Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2023 – 07:13 pm GMT

PDB ID	:	8PZY
Title	:	Intracellular leucine aminopeptidase of Pseudomonas aeruginosa PA14 - hexameric assembly with manganese bound
Authors	:	Simpson, M.C.; Czekster, C.M.; Harding, C.J.
Deposited on	:	2023-07-27
Resolution	:	1.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

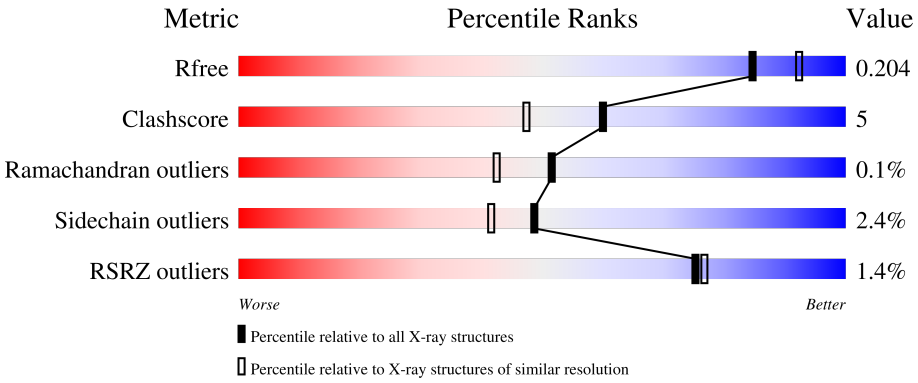
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	517	91% 6%
1	B	517	89% 7%
1	C	517	91% 5%
1	D	517	87% 9%
1	E	517	2% 86% 9%

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Mol	Chain	Length	Quality of chain
1	F	517	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	F	604	-	-	-	X
8	P03	F	606	-	-	X	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 24801 atoms, of which 144 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Probable cytosol aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	1	1	0
			3711	2348	649	699	15			
1	B	499	Total	C	N	O	S	0	2	0
			3719	2353	652	699	15			
1	C	499	Total	C	N	O	S	0	2	0
			3719	2353	652	699	15			
1	D	499	Total	C	N	O	S	0	2	0
			3719	2353	652	699	15			
1	E	499	Total	C	N	O	S	0	2	0
			3719	2353	652	699	15			
1	F	499	Total	C	N	O	S	0	1	0
			3711	2348	649	699	15			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q02RY8
A	1	HIS	-	expression tag	UNP Q02RY8
A	2	HIS	-	expression tag	UNP Q02RY8
A	3	HIS	-	expression tag	UNP Q02RY8
A	4	HIS	-	expression tag	UNP Q02RY8
A	5	HIS	-	expression tag	UNP Q02RY8
A	6	HIS	-	expression tag	UNP Q02RY8
A	7	ASP	-	expression tag	UNP Q02RY8
A	8	TYR	-	expression tag	UNP Q02RY8
A	9	ASP	-	expression tag	UNP Q02RY8
A	10	ILE	-	expression tag	UNP Q02RY8
A	11	PRO	-	expression tag	UNP Q02RY8
A	12	THR	-	expression tag	UNP Q02RY8
A	13	THR	-	expression tag	UNP Q02RY8
A	14	GLU	-	expression tag	UNP Q02RY8
A	15	ASN	-	expression tag	UNP Q02RY8
A	16	LEU	-	expression tag	UNP Q02RY8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	17	TYR	-	expression tag	UNP Q02RY8
A	18	PHE	-	expression tag	UNP Q02RY8
A	19	GLN	-	expression tag	UNP Q02RY8
A	20	GLY	-	expression tag	UNP Q02RY8
A	21	GLY	-	expression tag	UNP Q02RY8
B	0	MET	-	initiating methionine	UNP Q02RY8
B	1	HIS	-	expression tag	UNP Q02RY8
B	2	HIS	-	expression tag	UNP Q02RY8
B	3	HIS	-	expression tag	UNP Q02RY8
B	4	HIS	-	expression tag	UNP Q02RY8
B	5	HIS	-	expression tag	UNP Q02RY8
B	6	HIS	-	expression tag	UNP Q02RY8
B	7	ASP	-	expression tag	UNP Q02RY8
B	8	TYR	-	expression tag	UNP Q02RY8
B	9	ASP	-	expression tag	UNP Q02RY8
B	10	ILE	-	expression tag	UNP Q02RY8
B	11	PRO	-	expression tag	UNP Q02RY8
B	12	THR	-	expression tag	UNP Q02RY8
B	13	THR	-	expression tag	UNP Q02RY8
B	14	GLU	-	expression tag	UNP Q02RY8
B	15	ASN	-	expression tag	UNP Q02RY8
B	16	LEU	-	expression tag	UNP Q02RY8
B	17	TYR	-	expression tag	UNP Q02RY8
B	18	PHE	-	expression tag	UNP Q02RY8
B	19	GLN	-	expression tag	UNP Q02RY8
B	20	GLY	-	expression tag	UNP Q02RY8
B	21	GLY	-	expression tag	UNP Q02RY8
C	0	MET	-	initiating methionine	UNP Q02RY8
C	1	HIS	-	expression tag	UNP Q02RY8
C	2	HIS	-	expression tag	UNP Q02RY8
C	3	HIS	-	expression tag	UNP Q02RY8
C	4	HIS	-	expression tag	UNP Q02RY8
C	5	HIS	-	expression tag	UNP Q02RY8
C	6	HIS	-	expression tag	UNP Q02RY8
C	7	ASP	-	expression tag	UNP Q02RY8
C	8	TYR	-	expression tag	UNP Q02RY8
C	9	ASP	-	expression tag	UNP Q02RY8
C	10	ILE	-	expression tag	UNP Q02RY8
C	11	PRO	-	expression tag	UNP Q02RY8
C	12	THR	-	expression tag	UNP Q02RY8
C	13	THR	-	expression tag	UNP Q02RY8
C	14	GLU	-	expression tag	UNP Q02RY8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	15	ASN	-	expression tag	UNP Q02RY8
C	16	LEU	-	expression tag	UNP Q02RY8
C	17	TYR	-	expression tag	UNP Q02RY8
C	18	PHE	-	expression tag	UNP Q02RY8
C	19	GLN	-	expression tag	UNP Q02RY8
C	20	GLY	-	expression tag	UNP Q02RY8
C	21	GLY	-	expression tag	UNP Q02RY8
D	0	MET	-	initiating methionine	UNP Q02RY8
D	1	HIS	-	expression tag	UNP Q02RY8
D	2	HIS	-	expression tag	UNP Q02RY8
D	3	HIS	-	expression tag	UNP Q02RY8
D	4	HIS	-	expression tag	UNP Q02RY8
D	5	HIS	-	expression tag	UNP Q02RY8
D	6	HIS	-	expression tag	UNP Q02RY8
D	7	ASP	-	expression tag	UNP Q02RY8
D	8	TYR	-	expression tag	UNP Q02RY8
D	9	ASP	-	expression tag	UNP Q02RY8
D	10	ILE	-	expression tag	UNP Q02RY8
D	11	PRO	-	expression tag	UNP Q02RY8
D	12	THR	-	expression tag	UNP Q02RY8
D	13	THR	-	expression tag	UNP Q02RY8
D	14	GLU	-	expression tag	UNP Q02RY8
D	15	ASN	-	expression tag	UNP Q02RY8
D	16	LEU	-	expression tag	UNP Q02RY8
D	17	TYR	-	expression tag	UNP Q02RY8
D	18	PHE	-	expression tag	UNP Q02RY8
D	19	GLN	-	expression tag	UNP Q02RY8
D	20	GLY	-	expression tag	UNP Q02RY8
D	21	GLY	-	expression tag	UNP Q02RY8
E	0	MET	-	initiating methionine	UNP Q02RY8
E	1	HIS	-	expression tag	UNP Q02RY8
E	2	HIS	-	expression tag	UNP Q02RY8
E	3	HIS	-	expression tag	UNP Q02RY8
E	4	HIS	-	expression tag	UNP Q02RY8
E	5	HIS	-	expression tag	UNP Q02RY8
E	6	HIS	-	expression tag	UNP Q02RY8
E	7	ASP	-	expression tag	UNP Q02RY8
E	8	TYR	-	expression tag	UNP Q02RY8
E	9	ASP	-	expression tag	UNP Q02RY8
E	10	ILE	-	expression tag	UNP Q02RY8
E	11	PRO	-	expression tag	UNP Q02RY8
E	12	THR	-	expression tag	UNP Q02RY8

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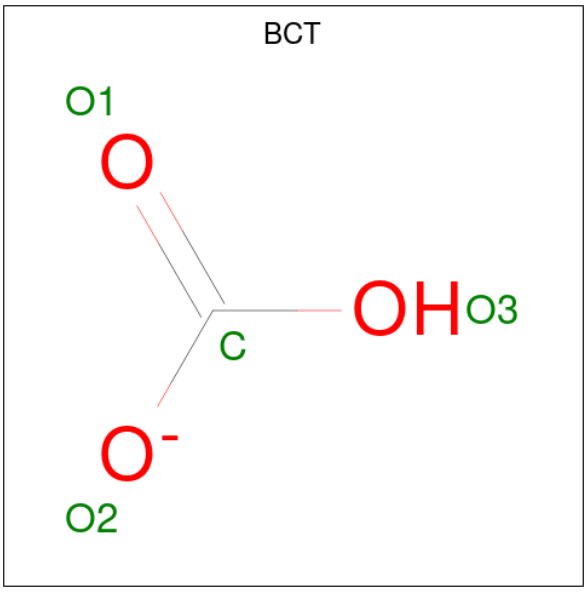
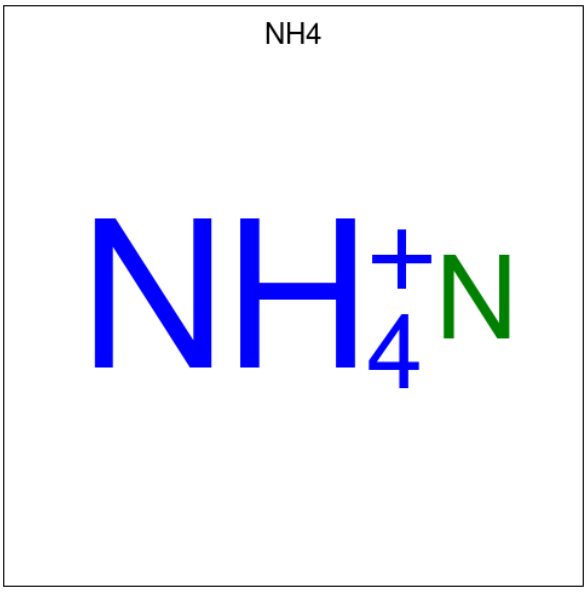
Chain	Residue	Modelled	Actual	Comment	Reference
E	13	THR	-	expression tag	UNP Q02RY8
E	14	GLU	-	expression tag	UNP Q02RY8
E	15	ASN	-	expression tag	UNP Q02RY8
E	16	LEU	-	expression tag	UNP Q02RY8
E	17	TYR	-	expression tag	UNP Q02RY8
E	18	PHE	-	expression tag	UNP Q02RY8
E	19	GLN	-	expression tag	UNP Q02RY8
E	20	GLY	-	expression tag	UNP Q02RY8
E	21	GLY	-	expression tag	UNP Q02RY8
F	0	MET	-	initiating methionine	UNP Q02RY8
F	1	HIS	-	expression tag	UNP Q02RY8
F	2	HIS	-	expression tag	UNP Q02RY8
F	3	HIS	-	expression tag	UNP Q02RY8
F	4	HIS	-	expression tag	UNP Q02RY8
F	5	HIS	-	expression tag	UNP Q02RY8
F	6	HIS	-	expression tag	UNP Q02RY8
F	7	ASP	-	expression tag	UNP Q02RY8
F	8	TYR	-	expression tag	UNP Q02RY8
F	9	ASP	-	expression tag	UNP Q02RY8
F	10	ILE	-	expression tag	UNP Q02RY8
F	11	PRO	-	expression tag	UNP Q02RY8
F	12	THR	-	expression tag	UNP Q02RY8
F	13	THR	-	expression tag	UNP Q02RY8
F	14	GLU	-	expression tag	UNP Q02RY8
F	15	ASN	-	expression tag	UNP Q02RY8
F	16	LEU	-	expression tag	UNP Q02RY8
F	17	TYR	-	expression tag	UNP Q02RY8
F	18	PHE	-	expression tag	UNP Q02RY8
F	19	GLN	-	expression tag	UNP Q02RY8
F	20	GLY	-	expression tag	UNP Q02RY8
F	21	GLY	-	expression tag	UNP Q02RY8

- Molecule 2 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



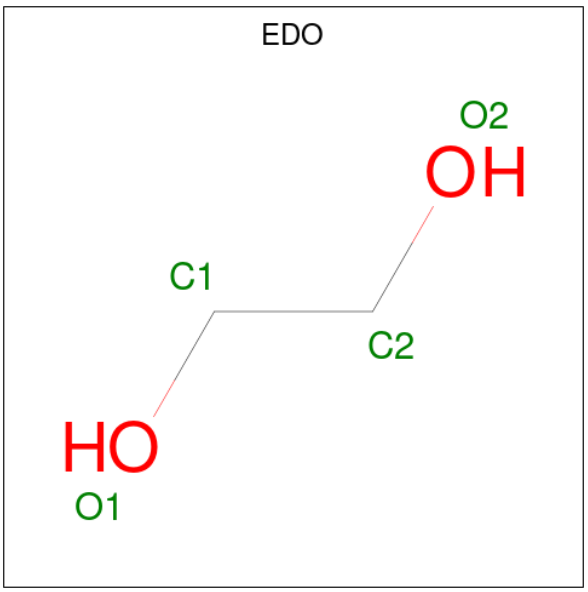
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			5	1	1	3		
2	B	1	Total	C	H	O	0	0
			5	1	1	3		
2	C	1	Total	C	H	O	0	0
			5	1	1	3		
2	D	1	Total	C	H	O	0	0
			5	1	1	3		
2	E	1	Total	C	H	O	0	0
			5	1	1	3		
2	F	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 3 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



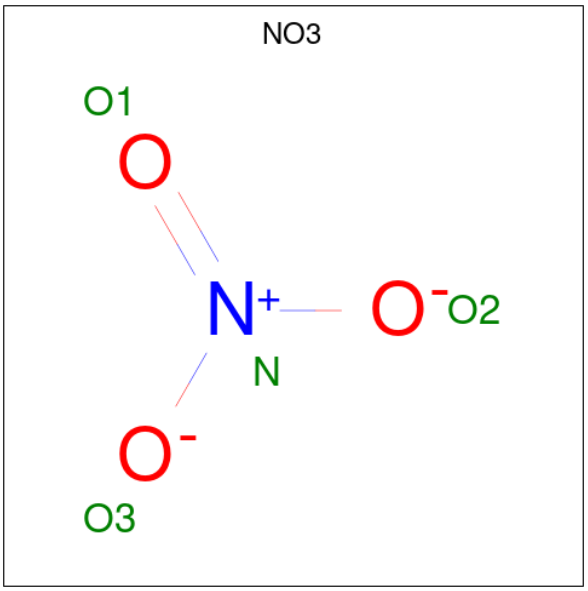
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total H N 5 4 1	0	0
3	A	1	Total H N 5 4 1	0	0
3	A	1	Total H N 5 4 1	0	0
3	A	1	Total H N 5 4 1	0	0
3	B	1	Total H N 5 4 1	0	0
3	B	1	Total H N 5 4 1	0	0
3	C	1	Total H N 5 4 1	0	0
3	C	1	Total H N 5 4 1	0	0
3	C	1	Total H N 5 4 1	0	0
3	C	1	Total H N 5 4 1	0	0
3	D	1	Total H N 5 4 1	0	0
3	E	1	Total H N 5 4 1	0	0
3	E	1	Total H N 5 4 1	0	0
3	F	1	Total H N 5 4 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	E	1	Total	C	H	O	0	0
			10	2	6	2		
4	F	1	Total	C	H	O	0	0
			10	2	6	2		
4	F	1	Total	C	H	O	0	0
			10	2	6	2		
4	F	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N O 4 1 3	0	0

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

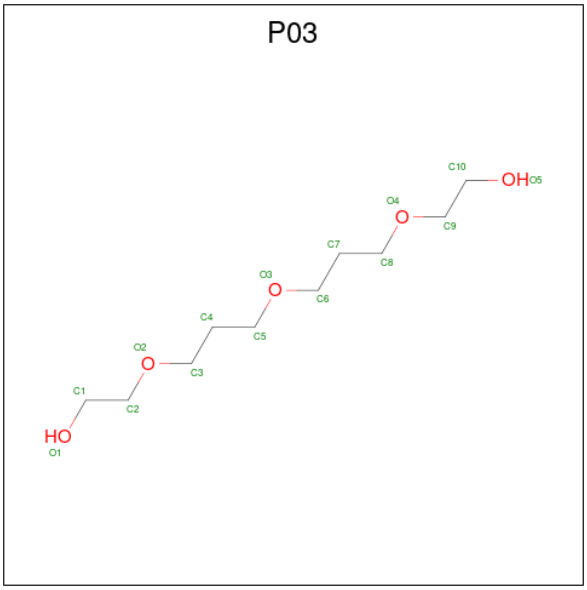
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Mn 2 2	0	0
6	B	2	Total Mn 2 2	0	0
6	C	2	Total Mn 2 2	0	0
6	D	2	Total Mn 2 2	0	0
6	E	2	Total Mn 2 2	0	0
6	F	2	Total Mn 2 2	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0

- Molecule 8 is 2-[3-[3-(2-hydroxyethoxy)propoxy]propoxy]ethanol (three-letter code: P03)

(formula: $C_{10}H_{22}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	1	Total	C	H	O	0	0
			37	10	22	5		

- Molecule 9 is water.

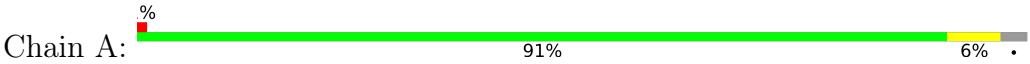
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	378	Total	O	0	0
			378	378		
9	B	377	Total	O	0	0
			377	377		
9	C	395	Total	O	0	0
			395	395		
9	D	362	Total	O	0	0
			362	362		
9	E	376	Total	O	0	0
			376	376		
9	F	361	Total	O	0	0
			361	361		

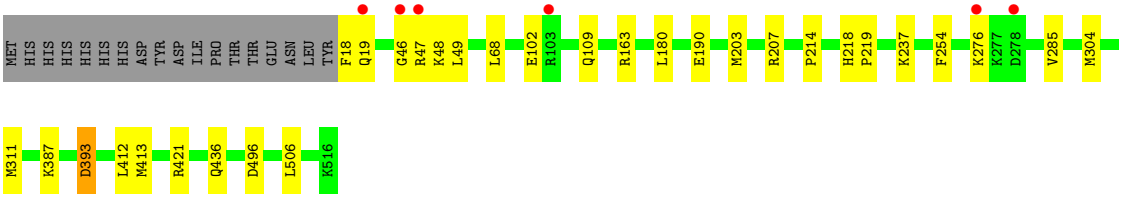
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Probable cytosol aminopeptidase

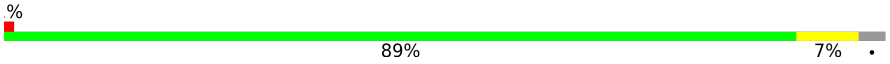
Chain A:

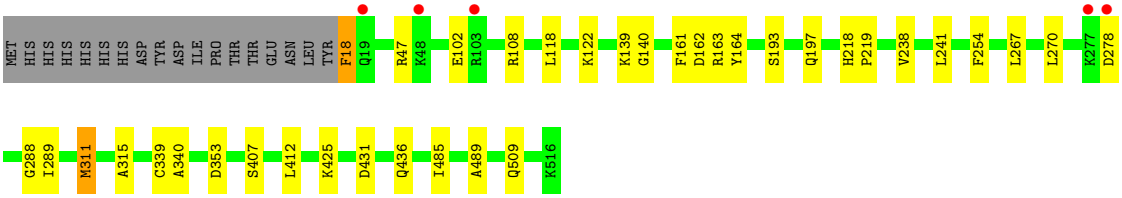




• Molecule 1: Probable cytosol aminopeptidase

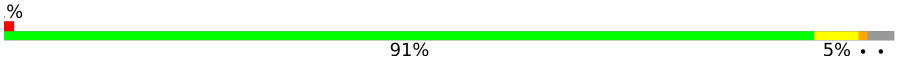
Chain B:

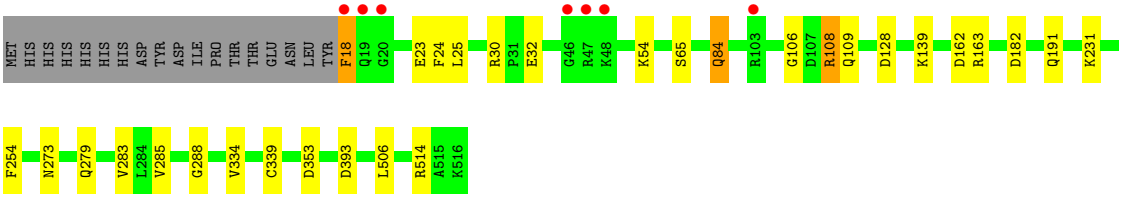




• Molecule 1: Probable cytosol aminopeptidase

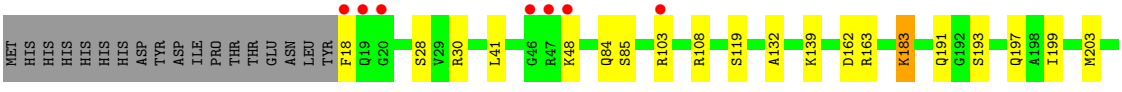
Chain C:

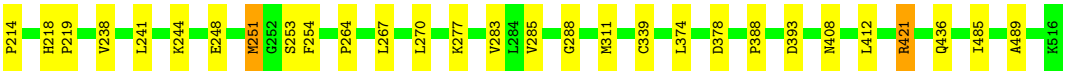




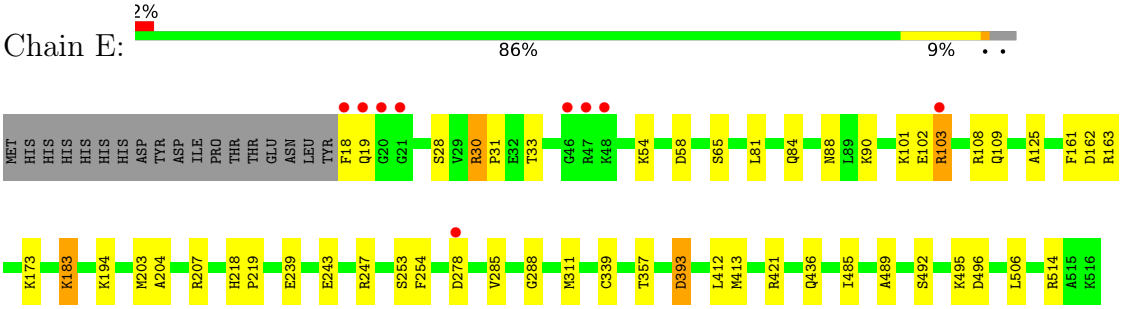
• Molecule 1: Probable cytosol aminopeptidase

Chain D:

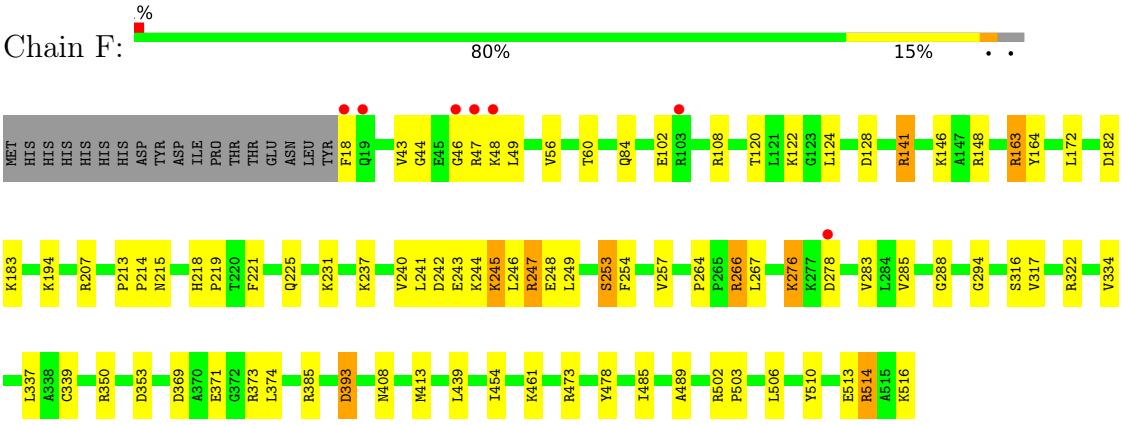




• Molecule 1: Probable cytosol aminopeptidase



• Molecule 1: Probable cytosol aminopeptidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.53Å 183.03Å 316.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.75 – 1.97 54.25 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.75-1.97) 100.0 (54.25-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 1.97Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.176 , 0.204 0.180 , 0.204	Depositor DCC
R_{free} test set	17956 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	24801	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9719e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: P03, NH4, BCT, NO3, MN, NA, EDO

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	0.44	0/3764	0.63	0/5079
1	B	0.43	0/3775	0.64	0/5093
1	C	0.41	0/3775	0.62	0/5093
1	D	0.41	0/3775	0.64	0/5093
1	E	0.43	0/3775	0.65	0/5093
1	F	0.53	0/3764	0.68	0/5079
All	All	0.44	0/22628	0.64	0/30530

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	13
All	All	0	14

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	421	ARG	Sidechain
1	F	141	ARG	Sidechain
1	F	148	ARG	Sidechain
1	F	163	ARG	Sidechain
1	F	207	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	247	ARG	Sidechain
1	F	266	ARG	Sidechain
1	F	322	ARG	Sidechain
1	F	350	ARG	Sidechain
1	F	373	ARG	Sidechain
1	F	385	ARG	Sidechain
1	F	473	ARG	Sidechain
1	F	502	ARG	Sidechain
1	F	514	ARG	Sidechain

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	3711	0	3834	22	0
1	B	3719	0	3847	29	0
1	C	3719	0	3847	26	0
1	D	3719	0	3847	38	0
1	E	3719	0	3847	43	0
1	F	3711	0	3834	55	0
2	A	4	1	1	0	0
2	B	4	1	1	0	0
2	C	4	1	1	0	0
2	D	4	1	1	0	0
2	E	4	1	1	0	0
2	F	4	1	0	0	0
3	A	4	16	0	1	0
3	B	2	8	0	0	0
3	C	4	16	0	1	0
3	D	1	4	0	0	0
3	E	2	8	0	1	0
3	F	1	4	0	0	0
4	A	8	12	12	1	0
4	B	12	18	18	2	0
4	D	4	6	6	0	0
4	E	4	6	6	3	0
4	F	12	18	18	2	0
5	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
7	A	1	0	0	0	0
8	F	15	22	22	12	0
9	A	378	0	0	6	0
9	B	377	0	0	6	0
9	C	395	0	0	6	0
9	D	362	0	0	3	0
9	E	376	0	0	5	0
9	F	361	0	0	4	0
All	All	24657	144	23143	209	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 (209) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:GLN:HG3	3:E:604:NH4:N	1.91	0.86
1:E:28:SER:HB3	1:E:183:LYS:HD3	1.59	0.84
1:D:183:LYS:HD3	1:D:183:LYS:H	1.44	0.83
1:B:425:LYS:HE3	4:B:604:EDO:H11	1.59	0.81
1:D:30:ARG:HG3	1:D:30:ARG:HH11	1.45	0.81
1:E:183:LYS:H	1:E:183:LYS:HE2	1.44	0.80
1:A:47:ARG:HD2	1:A:68:LEU:HB3	1.66	0.76
1:A:109:GLN:HG3	3:A:602:NH4:N	1.99	0.76
1:E:18:PHE:HB3	1:E:204:ALA:HB1	1.68	0.76
1:C:279:GLN:HB2	9:C:785:HOH:O	1.86	0.75
1:F:44:GLY:HA3	8:F:606:P03:H7	1.68	0.74
1:C:109:GLN:HG3	3:C:603:NH4:N	2.03	0.74
1:F:49:LEU:HA	8:F:606:P03:H6	1.69	0.73
1:E:183:LYS:H	1:E:183:LYS:CE	2.01	0.73
1:D:183:LYS:H	1:D:183:LYS:CD	2.02	0.72
1:F:44:GLY:H	8:F:606:P03:C6	2.03	0.72
1:B:139:LYS:HD2	1:B:139:LYS:C	2.10	0.71
1:A:237:LYS:HE2	9:A:763:HOH:O	1.91	0.69
1:C:106:GLY:H	1:C:109:GLN:NE2	1.89	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:LYS:HD3	1:D:183:LYS:N	2.08	0.68
1:A:47:ARG:HG2	9:A:704:HOH:O	1.94	0.67
1:F:44:GLY:H	8:F:606:P03:H6A	1.59	0.67
1:E:30:ARG:HD3	1:E:31:PRO:HD2	1.76	0.67
1:F:294:GLY:HA2	1:F:369:ASP:OD1	1.95	0.67
1:B:163[B]:ARG:NH1	9:B:703:HOH:O	2.26	0.67
1:C:84:GLN:H	4:E:601:EDO:H11	1.60	0.67
1:F:47:ARG:NH2	9:F:701:HOH:O	2.29	0.66
1:A:47:ARG:N	9:A:704:HOH:O	2.29	0.66
1:C:106:GLY:H	1:C:109:GLN:HE21	1.44	0.66
1:A:163:ARG:NH2	9:A:703:HOH:O	2.28	0.65
1:D:191:GLN:HG3	9:D:1036:HOH:O	1.97	0.64
1:F:47:ARG:HH11	1:F:47:ARG:HG2	1.63	0.64
1:B:139:LYS:HD2	1:B:140:GLY:N	2.14	0.62
1:B:509:GLN:HE21	4:B:604:EDO:H21	1.66	0.61
1:D:30:ARG:HG3	1:D:30:ARG:NH1	2.13	0.61
1:E:162:ASP:H	1:E:163[B]:ARG:HE	1.49	0.61
1:F:244:LYS:O	1:F:248:GLU:HG3	2.01	0.61
1:F:44:GLY:CA	8:F:606:P03:H7	2.31	0.60
1:B:407:SER:HB3	1:F:461:LYS:HE3	1.83	0.60
1:E:495:LYS:HG3	1:E:496:ASP:OD1	2.02	0.60
1:E:163[B]:ARG:NH1	9:E:704:HOH:O	2.34	0.60
1:F:102:GLU:HB2	9:F:731:HOH:O	2.01	0.60
1:D:162:ASP:H	1:D:163[B]:ARG:HE	1.49	0.59
1:F:513:GLU:HG3	4:F:603:EDO:O1	2.03	0.59
1:C:231:LYS:NZ	9:C:706:HOH:O	2.36	0.59
1:F:44:GLY:H	8:F:606:P03:C7	2.16	0.58
1:B:161:PHE:CE1	1:B:163[B]:ARG:HD2	2.39	0.58
1:C:191:GLN:HG3	9:C:1086:HOH:O	2.04	0.58
1:D:408:ASN:OD1	1:D:408:ASN:N	2.35	0.58
1:E:162:ASP:H	1:E:163[B]:ARG:HH21	1.52	0.57
1:B:102:GLU:HB2	9:B:826:HOH:O	2.03	0.57
1:C:108:ARG:HD2	9:C:1027:HOH:O	2.04	0.57
1:C:273:ASN:HB3	9:C:936:HOH:O	2.03	0.57
1:F:122:LYS:HD3	1:F:172:LEU:HD11	1.86	0.57
1:E:161:PHE:CE1	1:E:163[B]:ARG:HD2	2.40	0.56
1:C:84:GLN:H	4:E:601:EDO:C1	2.19	0.56
1:F:316:SER:HB2	1:F:503:PRO:HD2	1.87	0.56
1:F:241:LEU:HD12	1:F:267:LEU:HD23	1.89	0.55
1:F:276:LYS:HB3	1:F:278:ASP:OD1	2.06	0.55
1:E:243:GLU:OE1	1:E:247:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ARG:NH2	9:B:705:HOH:O	2.37	0.55
1:E:183:LYS:H	1:E:183:LYS:CD	2.20	0.55
1:F:243:GLU:H	4:F:604:EDO:H22	1.72	0.55
1:C:162:ASP:H	1:C:163[B]:ARG:HE	1.52	0.54
1:C:30:ARG:NE	1:C:32:GLU:OE2	2.40	0.54
1:F:49:LEU:CA	8:F:606:P03:H6	2.37	0.54
1:A:46:GLY:O	1:A:47:ARG:HD3	2.07	0.54
1:D:103:ARG:HH11	1:D:103:ARG:HG2	1.73	0.54
1:F:47:ARG:HG2	1:F:47:ARG:NH1	2.23	0.53
1:F:257:VAL:HG22	1:F:371:GLU:HB2	1.90	0.53
1:B:485:ILE:HD12	1:B:489:ALA:HB2	1.91	0.53
1:B:193:SER:O	1:B:197:GLN:HG3	2.08	0.53
1:B:163[B]:ARG:HE	1:B:163[B]:ARG:H	1.57	0.53
1:B:118:LEU:HG	1:B:122:LYS:HE3	1.92	0.52
1:F:253:SER:HB2	1:F:374:LEU:O	2.09	0.52
1:E:33:THR:O	1:E:90:LYS:HD3	2.09	0.52
1:F:46:GLY:H	8:F:606:P03:C1	2.23	0.52
1:D:162:ASP:OD1	1:D:163[B]:ARG:NH2	2.44	0.51
1:D:251:MET:HB3	1:D:378:ASP:OD2	2.09	0.51
1:E:514:ARG:HH11	1:E:514:ARG:HG2	1.75	0.51
1:A:285:VAL:O	1:A:393:ASP:HA	2.10	0.51
1:F:163:ARG:HG2	1:F:164:TYR:CE2	2.45	0.51
1:F:221:PHE:O	1:F:225:GLN:HG2	2.11	0.51
1:A:102:GLU:HA	1:A:102:GLU:OE1	2.11	0.51
1:C:23:GLU:HG3	1:C:25:LEU:HD21	1.92	0.51
1:F:43:VAL:HG13	8:F:606:P03:H5	1.92	0.51
1:A:102:GLU:HB2	9:A:768:HOH:O	2.10	0.50
1:A:304:MET:O	1:A:304:MET:HG2	2.11	0.50
1:F:513:GLU:HA	1:F:516:LYS:HD2	1.93	0.50
1:A:214:PRO:HG2	1:F:353:ASP:OD1	2.11	0.50
1:C:18:PHE:HB3	9:C:732:HOH:O	2.12	0.50
1:E:28:SER:HB3	1:E:183:LYS:CD	2.38	0.50
1:D:48:LYS:O	1:D:48:LYS:HG3	2.10	0.50
1:D:28:SER:HB3	1:D:183:LYS:HD3	1.94	0.50
1:E:163[B]:ARG:HE	1:E:163[B]:ARG:H	1.60	0.50
1:B:162:ASP:H	1:B:163[B]:ARG:HE	1.60	0.49
1:D:238:VAL:HG22	1:D:270:LEU:CD2	2.42	0.49
1:D:163[B]:ARG:NH1	9:D:703:HOH:O	2.43	0.49
1:F:18:PHE:HB2	9:F:748:HOH:O	2.12	0.49
1:D:199:ILE:O	1:D:203:MET:HG3	2.13	0.49
1:D:285:VAL:O	1:D:393:ASP:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:ARG:HD2	9:F:992:HOH:O	2.12	0.49
1:D:28:SER:HB3	1:D:183:LYS:CD	2.42	0.49
1:E:103:ARG:HD2	1:E:103:ARG:O	2.12	0.49
1:C:139:LYS:HD2	1:C:139:LYS:C	2.33	0.48
1:F:245:LYS:HE3	1:F:249:LEU:HG	1.95	0.48
1:F:285:VAL:O	1:F:393:ASP:HA	2.14	0.48
1:E:84:GLN:HB2	4:E:601:EDO:H22	1.96	0.47
1:B:162:ASP:H	1:B:163[B]:ARG:HH21	1.62	0.47
1:C:514:ARG:HG2	1:C:514:ARG:HH11	1.80	0.47
1:D:251:MET:HB3	1:D:378:ASP:CG	2.35	0.47
1:B:164:TYR:OH	9:B:701:HOH:O	2.20	0.47
1:D:241:LEU:HD12	1:D:267:LEU:HD23	1.96	0.47
1:E:30:ARG:HD3	1:E:30:ARG:HA	1.63	0.47
1:E:102:GLU:HA	1:E:102:GLU:OE1	2.14	0.46
1:D:264:PRO:HB3	9:D:702:HOH:O	2.14	0.46
1:A:412:LEU:O	1:A:436:GLN:HA	2.15	0.46
1:D:218:HIS:HB2	1:D:219:PRO:CD	2.45	0.46
1:E:163[B]:ARG:NH1	9:E:710:HOH:O	2.48	0.46
1:F:242:ASP:O	1:F:246:LEU:HG	2.16	0.46
1:B:311:MET:HE1	1:B:315:ALA:HB2	1.97	0.46
1:E:253:SER:HB2	1:E:357:THR:HG22	1.98	0.45
1:E:506:LEU:C	1:E:506:LEU:HD23	2.36	0.45
1:F:413:MET:HB3	1:F:439:LEU:HD11	1.98	0.45
1:D:253:SER:OG	1:D:374:LEU:O	2.30	0.45
1:D:103:ARG:HG2	1:D:103:ARG:NH1	2.30	0.45
1:B:18:PHE:HB3	9:B:703:HOH:O	2.16	0.45
1:E:514:ARG:HG2	1:E:514:ARG:NH1	2.30	0.45
1:C:514:ARG:HG2	1:C:514:ARG:NH1	2.32	0.45
1:F:141:ARG:HB3	1:F:146:LYS:HG3	1.98	0.45
1:F:485:ILE:HD12	1:F:489:ALA:HB2	1.99	0.45
1:D:288:GLY:O	1:D:339:CYS:HA	2.17	0.45
1:E:162:ASP:N	1:E:163[B]:ARG:HH21	2.15	0.44
1:F:316:SER:CB	1:F:503:PRO:HD2	2.47	0.44
1:C:288:GLY:O	1:C:339:CYS:HA	2.18	0.44
1:F:213:PRO:HB2	1:F:215:ASN:OD1	2.18	0.44
1:C:353:ASP:OD1	1:F:214:PRO:HG2	2.17	0.44
1:A:218:HIS:HB2	1:A:219:PRO:CD	2.48	0.44
1:B:288:GLY:O	1:B:339:CYS:HA	2.18	0.44
1:D:283:VAL:HG23	1:D:388:PRO:HB3	1.98	0.44
1:A:48:LYS:N	1:A:48:LYS:HD2	2.33	0.44
1:D:238:VAL:HG22	1:D:270:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:ALA:HA	1:E:173:LYS:HG3	2.00	0.44
1:D:485:ILE:HD12	1:D:489:ALA:HB2	1.99	0.44
1:C:163[B]:ARG:H	1:C:163[B]:ARG:HG2	1.40	0.43
1:D:193:SER:O	1:D:197:GLN:HG3	2.18	0.43
1:F:56:VAL:O	1:F:60:THR:HG23	2.19	0.43
1:E:163[B]:ARG:CZ	9:E:710:HOH:O	2.67	0.43
1:E:239:GLU:OE1	9:E:701:HOH:O	2.20	0.43
1:E:285:VAL:O	1:E:393:ASP:HA	2.19	0.43
1:C:506:LEU:C	1:C:506:LEU:HD23	2.39	0.43
1:F:243:GLU:HG2	1:F:247:ARG:HH12	1.83	0.43
1:F:288:GLY:O	1:F:339:CYS:HA	2.19	0.43
1:F:510:TYR:O	1:F:514:ARG:HG2	2.18	0.43
1:B:289:ILE:HA	1:B:340:ALA:O	2.18	0.43
1:D:277:LYS:HD3	1:D:277:LYS:HA	1.95	0.43
1:E:485:ILE:HD12	1:E:489:ALA:HB2	2.01	0.42
1:E:54:LYS:NZ	1:E:58:ASP:OD2	2.52	0.42
1:E:194:LYS:HE3	9:E:1035:HOH:O	2.18	0.42
1:A:203:MET:O	1:A:207:ARG:HG3	2.20	0.42
1:B:241:LEU:HD12	1:B:267:LEU:HD23	2.00	0.42
1:F:44:GLY:N	8:F:606:P03:C6	2.77	0.42
1:B:412:LEU:O	1:B:436:GLN:HA	2.19	0.42
1:C:23:GLU:CG	1:C:25:LEU:HD21	2.50	0.42
1:E:183:LYS:HE2	1:E:183:LYS:N	2.22	0.42
1:A:18:PHE:CG	1:A:19:GLN:N	2.87	0.42
1:A:190:GLU:OE2	1:A:190:GLU:HA	2.20	0.42
1:B:47:ARG:O	9:B:702:HOH:O	2.21	0.42
1:F:264:PRO:HB2	1:F:266:ARG:HH12	1.84	0.42
1:A:180:LEU:O	4:A:603:EDO:H12	2.20	0.42
1:B:238:VAL:HG22	1:B:270:LEU:CD2	2.50	0.42
1:F:240:VAL:CG1	1:F:266:ARG:HD2	2.50	0.42
1:E:183:LYS:CD	1:E:183:LYS:N	2.83	0.42
1:F:49:LEU:N	8:F:606:P03:H6	2.34	0.42
1:B:108:ARG:NH1	1:B:431:ASP:OD2	2.51	0.41
1:E:203:MET:O	1:E:207:ARG:HG3	2.20	0.41
1:F:237:LYS:HD3	1:F:237:LYS:HA	1.80	0.41
1:A:276:LYS:HD3	1:A:276:LYS:HA	1.76	0.41
1:F:506:LEU:HD23	1:F:506:LEU:C	2.41	0.41
1:D:218:HIS:HB2	1:D:219:PRO:HD2	2.01	0.41
1:E:218:HIS:HB2	1:E:219:PRO:CD	2.50	0.41
1:E:288:GLY:O	1:E:339:CYS:HA	2.20	0.41
1:D:41:LEU:HD23	1:D:132:ALA:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:LYS:NZ	1:D:248:GLU:OE2	2.53	0.41
1:F:218:HIS:HB2	1:F:219:PRO:CD	2.50	0.41
1:C:24:PHE:C	1:C:25:LEU:HD23	2.41	0.41
1:C:283:VAL:HG22	1:C:334:VAL:HB	2.01	0.41
1:E:162:ASP:H	1:E:163[B]:ARG:NH2	2.18	0.41
1:E:412:LEU:O	1:E:436:GLN:HA	2.20	0.41
1:D:421:ARG:HA	1:D:421:ARG:HD3	1.81	0.41
1:A:506:LEU:HD23	1:A:506:LEU:C	2.41	0.41
1:B:218:HIS:HB2	1:B:219:PRO:CD	2.51	0.41
1:B:353:ASP:OD1	1:D:214:PRO:HG2	2.21	0.41
1:C:32:GLU:H	1:C:32:GLU:CD	2.24	0.41
1:D:412:LEU:O	1:D:436:GLN:HA	2.21	0.41
1:F:120:THR:O	1:F:124:LEU:HG	2.21	0.41
1:B:163[B]:ARG:H	1:B:163[B]:ARG:HG2	1.51	0.41
1:E:81:LEU:HD23	1:E:81:LEU:C	2.42	0.41
1:F:48:LYS:O	8:F:606:P03:H7A	2.21	0.41
1:F:241:LEU:HD22	1:F:245:LYS:HG2	2.03	0.41
1:A:496:ASP:HB2	9:A:771:HOH:O	2.21	0.40
1:C:285:VAL:O	1:C:393:ASP:HA	2.21	0.40
1:F:283:VAL:HG22	1:F:334:VAL:HB	2.03	0.40
1:D:183:LYS:H	1:D:183:LYS:CE	2.35	0.40
1:F:317:VAL:HB	1:F:337:LEU:HD21	2.03	0.40
1:D:30:ARG:HA	1:D:30:ARG:HD2	1.90	0.40
1:E:278:ASP:OD1	1:E:278:ASP:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	498/517 (96%)	483 (97%)	14 (3%)	1 (0%)	47 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	499/517 (96%)	488 (98%)	11 (2%)	0	100	100
1	C	499/517 (96%)	488 (98%)	10 (2%)	1 (0%)	47	38
1	D	499/517 (96%)	489 (98%)	9 (2%)	1 (0%)	47	38
1	E	499/517 (96%)	489 (98%)	10 (2%)	0	100	100
1	F	498/517 (96%)	486 (98%)	11 (2%)	1 (0%)	47	38
All	All	2992/3102 (96%)	2923 (98%)	65 (2%)	4 (0%)	51	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	F	84	GLN
1	C	84	GLN
1	D	84	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	380/397 (96%)	374 (98%)	6 (2%)	62	56
1	B	381/397 (96%)	377 (99%)	4 (1%)	76	73
1	C	381/397 (96%)	374 (98%)	7 (2%)	59	51
1	D	381/397 (96%)	371 (97%)	10 (3%)	46	37
1	E	381/397 (96%)	368 (97%)	13 (3%)	37	25
1	F	380/397 (96%)	366 (96%)	14 (4%)	34	22
All	All	2284/2382 (96%)	2230 (98%)	54 (2%)	49	41

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	PHE
1	A	311	MET

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Mol	Chain	Res	Type
1	A	387	LYS
1	A	393	ASP
1	A	413	MET
1	A	421	ARG
1	B	18	PHE
1	B	254	PHE
1	B	278	ASP
1	B	311	MET
1	C	18	PHE
1	C	54	LYS
1	C	65	SER
1	C	108	ARG
1	C	128	ASP
1	C	182	ASP
1	C	254	PHE
1	D	18	PHE
1	D	85	SER
1	D	108	ARG
1	D	119	SER
1	D	139	LYS
1	D	183	LYS
1	D	251	MET
1	D	254	PHE
1	D	311	MET
1	D	421	ARG
1	E	19	GLN
1	E	30	ARG
1	E	65	SER
1	E	88	ASN
1	E	101	LYS
1	E	103	ARG
1	E	108	ARG
1	E	183	LYS
1	E	254	PHE
1	E	311	MET
1	E	393	ASP
1	E	413	MET
1	E	492	SER
1	F	108	ARG
1	F	128	ASP
1	F	182	ASP
1	F	183	LYS

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Mol	Chain	Res	Type
1	F	194	LYS
1	F	231	LYS
1	F	245	LYS
1	F	253	SER
1	F	254	PHE
1	F	276	LYS
1	F	393	ASP
1	F	408	ASN
1	F	454	ILE
1	F	478	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	C	109	GLN
1	C	191	GLN
1	E	191	GLN
1	F	408	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 45 ligands modelled in this entry, 14 are modelled with single atom and 13 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
2	BCT	A	601	-	2,3,3	1.12	0	2,3,3	4.28	1 (50%)
2	BCT	E	602	-	2,3,3	1.04	0	2,3,3	4.25	2 (100%)
2	BCT	C	601	-	2,3,3	1.04	0	2,3,3	4.29	2 (100%)
4	EDO	B	605	-	3,3,3	0.53	0	2,2,2	0.30	0
4	EDO	D	603	-	3,3,3	0.52	0	2,2,2	0.30	0
4	EDO	F	603	-	3,3,3	0.16	0	2,2,2	0.12	0
5	NO3	A	605	-	1,3,3	1.04	0	0,3,3	-	-
4	EDO	B	603	-	3,3,3	0.61	0	2,2,2	0.41	0
2	BCT	F	601	-	2,3,3	1.02	0	2,3,3	0.41	0
4	EDO	A	603	-	3,3,3	0.54	0	2,2,2	0.13	0
4	EDO	F	605	-	3,3,3	0.16	0	2,2,2	0.09	0
8	P03	F	606	-	14,14,14	0.19	0	13,13,13	0.25	0
2	BCT	B	602	-	2,3,3	1.24	0	2,3,3	3.72	1 (50%)
4	EDO	B	604	-	3,3,3	0.66	0	2,2,2	0.06	0
4	EDO	F	604	-	3,3,3	0.12	0	2,2,2	0.27	0
4	EDO	E	601	-	3,3,3	0.52	0	2,2,2	0.88	0
4	EDO	A	608	-	3,3,3	0.60	0	2,2,2	0.13	0
2	BCT	D	601	-	2,3,3	1.27	0	2,3,3	4.00	2 (100%)

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
4	EDO	B	605	-	-	1/1/1/1	-
4	EDO	F	603	-	-	0/1/1/1	-
4	EDO	B	603	-	-	1/1/1/1	-
4	EDO	A	603	-	-	0/1/1/1	-
4	EDO	F	605	-	-	1/1/1/1	-
8	P03	F	606	-	-	6/12/12/12	-
4	EDO	B	604	-	-	0/1/1/1	-
4	EDO	F	604	-	-	0/1/1/1	-
4	EDO	E	601	-	-	0/1/1/1	-
4	EDO	A	608	-	-	0/1/1/1	-
4	EDO	D	603	-	-	1/1/1/1	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	BCT	O2-C-O1	5.80	134.59	119.55
2	E	602	BCT	O2-C-O1	5.39	133.52	119.55
2	C	601	BCT	O2-C-O1	5.35	133.43	119.55
2	D	601	BCT	O2-C-O1	5.20	133.03	119.55
2	B	602	BCT	O2-C-O1	5.08	132.73	119.55
2	C	601	BCT	O3-C-O1	-2.87	112.11	119.55
2	E	602	BCT	O3-C-O1	-2.66	112.65	119.55
2	D	601	BCT	O3-C-O1	-2.24	113.74	119.55

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	606	P03	C3-C4-C5-O3
8	F	606	P03	C6-C7-C8-O4
4	D	603	EDO	O1-C1-C2-O2
8	F	606	P03	C4-C3-O2-C2
8	F	606	P03	O1-C1-C2-O2
4	B	603	EDO	O1-C1-C2-O2
4	F	605	EDO	O1-C1-C2-O2
8	F	606	P03	C7-C6-O3-C5
4	B	605	EDO	O1-C1-C2-O2
8	F	606	P03	C10-C9-O4-C8

There are no ring outliers.

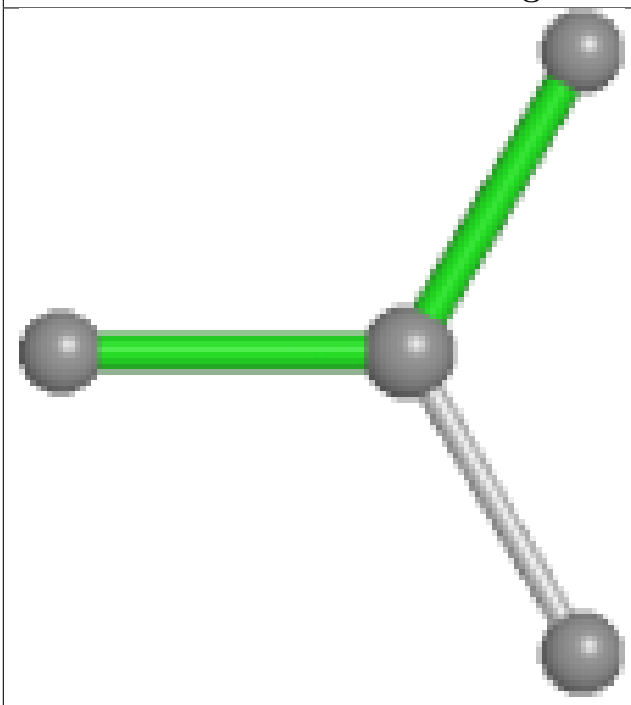
6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	603	EDO	1	0
4	A	603	EDO	1	0
8	F	606	P03	12	0
4	B	604	EDO	2	0
4	F	604	EDO	1	0
4	E	601	EDO	3	0

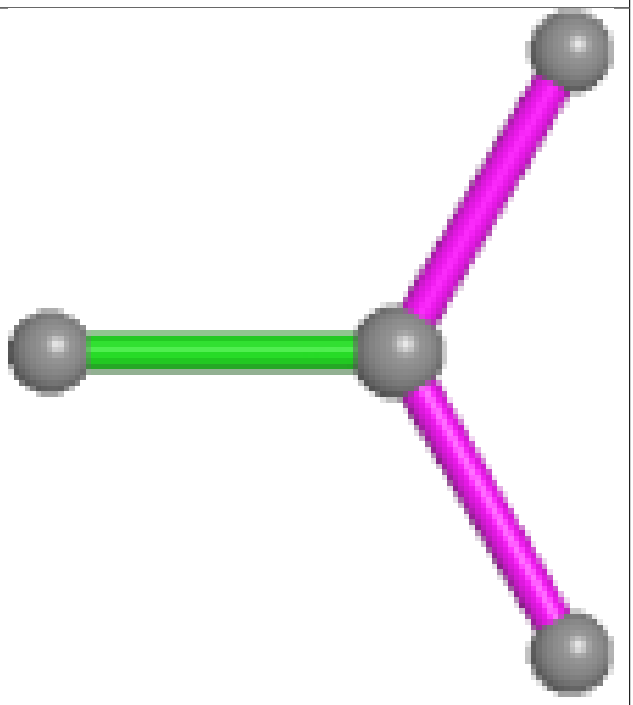
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

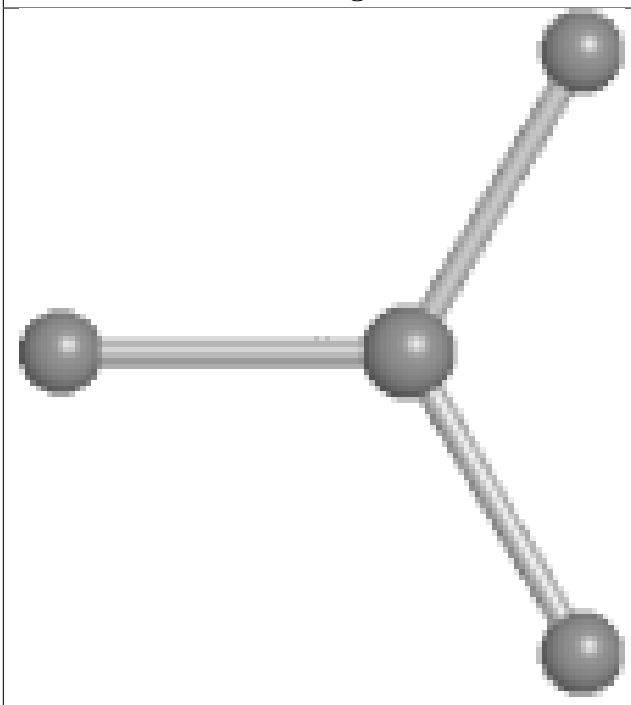
Ligand BCT A 601



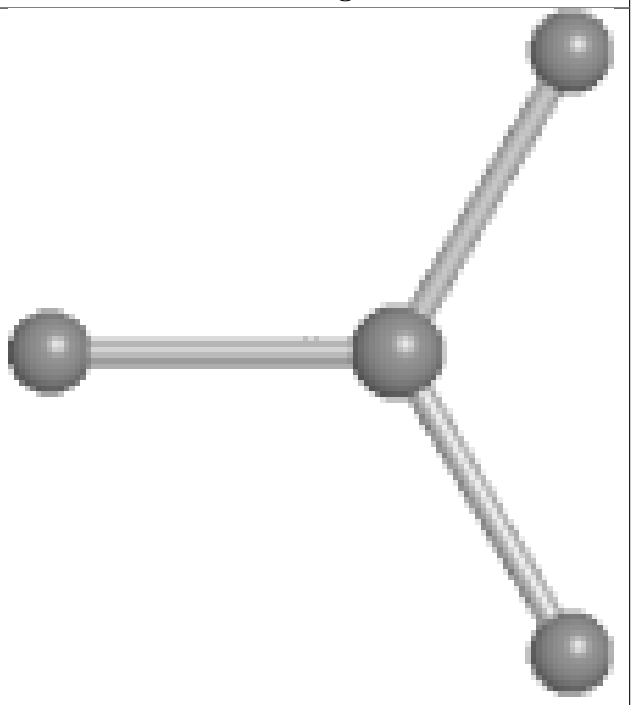
Bond lengths



Bond angles

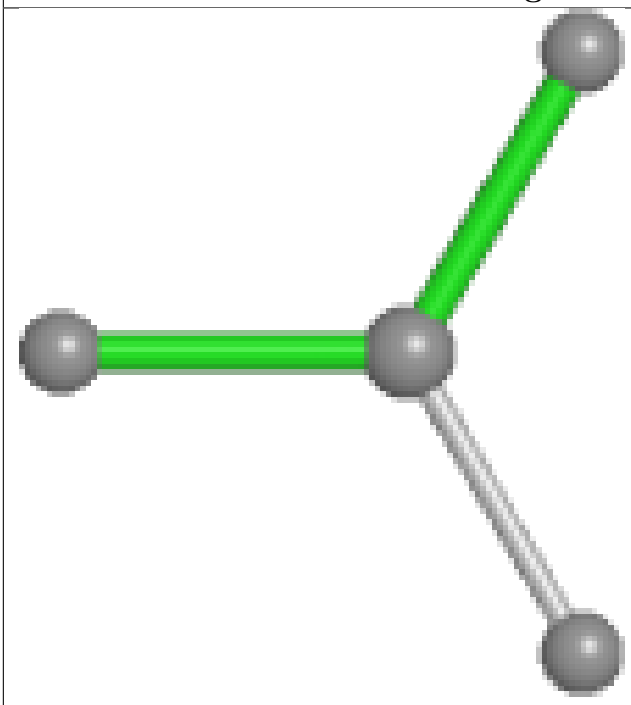


Torsions



Rings

Ligand BCT E 602



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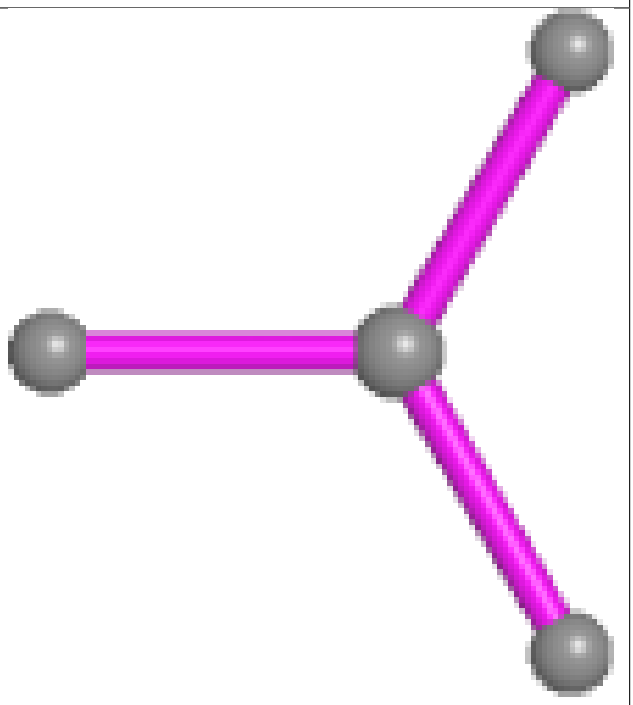
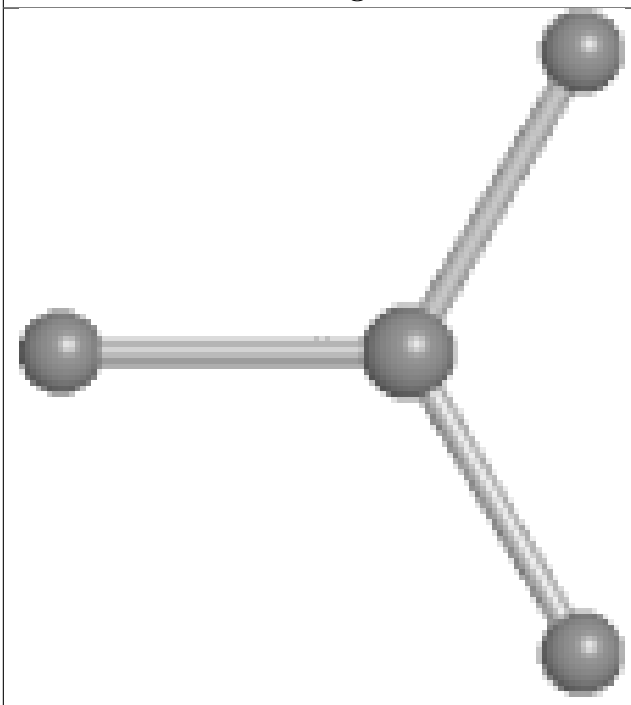


Bond angles



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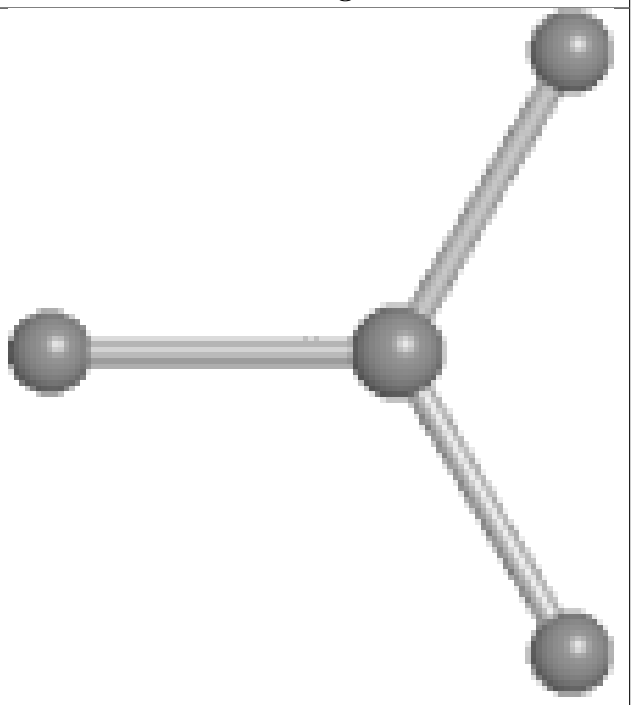
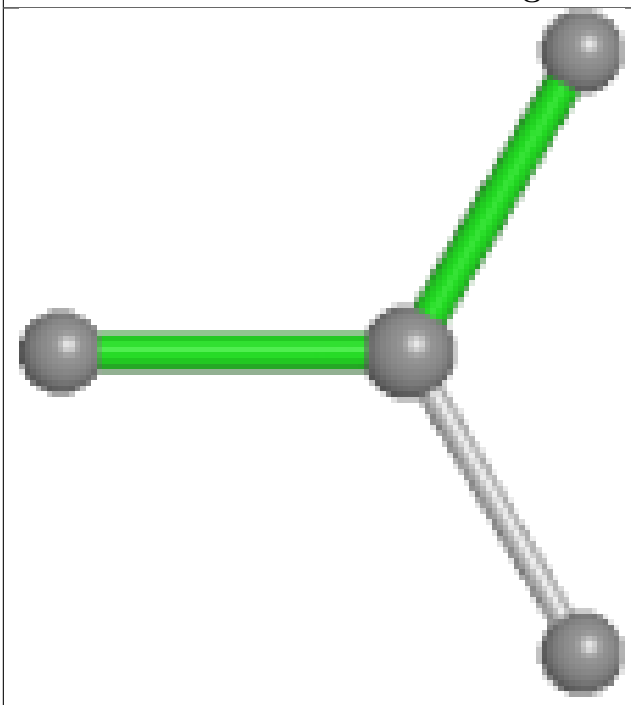
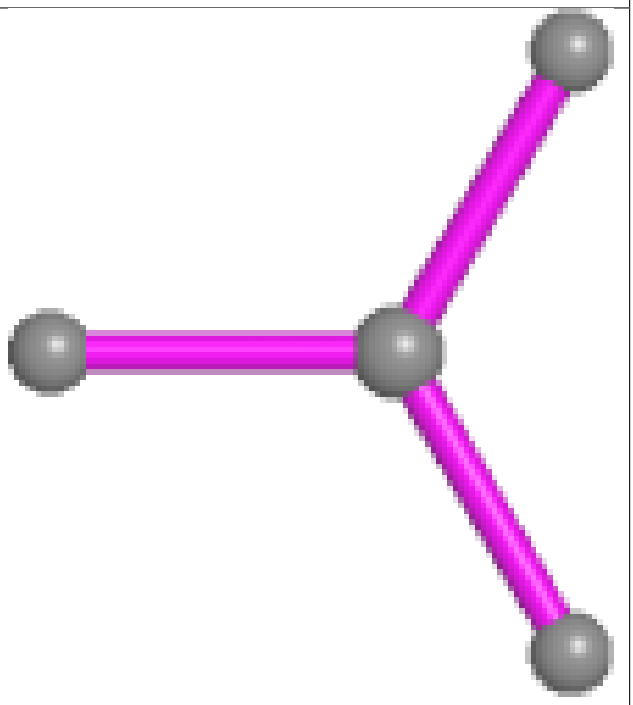


Rings

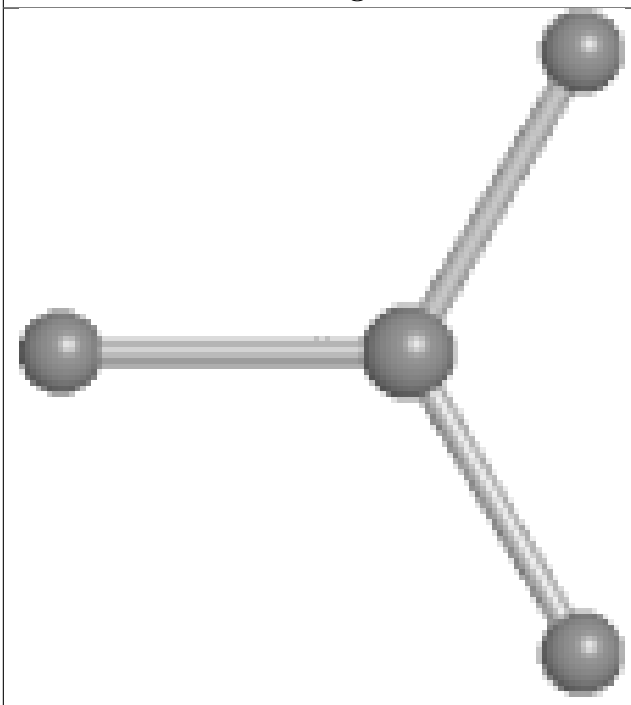
Ligand BCT C 601



Bond lengths



Bond angles



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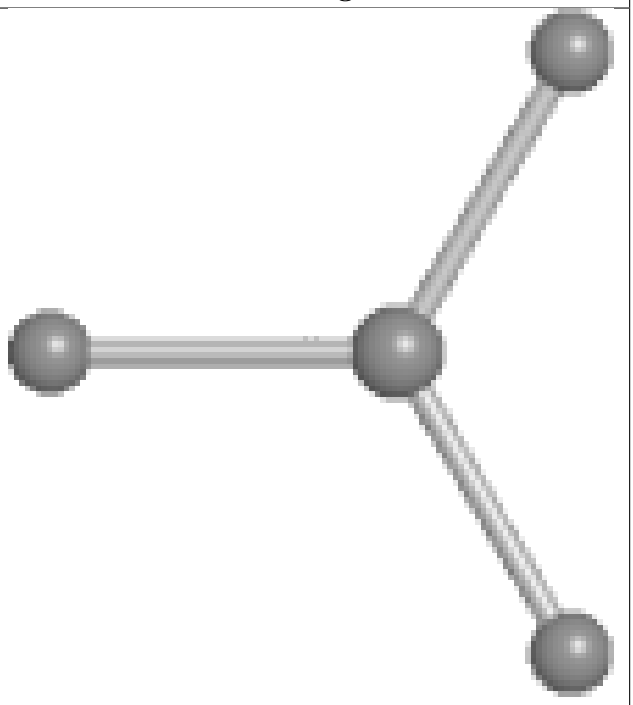
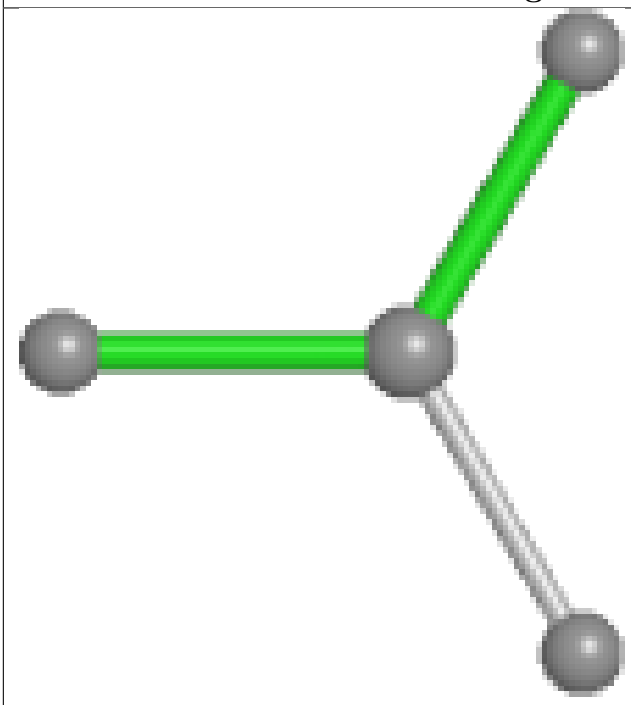
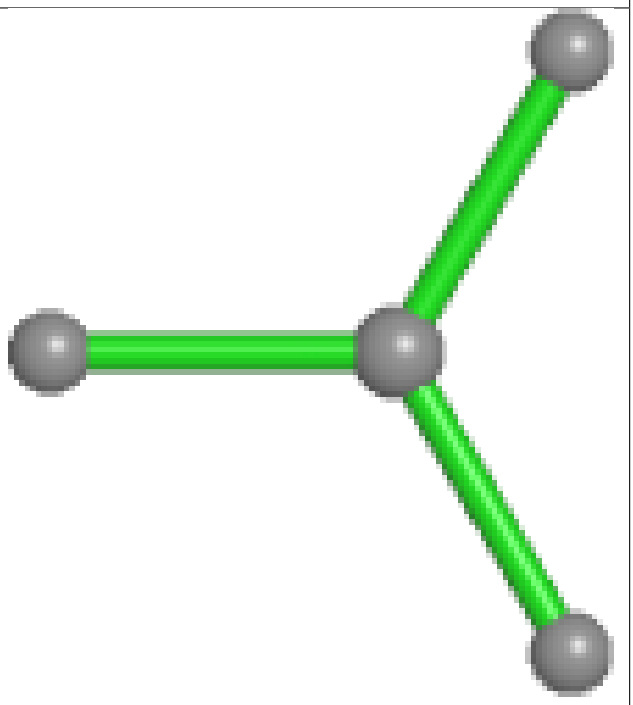


Rings

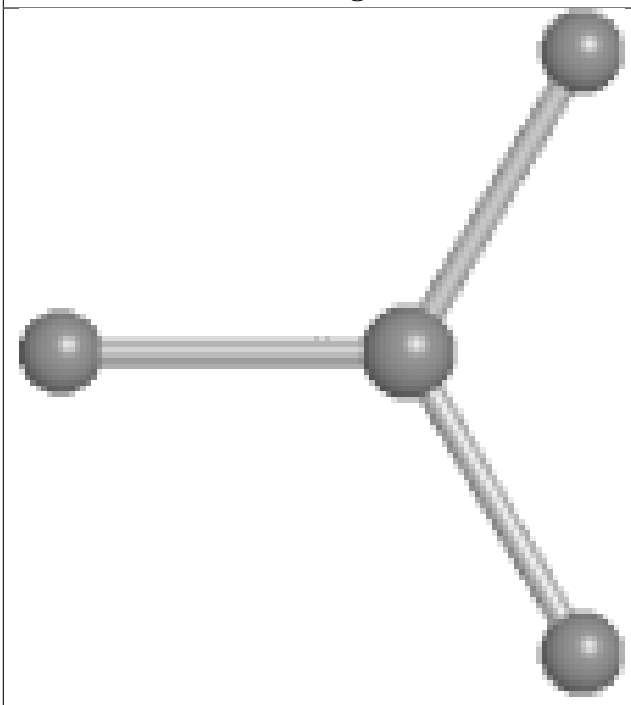
Ligand BCT F 601



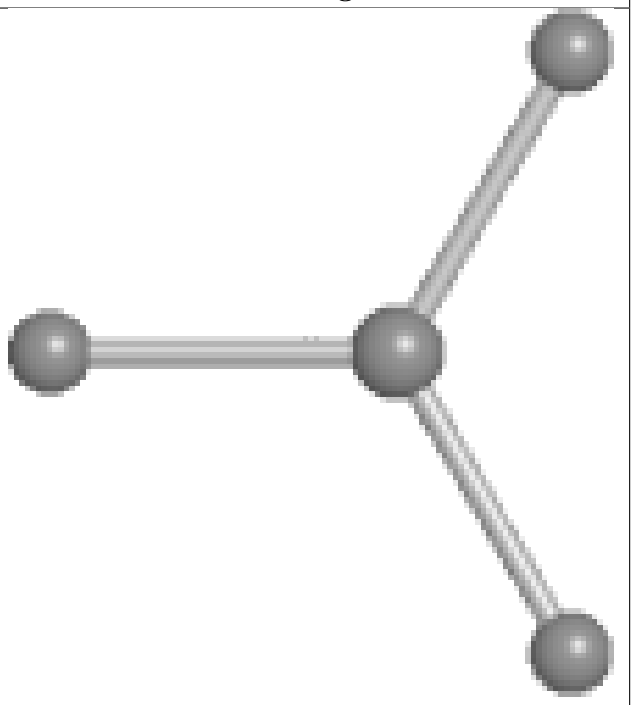
Bond lengths



Bond angles

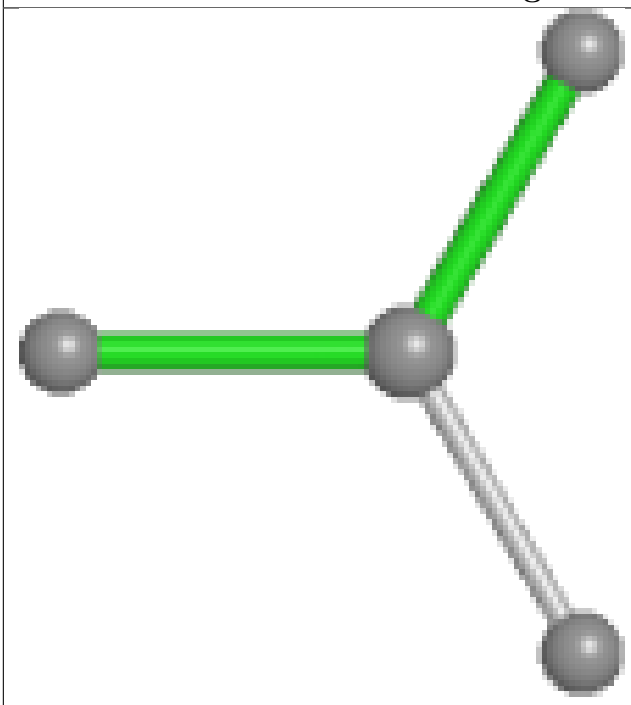


Torsions

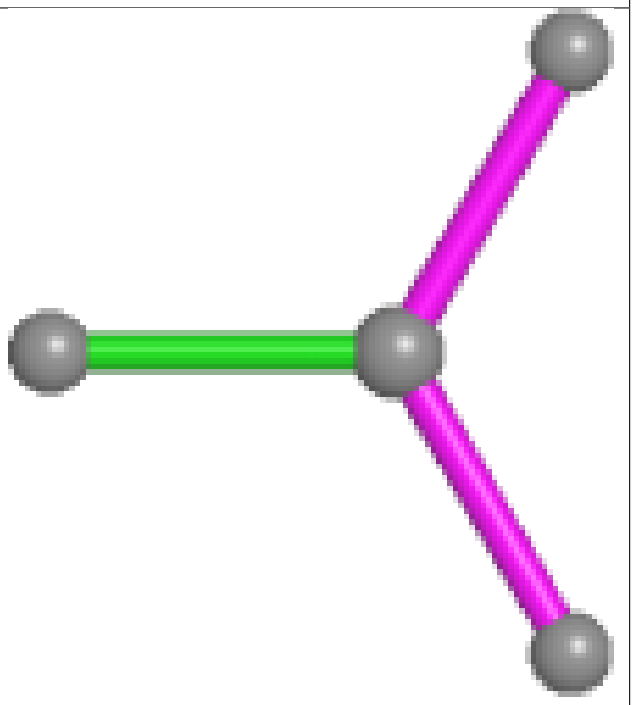


Rings

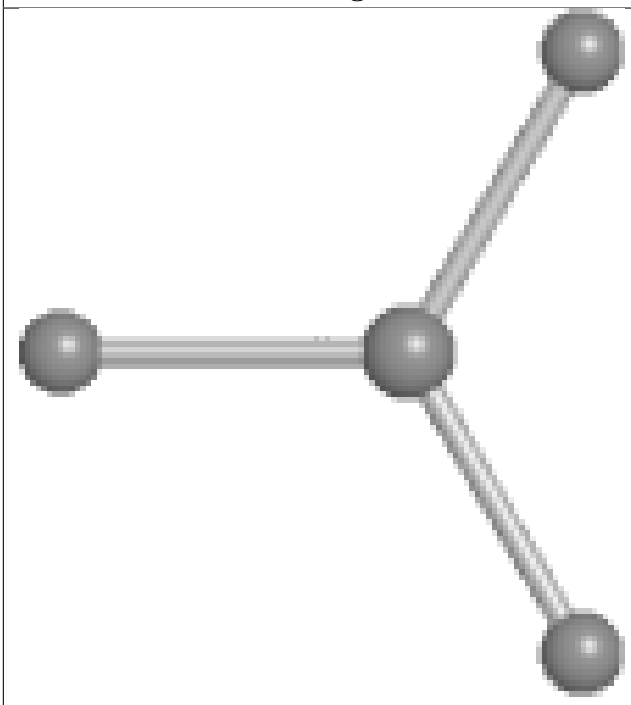
Ligand BCT B 602



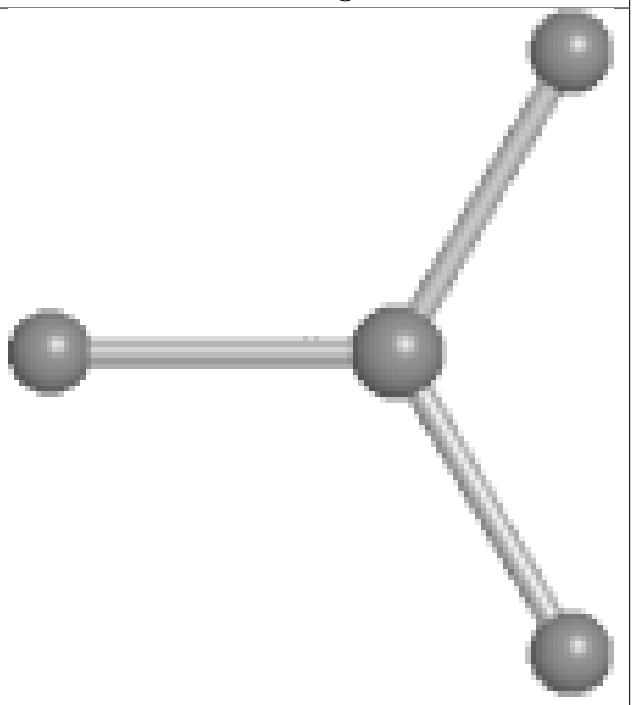
Bond lengths



Bond angles

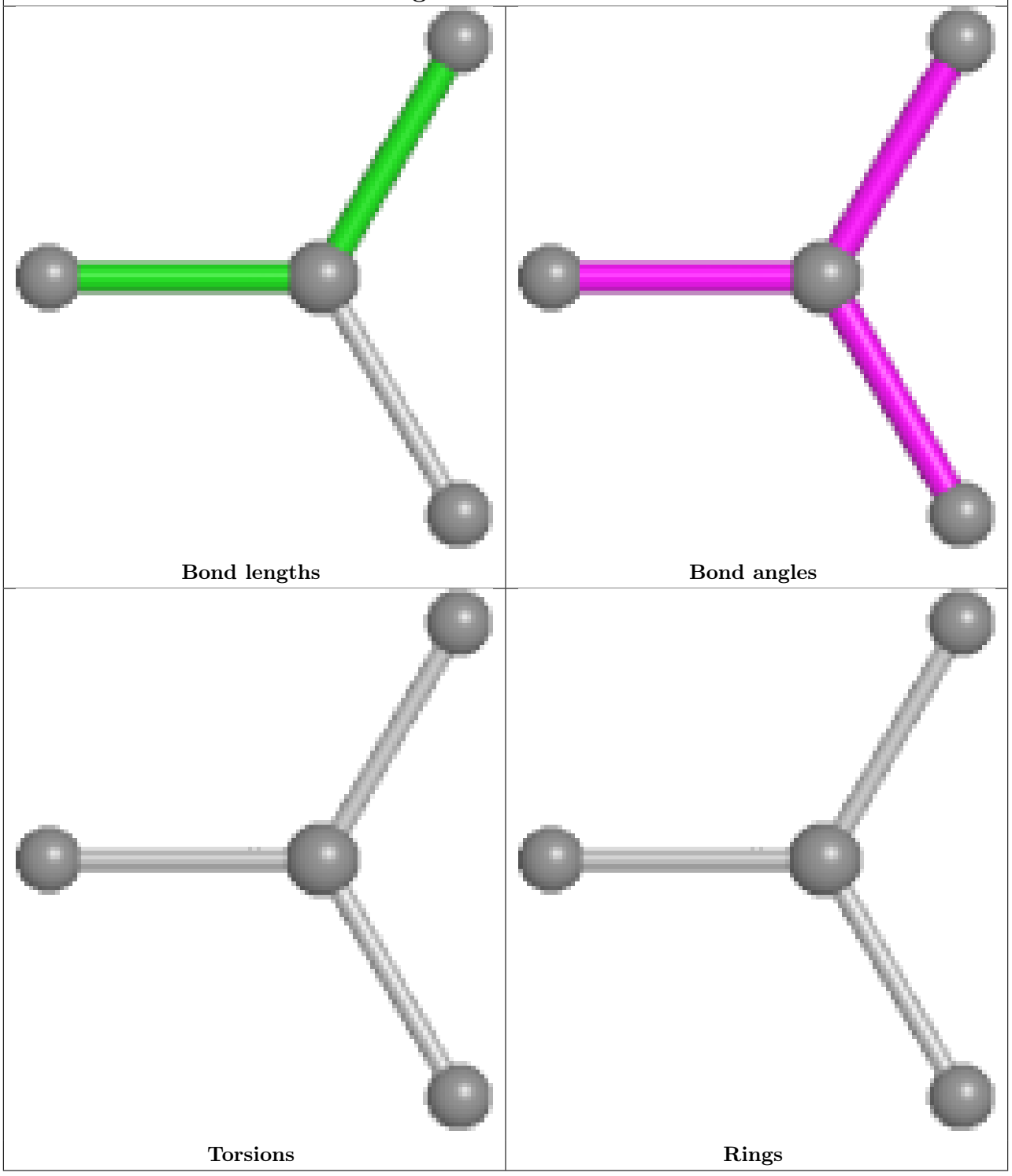


Torsions



Rings

Ligand BCT D 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	499/517 (96%)	-0.14	6 (1%)	79	80	33, 40, 60, 89	1 (0%)
1	B	499/517 (96%)	-0.15	5 (1%)	82	83	33, 41, 58, 85	0
1	C	499/517 (96%)	-0.12	7 (1%)	75	77	33, 42, 61, 88	0
1	D	499/517 (96%)	-0.09	7 (1%)	75	77	33, 42, 62, 86	0
1	E	499/517 (96%)	-0.09	9 (1%)	68	69	32, 41, 60, 82	0
1	F	499/517 (96%)	0.06	7 (1%)	75	77	32, 41, 60, 89	0
All	All	2994/3102 (96%)	-0.09	41 (1%)	75	77	32, 41, 60, 89	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	19	GLN	4.7
1	D	19	GLN	4.6
1	D	18	PHE	4.6
1	E	103	ARG	4.4
1	F	103	ARG	4.3
1	D	48	LYS	4.0
1	B	103	ARG	4.0
1	C	103	ARG	3.9
1	E	48	LYS	3.7
1	E	47	ARG	3.5
1	B	19	GLN	3.5
1	F	19	GLN	3.5
1	D	47	ARG	3.4
1	D	103	ARG	3.4
1	C	48	LYS	3.3
1	F	48	LYS	3.3
1	A	103	ARG	3.3
1	C	18	PHE	3.3
1	B	278	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	46	GLY	3.1
1	A	46	GLY	3.1
1	A	47	ARG	3.0
1	B	48	LYS	3.0
1	C	47	ARG	2.9
1	F	47	ARG	2.9
1	A	19	GLN	2.8
1	E	18	PHE	2.8
1	D	46	GLY	2.8
1	D	20	GLY	2.8
1	E	20	GLY	2.8
1	E	19	GLN	2.7
1	C	46	GLY	2.6
1	B	277	LYS	2.4
1	E	46	GLY	2.4
1	C	20	GLY	2.4
1	A	276	LYS	2.4
1	E	21	GLY	2.3
1	E	278	ASP	2.3
1	F	278	ASP	2.1
1	A	278	ASP	2.1
1	F	18	PHE	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	P03	F	606	15/15	0.53	0.52	65,78,84,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	F	604	4/4	0.75	0.42	55,66,77,79	0
4	EDO	B	604	4/4	0.79	0.26	48,59,73,73	0
3	NH4	E	603	1/1	0.80	0.19	44,52,52,52	0
4	EDO	B	603	4/4	0.81	0.18	54,65,73,73	0
3	NH4	A	602	1/1	0.81	0.09	49,58,58,58	0
4	EDO	F	605	4/4	0.84	0.43	50,60,69,73	0
4	EDO	F	603	4/4	0.85	0.26	46,59,71,73	0
3	NH4	A	604	1/1	0.86	0.19	44,53,53,53	0
4	EDO	A	603	4/4	0.86	0.39	54,64,69,77	0
3	NH4	C	602	1/1	0.88	0.24	46,55,55,55	0
4	EDO	A	608	4/4	0.88	0.21	54,65,67,71	0
4	EDO	D	603	4/4	0.89	0.14	50,60,68,71	0
3	NH4	D	602	1/1	0.90	0.27	46,55,55,55	0
3	NH4	A	607	1/1	0.90	0.11	50,60,60,60	0
3	NH4	E	604	1/1	0.90	0.14	58,69,69,69	0
3	NH4	C	603	1/1	0.90	0.11	50,60,60,60	0
4	EDO	E	601	4/4	0.91	0.41	56,67,76,76	0
5	NO3	A	605	4/4	0.92	0.31	62,62,67,67	0
3	NH4	B	601	1/1	0.92	0.26	53,64,64,64	0
3	NH4	C	605	1/1	0.93	0.11	50,60,60,60	0
7	NA	A	611	1/1	0.94	0.33	59,59,59,59	0
3	NH4	B	606	1/1	0.94	0.58	51,61,61,61	0
2	BCT	B	602	4/4	0.95	0.10	41,41,48,50	0
4	EDO	B	605	4/4	0.95	0.36	52,62,71,74	0
3	NH4	C	604	1/1	0.96	0.18	39,46,46,46	0
2	BCT	E	602	4/4	0.97	0.08	37,38,46,47	0
2	BCT	F	601	4/4	0.97	0.10	38,41,45,54	0
2	BCT	A	601	4/4	0.97	0.11	39,41,43,52	0
6	MN	C	606	1/1	0.98	0.10	35,35,35,35	0
6	MN	F	607	1/1	0.98	0.15	35,35,35,35	0
3	NH4	A	606	1/1	0.98	0.08	32,38,38,38	0
2	BCT	C	601	4/4	0.98	0.08	39,42,48,51	0
6	MN	B	608	1/1	0.99	0.10	36,36,36,36	0
3	NH4	F	602	1/1	0.99	0.13	32,38,38,38	0
6	MN	D	605	1/1	0.99	0.10	36,36,36,36	0
6	MN	E	605	1/1	0.99	0.10	34,34,34,34	0
2	BCT	D	601	4/4	0.99	0.07	39,41,49,51	0
6	MN	F	608	1/1	0.99	0.14	34,34,34,34	0
6	MN	A	609	1/1	0.99	0.12	33,33,33,33	0
6	MN	A	610	1/1	0.99	0.11	34,34,34,34	0
6	MN	D	604	1/1	1.00	0.10	35,35,35,35	0
6	MN	B	607	1/1	1.00	0.14	35,35,35,35	0

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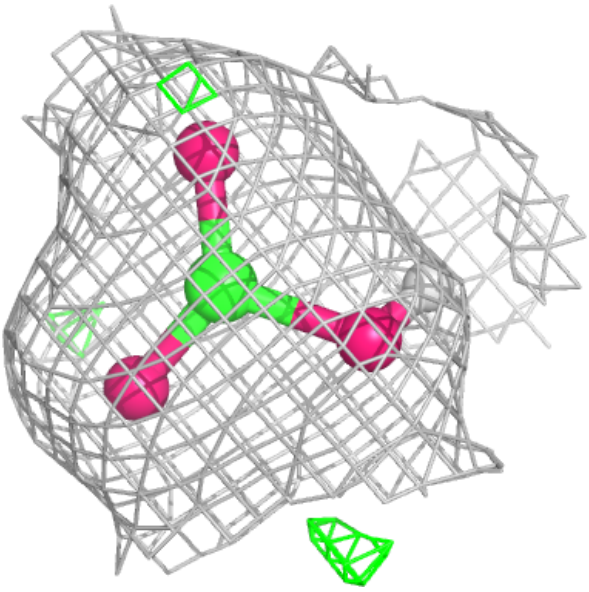
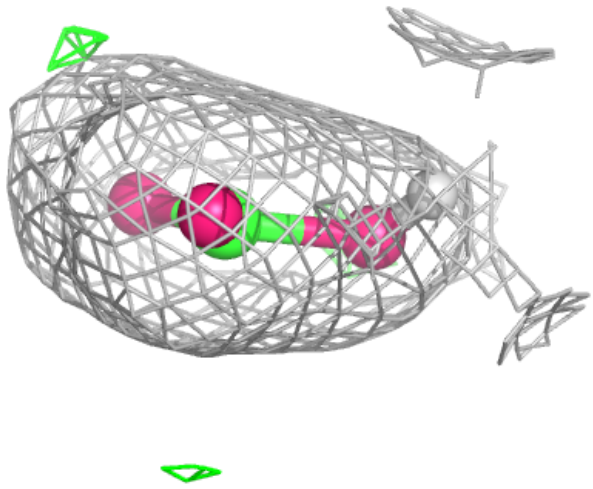
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MN	C	607	1/1	1.00	0.09	34,34,34,34	0
6	MN	E	606	1/1	1.00	0.10	34,34,34,34	0

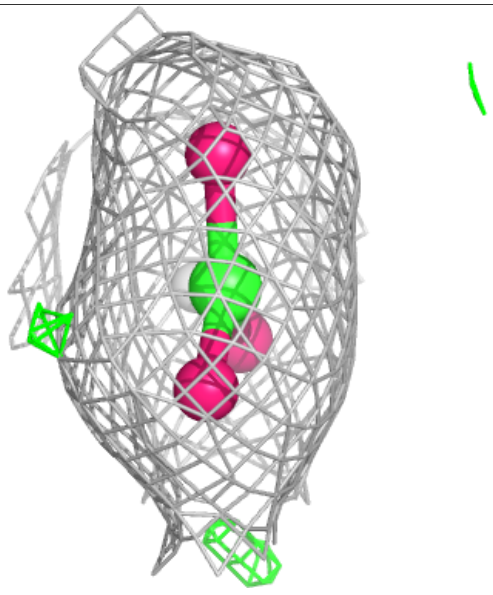
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BCT B 602:

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

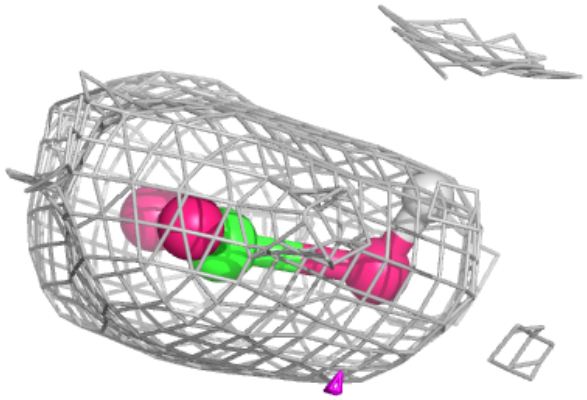


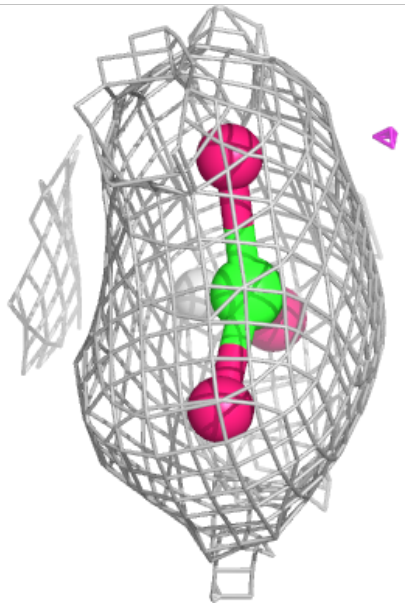




Electron density around BCT E 602:

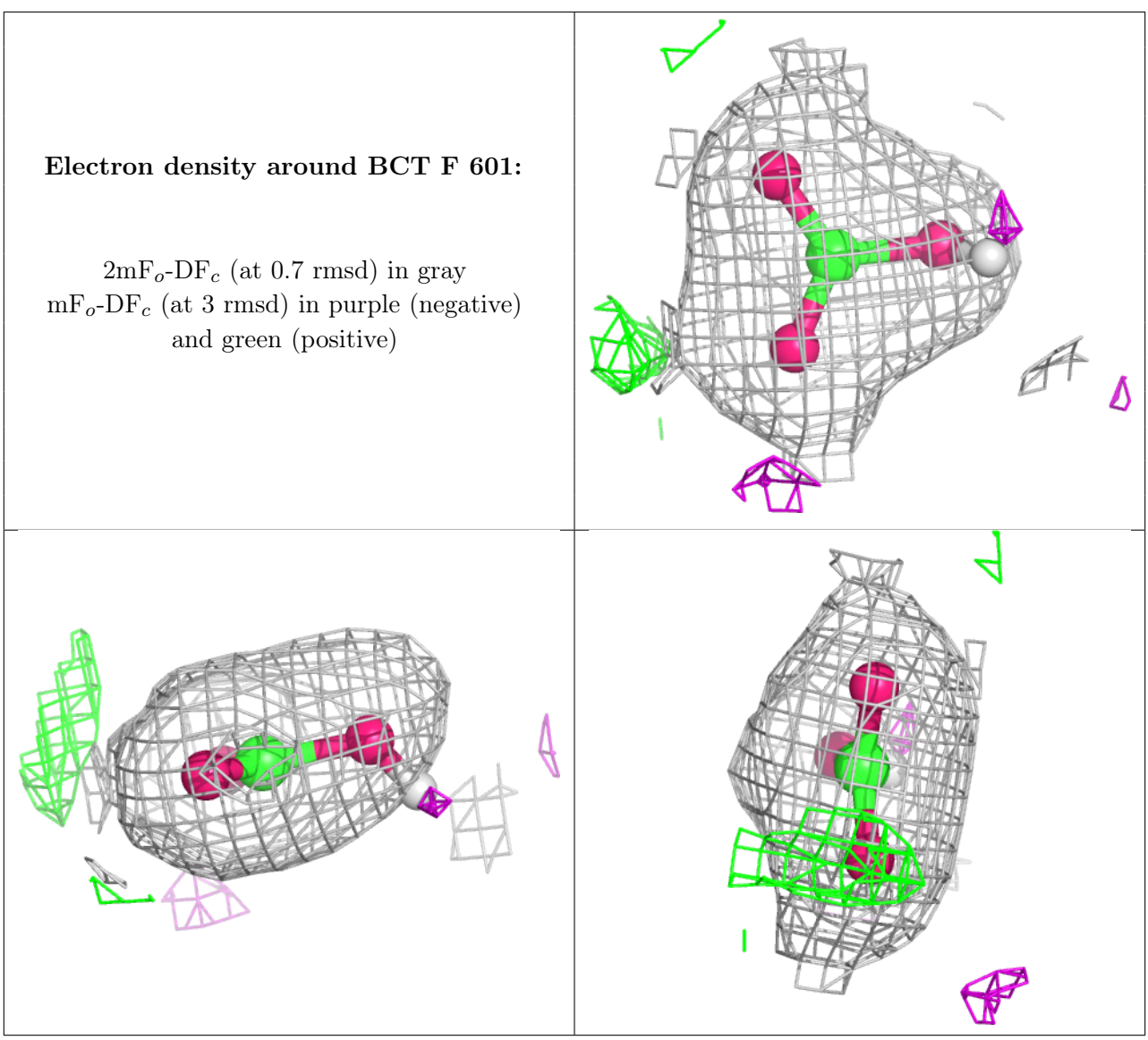
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





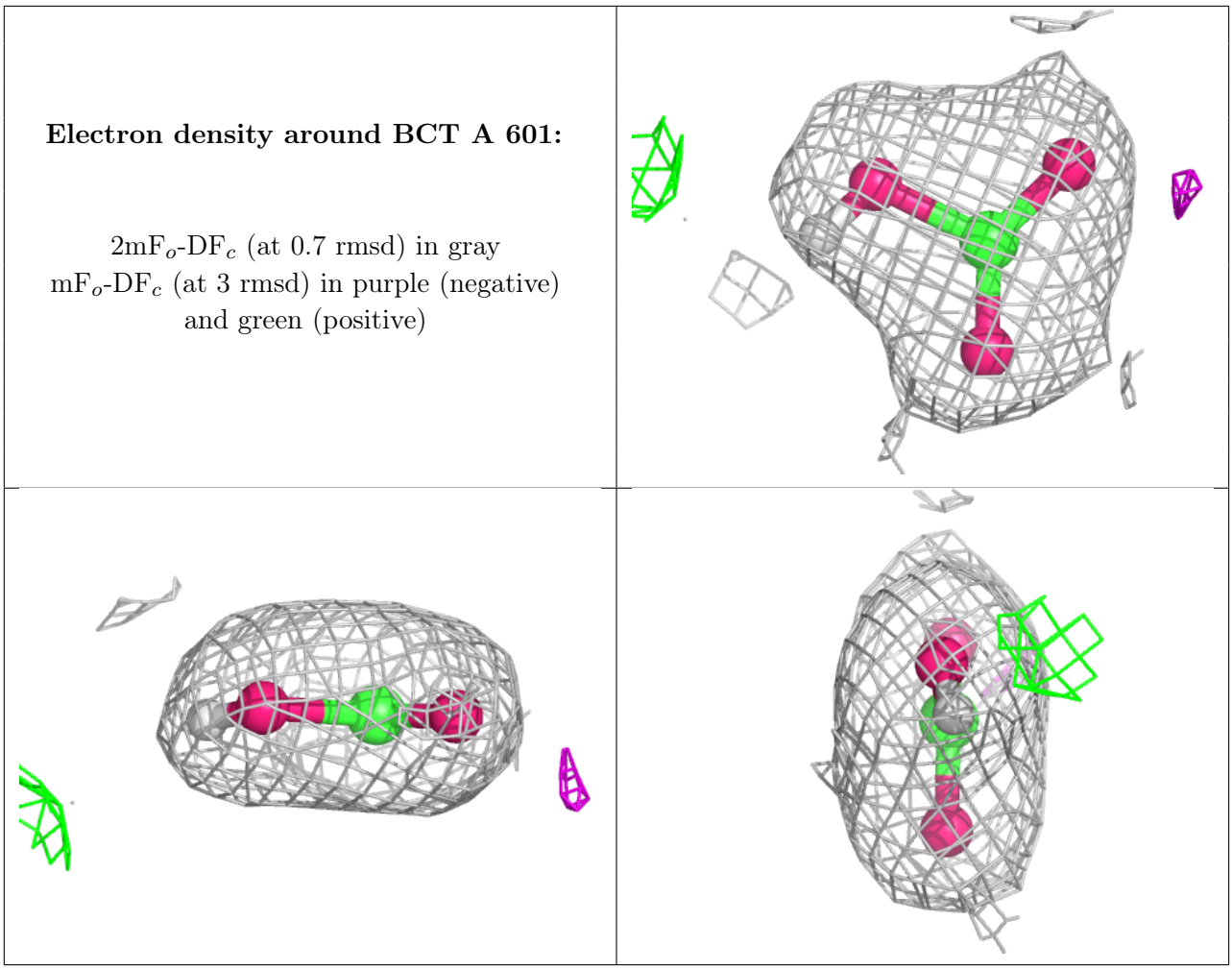
Electron density around BCT F 601:

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



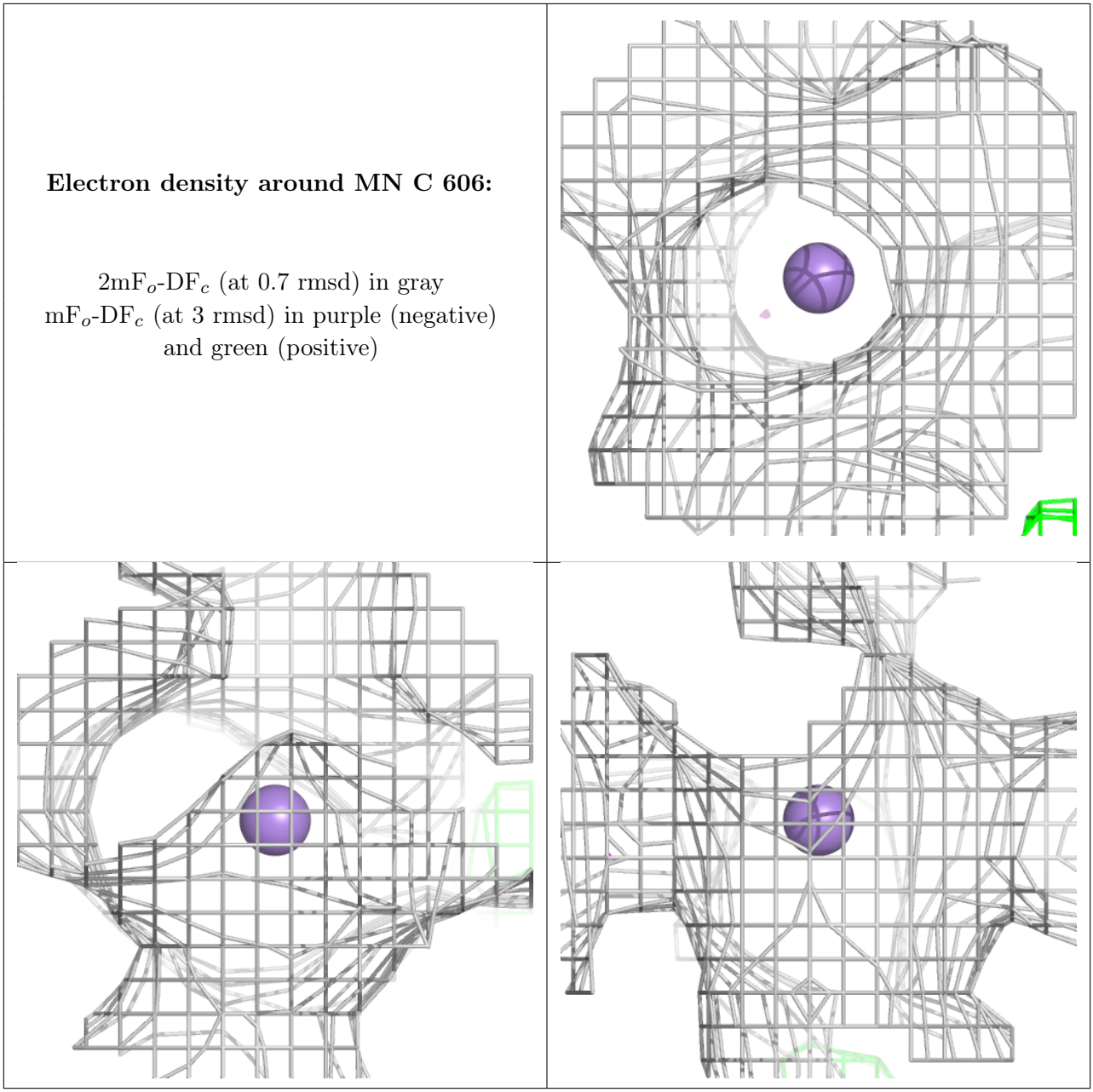
Electron density around BCT A 601:

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



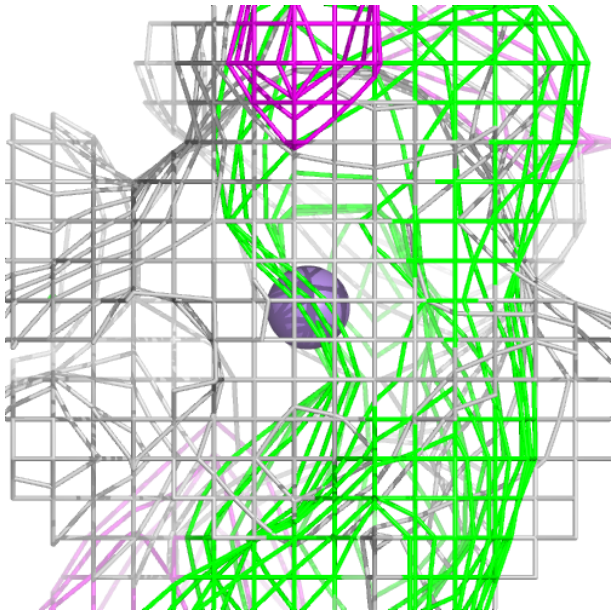
Electron density around MN C 606:

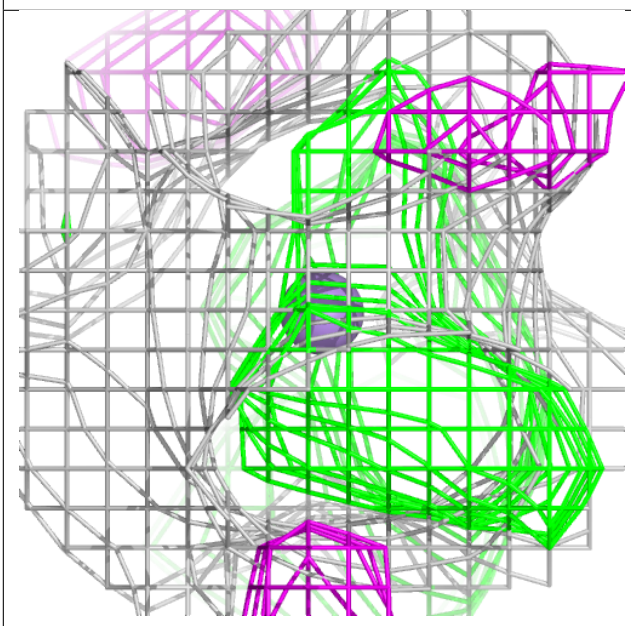
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

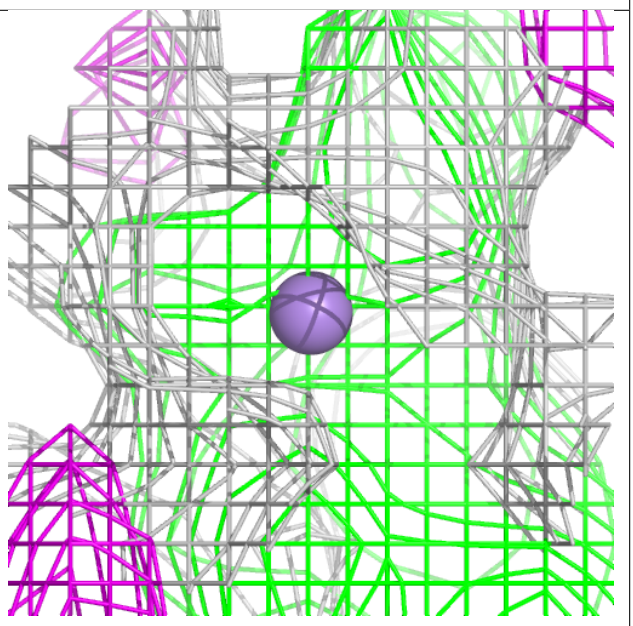


Electron density around MN F 607:

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

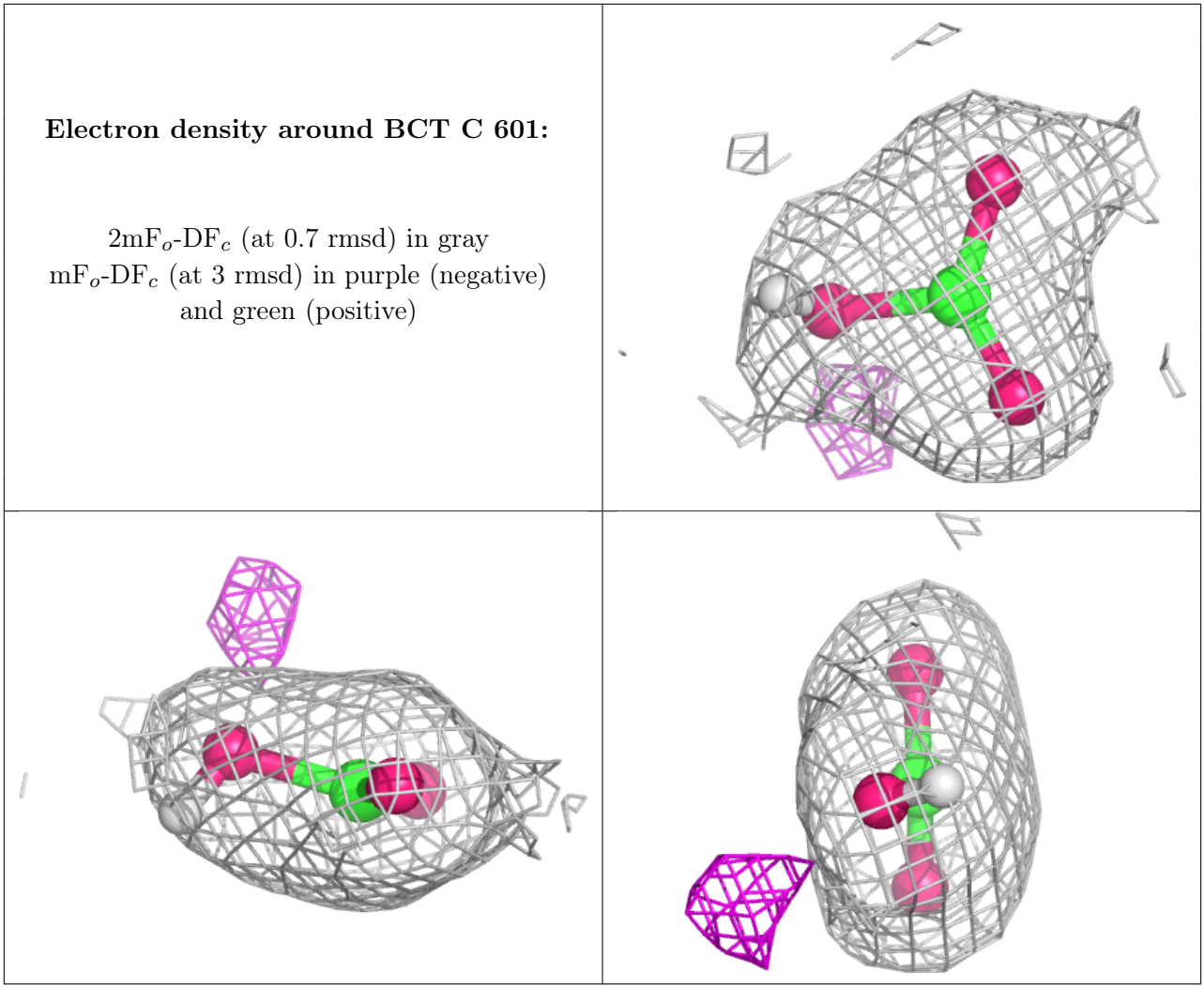






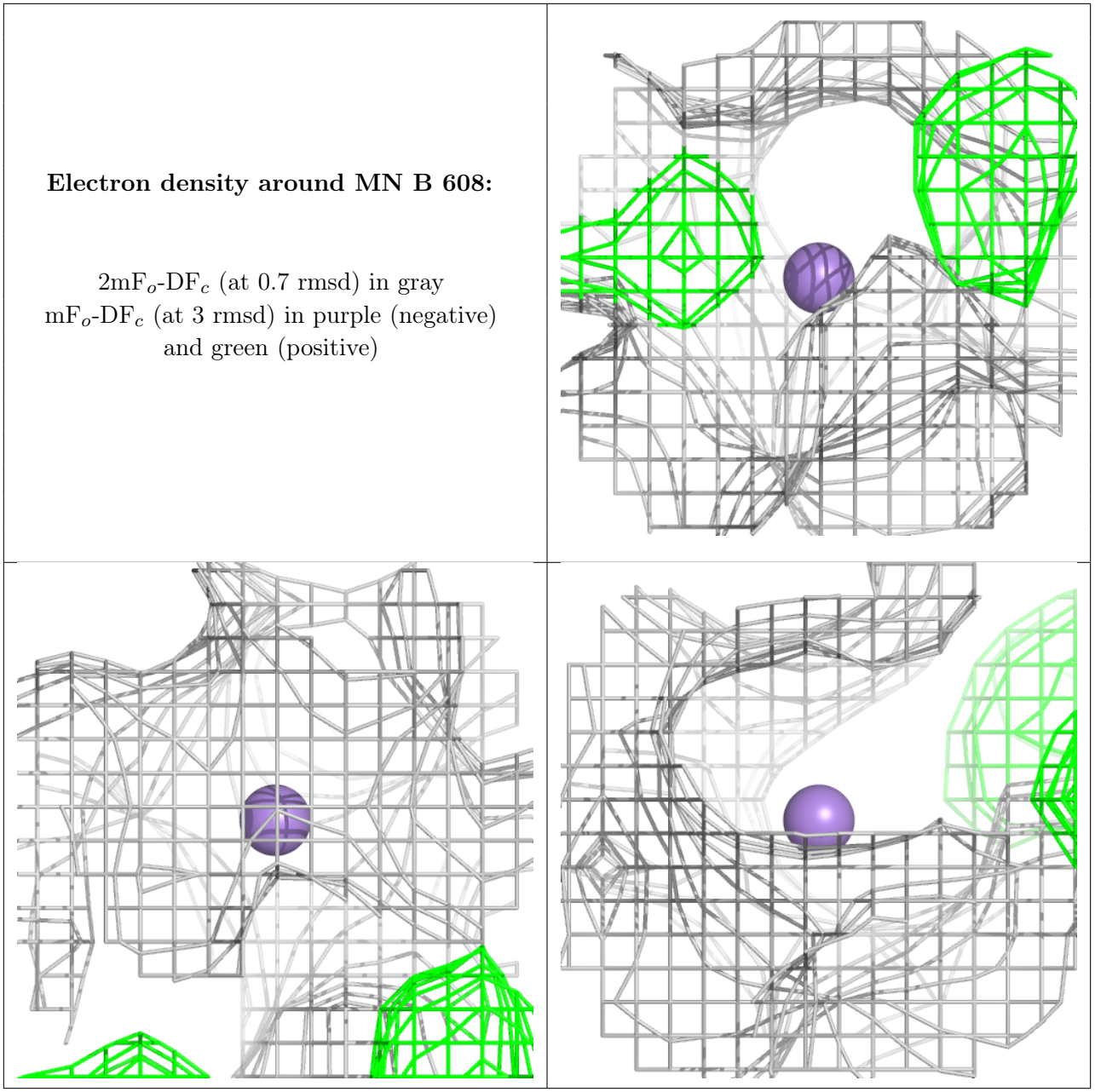
Electron density around BCT C 601:

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



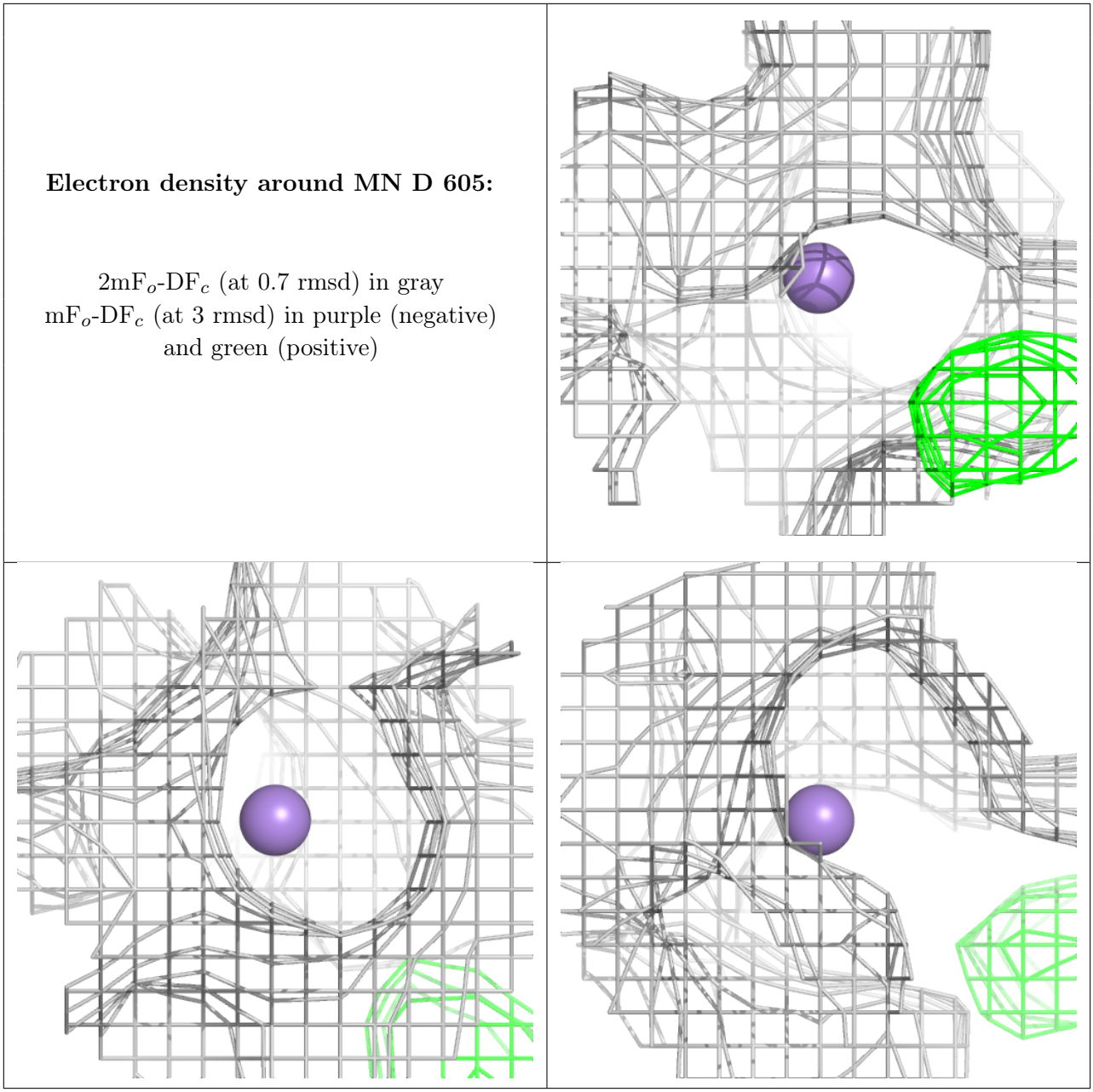
Electron density around MN B 608:

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



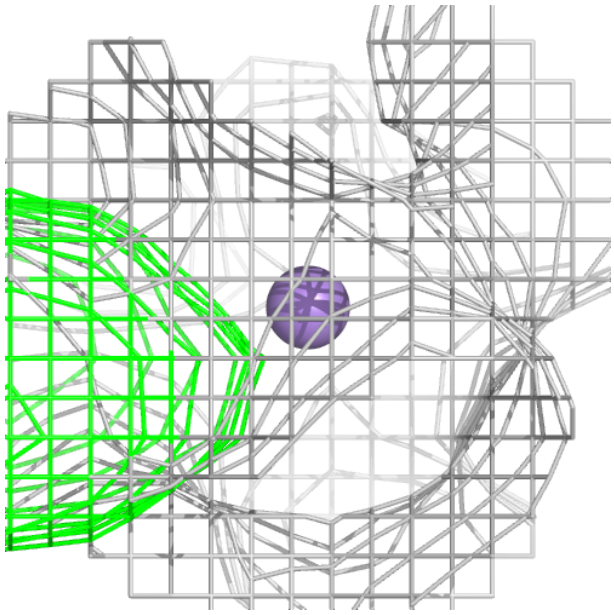
Electron density around MN D 605:

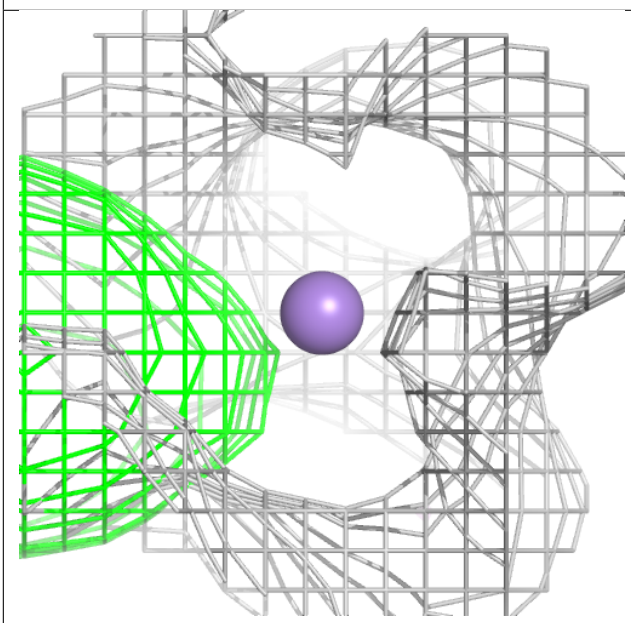
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

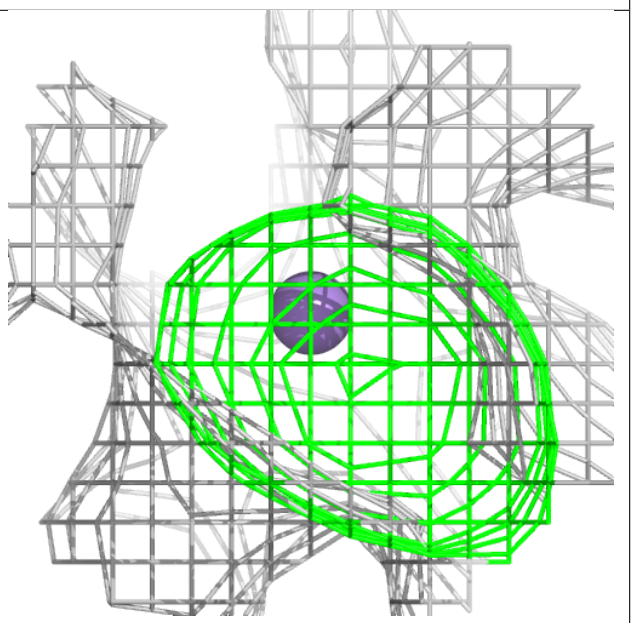


Electron density around MN E 605:

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

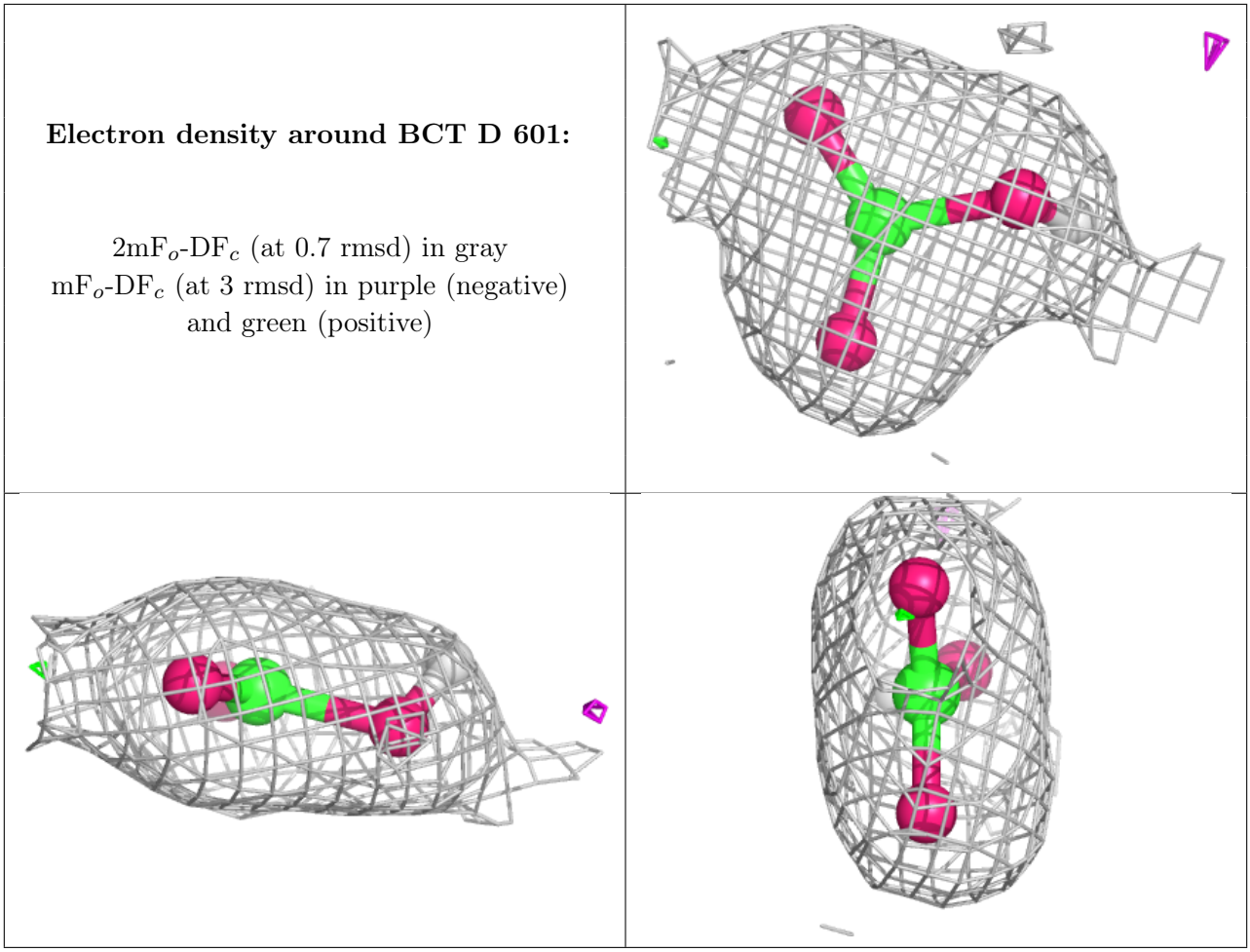






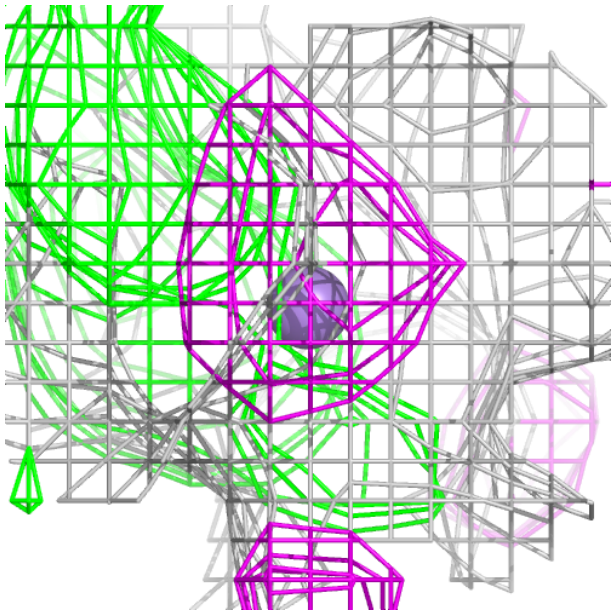
Electron density around BCT D 601:

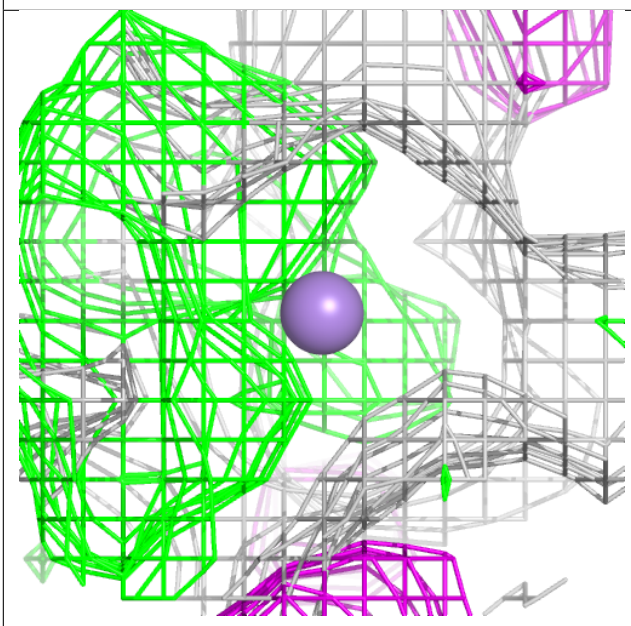
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

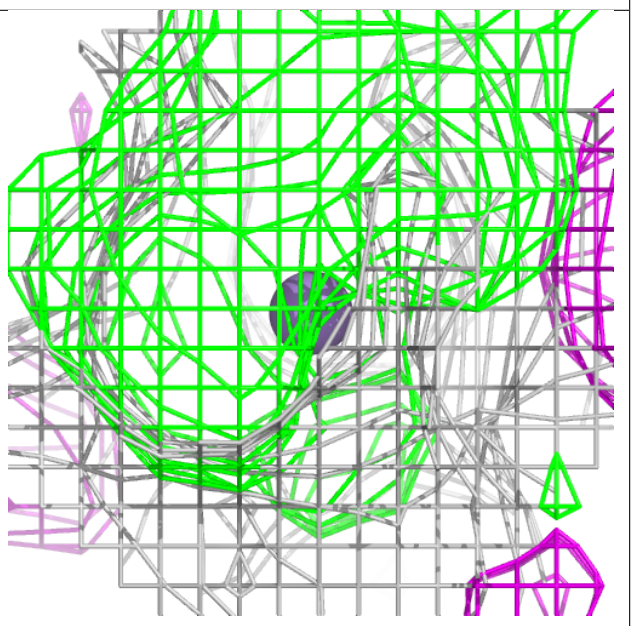


Electron density around MN F 608:

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

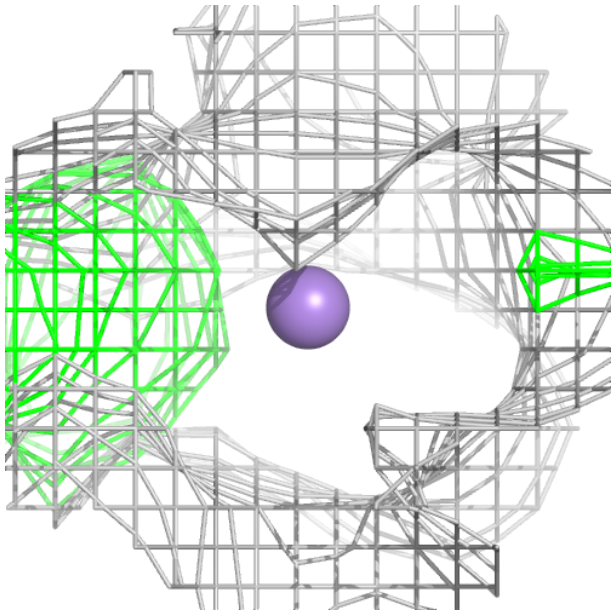


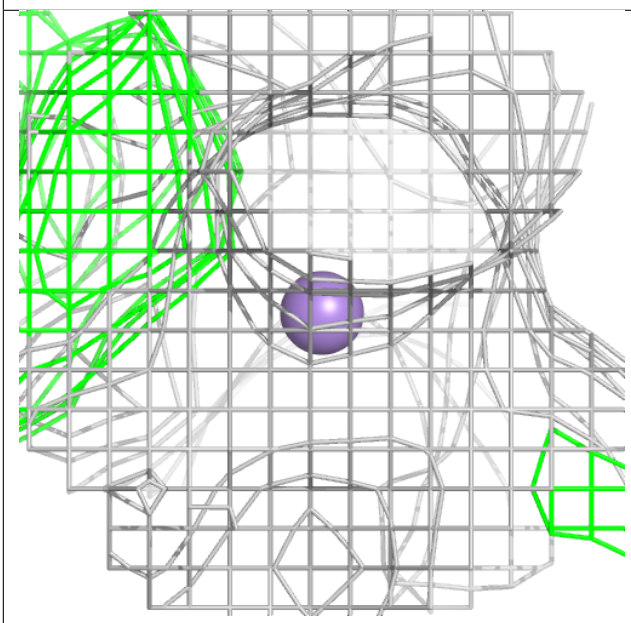


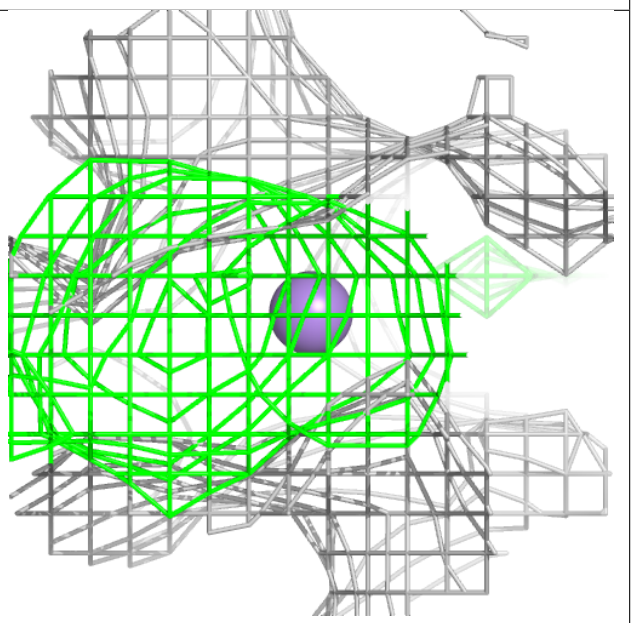


Electron density around MN A 609:

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

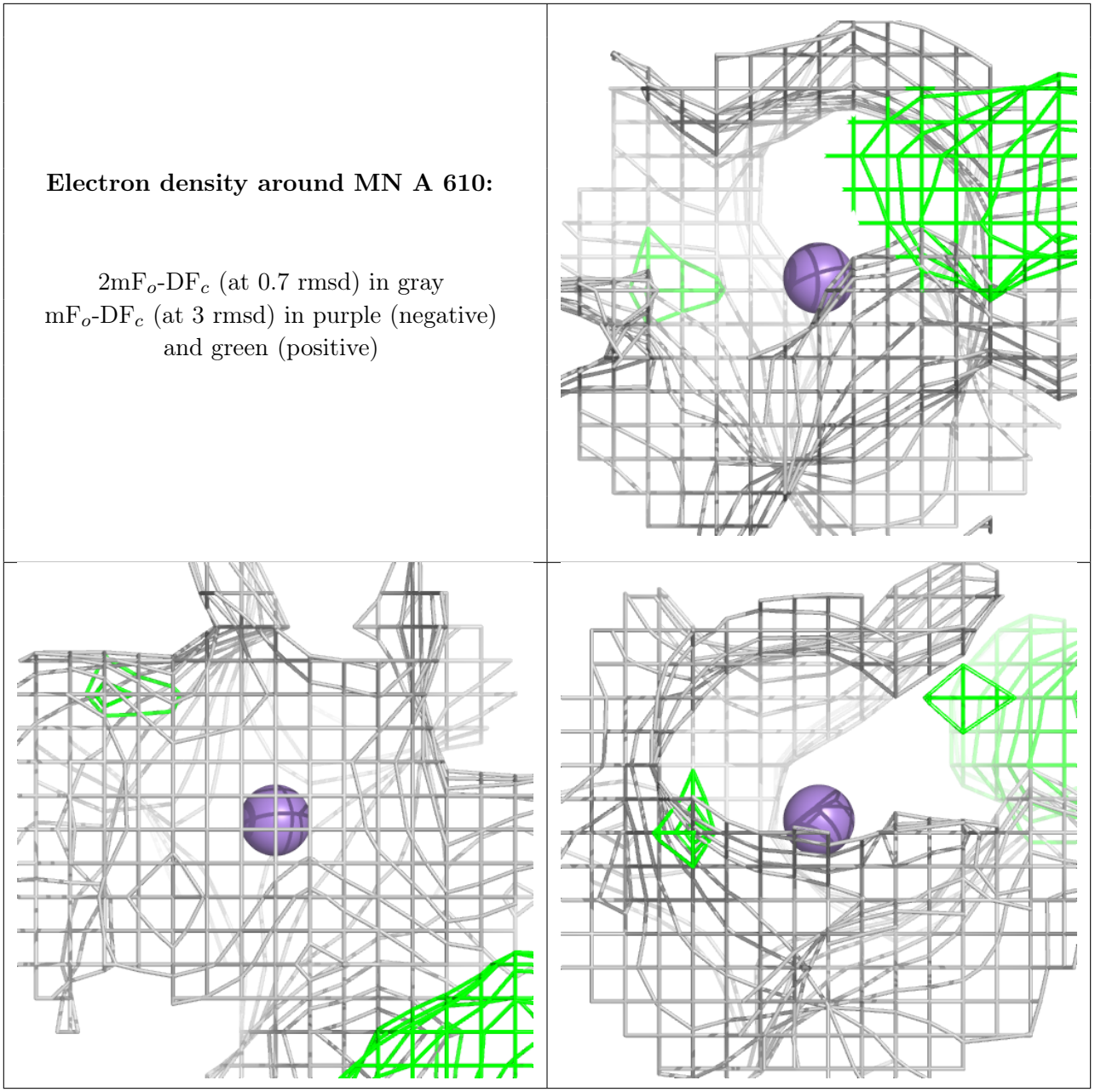






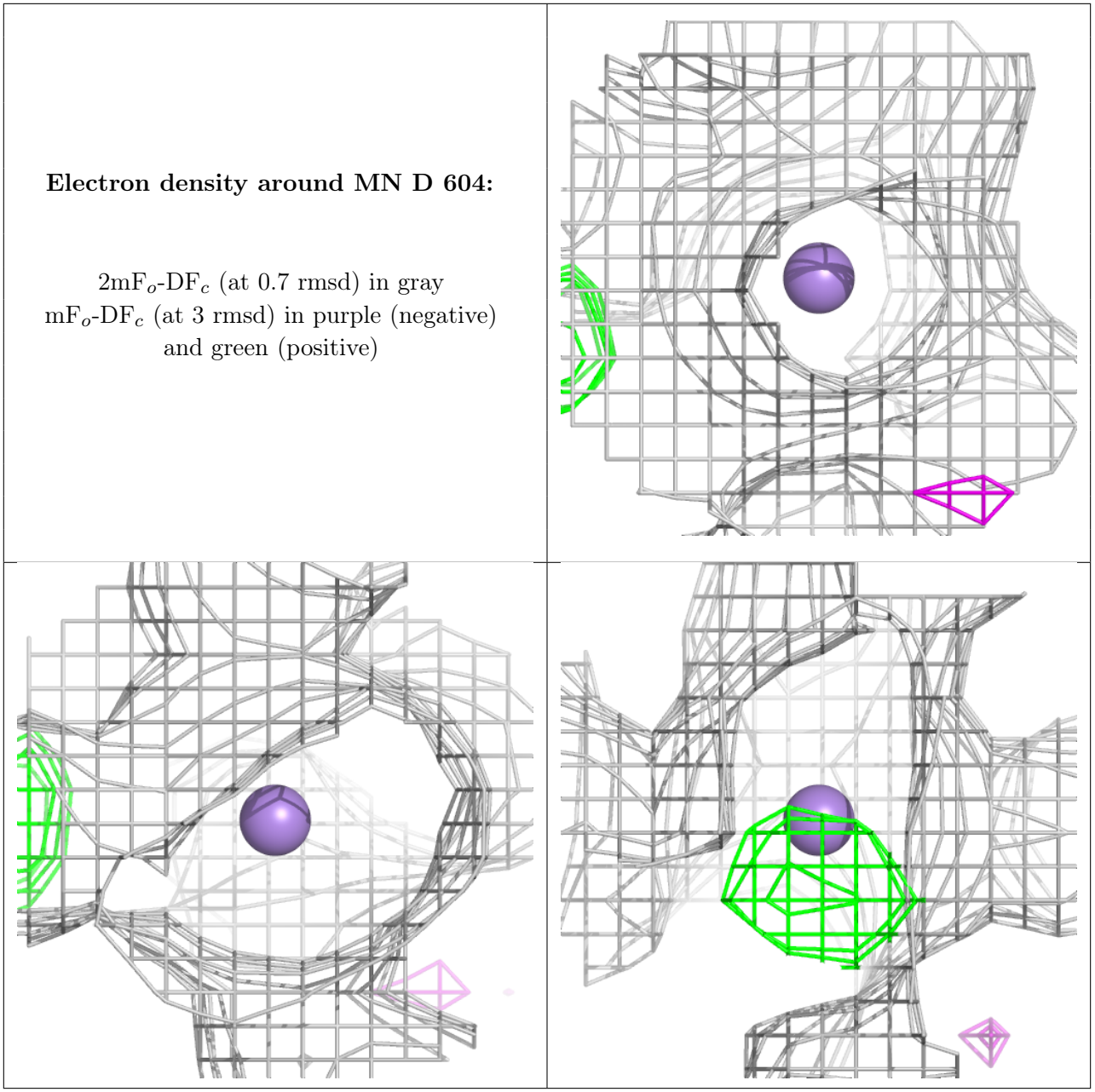
Electron density around MN A 610:

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



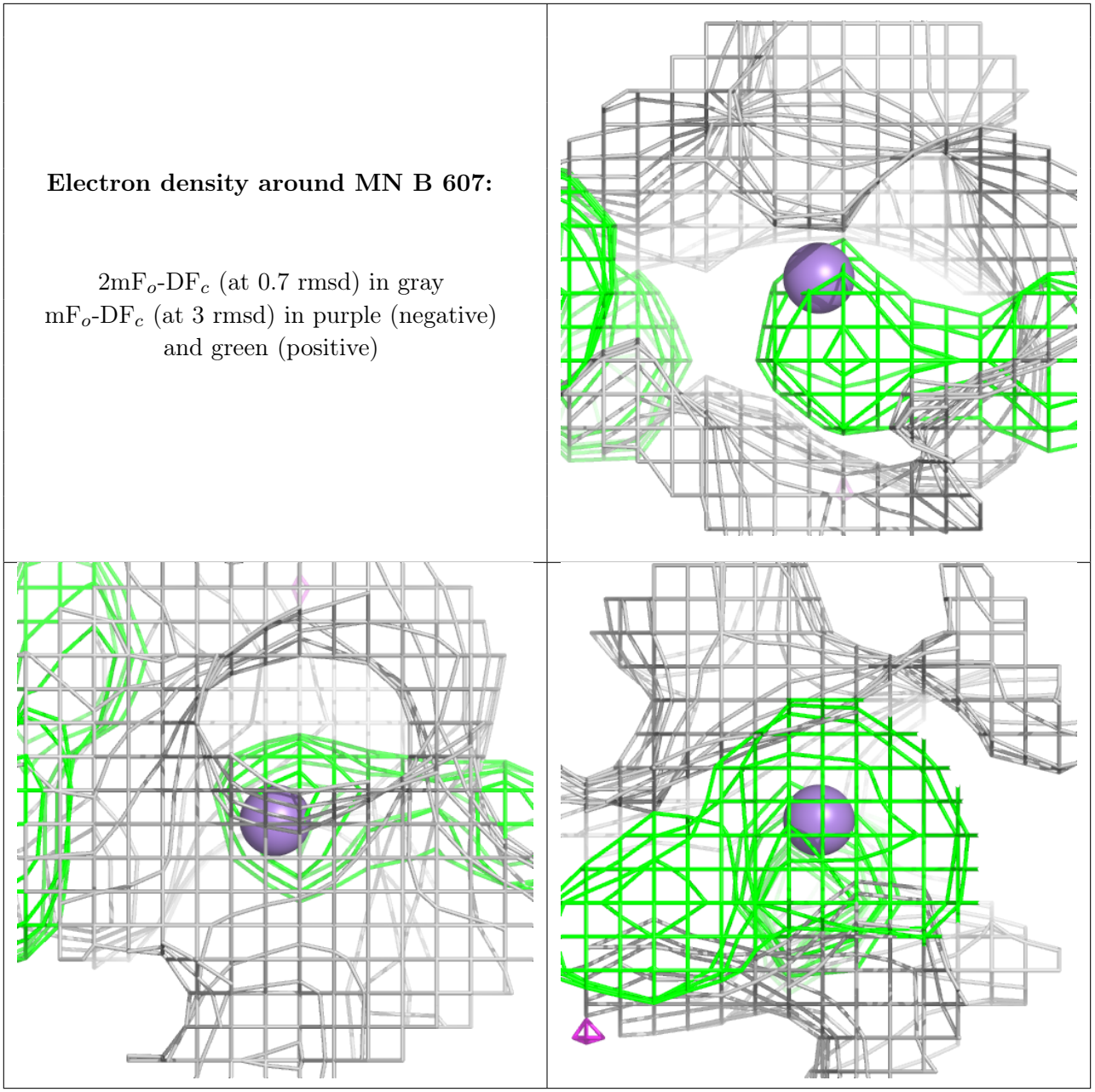
Electron density around MN D 604:

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



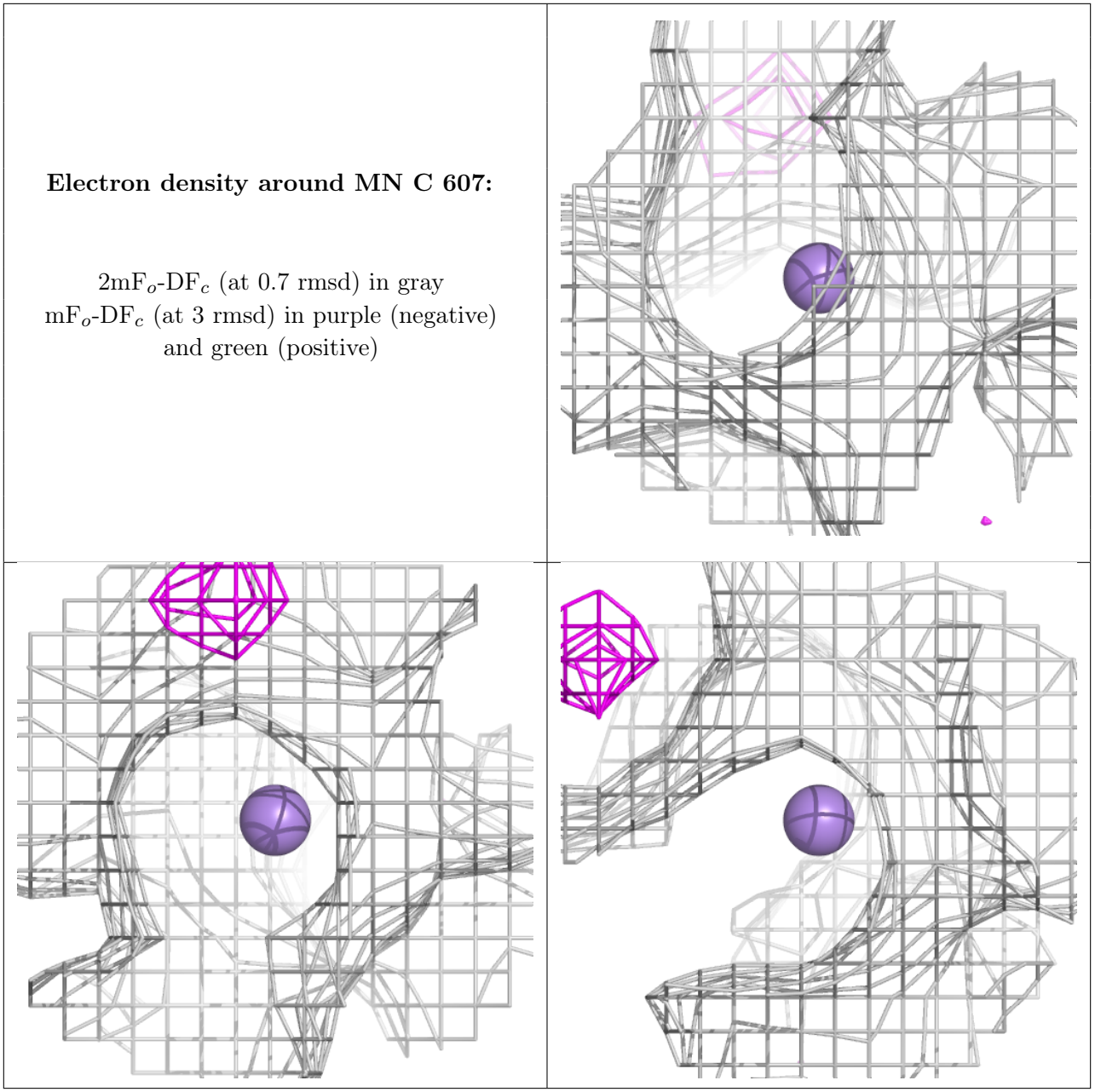
Electron density around MN B 607:

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



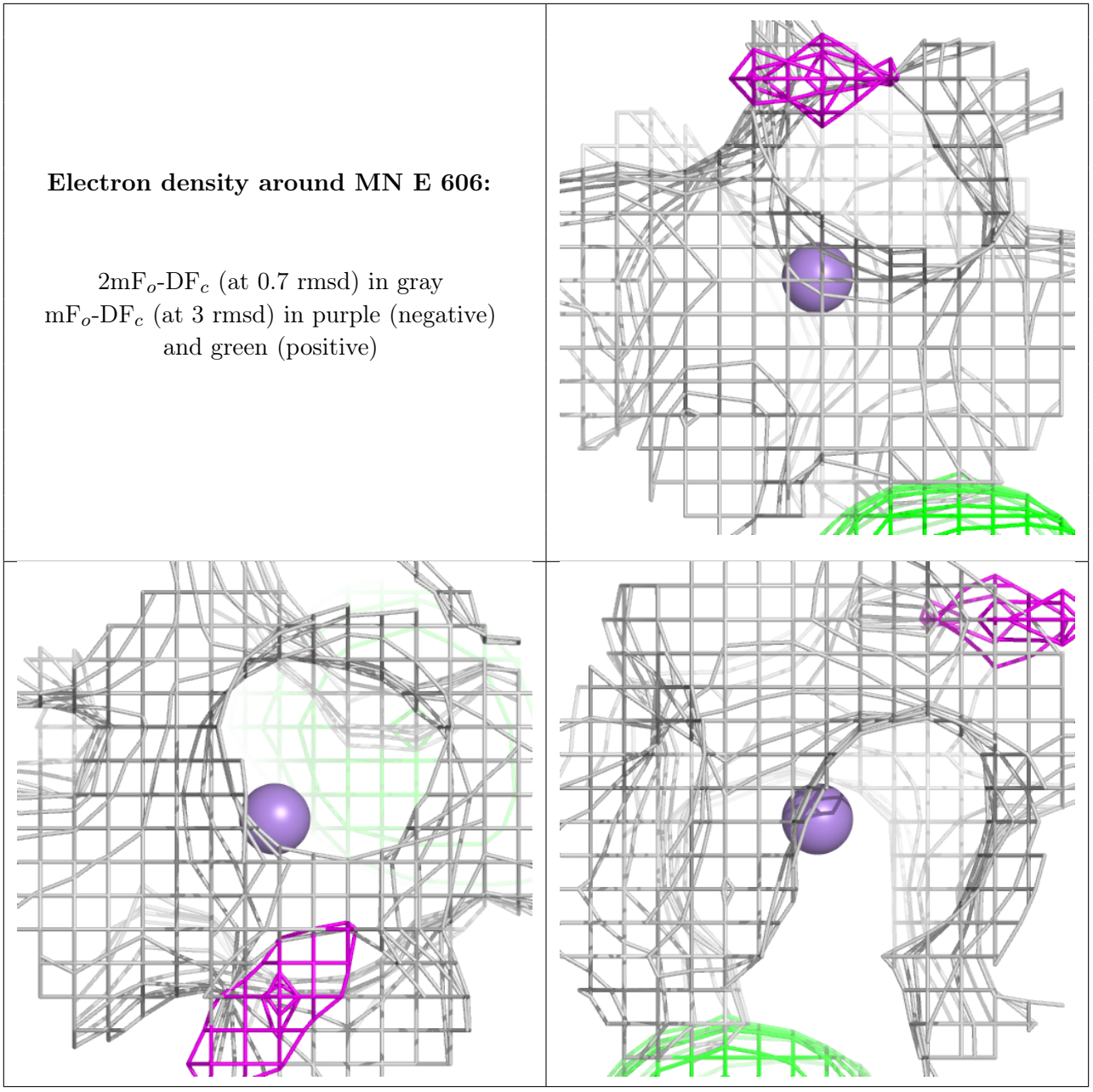
Electron density around MN C 607:

$2mF_o$-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 606:

$2mF_o$-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 (i)

There are no such residues in this entry.