Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2021 – 12:19 PM JST

PDB ID	:	7EEH
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 following versions of software and data (see references ⓘ) were used in the production of this report:

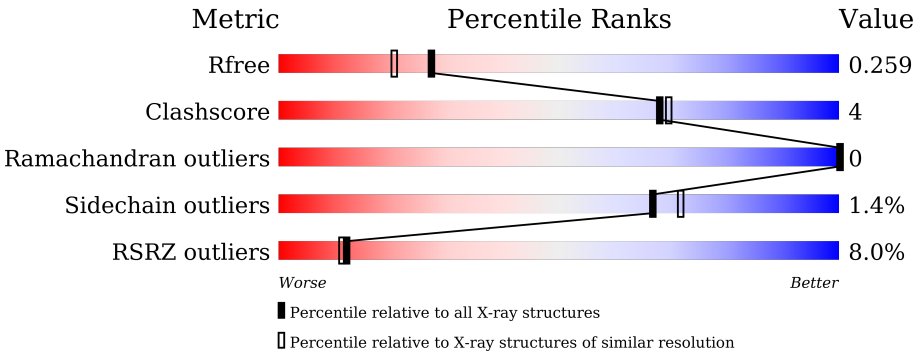
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	8% 79% 7% • 13%
1	B	309	5% 78% 9% • 12%
1	C	309	8% 81% 7% 12%
1	D	309	6% 83% • • 13%

2 Entry composition (i)

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.

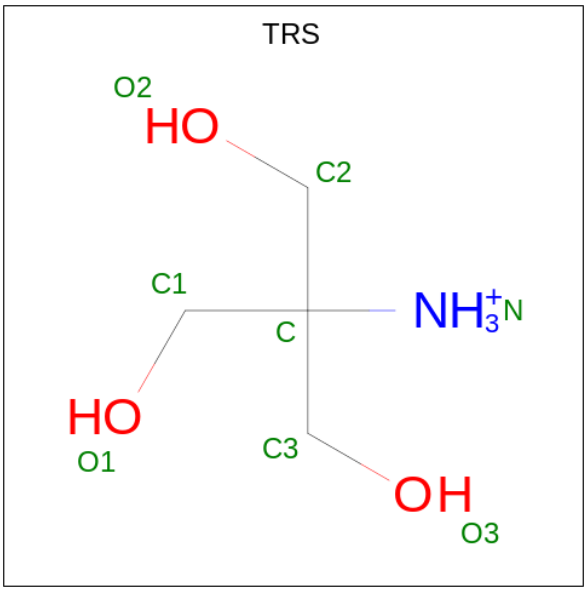
- Molecule 1 is a protein called TqaL.

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 (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



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

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

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

- Molecule 4 is water.

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

Continued on next page...

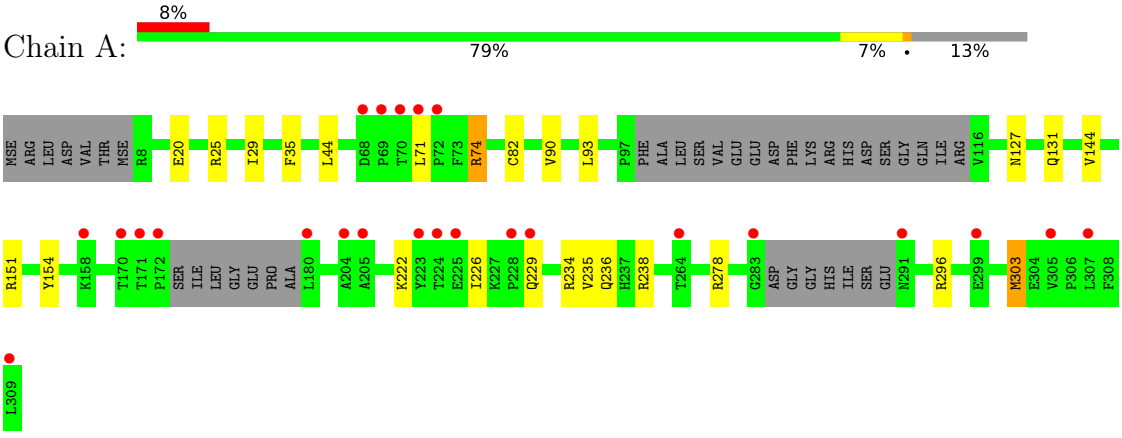
Continued from previous page...

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

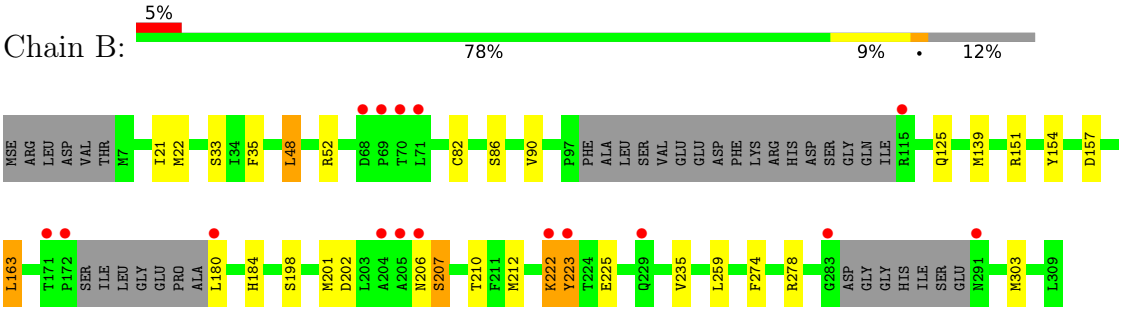
3 Residue-property plots (i)

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.

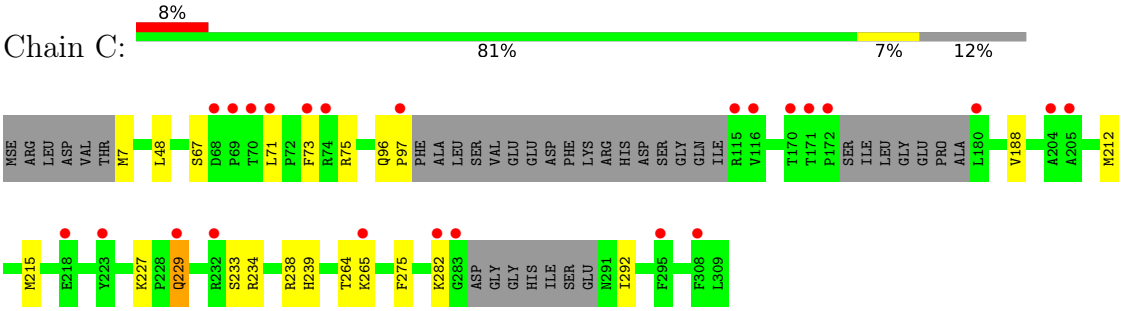
• Molecule 1: TqaL



• Molecule 1: TqaL

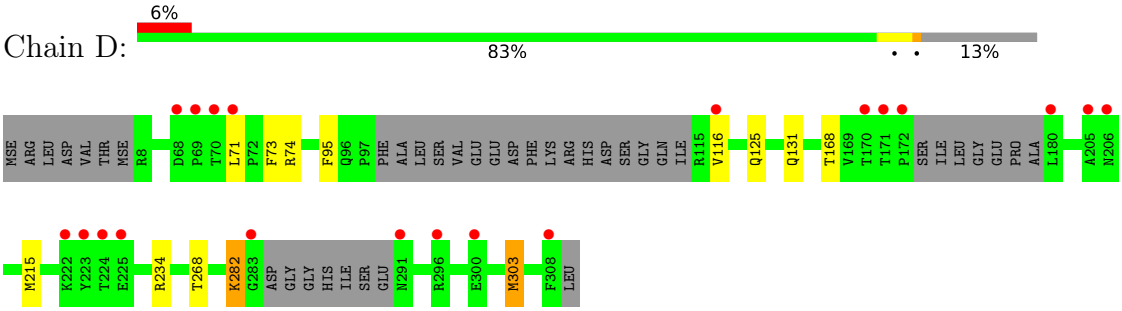


• Molecule 1: TqaL



• Molecule 1: TqaL

Chain D:


6%
83%
13%
MSE ARG LEU ASP VAL THR MSE R8 D68 P69 T70 L71 P72 F73 R74 F95 Q96 P97 PHE ALA LEU SER VAL GLU GLU ASP PHE LYS ARG HIS ASP SER GLY GLN ILE R115 V116 Q125 Q131 T168 V169 T170 T171 P172 SER ILE LEU GLY GLU PRO ALA L180 A205 N206
M215 K222 Y223 T224 E225 R234 T268 K282 G283 ASP GLY GLY HIS ILE SER GLU N291 R296 E300 M303 F308 LEU

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.85 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.232 , 0.261 0.232 , 0.259	Depositor DCC
R_{free} test set	2000 reflections (1.92%)	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 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.56$, $< L^2 > = 0.41$	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.*

[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: 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	0.40	0/2209	0.58	0/2973
1	B	0.38	0/2246	0.60	2/3021 (0.1%)
1	C	0.39	0/2232	0.60	1/3002 (0.0%)
1	D	0.39	0/2215	0.58	1/2981 (0.0%)
All	All	0.39	0/8902	0.59	4/11977 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	215	MSE	CG-SE-CE	6.06	112.23	98.90
1	B	48	LEU	CB-CG-CD2	-5.97	100.85	111.00
1	B	163	LEU	CA-CB-CG	-5.51	102.63	115.30
1	D	215	MSE	CG-SE-CE	5.29	110.54	98.90

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	2173	0	2148	16	0
1	B	2210	0	2185	23	0
1	C	2196	0	2167	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	0
4	D	93	0	0	0	0
All	All	9249	0	8697	66	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 (66) 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
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	239 (98%)	4 (2%)	62	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	249/269 (93%)	244 (98%)	5 (2%)	55 58
1	C	246/269 (91%)	244 (99%)	2 (1%)	81 86
1	D	245/269 (91%)	242 (99%)	3 (1%)	71 76
All	All	983/1076 (91%)	969 (99%)	14 (1%)	67 72

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ARG
1	A	229	GLN
1	A	234	ARG
1	A	303	MSE
1	B	151	ARG
1	B	180	LEU
1	B	207	SER
1	B	222	LYS
1	B	223	TYR
1	C	229	GLN
1	C	234	ARG
1	D	234	ARG
1	D	282	LYS
1	D	303	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	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 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	0.28	0	9,9,9	1.11	0
2	TRS	B	401	3	7,7,7	0.39	0	9,9,9	1.53	2 (22%)
2	TRS	A	401	3	7,7,7	0.21	0	9,9,9	0.97	0
2	TRS	C	401	3	7,7,7	0.15	0	9,9,9	0.95	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
2	TRS	D	401	3	-	0/9/9/9	-
2	TRS	B	401	3	-	5/9/9/9	-
2	TRS	A	401	3	-	3/9/9/9	-
2	TRS	C	401	3	-	3/9/9/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	TRS	C1-C-N	2.66	115.92	107.98
2	B	401	TRS	C3-C-C1	-2.16	104.11	110.81

There are no chirality outliers.

All (11) 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
2	C	401	TRS	C3-C-C2-O2
2	A	401	TRS	N-C-C1-O1
2	B	401	TRS	N-C-C1-O1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	TRS	1	0
2	C	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, 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	261/309 (84%)	0.54	24 (9%) 9 8	19, 29, 56, 68	0
1	B	262/309 (84%)	0.31	16 (6%) 21 20	17, 28, 55, 69	0
1	C	262/309 (84%)	0.60	24 (9%) 9 8	18, 31, 56, 75	0
1	D	261/309 (84%)	0.35	20 (7%) 13 12	17, 28, 56, 69	0
All	All	1046/1236 (84%)	0.45	84 (8%) 12 11	17, 29, 56, 75	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	THR	8.4
1	C	70	THR	8.0
1	C	204	ALA	7.1
1	D	70	THR	6.7
1	B	204	ALA	6.7
1	A	309	LEU	6.5
1	C	71	LEU	6.4
1	D	224	THR	6.4
1	B	283	GLY	6.2
1	B	70	THR	5.7
1	D	283	GLY	5.6
1	A	70	THR	5.5
1	D	225	GLU	5.5
1	D	180	LEU	5.3
1	C	68	ASP	5.1
1	D	223	TYR	4.6
1	A	223	TYR	4.4
1	C	172	PRO	4.3
1	A	180	LEU	4.2
1	C	116	VAL	4.1
1	D	71	LEU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	283	GLY	4.1
1	C	115	ARG	4.0
1	A	204	ALA	4.0
1	B	115	ARG	3.9
1	B	171	THR	3.9
1	B	223	TYR	3.9
1	D	206	ASN	3.9
1	A	291	ASN	3.7
1	B	291	ASN	3.7
1	A	283	GLY	3.7
1	A	69	PRO	3.7
1	B	71	LEU	3.7
1	C	170	THR	3.6
1	C	223	TYR	3.6
1	A	71	LEU	3.6
1	A	225	GLU	3.5
1	D	291	ASN	3.5
1	C	229	GLN	3.5
1	C	218	GLU	3.4
1	A	171	THR	3.4
1	D	205	ALA	3.4
1	D	171	THR	3.4
1	A	228	PRO	3.3
1	B	69	PRO	3.2
1	C	73	PHE	3.1
1	B	180	LEU	3.1
1	D	68	ASP	3.1
1	D	116	VAL	3.0
1	D	172	PRO	3.0
1	C	171	THR	2.9
1	B	229	GLN	2.8
1	D	222	LYS	2.8
1	C	69	PRO	2.8
1	D	69	PRO	2.8
1	C	205	ALA	2.8
1	C	180	LEU	2.7
1	C	295	PHE	2.6
1	C	232	ARG	2.6
1	B	172	PRO	2.6
1	A	307	LEU	2.5
1	D	170	THR	2.4
1	D	296	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	170	THR	2.3
1	A	158	LYS	2.3
1	B	206[A]	ASN	2.3
1	B	205	ALA	2.2
1	D	308	PHE	2.2
1	A	72	PRO	2.2
1	B	68	ASP	2.2
1	A	205	ALA	2.2
1	A	172	PRO	2.2
1	C	74	ARG	2.2
1	C	265	LYS	2.2
1	A	299	GLU	2.2
1	C	97	PRO	2.1
1	C	282	LYS	2.1
1	A	68	ASP	2.1
1	A	229	GLN	2.1
1	C	308	PHE	2.1
1	A	264	THR	2.1
1	B	222	LYS	2.0
1	D	300	GLU	2.0
1	A	305	VAL	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
2	TRS	C	401	8/8	0.69	0.23	26,45,50,59	0
2	TRS	A	401	8/8	0.85	0.32	27,32,38,42	0

Continued on next page...

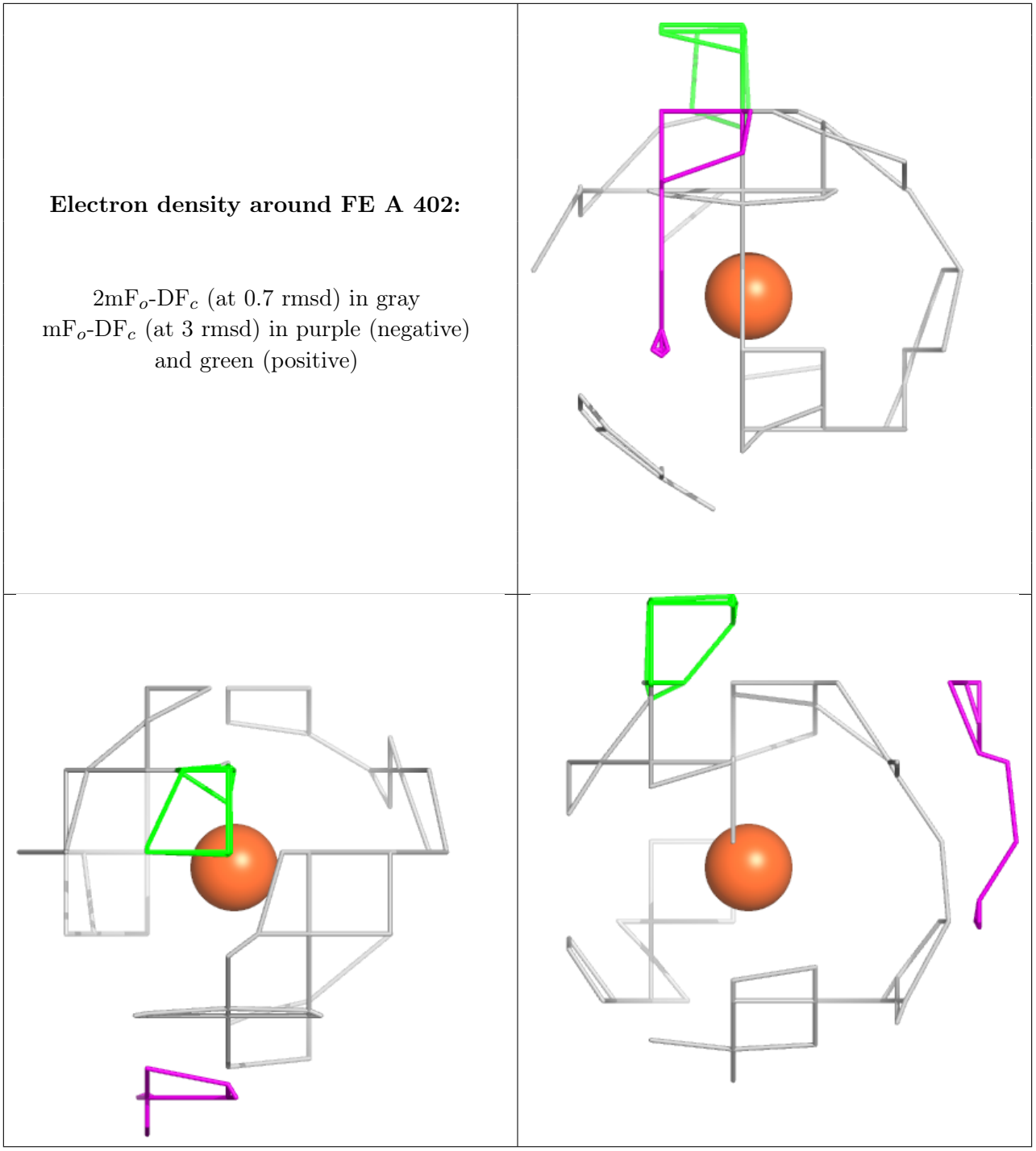
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TRS	B	401	8/8	0.89	0.24	26,35,45,49	0
2	TRS	D	401	8/8	0.89	0.23	24,31,37,43	0
3	FE	A	402	1/1	0.99	0.10	24,24,24,24	0
3	FE	B	402	1/1	0.99	0.13	24,24,24,24	0
3	FE	C	402	1/1	0.99	0.12	26,26,26,26	0
3	FE	D	402	1/1	1.00	0.12	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.

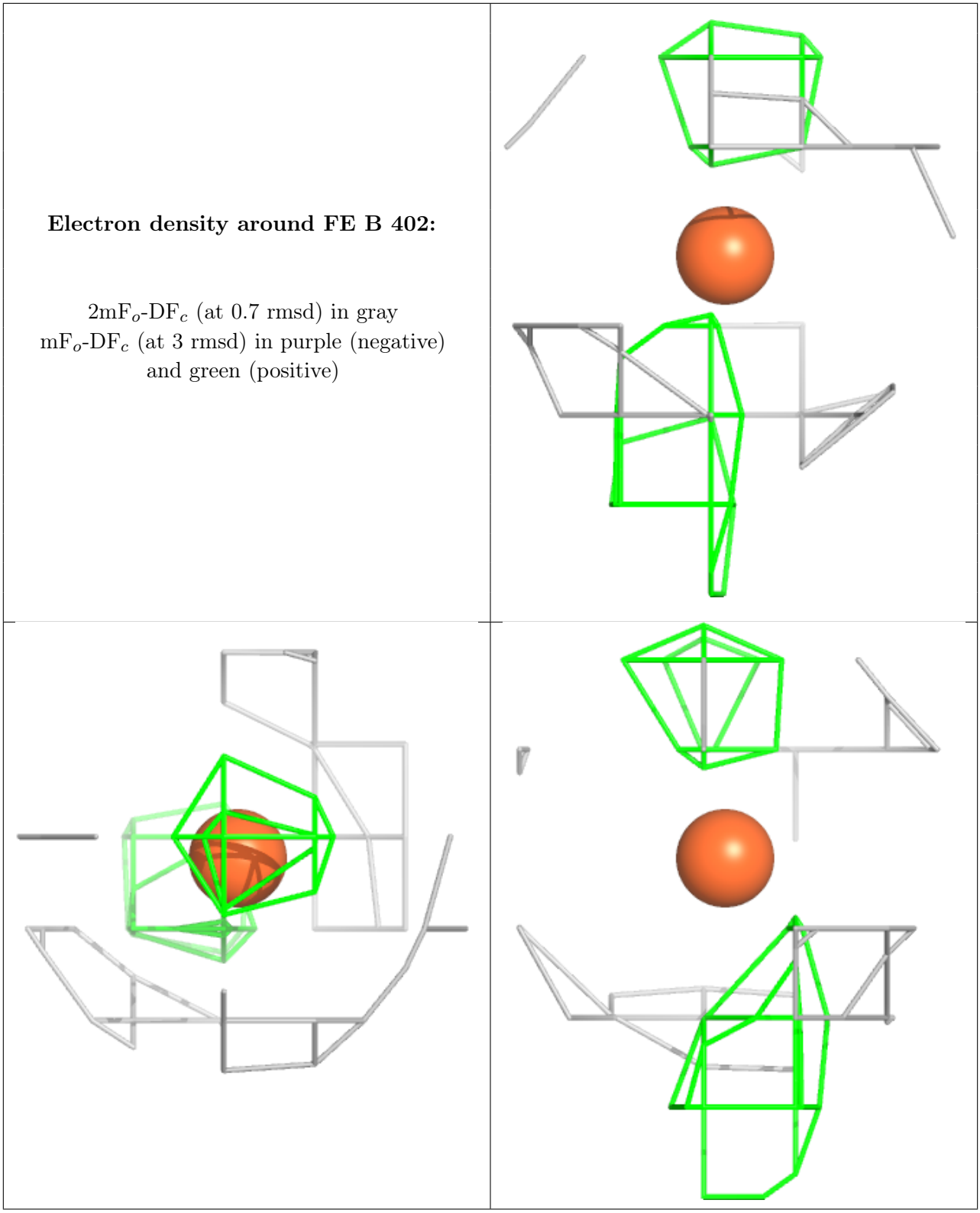
Electron density around FE A 402:

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



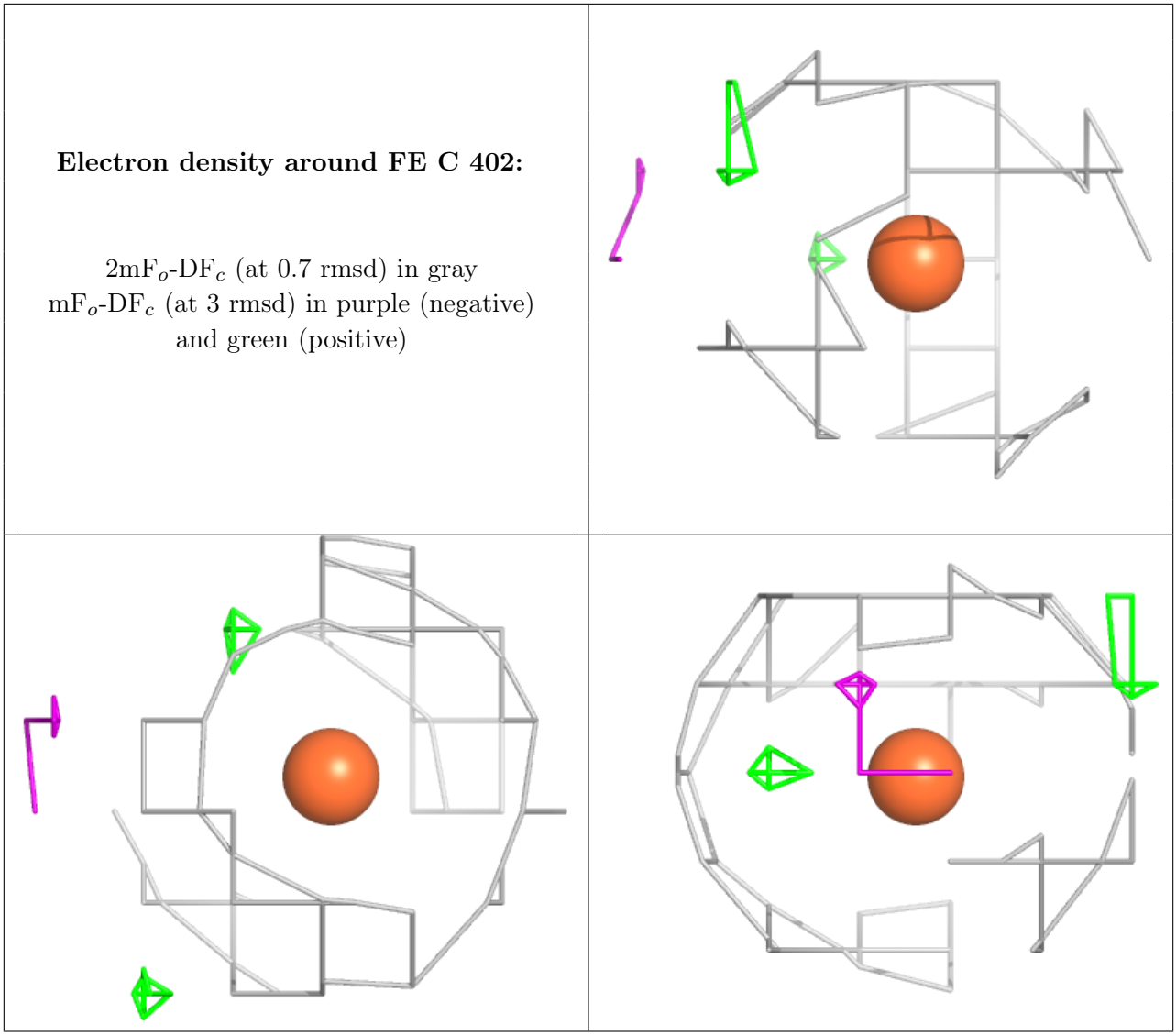
Electron density around FE B 402:

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



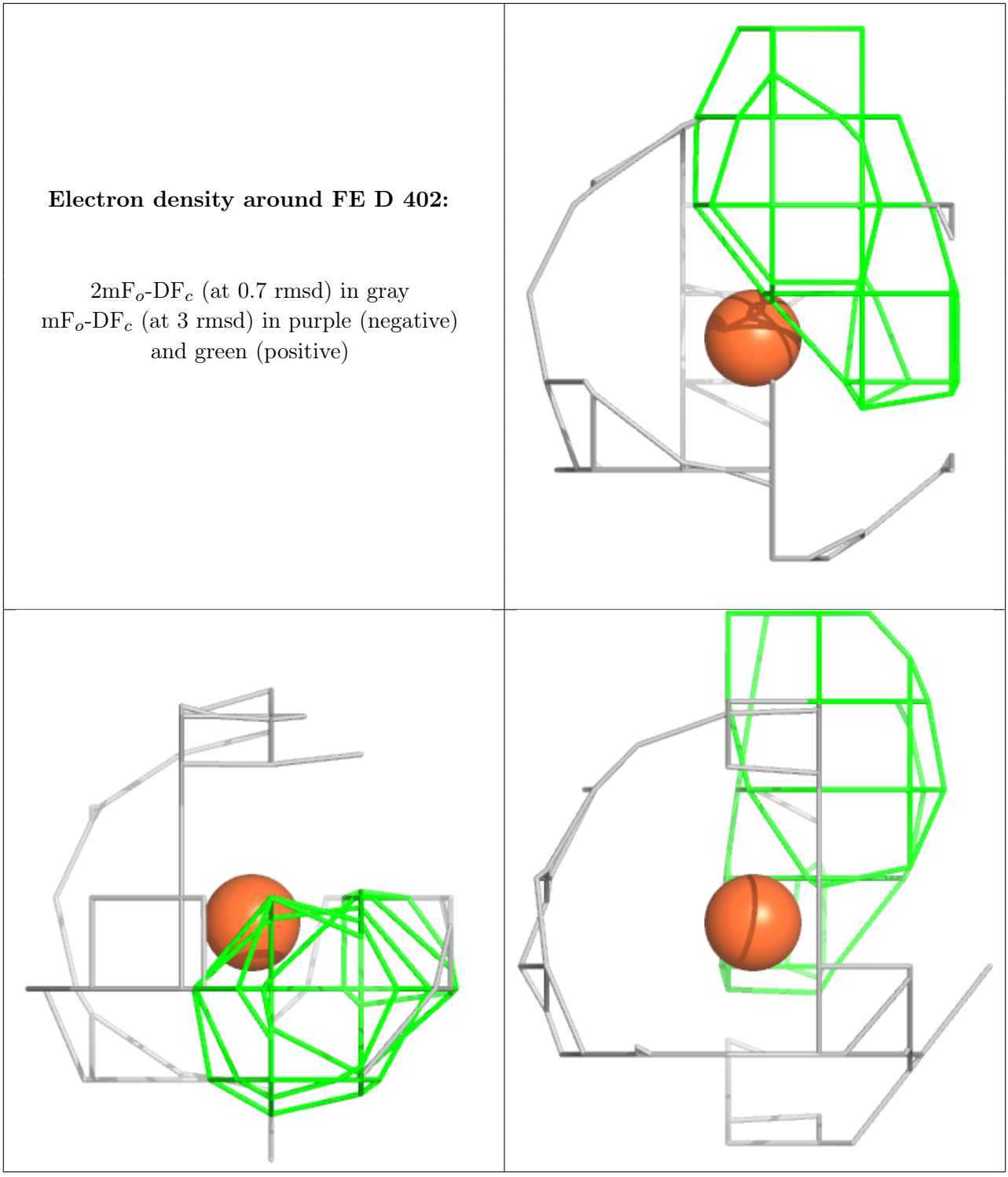
Electron density around FE C 402:

$2mF_o$-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 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.