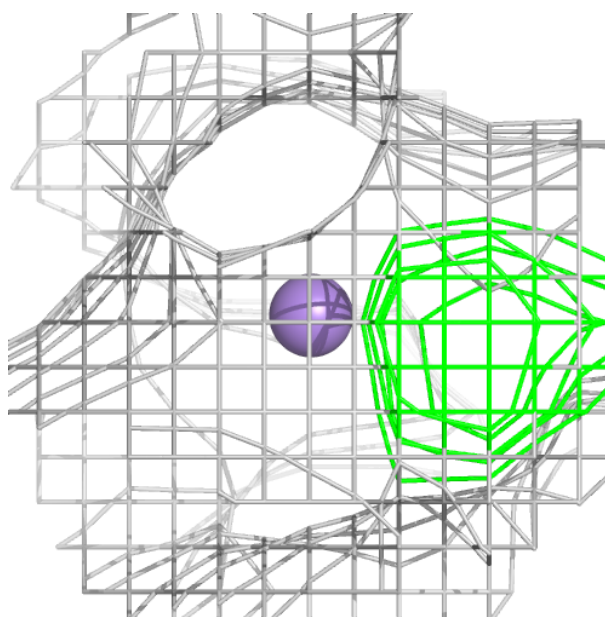
Electron density around MN K 402:

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



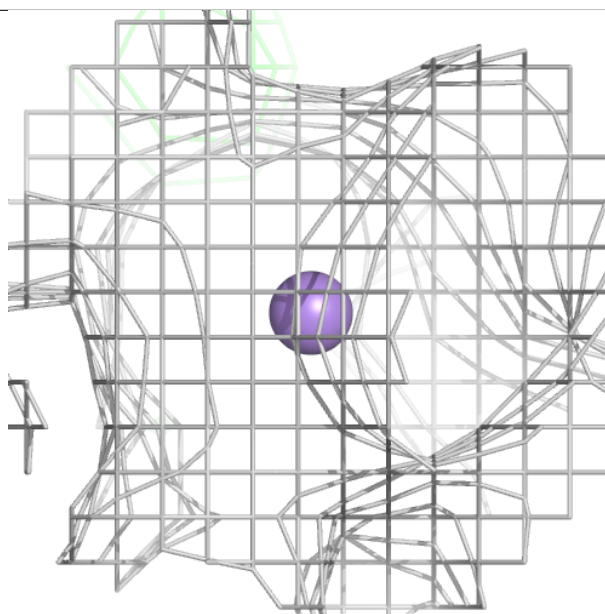
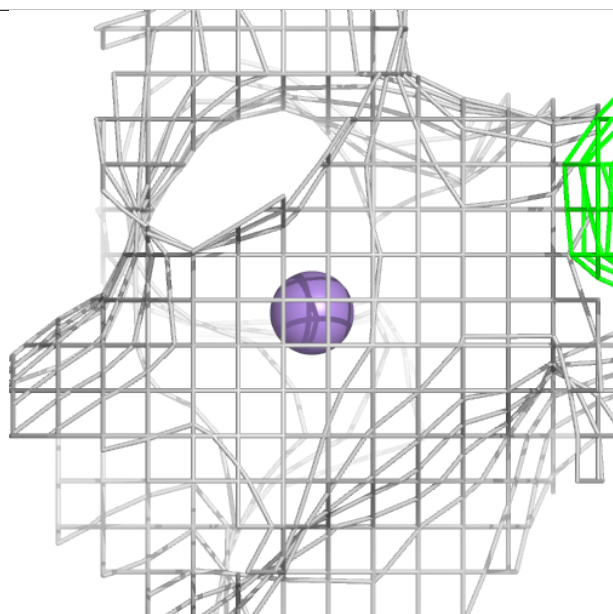
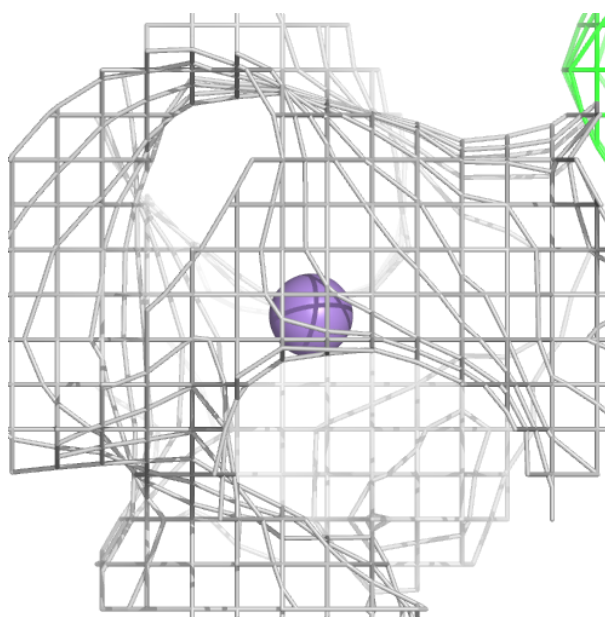
Electron density around MN P 401:

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



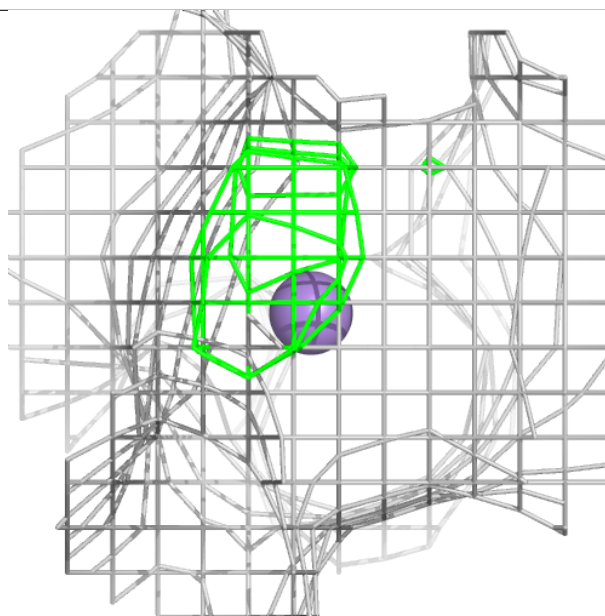
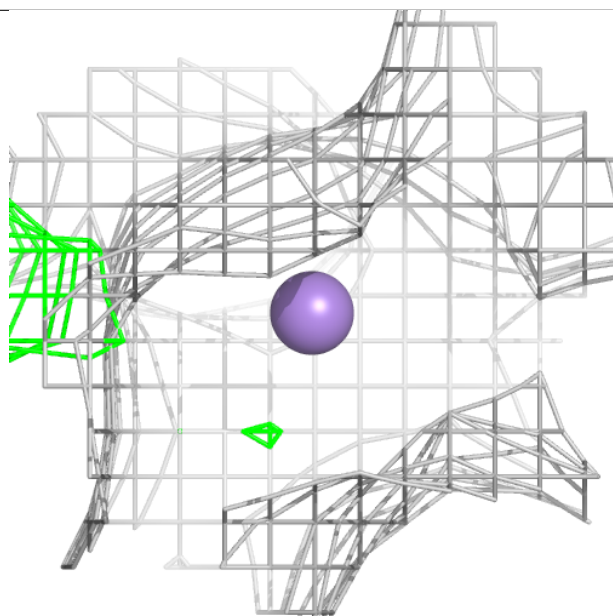
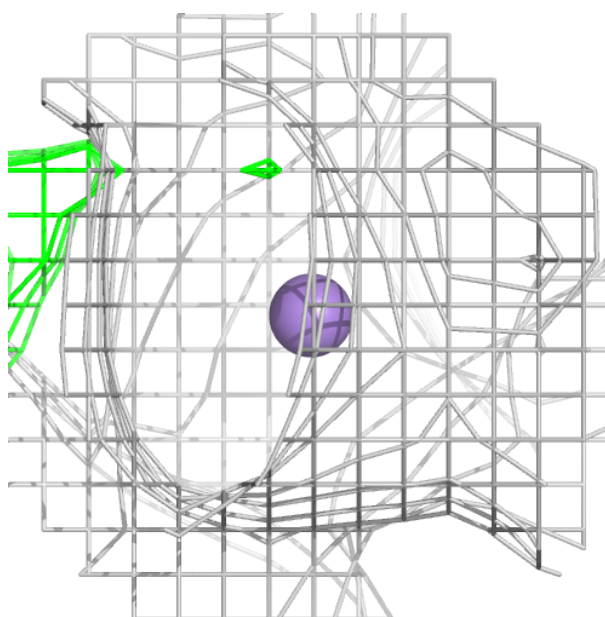
Electron density around MN S 401:

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



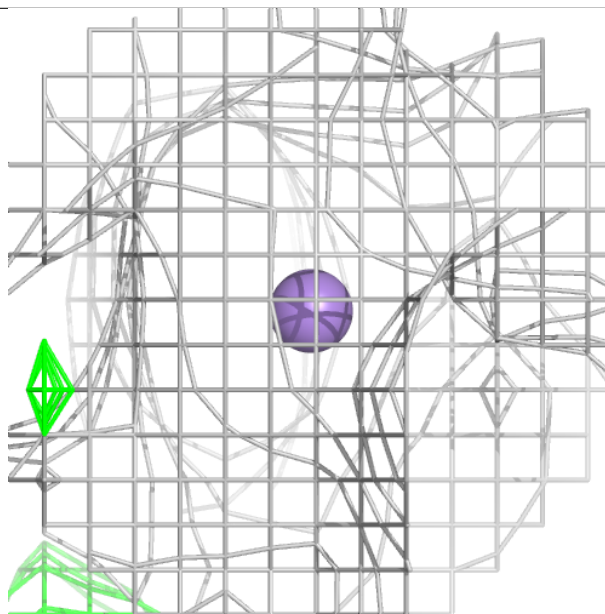
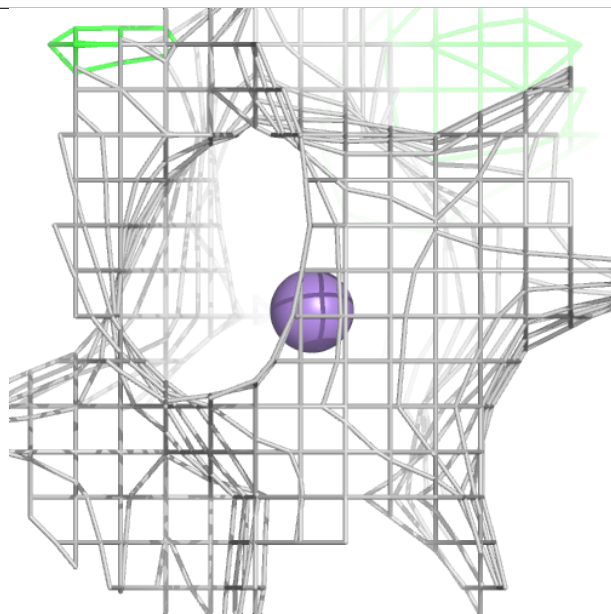
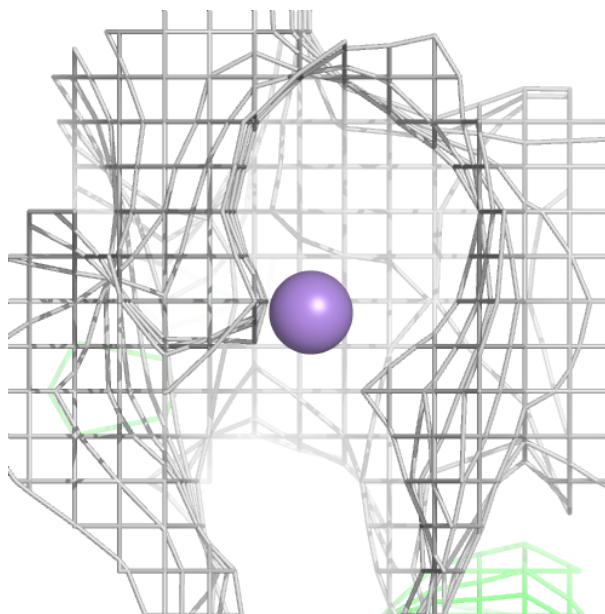
Electron density around MN S 402:

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



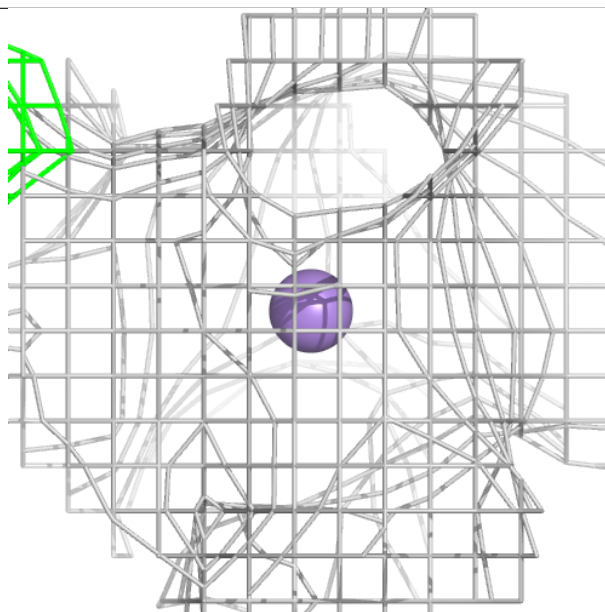
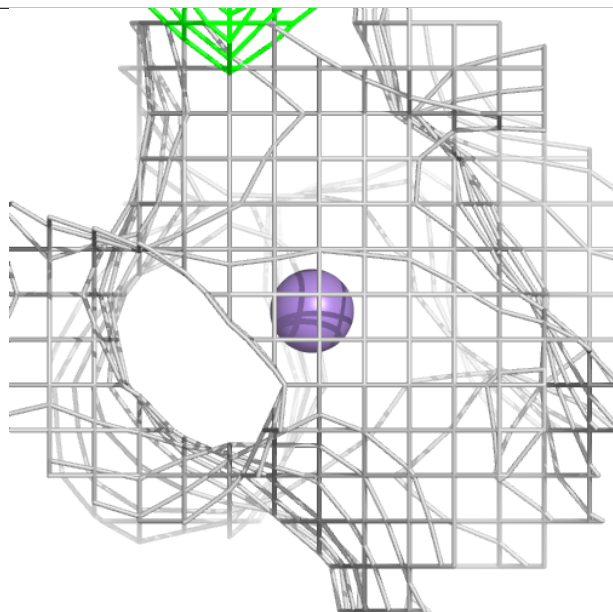
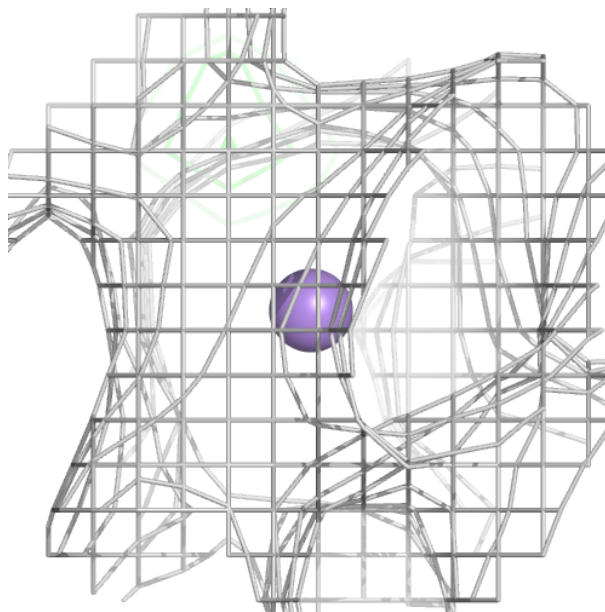
Electron density around MN R 402:

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



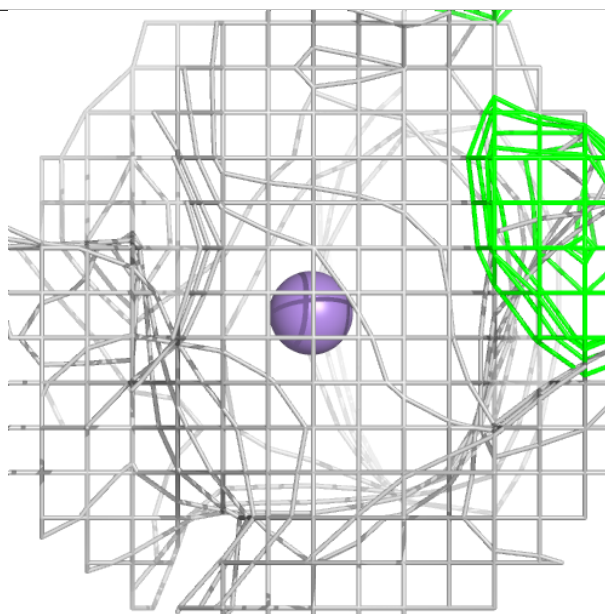
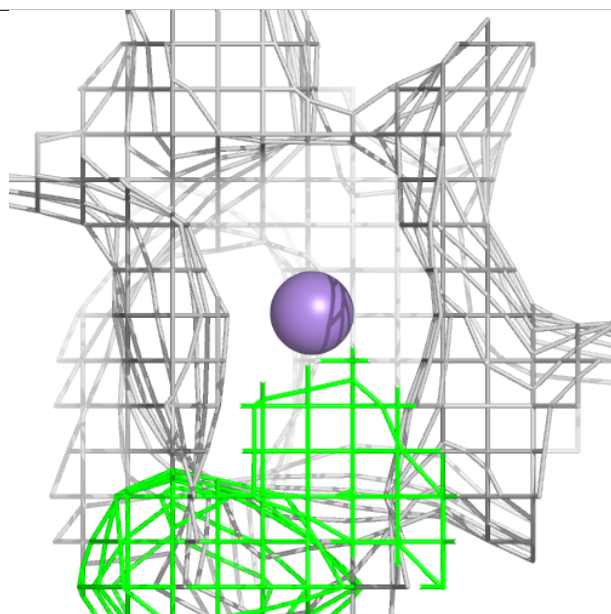
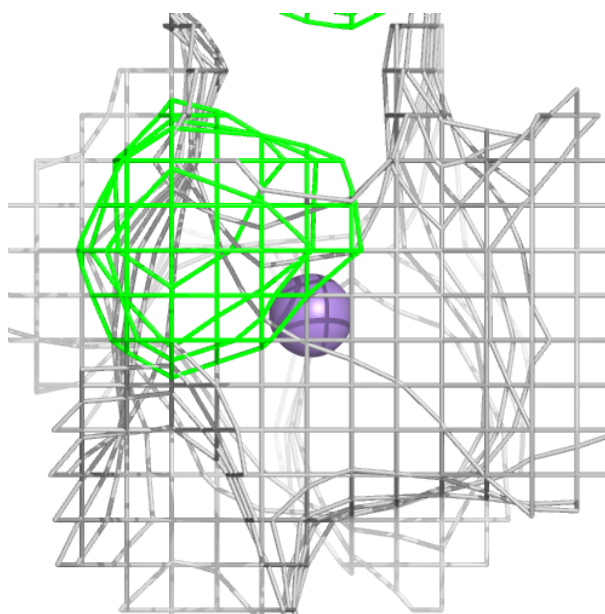
Electron density around MN G 401:

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



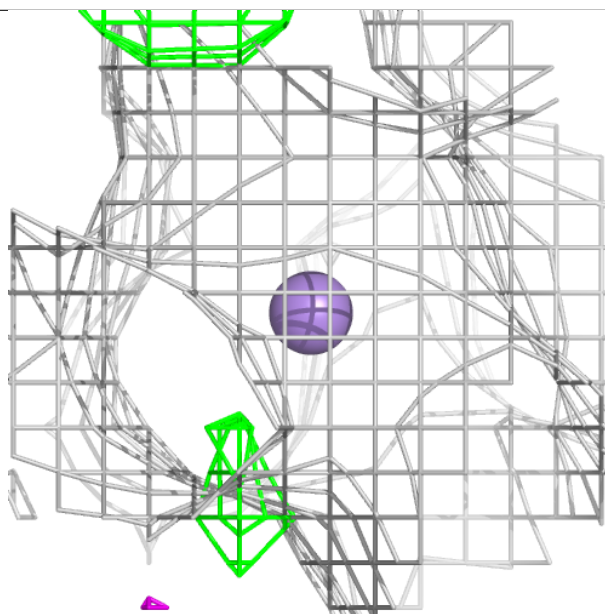
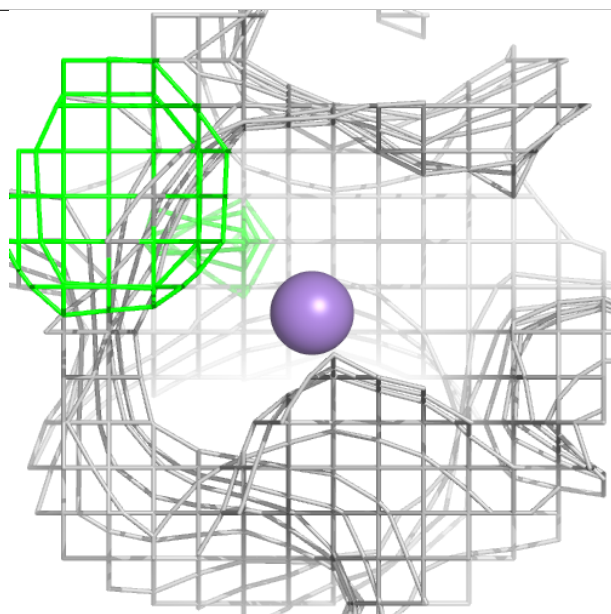
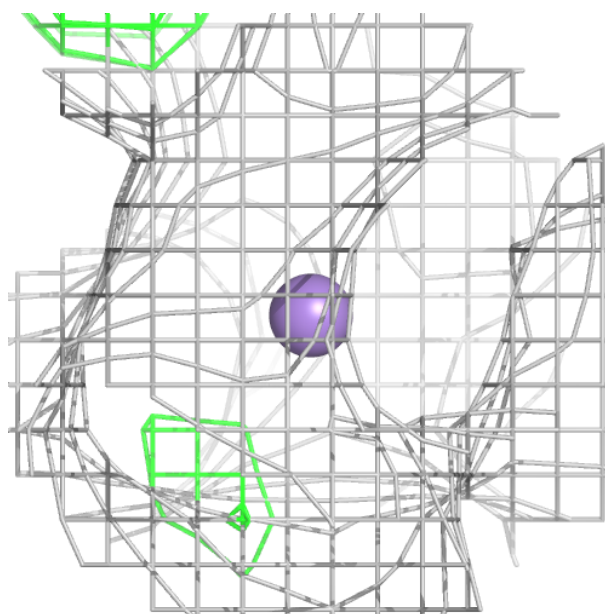
Electron density around MN G 402:

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



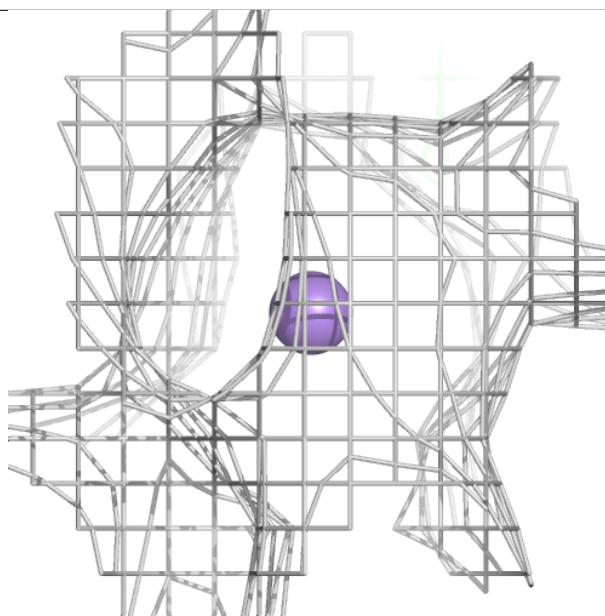
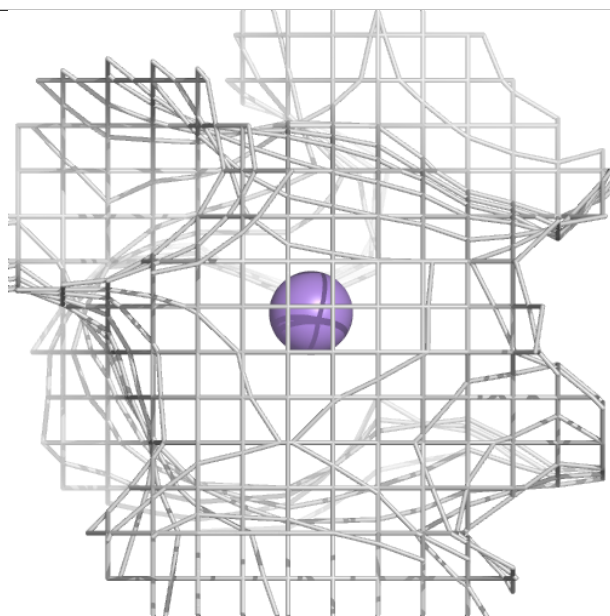
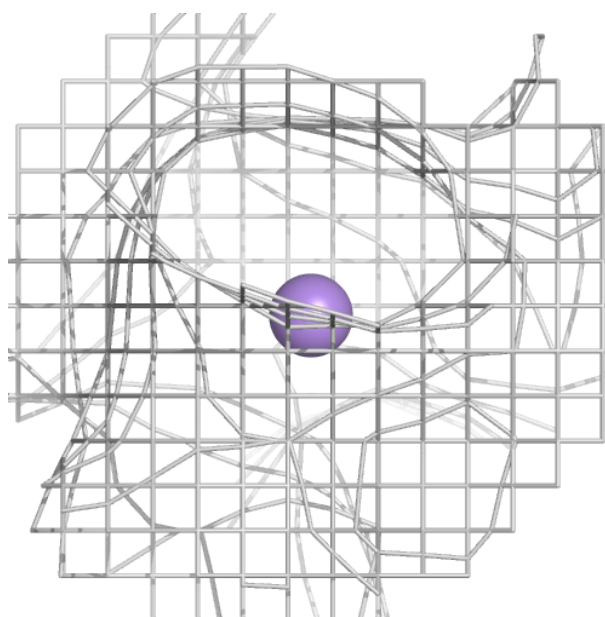
Electron density around MN H 401:

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



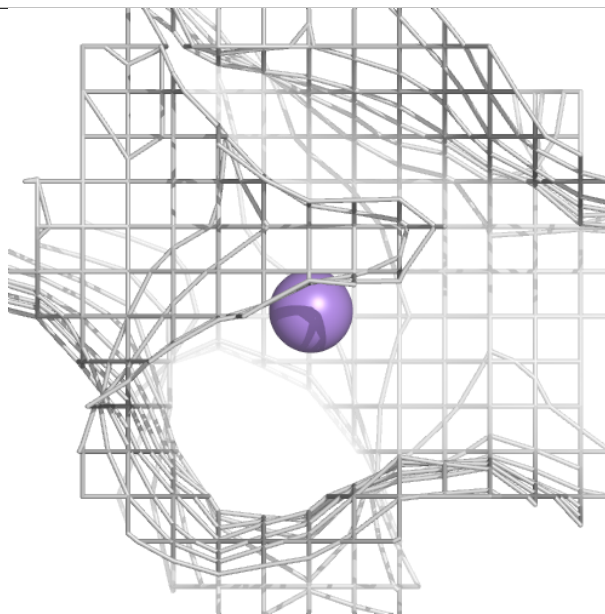
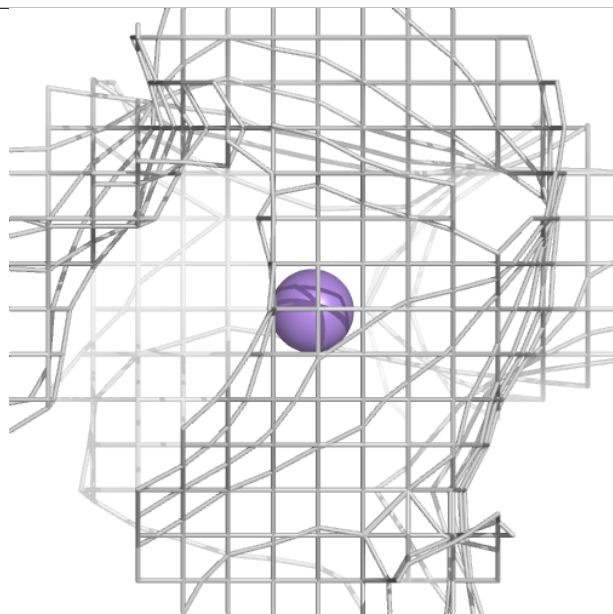
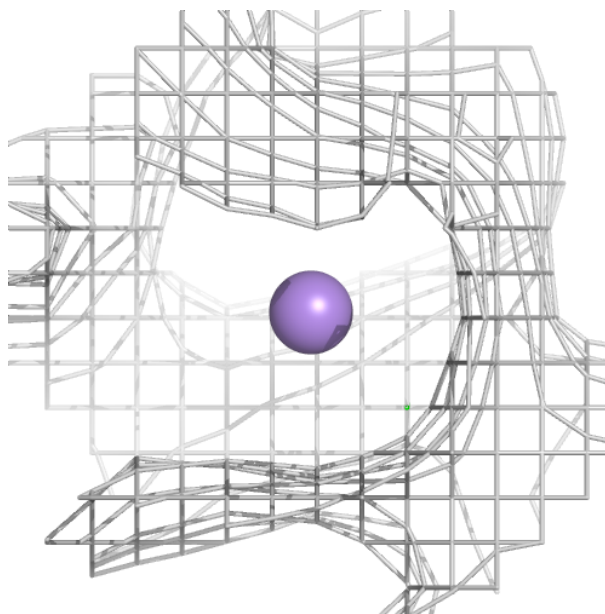
Electron density around MN H 402:

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



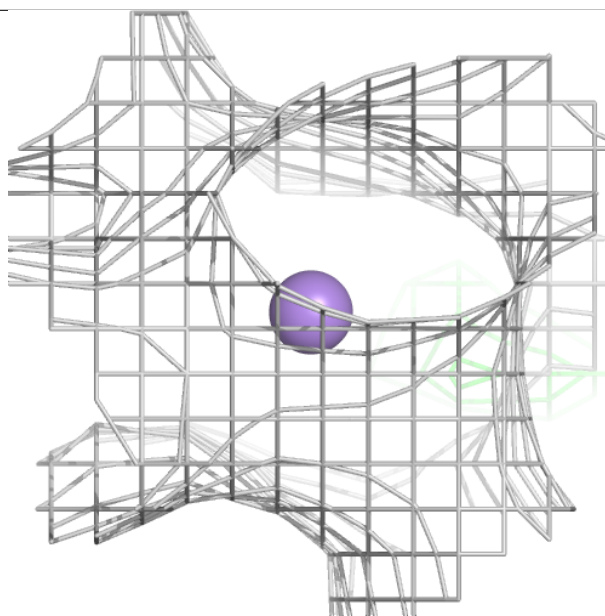
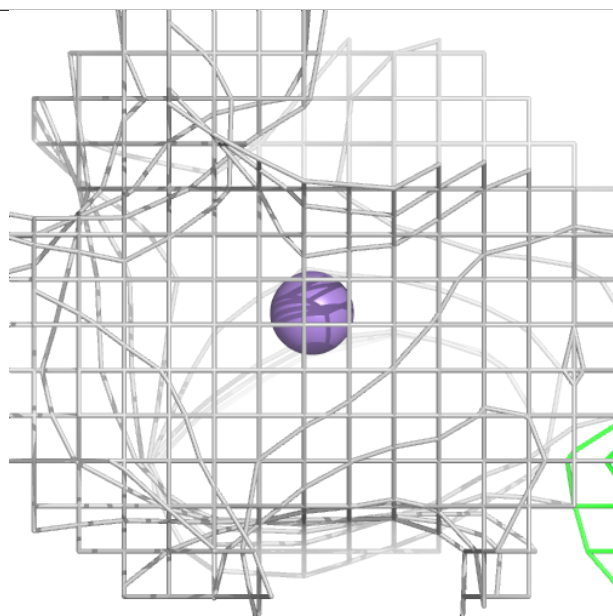
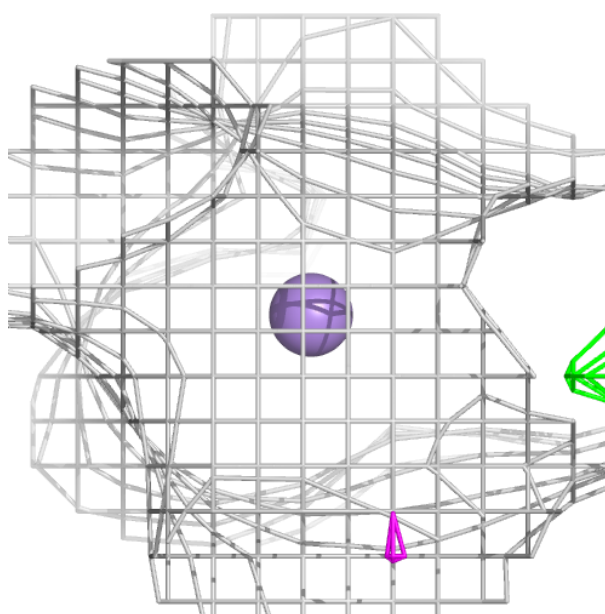
Electron density around MN U 401:

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



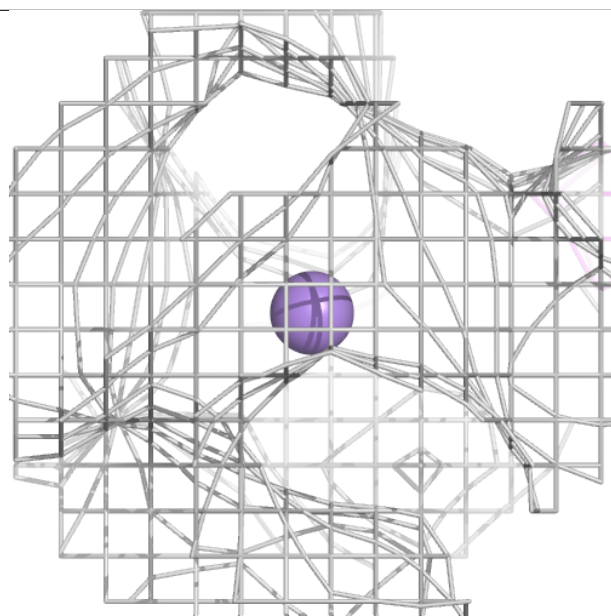
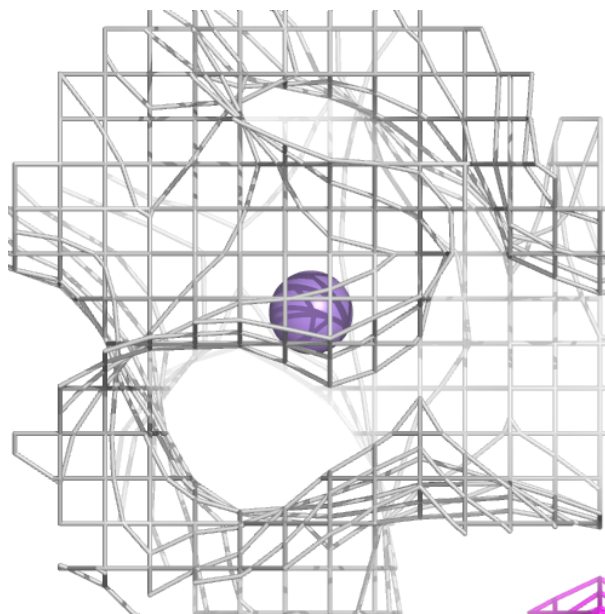
Electron density around MN U 402:

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



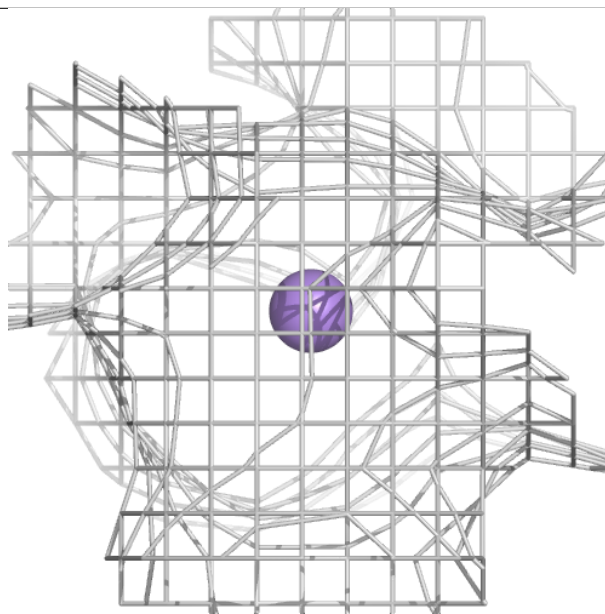
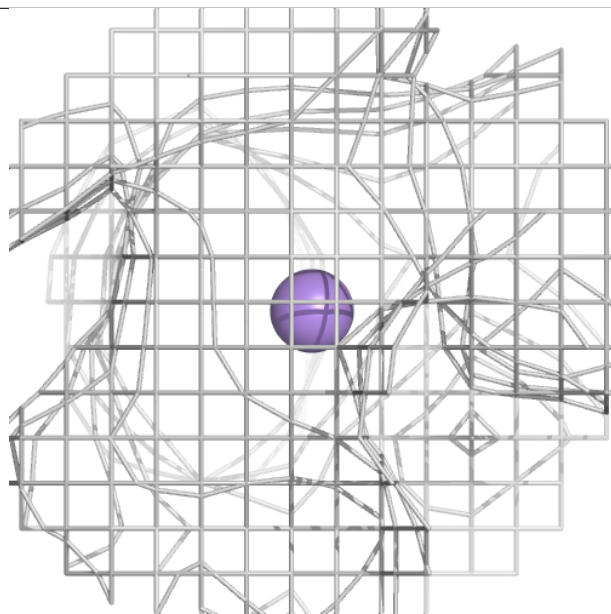
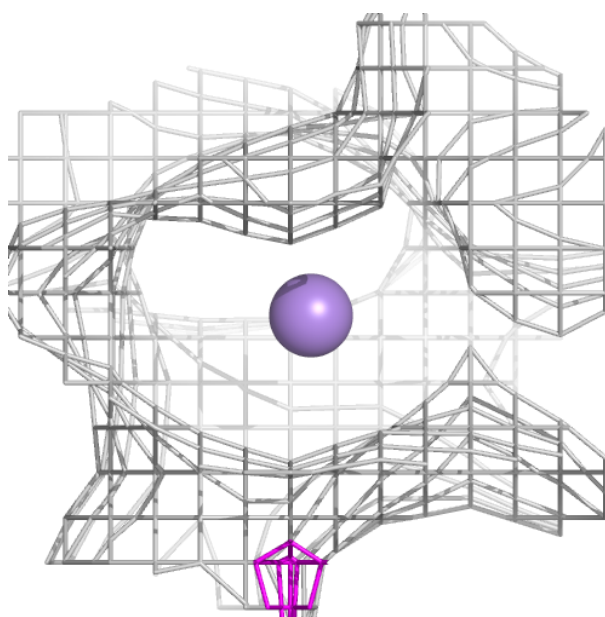
Electron density around MN I 401:

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



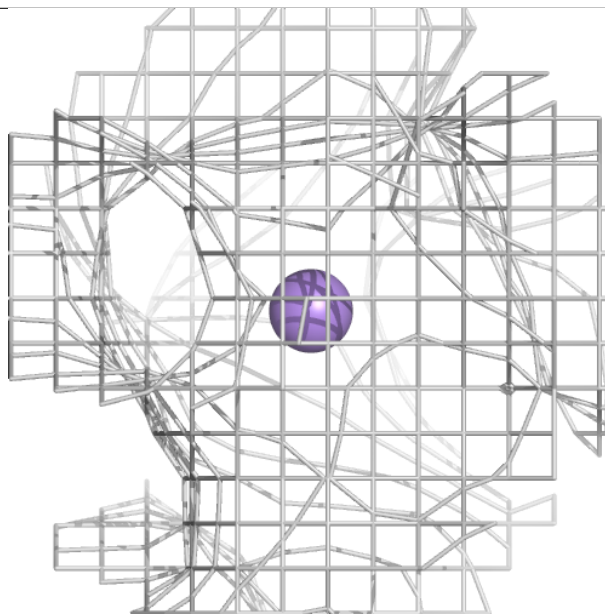
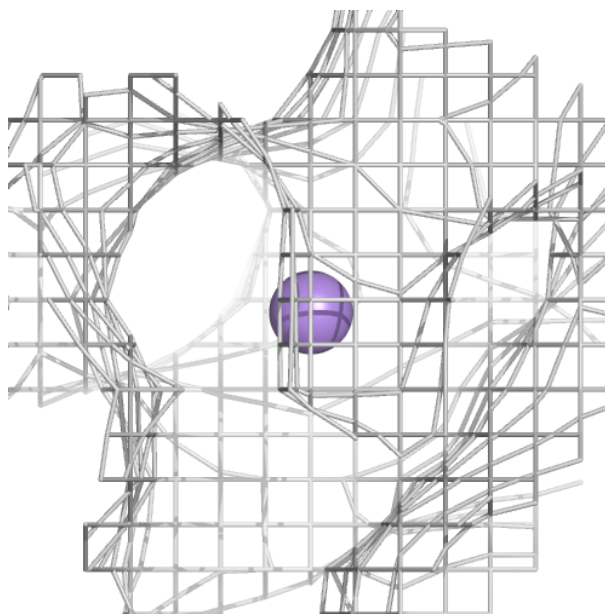
Electron density around MN I 402:

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



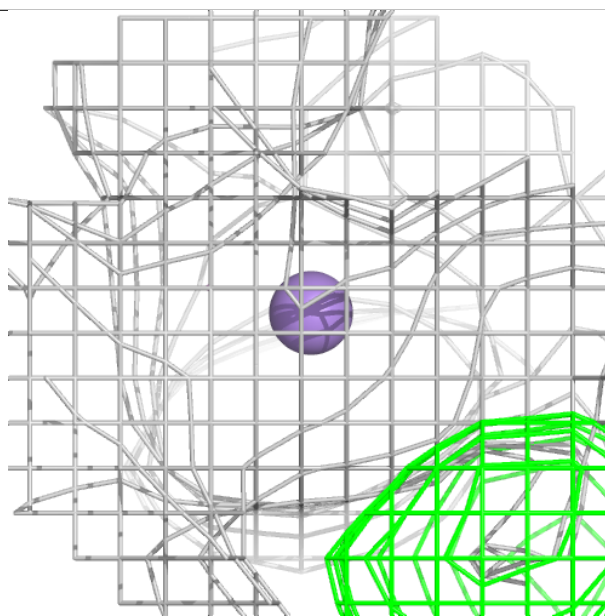
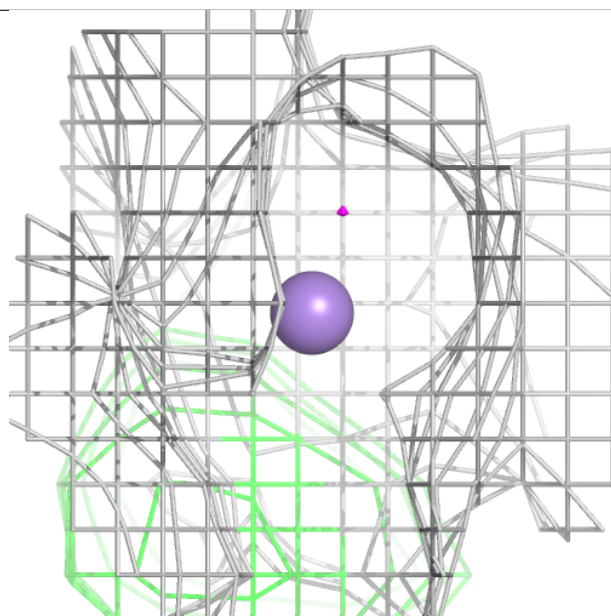
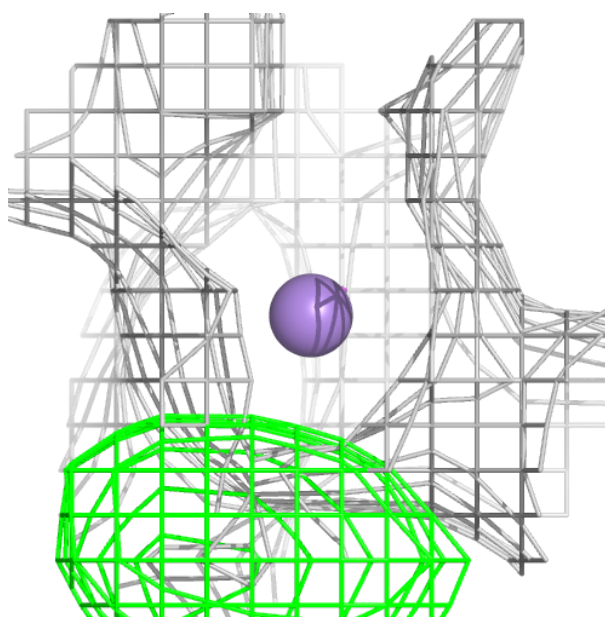
Electron density around MN J 401:

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



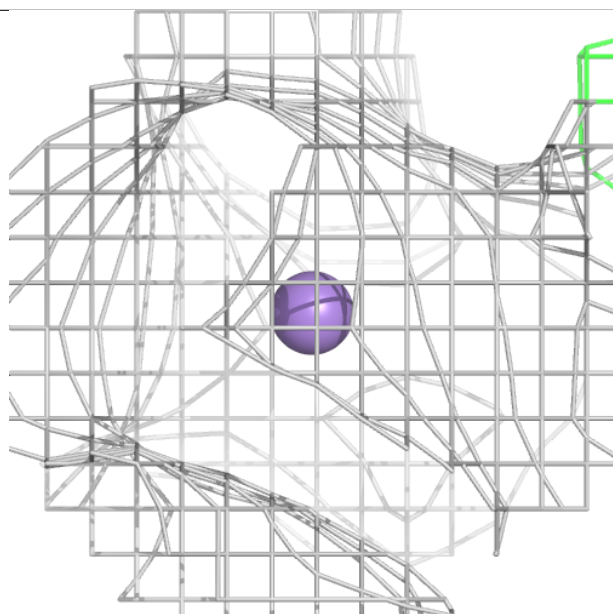
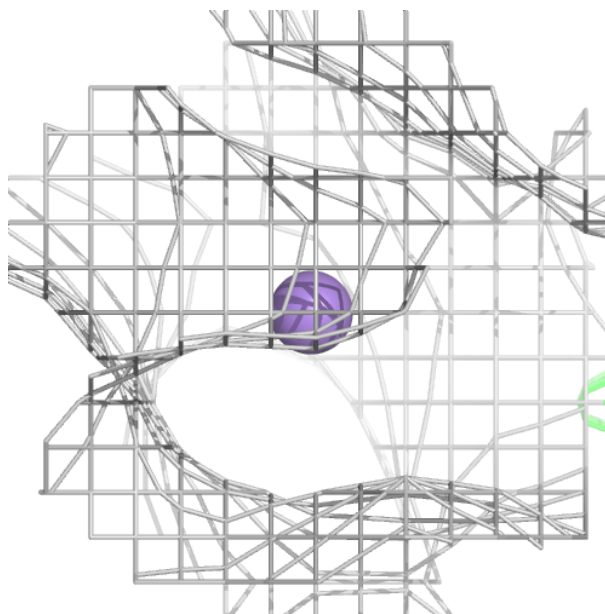
Electron density around MN J 402:

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



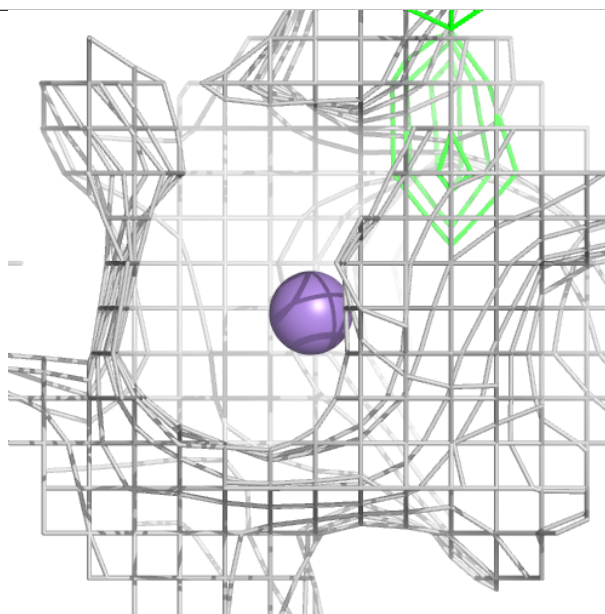
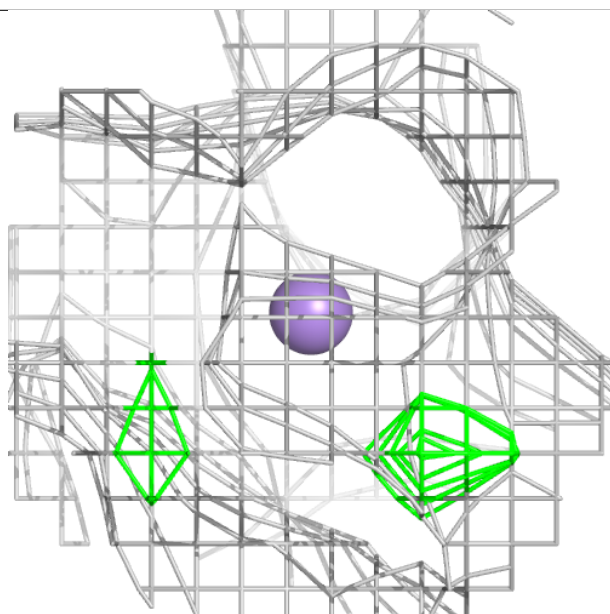
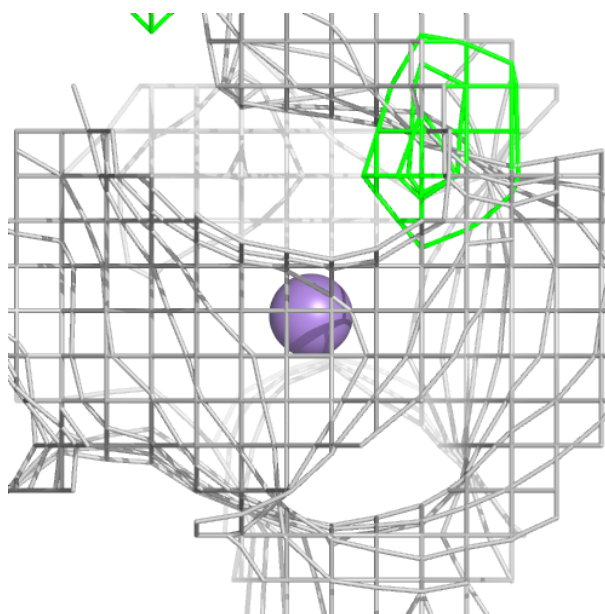
Electron density around MN X 401:

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



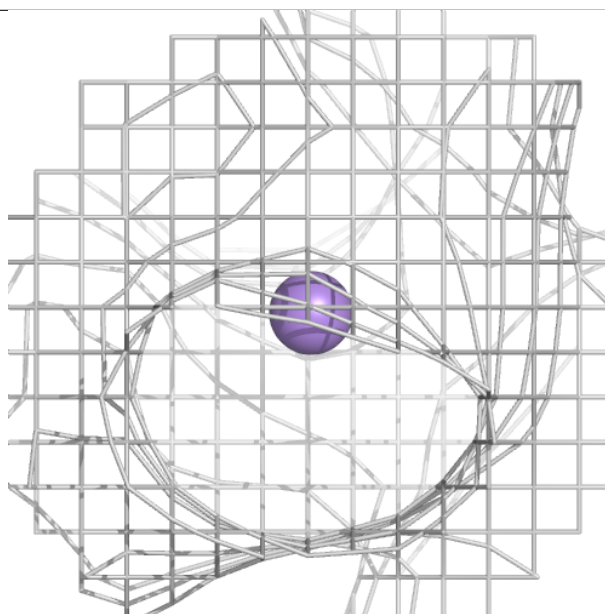
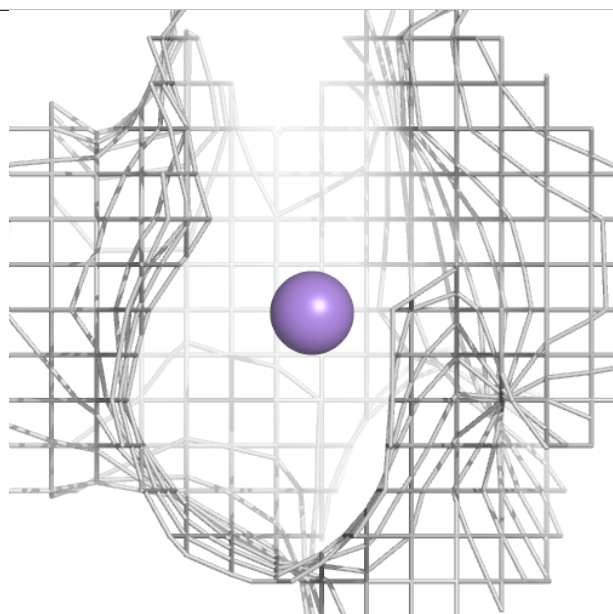
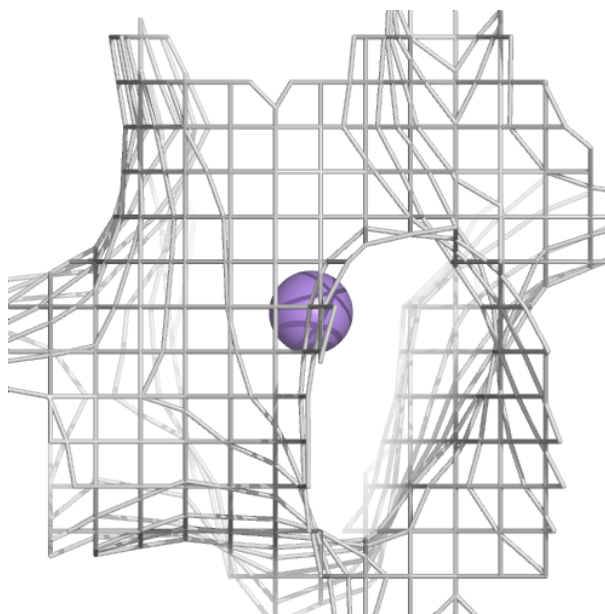
Electron density around MN K 401:

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



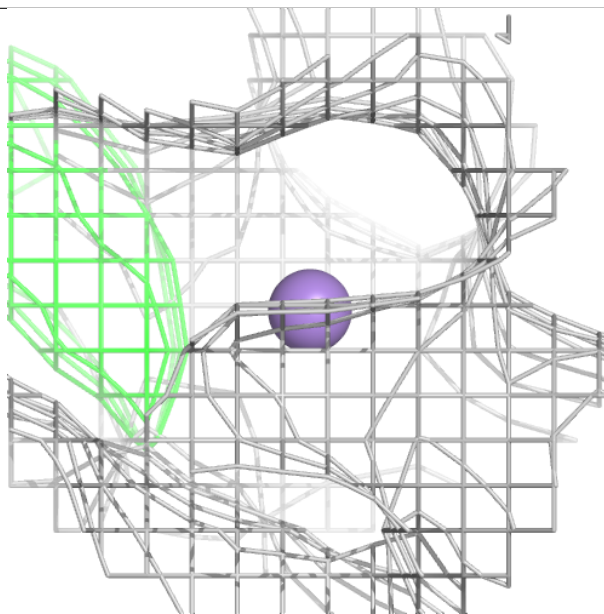
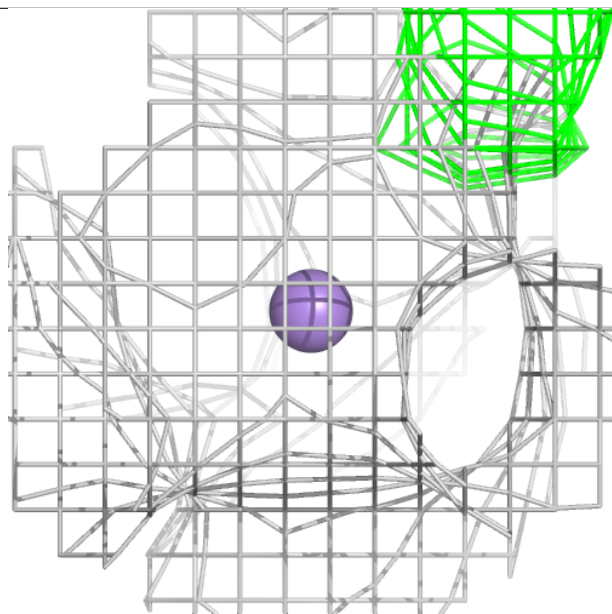
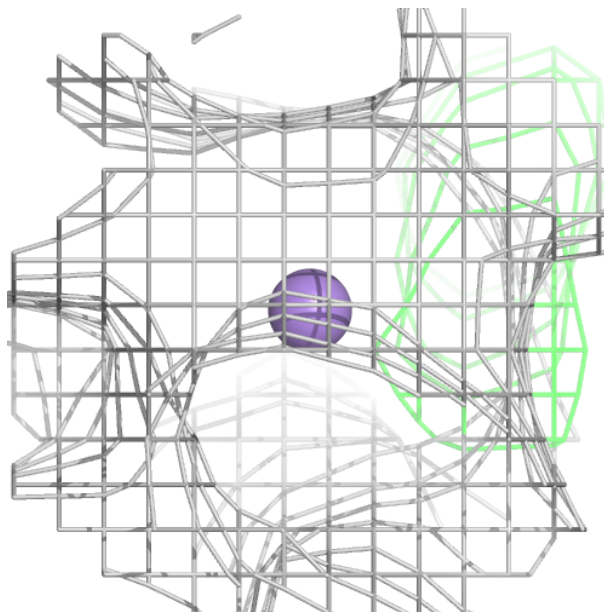
Electron density around MN A 402:

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



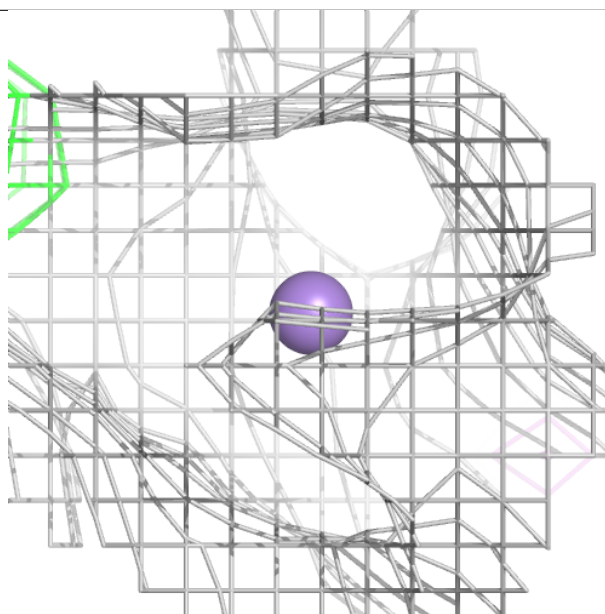
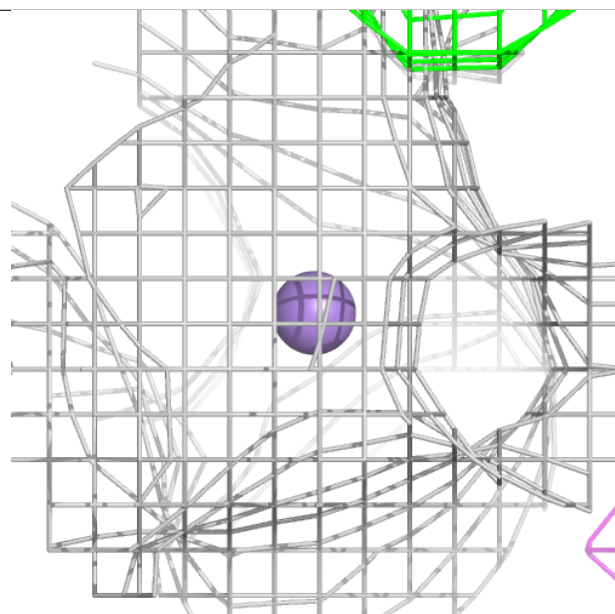
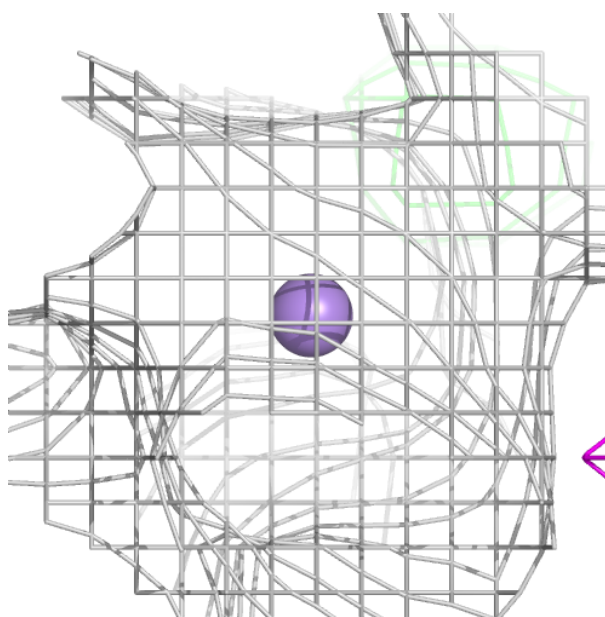
Electron density around MN L 401:

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



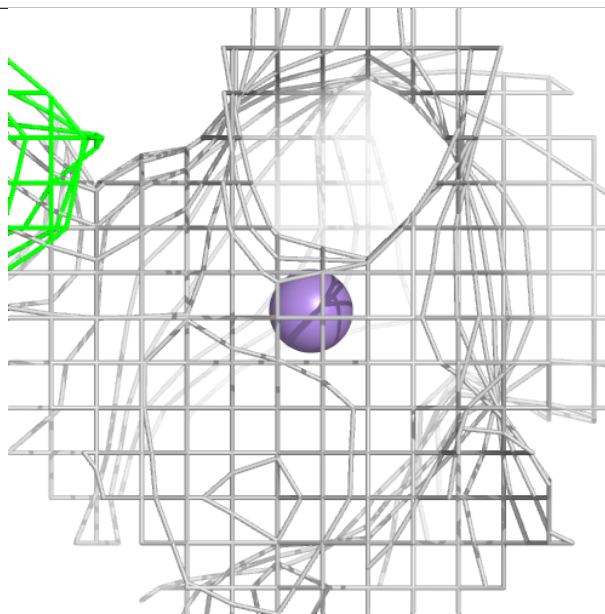
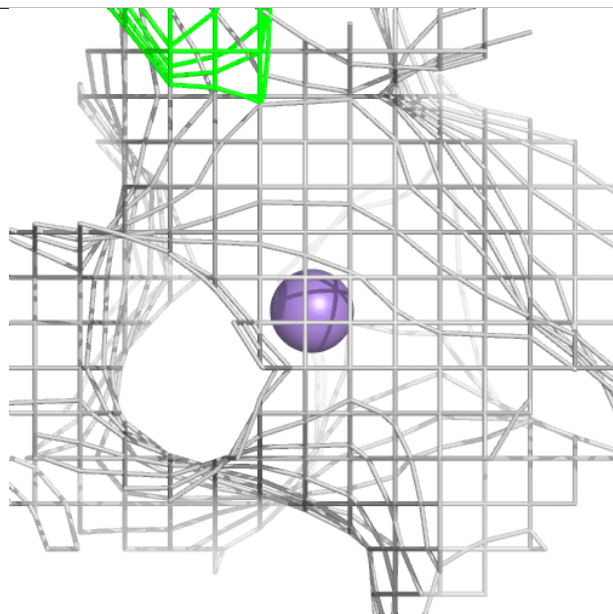
Electron density around MN B 401:

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



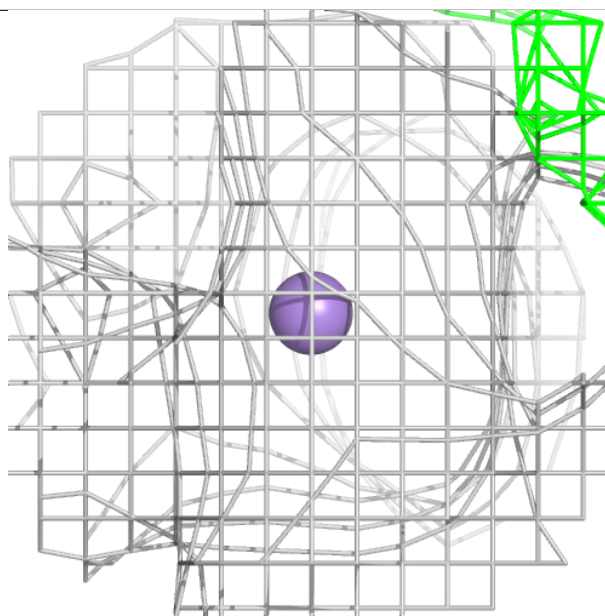
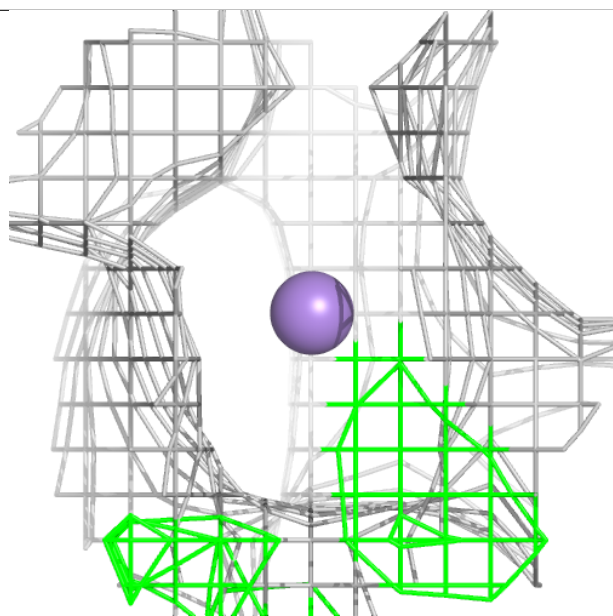
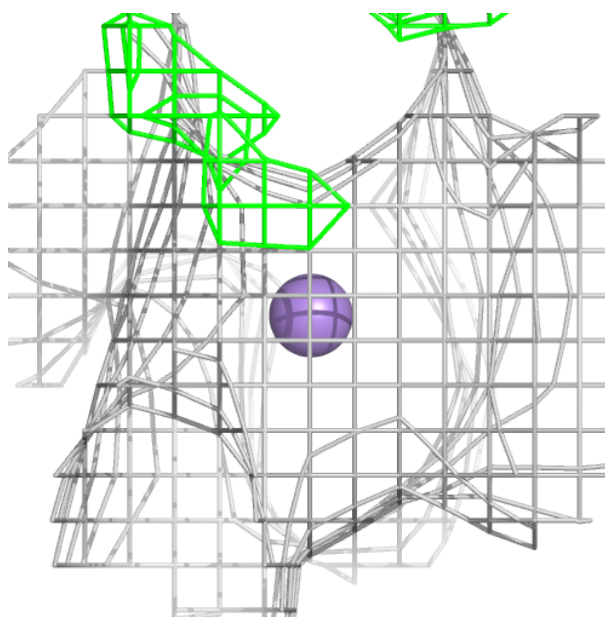
Electron density around MN D 401:

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



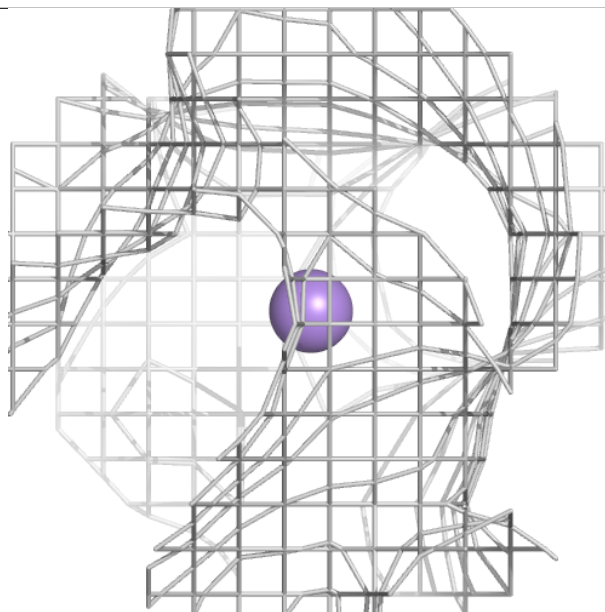
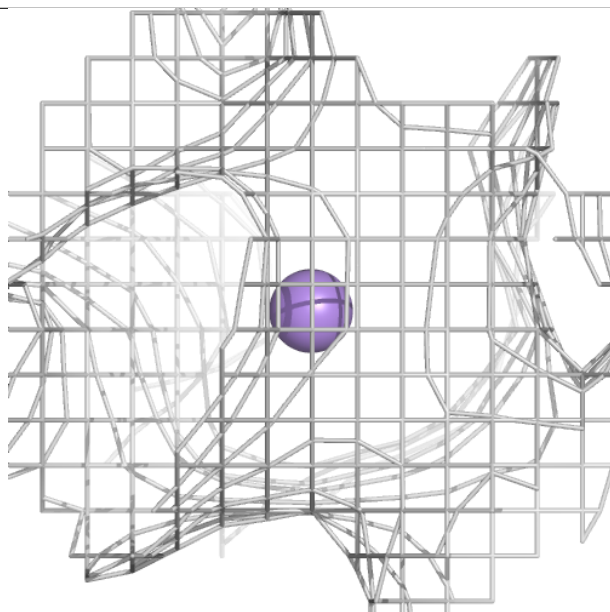
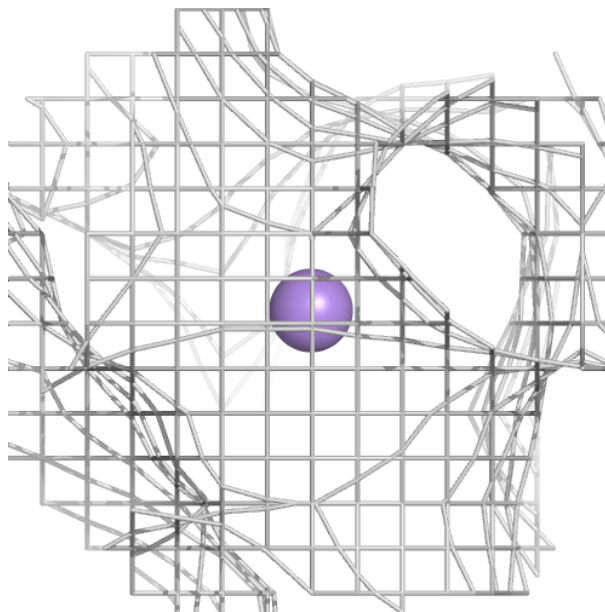
Electron density around MN D 402:

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



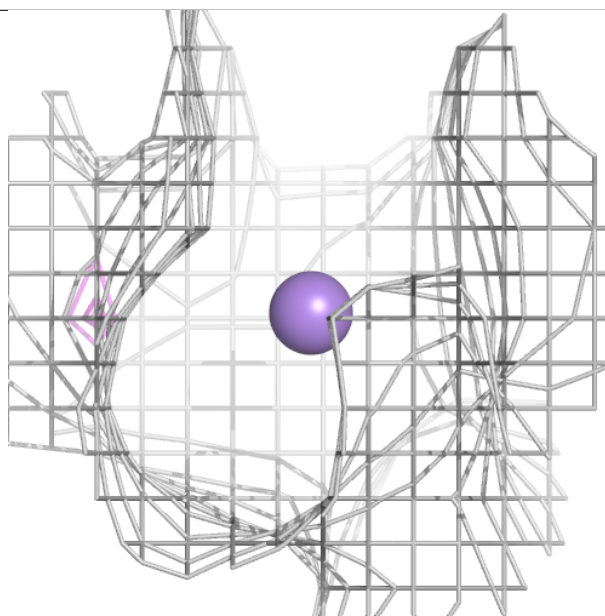
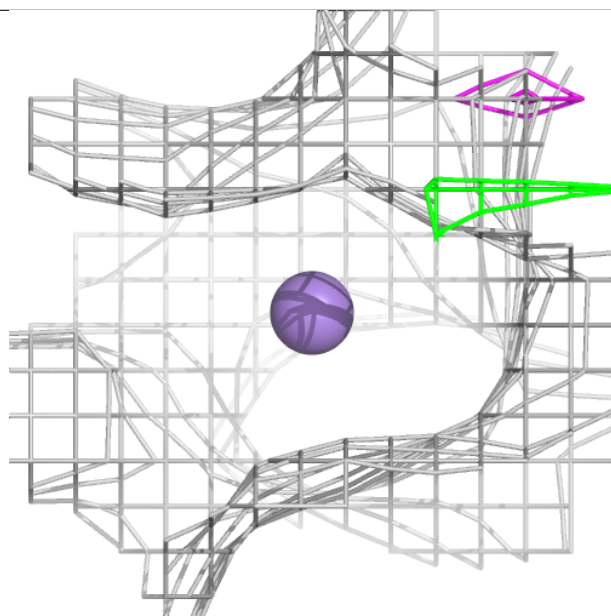
Electron density around MN A 401:

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



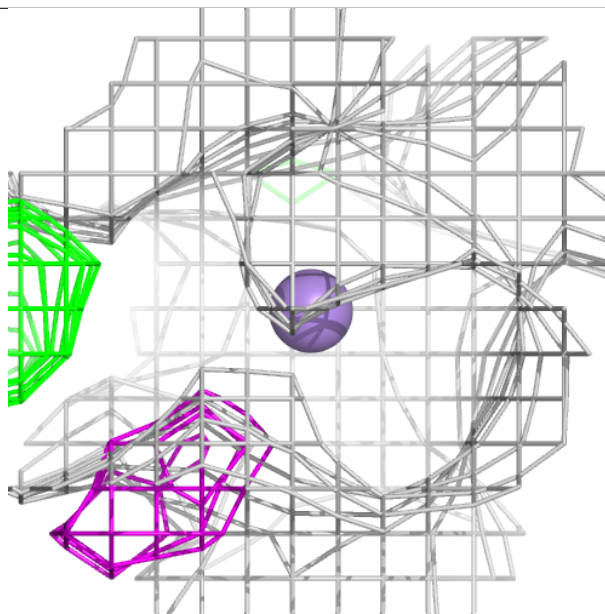
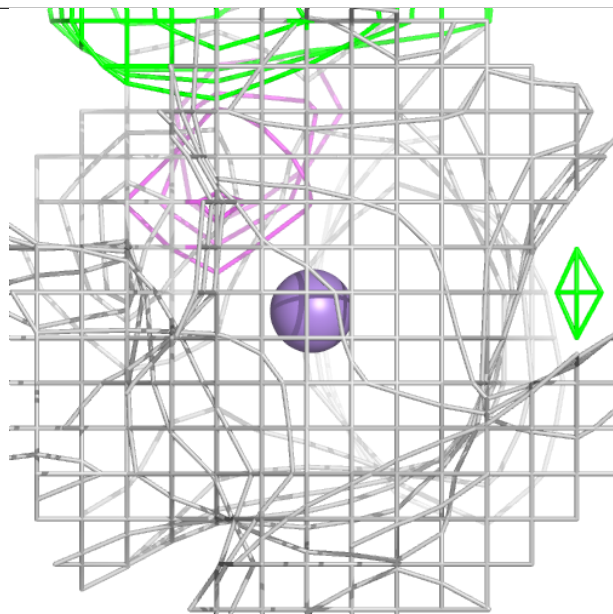
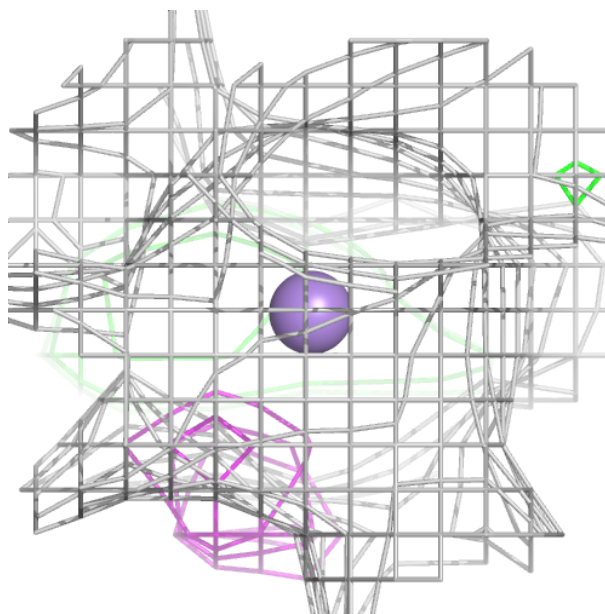
Electron density around MN N 402:

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



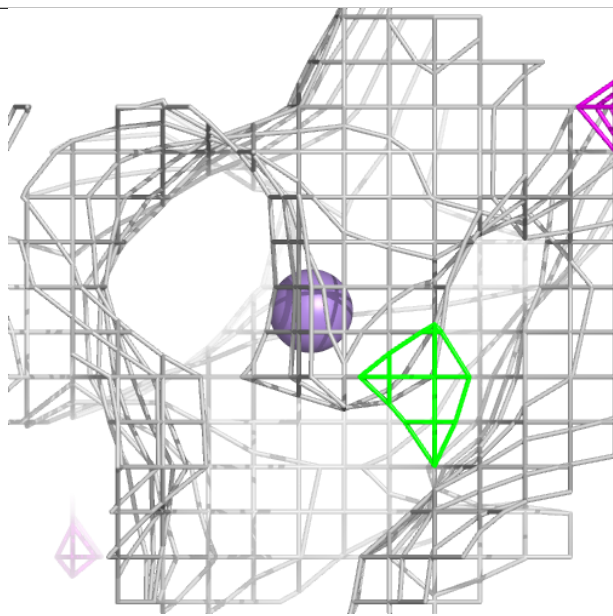
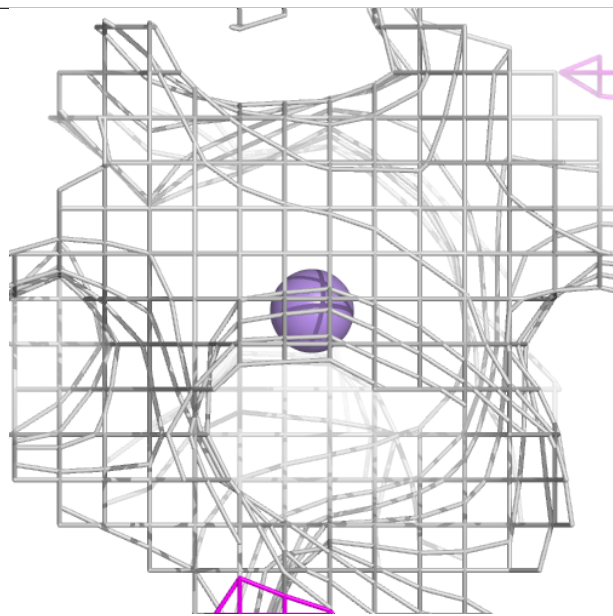
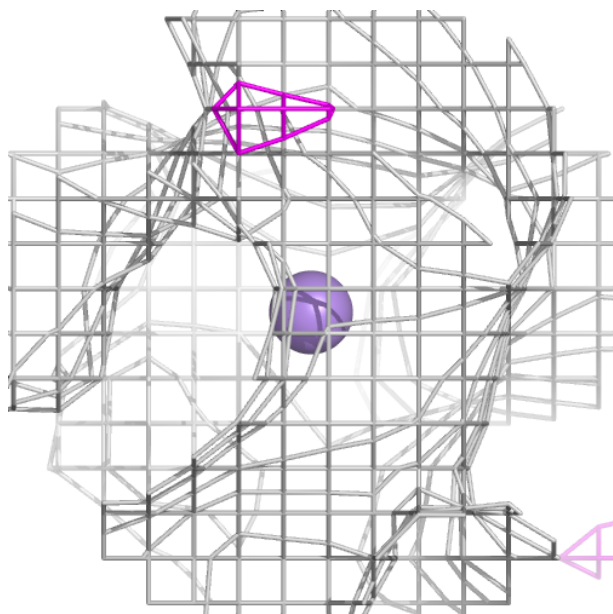
Electron density around MN E 402:

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



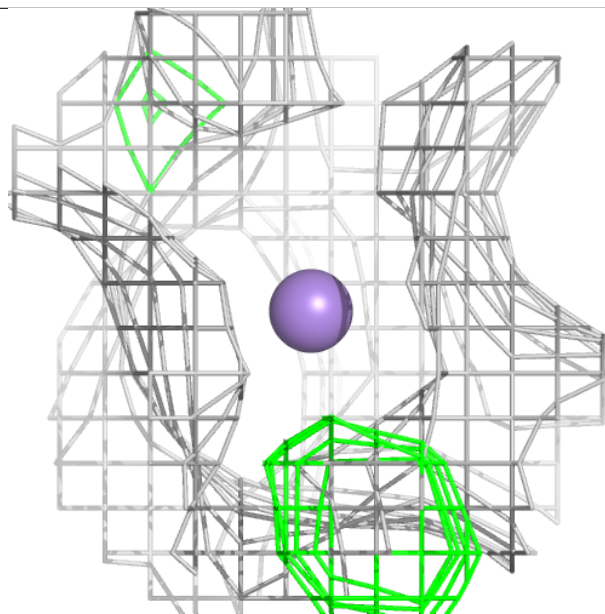
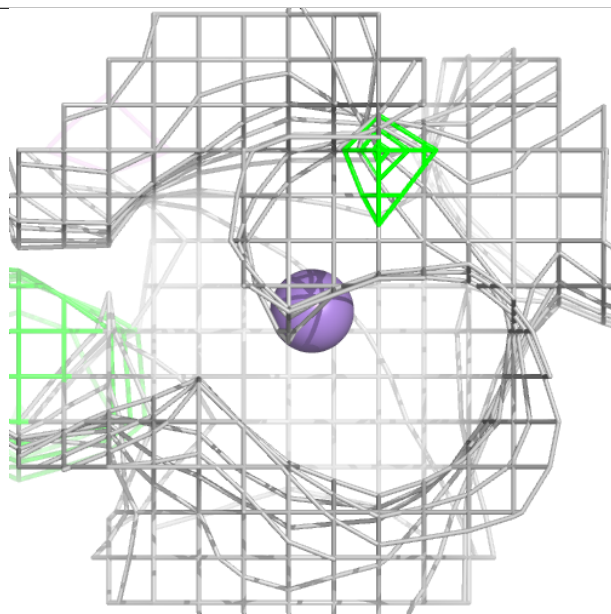
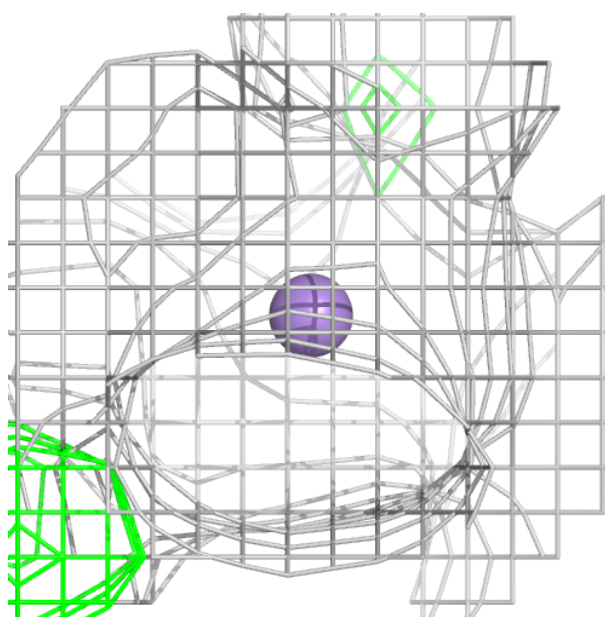
Electron density around MN F 401:

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



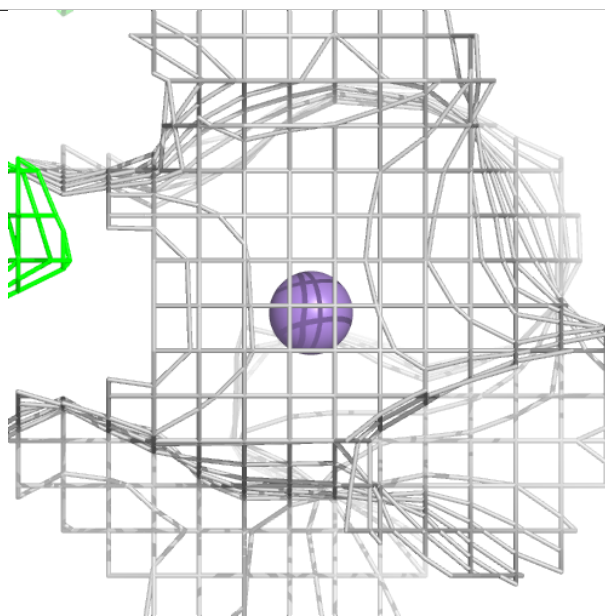
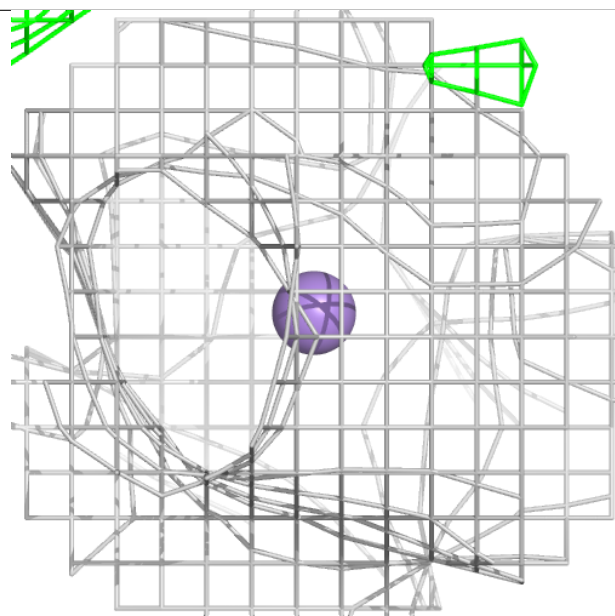
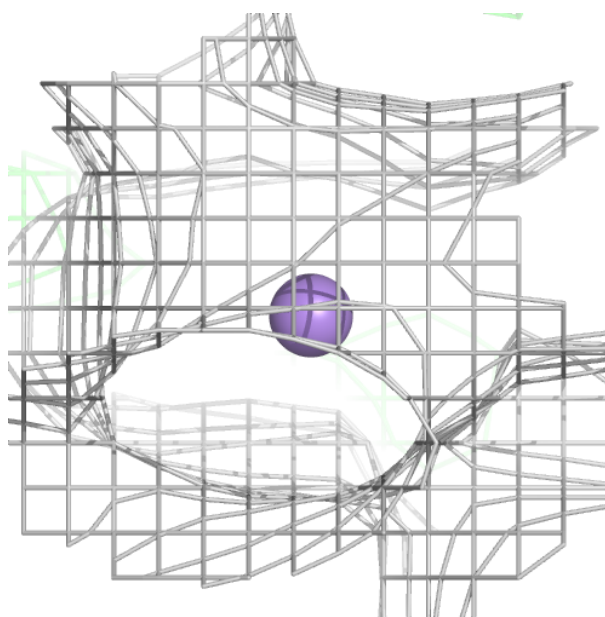
Electron density around MN F 402:

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



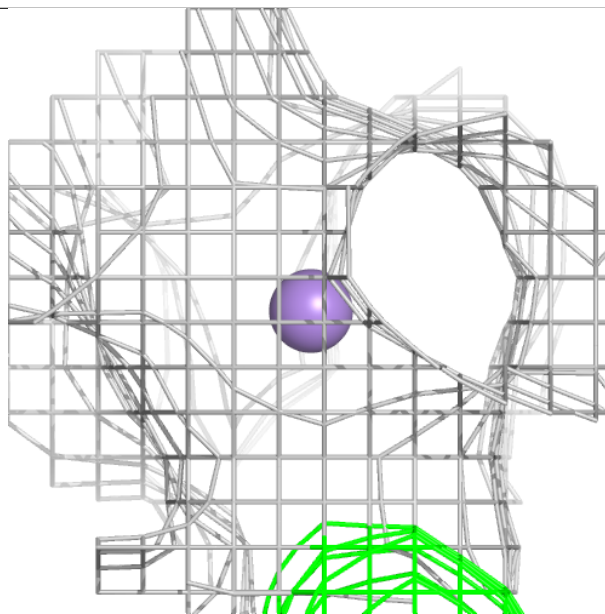
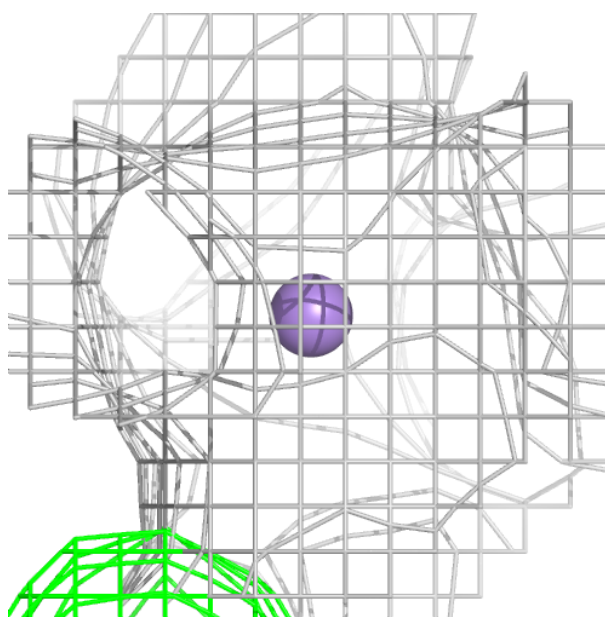
Electron density around MN P 402:

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



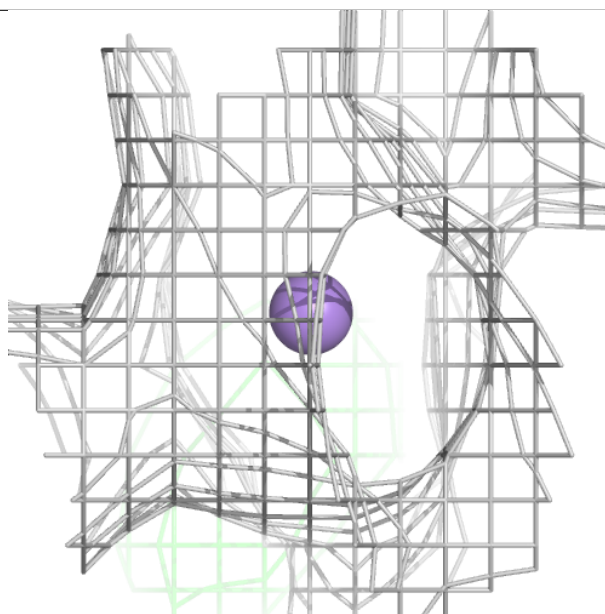
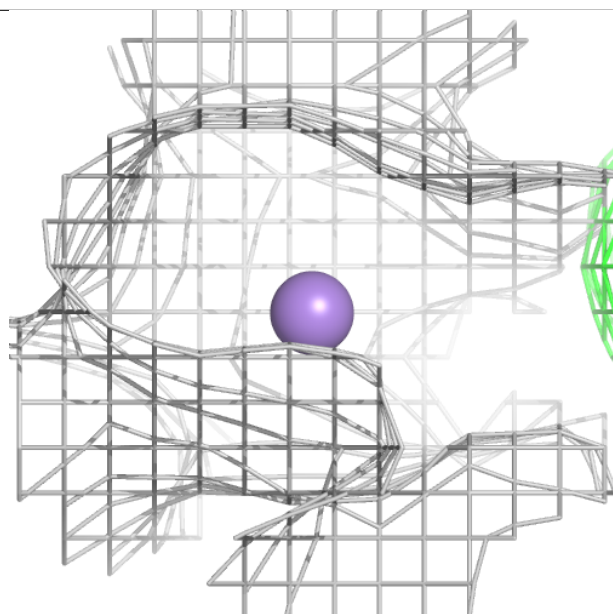
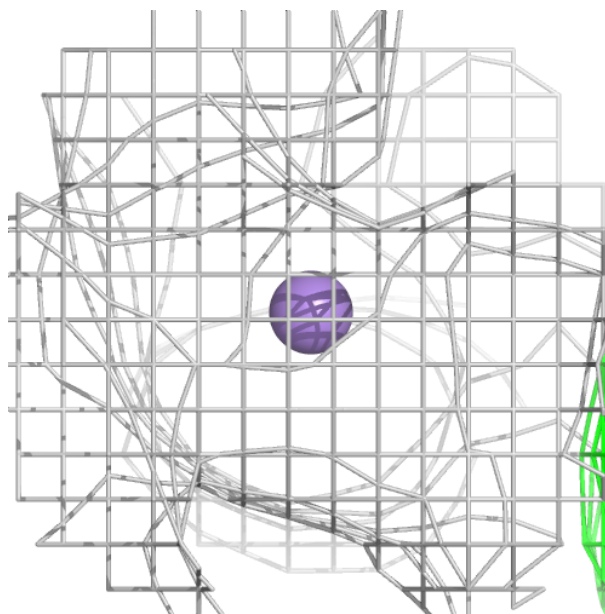
Electron density around MN Q 401:

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



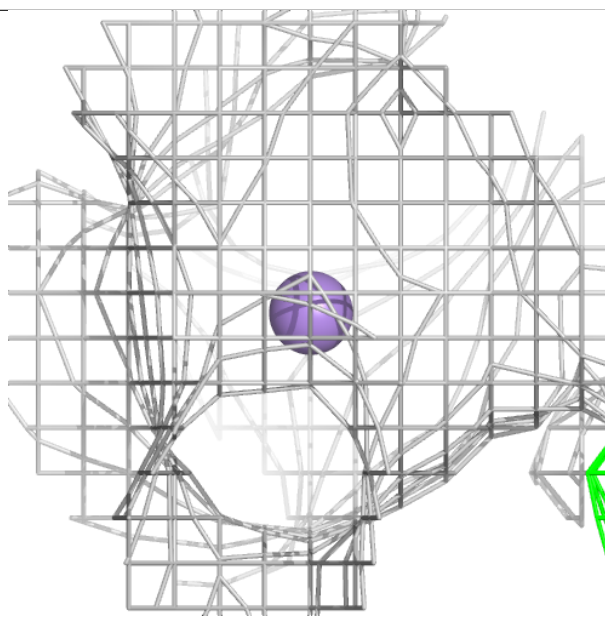
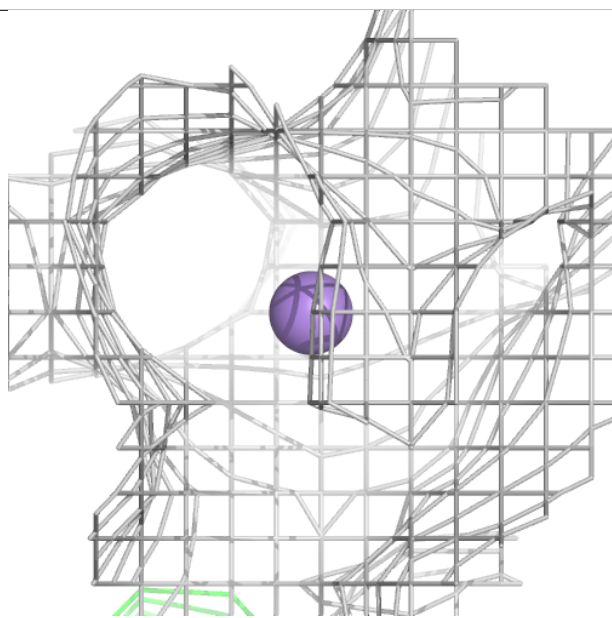
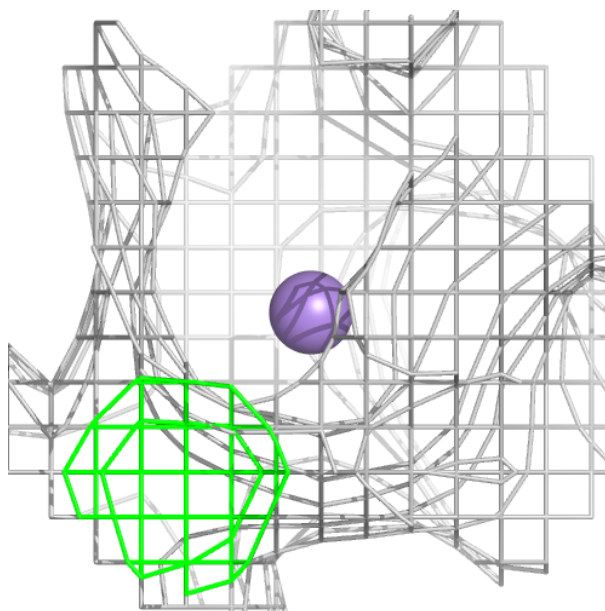
Electron density around MN Q 402:

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



Electron density around MN R 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.