wwPDB X-ray Structure Validation Summary Report (i)

Oct 25, 2026 – 04:25 PM JST

PDB ID	:	27DQ / pdb_000027dq
Title	:	Crystal structure of HPO from Pseudomonas
Authors	:	Cheng, Z.Y.; Han, X.; Li, Q.; Wei, H.L.; Hu, H.Y.; Xu, P.; Liu, W.; Tang, H.Z.
Deposited on	:	2026-05-27
Resolution	:	2.56 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 (i) 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 (1)) were used in the production of this report:

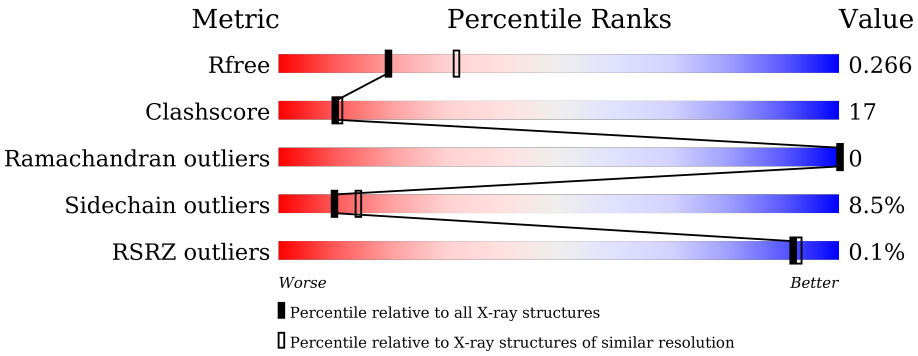
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	343	60% 35%
1	B	343	66% 29%
1	C	343	62% 32%
1	D	343	62% 30% 5%
1	E	343	59% 35%
1	F	343	58% 36%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15099 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 2,5-DHP dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2526	1602	421	481	22			
1	B	333	Total	C	N	O	S	0	0	0
			2518	1593	424	479	22			
1	C	330	Total	C	N	O	S	0	0	0
			2520	1595	426	477	22			
1	D	332	Total	C	N	O	S	0	0	0
			2522	1600	422	478	22			
1	E	332	Total	C	N	O	S	0	0	0
			2492	1575	415	480	22			
1	F	332	Total	C	N	O	S	0	0	0
			2436	1545	400	470	21			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	23	Total O 23 23	0	0
3	B	13	Total O 13 13	0	0
3	C	12	Total O 12 12	0	0
3	D	19	Total O 19 19	0	0
3	E	7	Total O 7 7	0	0
3	F	5	Total O 5 5	0	0

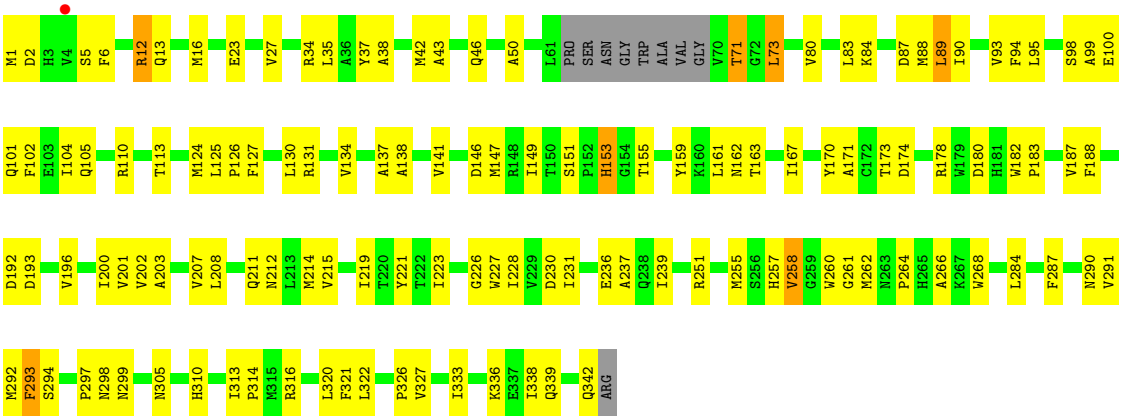
3 Residue-property plots (i)

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

• Molecule 1: 2,5-DHP dioxygenase

Chain A:

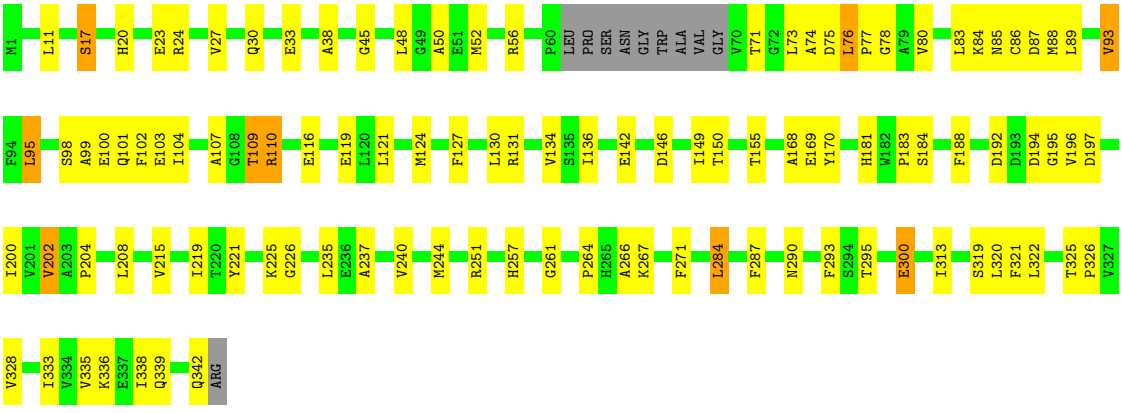




• Molecule 1: 2,5-DHP dioxygenase

Chain B:

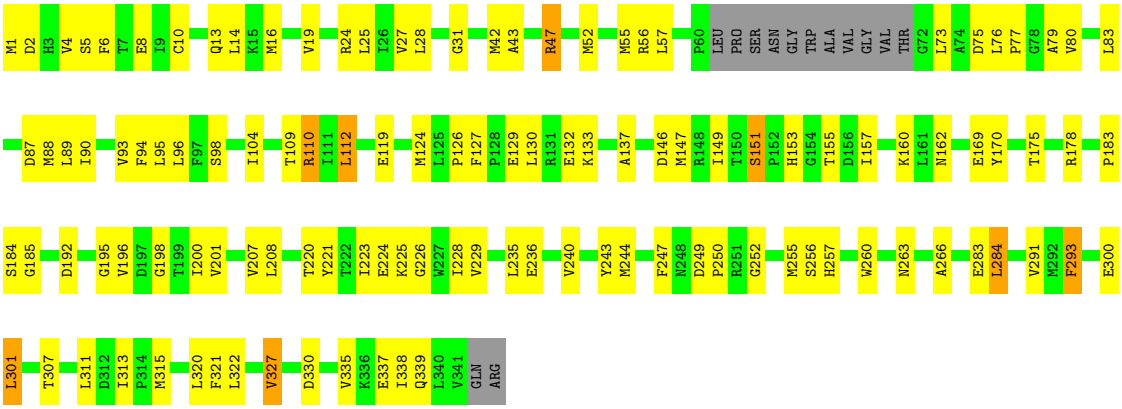




• Molecule 1: 2,5-DHP dioxygenase

Chain C:

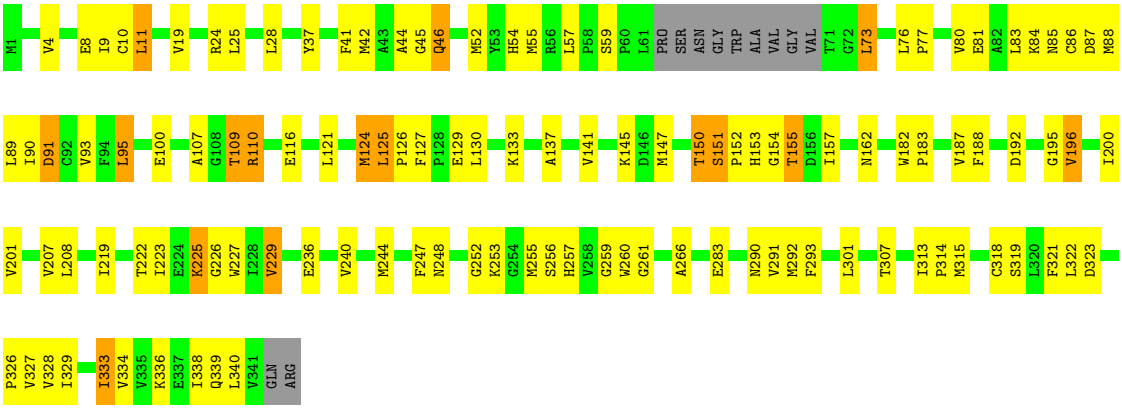




• Molecule 1: 2,5-DHP dioxygenase

Chain D:

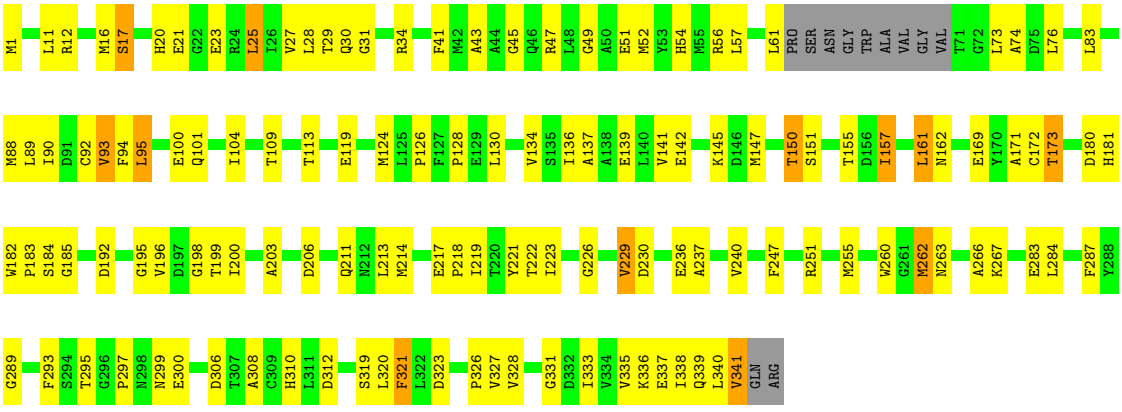




• Molecule 1: 2,5-DHP dioxygenase

Chain E:

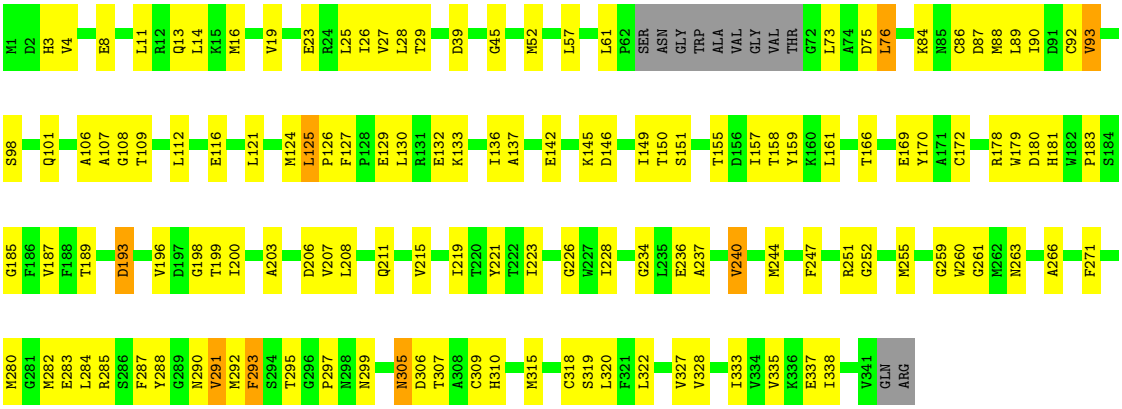




• Molecule 1: 2,5-DHP dioxygenase

Chain F:




M1 D2 H3 V4 E8 L11 R12 Q13 L14 K15 M16 V19 E23 R24 L25 I26 V27 L28 T29 D39 G45 M52 L57 L61 P62 SER ASN GLY TRP ALA VAL GLY VAL THR G72 L73 A74 D75 L76 K84 N85 C86 D87 M88 L89 I90 D91 C92 V93
S98 Q101 A106 A107 G108 T109 L112 E116 L121 M124 L125 P126 F127 P128 E129 L130 R131 E132 K133 I136 A137 E142 K145 D146 I149 T150 S151 T155 D156 I157 T158 Y159 K160 L161 T166 E169 Y170 A171 C172 R178 W179 D180 H181 W182 P183 S184
G185 F186 V187 F188 T189 D193 V196 D197 G198 T199 I200 A203 D206 V207 L208 Q211 V215 I219 T220 Y221 T222 I223 G226 W227 I228 G234 L235 E236 A237 V240 M244 F247 R251 G252 M255 G259 W260 G261 M262 N263 A266 F271
M280 G281 M282 E283 L284 R285 S286 F287 Y288 G289 N290 V291 M292 F293 S294 T295 G296 P297 N298 N299 N305 D306 T307 A308 C309 H310 M315 C318 S319 L320 F321 L322 V327 V328 I333 V334 V335 K336 E337 I338 V341 GLN ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.63Å 142.96Å 89.53Å 90.00° 107.72° 90.00°	Depositor
Resolution (Å)	28.14 – 2.56 28.14 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.14-2.56) 96.2 (28.14-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.57Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.223 , 0.277 0.236 , 0.266	Depositor DCC
R_{free} test set	3380 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	63.8	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.059 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15099	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: FE

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	0.50	0/2585	0.82	0/3521
1	B	0.62	0/2577	0.93	0/3511
1	C	0.61	0/2579	0.96	0/3508
1	D	0.54	0/2582	0.86	0/3515
1	E	0.71	0/2549	1.03	0/3475
1	F	0.61	0/2494	0.97	0/3409
All	All	0.60	0/15366	0.93	0/20939

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	2526	0	2420	84	0
1	B	2518	0	2406	77	0
1	C	2520	0	2434	86	0
1	D	2522	0	2424	88	0
1	E	2492	0	2374	87	0
1	F	2436	0	2268	93	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	23	0	0	1	0
3	B	13	0	0	0	0
3	C	12	0	0	0	0
3	D	19	0	0	1	0
3	E	7	0	0	1	0
3	F	5	0	0	0	0
All	All	15099	0	14326	509	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 17.

The worst 5 of 509 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:C:88:MET:HB2	1:C:110:ARG:HE	1.06	1.15
1:B:104:ILE:O	1:B:109:THR:HG23	1.55	1.07
1:E:73:LEU:HD12	1:E:95:LEU:HD21	1.35	1.01
1:B:74:ALA:HB2	1:B:100:GLU:OE1	1.63	0.99
1:B:169:GLU:HB3	1:B:184:SER:HB3	1.47	0.95

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	330/343 (96%)	319 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	329/343 (96%)	321 (98%)	8 (2%)	0	100	100
1	C	326/343 (95%)	317 (97%)	9 (3%)	0	100	100
1	D	328/343 (96%)	314 (96%)	14 (4%)	0	100	100
1	E	328/343 (96%)	317 (97%)	11 (3%)	0	100	100
1	F	328/343 (96%)	319 (97%)	9 (3%)	0	100	100
All	All	1969/2058 (96%)	1907 (97%)	62 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	267/285 (94%)	246 (92%)	21 (8%)	11	16
1	B	266/285 (93%)	247 (93%)	19 (7%)	13	19
1	C	269/285 (94%)	247 (92%)	22 (8%)	10	15
1	D	268/285 (94%)	242 (90%)	26 (10%)	8	10
1	E	263/285 (92%)	236 (90%)	27 (10%)	7	8
1	F	249/285 (87%)	229 (92%)	20 (8%)	11	16
All	All	1582/1710 (92%)	1447 (92%)	135 (8%)	10	14

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	11	LEU
1	F	93	VAL
1	F	293	PHE
1	C	175	THR
1	C	151	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	238	GLN
1	E	30	GLN
1	F	238	GLN
1	D	290	ASN
1	E	101	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (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	334/343 (97%)	-1.29	1 (0%) 90 91	47, 69, 87, 103	0
1	B	333/343 (97%)	-1.26	0 100 100	49, 69, 86, 102	0
1	C	330/343 (96%)	-1.24	0 100 100	42, 65, 86, 105	0
1	D	332/343 (96%)	-1.30	0 100 100	46, 67, 86, 101	0
1	E	332/343 (96%)	-1.24	0 100 100	48, 76, 99, 108	0
1	F	332/343 (96%)	-1.22	0 100 100	51, 83, 108, 120	0
All	All	1993/2058 (96%)	-1.26	1 (0%) 92 93	42, 71, 96, 120	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	VAL	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

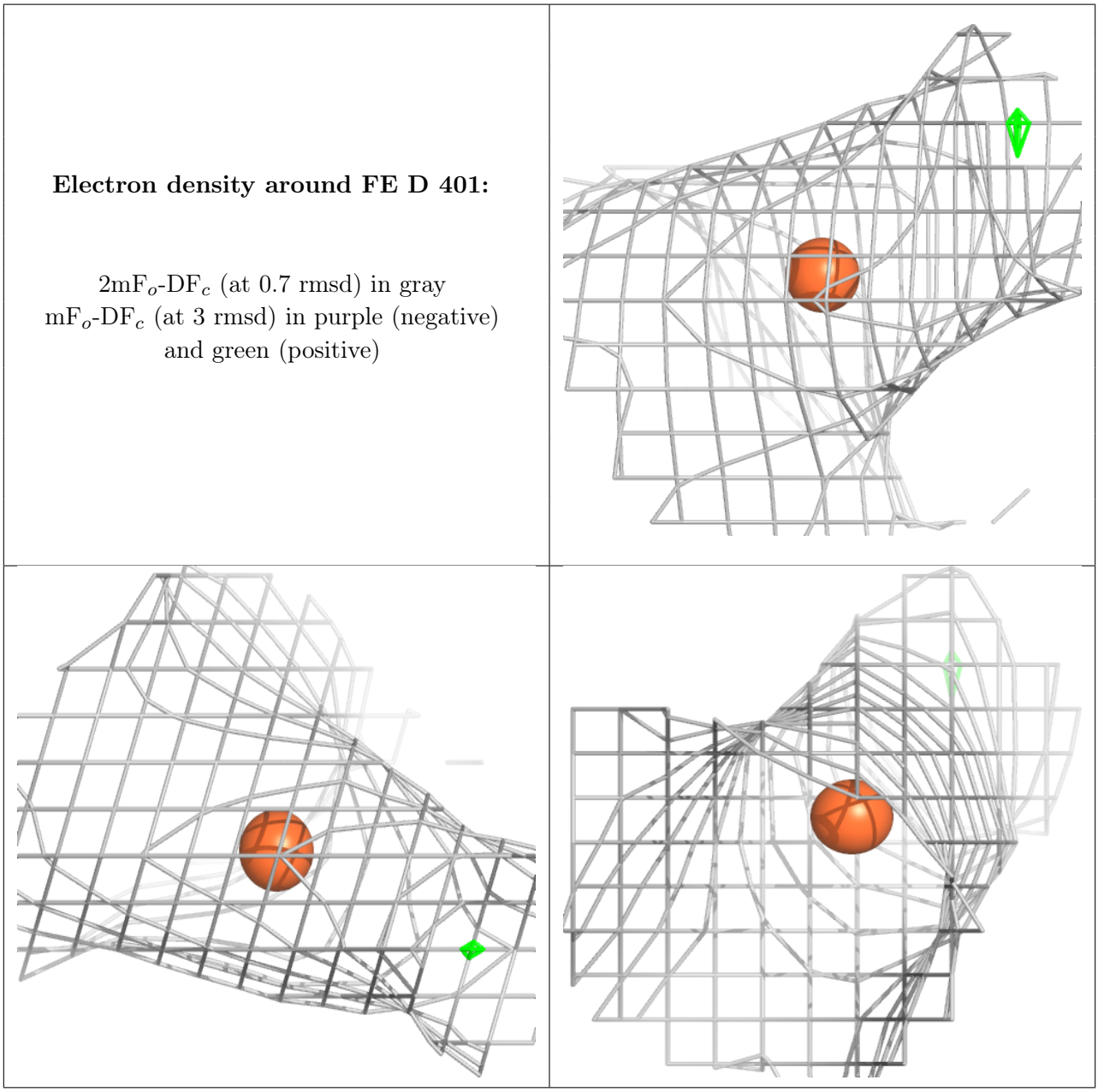
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	FE	D	401	1/1	0.98	0.04	108,108,108,108	0
2	FE	B	401	1/1	0.99	0.02	157,157,157,157	0
2	FE	C	401	1/1	0.99	0.04	131,131,131,131	0
2	FE	A	401	1/1	0.99	0.03	121,121,121,121	0
2	FE	E	401	1/1	0.99	0.03	147,147,147,147	0
2	FE	F	401	1/1	0.99	0.03	160,160,160,160	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.

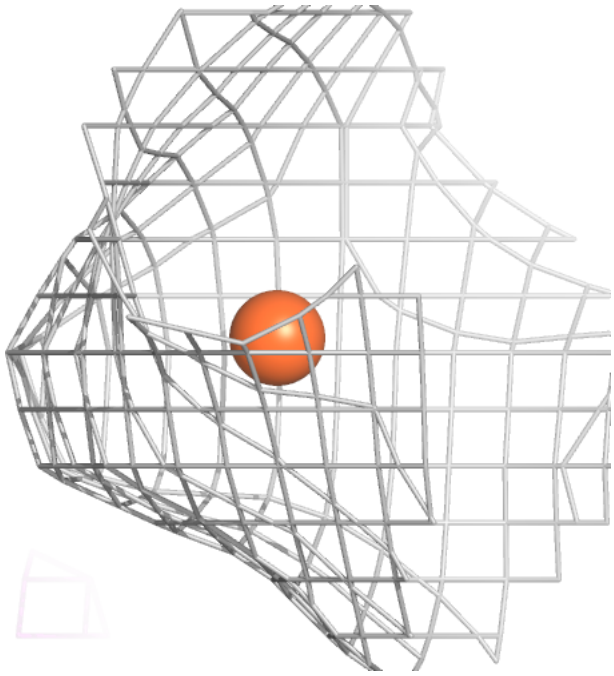
Electron density around FE D 401:

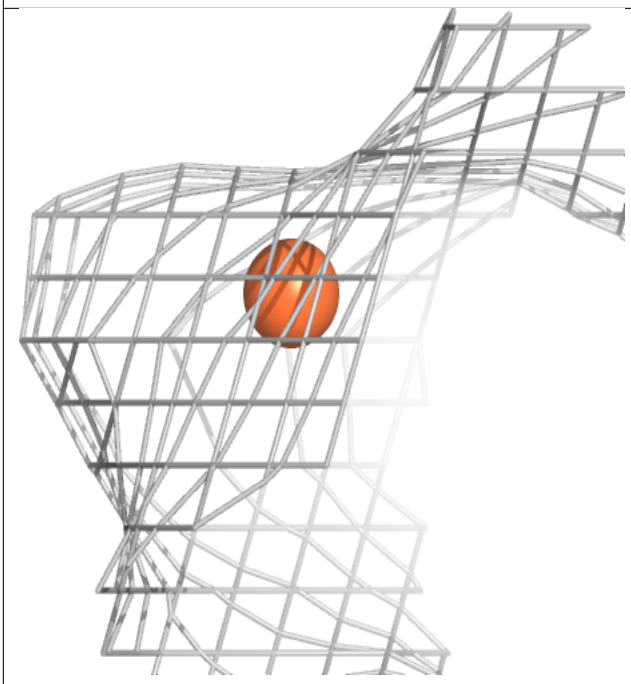
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

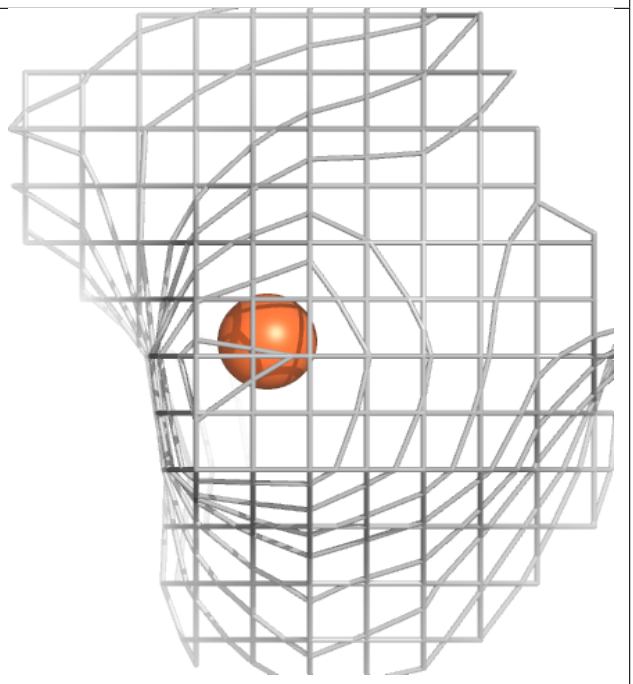


Electron density around FE B 401:

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

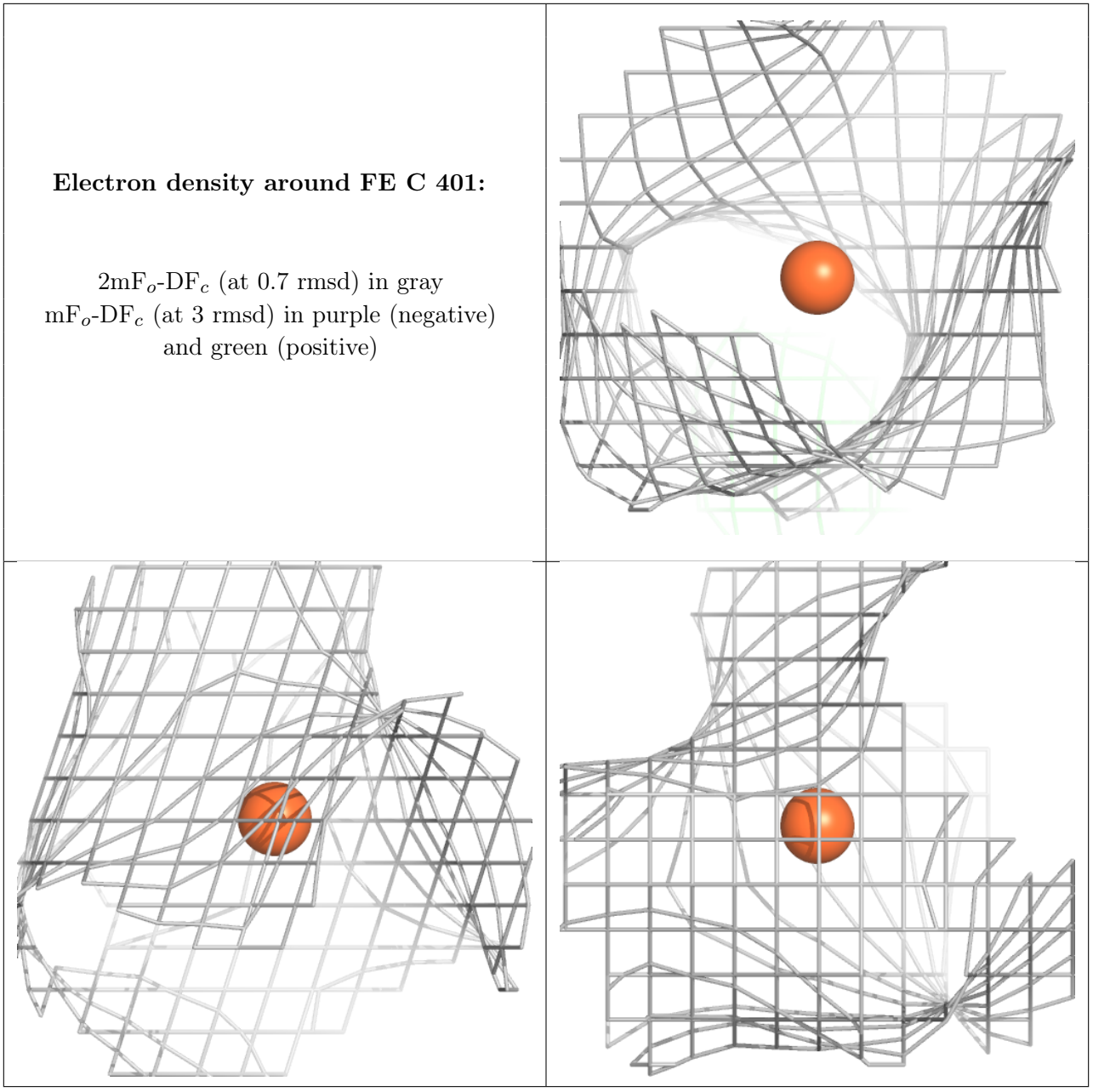






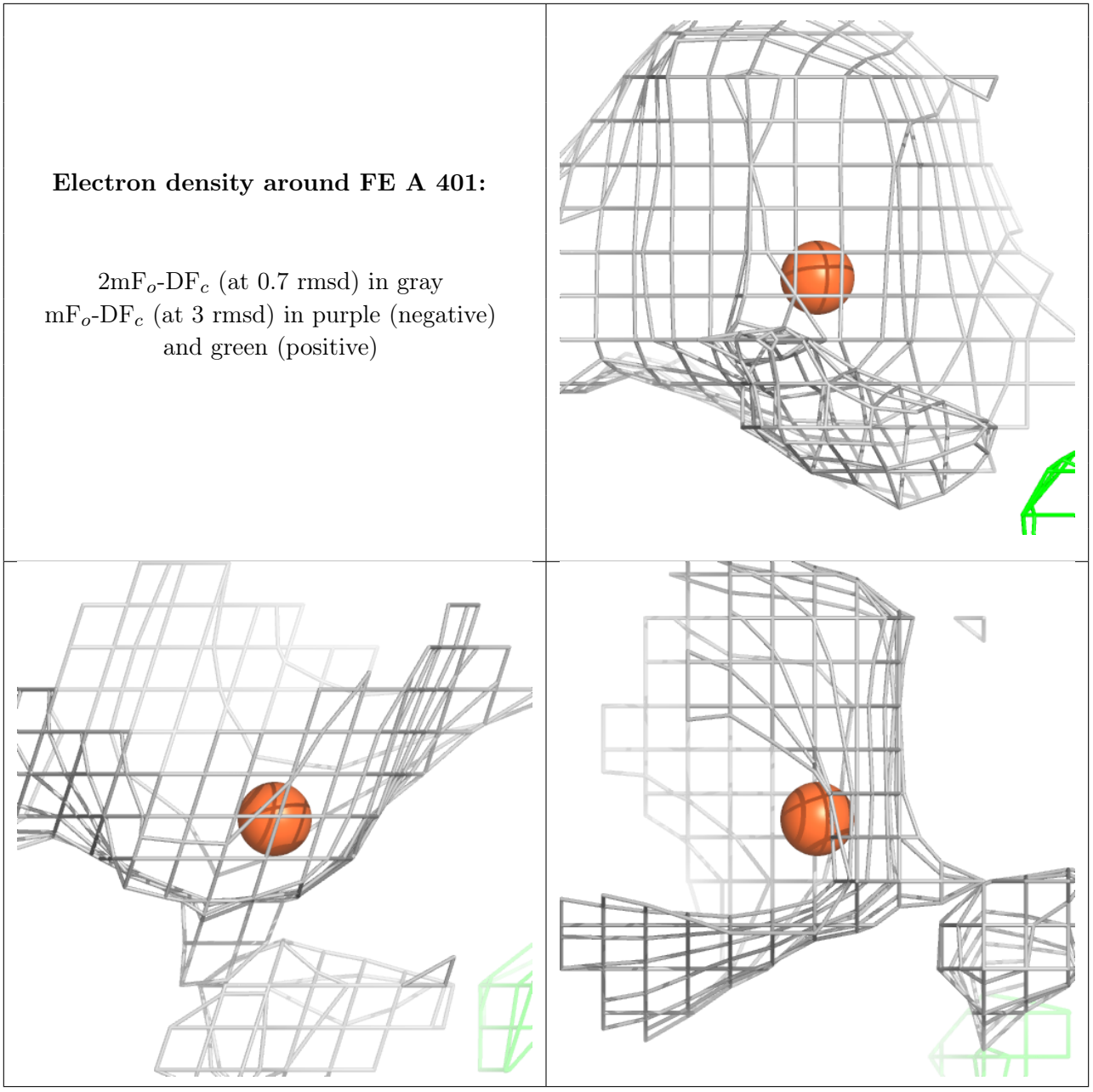
Electron density around FE C 401:

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



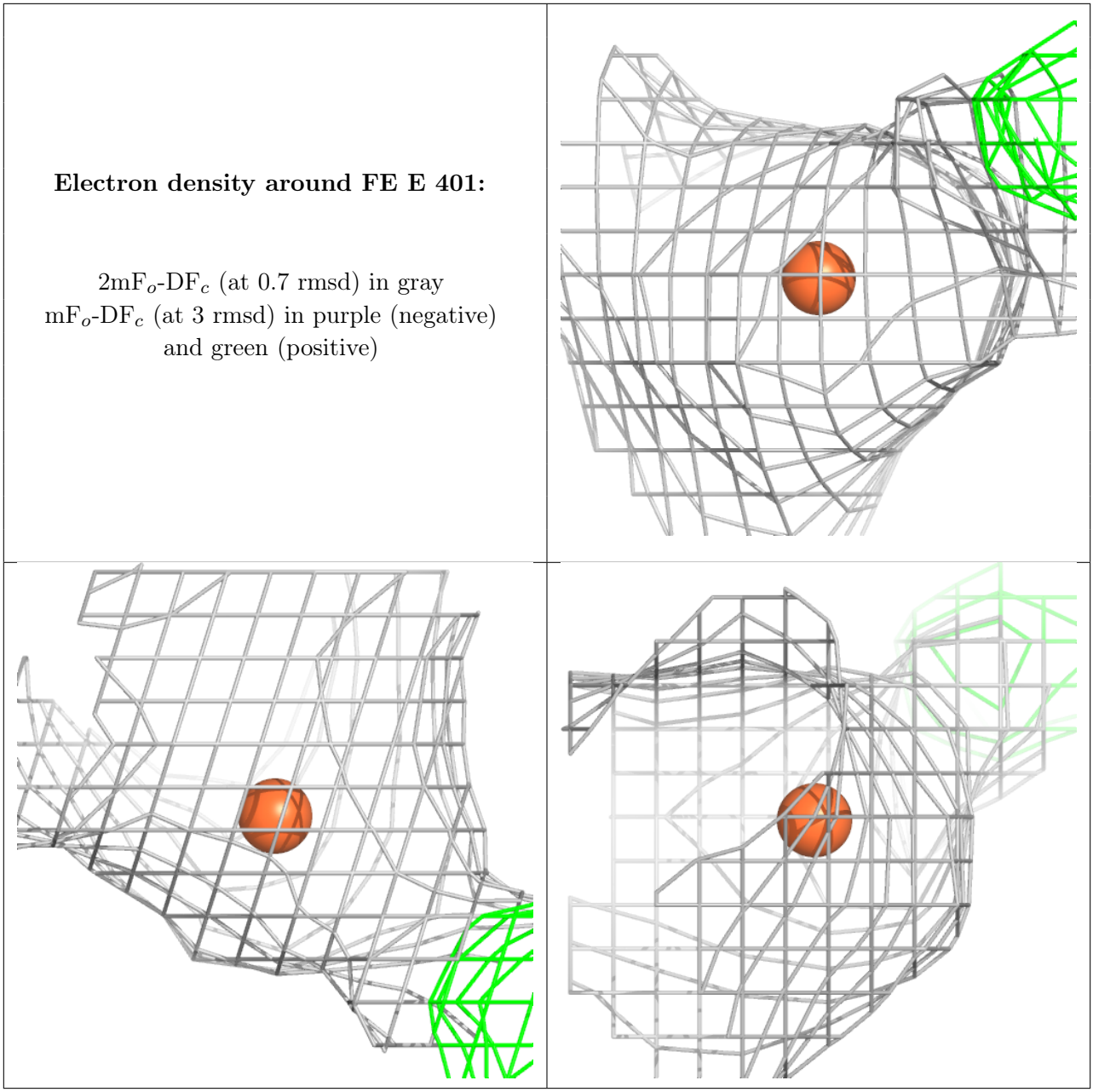
Electron density around FE A 401:

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



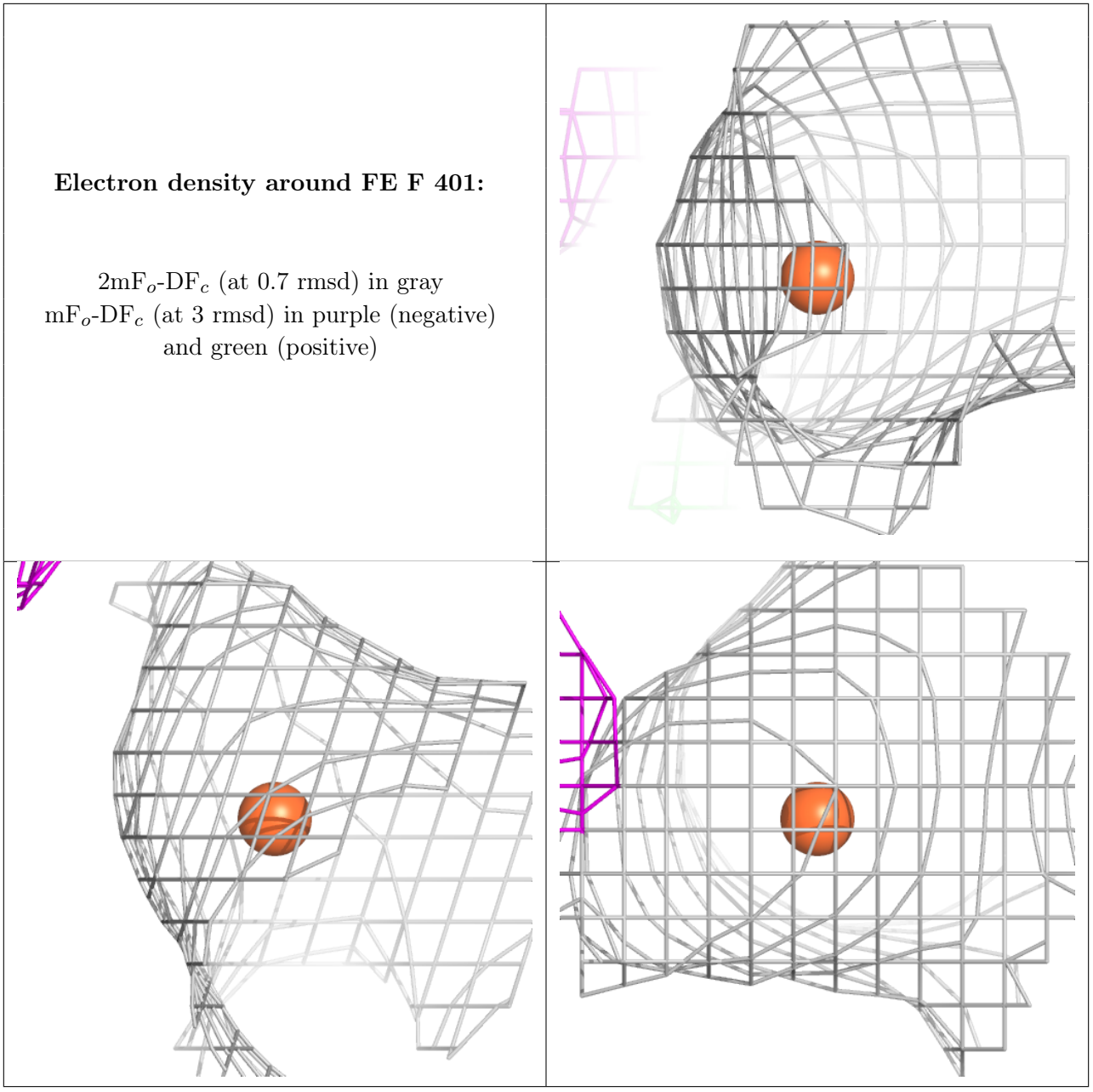
Electron density around FE E 401:

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



Electron density around FE F 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.