



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:53 AM UTC

PDB ID : 7EEH / pdb_00007eeh
Title : Selenomethionine labeled Fe(II)/(alpha)ketoglutarate-dependent dioxygenase TqaL
Authors : Bunno, R.; Mori, T.; Awakawa, T.; Abe, I.
Deposited on : 2021-03-18
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

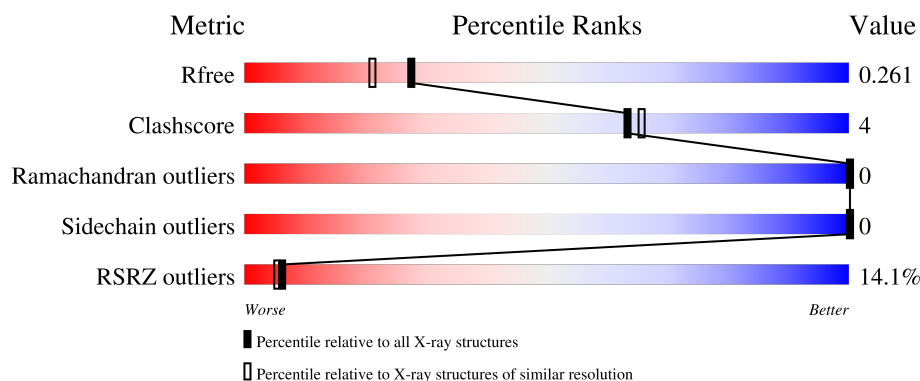
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	12% 79% 8% 13%
1	B	309	10% 78% 9% 12%
1	C	309	14% 81% 7% 12%
1	D	309	12% 83% • 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9249 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.

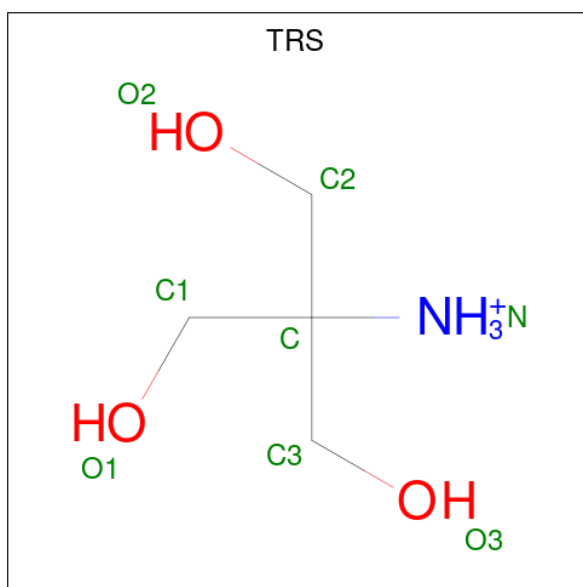
- Molecule 1 is a protein called TqaL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	Se	0	0	0
			2173	1375	385	401	3	9			
1	B	272	Total	C	N	O	S	Se	0	1	0
			2210	1394	393	410	3	10			
1	C	272	Total	C	N	O	S	Se	0	0	0
			2196	1386	390	407	3	10			
1	D	270	Total	C	N	O	S	Se	0	0	0
			2179	1377	386	404	3	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q8X0D9
A	7	MSE	LYS	engineered mutation	UNP Q8X0D9
B	1	MSE	-	initiating methionine	UNP Q8X0D9
B	7	MSE	LYS	engineered mutation	UNP Q8X0D9
C	1	MSE	-	initiating methionine	UNP Q8X0D9
C	7	MSE	LYS	engineered mutation	UNP Q8X0D9
D	1	MSE	-	initiating methionine	UNP Q8X0D9
D	7	MSE	LYS	engineered mutation	UNP Q8X0D9

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		

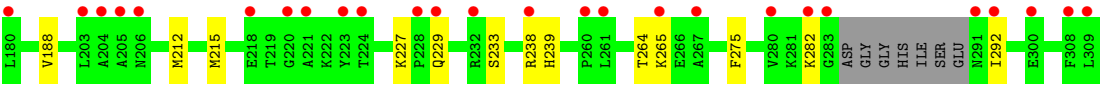
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	125	Total	O	0	0
			125	125		

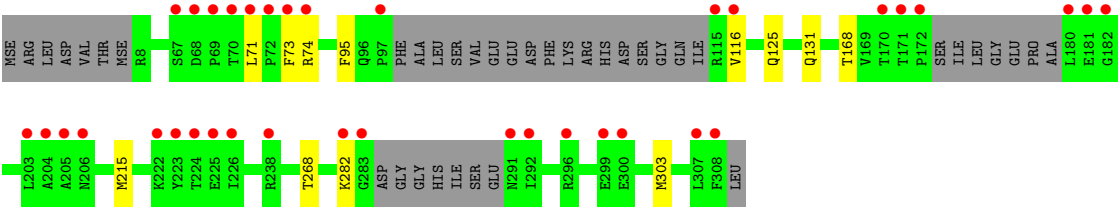
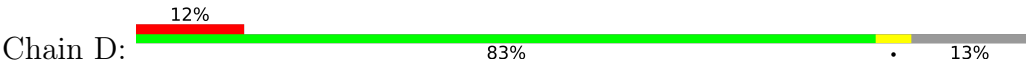
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	123	Total 123	O 123	0	0
4	C	114	Total 114	O 114	0	0
4	D	93	Total 93	O 93	0	0



● Molecule 1: TqaL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.75Å 99.49Å 193.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 2.00 48.48 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.48-2.00) 99.7 (48.48-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.232 , 0.261 0.233 , 0.261	Depositor DCC
R_{free} test set	2000 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.41$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9249	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 48.90 % 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 8.0522e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, 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	0.37	0/2209	0.54	0/2973
1	B	0.39	1/2246 (0.0%)	0.54	0/3021
1	C	0.37	0/2232	0.55	1/3002 (0.0%)
1	D	0.37	0/2215	0.54	1/2981 (0.0%)
All	All	0.38	1/8902 (0.0%)	0.54	2/11977 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	139	MSE	C-O	-5.51	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	MSE	CG-SE-CE	6.05	112.23	98.92
1	D	215	MSE	CG-SE-CE	5.28	110.54	98.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2173	0	2148	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2210	0	2185	23	0
1	C	2196	0	2167	19	0
1	D	2179	0	2154	10	0
2	A	8	0	11	0	0
2	B	8	0	10	1	0
2	C	8	0	11	1	0
2	D	8	0	11	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	125	0	0	2	0
4	B	123	0	0	1	0
4	C	114	0	0	4	0
4	D	93	0	0	0	0
All	All	9249	0	8697	70	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 4.

All (70) 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:B:86:SER:OG	1:B:157:ASP:OD2	2.12	0.67
1:D:282:LYS:HD2	1:D:282:LYS:H	1.60	0.65
1:B:163:LEU:HD13	1:B:274:PHE:CE2	2.32	0.65
1:A:296:ARG:NH1	4:A:501:HOH:O	2.32	0.62
1:C:265:LYS:NZ	4:C:501:HOH:O	2.28	0.61
1:B:210:THR:HB	1:B:235:VAL:HG12	1.83	0.60
1:C:238:ARG:HH21	1:C:239:HIS:HE1	1.49	0.60
1:D:131:GLN:HG2	1:D:303:MSE:HE2	1.85	0.59
1:C:282:LYS:HG3	1:C:292:ILE:HD12	1.85	0.59
1:D:282:LYS:HD2	1:D:282:LYS:N	2.18	0.58
1:B:207:SER:HB2	1:B:259:LEU:HB2	1.86	0.57
2:C:401:TRS:O1	2:C:401:TRS:O2	2.20	0.57
1:A:35:PHE:CD1	1:A:235:VAL:HG21	2.40	0.56
1:D:71:LEU:HD13	1:D:74:ARG:HD3	1.87	0.56
1:C:238:ARG:HH21	1:C:239:HIS:CE1	2.23	0.55
1:C:71:LEU:HD11	1:C:73:PHE:HB2	1.90	0.54
1:A:29:ILE:HD11	1:A:144:VAL:HG22	1.90	0.53
1:A:131:GLN:HG2	1:A:303:MSE:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:MSE:N	4:C:504:HOH:O	2.41	0.53
1:C:282:LYS:N	1:C:282:LYS:HD2	2.24	0.53
1:B:154:TYR:CD2	1:B:278:ARG:HG3	2.44	0.53
1:C:212:MSE:HE3	1:C:233:SER:OG	2.09	0.52
1:B:21:ILE:HG21	1:B:139:MSE:HE2	1.91	0.52
1:B:163:LEU:CD1	1:B:274:PHE:CD2	2.93	0.51
1:B:163:LEU:CD1	1:B:274:PHE:CE2	2.94	0.51
1:B:222:LYS:HB2	1:B:225:GLU:OE1	2.12	0.50
1:D:95:PHE:CZ	1:D:116:VAL:HG21	2.46	0.49
1:C:229:GLN:H	1:C:229:GLN:CD	2.21	0.48
1:B:35:PHE:CD1	1:B:235:VAL:HG21	2.49	0.48
1:B:125:GLN:O	1:B:303:MSE:HE2	2.14	0.47
1:C:264:THR:OG1	1:C:265:LYS:HD2	2.15	0.47
1:A:82:CYS:HB2	1:A:93:LEU:HD11	1.97	0.47
1:B:22:MSE:HE3	1:B:139:MSE:HE3	1.97	0.47
1:C:67:SER:OG	1:C:75:ARG:HG2	2.15	0.47
1:A:154:TYR:CD2	1:A:278:ARG:HG3	2.50	0.47
1:B:21:ILE:CG2	1:B:139:MSE:HE2	2.45	0.47
1:C:71:LEU:HD12	1:C:73:PHE:H	1.80	0.46
1:C:188:VAL:HG11	1:C:275:PHE:HB3	1.98	0.46
1:B:163:LEU:HD13	1:B:274:PHE:CD2	2.50	0.46
1:B:202:ASP:O	1:B:207:SER:HB3	2.15	0.46
1:A:71:LEU:HD12	1:A:74:ARG:HG2	1.98	0.46
1:D:71:LEU:HD23	1:D:73:PHE:H	1.81	0.46
1:A:82:CYS:O	1:A:90:VAL:HA	2.16	0.45
1:C:75:ARG:NH1	4:C:508:HOH:O	2.50	0.45
1:A:236:GLN:OE1	1:A:238:ARG:NH1	2.50	0.44
1:A:204:ALA:C	1:A:206:ASN:H	2.25	0.44
1:B:206[B]:ASN:ND2	1:B:223:TYR:OH	2.51	0.44
1:B:198:SER:CB	1:B:201:MSE:HE2	2.48	0.44
1:C:282:LYS:NZ	4:C:510:HOH:O	2.51	0.44
1:A:20:GLU:HG2	1:A:44:LEU:HD21	2.00	0.43
1:A:127:ASN:O	1:A:131:GLN:HG3	2.18	0.43
1:A:131:GLN:HG2	1:A:303:MSE:CE	2.47	0.43
1:C:96:GLN:HA	1:C:97:PRO:HD3	1.90	0.43
1:D:131:GLN:HG2	1:D:303:MSE:CE	2.48	0.43
1:A:151:ARG:HG2	4:A:608:HOH:O	2.19	0.42
1:D:168:THR:O	1:D:268:THR:HA	2.20	0.42
1:C:227:LYS:HB3	1:C:229:GLN:OE1	2.20	0.42
1:C:48:LEU:HD23	1:C:48:LEU:HA	1.79	0.42
1:D:95:PHE:CE2	1:D:116:VAL:HG21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:O	1:A:226:ILE:HG23	2.20	0.41
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.66	0.41
1:A:235:VAL:HG22	1:A:236:GLN:N	2.36	0.41
1:B:184:HIS:CE1	2:B:401:TRS:O3	2.74	0.41
1:B:198:SER:OG	1:B:201:MSE:HE2	2.20	0.41
1:D:125:GLN:O	1:D:303:MSE:HE3	2.21	0.41
1:B:33:SER:HB3	1:B:212:MSE:HE1	2.03	0.41
1:C:78:ASN:C	1:C:120:VAL:HG23	2.46	0.41
1:B:52:ARG:NE	4:B:507:HOH:O	2.51	0.40
1:A:25:ARG:O	1:A:29:ILE:HG12	2.21	0.40
1:B:82:CYS:O	1:B:90:VAL:HA	2.21	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	262/309 (85%)	254 (97%)	8 (3%)	0	100	100
1	B	265/309 (86%)	258 (97%)	7 (3%)	0	100	100
1	C	264/309 (85%)	261 (99%)	3 (1%)	0	100	100
1	D	262/309 (85%)	256 (98%)	6 (2%)	0	100	100
All	All	1053/1236 (85%)	1029 (98%)	24 (2%)	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	243/269 (90%)	243 (100%)	0	100	100
1	B	249/269 (93%)	249 (100%)	0	100	100
1	C	246/269 (91%)	246 (100%)	0	100	100
1	D	245/269 (91%)	245 (100%)	0	100	100
All	All	983/1076 (91%)	983 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	B	121	GLN
1	B	230	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	TRS	D	401	3	7,7,7	0.30	0	9,9,9	1.23	0
2	TRS	C	401	3	7,7,7	0.17	0	9,9,9	1.07	1 (11%)
2	TRS	A	401	3	7,7,7	0.22	0	9,9,9	1.07	0
2	TRS	B	401	3	7,7,7	0.43	0	9,9,9	1.72	3 (33%)

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
2	TRS	D	401	3	-	0/9/9/9	-
2	TRS	C	401	3	-	4/9/9/9	-
2	TRS	A	401	3	-	3/9/9/9	-
2	TRS	B	401	3	-	6/9/9/9	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	TRS	C1-C-N	3.04	115.92	108.17
2	B	401	TRS	C3-C-C1	-2.46	104.11	110.66
2	C	401	TRS	C2-C-N	2.14	113.63	108.17
2	B	401	TRS	O3-C3-C	-2.04	105.20	110.88

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	TRS	C1-C-C2-O2
2	C	401	TRS	N-C-C2-O2
2	B	401	TRS	C2-C-C1-O1
2	B	401	TRS	C1-C-C2-O2
2	A	401	TRS	C2-C-C1-O1
2	A	401	TRS	C3-C-C1-O1
2	B	401	TRS	C3-C-C1-O1
2	B	401	TRS	N-C-C2-O2

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Mol	Chain	Res	Type	Atoms
2	C	401	TRS	C3-C-C2-O2
2	A	401	TRS	N-C-C1-O1
2	B	401	TRS	N-C-C1-O1
2	B	401	TRS	C3-C-C2-O2
2	C	401	TRS	N-C-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	TRS	1	0
2	B	401	TRS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	261/309 (84%)	0.86	37 (14%) 6 5	19, 29, 56, 68	0
1	B	262/309 (84%)	0.43	32 (12%) 8 7	17, 28, 55, 69	1 (0%)
1	C	262/309 (84%)	0.89	42 (16%) 5 4	18, 31, 56, 75	0
1	D	261/309 (84%)	0.57	36 (13%) 6 6	17, 28, 56, 69	0
All	All	1046/1236 (84%)	0.69	147 (14%) 6 5	17, 29, 56, 75	1 (0%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	180	LEU	7.4
1	C	204	ALA	7.1
1	A	180	LEU	6.9
1	B	204	ALA	6.4
1	C	71	LEU	6.4
1	C	180	LEU	6.4
1	A	204	ALA	6.3
1	D	70	THR	6.3
1	A	283	GLY	6.2
1	D	223	TYR	5.8
1	C	116	VAL	5.8
1	D	283	GLY	5.7
1	B	70	THR	5.6
1	D	308	PHE	5.6
1	A	71	LEU	5.5
1	D	224	THR	5.4
1	B	115	ARG	5.1
1	A	223	TYR	5.0
1	B	283	GLY	5.0
1	C	70	THR	4.9
1	C	68	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	69	PRO	4.8
1	B	71	LEU	4.7
1	C	291	ASN	4.7
1	A	205	ALA	4.6
1	D	205	ALA	4.5
1	B	180	LEU	4.5
1	C	283	GLY	4.5
1	D	225	GLU	4.4
1	D	116	VAL	4.3
1	B	69	PRO	4.3
1	B	205	ALA	4.3
1	B	203	LEU	4.2
1	D	71	LEU	4.1
1	C	115	ARG	4.1
1	A	224	THR	4.1
1	A	220	GLY	4.0
1	A	226	ILE	4.0
1	A	97	PRO	3.9
1	C	203	LEU	3.9
1	D	115	ARG	3.9
1	D	204	ALA	3.7
1	D	97	PRO	3.7
1	B	171	THR	3.7
1	A	309	LEU	3.6
1	A	69	PRO	3.6
1	D	300	GLU	3.6
1	C	205	ALA	3.6
1	B	223	TYR	3.5
1	C	172	PRO	3.5
1	B	300	GLU	3.5
1	D	69	PRO	3.4
1	D	206	ASN	3.4
1	D	307	LEU	3.4
1	C	170	THR	3.4
1	C	74	ARG	3.3
1	C	223	TYR	3.3
1	A	291	ASN	3.3
1	A	70	THR	3.3
1	B	206[A]	ASN	3.3
1	B	291	ASN	3.2
1	D	292	ILE	3.2
1	A	219	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	222	LYS	3.2
1	D	68	ASP	3.2
1	C	73	PHE	3.1
1	D	282	LYS	3.1
1	C	282	LYS	3.1
1	B	172	PRO	3.1
1	D	226	ILE	3.1
1	A	234	ARG	3.0
1	A	282	LYS	3.0
1	D	203	LEU	3.0
1	A	308	PHE	3.0
1	C	171	THR	2.9
1	C	232	ARG	2.9
1	A	72	PRO	2.8
1	C	72	PRO	2.8
1	D	296	ARG	2.8
1	A	307	LEU	2.8
1	D	171	THR	2.8
1	D	72	PRO	2.8
1	D	291	ASN	2.8
1	B	68	ASP	2.8
1	C	218	GLU	2.8
1	C	97	PRO	2.8
1	B	202	ASP	2.7
1	C	238	ARG	2.7
1	A	225	GLU	2.7
1	A	172	PRO	2.7
1	A	300	GLU	2.7
1	C	261	LEU	2.6
1	A	305	VAL	2.6
1	C	220	GLY	2.6
1	C	206	ASN	2.6
1	A	229	GLN	2.5
1	D	74	ARG	2.5
1	A	170	THR	2.5
1	D	172	PRO	2.5
1	C	308	PHE	2.5
1	D	170	THR	2.5
1	B	97	PRO	2.5
1	C	67	SER	2.5
1	A	116	VAL	2.5
1	C	229	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	282	LYS	2.5
1	D	67	SER	2.4
1	A	73	PHE	2.4
1	C	260	PRO	2.4
1	D	299	GLU	2.4
1	A	292	ILE	2.4
1	C	292	ILE	2.4
1	A	67	SER	2.4
1	D	182	GLY	2.4
1	B	265	LYS	2.4
1	D	238	ARG	2.4
1	B	226	ILE	2.3
1	B	116	VAL	2.3
1	C	300	GLU	2.3
1	C	265	LYS	2.3
1	A	255	LEU	2.3
1	D	181	GLU	2.2
1	A	171	THR	2.2
1	A	37	GLU	2.2
1	B	229	GLN	2.2
1	B	221	ALA	2.2
1	C	267	ALA	2.2
1	C	224	THR	2.2
1	B	292	ILE	2.1
1	C	228	PRO	2.1
1	A	211	PHE	2.1
1	C	85	PHE	2.1
1	A	296	ARG	2.1
1	B	232	ARG	2.1
1	B	308	PHE	2.1
1	C	309	LEU	2.1
1	B	225	GLU	2.1
1	B	299	GLU	2.1
1	B	72	PRO	2.1
1	D	73	PHE	2.1
1	B	159	TRP	2.1
1	C	159	TRP	2.1
1	A	181	GLU	2.0
1	A	295	PHE	2.0
1	C	280	VAL	2.0
1	C	221	ALA	2.0
1	B	158	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

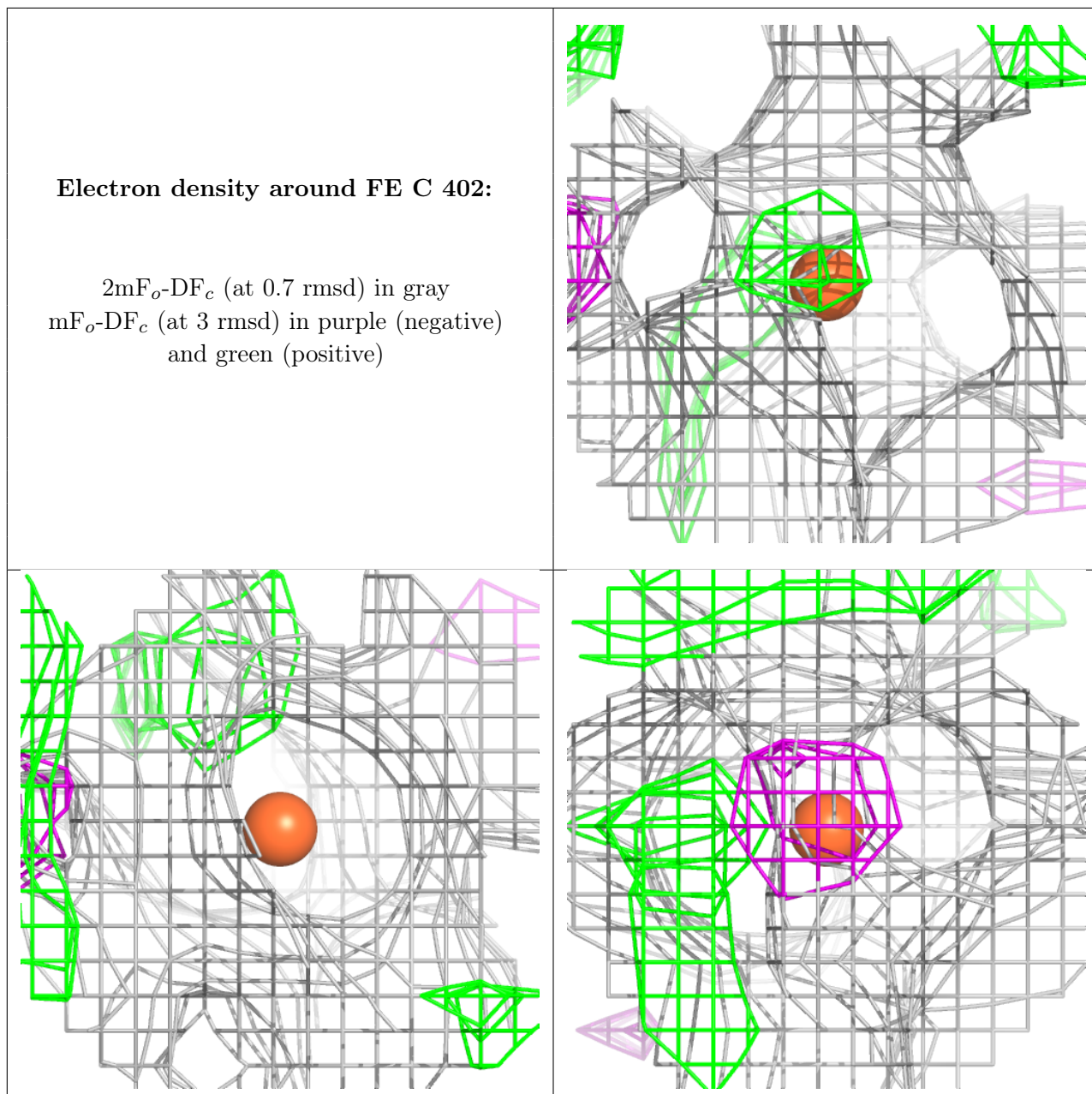
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TRS	C	401	8/8	0.73	0.22	26,45,50,59	0
2	TRS	B	401	8/8	0.81	0.19	26,35,45,49	0
2	TRS	A	401	8/8	0.81	0.16	27,32,38,42	0
2	TRS	D	401	8/8	0.84	0.16	24,31,37,43	0
3	FE	C	402	1/1	0.99	0.03	26,26,26,26	0
3	FE	B	402	1/1	1.00	0.04	24,24,24,24	0
3	FE	A	402	1/1	1.00	0.02	24,24,24,24	0
3	FE	D	402	1/1	1.00	0.04	22,22,22,22	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.

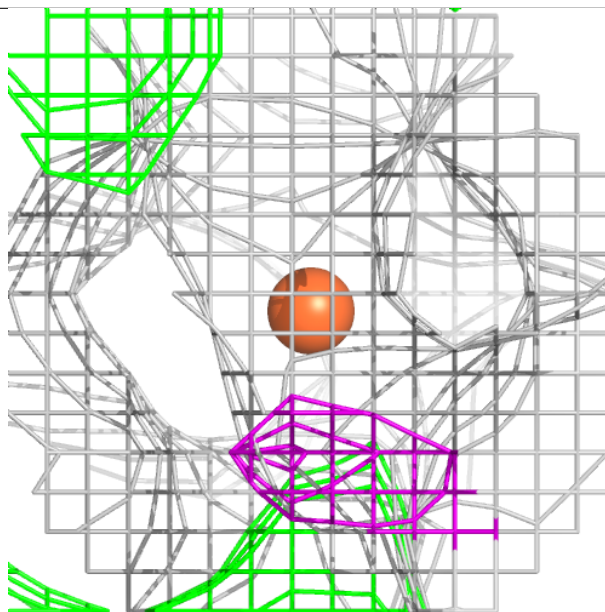
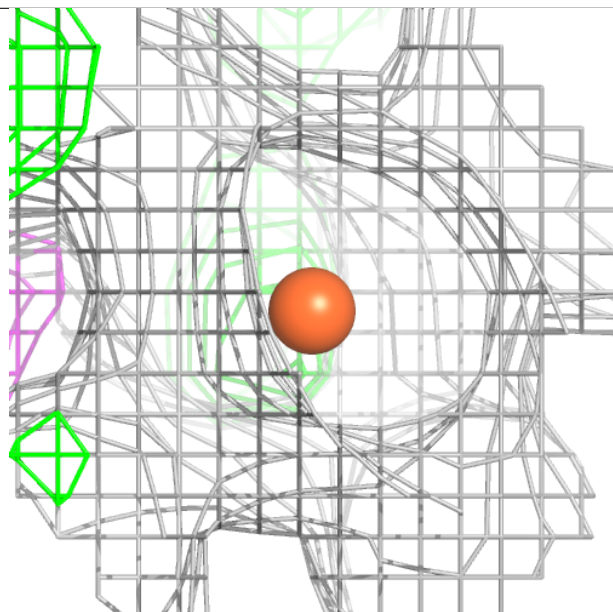
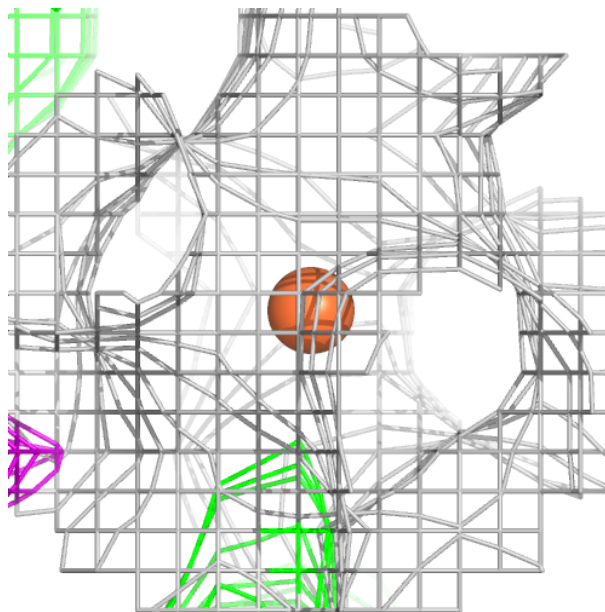
Electron density around FE C 402:

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



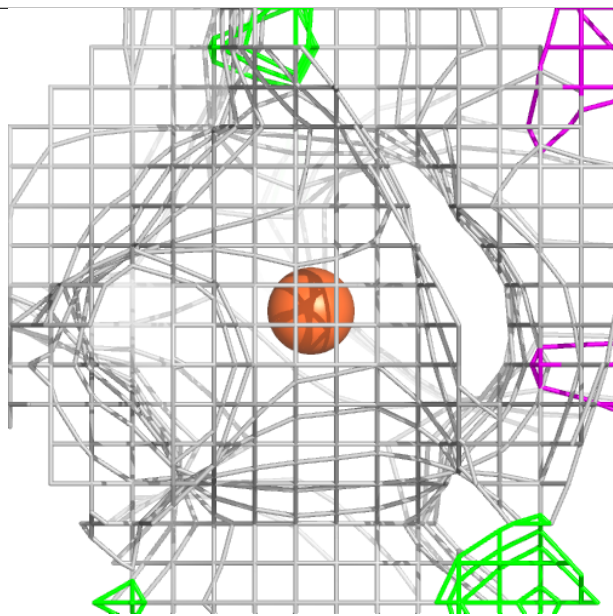
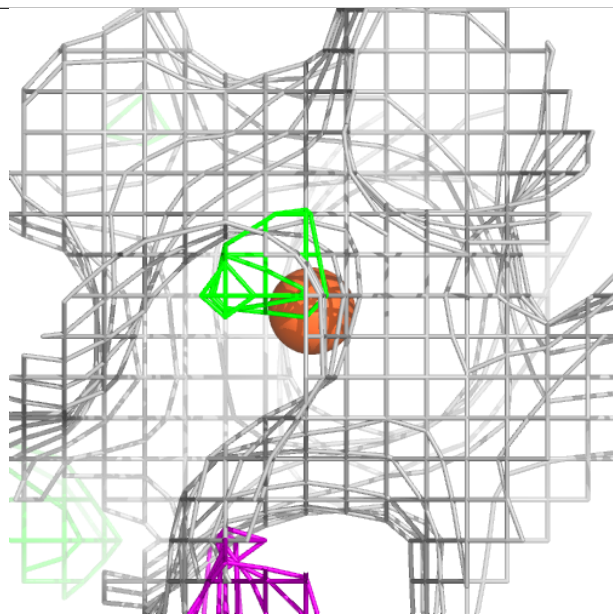
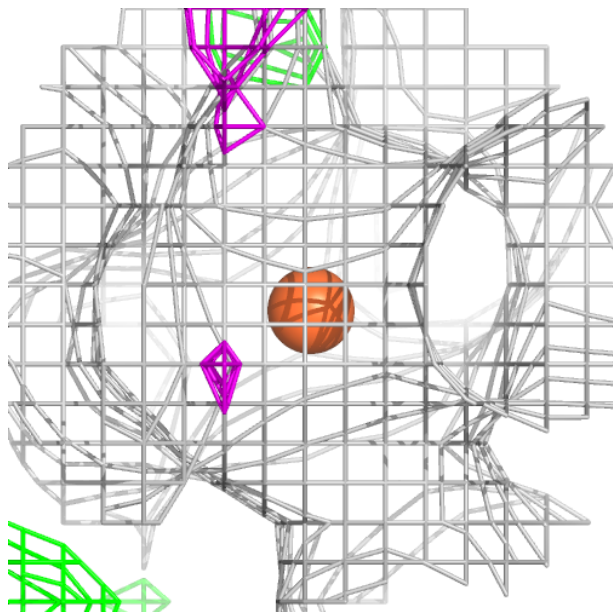
Electron density around FE B 402:

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



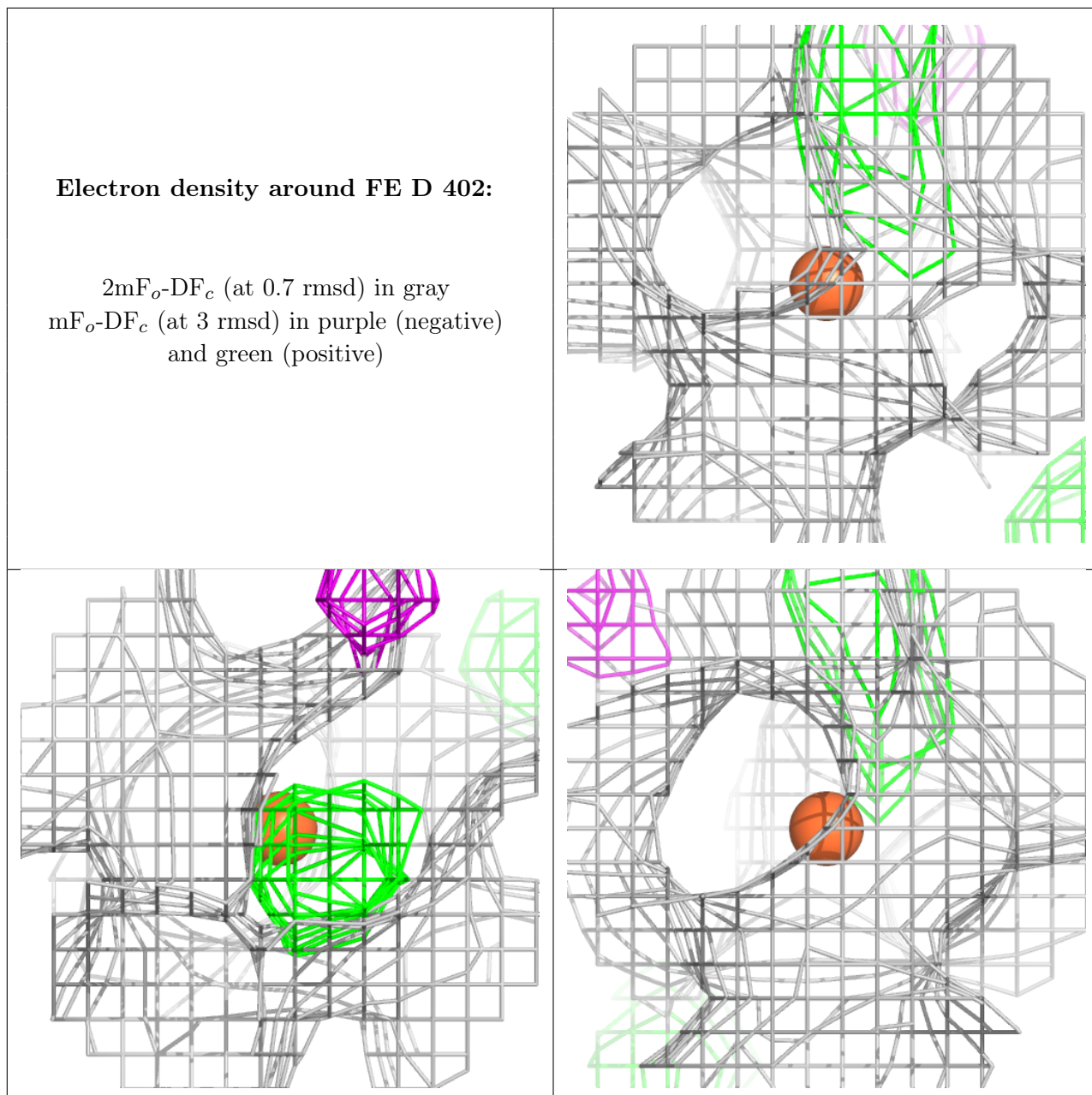
Electron density around FE A 402:

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



Electron density around FE D 402:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.