



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 10:37 AM BST

PDB ID : 6VSU
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

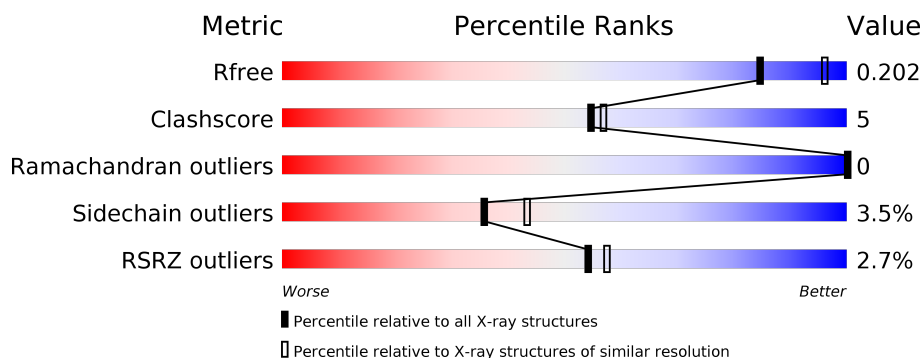
1 Overall quality at a glance

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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (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 on 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	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	321	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
1	C	321	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>31%</div> <div>..</div> </div> </div>
1	D	321	<div> <div></div> <div> <div></div> <div>88%</div> <div>10%</div> <div>..</div> </div> </div>
1	E	321	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>..</div> </div> </div>
1	F	321	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	321	 90% 8% .
1	H	321	 % 89% 10% .
1	I	321	 90% 7% ..
1	J	321	 % 88% 11% .
1	K	321	 % 88% 9% ..
1	L	321	 % 88% 10% ..
1	M	321	 10% 74% 23% ..
1	N	321	 % 87% 11% ..
1	O	321	 12% 79% 17% ..
1	P	321	 2% 89% 9% ..
1	Q	321	 % 88% 10% .
1	R	321	 % 89% 9% ..
1	S	321	 2% 89% 9% ..
1	T	321	 % 87% 11% ..
1	U	321	 3% 87% 11% ..
1	V	321	 7% 74% 22% ..
1	W	321	 9% 81% 17% ..
1	X	321	 % 87% 11% ..

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 (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	2	Total Mn 2 2	0	0
2	K	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0
2	W	2	Total Mn 2 2	0	0
2	N	2	Total Mn 2 2	0	0
2	X	2	Total Mn 2 2	0	0
2	S	2	Total Mn 2 2	0	0
2	J	2	Total Mn 2 2	0	0
2	E	2	Total Mn 2 2	0	0
2	V	2	Total Mn 2 2	0	0
2	A	2	Total Mn 2 2	0	0
2	R	2	Total Mn 2 2	0	0
2	M	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0
2	I	2	Total Mn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	U	2	Total 2	Mn 2	0	0
2	L	2	Total 2	Mn 2	0	0
2	G	2	Total 2	Mn 2	0	0
2	Q	2	Total 2	Mn 2	0	0
2	H	2	Total 2	Mn 2	0	0
2	C	2	Total 2	Mn 2	0	0
2	T	2	Total 2	Mn 2	0	0
2	O	2	Total 2	Mn 2	0	0
2	F	2	Total 2	Mn 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

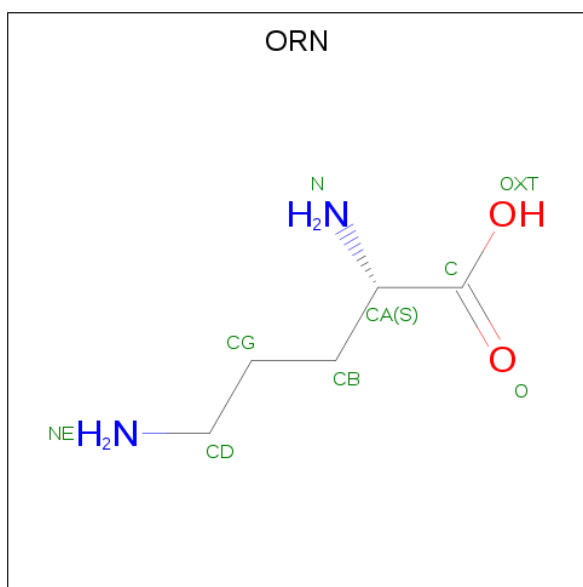
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total 1	Na 1	0	0
3	K	1	Total 1	Na 1	0	0
3	B	1	Total 1	Na 1	0	0
3	W	1	Total 1	Na 1	0	0
3	N	1	Total 1	Na 1	0	0
3	X	1	Total 1	Na 1	0	0
3	S	1	Total 1	Na 1	0	0
3	J	1	Total 1	Na 1	0	0
3	E	1	Total 1	Na 1	0	0
3	V	1	Total 1	Na 1	0	0

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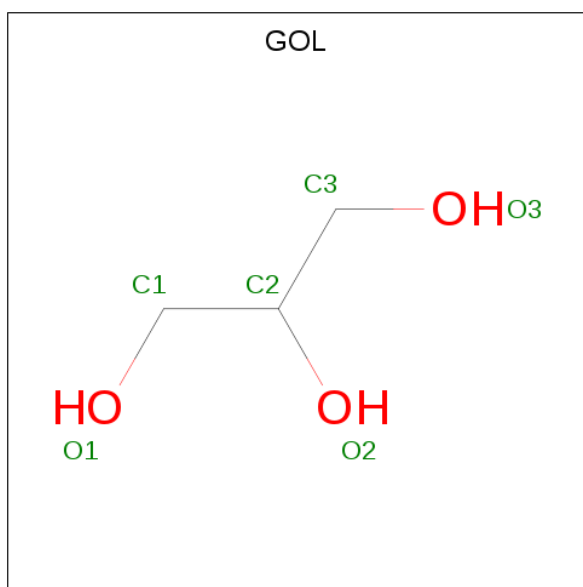
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	R	1	Total 1	Na 1	0	0
3	M	1	Total 1	Na 1	0	0
3	D	1	Total 1	Na 1	0	0
3	I	1	Total 1	Na 1	0	0
3	U	1	Total 1	Na 1	0	0
3	L	1	Total 1	Na 1	0	0
3	G	1	Total 1	Na 1	0	0
3	Q	1	Total 1	Na 1	0	0
3	H	1	Total 1	Na 1	0	0
3	C	1	Total 1	Na 1	0	0
3	T	1	Total 1	Na 1	0	0
3	O	1	Total 1	Na 1	0	0
3	F	1	Total 1	Na 1	0	0

- Molecule 4 is L-ornithine (three-letter code: ORN) (formula: $C_5H_{12}N_2O_2$) (labeled as "Ligand of Interest" by author).



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 (three-letter code: GOL) (formula: C₃H₈O₃).



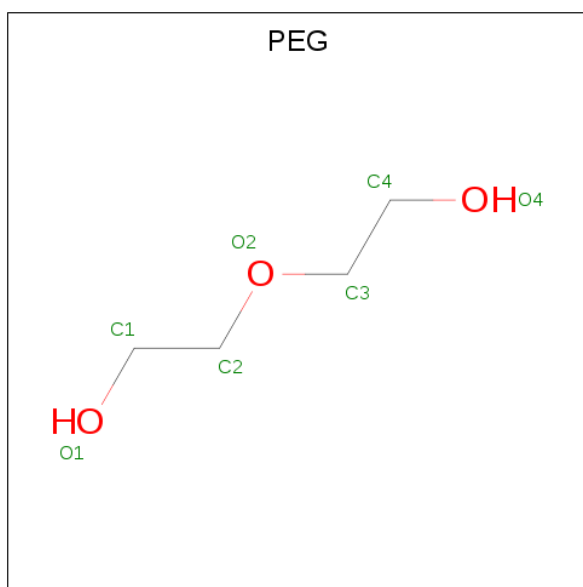
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	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 (three-letter code: 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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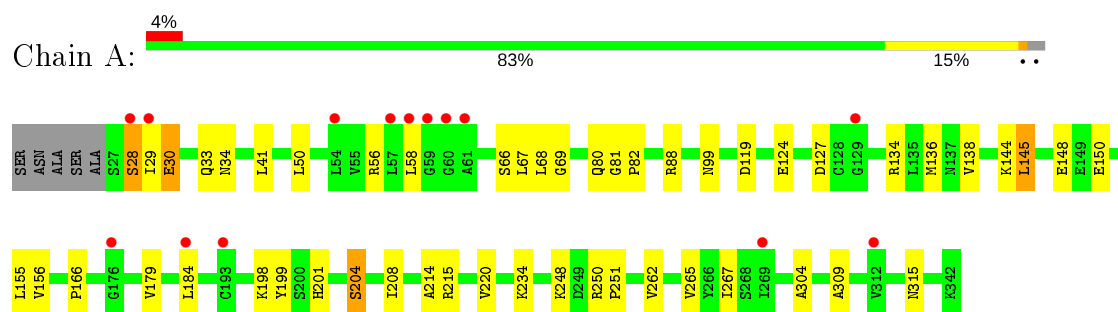
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	260	Total 260	O 260	0	0
7	I	265	Total 265	O 265	0	0
7	J	336	Total 336	O 336	0	0
7	K	276	Total 276	O 276	0	0
7	L	231	Total 231	O 231	0	0
7	M	61	Total 61	O 61	0	0
7	N	182	Total 182	O 182	0	0
7	O	79	Total 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

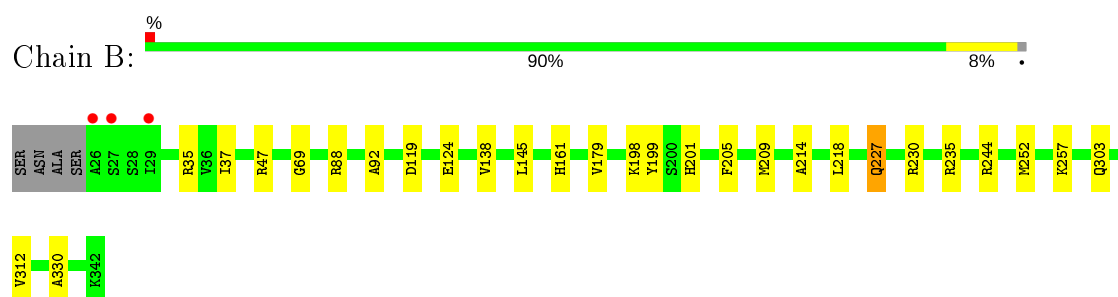
3 Residue-property plots [i](#)

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.

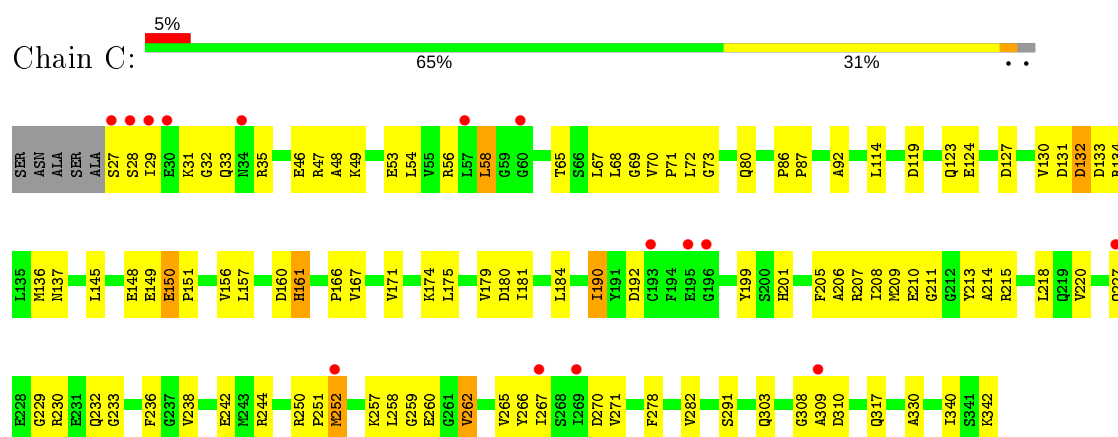
- Molecule 1: Arginase 1, mitochondrial




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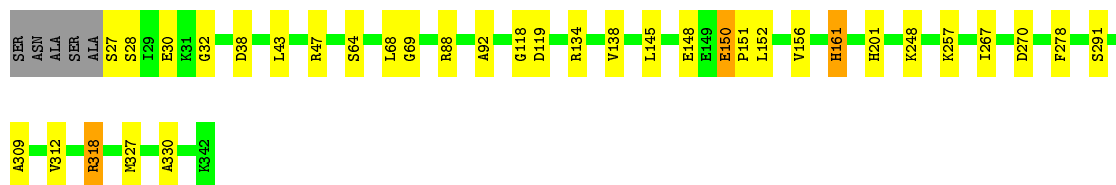


- Molecule 1: Arginase 1, mitochondrial




- Molecule 1: Arginase 1, mitochondrial

Chain D:  88% 10% ..




- Molecule 1: Arginase 1, mitochondrial

Chain E:  90% 8% ..




- Molecule 1: Arginase 1, mitochondrial

Chain F:  91% 7% .




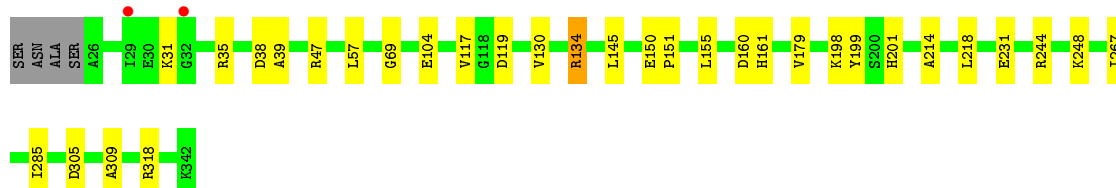
- Molecule 1: Arginase 1, mitochondrial

Chain G:  90% 8% .



- Molecule 1: Arginase 1, mitochondrial

Chain H:  89% 10% .

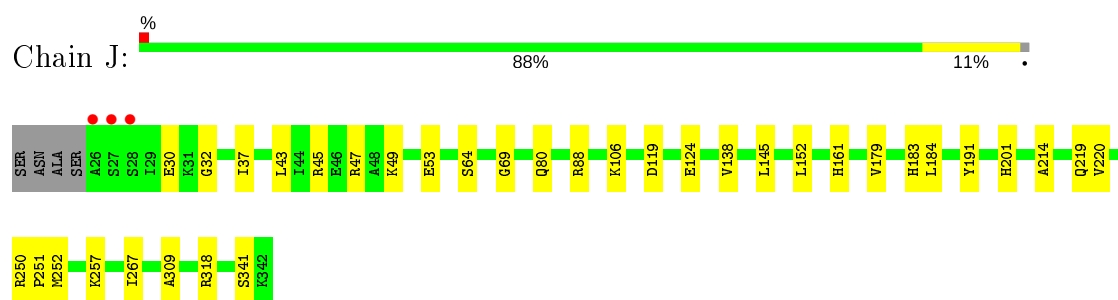


- Molecule 1: Arginase 1, mitochondrial

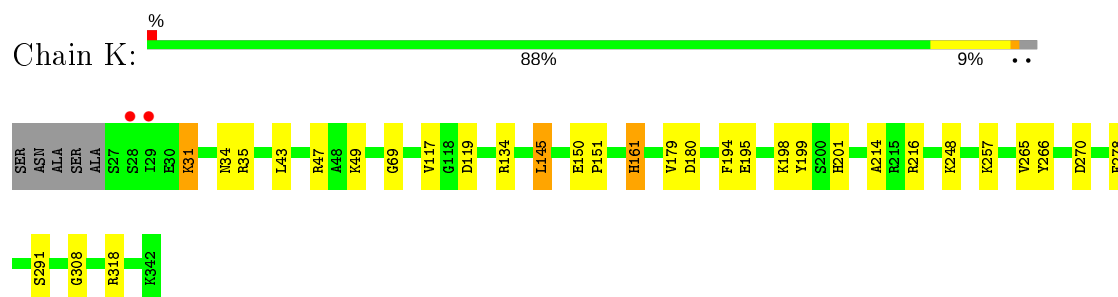
Chain I:  90% 7% ..



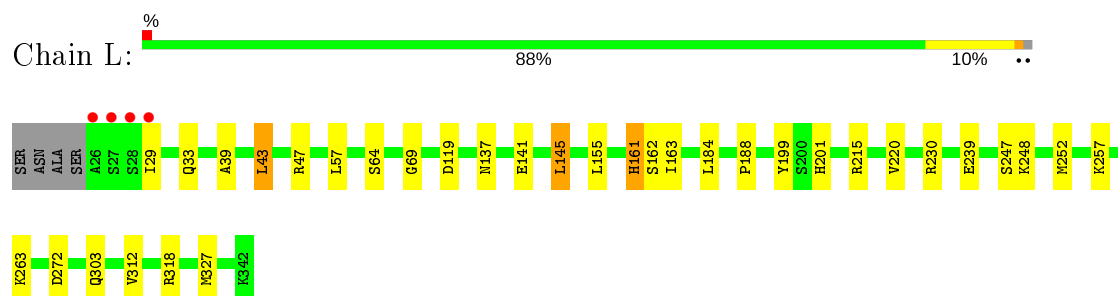
- Molecule 1: Arginase 1, mitochondrial



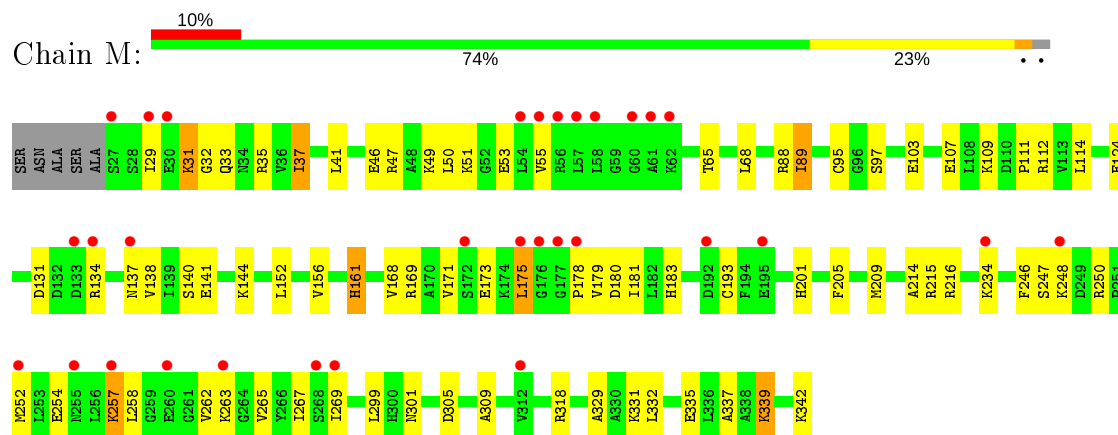
- Molecule 1: Arginase 1, mitochondrial



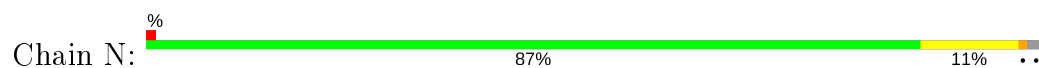
- Molecule 1: Arginase 1, mitochondrial

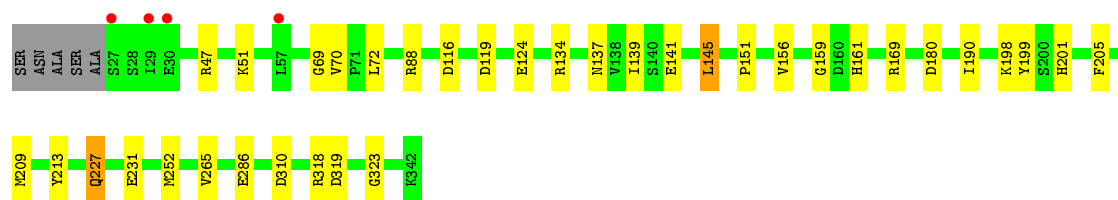


- Molecule 1: Arginase 1, mitochondrial

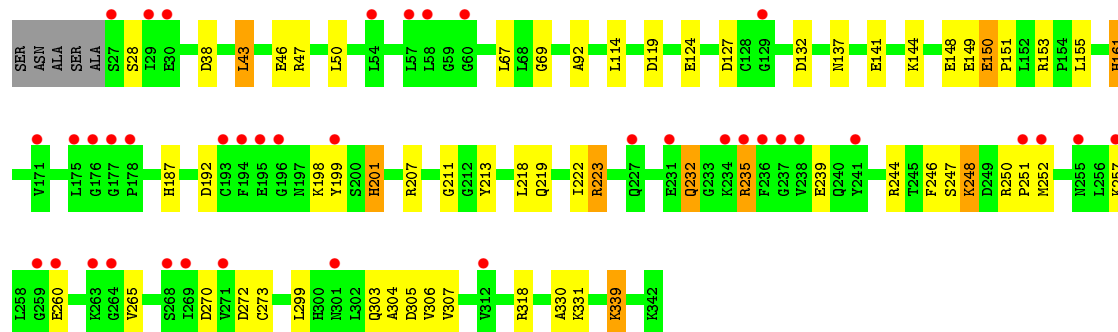
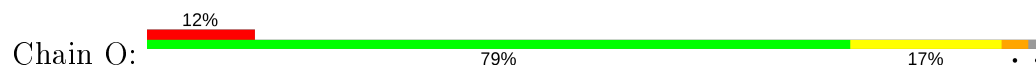


- Molecule 1: Arginase 1, mitochondrial

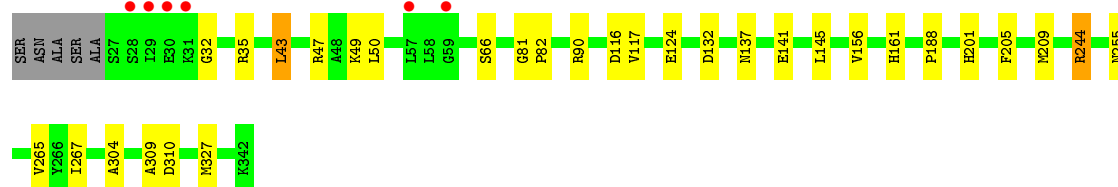
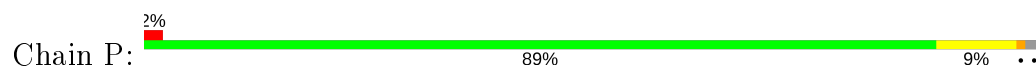




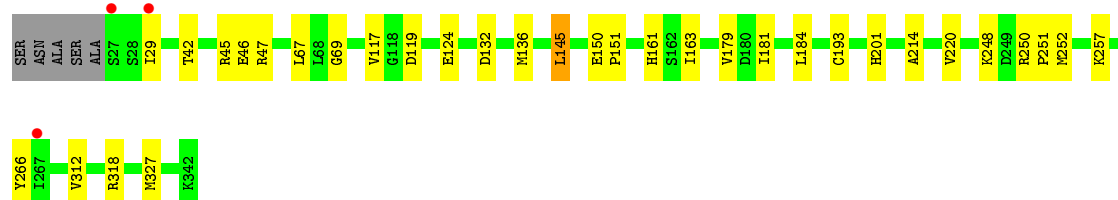
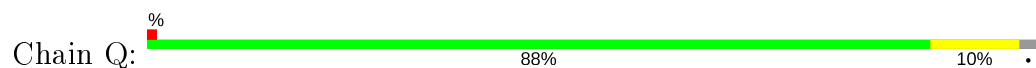
- Molecule 1: Arginase 1, mitochondrial



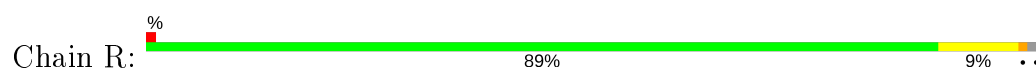
- Molecule 1: Arginase 1, mitochondrial



- Molecule 1: Arginase 1, mitochondrial

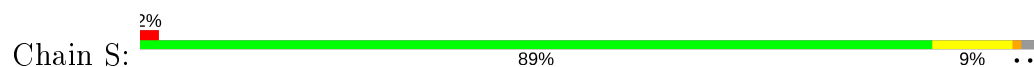


- Molecule 1: Arginase 1, mitochondrial

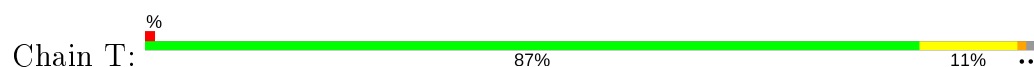




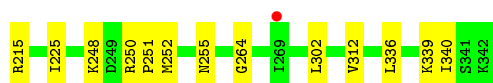
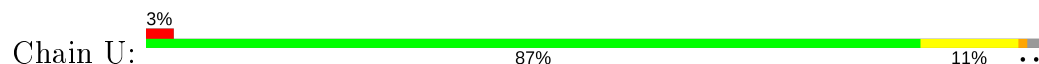
- Molecule 1: Arginase 1, mitochondrial



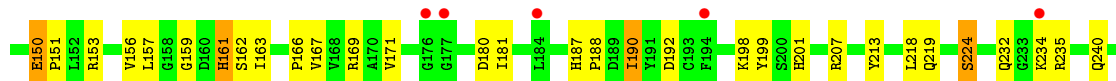
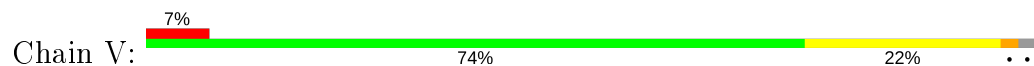
- Molecule 1: Arginase 1, mitochondrial




- Molecule 1: Arginase 1, mitochondrial

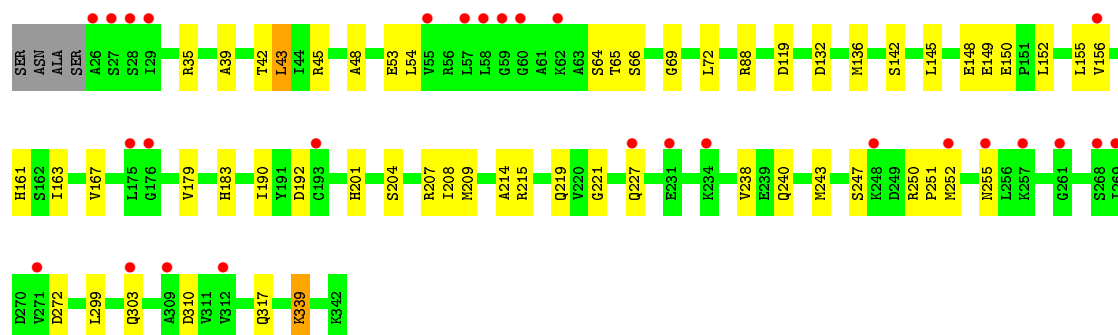


- Molecule 1: Arginase 1, mitochondrial




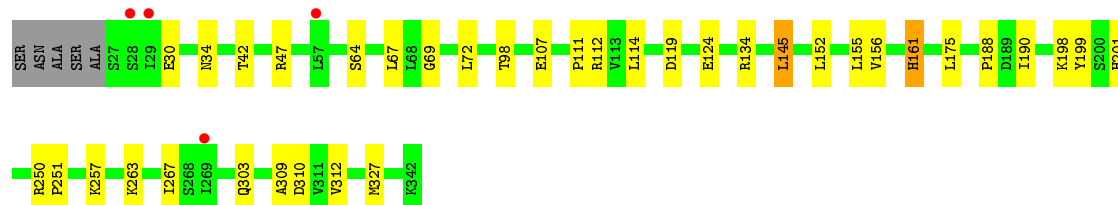
- Molecule 1: Arginase 1, mitochondrial

Chain W:  9% 81% 17% ..



- Molecule 1: Arginase 1, mitochondrial

Chain X:  87% 11% ..



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 29.95 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.97-2.25) 98.5 (29.95-2.25)	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	2236 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 , 45.1	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, GOL, MN, PEG, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.79	0/2468	0.93	0/3331
1	B	0.89	0/2465	0.95	0/3328
1	C	0.89	0/2476	1.00	0/3341
1	D	0.84	0/2460	0.93	0/3321
1	E	0.87	0/2470	0.94	0/3335
1	F	0.83	0/2468	0.92	0/3332
1	G	0.87	0/2469	0.95	0/3333
1	H	0.88	0/2465	0.94	0/3328
1	I	0.84	0/2460	0.94	0/3321
1	J	0.87	0/2465	0.96	0/3328
1	K	0.93	0/2460	0.99	0/3321
1	L	0.95	0/2465	0.94	0/3328
1	M	0.81	0/2460	0.88	0/3321
1	N	0.82	0/2460	0.92	0/3321
1	O	0.81	0/2460	0.91	1/3321 (0.0%)
1	P	0.79	0/2460	0.90	0/3321
1	Q	0.84	0/2460	0.93	0/3321
1	R	0.77	0/2471	0.91	0/3335
1	S	0.85	0/2460	0.94	0/3321
1	T	0.84	0/2471	0.93	0/3336
1	U	0.83	0/2468	0.93	0/3332
1	V	0.97	0/2460	1.03	0/3321
1	W	0.82	0/2465	0.92	0/3328
1	X	0.84	0/2460	0.93	0/3321
All	All	0.85	0/59146	0.94	1/79846 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	38	ASP	CB-CA-C	5.03	120.45	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2426	0	2446	32	0
1	B	2426	0	2442	18	0
1	C	2431	0	2455	67	0
1	D	2421	0	2437	22	0
1	E	2431	0	2444	20	0
1	F	2426	0	2443	18	0
1	G	2427	0	2443	19	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	17	0
1	L	2426	0	2442	25	0
1	M	2421	0	2437	80	0
1	N	2421	0	2437	18	0
1	O	2421	0	2437	48	0
1	P	2421	0	2437	23	0
1	Q	2421	0	2437	16	0
1	R	2429	0	2450	23	0
1	S	2421	0	2437	17	0
1	T	2432	0	2447	21	0
1	U	2426	0	2448	24	0
1	V	2421	0	2437	47	0
1	W	2426	0	2442	29	0
1	X	2421	0	2437	29	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	0	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	3	0
7	A	126	0	0	1	0
7	B	240	0	0	1	0
7	C	138	0	0	4	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	4	0
7	H	260	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	265	0	0	4	0
7	J	336	0	0	4	0
7	K	276	0	0	2	0
7	L	231	0	0	5	0
7	M	61	0	0	3	0
7	N	182	0	0	1	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	7	0
7	W	107	0	0	3	0
7	X	152	0	0	2	0
All	All	63508	0	58982	616	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (616) 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	1.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:50:LEU:N	1:M:50:LEU:HD23	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:HD23	1:M:175:LEU:N	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:L:327:MET:HE3	7:L:639:HOH:O	1.90	0.72
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
1:M:33:GLN:O	1:M:37:ILE:HG13	1.91	0.71
1:C:136[A]:MET:HE3	1:C:166:PRO:HG3	1.72	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:O:43:LEU:HG	1:O:47:ARG:NH1	2.05	0.70
1:M:107:GLU:OE2	1:M:109:LYS:N	2.25	0.69
1:M:47:ARG:NH1	1:P:124:GLU:HG2	2.07	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:HA	1:B:227:GLN:OE1	1.92	0.68
1:P:327:MET:HE3	7:P:646:HOH:O	1.94	0.67
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:327:MET:HE3	7:F:595:HOH:O	2.03	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: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
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:HH21	1:E:134:ARG:HG2	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:M:49:LYS:HZ1	1:M:50:LEU:HD21	1.69	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:U:124:GLU:HB3	1:X:47:ARG:HD2	1.88	0.55
1:M:299:LEU:O	1:M:339:LYS:NZ	2.25	0.55
1:D:43:LEU:HG	1:D:47:ARG:HH11	1.71	0.55
1:K:198:LYS:HE2	1:K:199:TYR:CE2	2.41	0.55
1:K:34:ASN:OD1	1:K:134:ARG:NH1	2.31	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:M:49:LYS:NZ	1:M:50:LEU:CD2	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:124:GLU:HG2	1:Q:47:ARG:CZ	2.38	0.54
1:N:88:ARG:NE	7:N:502:HOH:O	2.41	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
1:N:69:GLY:HA3	1:N:119:ASP:OD1	2.08	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:V:219:GLN:OE1	1:V:240:GLN:HG2	2.09	0.52
1:U:47:ARG:HD2	1:X:124:GLU:HB3	1.92	0.52
1:K:179:VAL:O	1:K:214:ALA:HA	2.10	0.52
1:I:124:GLU:HG2	1:L:47:ARG:CZ	2.39	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:179:VAL:O	1:T:214:ALA:HA	2.10	0.52
1:T:67:LEU:O	1:T:117:VAL:HG22	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	1:G:134:ARG:HG2	2.24	0.51
1:V:192:ASP:O	1:V:207:ARG:NH1	2.41	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:I:327:MET:HE3	7:I:596:HOH:O	2.09	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:PRO:HB2	1:G:87:PRO:HD3	1.94	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
1:L:184:LEU:HD23	1:L:220:VAL:HB	1.94	0.49
1:V:169:ARG:HG3	1:V:213:TYR:CZ	2.48	0.49
1:V:58:LEU:HA	7:V:555:HOH:O	2.13	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:HH11	1:W:88:ARG:HG3	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: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:M:49:LYS:HZ3	1:M:50:LEU:HD21	1.78	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:V:190:ILE:O	1:V:190:ILE:HG23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:49:LYS:HZ3	1:M:50:LEU:CD2	2.25	0.48
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:103:GLU:HG3	1:M:335:GLU:OE2	2.14	0.47
1:M:37:ILE:CG2	1:M:138:VAL:HG22	2.44	0.47
1:O:46:GLU:CD	1:R:35:ARG:HD3	2.35	0.47
1:O:67:LEU:HG	1:O:114:LEU:HD11	1.96	0.47
1:C:132:ASP:O	1:C:136[A]:MET:HG2	2.13	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:C:32:GLY:HA2	1:C:35:ARG:HD3	1.95	0.47
1:M:179:VAL:O	1:M:214:ALA:HA	2.15	0.47
1:R:218:LEU:HD12	1:R:218:LEU:N	2.29	0.47
1:U:161:HIS:CD2	1:U:312:VAL:HG21	2.49	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
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:C:67:LEU:HD13	1:C:157:LEU:HD11	1.96	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: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
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:X:155:LEU:C	1:X:155:LEU:HD23	2.35	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:O:155:LEU:C	1:O:155:LEU:HD23	2.35	0.46
1:U:51:LYS:HE3	1:U:116:ASP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:327:MET:HE3	7:D:647:HOH:O	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
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:J:49:LYS:NZ	1:J:53:GLU:OE1	2.39	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:Q:42:THR:O	1:Q:46:GLU:HG2	2.16	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:B:47:ARG:HD2	1:E:124:GLU:HB3	1.98	0.46
1:A:41:LEU:HD21	1:A:138:VAL:HG13	1.98	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:I:62:LYS:NZ	7:I:510:HOH:O	2.45	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:S:28:SER:OG	1:S:28:SER:O	2.33	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:49:LYS:HZ3	1:M:49:LYS:HB3	1.81	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:C:167:VAL:O	1:C:171:VAL:HG23	2.16	0.45
1:A:50:LEU:HD21	1:D:32:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:92:ALA:HB3	1:O:330:ALA:HB2	1.97	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:W:272:ASP:C	1:W:272:ASP:OD1	2.54	0.45
1:X:327:MET:HE3	7:X:633:HOH:O	2.17	0.45
1:A:88:ARG:HD2	7:A:609:HOH:O	2.16	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: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:156:VAL:O	1:P:310:ASP:HA	2.17	0.45
1:P:43:LEU:HD12	1:P:47:ARG:HD3	1.99	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
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: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:Q:327:MET:HE3	7:Q:596:HOH:O	2.17	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: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:267:ILE:O	1:T:309:ALA:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:29:ILE:O	1:T:33:GLN:HG3	2.18	0.44
1:X:34:ASN:ND2	1:X:134:ARG:HH22	2.16	0.44
1:C:342:LYS:NZ	7:C:512:HOH:O	2.41	0.44
1:L:272:ASP:C	1:L:272:ASP:OD1	2.56	0.44
1:L:239:GLU:HB3	6:L:408:PEG:H42	1.99	0.44
1:O:192:ASP:HA	7:O:563:HOH:O	2.17	0.44
1:O:161:HIS:CB	1:O:201:HIS:HB2	2.47	0.44
1:O:248:LYS:HA	1:O:248:LYS:HE3	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:V:249:ASP:O	1:V:253:LEU:HG	2.18	0.44
1:V:72:LEU:O	1:V:159:GLY:HA2	2.17	0.44
1:S:88:ARG:NH2	1:V:88:ARG:NH2	2.66	0.44
1:X:112:ARG:HB2	1:X:112:ARG:HE	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:U:248:LYS:NZ	7:U:516:HOH:O	2.51	0.44
1:U:81:GLY:N	1:U:82:PRO:CD	2.81	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: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:NH2	1:E:134:ARG:HG2	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: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:HA	1:S:34:ASN:HD22	1.67	0.43
1:C:257:LYS:HE2	1:C:303:GLN:CB	2.43	0.43
1:E:155:LEU:C	1:E:155:LEU:HD23	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:48:ALA:O	1:W:149:GLU:HG3	2.18	0.43
1:L:161:HIS:CD2	1:L:312:VAL:HG21	2.53	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:M:33:GLN:O	1:M:37:ILE:CG1	2.61	0.43
1:C:206:ALA:O	1:C:210:GLU:CG	2.60	0.43
1:C:65:THR:OG1	1:C:340:ILE:HB	2.19	0.43
1:L:230:ARG:HG2	1:L:230:ARG:HH11	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:M:124:GLU:HG2	1:P:47:ARG:CZ	2.49	0.43
1:T:169:ARG:O	1:T:173:GLU:HG3	2.19	0.43
1:T:72:LEU:O	1:T:159:GLY:HA2	2.18	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: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:A:315:ASN:C	1:A:315:ASN:OD1	2.57	0.42
1:H:155:LEU:C	1:H:155:LEU:HD23	2.39	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:D:38:ASP:OD2	1:R:35:ARG:NE	2.51	0.42
1:U:37:ILE:HG23	1:U:138:VAL:HG22	2.00	0.42
1:A:68:LEU:O	1:A:156:VAL:HA	2.19	0.42
1:A:80:GLN:C	1:A:82:PRO:HD2	2.39	0.42
1:C:259:GLY:HA2	1:C:262:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:OG	1:A:28:SER:O	2.32	0.42
1:C:92:ALA:HB3	1:C:330:ALA:HB2	2.00	0.42
1:C:47:ARG:NH2	1:F:124:GLU:HG2	2.34	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:C:160:ASP:OD1	1:C:160:ASP:C	2.58	0.42
1:G:267:ILE:O	1:G:309:ALA:HA	2.19	0.42
1:G:51:LYS:HE2	7:G:711:HOH:O	2.20	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:W:299:LEU:O	1:W:339:LYS:NZ	2.37	0.42
1:B:69:GLY:HA3	1:B:119:ASP:OD1	2.19	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:HA	1:A:145:LEU:HD12	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
1:R:107:GLU:OE1	7:R:502:HOH:O	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:32:GLY:HA3	1:V:50:LEU:HD21	2.02	0.42
1:C:133:ASP:O	1:C:137:ASN:ND2	2.36	0.41
1:C:71:PRO:O	1:C:123:GLN:NE2	2.52	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: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:X:72:LEU:HD23	1:X:72:LEU:C	2.41	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: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
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:J:184:LEU:HD23	1:J:220:VAL:HB	2.03	0.41
1:M:175:LEU:CD2	1:M:175:LEU:N	2.73	0.41
1:O:187:HIS:CE1	7:O:509:HOH:O	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:145:LEU:HA	1:Q:145:LEU:HD12	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: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: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:N:205:PHE:O	1:N:209:MET:HG2	2.21	0.41
1:N:286:GLU:OE2	1:O:331:LYS:NZ	2.46	0.41
1:N:124:GLU:HB3	1:Q:47:ARG:HD2	2.01	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:X:250:ARG:HB3	1:X:251:PRO:HD3	2.03	0.41
1:C:252:MET:SD	1:C:252:MET:O	2.78	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:P:66:SER:OG	1:P:117:VAL:HG13	2.21	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:C:230:ARG:HH22	1:C:242:GLU:CD	2.24	0.40
1:H:267:ILE:O	1:H:309:ALA:HA	2.21	0.40
1:K:198:LYS:HE2	1:K:199:TYR:CZ	2.56	0.40
1:L:155:LEU:C	1:L:155:LEU:HD23	2.41	0.40
1:L:163:ILE:HD11	1:L:312:VAL:HG12	2.03	0.40
1:L:64:SER:HB3	7:L:574:HOH:O	2.20	0.40
1:M:168:VAL:HG11	1:M:181:ILE:HD11	2.03	0.40
1:M:31:LYS:HD3	1:U:148:GLU:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:257:LYS:NZ	7:J:521:HOH:O	2.53	0.40
1:A:81:GLY:N	1:A:82:PRO:CD	2.85	0.40
1:E:198:LYS:HE3	1:E:199:TYR:CE2	2.56	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
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:O:246:PHE:O	1:O:247:SER:C	2.59	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:W:72:LEU:HD23	1:W:72:LEU:C	2.42	0.40
1:X:327:MET:HA	1:X:327:MET:HE3	2.03	0.40
1:A:29:ILE:O	1:A:33:GLN:HG3	2.21	0.40
1:C:192:ASP:O	1:C:207:ARG:NH2	2.44	0.40
1:C:49:LYS:O	1:C:53:GLU:HG3	2.21	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	255 (96%)	10 (4%)	33	39
1	B	264/267 (99%)	258 (98%)	6 (2%)	50	59
1	C	266/267 (100%)	249 (94%)	17 (6%)	17	16
1	D	264/267 (99%)	254 (96%)	10 (4%)	33	39
1	E	264/267 (99%)	256 (97%)	8 (3%)	41	50
1	F	265/267 (99%)	258 (97%)	7 (3%)	46	55
1	G	265/267 (99%)	259 (98%)	6 (2%)	50	59
1	H	264/267 (99%)	253 (96%)	11 (4%)	30	34
1	I	264/267 (99%)	256 (97%)	8 (3%)	41	50
1	J	264/267 (99%)	258 (98%)	6 (2%)	50	59
1	K	264/267 (99%)	256 (97%)	8 (3%)	41	50
1	L	264/267 (99%)	255 (97%)	9 (3%)	37	45
1	M	264/267 (99%)	248 (94%)	16 (6%)	18	18
1	N	264/267 (99%)	255 (97%)	9 (3%)	37	45
1	O	264/267 (99%)	249 (94%)	15 (6%)	20	20
1	P	264/267 (99%)	258 (98%)	6 (2%)	50	59
1	Q	264/267 (99%)	254 (96%)	10 (4%)	33	39
1	R	265/267 (99%)	257 (97%)	8 (3%)	41	50
1	S	264/267 (99%)	256 (97%)	8 (3%)	41	50
1	T	265/267 (99%)	256 (97%)	9 (3%)	37	45
1	U	265/267 (99%)	259 (98%)	6 (2%)	50	59
1	V	264/267 (99%)	252 (96%)	12 (4%)	27	31
1	W	264/267 (99%)	250 (95%)	14 (5%)	22	23
1	X	264/267 (99%)	259 (98%)	5 (2%)	57	66
All	All	6344/6408 (99%)	6120 (96%)	224 (4%)	36	43

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	30	GLU
1	A	58	LEU
1	A	66	SER
1	A	127	ASP
1	A	145	LEU

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Mol	Chain	Res	Type
1	A	201	HIS
1	A	204	SER
1	A	234	LYS
1	A	248	LYS
1	B	35	ARG
1	B	145	LEU
1	B	201	HIS
1	B	227	GLN
1	B	244	ARG
1	B	252	MET
1	C	27	SER
1	C	28	SER
1	C	31	LYS
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	201	HIS
1	C	227	GLN
1	C	244	ARG
1	C	252	MET
1	C	262	VAL
1	D	27	SER
1	D	28	SER
1	D	30	GLU
1	D	145	LEU
1	D	150	GLU
1	D	161	HIS
1	D	201	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	201	HIS

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Mol	Chain	Res	Type
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	201	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	201	HIS
1	G	244	ARG
1	H	31	LYS
1	H	35	ARG
1	H	38	ASP
1	H	57	LEU
1	H	134	ARG
1	H	145	LEU
1	H	160	ASP
1	H	161	HIS
1	H	201	HIS
1	H	244	ARG
1	H	318	ARG
1	I	43	LEU
1	I	134	ARG
1	I	145	LEU
1	I	150	GLU
1	I	151	PRO
1	I	161	HIS
1	I	201	HIS
1	I	318	ARG
1	J	30	GLU
1	J	145	LEU
1	J	161	HIS
1	J	201	HIS
1	J	252	MET
1	J	318	ARG
1	K	31	LYS

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Mol	Chain	Res	Type
1	K	145	LEU
1	K	150	GLU
1	K	151	PRO
1	K	161	HIS
1	K	201	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	201	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	89	ILE
1	M	161	HIS
1	M	175	LEU
1	M	193	CYS
1	M	201	HIS
1	M	216	ARG
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	134	ARG
1	N	145	LEU
1	N	151	PRO
1	N	161	HIS
1	N	190	ILE
1	N	201	HIS
1	N	227	GLN
1	N	252	MET
1	N	318	ARG
1	O	28	SER

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Mol	Chain	Res	Type
1	O	43	LEU
1	O	132	ASP
1	O	149	GLU
1	O	150	GLU
1	O	161	HIS
1	O	201	HIS
1	O	223	ARG
1	O	232	GLN
1	O	235	ARG
1	O	248	LYS
1	O	252	MET
1	O	260	GLU
1	O	318	ARG
1	O	339	LYS
1	P	43	LEU
1	P	145	LEU
1	P	161	HIS
1	P	201	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	201	HIS
1	Q	248	LYS
1	Q	252	MET
1	Q	257	LYS
1	Q	318	ARG
1	R	31	LYS
1	R	35	ARG
1	R	66	SER
1	R	145	LEU
1	R	161	HIS
1	R	201	HIS
1	R	257	LYS
1	R	260	GLU
1	S	28	SER
1	S	145	LEU
1	S	151	PRO
1	S	161	HIS

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Mol	Chain	Res	Type
1	S	201	HIS
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	201	HIS
1	T	234	LYS
1	T	252	MET
1	T	318	ARG
1	U	27	SER
1	U	145	LEU
1	U	150	GLU
1	U	161	HIS
1	U	201	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	201	HIS
1	V	224	SER
1	V	234	LYS
1	V	252	MET
1	W	43	LEU
1	W	53	GLU
1	W	54	LEU
1	W	66	SER
1	W	148	GLU
1	W	150	GLU
1	W	161	HIS
1	W	190	ILE
1	W	201	HIS
1	W	215	ARG
1	W	247	SER

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Mol	Chain	Res	Type
1	W	252	MET
1	W	255	ASN
1	W	339	LYS
1	X	30	GLU
1	X	107	GLU
1	X	145	LEU
1	X	161	HIS
1	X	201	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	GLN
1	B	303	GLN
1	F	80	GLN
1	G	137	ASN
1	H	137	ASN
1	J	80	GLN
1	L	303	GLN
1	O	232	GLN
1	Q	255	ASN
1	S	34	ASN
1	V	137	ASN
1	W	227	GLN
1	X	34	ASN
1	X	137	ASN
1	X	255	ASN
1	X	303	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	F	404	-	5,5,5	0.16	0	5,5,5	0.49	0
5	GOL	W	405	-	5,5,5	0.14	0	5,5,5	0.40	0
4	ORN	A	404	-	4,8,8	0.90	0	3,9,9	0.43	0
4	ORN	U	405	-	4,8,8	0.39	0	3,9,9	0.18	0
5	GOL	T	404	-	5,5,5	0.08	0	5,5,5	0.27	0
5	GOL	P	403	-	5,5,5	0.09	0	5,5,5	0.30	0
5	GOL	Q	403	-	5,5,5	0.18	0	5,5,5	0.37	0
5	GOL	B	405	-	5,5,5	0.20	0	5,5,5	0.53	0
5	GOL	H	404	-	5,5,5	0.21	0	5,5,5	0.43	0
5	GOL	I	404	-	5,5,5	0.17	0	5,5,5	0.44	0
6	PEG	L	406	-	6,6,6	0.23	0	5,5,5	0.10	0
5	GOL	L	405	-	5,5,5	0.27	0	5,5,5	0.59	0
5	GOL	J	405	-	5,5,5	0.15	0	5,5,5	0.45	0
4	ORN	K	406	-	4,8,8	1.02	1 (25%)	3,9,9	0.37	0
6	PEG	G	406	-	6,6,6	0.41	0	5,5,5	0.31	0
5	GOL	B	403	-	5,5,5	0.16	0	5,5,5	0.35	0
4	ORN	E	404	-	4,8,8	0.41	0	3,9,9	0.31	0
5	GOL	C	403	-	5,5,5	0.26	0	5,5,5	0.90	0
5	GOL	S	405	-	5,5,5	0.23	0	5,5,5	0.60	0
5	GOL	L	403	-	5,5,5	0.20	0	5,5,5	0.36	0
5	GOL	K	403	-	5,5,5	0.17	0	5,5,5	0.46	0
5	GOL	N	403	-	5,5,5	0.15	0	5,5,5	0.40	0
5	GOL	D	405	-	5,5,5	0.22	0	5,5,5	0.50	0
5	GOL	G	405	-	5,5,5	0.25	0	5,5,5	0.51	0
5	GOL	G	408	-	5,5,5	0.17	0	5,5,5	0.49	0
5	GOL	E	405	-	5,5,5	0.09	0	5,5,5	0.30	0
5	GOL	U	403	-	5,5,5	0.17	0	5,5,5	0.41	0
5	GOL	K	405	-	5,5,5	0.17	0	5,5,5	0.52	0
4	ORN	G	404	-	4,8,8	0.31	0	3,9,9	0.39	0
5	GOL	R	404	-	5,5,5	0.11	0	5,5,5	0.29	0
4	ORN	V	404	-	4,8,8	0.35	0	3,9,9	0.35	0
5	GOL	W	403	-	5,5,5	0.17	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	L	408	-	6,6,6	0.14	0	5,5,5	0.21	0
4	ORN	C	405	-	4,8,8	0.50	0	3,9,9	0.36	0
4	ORN	P	405	-	4,8,8	0.87	0	3,9,9	0.43	0
5	GOL	I	405	-	5,5,5	0.09	0	5,5,5	0.35	0
5	GOL	D	403	-	5,5,5	0.13	0	5,5,5	0.30	0
5	GOL	J	404	-	5,5,5	0.31	0	5,5,5	0.55	0
5	GOL	H	403	-	5,5,5	0.13	0	5,5,5	0.32	0
4	ORN	F	405	-	4,8,8	0.36	0	3,9,9	0.24	0
6	PEG	G	407	-	6,6,6	0.39	0	5,5,5	0.26	0
6	PEG	L	407	-	6,6,6	0.18	0	5,5,5	0.14	0
5	GOL	S	403	-	5,5,5	0.12	0	5,5,5	0.43	0
5	GOL	E	406	-	5,5,5	0.17	0	5,5,5	0.43	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	F	404	-	-	2/4/4/4	-
5	GOL	W	405	-	-	2/4/4/4	-
4	ORN	A	404	-	-	0/4/8/8	-
4	ORN	U	405	-	-	0/4/8/8	-
5	GOL	T	404	-	-	4/4/4/4	-
5	GOL	P	403	-	-	4/4/4/4	-
5	GOL	Q	403	-	-	4/4/4/4	-
5	GOL	B	405	-	-	2/4/4/4	-
5	GOL	H	404	-	-	0/4/4/4	-
5	GOL	I	404	-	-	0/4/4/4	-
6	PEG	L	406	-	-	3/4/4/4	-
5	GOL	L	405	-	-	0/4/4/4	-
5	GOL	J	405	-	-	2/4/4/4	-
4	ORN	K	406	-	-	0/4/8/8	-
6	PEG	G	406	-	-	2/4/4/4	-
5	GOL	B	403	-	-	2/4/4/4	-
4	ORN	E	404	-	-	0/4/8/8	-
5	GOL	C	403	-	-	3/4/4/4	-
5	GOL	S	405	-	-	2/4/4/4	-
5	GOL	L	403	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	K	403	-	-	2/4/4/4	-
5	GOL	N	403	-	-	2/4/4/4	-
5	GOL	D	405	-	-	0/4/4/4	-
5	GOL	G	405	-	-	2/4/4/4	-
5	GOL	G	408	-	-	1/4/4/4	-
5	GOL	E	405	-	-	2/4/4/4	-
5	GOL	U	403	-	-	0/4/4/4	-
5	GOL	K	405	-	-	1/4/4/4	-
4	ORN	G	404	-	-	0/4/8/8	-
5	GOL	R	404	-	-	4/4/4/4	-
4	ORN	V	404	-	-	1/4/8/8	-
5	GOL	W	403	-	-	4/4/4/4	-
6	PEG	L	408	-	-	0/4/4/4	-
4	ORN	C	405	-	-	0/4/8/8	-
4	ORN	P	405	-	-	0/4/8/8	-
5	GOL	I	405	-	-	4/4/4/4	-
5	GOL	D	403	-	-	2/4/4/4	-
5	GOL	J	404	-	-	0/4/4/4	-
5	GOL	H	403	-	-	1/4/4/4	-
4	ORN	F	405	-	-	1/4/8/8	-
6	PEG	G	407	-	-	2/4/4/4	-
6	PEG	L	407	-	-	1/4/4/4	-
5	GOL	S	403	-	-	2/4/4/4	-
5	GOL	E	406	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	406	ORN	CA-N	2.01	1.51	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	S	405	GOL	O1-C1-C2-C3
5	T	404	GOL	O1-C1-C2-O2
5	T	404	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	T	404	GOL	C1-C2-C3-O3
5	J	405	GOL	O1-C1-C2-O2
5	J	405	GOL	O1-C1-C2-C3
5	N	403	GOL	O1-C1-C2-O2
5	N	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	D	403	GOL	C1-C2-C3-O3
5	E	406	GOL	O1-C1-C2-O2
5	E	406	GOL	O1-C1-C2-C3
5	K	403	GOL	O1-C1-C2-C3
5	E	405	GOL	O1-C1-C2-C3
5	S	403	GOL	O1-C1-C2-C3
5	W	403	GOL	O1-C1-C2-O2
5	W	403	GOL	C1-C2-C3-O3
5	P	403	GOL	O1-C1-C2-C3
5	C	403	GOL	O1-C1-C2-C3
5	I	405	GOL	C1-C2-C3-O3
5	S	405	GOL	O1-C1-C2-O2
5	S	403	GOL	O1-C1-C2-O2
5	W	405	GOL	O1-C1-C2-C3
5	B	405	GOL	O1-C1-C2-C3
5	B	403	GOL	O1-C1-C2-C3
5	E	406	GOL	C1-C2-C3-O3
5	W	403	GOL	O1-C1-C2-C3
5	F	404	GOL	C1-C2-C3-O3
5	P	403	GOL	C1-C2-C3-O3
5	Q	403	GOL	O1-C1-C2-C3
5	Q	403	GOL	C1-C2-C3-O3
5	G	405	GOL	O1-C1-C2-C3
5	I	405	GOL	O1-C1-C2-C3
5	T	404	GOL	O2-C2-C3-O3
5	R	404	GOL	O2-C2-C3-O3
5	D	403	GOL	O2-C2-C3-O3
5	K	403	GOL	O1-C1-C2-O2
5	E	405	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	C	403	GOL	O1-C1-C2-O2
5	G	405	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	I	405	GOL	O2-C2-C3-O3
4	V	404	ORN	CA-CB-CG-CD
6	L	407	PEG	O2-C3-C4-O4
6	L	406	PEG	O1-C1-C2-O2
6	L	406	PEG	O2-C3-C4-O4
6	G	407	PEG	O1-C1-C2-O2
5	B	405	GOL	O1-C1-C2-O2
5	W	403	GOL	O2-C2-C3-O3
5	L	403	GOL	O1-C1-C2-O2
5	H	403	GOL	O2-C2-C3-O3
5	Q	403	GOL	O2-C2-C3-O3
6	G	406	PEG	C4-C3-O2-C2
5	C	403	GOL	O2-C2-C3-O3
6	L	406	PEG	C4-C3-O2-C2
6	G	406	PEG	C1-C2-O2-C3
5	W	405	GOL	O1-C1-C2-O2
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
5	L	403	GOL	C1-C2-C3-O3
5	G	408	GOL	O1-C1-C2-C3
5	L	403	GOL	O2-C2-C3-O3
5	K	405	GOL	O2-C2-C3-O3
6	G	407	PEG	C1-C2-O2-C3
5	L	403	GOL	O1-C1-C2-C3
4	F	405	ORN	N-CA-CB-CG

There are no ring outliers.

14 monomers are involved in 20 short contacts:

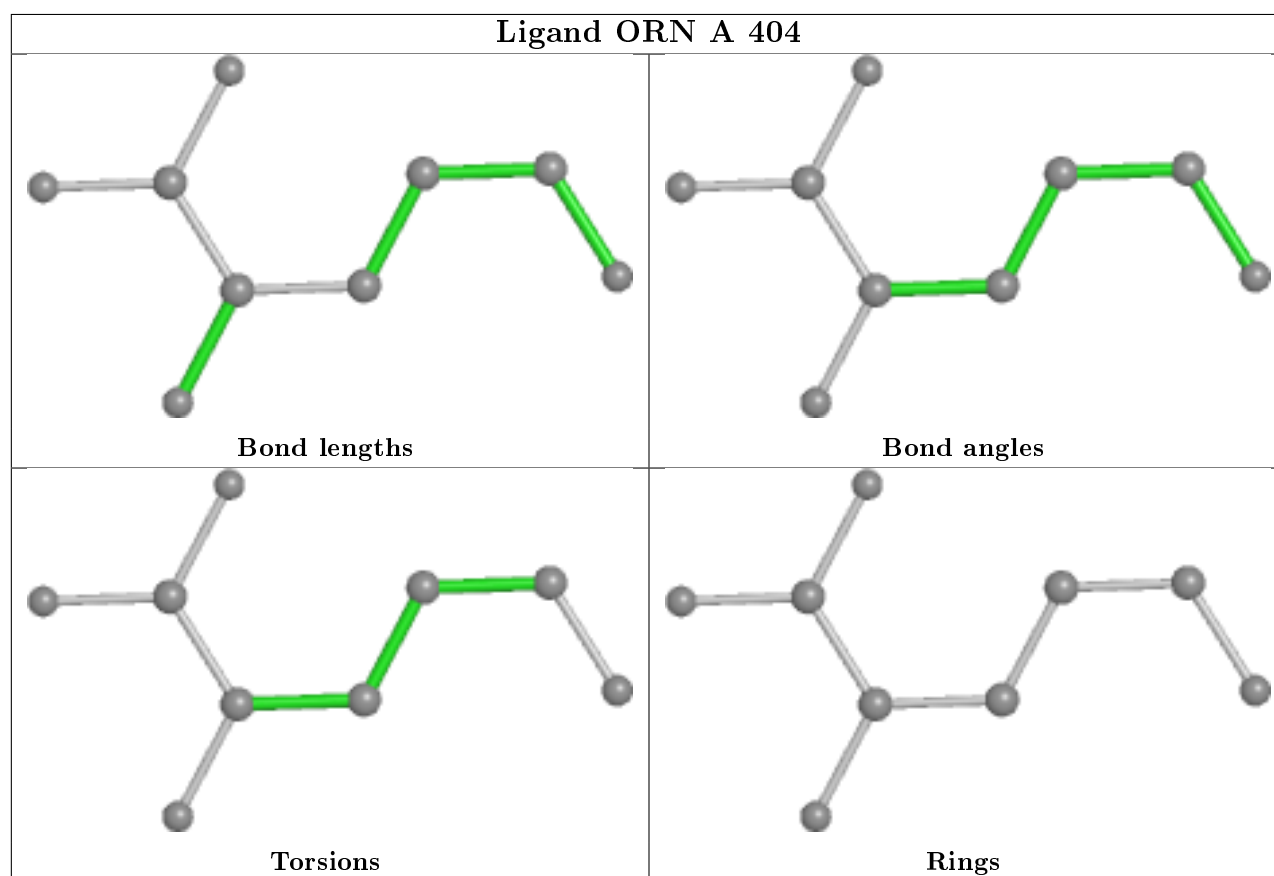
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	U	405	ORN	3	0
5	J	405	GOL	1	0
4	E	404	ORN	1	0
5	C	403	GOL	3	0
5	G	408	GOL	1	0
5	K	405	GOL	1	0
4	G	404	ORN	1	0
5	R	404	GOL	1	0
4	V	404	ORN	1	0
6	L	408	PEG	1	0

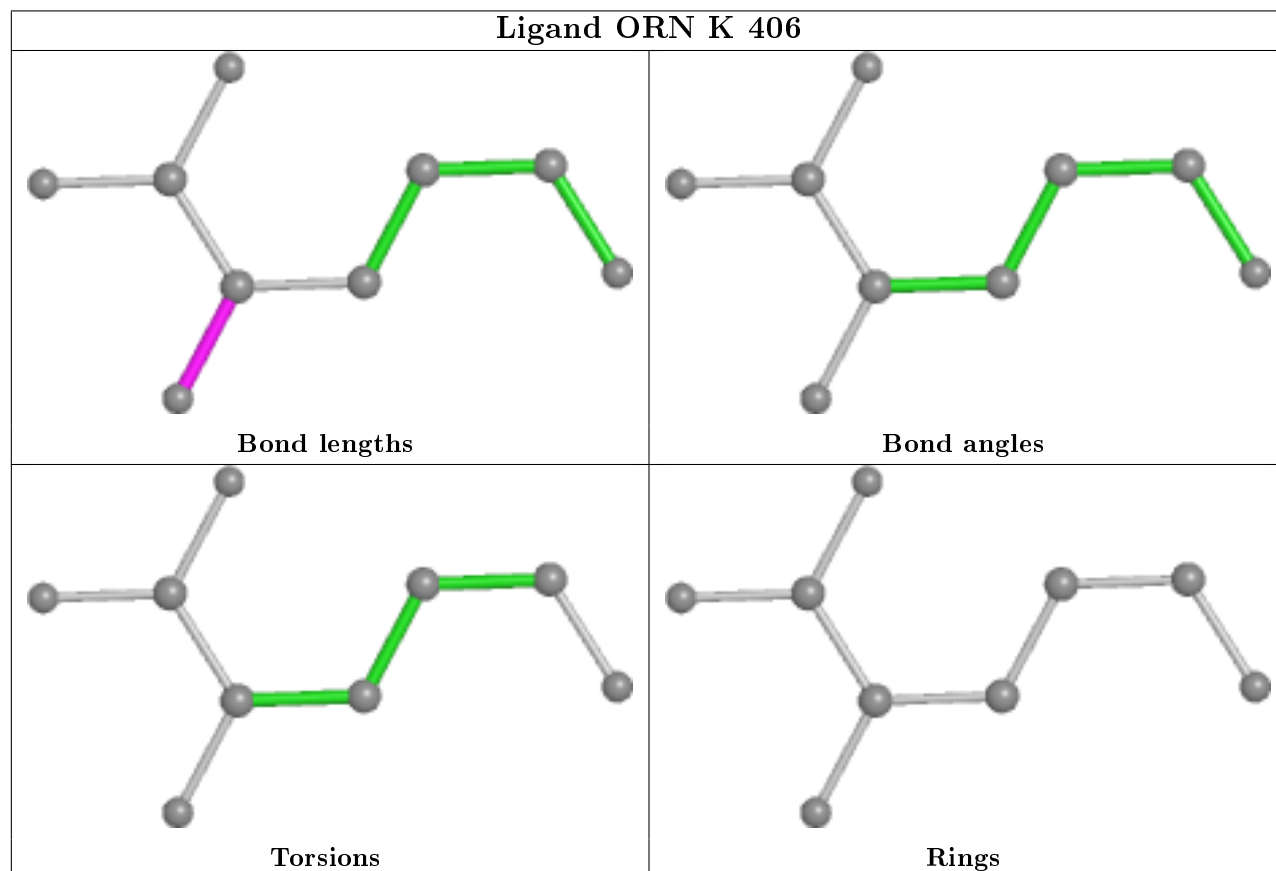
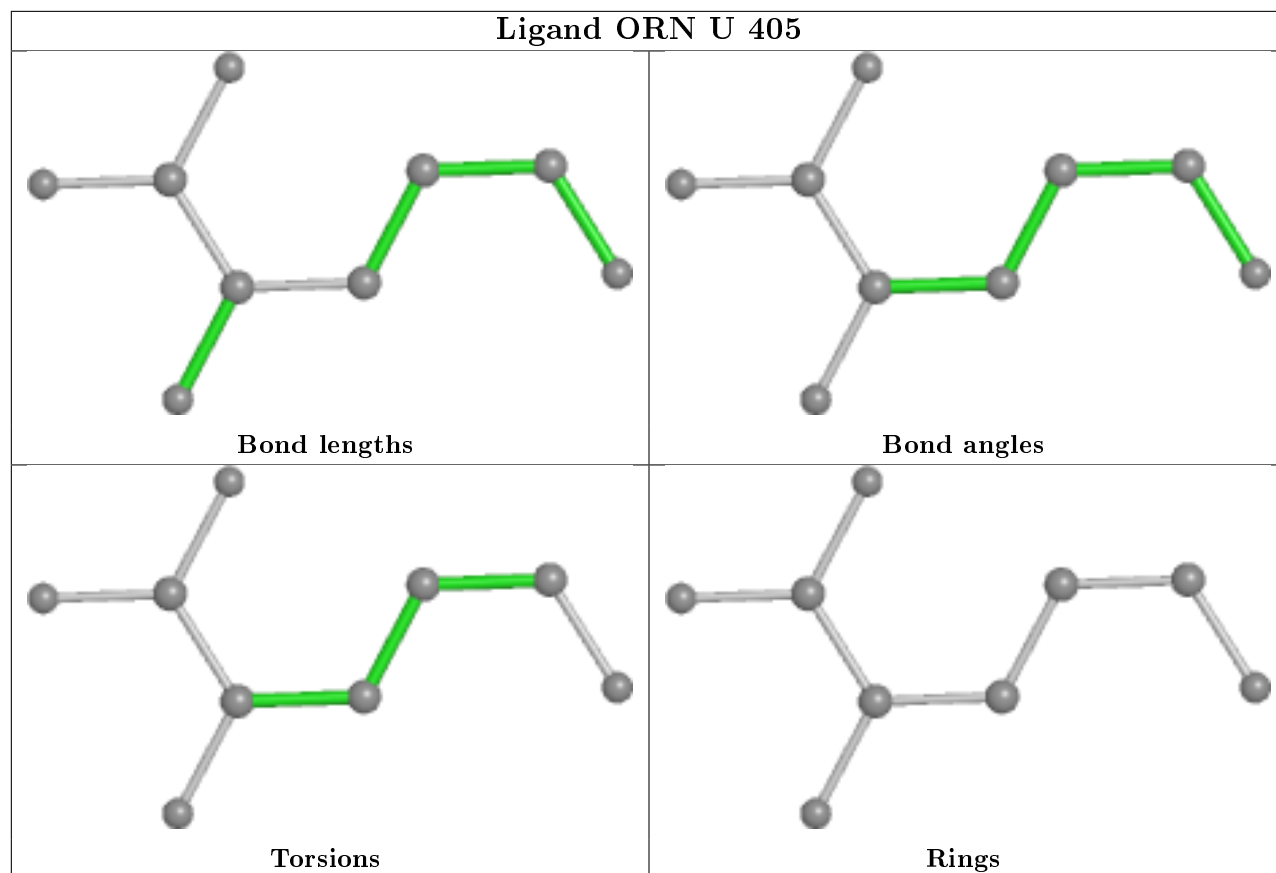
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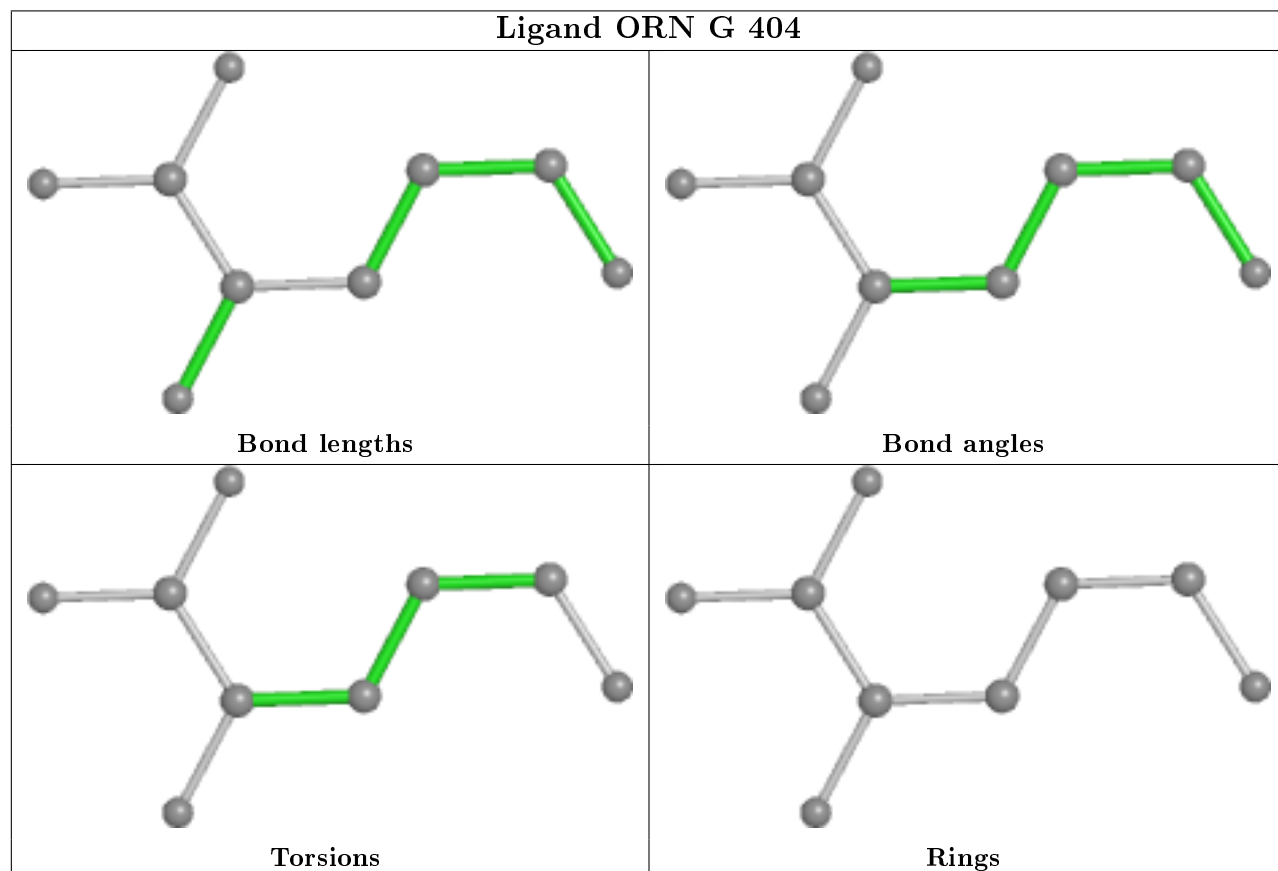
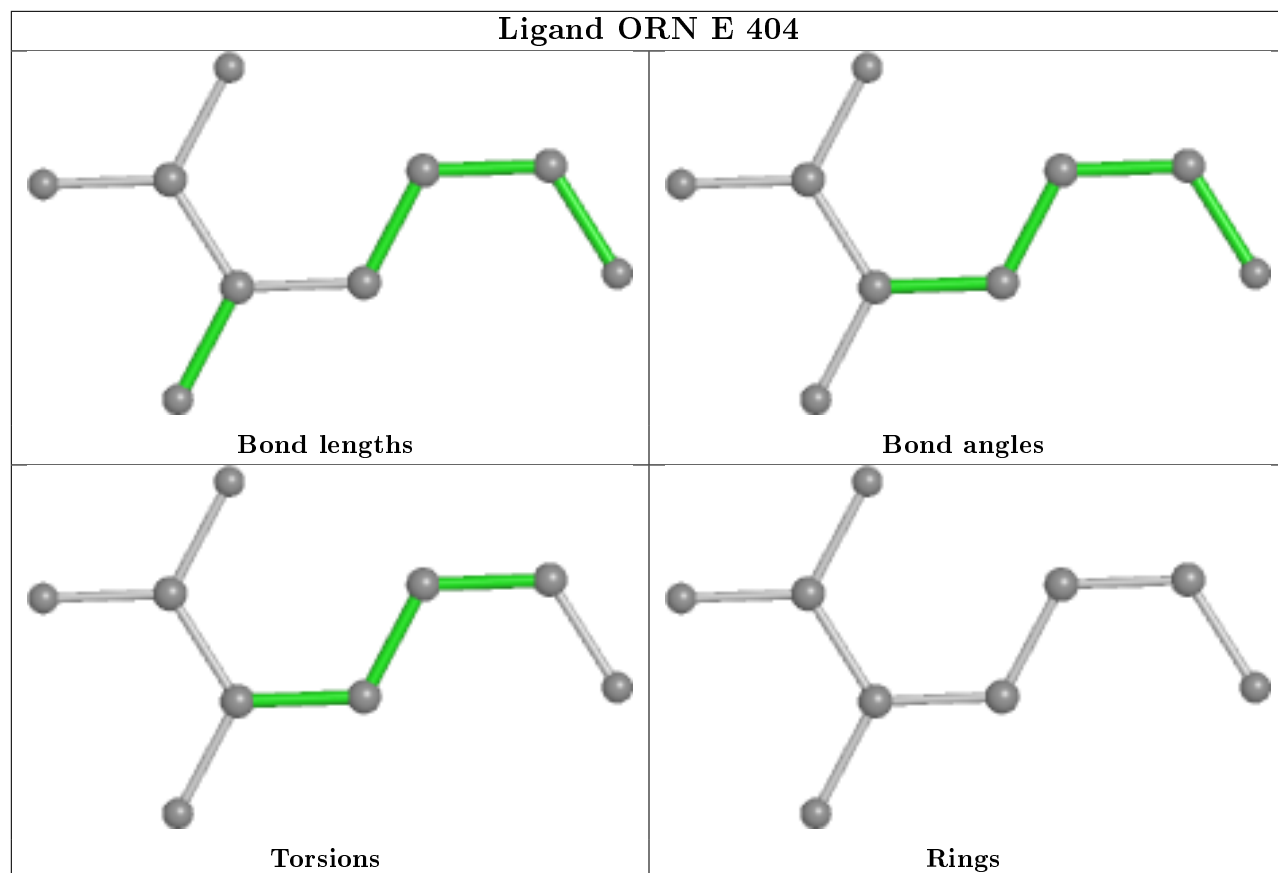
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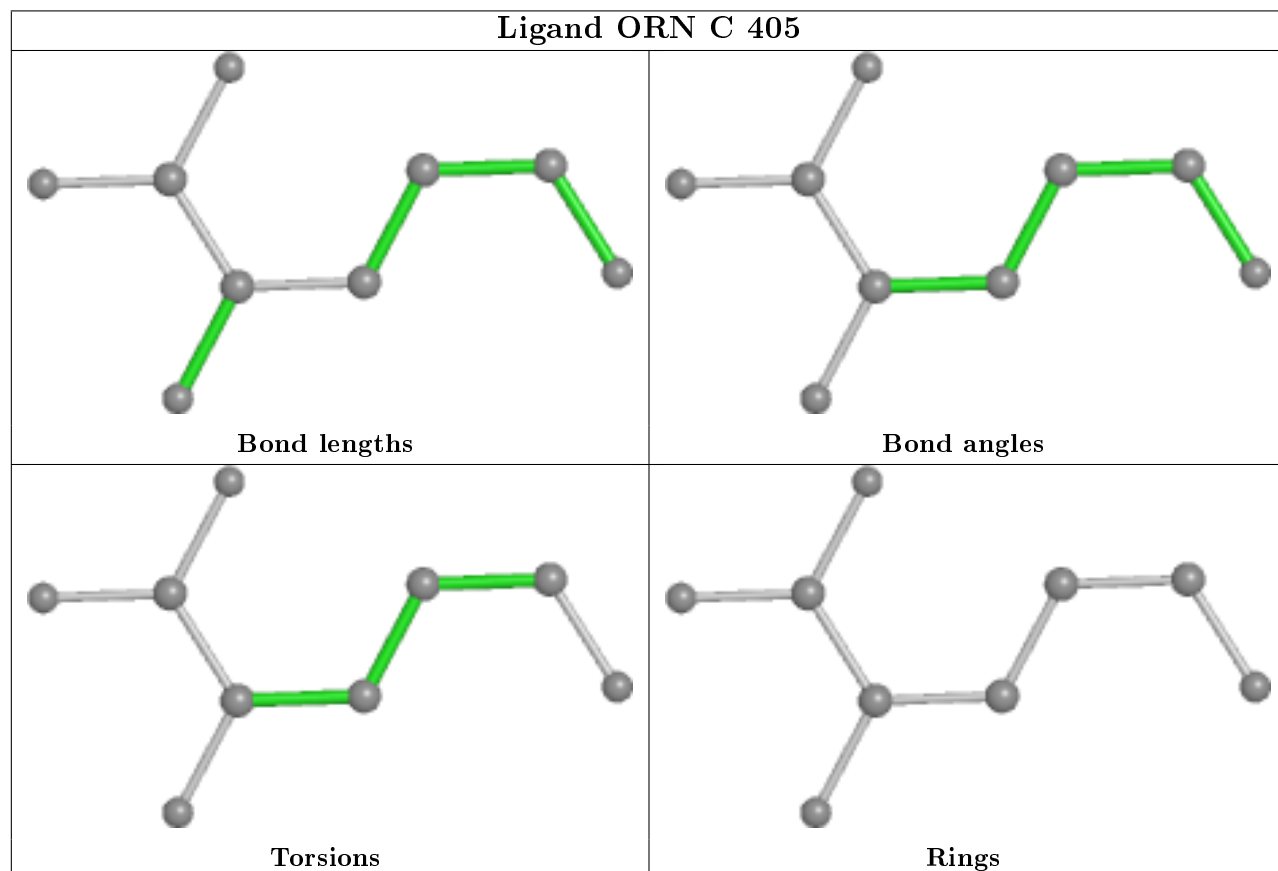
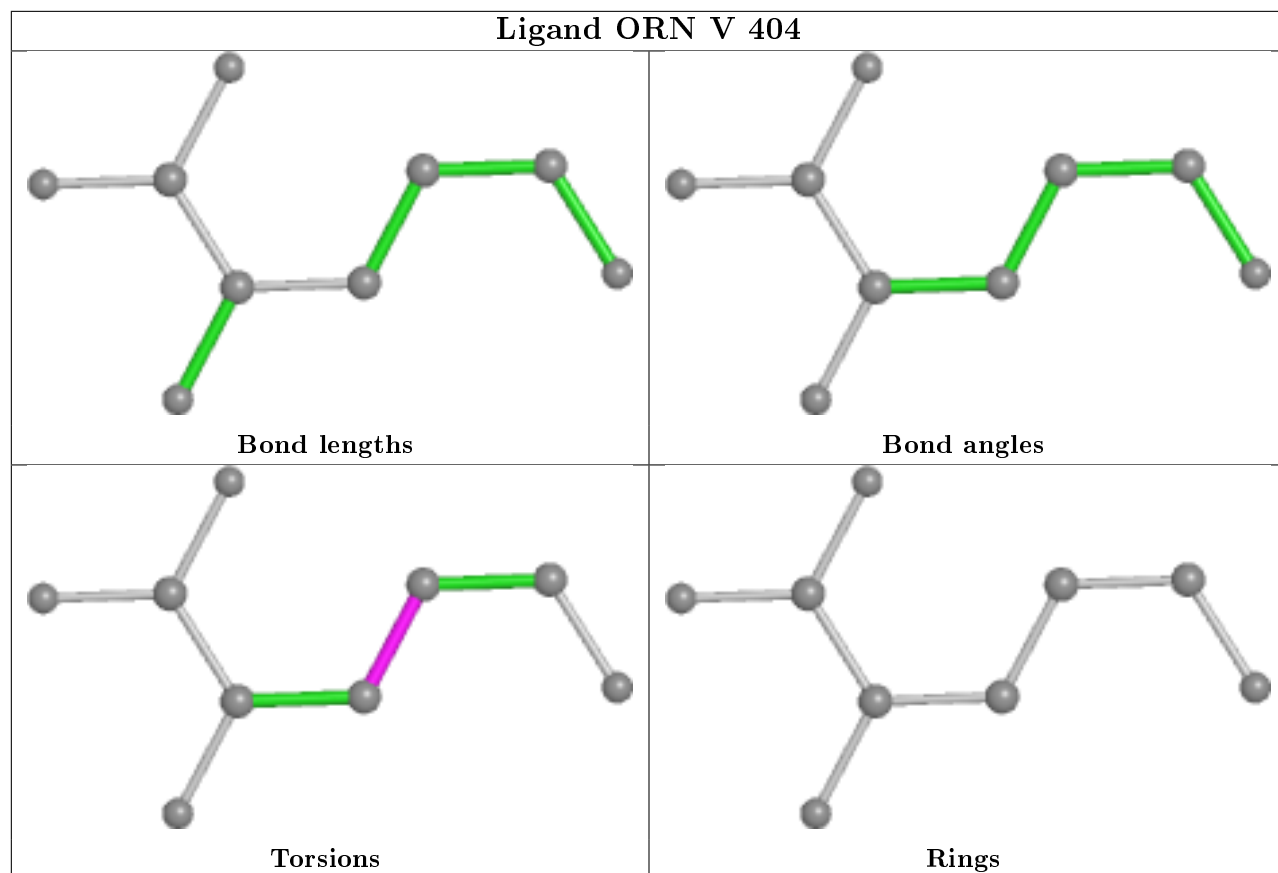
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	405	ORN	1	0
4	P	405	ORN	2	0
4	F	405	ORN	1	0
6	L	407	PEG	2	0

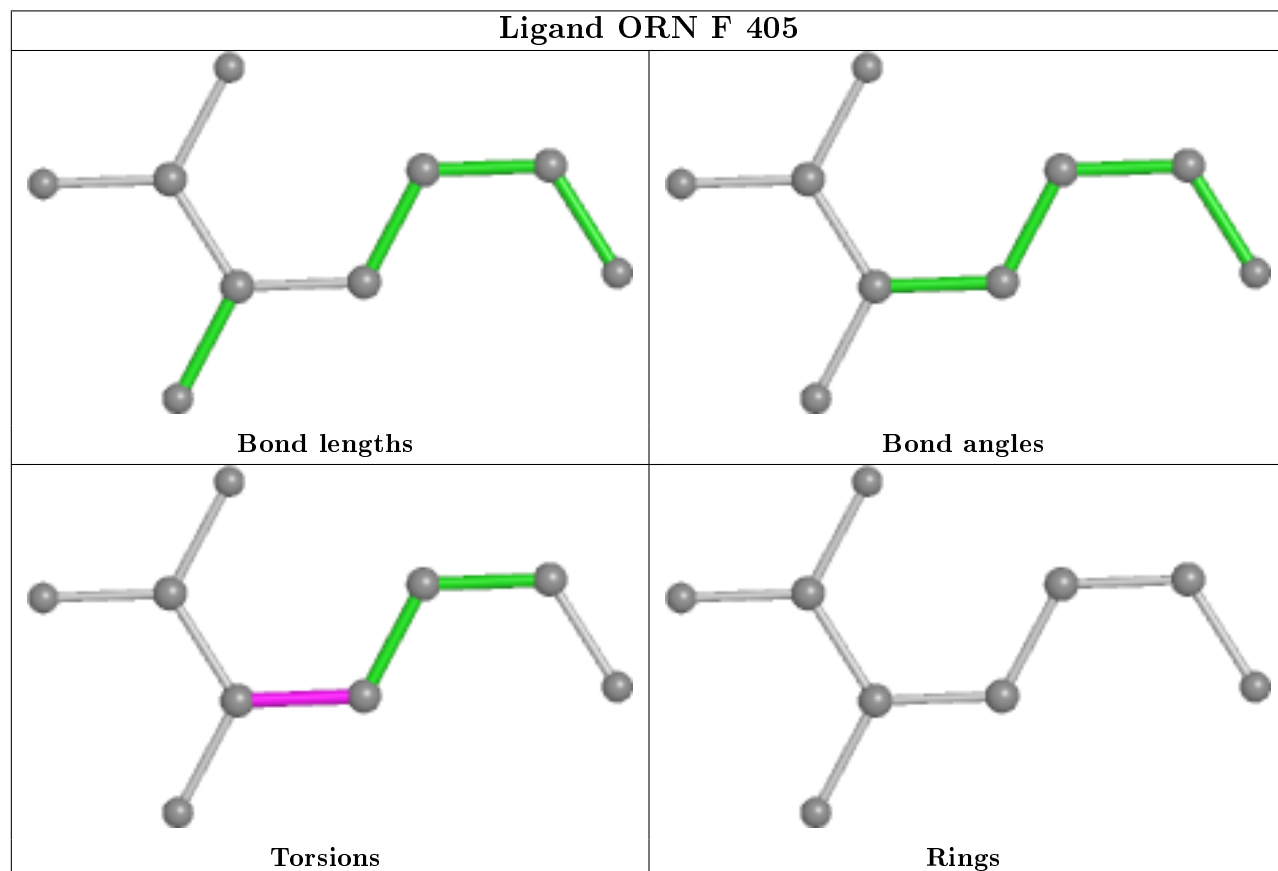
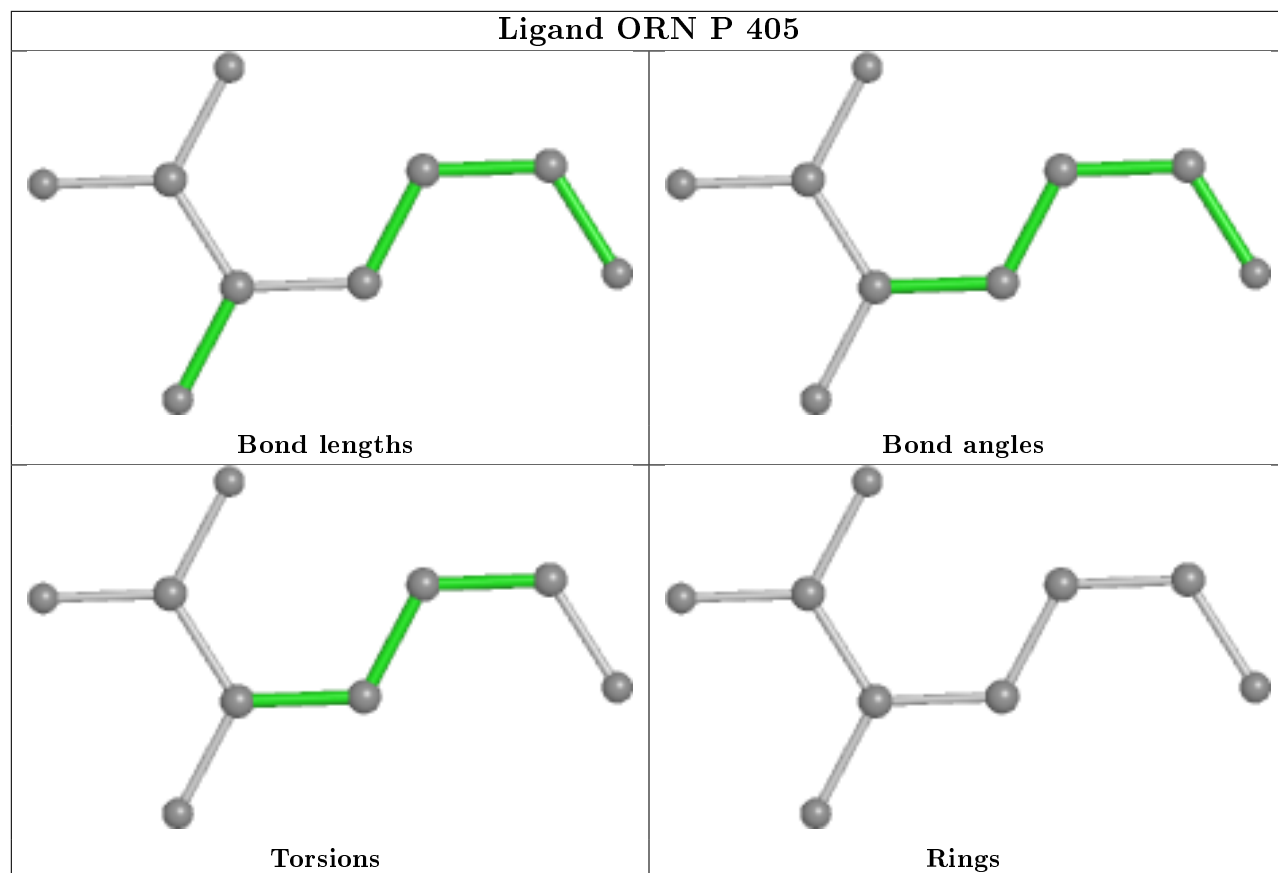
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	316/321 (98%)	0.03	14 (4%) 34 37	25, 54, 91, 116	0
1	B	317/321 (98%)	-0.53	3 (0%) 84 85	21, 33, 56, 95	0
1	C	316/321 (98%)	0.17	15 (4%) 31 34	26, 59, 84, 125	0
1	D	316/321 (98%)	-0.58	0 100 100	18, 31, 54, 96	0
1	E	318/321 (99%)	-0.60	4 (1%) 77 79	16, 24, 38, 86	0
1	F	316/321 (98%)	-0.55	2 (0%) 89 89	18, 31, 53, 80	0
1	G	316/321 (98%)	-0.67	0 100 100	15, 25, 40, 58	0
1	H	317/321 (98%)	-0.53	2 (0%) 89 89	17, 31, 54, 69	0
1	I	316/321 (98%)	-0.61	0 100 100	17, 32, 53, 78	0
1	J	317/321 (98%)	-0.62	3 (0%) 84 85	17, 25, 40, 93	0
1	K	316/321 (98%)	-0.55	2 (0%) 89 89	20, 33, 51, 82	0
1	L	317/321 (98%)	-0.46	4 (1%) 77 79	20, 36, 57, 74	0
1	M	316/321 (98%)	0.50	31 (9%) 7 8	38, 74, 117, 145	0
1	N	316/321 (98%)	-0.39	4 (1%) 77 79	26, 43, 66, 93	0
1	O	316/321 (98%)	0.43	39 (12%) 4 3	32, 69, 106, 124	0
1	P	316/321 (98%)	-0.36	6 (1%) 66 69	24, 43, 73, 115	0
1	Q	316/321 (98%)	-0.48	3 (0%) 84 85	22, 38, 61, 94	0
1	R	316/321 (98%)	-0.38	3 (0%) 84 85	22, 39, 64, 118	0
1	S	316/321 (98%)	-0.36	7 (2%) 62 65	23, 40, 67, 95	0
1	T	318/321 (99%)	-0.37	3 (0%) 84 85	22, 41, 63, 88	0
1	U	316/321 (98%)	-0.21	9 (2%) 53 55	23, 46, 77, 117	0
1	V	316/321 (98%)	0.33	21 (6%) 18 20	38, 59, 79, 90	0
1	W	317/321 (98%)	0.27	28 (8%) 10 11	29, 63, 92, 103	0
1	X	316/321 (98%)	-0.27	4 (1%) 77 79	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%)	-0.28	207 (2%) 54 57	15, 40, 81, 145	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	29	ILE	6.7
1	O	234	LYS	6.1
1	E	26	ALA	6.1
1	M	57	LEU	5.9
1	A	58	LEU	5.9
1	V	177	GLY	5.8
1	T	25	SER	5.6
1	O	29	ILE	5.1
1	A	57	LEU	4.8
1	O	196	GLY	4.7
1	Q	29	ILE	4.6
1	J	26	ALA	4.6
1	M	177	GLY	4.5
1	T	26	ALA	4.5
1	V	29	ILE	4.4
1	M	60	GLY	4.1
1	O	58	LEU	4.1
1	M	61	ALA	4.1
1	M	263	LYS	4.1
1	U	60	GLY	4.0
1	A	59	GLY	3.9
1	O	30	GLU	3.9
1	V	27	SER	3.9
1	O	175	LEU	3.9
1	V	176	GLY	3.8
1	U	27	SER	3.8
1	W	60	GLY	3.8
1	W	227	GLN	3.8
1	R	27	SER	3.8
1	H	29	ILE	3.7
1	C	30	GLU	3.7
1	O	257	LYS	3.7
1	O	259	GLY	3.7
1	O	176	GLY	3.6
1	W	234	LYS	3.6
1	O	57	LEU	3.6
1	C	28	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	V	257	LYS	3.6
1	W	257	LYS	3.5
1	V	252	MET	3.5
1	P	29	ILE	3.5
1	M	269	ILE	3.4
1	O	54	LEU	3.4
1	U	29	ILE	3.4
1	W	29	ILE	3.4
1	M	62	LYS	3.4
1	W	27	SER	3.4
1	B	27	SER	3.4
1	A	60	GLY	3.4
1	O	129	GLY	3.4
1	A	269	ILE	3.4
1	P	28	SER	3.3
1	V	55	VAL	3.3
1	M	176	GLY	3.3
1	M	29	ILE	3.3
1	W	26	ALA	3.3
1	M	312	VAL	3.3
1	E	25	SER	3.2
1	M	175	LEU	3.2
1	V	57	LEU	3.2
1	A	176	GLY	3.2
1	W	59	GLY	3.2
1	B	26	ALA	3.2
1	P	31	LYS	3.2
1	O	195	GLU	3.2
1	V	30	GLU	3.2
1	M	257	LYS	3.2
1	W	269	ILE	3.1
1	A	312	VAL	3.1
1	O	227	GLN	3.1
1	X	57	LEU	3.1
1	M	137	ASN	3.1
1	C	193	CYS	3.1
1	O	236	PHE	3.1
1	S	29	ILE	3.1
1	E	27	SER	3.0
1	S	30	GLU	3.0
1	M	56	ARG	3.0
1	S	31	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	O	178	PRO	3.0
1	V	267	ILE	3.0
1	W	252	MET	2.9
1	O	199	TYR	2.9
1	S	60	GLY	2.9
1	Q	27	SER	2.9
1	M	55	VAL	2.9
1	N	29	ILE	2.9
1	A	193	CYS	2.9
1	O	193	CYS	2.9
1	W	312	VAL	2.9
1	S	28	SER	2.9
1	M	260	GLU	2.9
1	P	57	LEU	2.9
1	S	27	SER	2.8
1	O	255	ASN	2.8
1	N	27	SER	2.8
1	V	312	VAL	2.8
1	M	27	SER	2.8
1	W	268	SER	2.8
1	L	27	SER	2.7
1	X	28	SER	2.7
1	O	252	MET	2.7
1	O	231	GLU	2.7
1	F	29	ILE	2.7
1	V	269	ILE	2.7
1	C	309	ALA	2.7
1	R	29	ILE	2.7
1	W	303	GLN	2.7
1	U	28	SER	2.7
1	O	301	ASN	2.7
1	W	231	GLU	2.7
1	C	34	ASN	2.7
1	M	54	LEU	2.7
1	M	58	LEU	2.7
1	V	234	LYS	2.6
1	W	57	LEU	2.6
1	C	252	MET	2.6
1	W	176	GLY	2.6
1	N	57	LEU	2.6
1	O	194	PHE	2.6
1	C	227	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	V	309	ALA	2.6
1	C	269	ILE	2.6
1	M	30	GLU	2.5
1	M	255	ASN	2.5
1	J	27	SER	2.5
1	C	27	SER	2.5
1	S	57	LEU	2.5
1	O	171	VAL	2.5
1	U	269	ILE	2.5
1	O	268	SER	2.4
1	O	241	TYR	2.4
1	U	176	GLY	2.4
1	X	269	ILE	2.4
1	U	156	VAL	2.4
1	B	29	ILE	2.4
1	M	234	LYS	2.4
1	R	30	GLU	2.4
1	U	131	ASP	2.4
1	A	29	ILE	2.4
1	W	58	LEU	2.4
1	C	195	GLU	2.4
1	A	54	LEU	2.4
1	M	178	PRO	2.4
1	O	251	PRO	2.4
1	M	248	LYS	2.4
1	O	263	LYS	2.4
1	O	177	GLY	2.4
1	J	28	SER	2.4
1	T	29	ILE	2.3
1	W	309	ALA	2.3
1	M	192	ASP	2.3
1	F	30	GLU	2.3
1	L	29	ILE	2.3
1	O	260	GLU	2.3
1	X	29	ILE	2.3
1	O	312	VAL	2.3
1	K	29	ILE	2.3
1	L	26	ALA	2.3
1	W	248	LYS	2.3
1	W	28	SER	2.3
1	C	57	LEU	2.3
1	W	175	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	V	194	PHE	2.3
1	C	60	GLY	2.2
1	U	129	GLY	2.2
1	W	193	CYS	2.2
1	W	156	VAL	2.2
1	M	134	ARG	2.2
1	M	268	SER	2.2
1	O	237	GLY	2.2
1	A	28	SER	2.2
1	C	196	GLY	2.2
1	H	32	GLY	2.2
1	O	60	GLY	2.2
1	O	269	ILE	2.2
1	M	252	MET	2.2
1	M	195	GLU	2.2
1	V	311	VAL	2.2
1	P	30	GLU	2.1
1	A	129	GLY	2.1
1	V	60	GLY	2.1
1	W	62	LYS	2.1
1	E	29	ILE	2.1
1	W	261	GLY	2.1
1	M	133	ASP	2.1
1	V	127	ASP	2.1
1	O	271	VAL	2.1
1	W	55	VAL	2.1
1	P	59	GLY	2.1
1	W	271	VAL	2.1
1	L	28	SER	2.1
1	M	172	SER	2.1
1	O	27	SER	2.1
1	O	264	GLY	2.1
1	V	248	LYS	2.1
1	A	184	LEU	2.1
1	W	255	ASN	2.1
1	A	61	ALA	2.1
1	N	30	GLU	2.0
1	Q	267	ILE	2.0
1	V	184	LEU	2.0
1	K	28	SER	2.0
1	O	235	ARG	2.0
1	O	238	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	V	36	VAL	2.0
1	C	267	ILE	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 monosaccharides 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(\AA^2)	Q<0.9
4	ORN	V	404	9/9	0.57	0.36	45,56,67,68	9
4	ORN	C	405	9/9	0.62	0.26	56,58,67,68	0
4	ORN	P	405	9/9	0.68	0.27	52,57,70,73	0
5	GOL	W	405	6/6	0.69	0.24	70,72,78,79	0
4	ORN	K	406	9/9	0.73	0.19	42,49,53,54	0
5	GOL	E	406	6/6	0.75	0.17	69,73,74,75	0
6	PEG	G	406	7/7	0.78	0.19	62,65,68,69	0
4	ORN	E	404	9/9	0.80	0.21	50,55,58,61	0
2	MN	O	401	1/1	0.80	0.08	57,57,57,57	0
6	PEG	L	406	7/7	0.81	0.15	57,66,78,79	0
6	PEG	G	407	7/7	0.81	0.18	52,59,63,64	0
5	GOL	H	404	6/6	0.82	0.17	51,57,62,62	0
4	ORN	F	405	9/9	0.82	0.21	45,52,60,61	0
4	ORN	U	405	9/9	0.83	0.21	55,58,70,74	0
5	GOL	K	405	6/6	0.84	0.32	50,58,64,66	0
5	GOL	C	403	6/6	0.84	0.22	53,57,65,66	0
6	PEG	L	408	7/7	0.85	0.18	71,73,75,75	0
5	GOL	S	403	6/6	0.85	0.23	54,70,72,73	0
5	GOL	F	404	6/6	0.85	0.24	54,59,61,70	0
5	GOL	W	403	6/6	0.86	0.18	55,64,68,71	0
5	GOL	J	404	6/6	0.86	0.17	33,40,45,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	Q	403	6/6	0.86	0.18	45,58,62,62	0
4	ORN	G	404	9/9	0.87	0.17	48,53,57,58	0
5	GOL	N	403	6/6	0.87	0.16	61,65,73,74	0
4	ORN	A	404	9/9	0.87	0.14	41,48,58,60	0
2	MN	O	402	1/1	0.87	0.10	63,63,63,63	0
5	GOL	L	403	6/6	0.87	0.18	40,51,55,55	0
5	GOL	G	408	6/6	0.87	0.19	53,62,67,68	0
5	GOL	B	403	6/6	0.87	0.14	50,57,61,64	0
5	GOL	J	405	6/6	0.88	0.23	49,51,55,57	0
5	GOL	H	403	6/6	0.89	0.16	49,56,59,67	0
5	GOL	P	403	6/6	0.91	0.18	61,65,67,75	0
5	GOL	L	405	6/6	0.91	0.18	42,49,53,56	0
2	MN	C	402	1/1	0.91	0.04	48,48,48,48	0
3	NA	O	403	1/1	0.91	0.17	62,62,62,62	0
5	GOL	S	405	6/6	0.91	0.20	54,57,60,61	0
5	GOL	K	403	6/6	0.91	0.14	56,66,67,76	0
5	GOL	E	405	6/6	0.92	0.17	37,48,51,58	0
5	GOL	U	403	6/6	0.92	0.13	47,51,56,56	0
5	GOL	R	404	6/6	0.92	0.27	59,61,63,66	0
5	GOL	D	403	6/6	0.93	0.14	46,55,56,61	0
5	GOL	I	405	6/6	0.93	0.36	55,59,61,62	0
5	GOL	I	404	6/6	0.93	0.14	51,53,56,57	0
3	NA	C	404	1/1	0.94	0.20	44,44,44,44	0
3	NA	M	403	1/1	0.94	0.12	50,50,50,50	0
2	MN	C	401	1/1	0.94	0.11	45,45,45,45	0
5	GOL	G	405	6/6	0.94	0.15	34,38,39,41	0
6	PEG	L	407	7/7	0.95	0.18	52,55,61,61	0
3	NA	W	404	1/1	0.95	0.14	47,47,47,47	0
5	GOL	D	405	6/6	0.95	0.10	36,41,46,47	0
3	NA	Q	404	1/1	0.95	0.08	33,33,33,33	0
5	GOL	B	405	6/6	0.96	0.14	41,45,46,48	0
5	GOL	T	404	6/6	0.96	0.13	55,60,62,67	0
3	NA	N	404	1/1	0.97	0.20	38,38,38,38	0
3	NA	X	403	1/1	0.97	0.10	39,39,39,39	0
2	MN	W	402	1/1	0.97	0.05	49,49,49,49	0
2	MN	V	402	1/1	0.98	0.04	48,48,48,48	0
2	MN	W	401	1/1	0.98	0.03	48,48,48,48	0
2	MN	M	401	1/1	0.98	0.06	45,45,45,45	0
3	NA	T	403	1/1	0.98	0.08	38,38,38,38	0
3	NA	H	405	1/1	0.98	0.07	34,34,34,34	0
3	NA	S	404	1/1	0.98	0.16	42,42,42,42	0
2	MN	V	401	1/1	0.98	0.05	42,42,42,42	0

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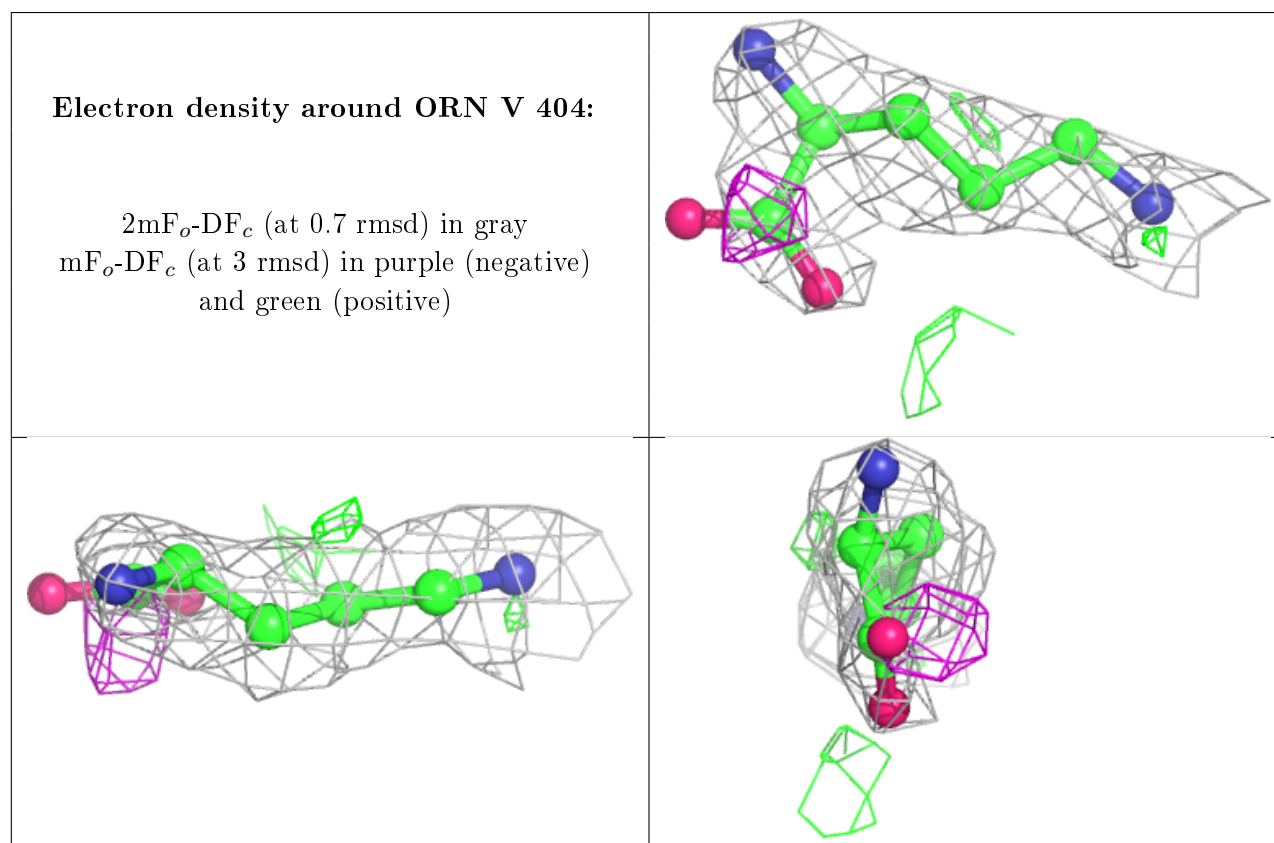
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	V	403	1/1	0.98	0.15	38,38,38,38	0
3	NA	U	404	1/1	0.98	0.27	44,44,44,44	0
3	NA	I	403	1/1	0.98	0.07	33,33,33,33	0
2	MN	T	401	1/1	0.98	0.07	31,31,31,31	0
3	NA	B	404	1/1	0.98	0.07	31,31,31,31	0
3	NA	P	404	1/1	0.98	0.06	43,43,43,43	0
3	NA	A	403	1/1	0.99	0.10	34,34,34,34	0
3	NA	L	404	1/1	0.99	0.09	36,36,36,36	0
3	NA	E	403	1/1	0.99	0.07	32,32,32,32	0
2	MN	M	402	1/1	0.99	0.04	54,54,54,54	0
2	MN	U	401	1/1	0.99	0.08	32,32,32,32	0
2	MN	N	401	1/1	0.99	0.07	35,35,35,35	0
2	MN	B	402	1/1	0.99	0.07	36,36,36,36	0
3	NA	F	403	1/1	0.99	0.06	30,30,30,30	0
3	NA	G	403	1/1	0.99	0.12	29,29,29,29	0
2	MN	S	402	1/1	0.99	0.07	38,38,38,38	0
2	MN	P	401	1/1	0.99	0.08	29,29,29,29	0
2	MN	T	402	1/1	0.99	0.09	36,36,36,36	0
2	MN	U	402	1/1	0.99	0.06	42,42,42,42	0
2	MN	E	401	1/1	0.99	0.12	21,21,21,21	0
2	MN	S	401	1/1	0.99	0.08	28,28,28,28	0
3	NA	K	404	1/1	0.99	0.09	34,34,34,34	0
2	MN	X	402	1/1	0.99	0.07	37,37,37,37	0
2	MN	H	401	1/1	0.99	0.09	25,25,25,25	0
2	MN	A	402	1/1	0.99	0.07	41,41,41,41	0
2	MN	D	401	1/1	0.99	0.07	26,26,26,26	0
2	MN	P	402	1/1	0.99	0.07	39,39,39,39	0
2	MN	N	402	1/1	0.99	0.06	41,41,41,41	0
2	MN	X	401	1/1	0.99	0.07	32,32,32,32	0
2	MN	K	402	1/1	0.99	0.07	32,32,32,32	0
2	MN	R	402	1/1	0.99	0.06	34,34,34,34	0
3	NA	R	403	1/1	0.99	0.07	33,33,33,33	0
3	NA	D	404	1/1	0.99	0.10	38,38,38,38	0
3	NA	J	403	1/1	0.99	0.18	29,29,29,29	0
2	MN	R	401	1/1	0.99	0.07	27,27,27,27	0
2	MN	K	401	1/1	1.00	0.05	24,24,24,24	0
2	MN	B	401	1/1	1.00	0.06	31,31,31,31	0
2	MN	I	401	1/1	1.00	0.09	22,22,22,22	0
2	MN	F	401	1/1	1.00	0.08	23,23,23,23	0
2	MN	A	401	1/1	1.00	0.08	32,32,32,32	0
2	MN	L	402	1/1	1.00	0.07	39,39,39,39	0
2	MN	E	402	1/1	1.00	0.07	25,25,25,25	0

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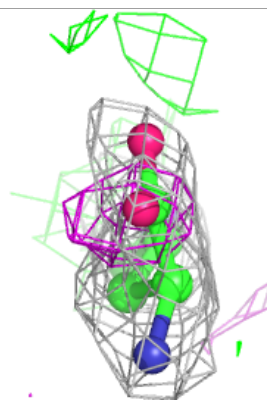
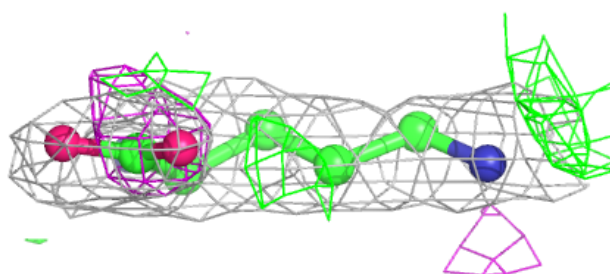
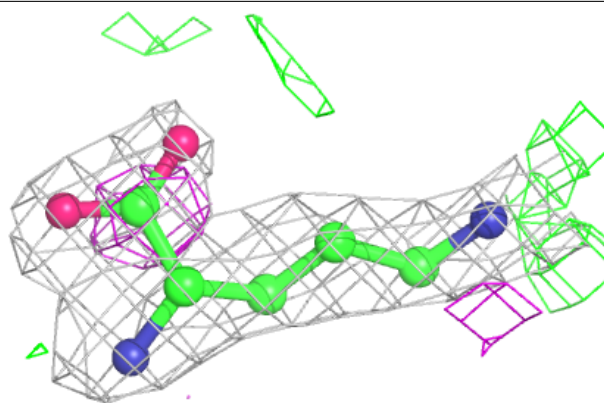
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	F	402	1/1	1.00	0.07	31,31,31,31	0
2	MN	H	402	1/1	1.00	0.07	31,31,31,31	0
2	MN	Q	402	1/1	1.00	0.07	33,33,33,33	0
2	MN	Q	401	1/1	1.00	0.09	29,29,29,29	0
2	MN	I	402	1/1	1.00	0.06	30,30,30,30	0
2	MN	G	401	1/1	1.00	0.09	21,21,21,21	0
2	MN	L	401	1/1	1.00	0.06	30,30,30,30	0
2	MN	J	401	1/1	1.00	0.08	21,21,21,21	0
2	MN	D	402	1/1	1.00	0.06	33,33,33,33	0
2	MN	G	402	1/1	1.00	0.07	27,27,27,27	0
2	MN	J	402	1/1	1.00	0.06	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.

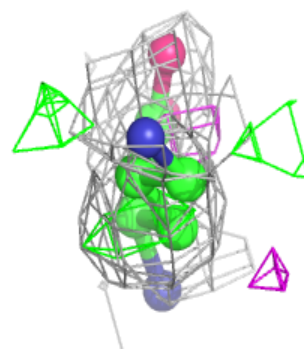
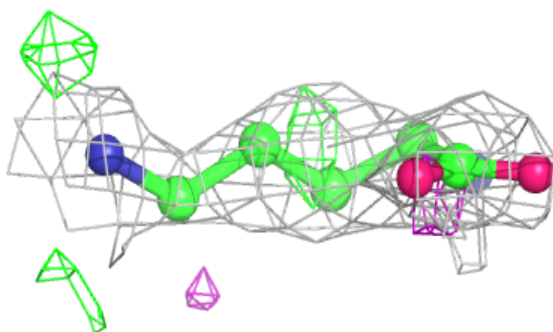
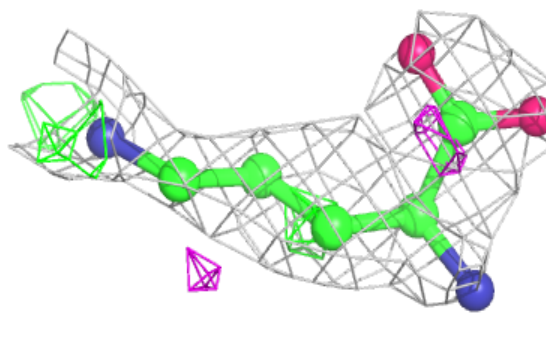


Electron density around ORN C 405:

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

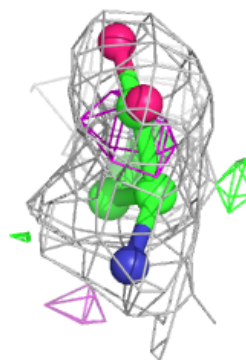
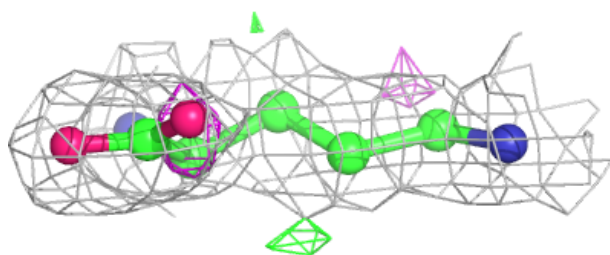
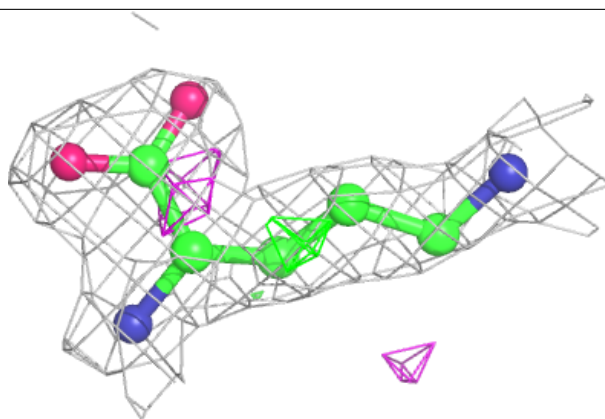
**Electron density around ORN P 405:**

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

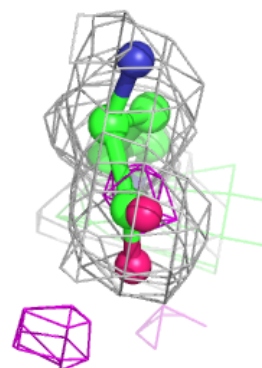
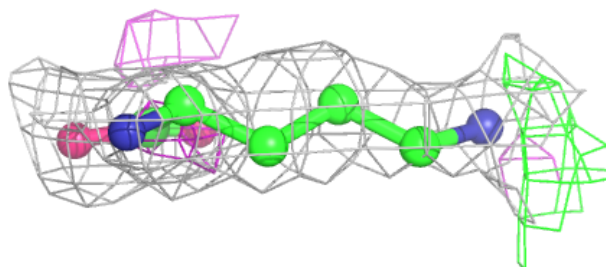
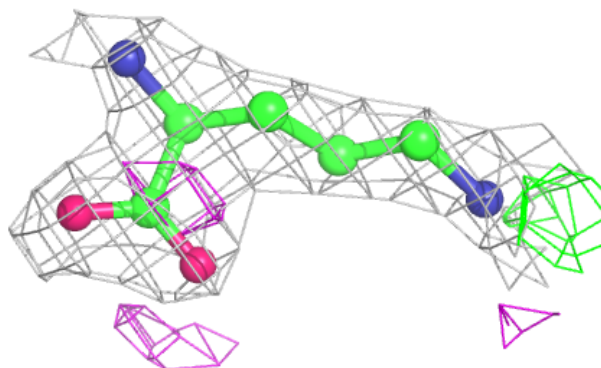


Electron density around ORN K 406:

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

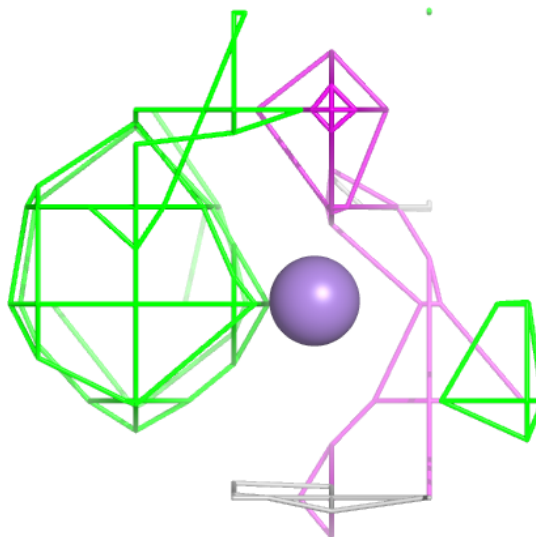
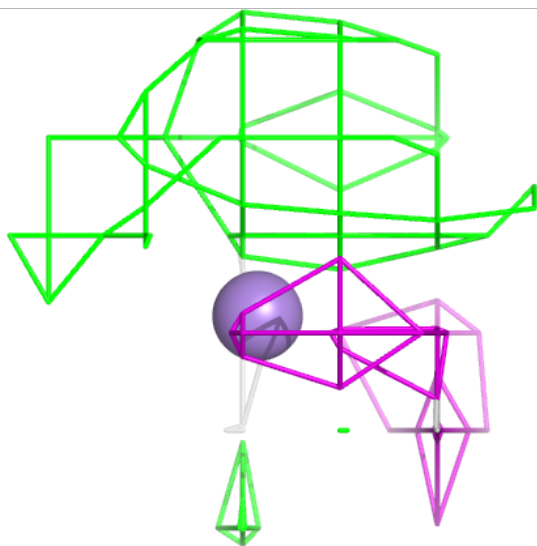
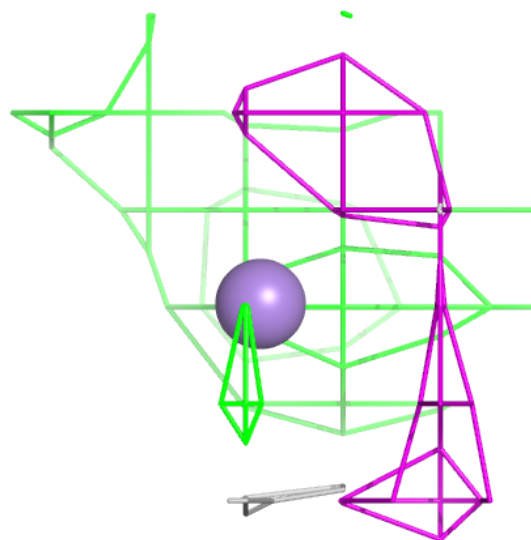
**Electron density around ORN E 404:**

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



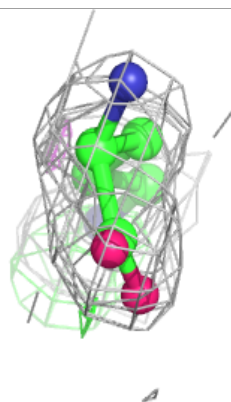
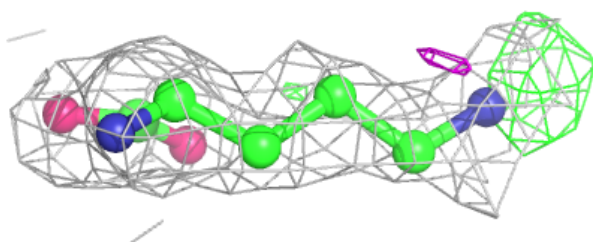
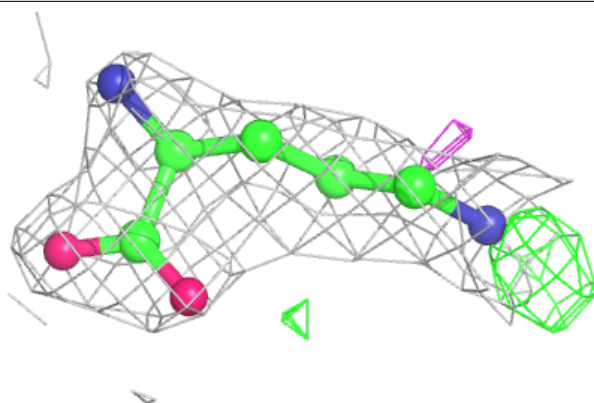
Electron density around MN O 401:

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

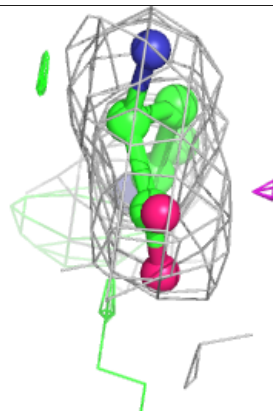
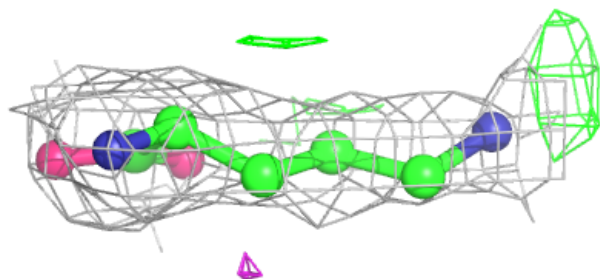
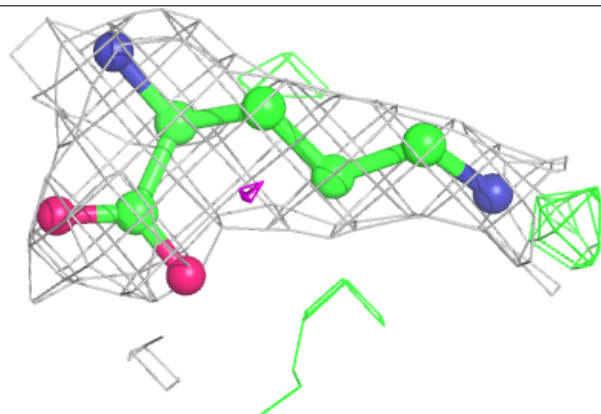


Electron density around ORN F 405:

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

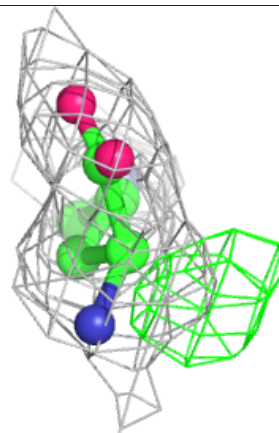
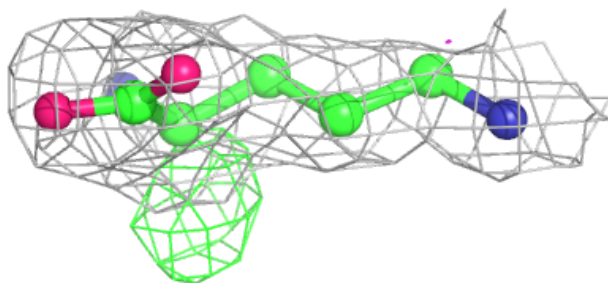
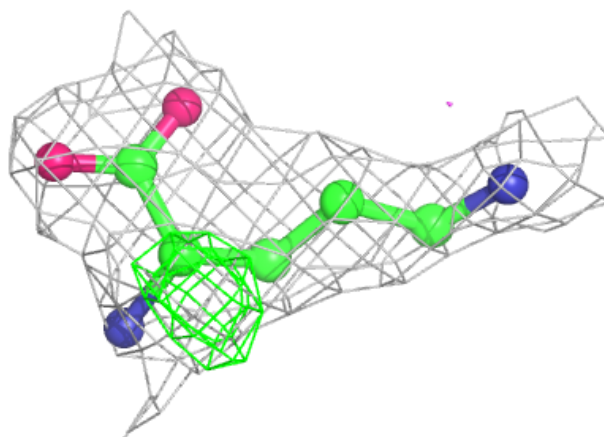
**Electron density around ORN U 405:**

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

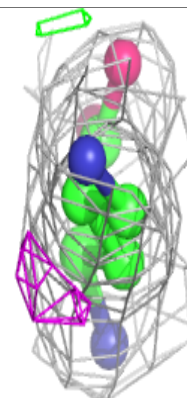
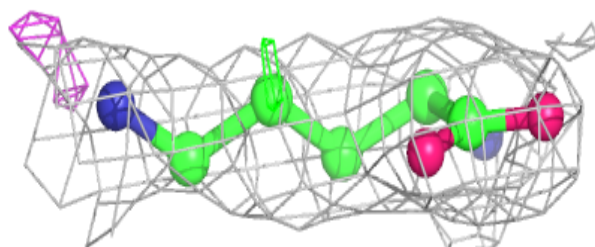
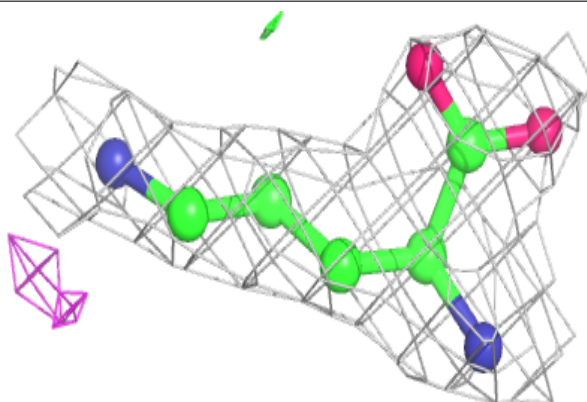


Electron density around ORN G 404:

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

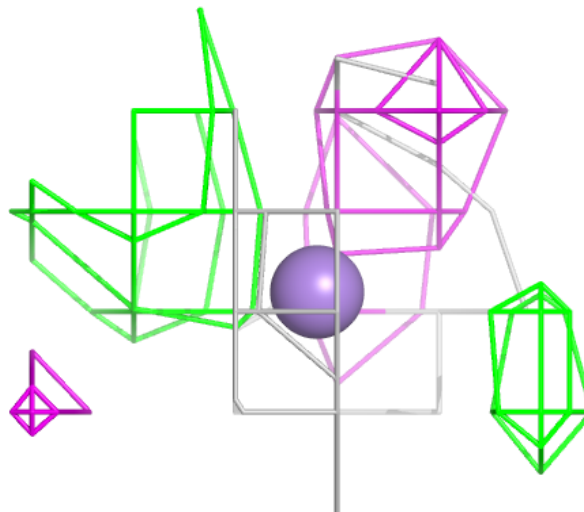
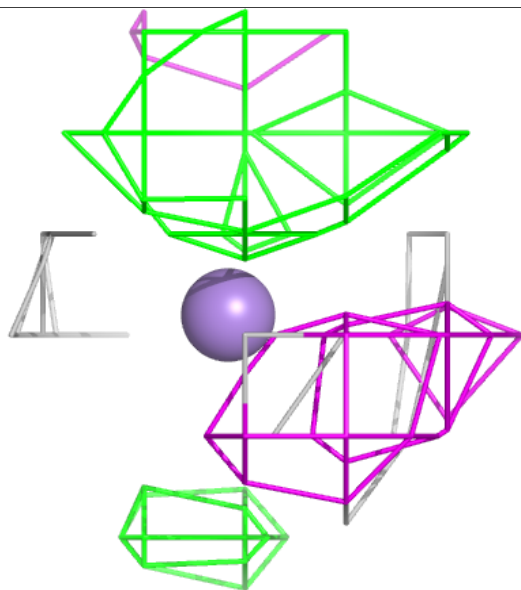
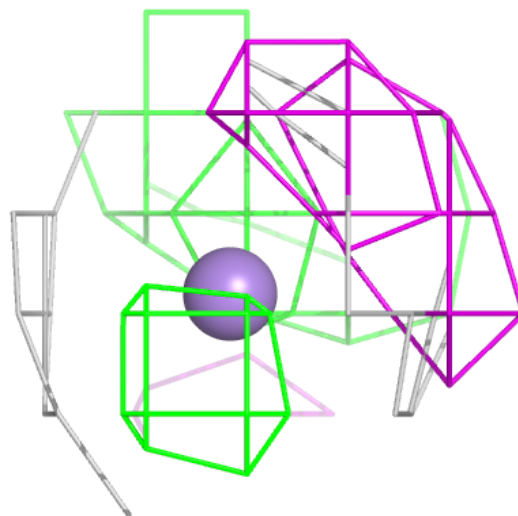
**Electron density around ORN A 404:**

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



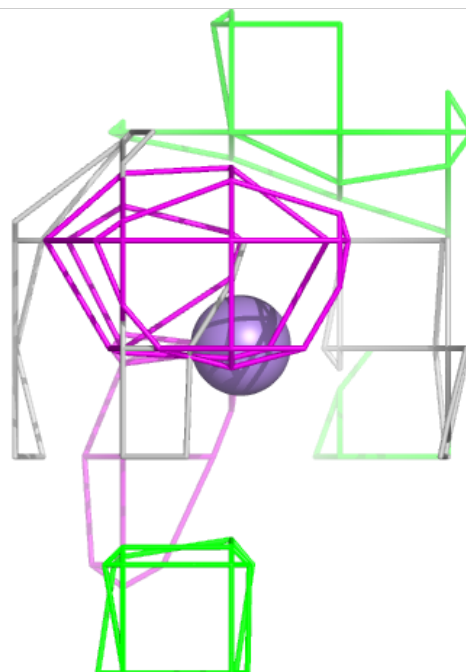
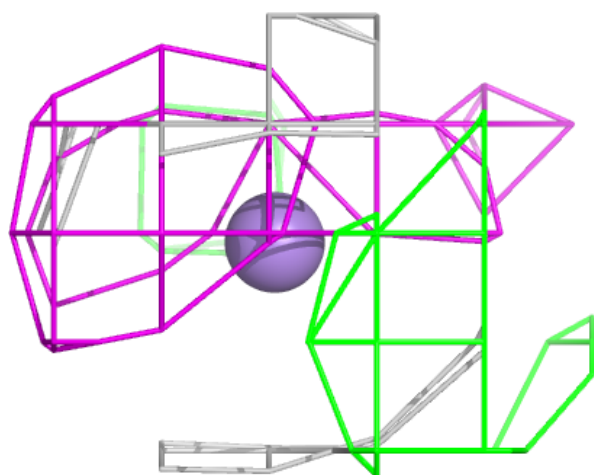
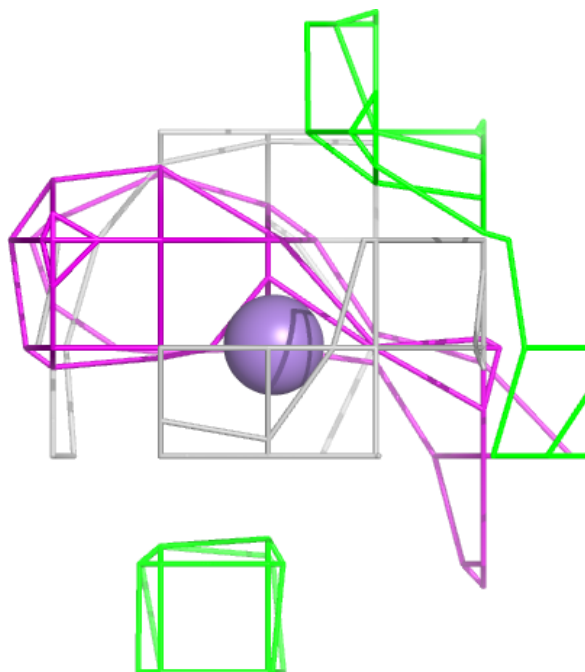
Electron density around MN O 402:

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



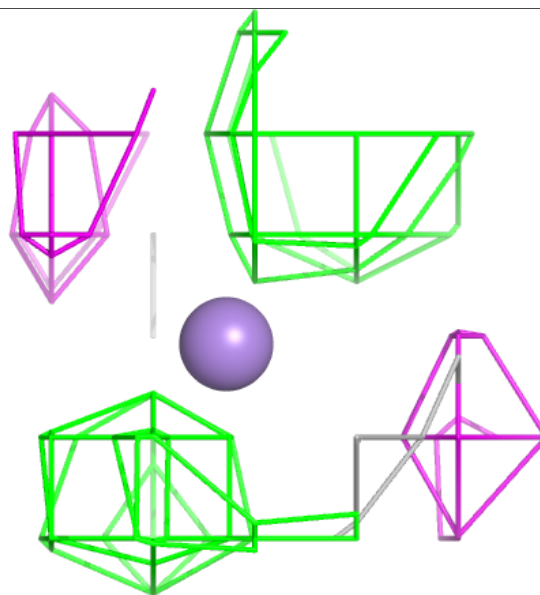
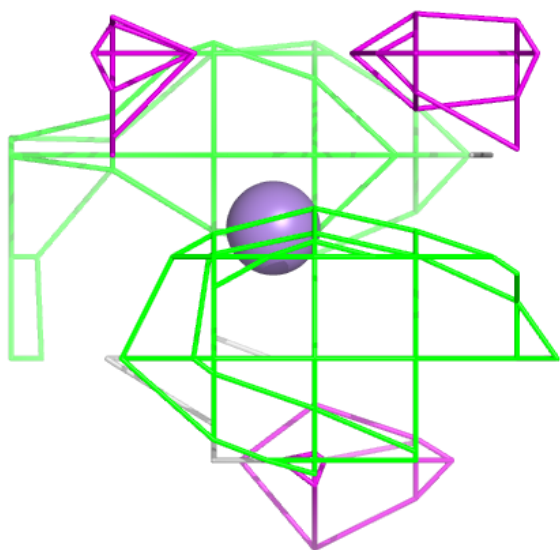
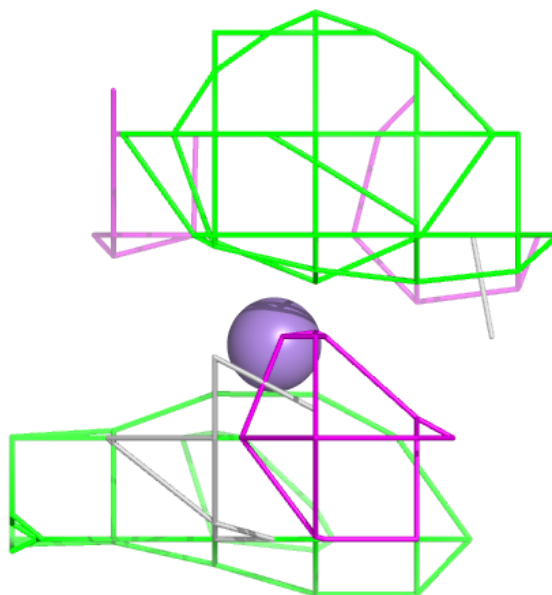
Electron density around MN C 402:

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



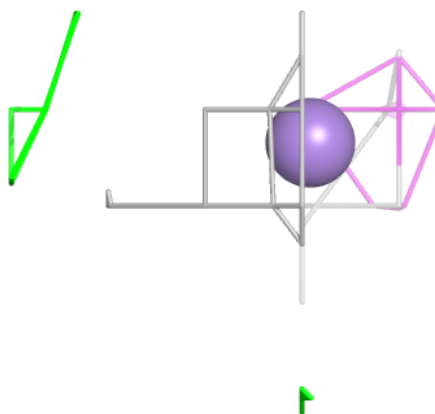
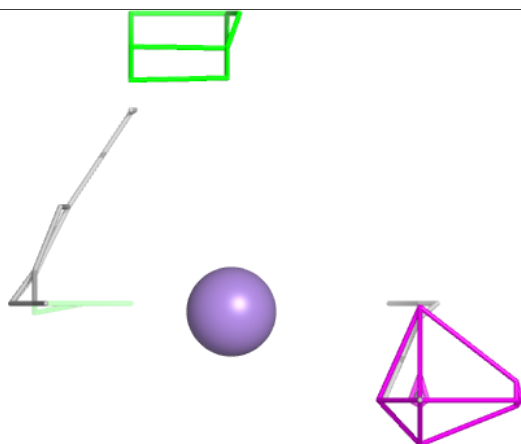
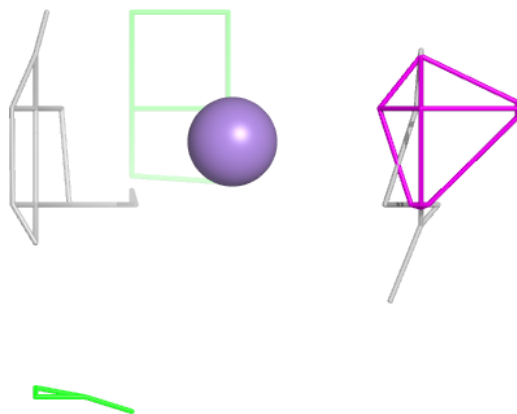
Electron density around MN C 401:

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



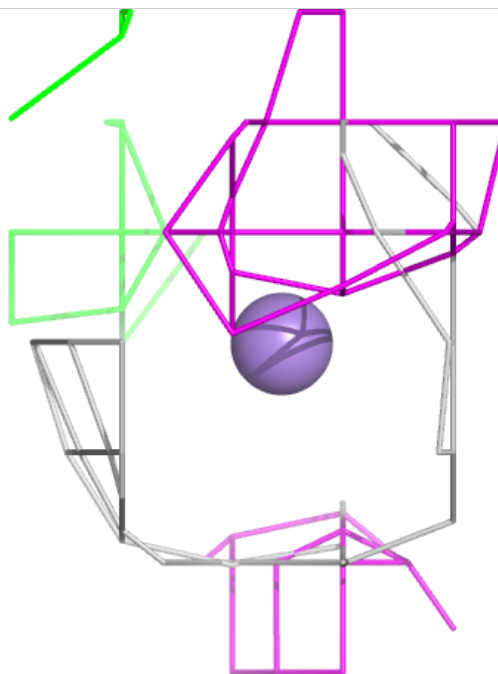
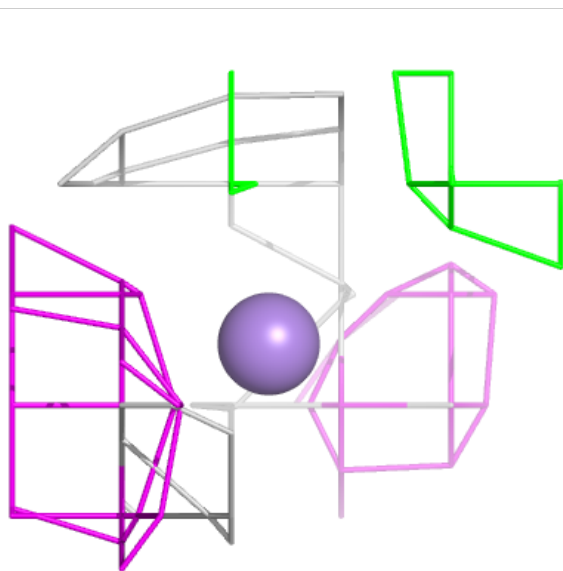
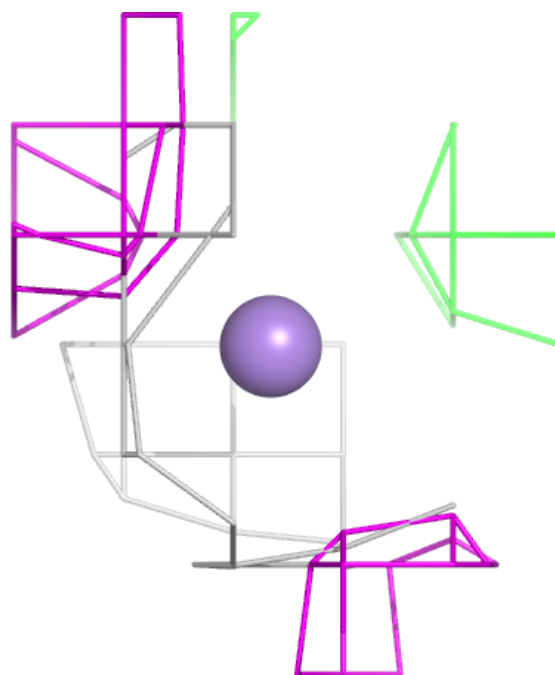
Electron density around MN W 402:

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



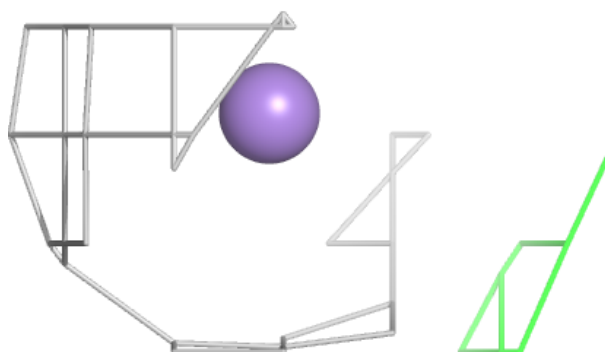
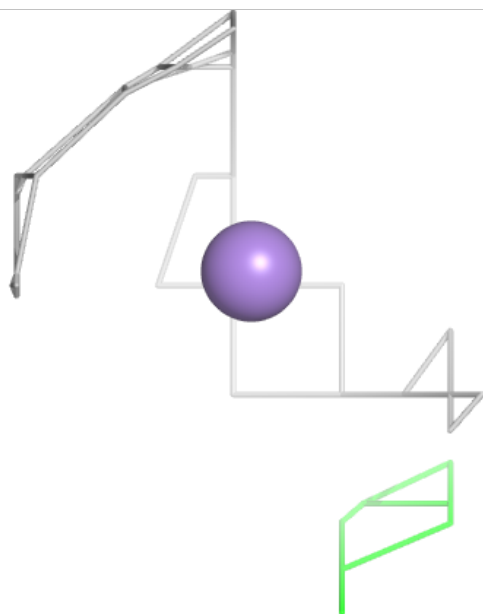
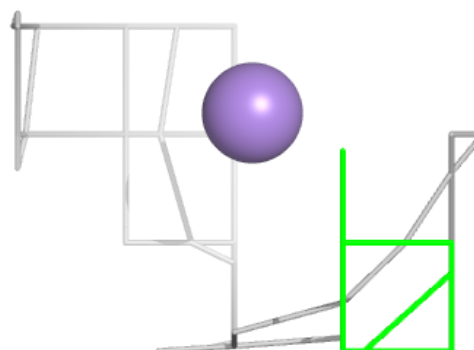
Electron density around MN V 402:

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



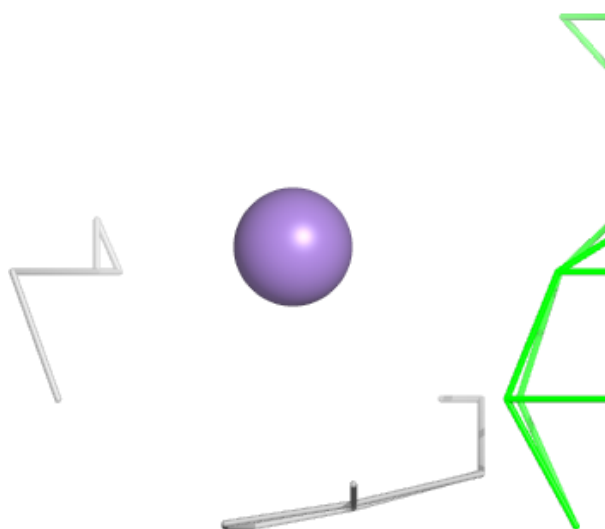
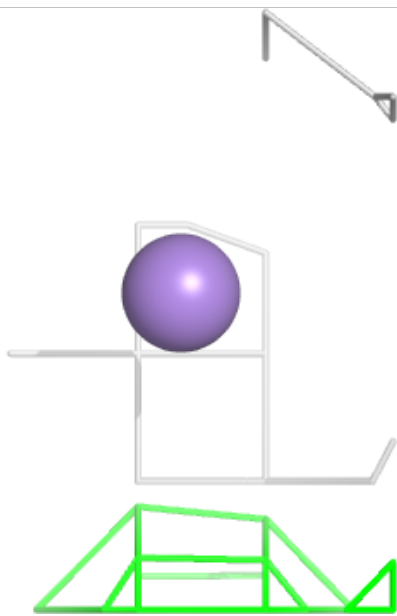
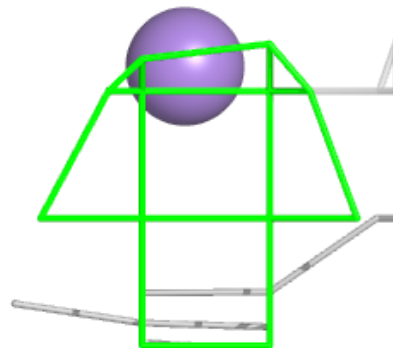
Electron density around MN W 401:

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



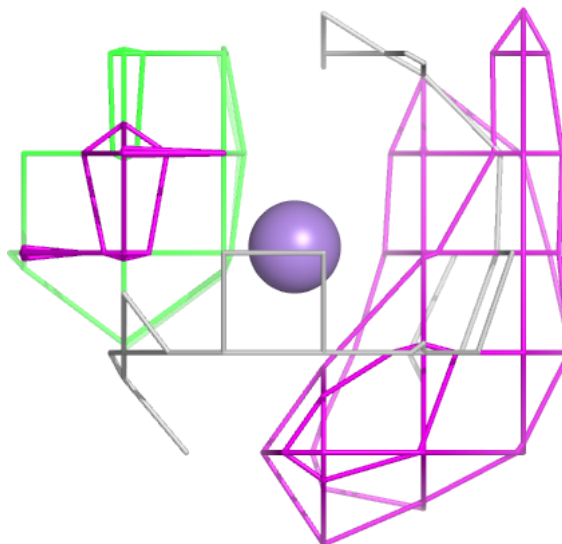
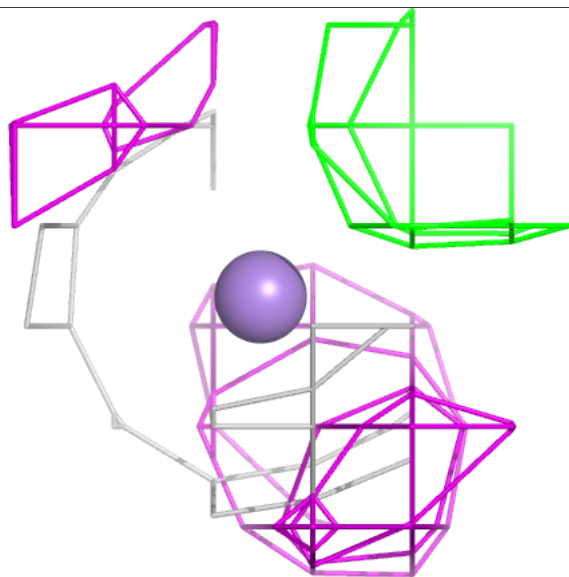
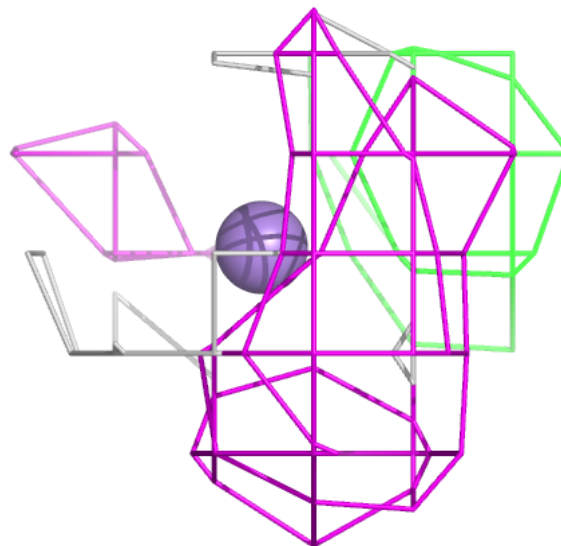
Electron density around MN M 401:

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



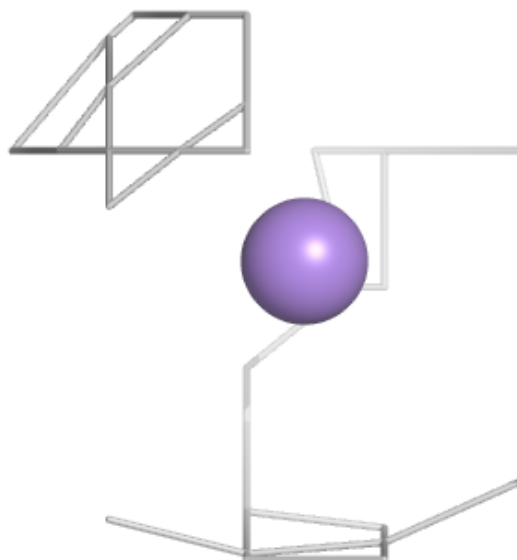
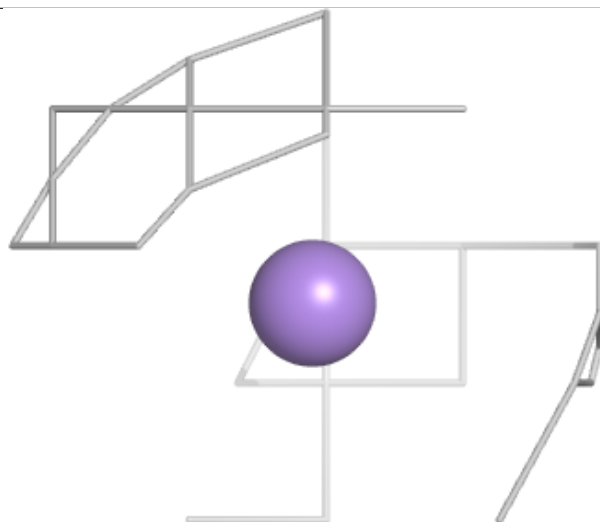
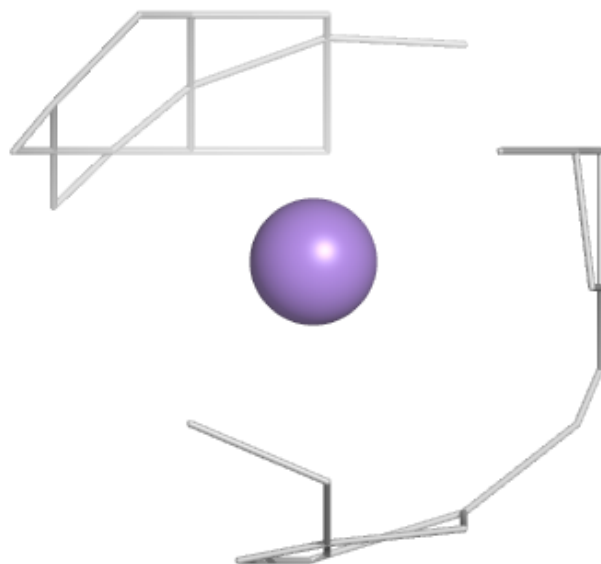
Electron density around MN V 401:

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



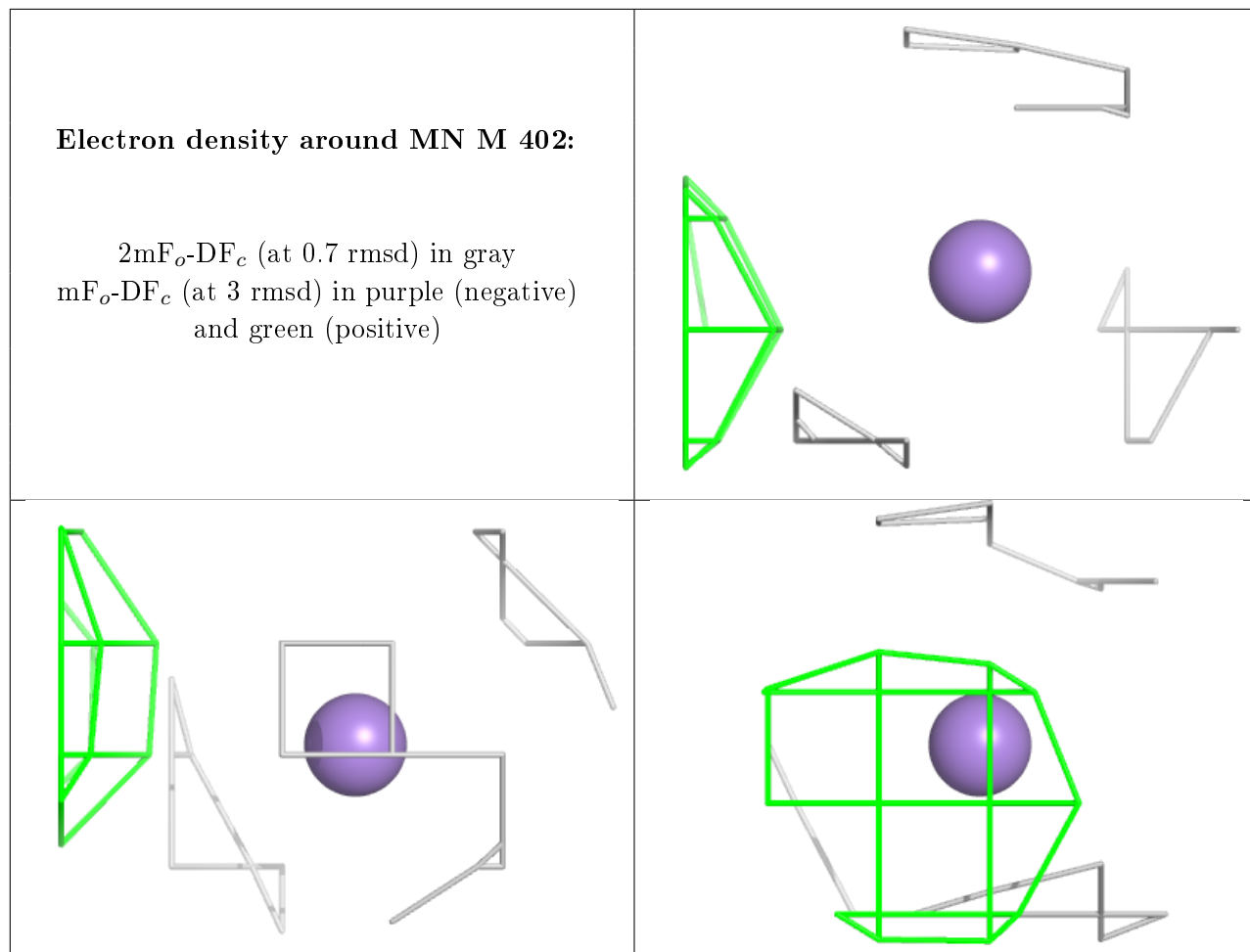
Electron density around MN T 401:

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



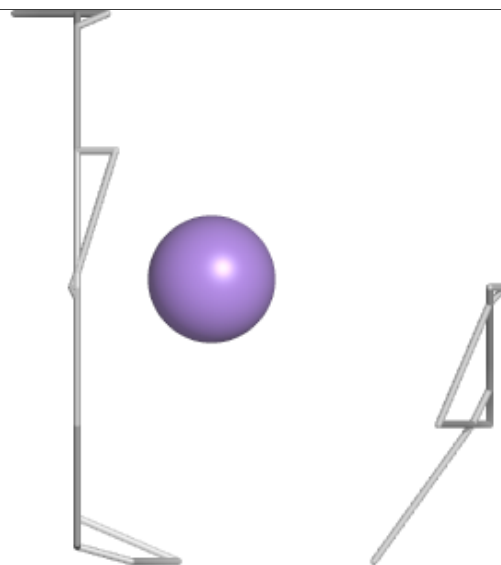
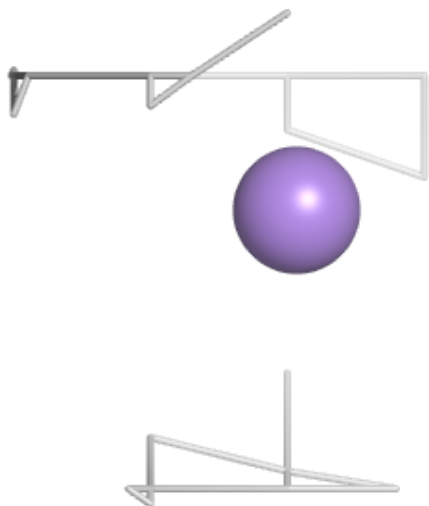
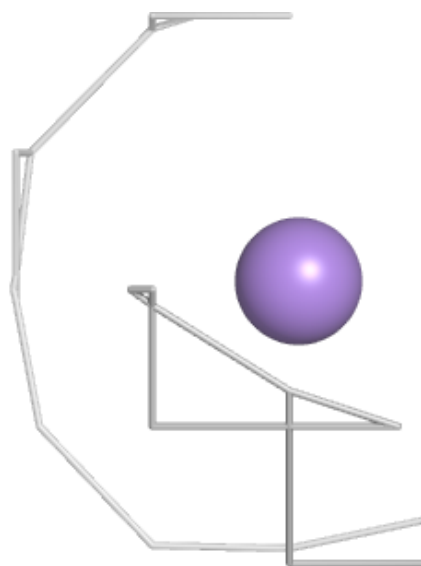
Electron density around MN M 402:

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



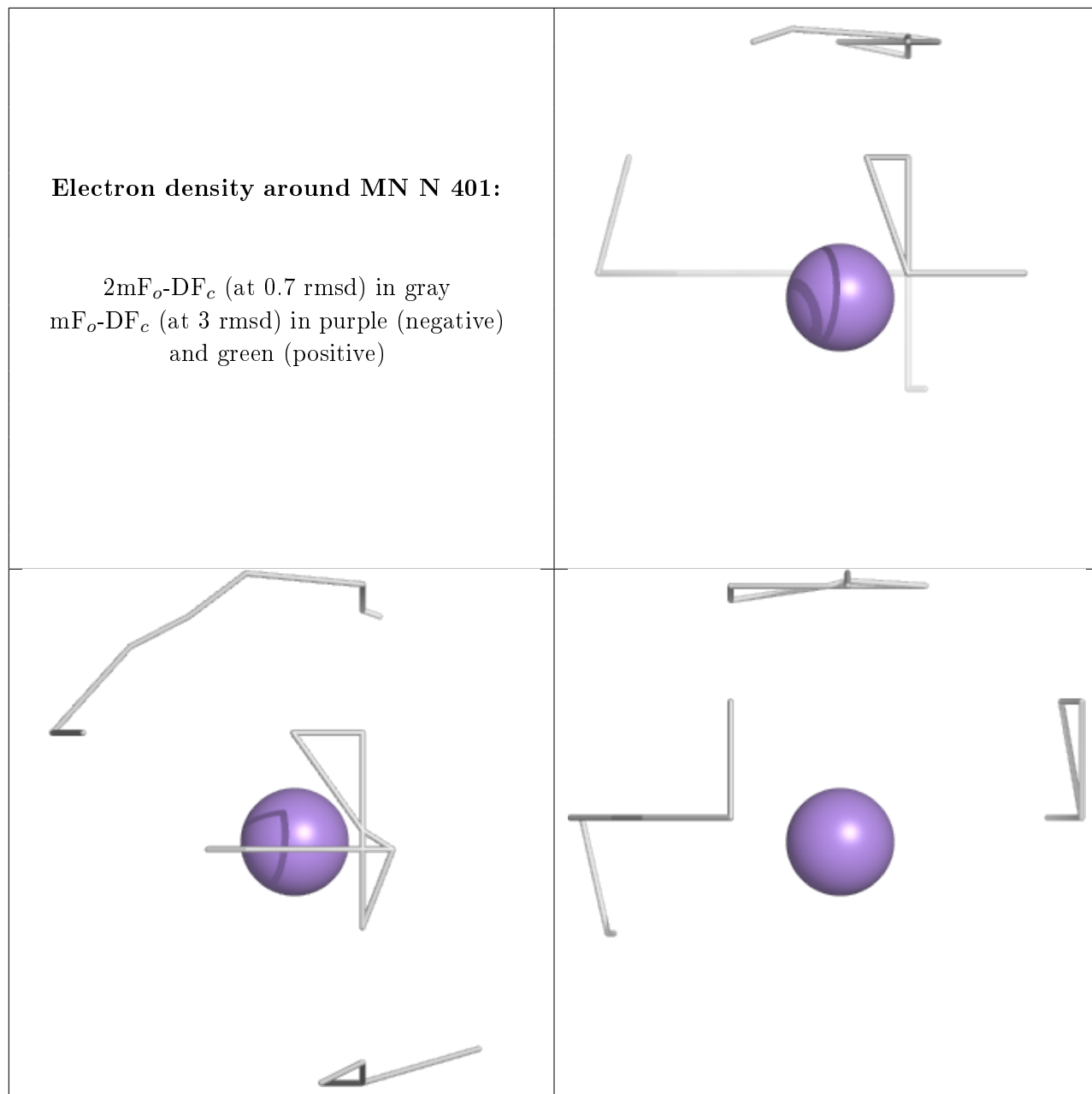
Electron density around MN U 401:

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



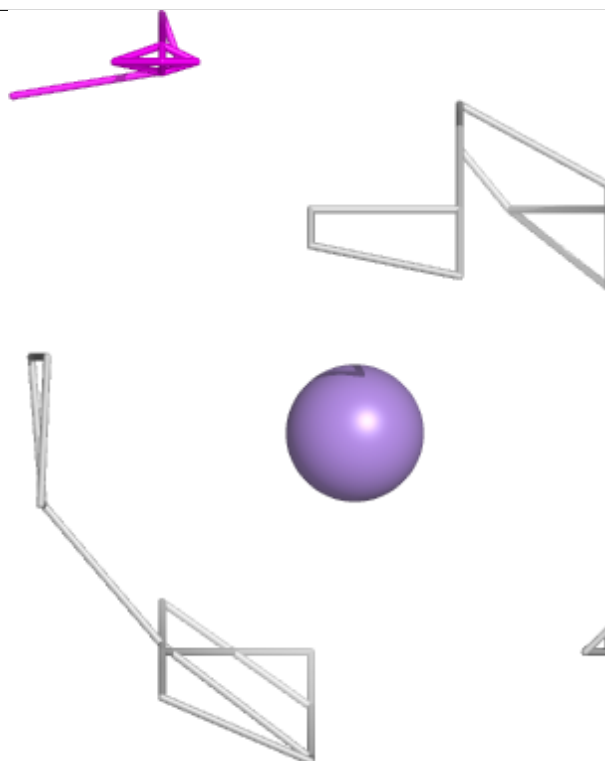
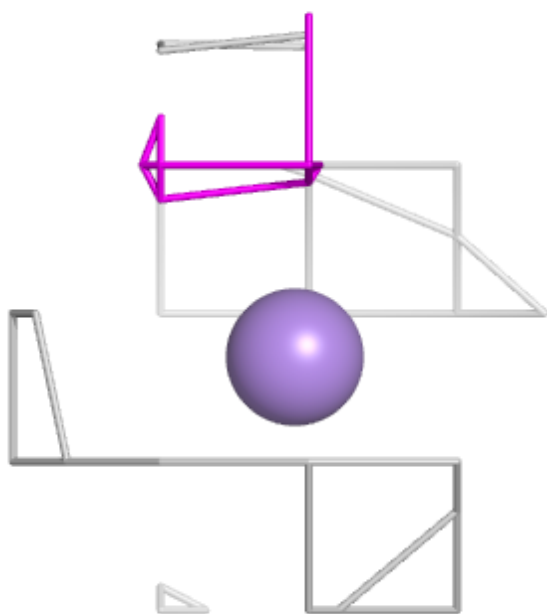
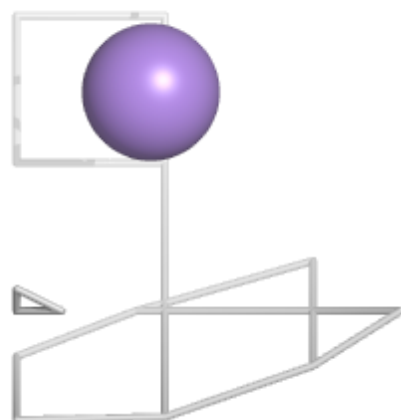
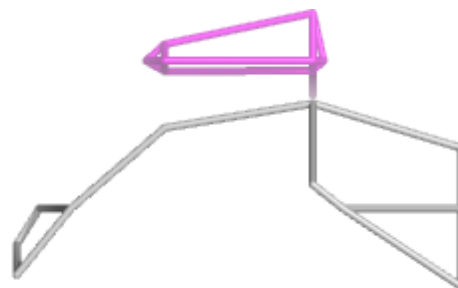
Electron density around MN N 401:

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



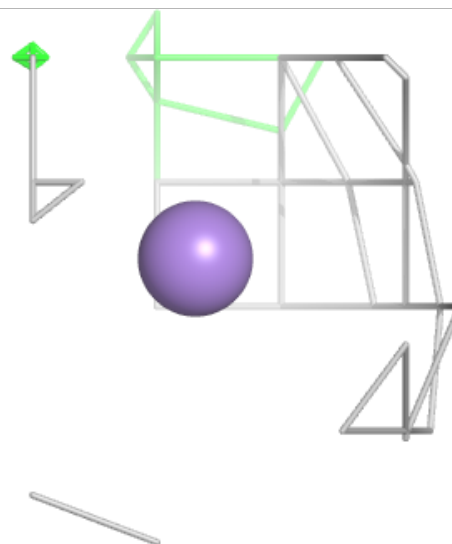
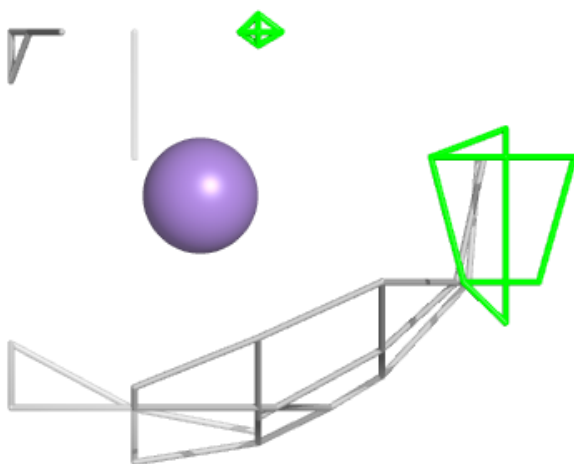
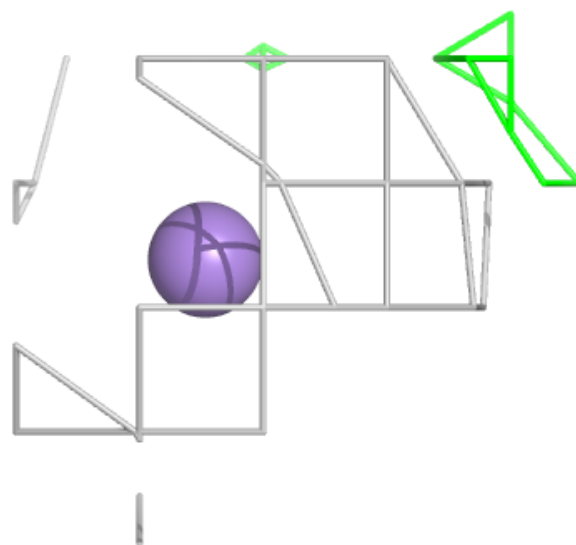
Electron density around MN B 402:

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



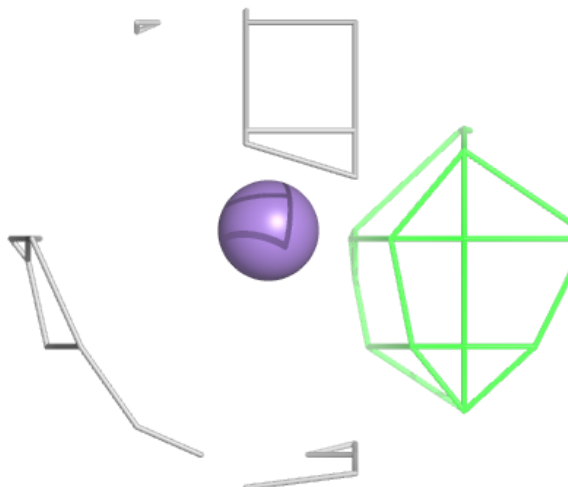
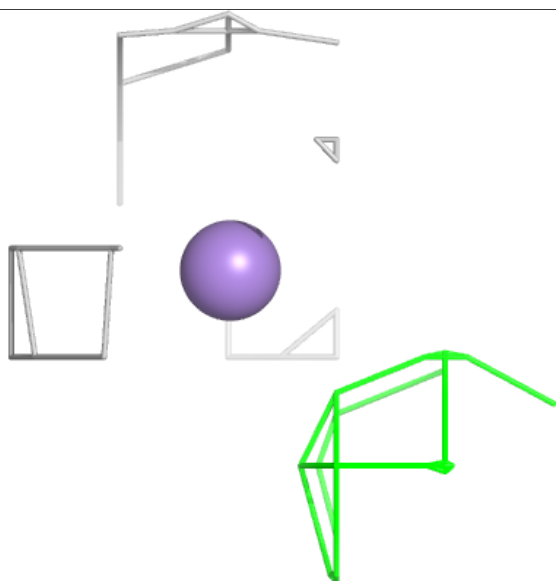
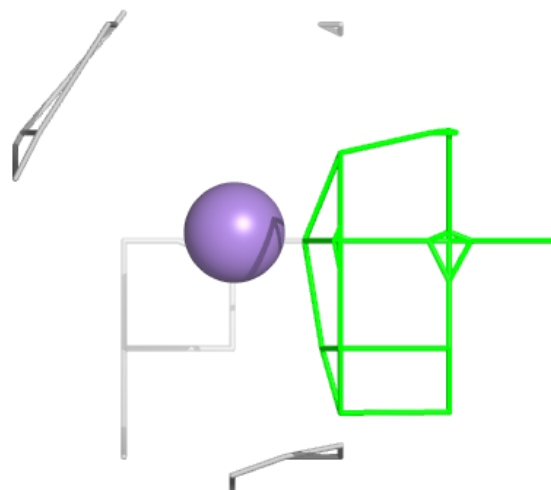
Electron density around MN S 402:

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



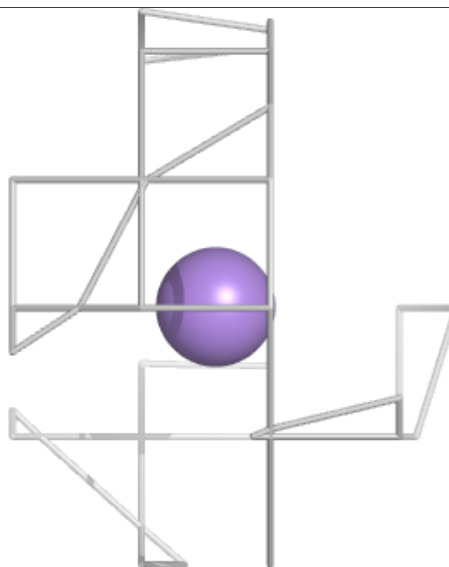
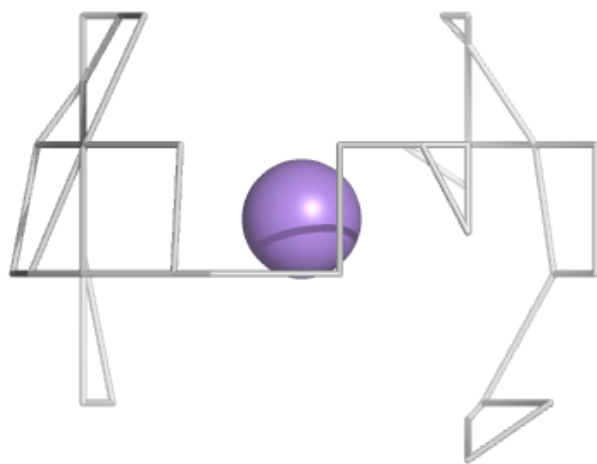
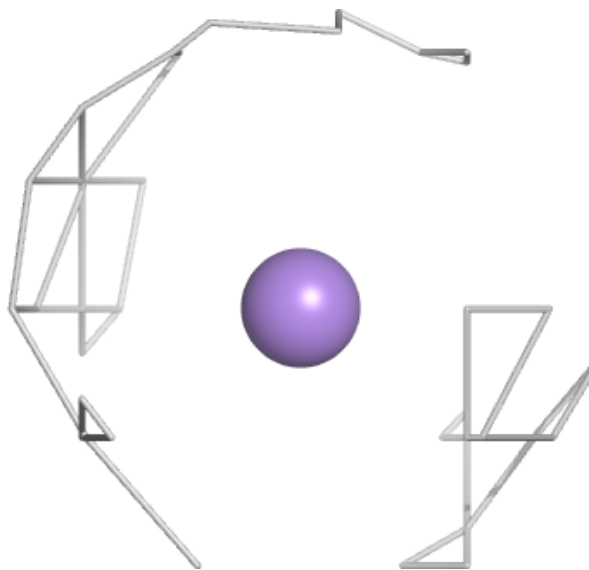
Electron density around MN P 401:

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



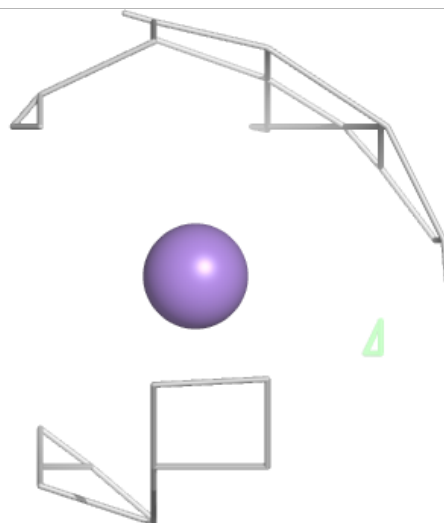
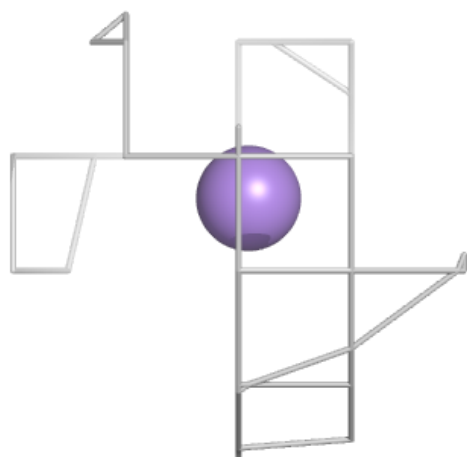
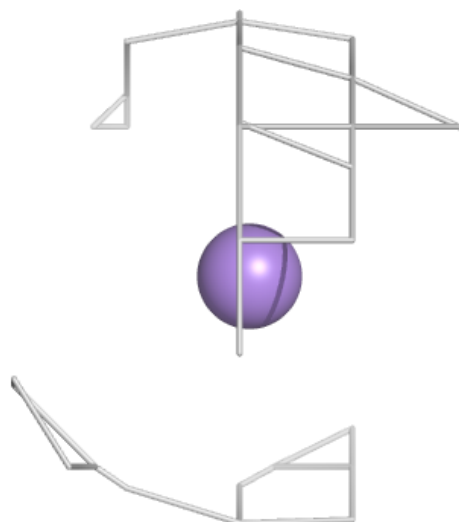
Electron density around MN T 402:

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



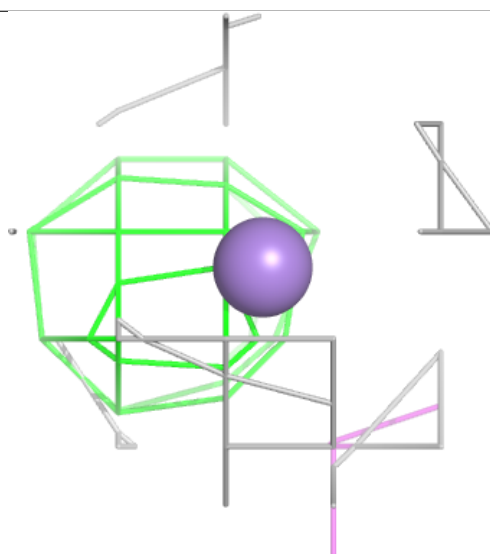
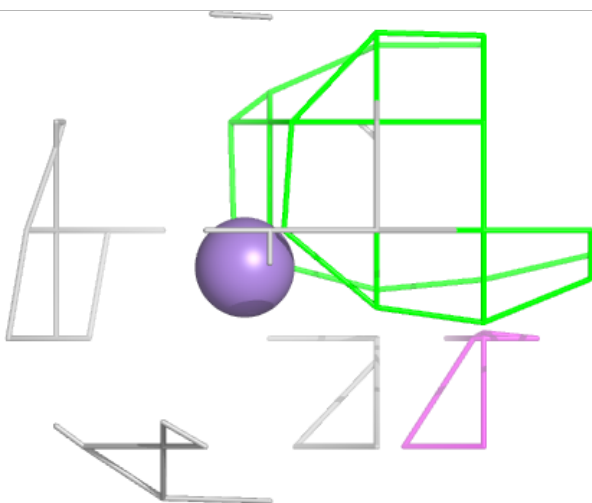
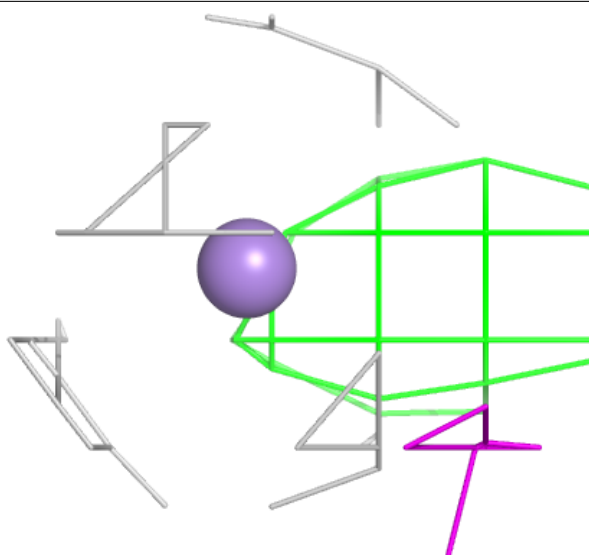
Electron density around MN U 402:

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



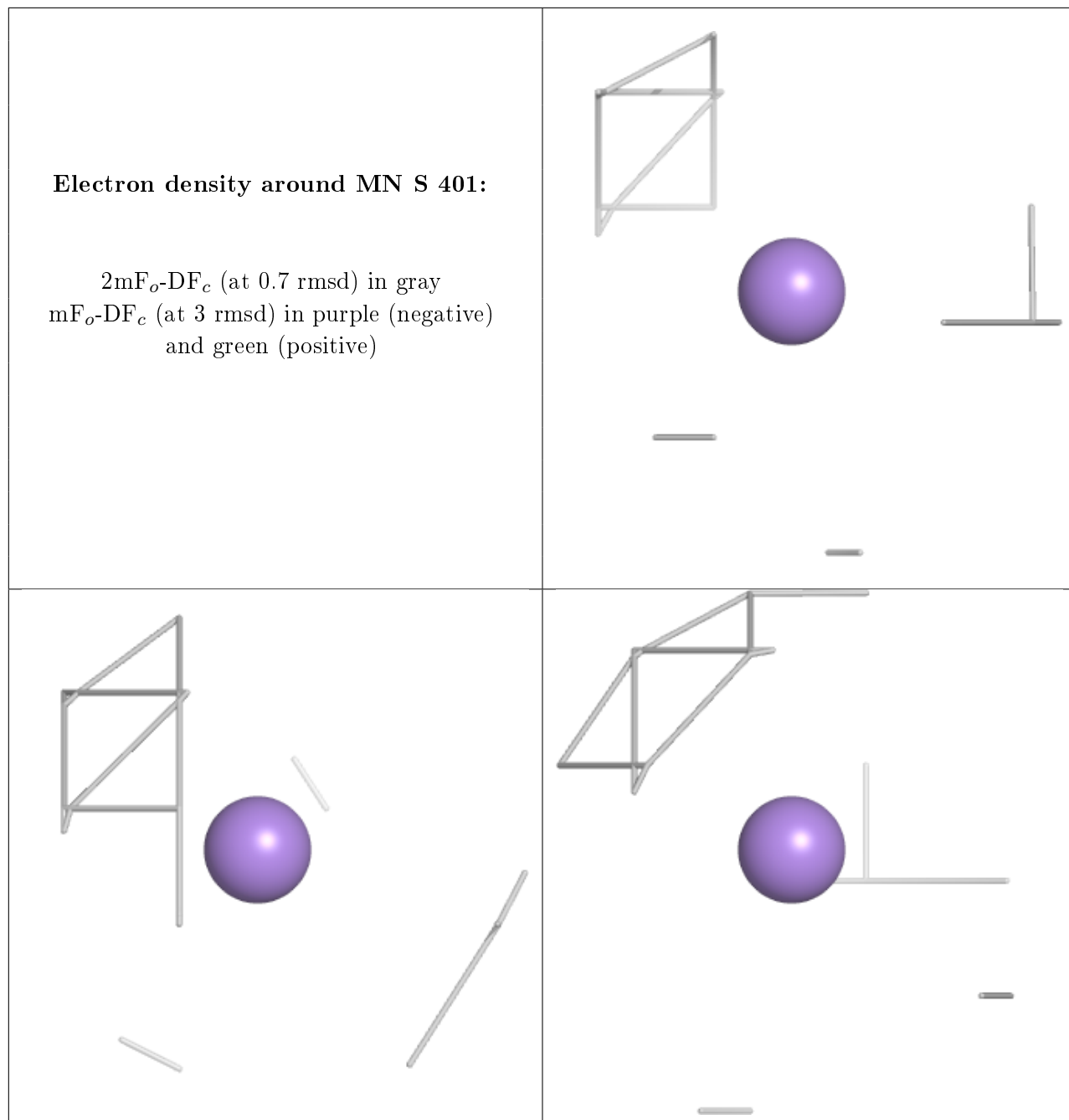
Electron density around MN E 401:

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



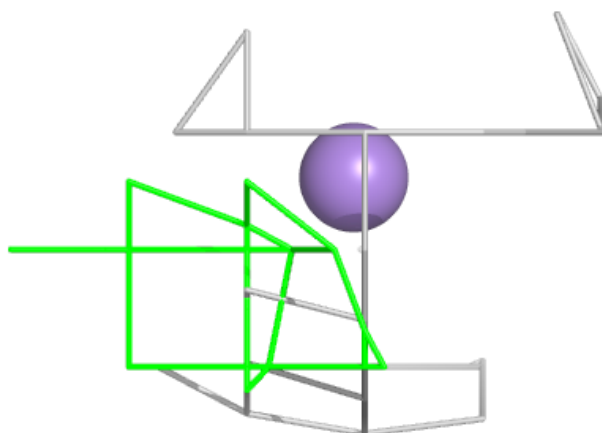
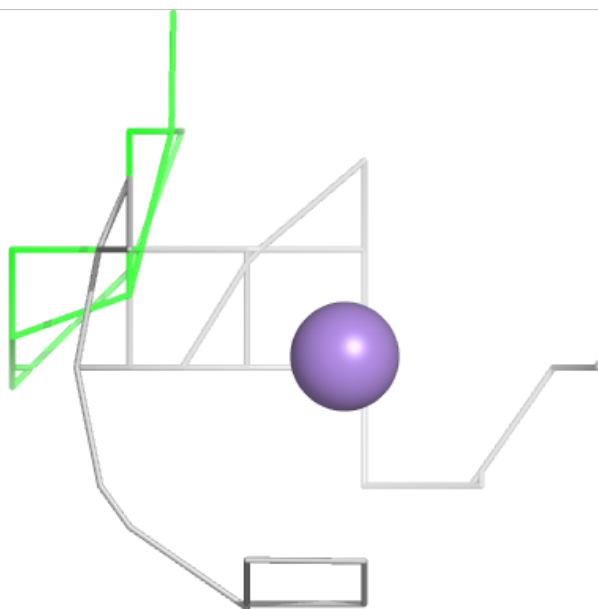
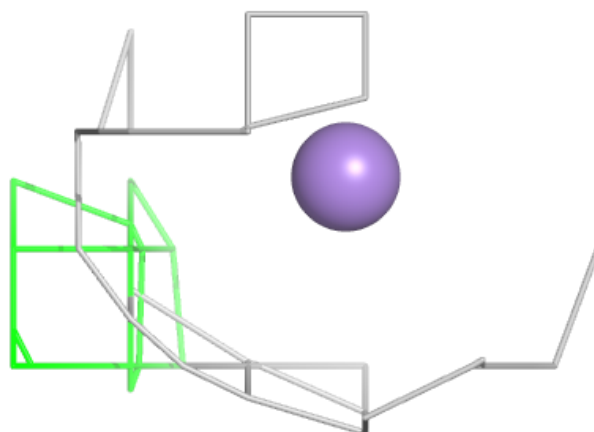
Electron density around MN S 401:

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



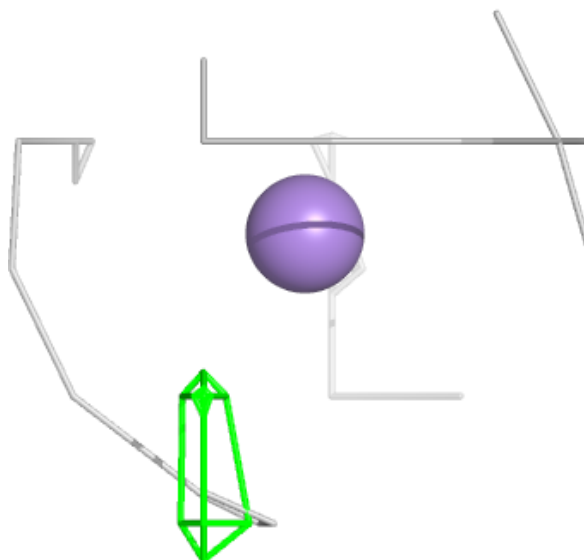
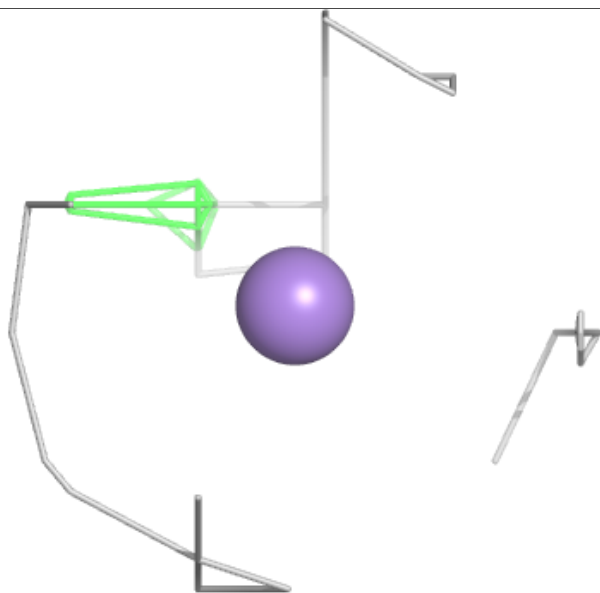
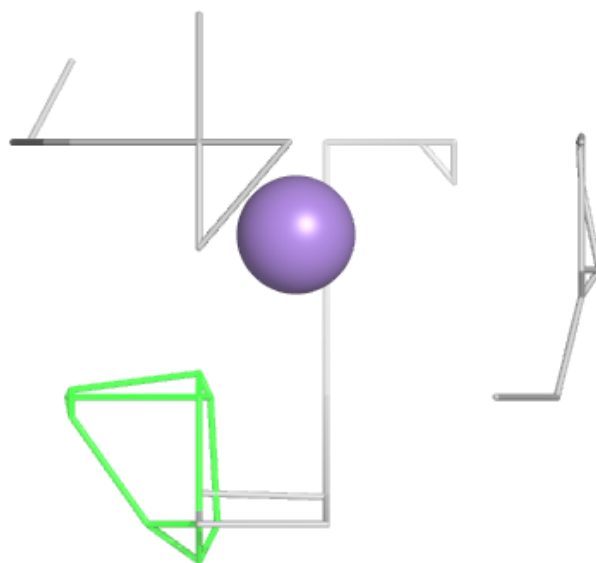
Electron density around MN X 402:

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



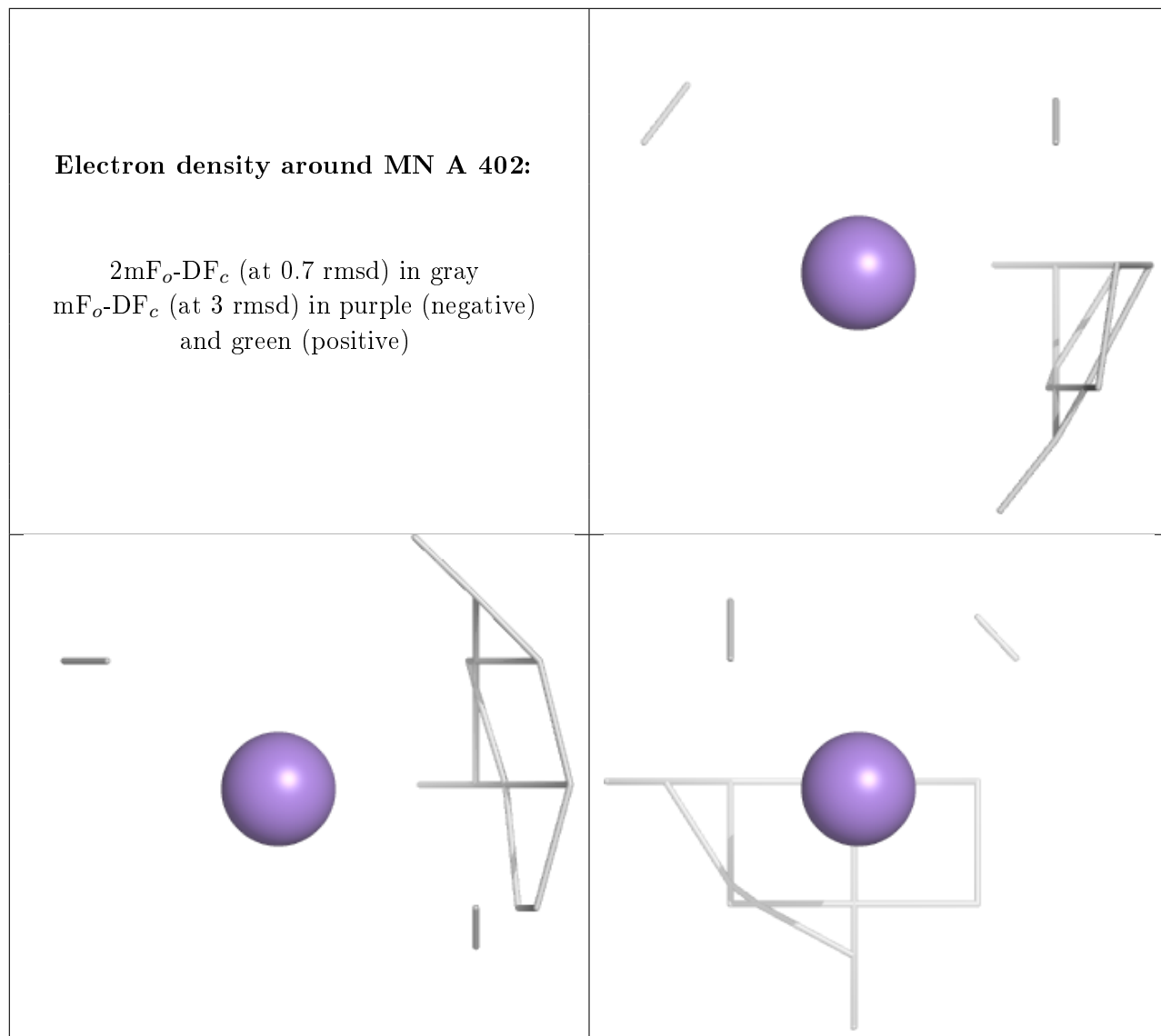
Electron density around MN H 401:

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



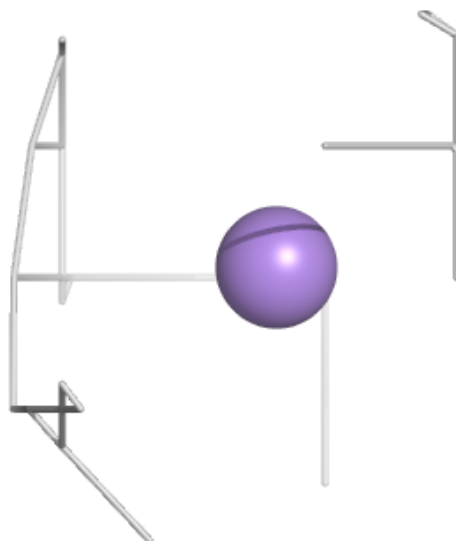
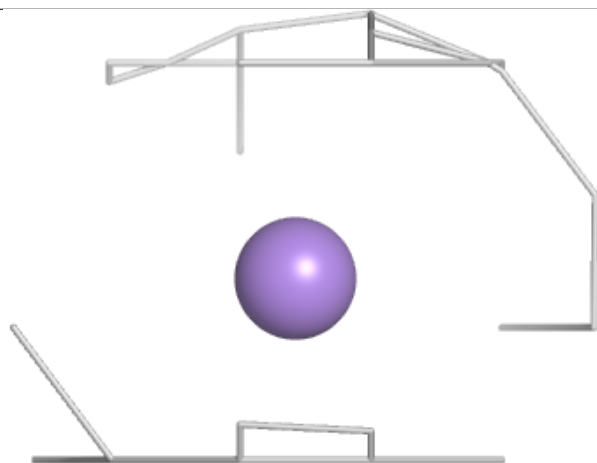
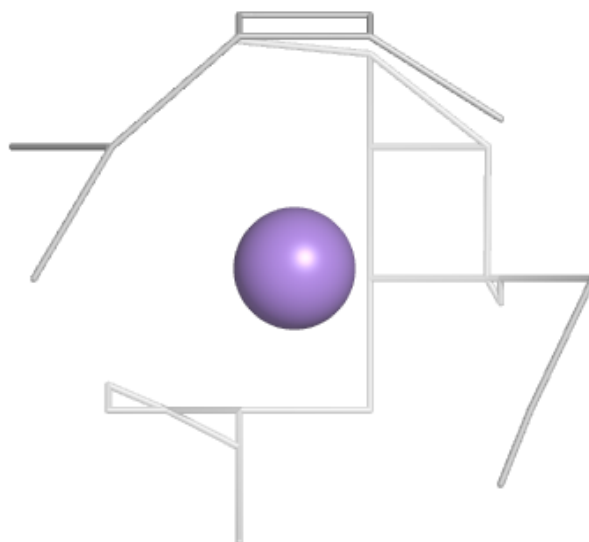
Electron density around MN A 402:

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



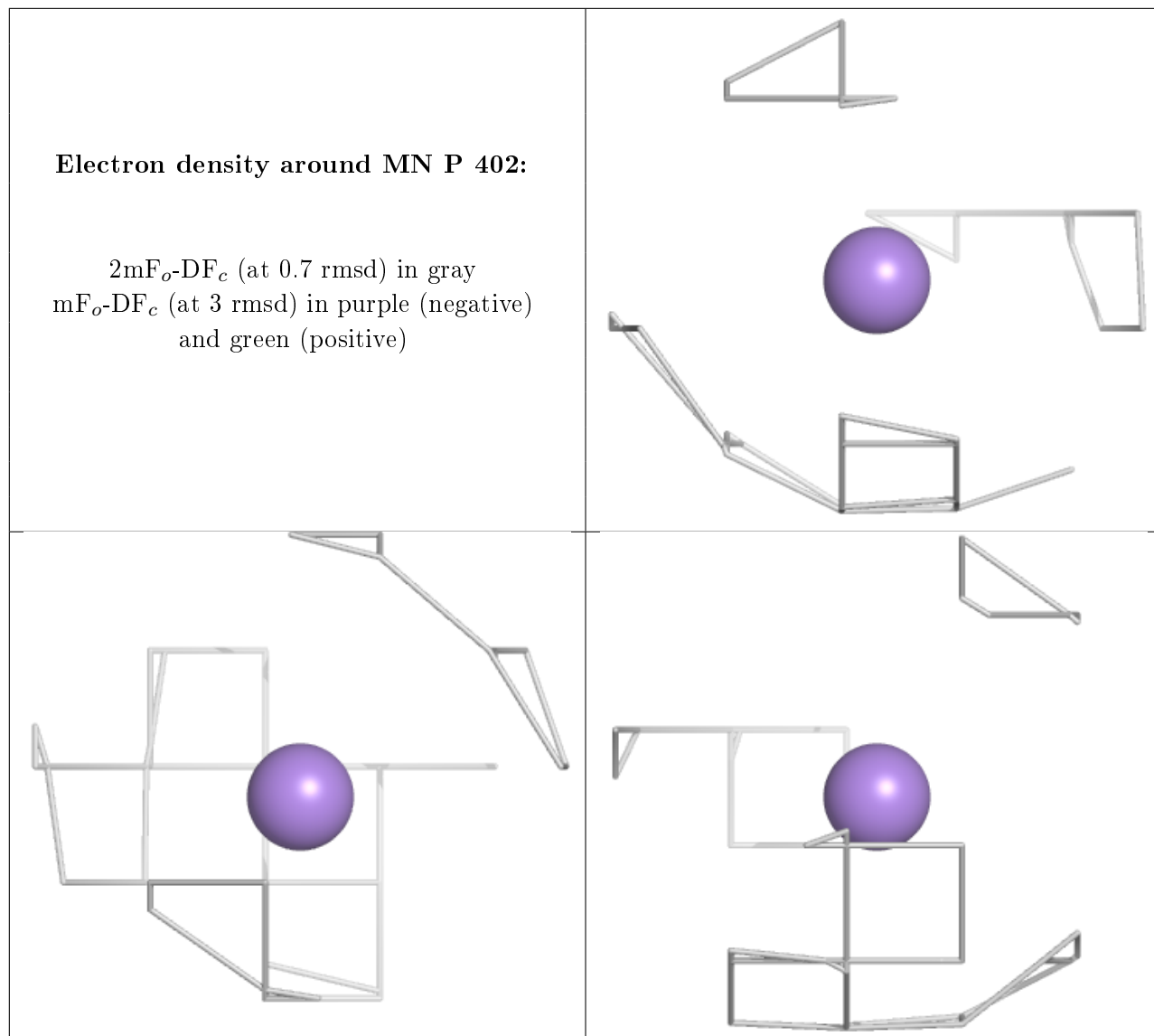
Electron density around MN D 401:

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



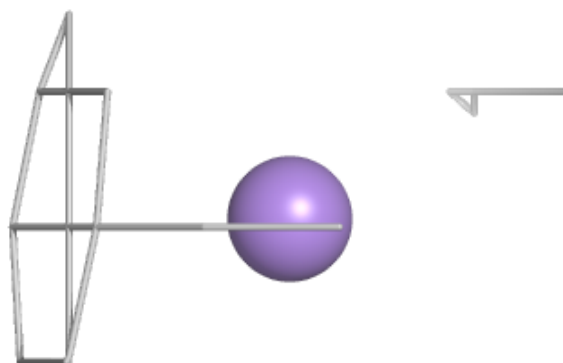
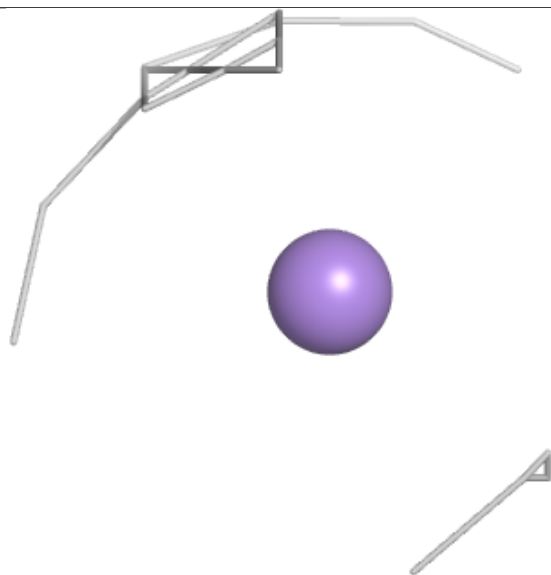
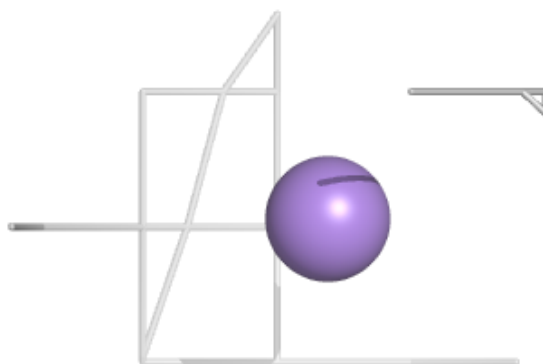
Electron density around MN P 402:

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



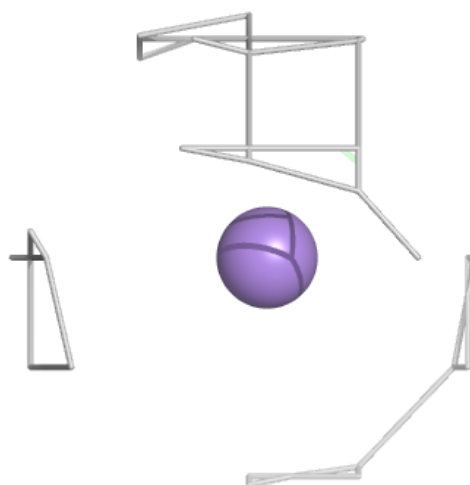
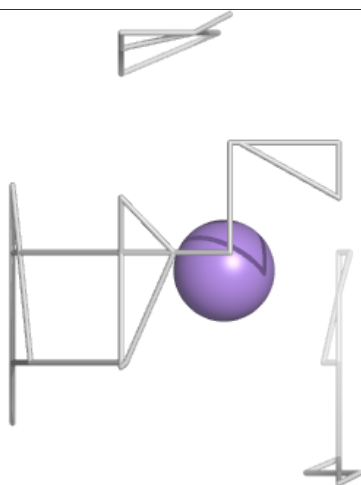
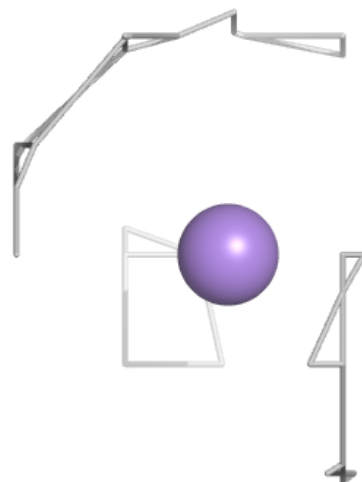
Electron density around MN N 402:

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



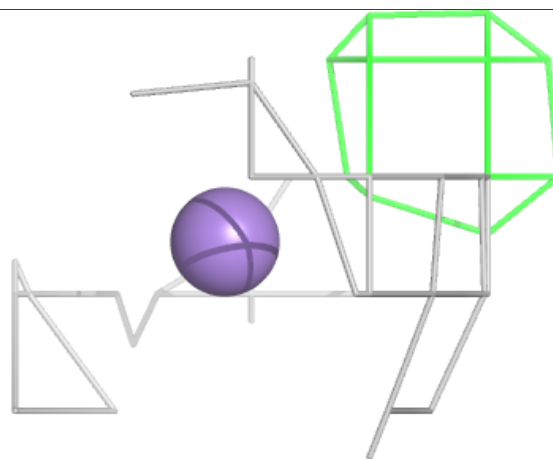
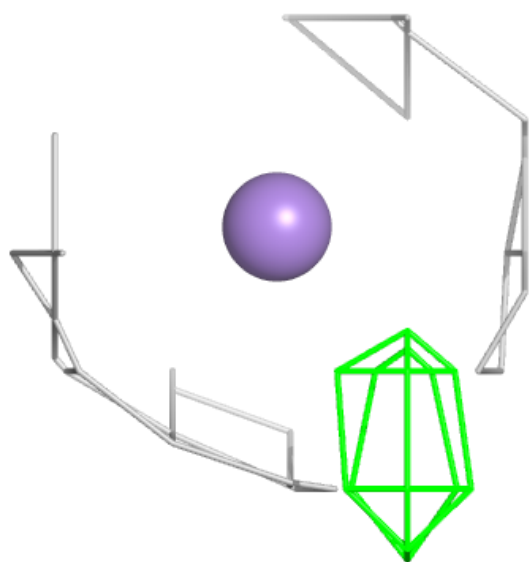
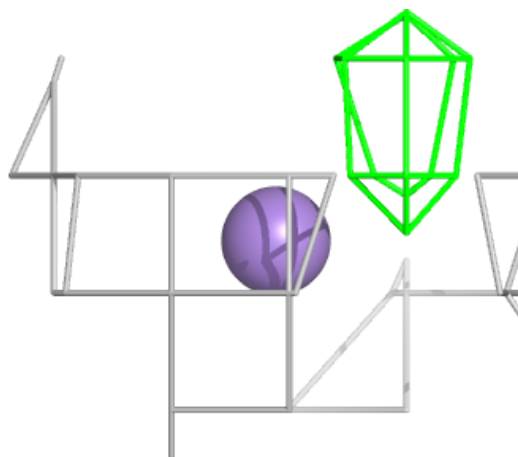
Electron density around MN X 401:

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



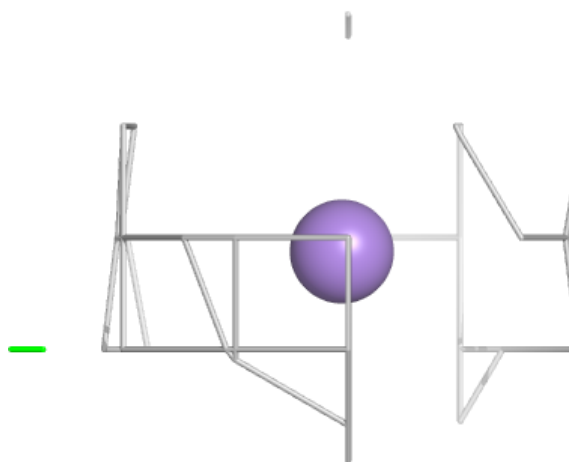
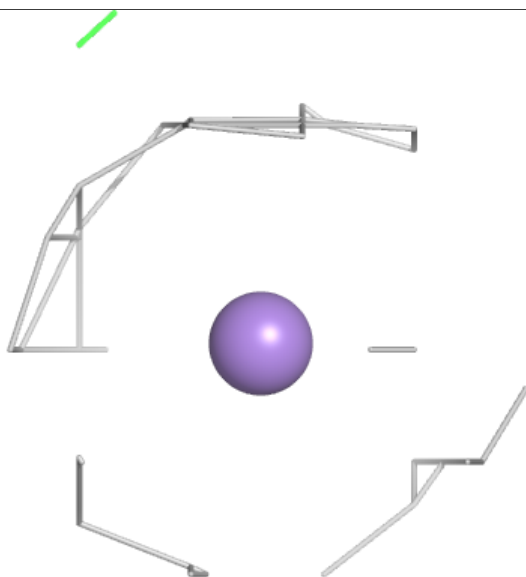
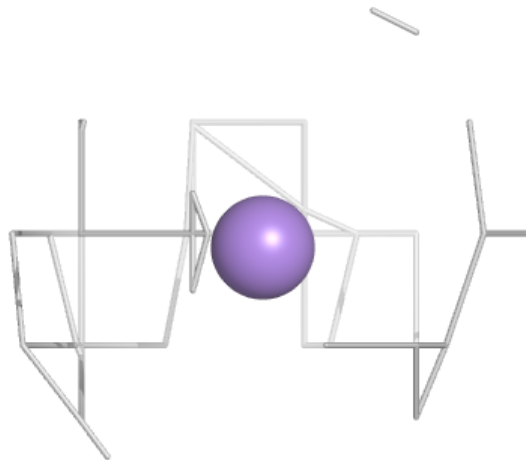
Electron density around MN K 402:

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



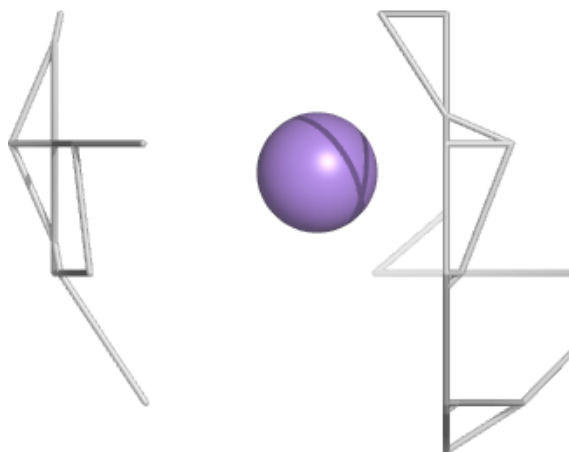
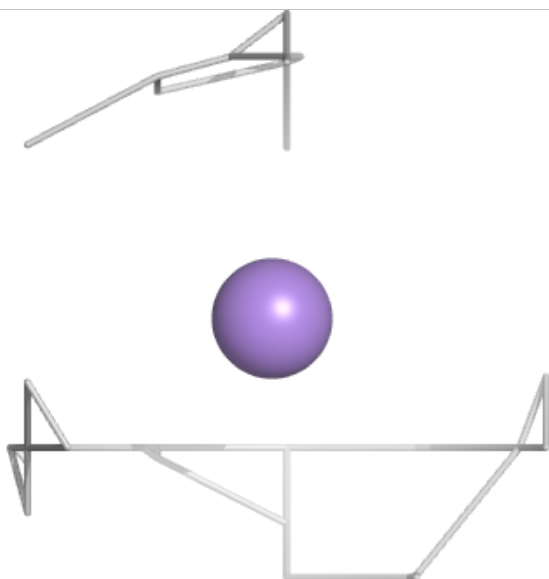
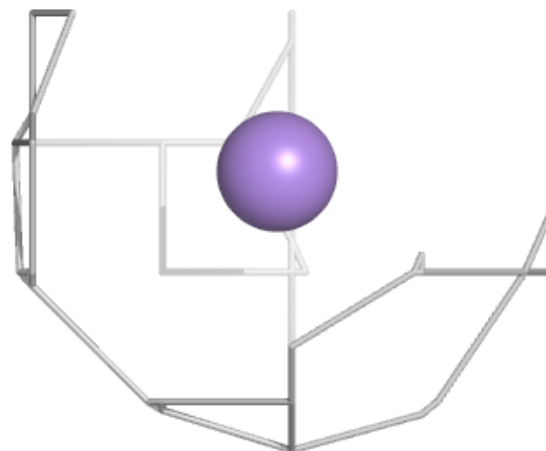
Electron density around MN R 402:

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



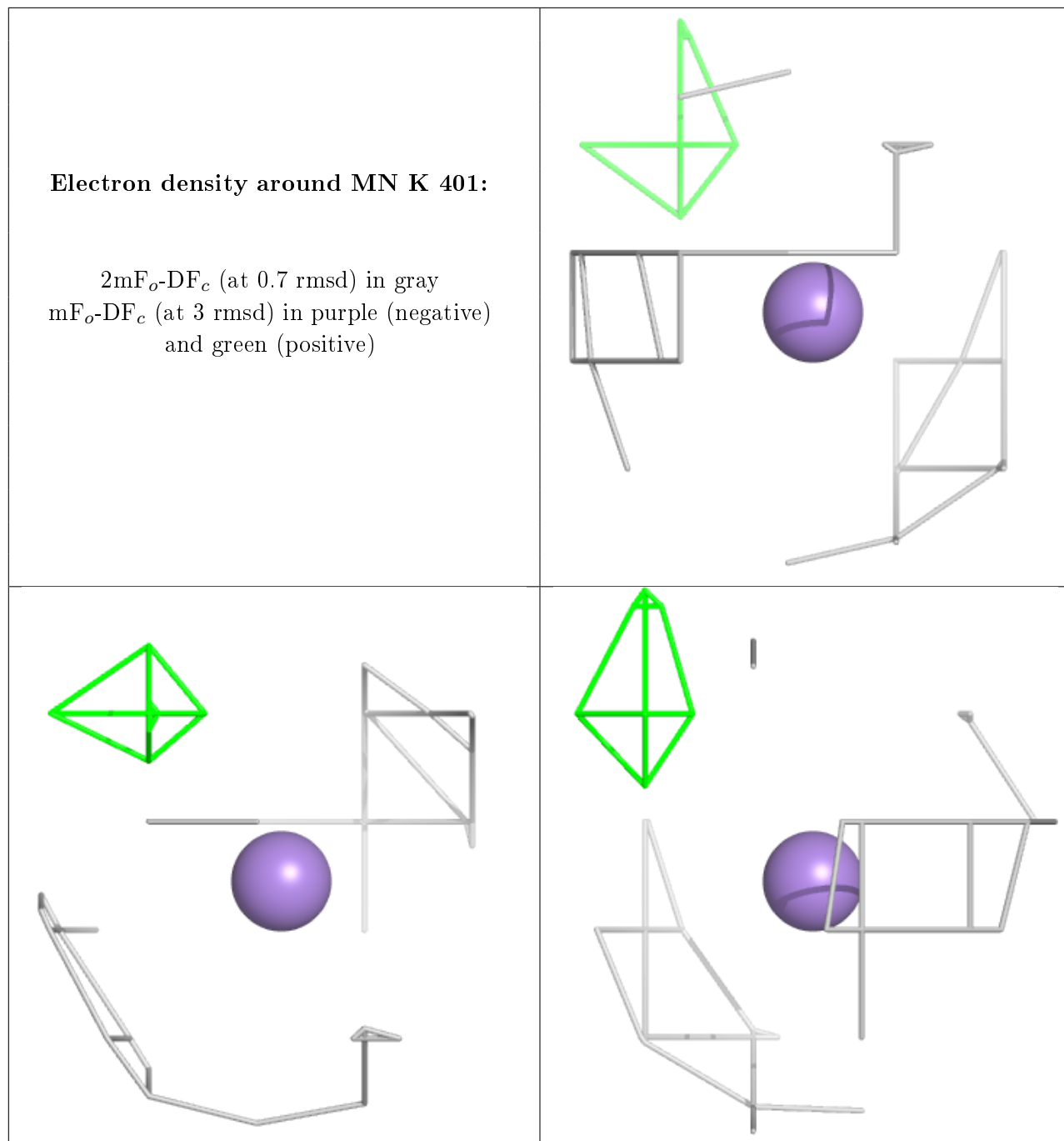
Electron density around MN R 401:

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



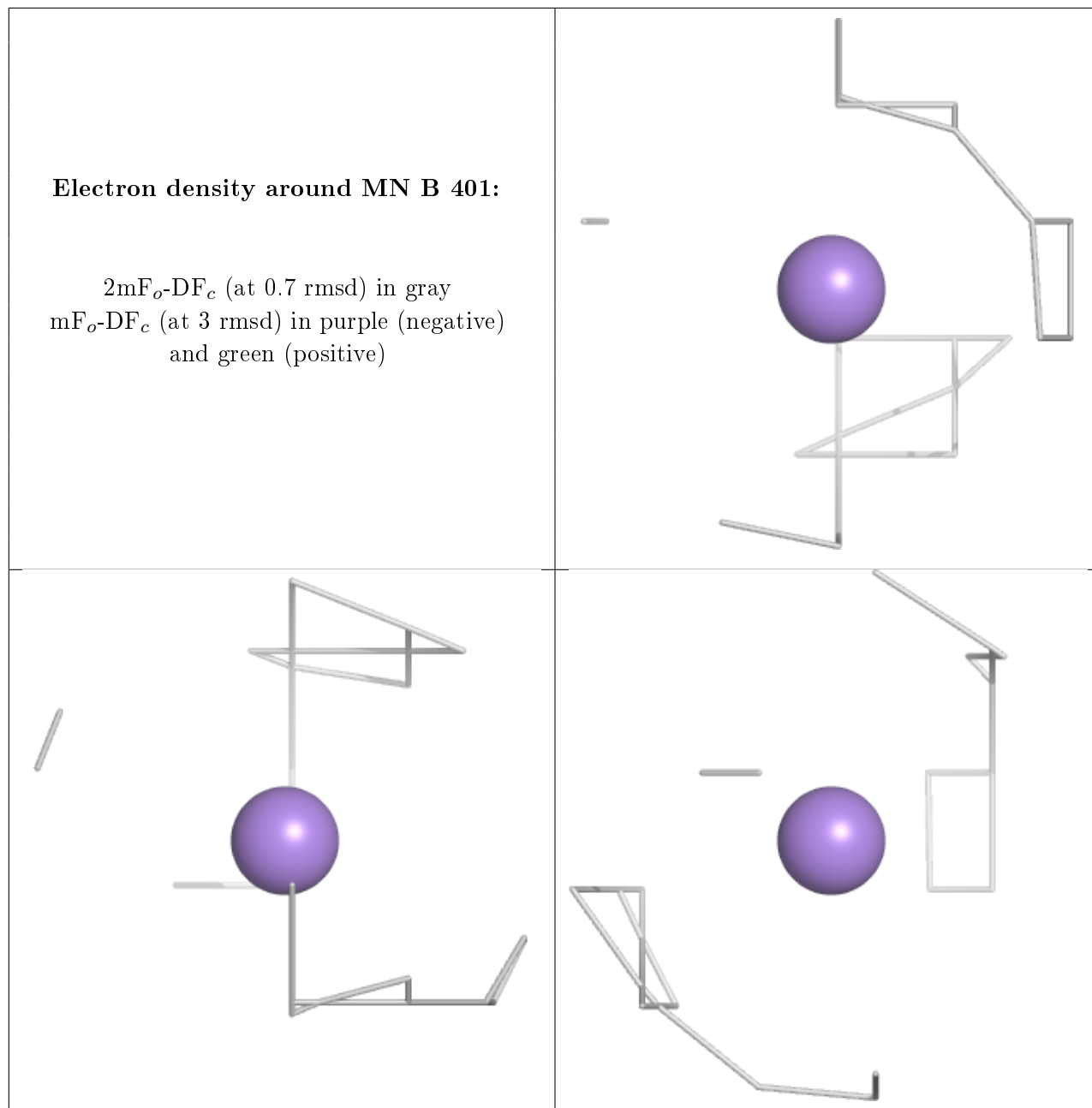
Electron density around MN K 401:

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



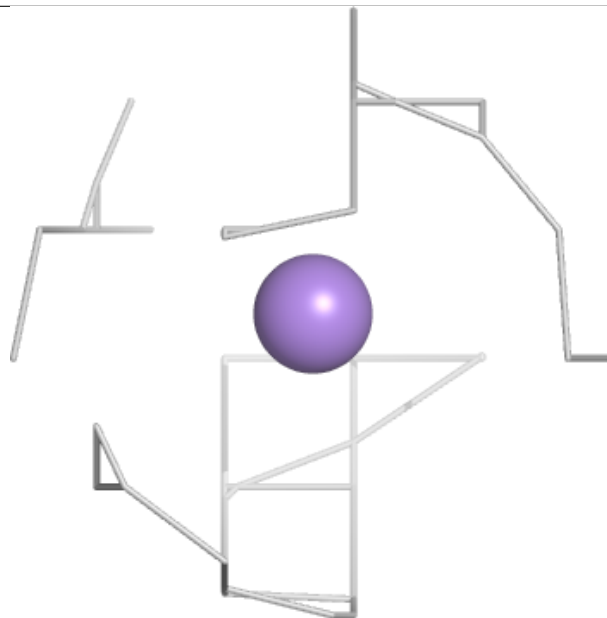
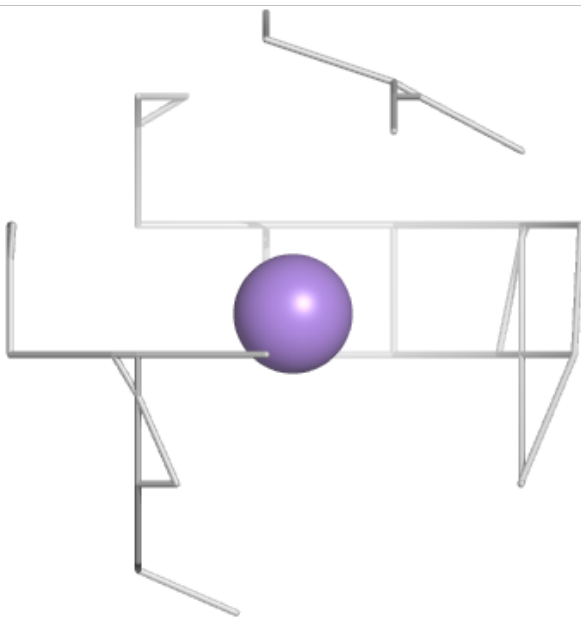
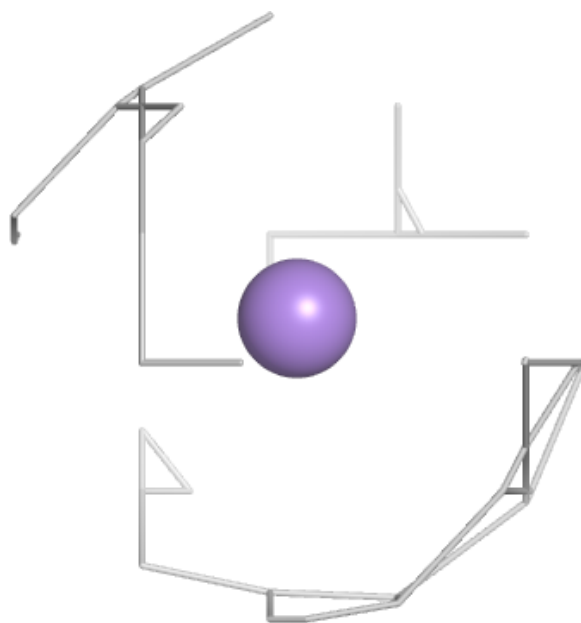
Electron density around MN B 401:

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



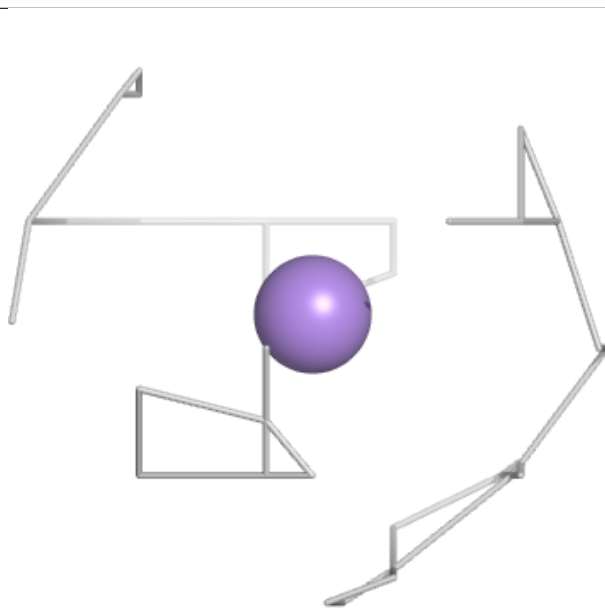
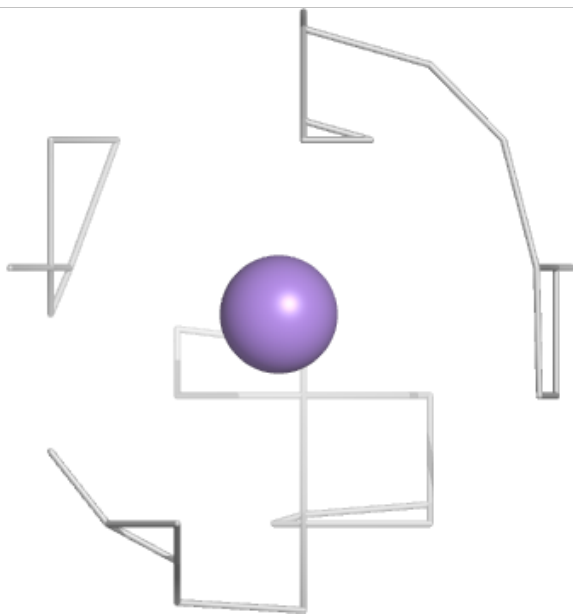
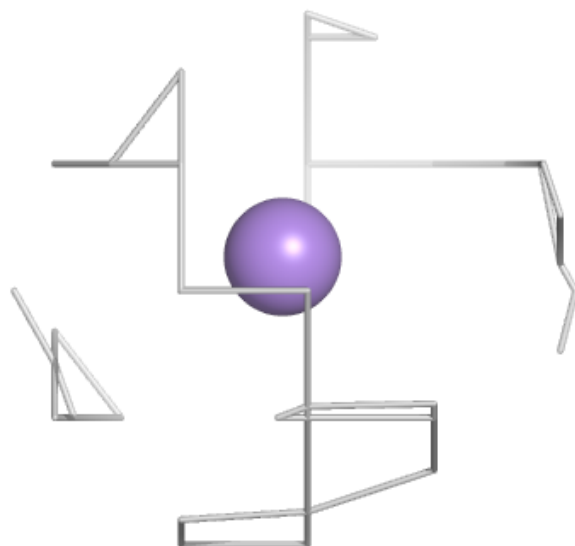
Electron density around MN I 401:

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



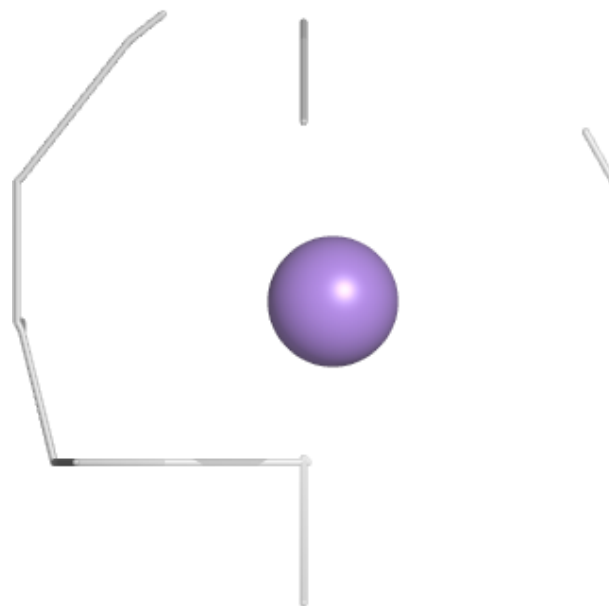
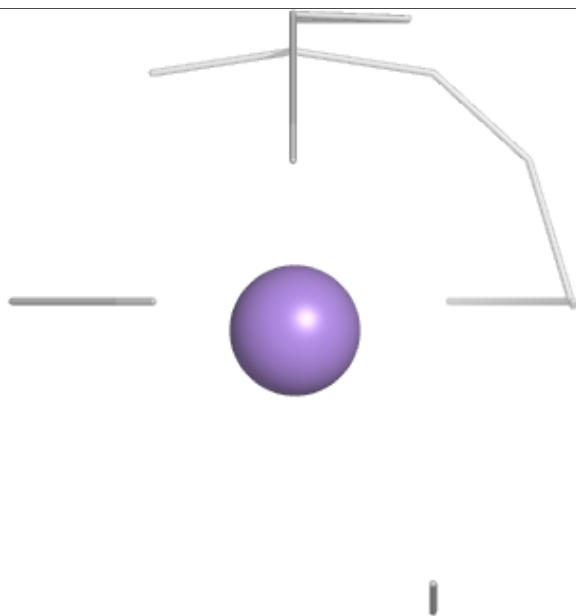
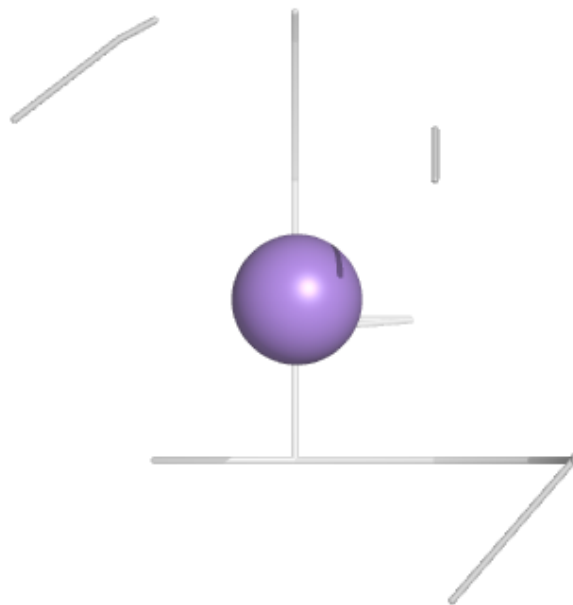
Electron density around MN F 401:

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



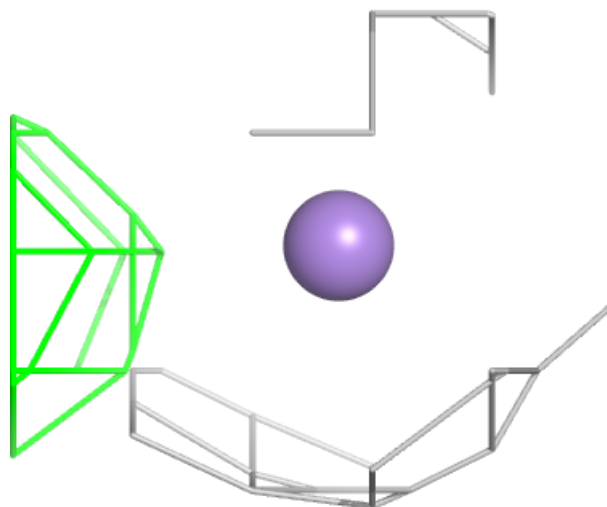
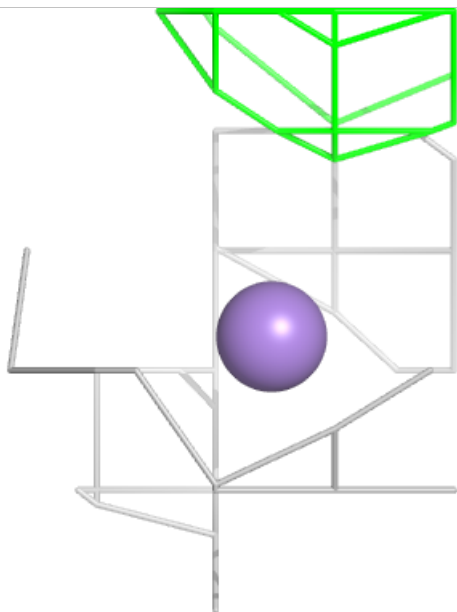
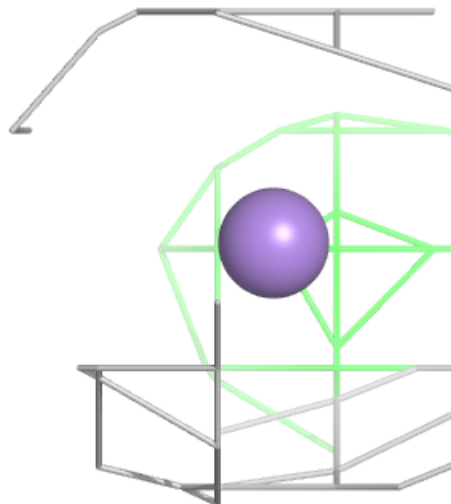
Electron density around MN A 401:

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



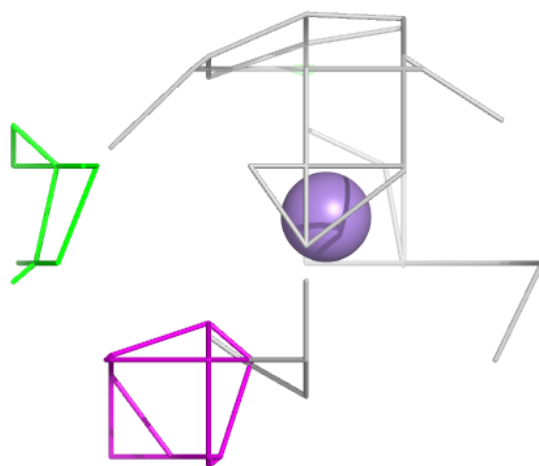
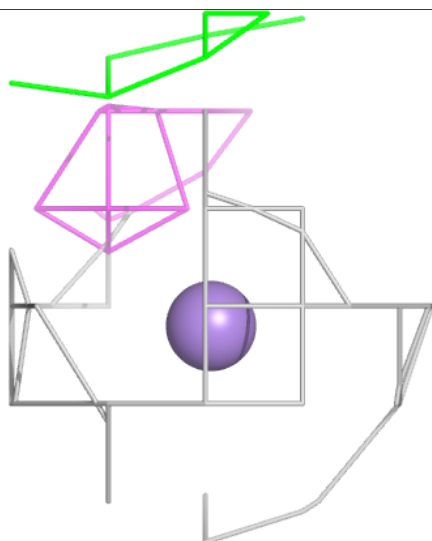
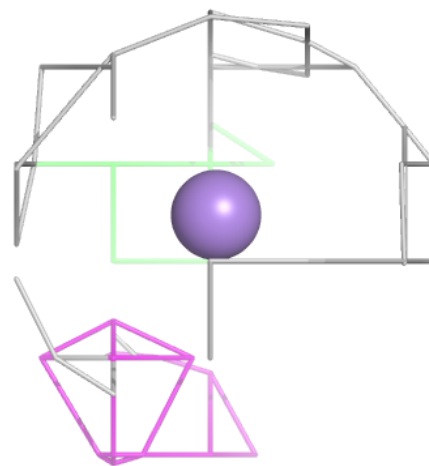
Electron density around MN L 402:

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



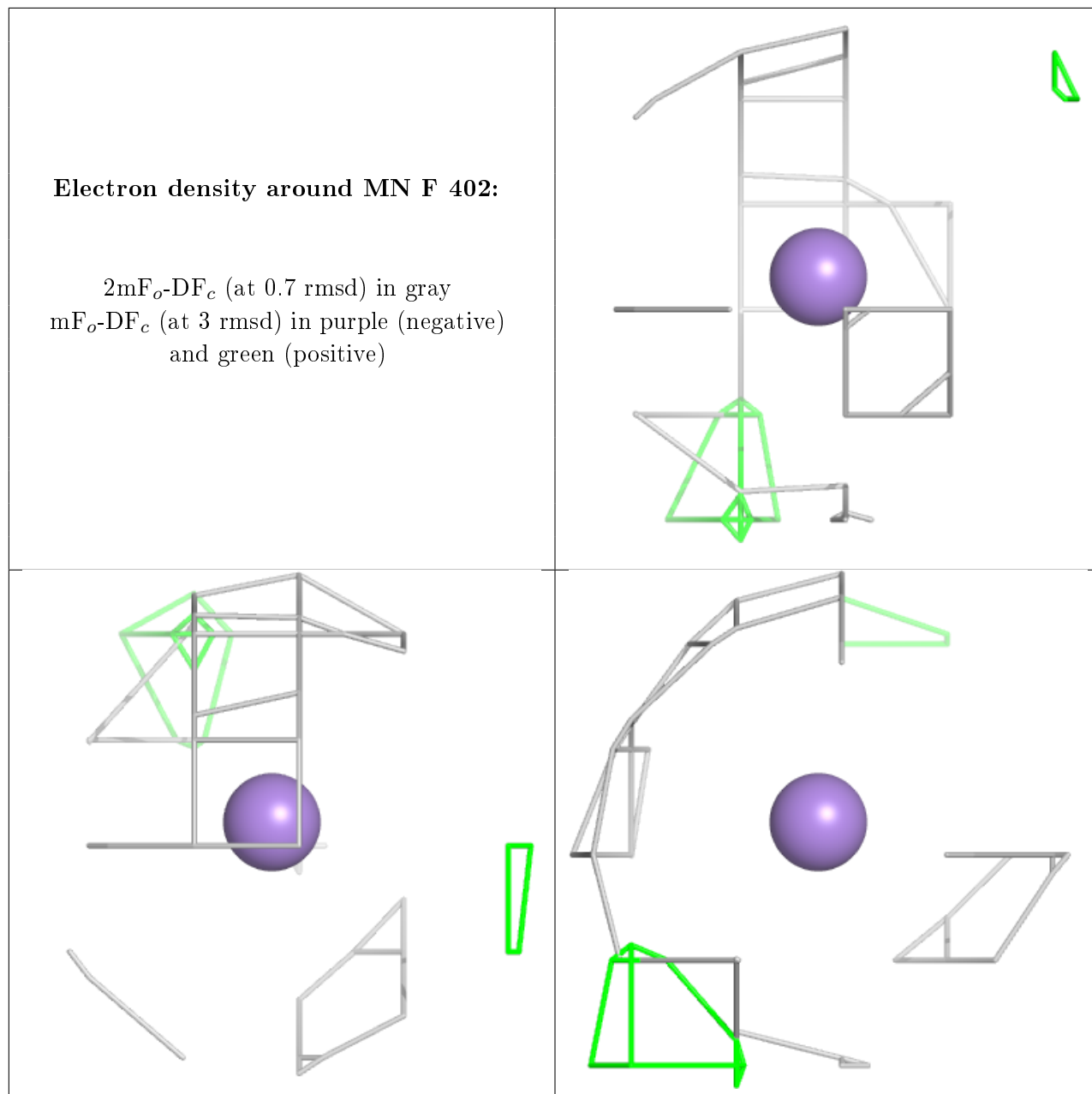
Electron density around MN E 402:

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



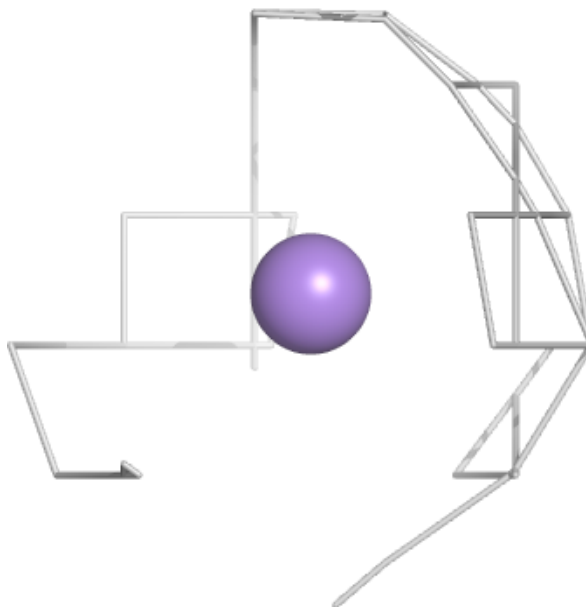
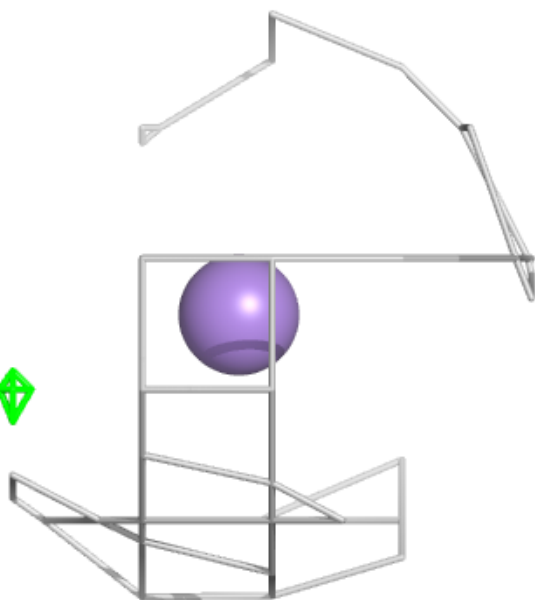
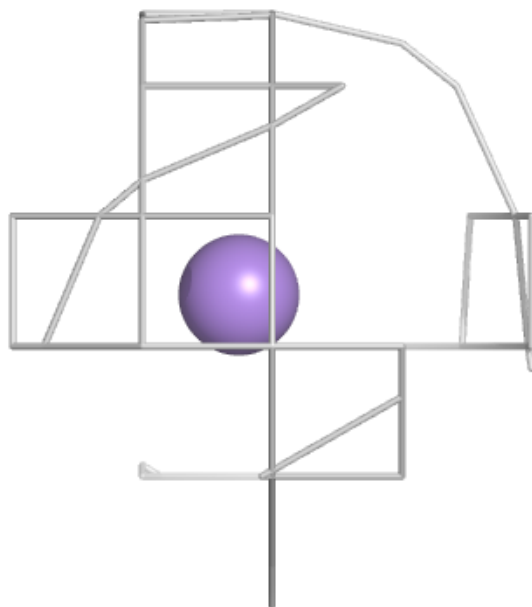
Electron density around MN F 402:

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



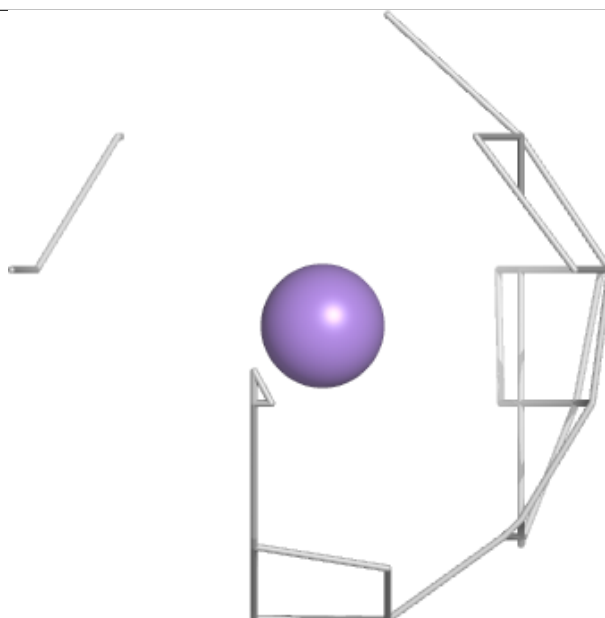
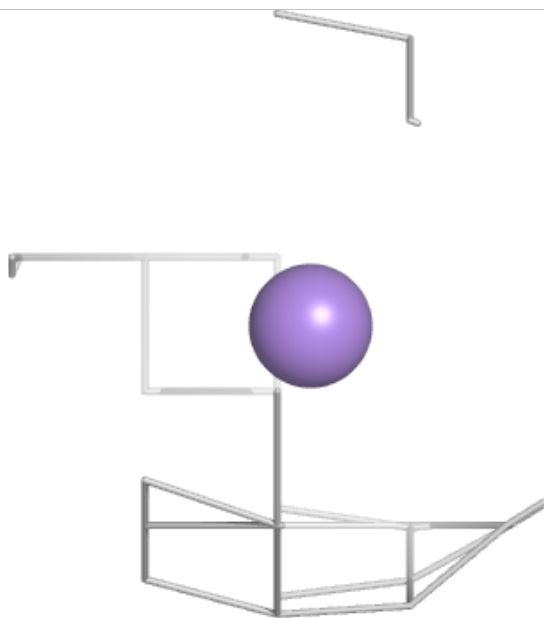
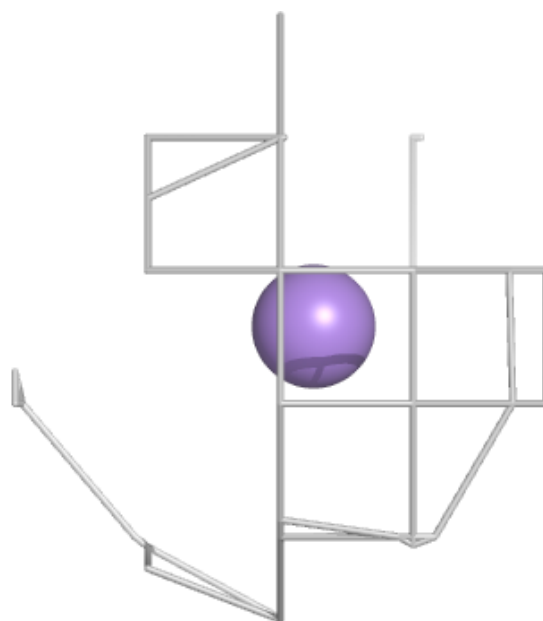
Electron density around MN H 402:

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



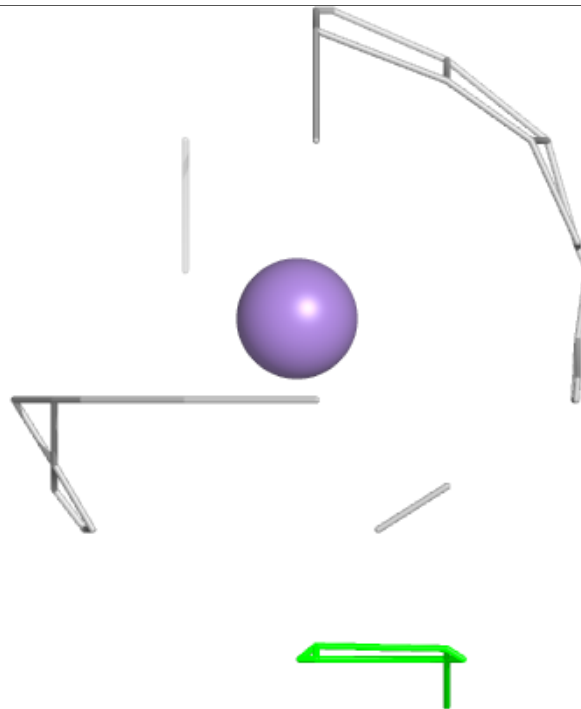
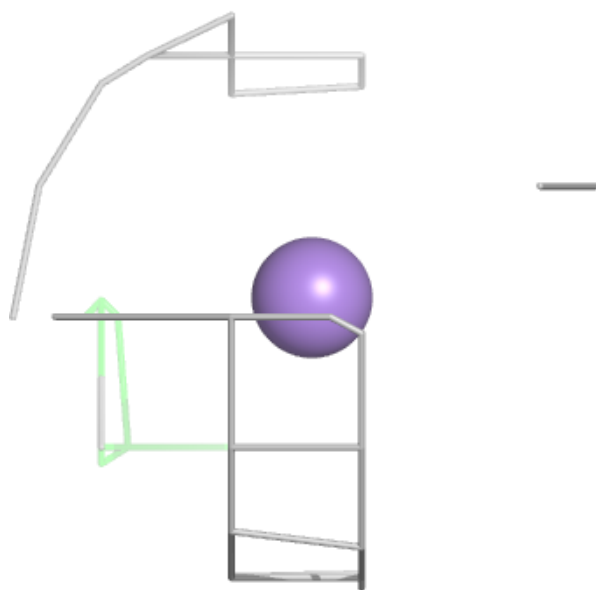
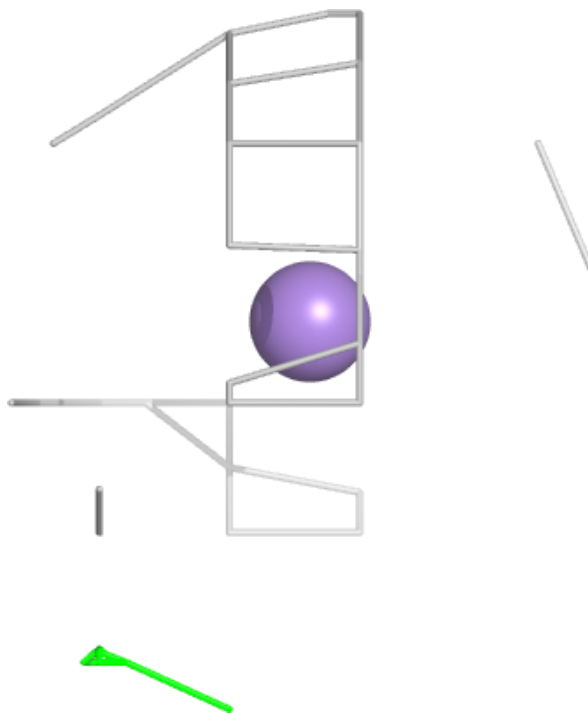
Electron density around MN Q 402:

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



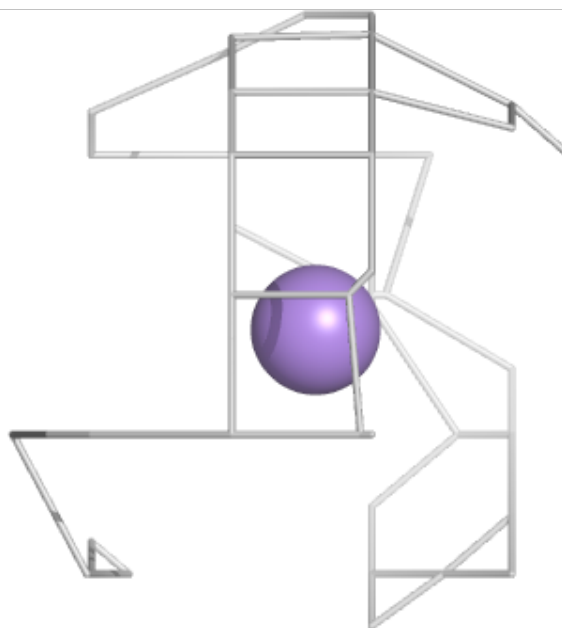
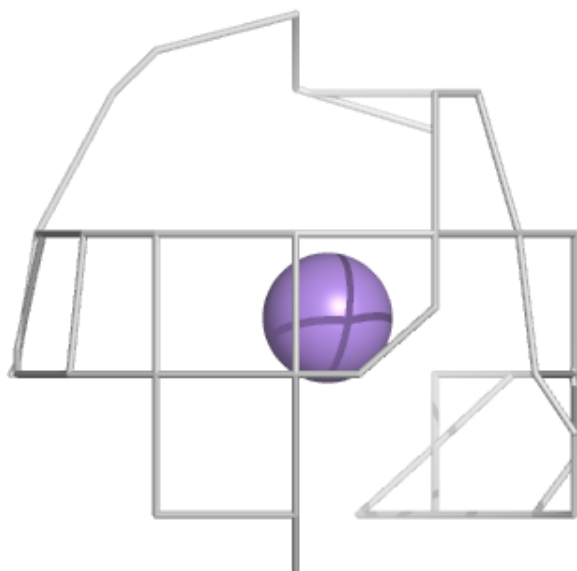
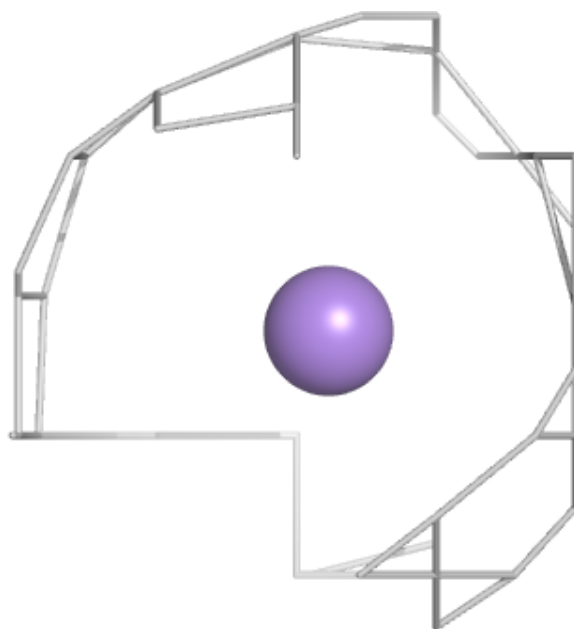
Electron density around MN Q 401:

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



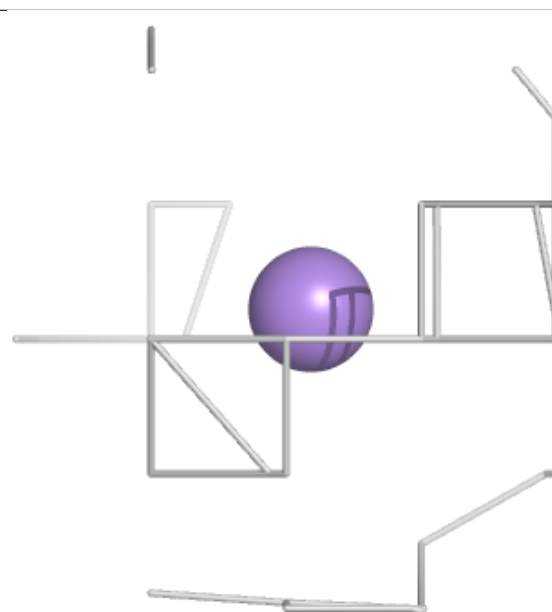
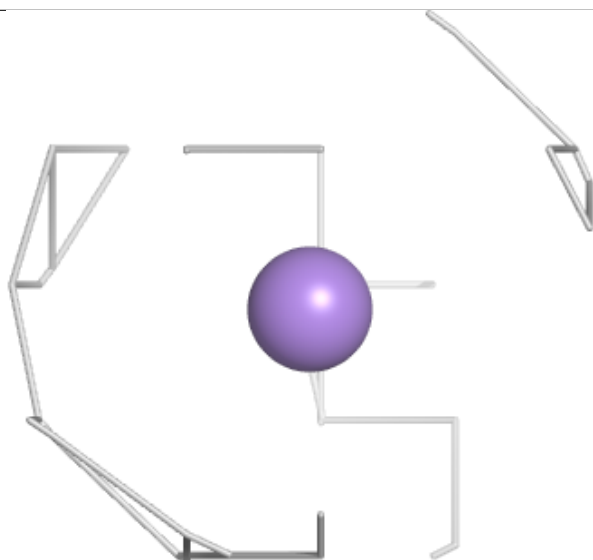
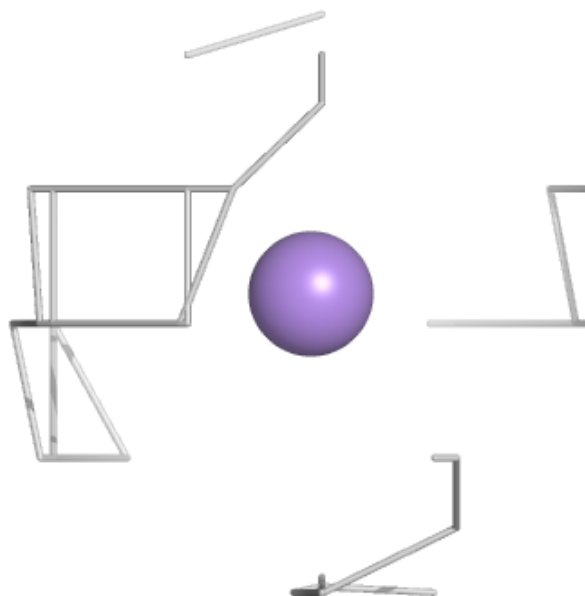
Electron density around MN I 402:

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



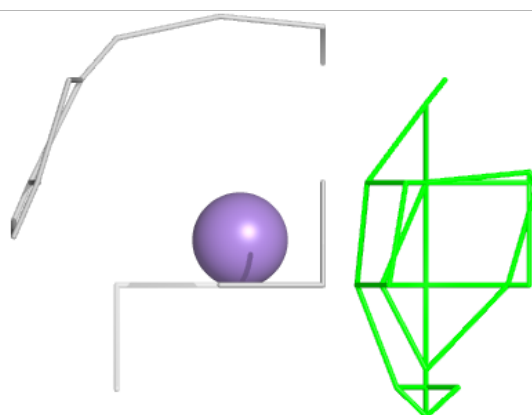
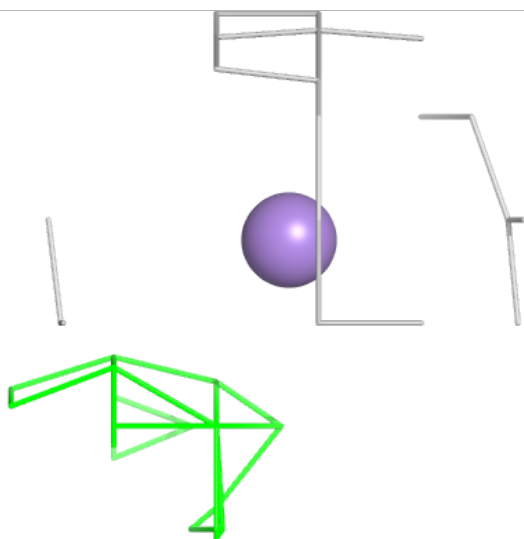
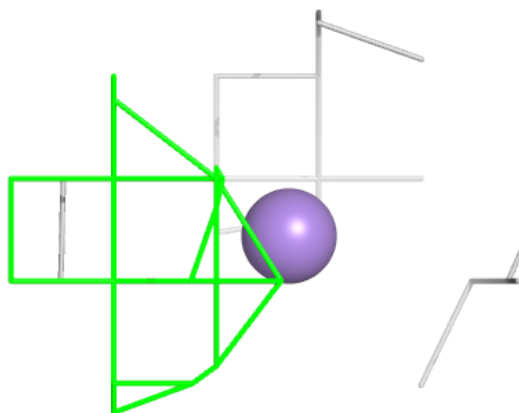
Electron density around MN G 401:

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



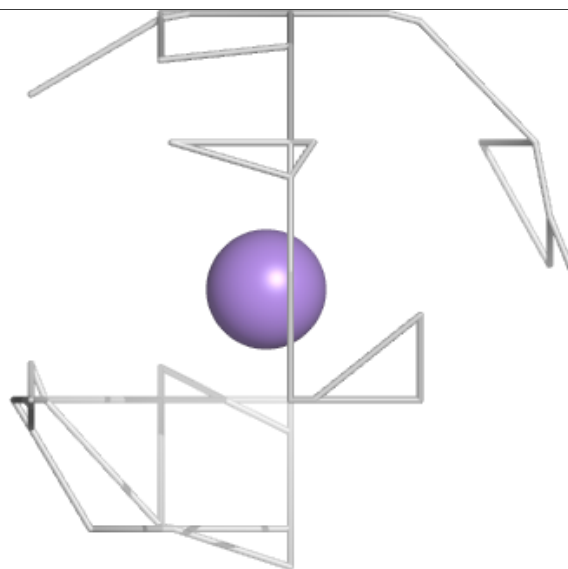
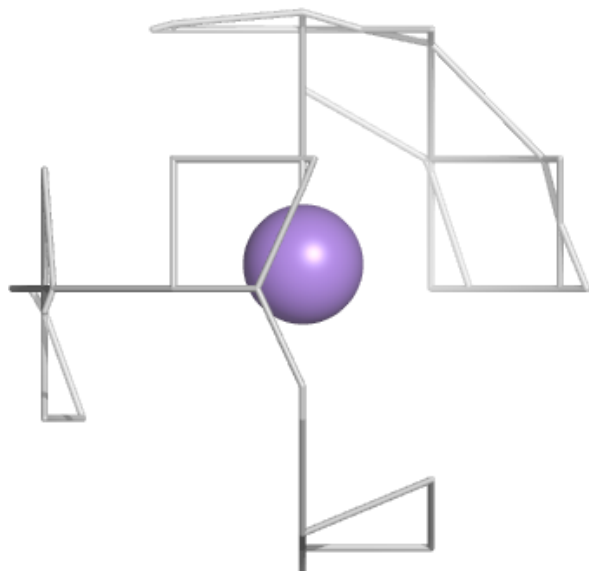
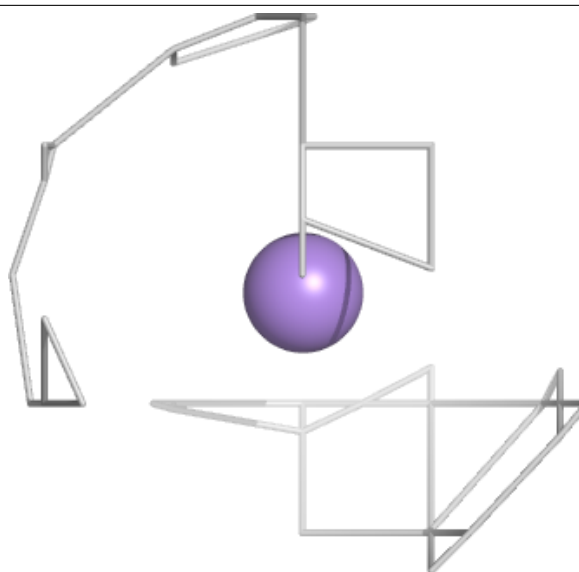
Electron density around MN L 401:

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



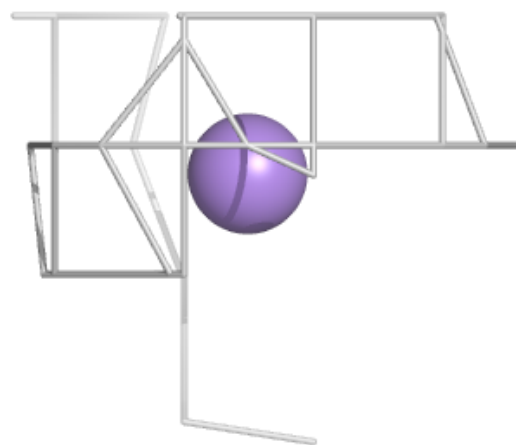
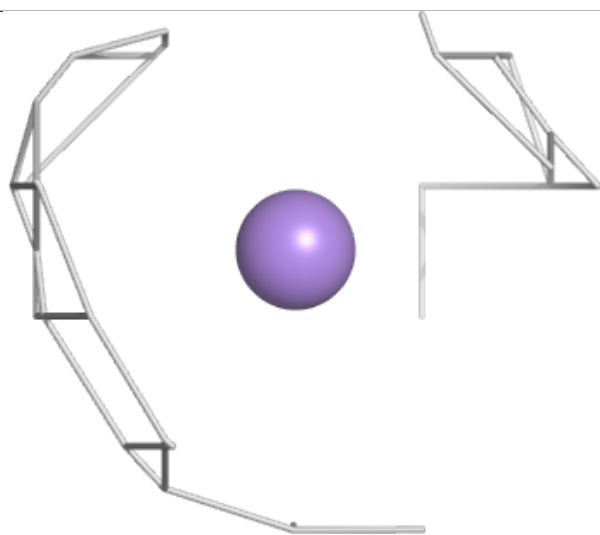
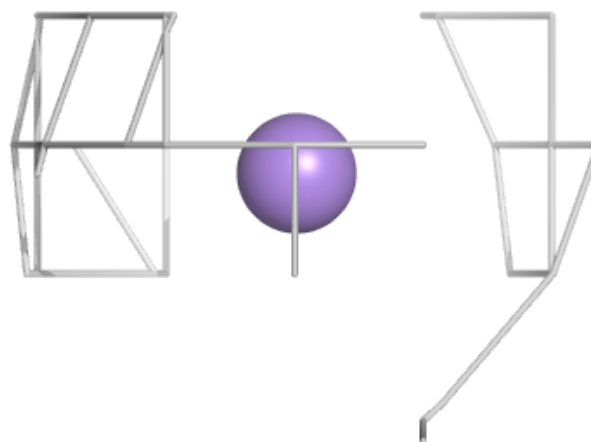
Electron density around MN J 401:

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



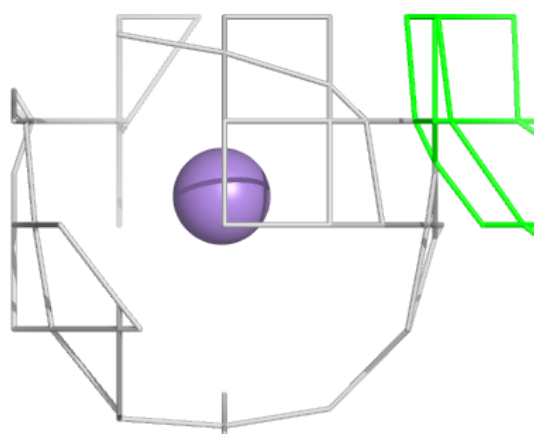
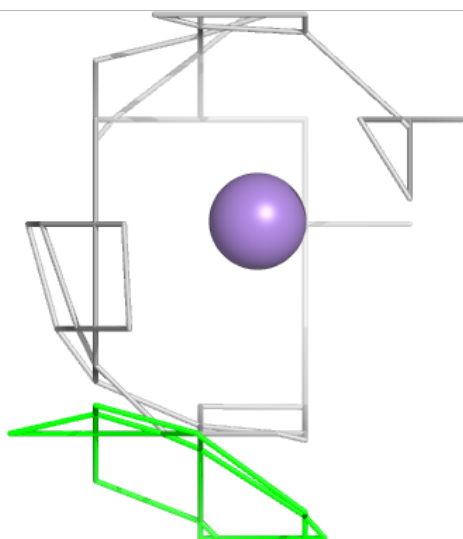
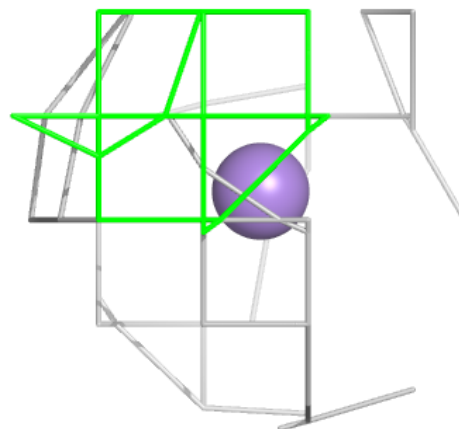
Electron density around MN D 402:

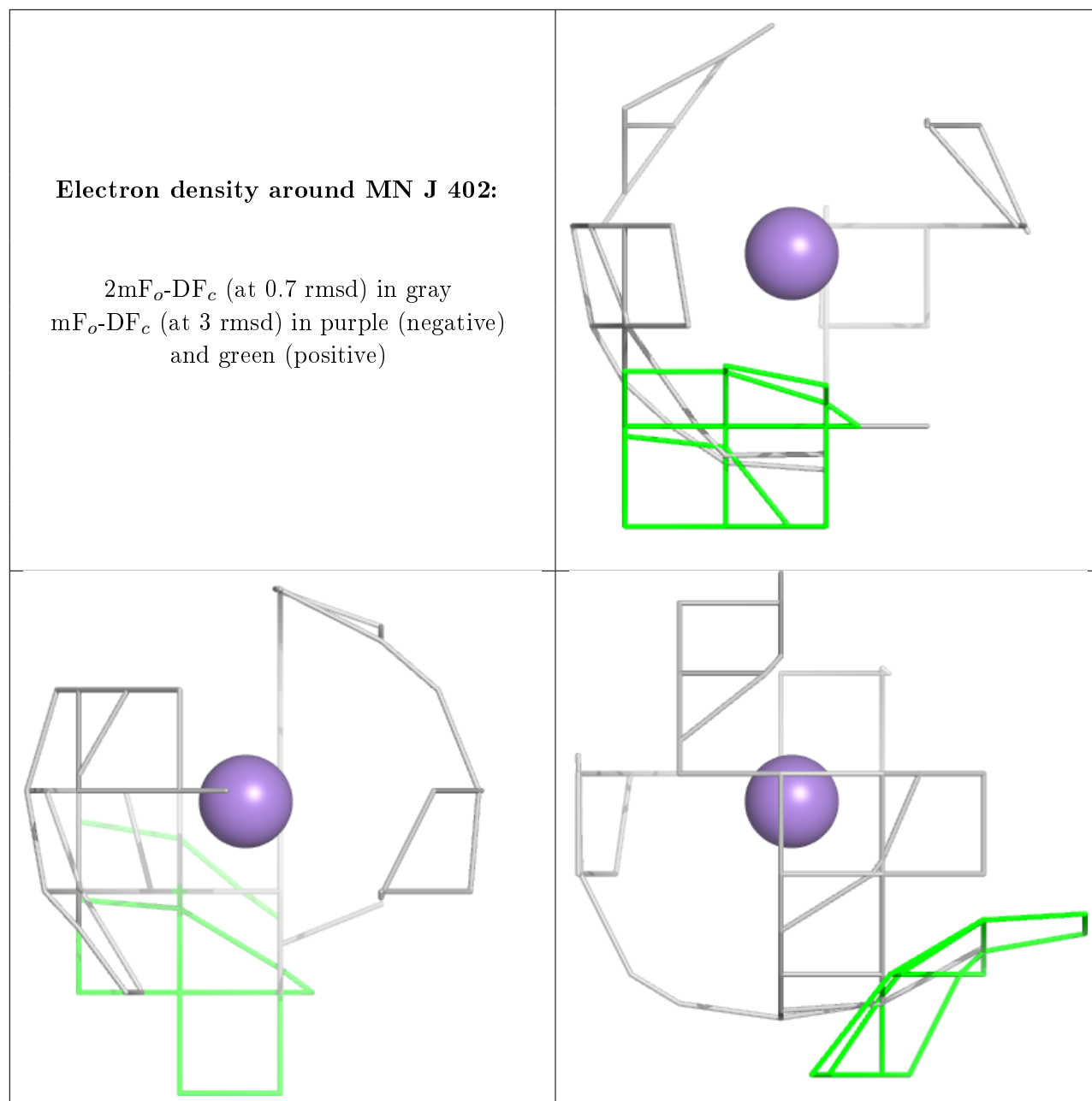
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MN 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.