



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2020 – 07:15 PM BST

PDB ID : 6LVV
Title : N, N-dimethylformamidase
Authors : Arya, C.K.; Ramaswamy, S.; Kutti, R.V.; Gurunath, R.
Deposited on : 2020-02-05
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	2.13.1
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

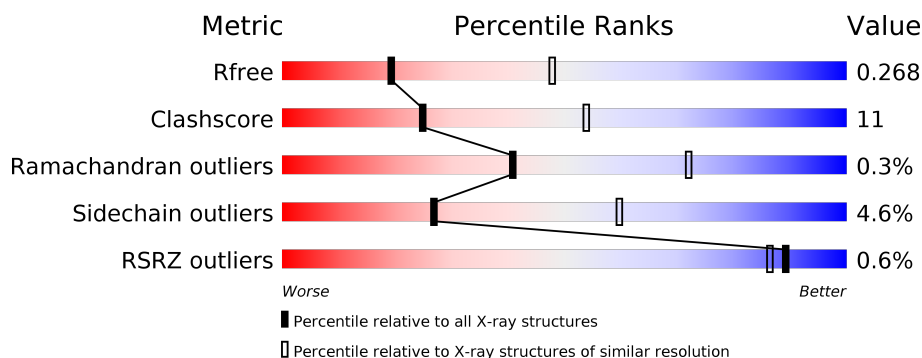
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	775	<div> <div>76%</div> <div>21%</div> <div>..</div> </div>
1	C	775	<div> <div>%</div> <div>77%</div> <div>20%</div> <div>..</div> </div>
1	E	775	<div> <div>%</div> <div>77%</div> <div>20%</div> <div>..</div> </div>
1	G	775	<div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	I	775	<div> <div>76%</div> <div>21%</div> <div>..</div> </div>
1	K	775	<div> <div>%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	M	775	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>77%</div><div>20%</div><div>• •</div></div></div>
1	O	775	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>76%</div><div>22%</div><div>• •</div></div></div>
2	B	132	<div><div><div>3%</div><div><div></div><div></div><div></div></div><div>72%</div><div>20%</div><div>• 5%</div></div></div>
2	D	132	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>78%</div><div>14%</div><div>• 5%</div></div></div>
2	F	132	<div><div><div></div><div><div></div><div></div><div></div></div><div>75%</div><div>17%</div><div>• 5%</div></div></div>
2	H	132	<div><div><div></div><div><div></div><div></div><div></div></div><div>70%</div><div>21%</div><div>• 5%</div></div></div>
2	J	132	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>71%</div><div>19%</div><div>5% 5%</div></div></div>
2	L	132	<div><div><div></div><div><div></div><div></div><div></div></div><div>79%</div><div>14%</div><div>• 5%</div></div></div>
2	N	132	<div><div><div></div><div><div></div><div></div><div></div></div><div>77%</div><div>16%</div><div>• 5%</div></div></div>
2	P	132	<div><div><div></div><div><div></div><div></div><div></div></div><div>71%</div><div>20%</div><div>• 5%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 56839 atoms, of which 48 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 N,N-dimethylformamidase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			
1	C	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			
1	E	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			
1	G	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			
1	I	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			
1	K	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			
1	M	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			
1	O	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	763	LYS	-	expression tag	UNP I6NT79
A	764	LEU	-	expression tag	UNP I6NT79
A	765	ALA	-	expression tag	UNP I6NT79
A	766	ALA	-	expression tag	UNP I6NT79
A	767	ALA	-	expression tag	UNP I6NT79
A	768	LEU	-	expression tag	UNP I6NT79
A	769	GLU	-	expression tag	UNP I6NT79
A	770	HIS	-	expression tag	UNP I6NT79
A	771	HIS	-	expression tag	UNP I6NT79
A	772	HIS	-	expression tag	UNP I6NT79
A	773	HIS	-	expression tag	UNP I6NT79
A	774	HIS	-	expression tag	UNP I6NT79
A	775	HIS	-	expression tag	UNP I6NT79

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Chain	Residue	Modelled	Actual	Comment	Reference
C	763	LYS	-	expression tag	UNP I6NT79
C	764	LEU	-	expression tag	UNP I6NT79
C	765	ALA	-	expression tag	UNP I6NT79
C	766	ALA	-	expression tag	UNP I6NT79
C	767	ALA	-	expression tag	UNP I6NT79
C	768	LEU	-	expression tag	UNP I6NT79
C	769	GLU	-	expression tag	UNP I6NT79
C	770	HIS	-	expression tag	UNP I6NT79
C	771	HIS	-	expression tag	UNP I6NT79
C	772	HIS	-	expression tag	UNP I6NT79
C	773	HIS	-	expression tag	UNP I6NT79
C	774	HIS	-	expression tag	UNP I6NT79
C	775	HIS	-	expression tag	UNP I6NT79
E	763	LYS	-	expression tag	UNP I6NT79
E	764	LEU	-	expression tag	UNP I6NT79
E	765	ALA	-	expression tag	UNP I6NT79
E	766	ALA	-	expression tag	UNP I6NT79
E	767	ALA	-	expression tag	UNP I6NT79
E	768	LEU	-	expression tag	UNP I6NT79
E	769	GLU	-	expression tag	UNP I6NT79
E	770	HIS	-	expression tag	UNP I6NT79
E	771	HIS	-	expression tag	UNP I6NT79
E	772	HIS	-	expression tag	UNP I6NT79
E	773	HIS	-	expression tag	UNP I6NT79
E	774	HIS	-	expression tag	UNP I6NT79
E	775	HIS	-	expression tag	UNP I6NT79
G	763	LYS	-	expression tag	UNP I6NT79
G	764	LEU	-	expression tag	UNP I6NT79
G	765	ALA	-	expression tag	UNP I6NT79
G	766	ALA	-	expression tag	UNP I6NT79
G	767	ALA	-	expression tag	UNP I6NT79
G	768	LEU	-	expression tag	UNP I6NT79
G	769	GLU	-	expression tag	UNP I6NT79
G	770	HIS	-	expression tag	UNP I6NT79
G	771	HIS	-	expression tag	UNP I6NT79
G	772	HIS	-	expression tag	UNP I6NT79
G	773	HIS	-	expression tag	UNP I6NT79
G	774	HIS	-	expression tag	UNP I6NT79
G	775	HIS	-	expression tag	UNP I6NT79
I	763	LYS	-	expression tag	UNP I6NT79
I	764	LEU	-	expression tag	UNP I6NT79
I	765	ALA	-	expression tag	UNP I6NT79

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Chain	Residue	Modelled	Actual	Comment	Reference
I	766	ALA	-	expression tag	UNP I6NT79
I	767	ALA	-	expression tag	UNP I6NT79
I	768	LEU	-	expression tag	UNP I6NT79
I	769	GLU	-	expression tag	UNP I6NT79
I	770	HIS	-	expression tag	UNP I6NT79
I	771	HIS	-	expression tag	UNP I6NT79
I	772	HIS	-	expression tag	UNP I6NT79
I	773	HIS	-	expression tag	UNP I6NT79
I	774	HIS	-	expression tag	UNP I6NT79
I	775	HIS	-	expression tag	UNP I6NT79
K	763	LYS	-	expression tag	UNP I6NT79
K	764	LEU	-	expression tag	UNP I6NT79
K	765	ALA	-	expression tag	UNP I6NT79
K	766	ALA	-	expression tag	UNP I6NT79
K	767	ALA	-	expression tag	UNP I6NT79
K	768	LEU	-	expression tag	UNP I6NT79
K	769	GLU	-	expression tag	UNP I6NT79
K	770	HIS	-	expression tag	UNP I6NT79
K	771	HIS	-	expression tag	UNP I6NT79
K	772	HIS	-	expression tag	UNP I6NT79
K	773	HIS	-	expression tag	UNP I6NT79
K	774	HIS	-	expression tag	UNP I6NT79
K	775	HIS	-	expression tag	UNP I6NT79
M	763	LYS	-	expression tag	UNP I6NT79
M	764	LEU	-	expression tag	UNP I6NT79
M	765	ALA	-	expression tag	UNP I6NT79
M	766	ALA	-	expression tag	UNP I6NT79
M	767	ALA	-	expression tag	UNP I6NT79
M	768	LEU	-	expression tag	UNP I6NT79
M	769	GLU	-	expression tag	UNP I6NT79
M	770	HIS	-	expression tag	UNP I6NT79
M	771	HIS	-	expression tag	UNP I6NT79
M	772	HIS	-	expression tag	UNP I6NT79
M	773	HIS	-	expression tag	UNP I6NT79
M	774	HIS	-	expression tag	UNP I6NT79
M	775	HIS	-	expression tag	UNP I6NT79
O	763	LYS	-	expression tag	UNP I6NT79
O	764	LEU	-	expression tag	UNP I6NT79
O	765	ALA	-	expression tag	UNP I6NT79
O	766	ALA	-	expression tag	UNP I6NT79
O	767	ALA	-	expression tag	UNP I6NT79
O	768	LEU	-	expression tag	UNP I6NT79

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Chain	Residue	Modelled	Actual	Comment	Reference
O	769	GLU	-	expression tag	UNP I6NT79
O	770	HIS	-	expression tag	UNP I6NT79
O	771	HIS	-	expression tag	UNP I6NT79
O	772	HIS	-	expression tag	UNP I6NT79
O	773	HIS	-	expression tag	UNP I6NT79
O	774	HIS	-	expression tag	UNP I6NT79
O	775	HIS	-	expression tag	UNP I6NT79

- Molecule 2 is a protein called N,N-dimethylformamidase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			
2	D	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			
2	F	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			
2	H	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			
2	J	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			
2	L	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			
2	N	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			
2	P	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by author).

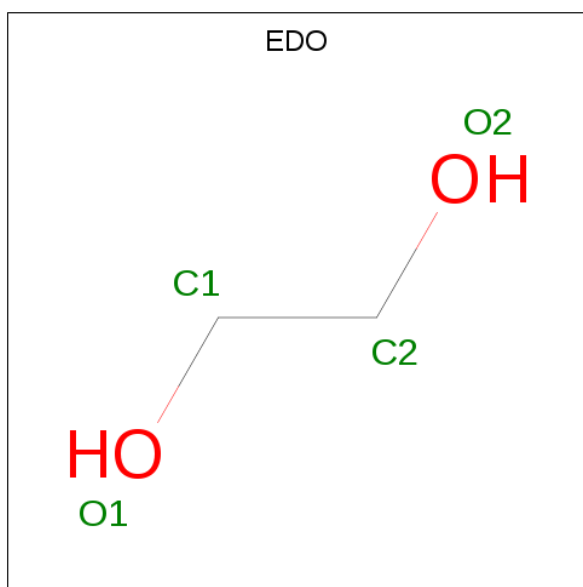
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Fe	0	0
			1	1		
3	K	1	Total	Fe	0	0
			1	1		
3	E	1	Total	Fe	0	0
			1	1		
3	I	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Fe 1	0	0
3	O	1	Total 1	Fe 1	0	0
3	M	1	Total 1	Fe 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	B	1	Total 10	C 2	H 6	O 2	0	0
4	D	1	Total 10	C 2	H 6	O 2	0	0
4	F	1	Total 10	C 2	H 6	O 2	0	0
4	H	1	Total 10	C 2	H 6	O 2	0	0
4	J	1	Total 10	C 2	H 6	O 2	0	0
4	L	1	Total 10	C 2	H 6	O 2	0	0
4	N	1	Total 10	C 2	H 6	O 2	0	0
4	P	1	Total 10	C 2	H 6	O 2	0	0

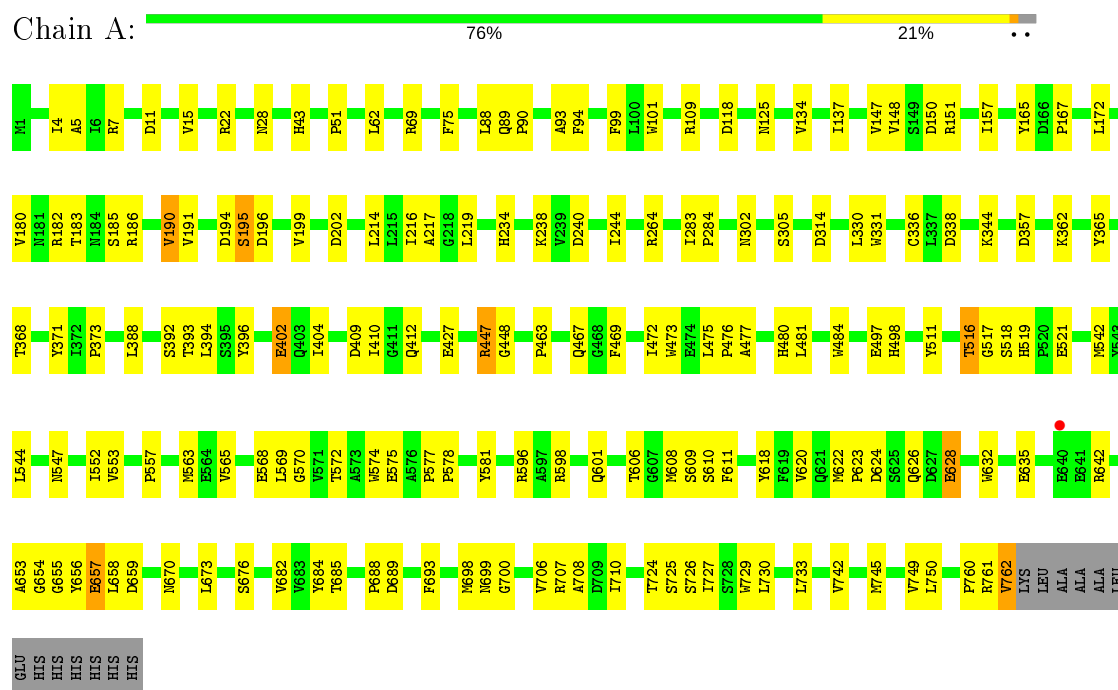
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total 22	O 22	0	0
5	B	1	Total 1	O 1	0	0
5	C	21	Total 21	O 21	0	0
5	E	21	Total 21	O 21	0	0
5	G	22	Total 22	O 22	0	0
5	H	1	Total 1	O 1	0	0
5	I	20	Total 20	O 20	0	0
5	J	1	Total 1	O 1	0	0
5	K	21	Total 21	O 21	0	0
5	M	22	Total 22	O 22	0	0
5	O	23	Total 23	O 23	0	0

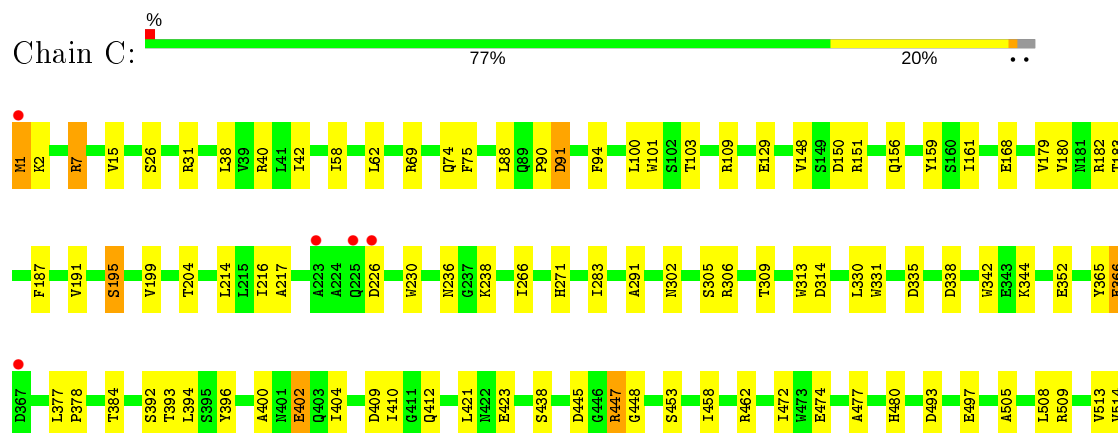
3 Residue-property plots

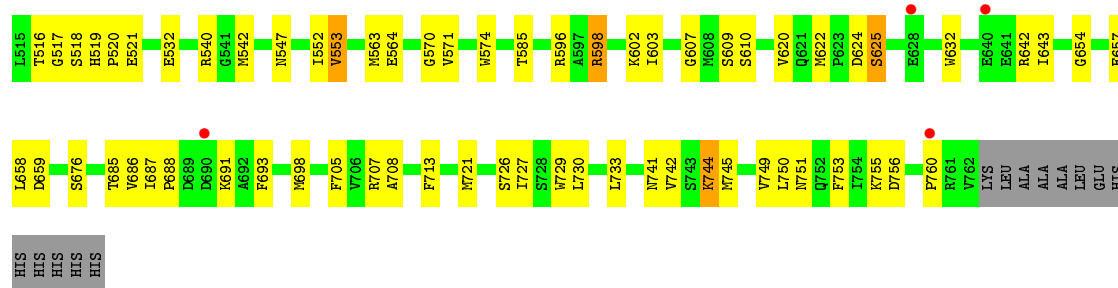
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: N,N-dimethylformamidase large subunit

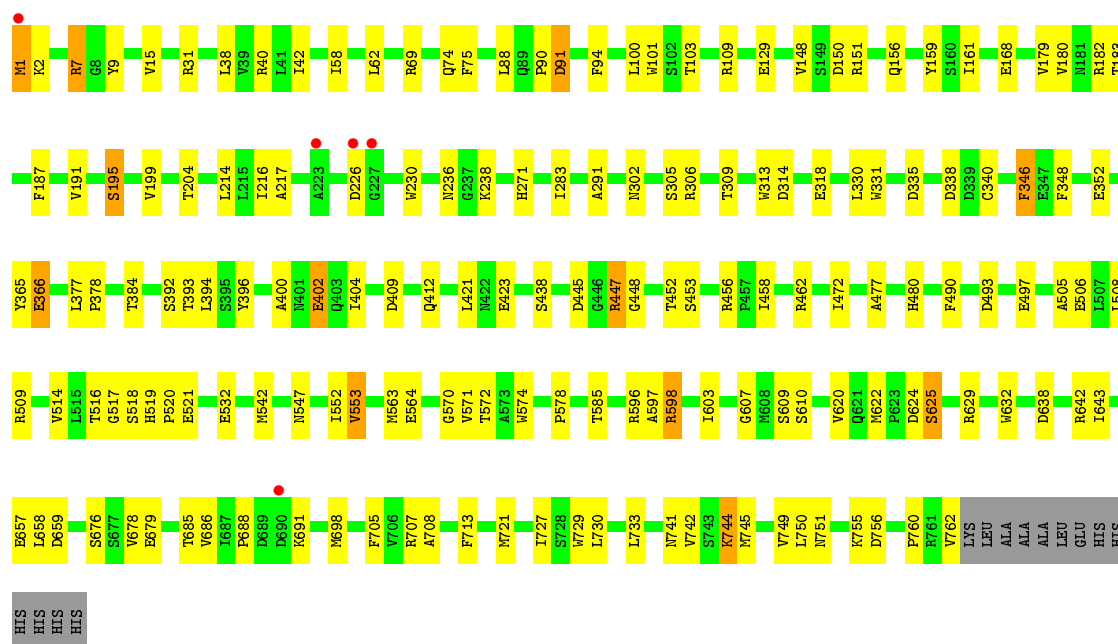
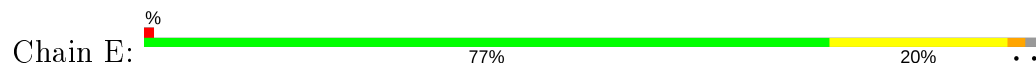


- Molecule 1: N,N-dimethylformamidase large subunit

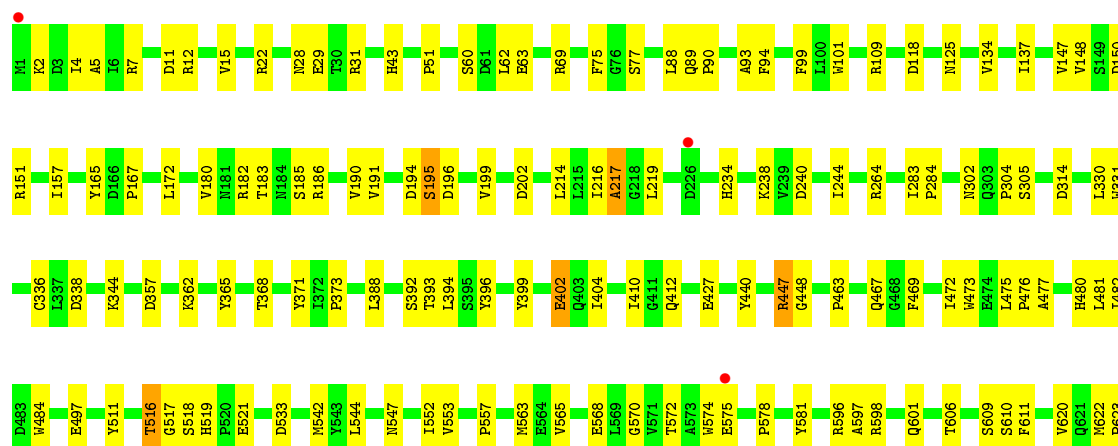
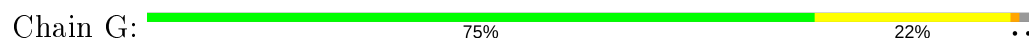


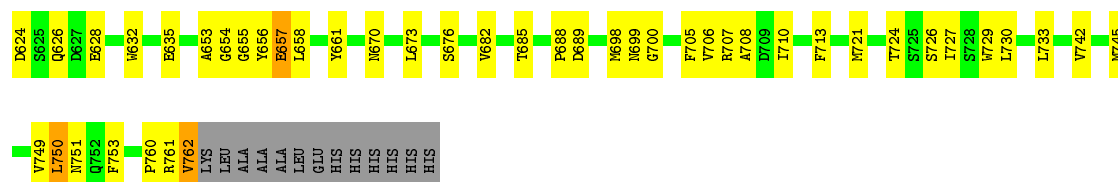


• Molecule 1: N,N-dimethylformamidase large subunit



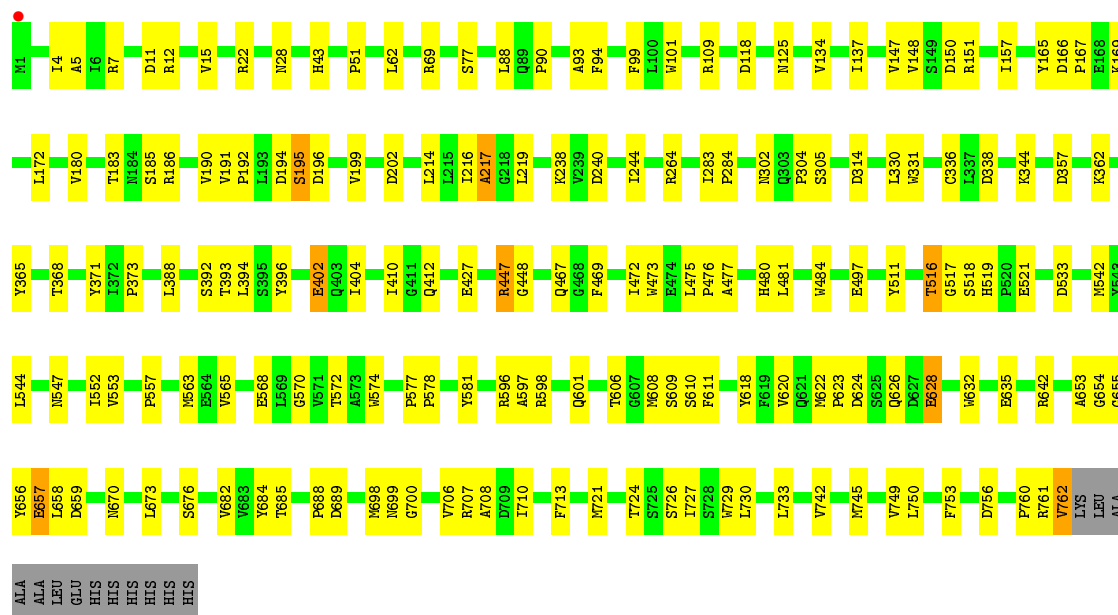
• Molecule 1: N,N-dimethylformamidase large subunit





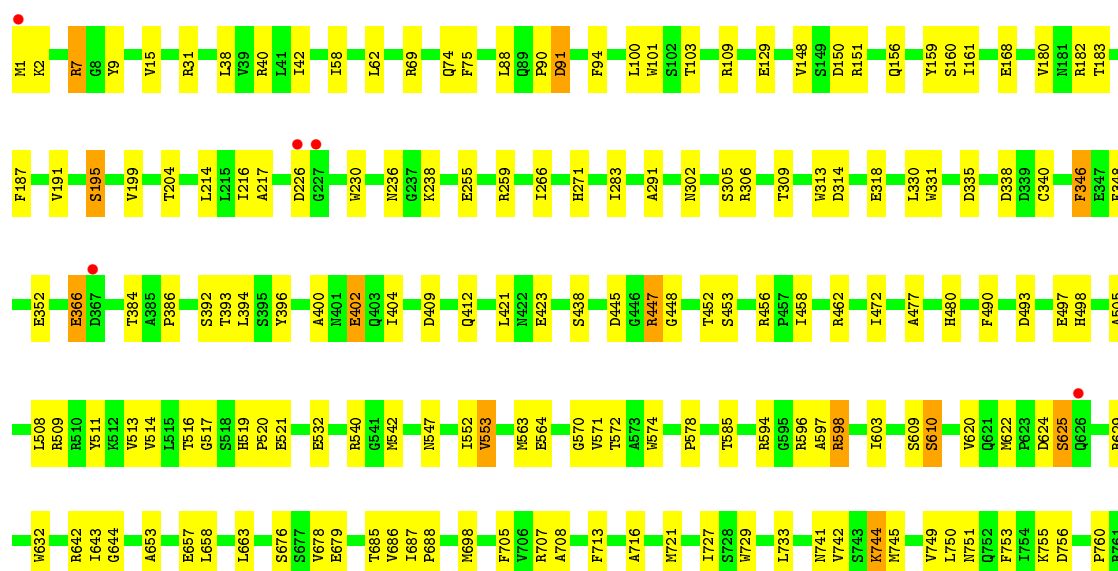
- Molecule 1: N,N-dimethylformamidase large subunit

Chain I: 76% 21% ..



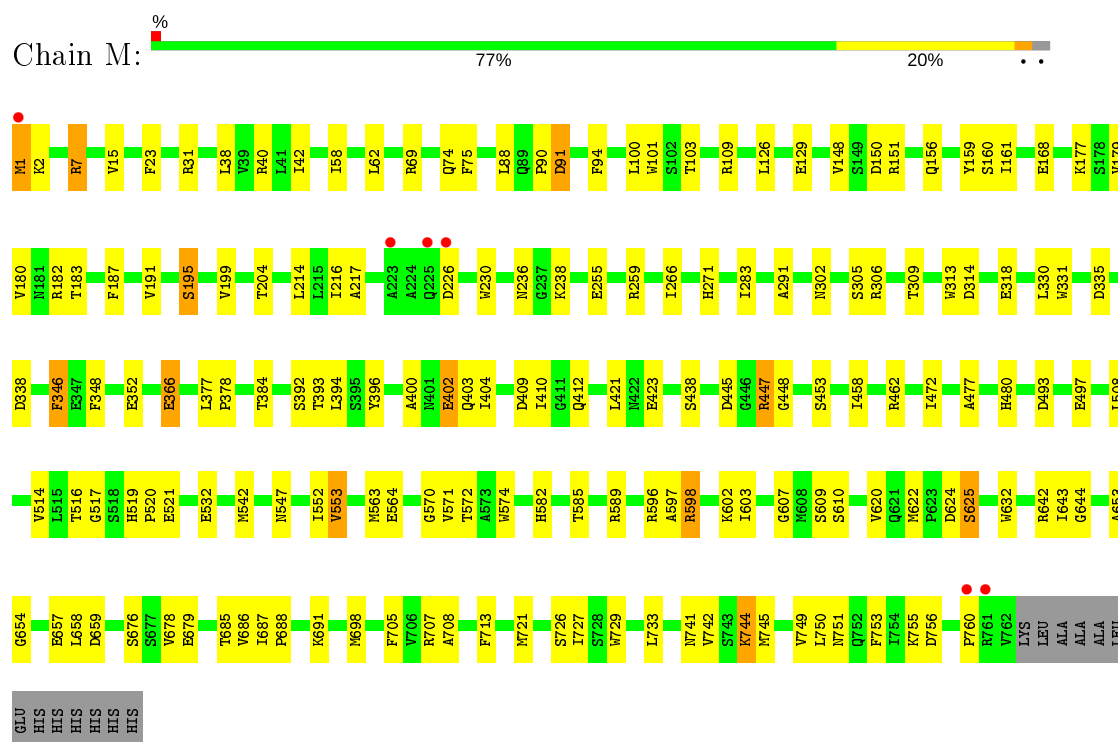
- Molecule 1: N,N-dimethylformamidase large subunit

Chain K: 76% 21% ..



V762
LYS
LEU
ALA
ALA
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

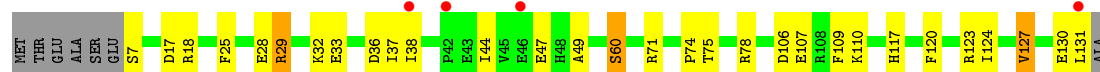
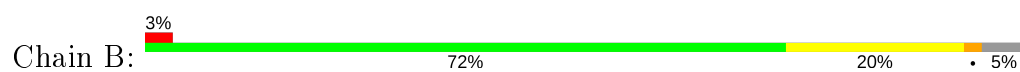
• Molecule 1: N,N-dimethylformamidase large subunit



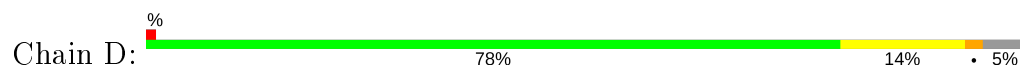
• Molecule 1: N,N-dimethylformamidase large subunit



• Molecule 2: N,N-dimethylformamidase small subunit



- Molecule 2: N,N-dimethylformamidase small subunit



- Molecule 2: N,N-dimethylformamidase small subunit



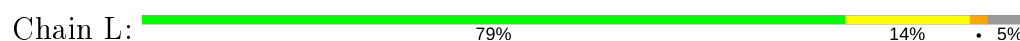
- Molecule 2: N,N-dimethylformamidase small subunit



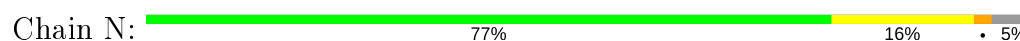
- Molecule 2: N,N-dimethylformamidase small subunit



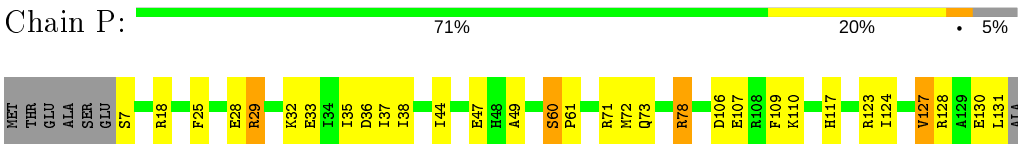
- Molecule 2: N,N-dimethylformamidase small subunit



- Molecule 2: N,N-dimethylformamidase small subunit



- Molecule 2: N,N-dimethylformamidase small subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	160.51Å 142.55Å 181.49Å 90.00° 92.92° 90.00°	Depositor
Resolution (Å)	49.47 – 2.80 49.47 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.47-2.80) 99.9 (49.47-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18rc6 _3830	Depositor
R, R_{free}	0.227 , 0.267 0.230 , 0.268	Depositor DCC
R_{free} test set	1923 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 22.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	56839	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 32.38 % 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 9.4942e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, 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	0.30	0/6157	0.48	0/8375
1	C	0.34	0/6157	0.49	0/8375
1	E	0.36	0/6157	0.49	0/8375
1	G	0.31	0/6157	0.48	0/8375
1	I	0.31	0/6157	0.48	0/8375
1	K	0.33	0/6157	0.48	0/8375
1	M	0.33	0/6157	0.49	0/8375
1	O	0.32	0/6157	0.48	0/8375
2	B	0.30	0/1117	0.43	0/1509
2	D	0.29	0/1117	0.41	0/1509
2	F	0.48	0/1117	0.44	0/1509
2	H	0.37	0/1117	0.46	0/1509
2	J	0.42	0/1117	0.48	0/1509
2	L	0.28	0/1117	0.41	0/1509
2	N	0.28	0/1117	0.42	0/1509
2	P	0.44	0/1117	0.49	0/1509
All	All	0.33	0/58192	0.48	0/79072

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5987	0	5637	139	0
1	C	5987	0	5637	133	0
1	E	5987	0	5637	150	0
1	G	5987	0	5637	143	0
1	I	5987	0	5637	148	0
1	K	5987	0	5637	142	0
1	M	5987	0	5637	142	0
1	O	5987	0	5637	147	0
2	B	1085	0	1010	18	0
2	D	1085	0	1010	16	0
2	F	1085	0	1010	25	0
2	H	1085	0	1010	23	0
2	J	1085	0	1010	22	0
2	L	1085	0	1010	13	0
2	N	1085	0	1010	15	0
2	P	1085	0	1010	22	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
4	B	4	6	6	0	0
4	D	4	6	6	0	0
4	F	4	6	6	0	0
4	H	4	6	6	0	0
4	J	4	6	6	0	0
4	L	4	6	6	0	0
4	N	4	6	6	0	0
4	P	4	6	6	0	0
5	A	22	0	0	0	0
5	B	1	0	0	0	0
5	C	21	0	0	1	0
5	E	21	0	0	0	0
5	G	22	0	0	0	0
5	H	1	0	0	1	0
5	I	20	0	0	0	0
5	J	1	0	0	0	0
5	K	21	0	0	4	0
5	M	22	0	0	1	0
5	O	23	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	56791	48	53224	1185	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 11.

The worst 5 of 1185 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:I:362:LYS:HE3	1:I:371:TYR:OH	1.44	1.16
1:I:688:PRO:HG2	1:K:688:PRO:HG2	1.28	1.15
1:E:506:GLU:HG3	1:I:756:ASP:HB2	1.39	1.05
1:E:688:PRO:HG2	1:G:688:PRO:HG2	1.35	1.03
1:M:688:PRO:HG2	1:O:688:PRO:HG2	1.41	0.99

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	760/775 (98%)	715 (94%)	43 (6%)	2 (0%)	41	72
1	C	760/775 (98%)	715 (94%)	44 (6%)	1 (0%)	51	81
1	E	760/775 (98%)	717 (94%)	42 (6%)	1 (0%)	51	81
1	G	760/775 (98%)	716 (94%)	41 (5%)	3 (0%)	34	66
1	I	760/775 (98%)	716 (94%)	41 (5%)	3 (0%)	34	66
1	K	760/775 (98%)	713 (94%)	46 (6%)	1 (0%)	51	81
1	M	760/775 (98%)	718 (94%)	41 (5%)	1 (0%)	51	81
1	O	760/775 (98%)	718 (94%)	39 (5%)	3 (0%)	34	66
2	B	123/132 (93%)	114 (93%)	8 (6%)	1 (1%)	19	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	123/132 (93%)	118 (96%)	5 (4%)	0	100	100
2	F	123/132 (93%)	117 (95%)	6 (5%)	0	100	100
2	H	123/132 (93%)	114 (93%)	8 (6%)	1 (1%)	19	49
2	J	123/132 (93%)	114 (93%)	8 (6%)	1 (1%)	19	49
2	L	123/132 (93%)	118 (96%)	5 (4%)	0	100	100
2	N	123/132 (93%)	118 (96%)	5 (4%)	0	100	100
2	P	123/132 (93%)	113 (92%)	10 (8%)	0	100	100
All	All	7064/7256 (97%)	6654 (94%)	392 (6%)	18 (0%)	41	72

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	635	GLU
1	G	635	GLU
1	I	635	GLU
1	O	635	GLU
1	A	761	ARG

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	621/631 (98%)	594 (96%)	27 (4%)	29	62
1	C	621/631 (98%)	596 (96%)	25 (4%)	31	65
1	E	621/631 (98%)	596 (96%)	25 (4%)	31	65
1	G	621/631 (98%)	591 (95%)	30 (5%)	25	58
1	I	621/631 (98%)	594 (96%)	27 (4%)	29	62
1	K	621/631 (98%)	596 (96%)	25 (4%)	31	65
1	M	621/631 (98%)	595 (96%)	26 (4%)	30	63
1	O	621/631 (98%)	593 (96%)	28 (4%)	27	60
2	B	111/117 (95%)	105 (95%)	6 (5%)	22	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	111/117 (95%)	104 (94%)	7 (6%)	18	46
2	F	111/117 (95%)	104 (94%)	7 (6%)	18	46
2	H	111/117 (95%)	104 (94%)	7 (6%)	18	46
2	J	111/117 (95%)	102 (92%)	9 (8%)	11	33
2	L	111/117 (95%)	104 (94%)	7 (6%)	18	46
2	N	111/117 (95%)	104 (94%)	7 (6%)	18	46
2	P	111/117 (95%)	104 (94%)	7 (6%)	18	46
All	All	5856/5984 (98%)	5586 (95%)	270 (5%)	27	60

5 of 270 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	699	ASN
1	I	620	VAL
1	O	410	ILE
1	G	751	ASN
1	I	150	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	480	HIS
1	I	480	HIS
1	O	480	HIS
1	G	519	HIS
1	C	465	HIS

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z > 2$
4	EDO	P	201	-	3,3,3	0.50	0	2,2,2	0.18	0
4	EDO	J	201	-	3,3,3	0.56	0	2,2,2	0.19	0
4	EDO	H	201	-	3,3,3	0.52	0	2,2,2	0.26	0
4	EDO	N	201	-	3,3,3	0.58	0	2,2,2	0.15	0
4	EDO	L	201	-	3,3,3	0.53	0	2,2,2	0.15	0
4	EDO	B	201	-	3,3,3	0.58	0	2,2,2	0.17	0
4	EDO	F	201	-	3,3,3	0.59	0	2,2,2	0.12	0
4	EDO	D	201	-	3,3,3	0.57	0	2,2,2	0.12	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
4	EDO	P	201	-	-	0/1/1/1	-
4	EDO	J	201	-	-	0/1/1/1	-
4	EDO	H	201	-	-	0/1/1/1	-
4	EDO	N	201	-	-	0/1/1/1	-
4	EDO	L	201	-	-	0/1/1/1	-
4	EDO	B	201	-	-	0/1/1/1	-
4	EDO	F	201	-	-	0/1/1/1	-
4	EDO	D	201	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	762/775 (98%)	-0.33	1 (0%) 95 95	13, 25, 49, 76	0
1	C	762/775 (98%)	-0.19	9 (1%) 79 73	15, 28, 51, 87	0
1	E	762/775 (98%)	-0.31	5 (0%) 87 84	13, 26, 49, 81	0
1	G	762/775 (98%)	-0.22	3 (0%) 92 91	13, 30, 56, 76	0
1	I	762/775 (98%)	-0.30	1 (0%) 95 95	14, 25, 48, 75	0
1	K	762/775 (98%)	-0.31	5 (0%) 87 84	13, 26, 49, 81	0
1	M	762/775 (98%)	-0.27	6 (0%) 86 81	13, 26, 49, 85	0
1	O	762/775 (98%)	-0.34	6 (0%) 86 81	14, 25, 49, 76	0
2	B	125/132 (94%)	0.17	4 (3%) 47 37	24, 33, 53, 62	0
2	D	125/132 (94%)	0.15	1 (0%) 86 81	27, 39, 54, 74	0
2	F	125/132 (94%)	0.06	0 100 100	27, 38, 54, 72	0
2	H	125/132 (94%)	0.28	0 100 100	28, 36, 57, 65	0
2	J	125/132 (94%)	0.10	1 (0%) 86 81	24, 33, 52, 63	0
2	L	125/132 (94%)	0.00	0 100 100	25, 36, 56, 63	0
2	N	125/132 (94%)	-0.03	0 100 100	23, 36, 54, 70	0
2	P	125/132 (94%)	0.10	0 100 100	20, 34, 53, 62	0
All	All	7096/7256 (97%)	-0.23	42 (0%) 89 86	13, 28, 52, 87	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	1	MET	4.2
1	E	1	MET	4.1
1	C	226	ASP	3.7
1	C	1	MET	3.4
1	K	367	ASP	3.2

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](#)

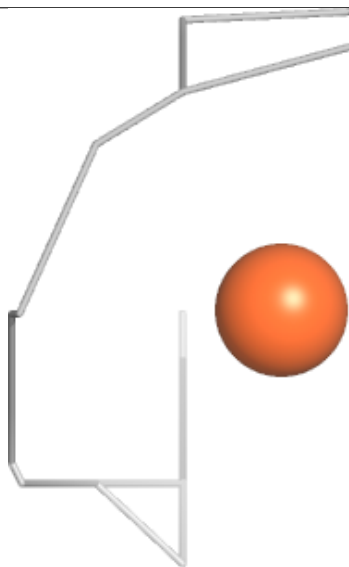
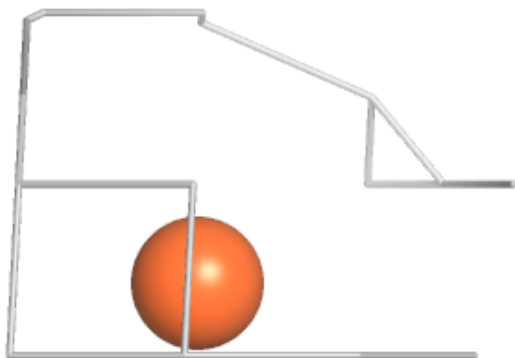
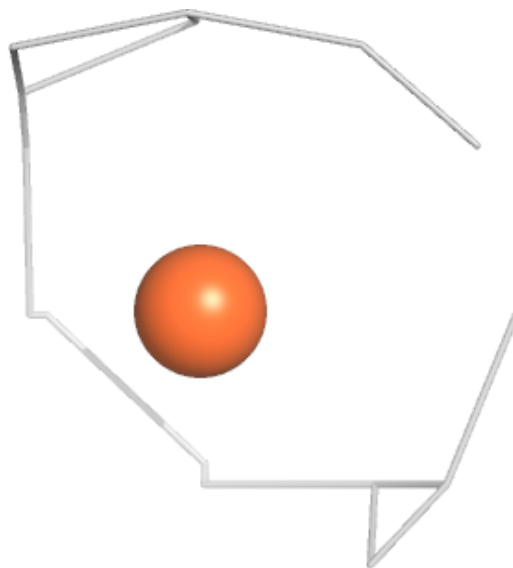
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	F	201	4/4	0.76	0.22	24,31,37,37	0
4	EDO	D	201	4/4	0.83	0.20	18,29,35,35	0
4	EDO	J	201	4/4	0.85	0.19	15,24,30,36	0
4	EDO	N	201	4/4	0.85	0.17	18,24,30,30	0
4	EDO	B	201	4/4	0.89	0.21	19,24,32,32	0
4	EDO	L	201	4/4	0.90	0.16	16,29,36,36	0
4	EDO	P	201	4/4	0.92	0.14	15,21,26,26	0
4	EDO	H	201	4/4	0.94	0.15	19,23,30,36	0
3	FE	K	801	1/1	0.97	0.05	17,17,17,17	0
3	FE	O	801	1/1	0.98	0.09	23,23,23,23	0
3	FE	G	801	1/1	0.98	0.09	23,23,23,23	0
3	FE	A	801	1/1	0.98	0.08	24,24,24,24	0
3	FE	I	801	1/1	0.99	0.13	21,21,21,21	0
3	FE	M	801	1/1	0.99	0.10	20,20,20,20	0
3	FE	E	801	1/1	0.99	0.08	17,17,17,17	0
3	FE	C	801	1/1	0.99	0.07	17,17,17,17	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.

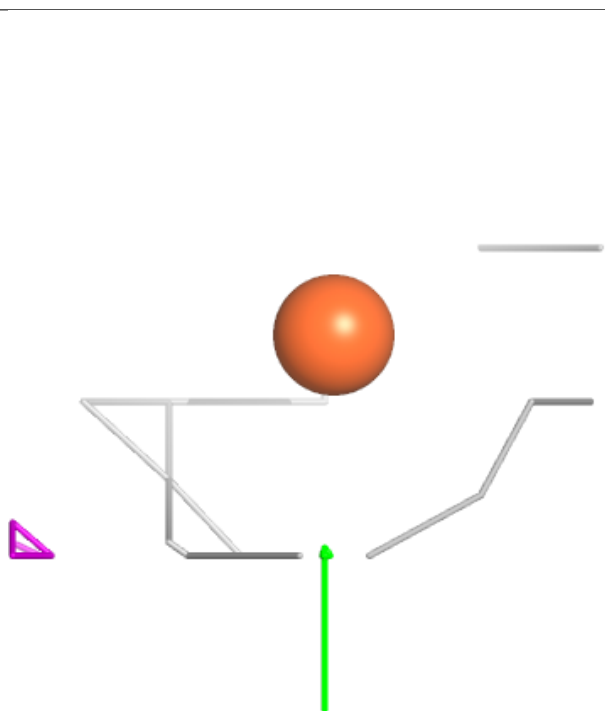
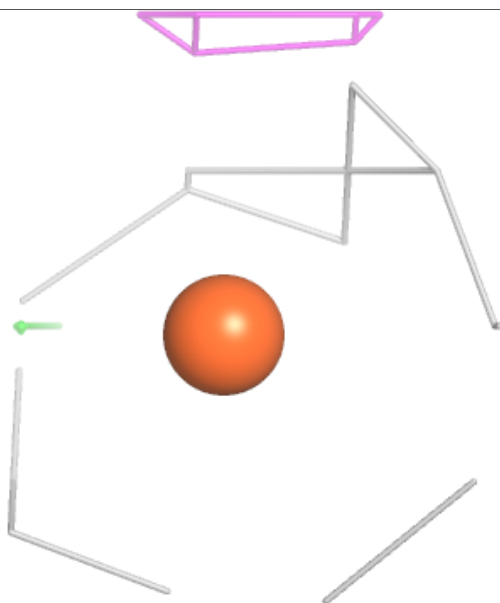
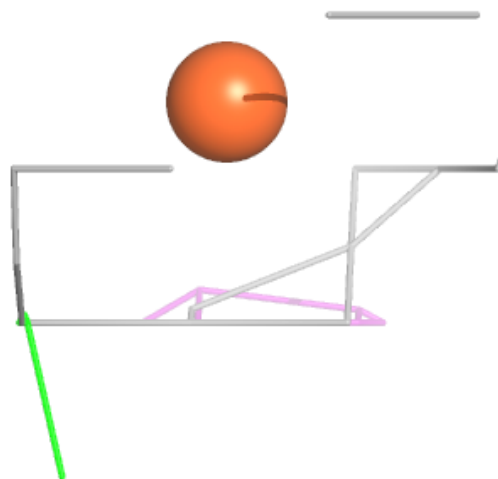
Electron density around FE K 801:

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



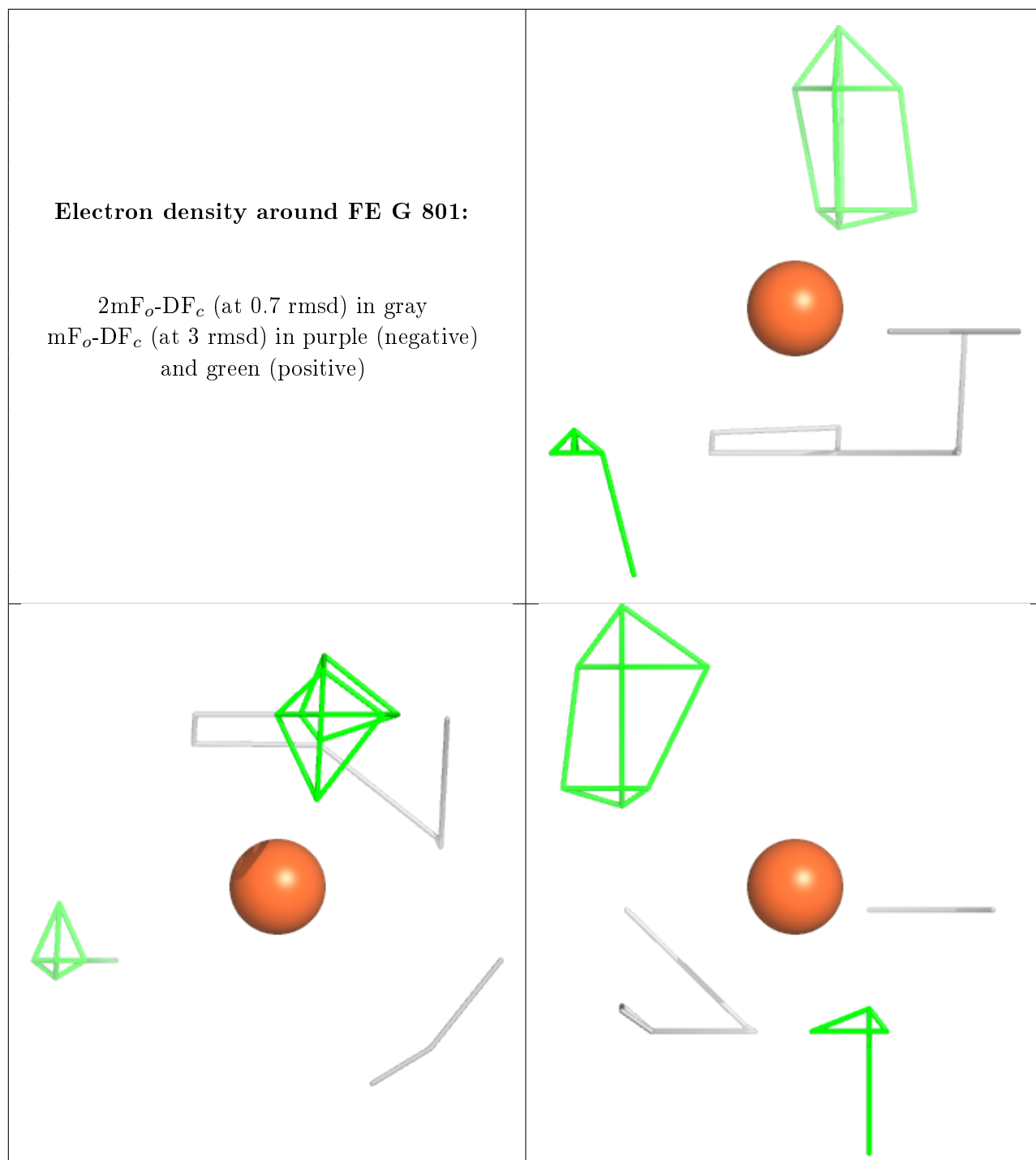
Electron density around FE O 801:

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



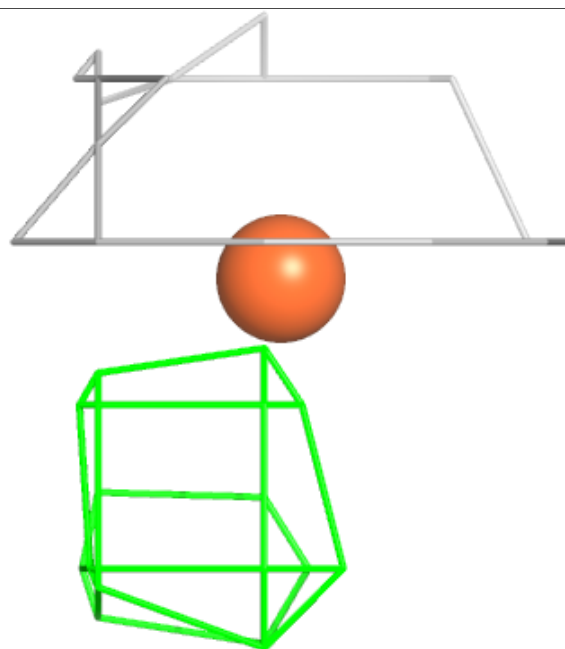
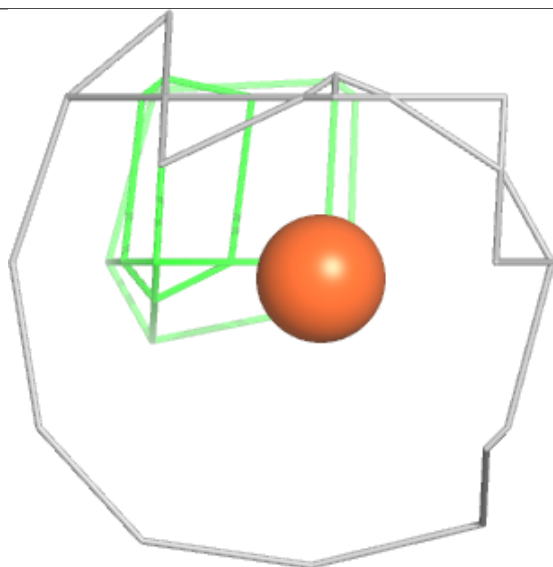
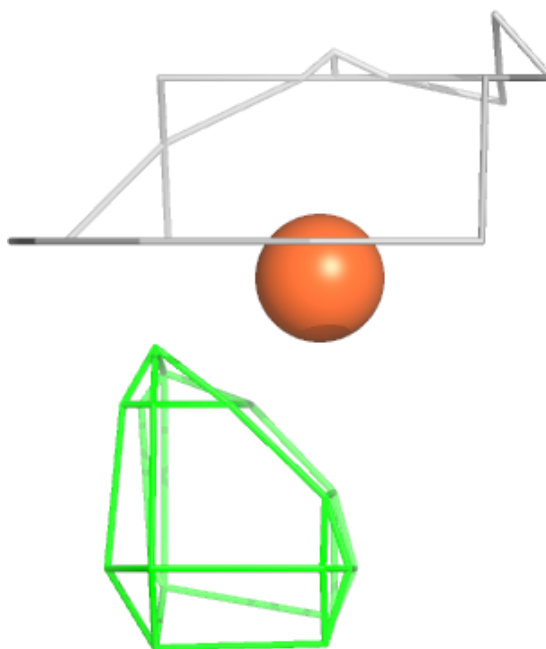
Electron density around FE G 801:

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



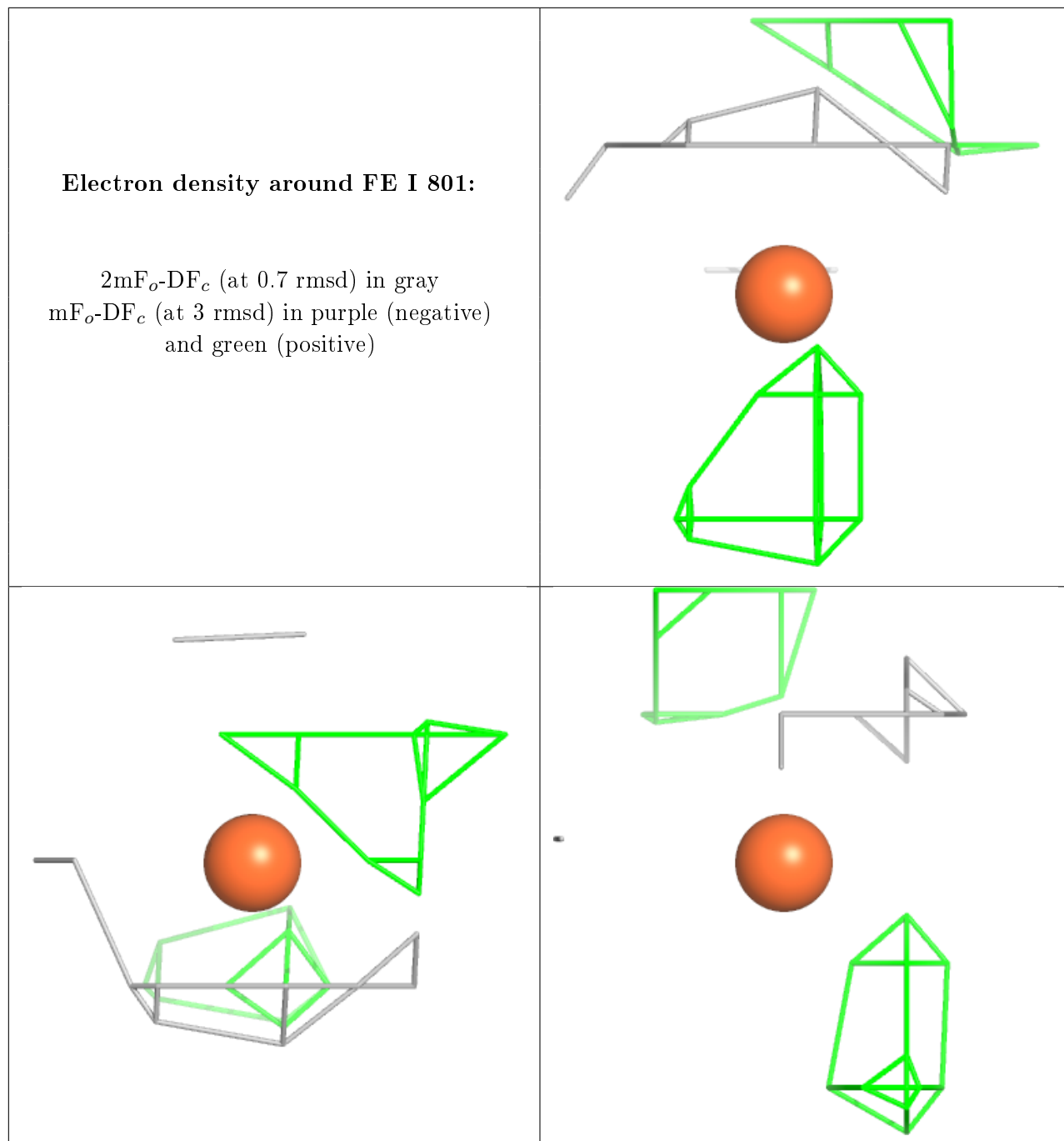
Electron density around FE A 801:

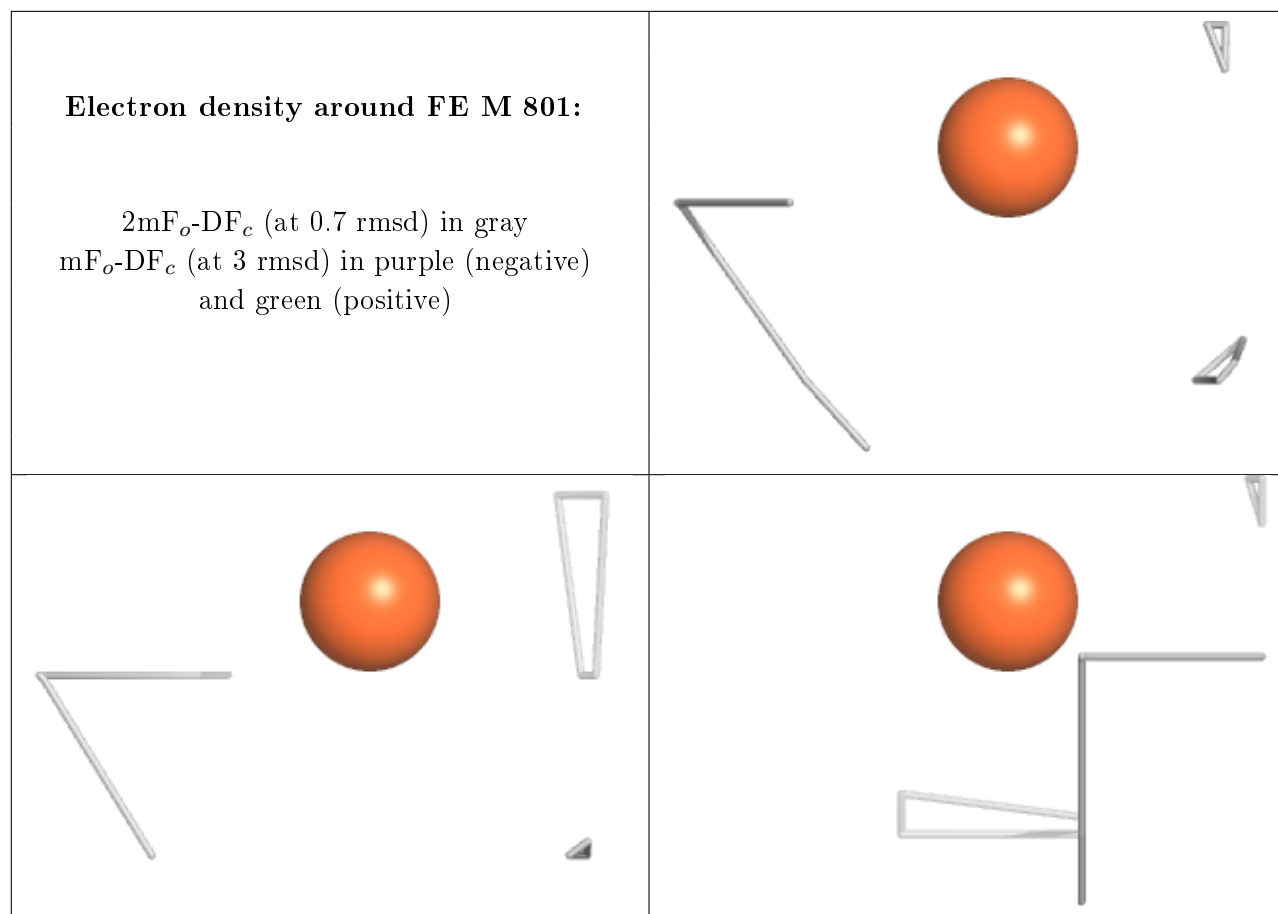
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE I 801:

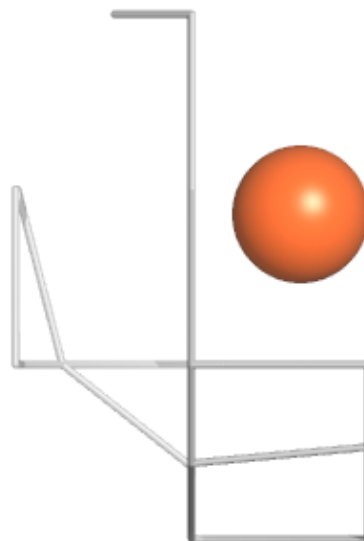
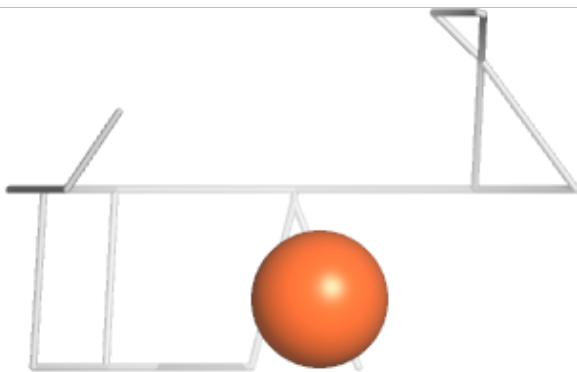
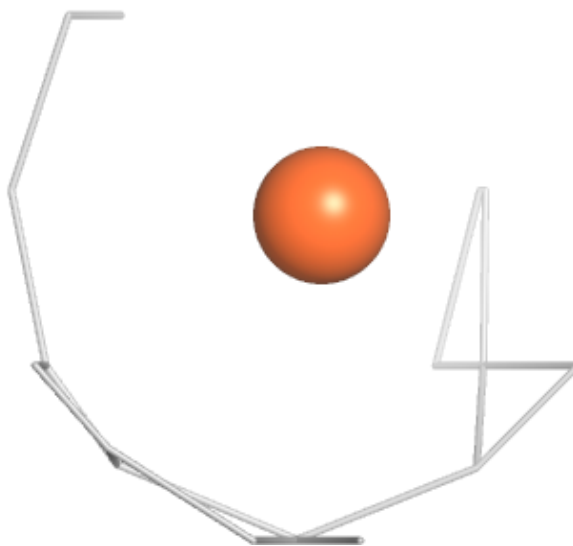
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

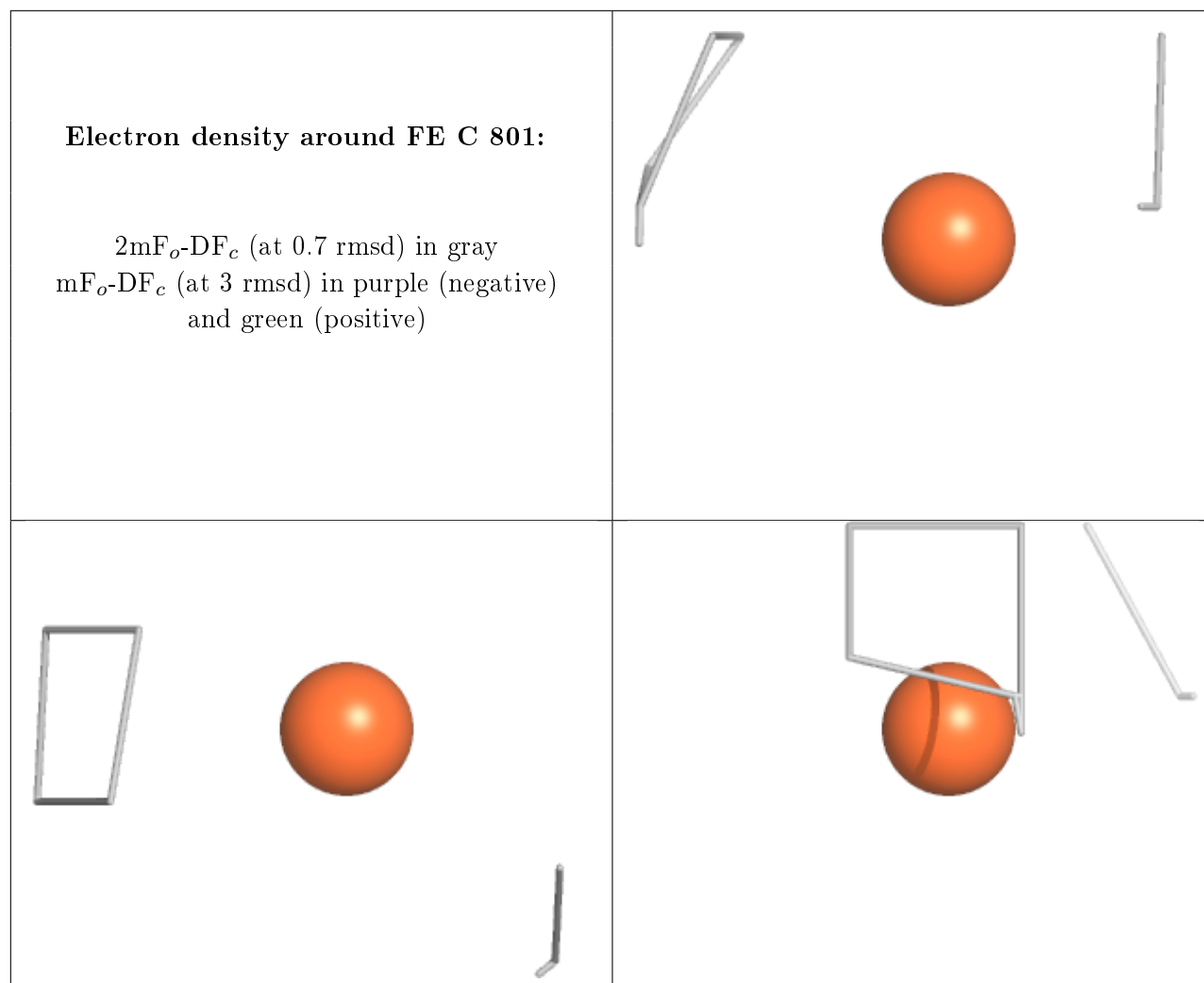




Electron density around FE E 801:

$2mF_o-DF_c$ (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.