Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2023 – 02:24 pm BST

PDB ID	:	7QTD
Title	:	Crystal Structure of the Fe(II)/alpha-ketoglutarate dependent dioxygenase PlaO1 in complex with iron and alpha-ketoglutarate
Authors	:	Lukat, P.; Daum, M.; Bechthold, A.; Einsle, O.
Deposited on	:	2022-01-14
Resolution	:	1.75 Å(reported)

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

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

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

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

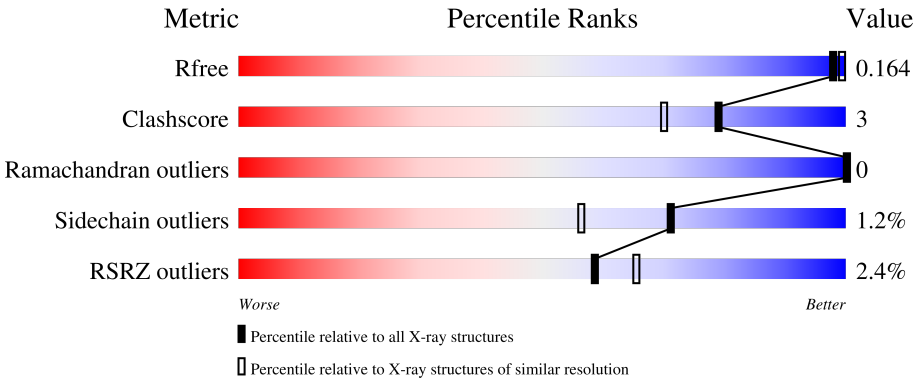
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	297	2% 89% • 6%
1	B	297	3% 86% 8% • 5%
1	C	297	3% 91% • 5%
1	D	297	% 88% 5% 7%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19738 atoms, of which 9194 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 PlaO1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	279	Total	C	H	N	O	S	0	23	0
			4678	1501	2309	432	432	4			
1	B	283	Total	C	H	N	O	S	0	18	0
			4651	1496	2297	426	429	3			
1	C	282	Total	C	H	N	O	S	0	24	0
			4698	1511	2321	427	435	4			
1	D	277	Total	C	H	N	O	S	0	15	0
			4529	1459	2229	420	417	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	GLY	-	expression tag	UNP Q2I752
A	290	LYS	-	expression tag	UNP Q2I752
A	291	LEU	-	expression tag	UNP Q2I752
A	292	GLU	-	expression tag	UNP Q2I752
A	293	ASN	-	expression tag	UNP Q2I752
A	294	LEU	-	expression tag	UNP Q2I752
A	295	TYR	-	expression tag	UNP Q2I752
A	296	PHE	-	expression tag	UNP Q2I752
A	297	GLN	-	expression tag	UNP Q2I752
B	289	GLY	-	expression tag	UNP Q2I752
B	290	LYS	-	expression tag	UNP Q2I752
B	291	LEU	-	expression tag	UNP Q2I752
B	292	GLU	-	expression tag	UNP Q2I752
B	293	ASN	-	expression tag	UNP Q2I752
B	294	LEU	-	expression tag	UNP Q2I752
B	295	TYR	-	expression tag	UNP Q2I752
B	296	PHE	-	expression tag	UNP Q2I752
B	297	GLN	-	expression tag	UNP Q2I752
C	289	GLY	-	expression tag	UNP Q2I752
C	290	LYS	-	expression tag	UNP Q2I752
C	291	LEU	-	expression tag	UNP Q2I752

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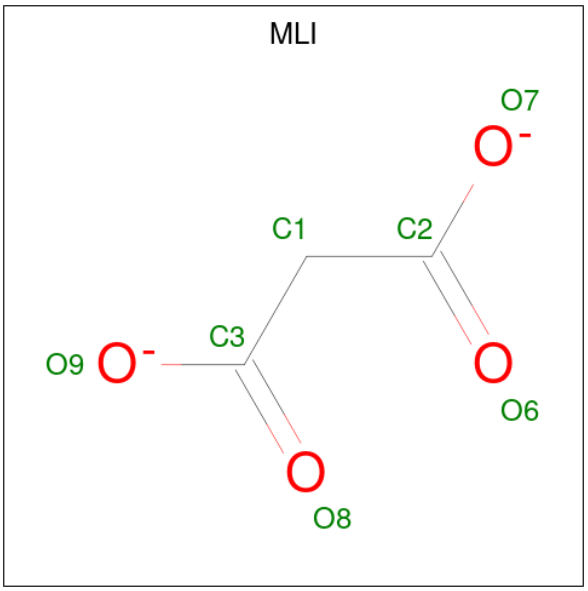
Chain	Residue	Modelled	Actual	Comment	Reference
C	292	GLU	-	expression tag	UNP Q2I752
C	293	ASN	-	expression tag	UNP Q2I752
C	294	LEU	-	expression tag	UNP Q2I752
C	295	TYR	-	expression tag	UNP Q2I752
C	296	PHE	-	expression tag	UNP Q2I752
C	297	GLN	-	expression tag	UNP Q2I752
D	289	GLY	-	expression tag	UNP Q2I752
D	290	LYS	-	expression tag	UNP Q2I752
D	291	LEU	-	expression tag	UNP Q2I752
D	292	GLU	-	expression tag	UNP Q2I752
D	293	ASN	-	expression tag	UNP Q2I752
D	294	LEU	-	expression tag	UNP Q2I752
D	295	TYR	-	expression tag	UNP Q2I752
D	296	PHE	-	expression tag	UNP Q2I752
D	297	GLN	-	expression tag	UNP Q2I752

- Molecule 2 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).

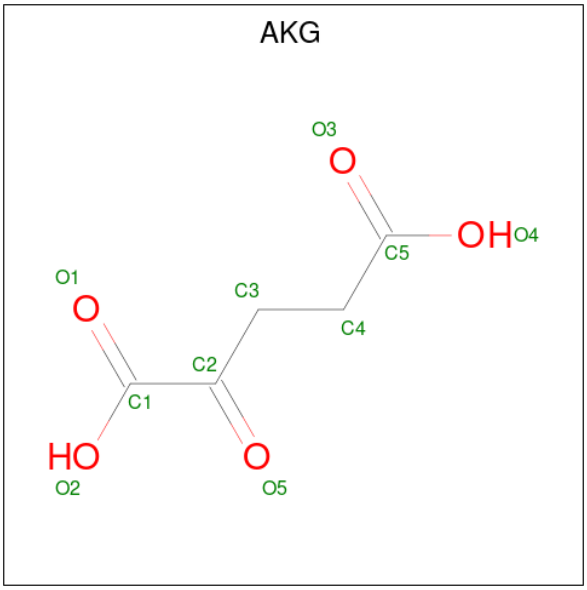


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			9	3	2	4		
2	C	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

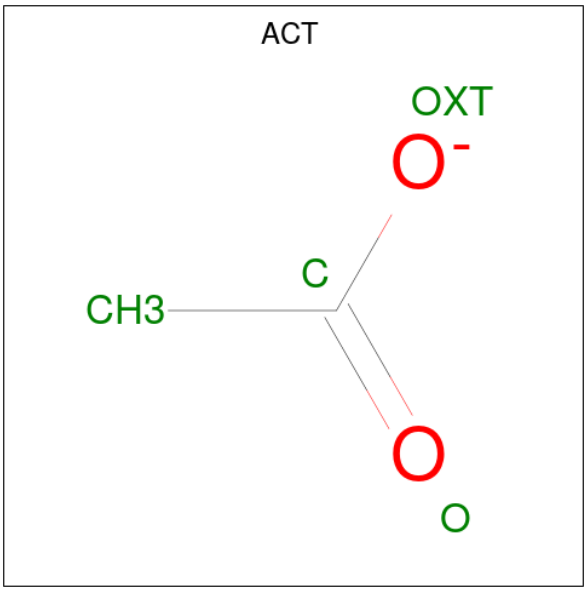
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe 1 1	0	0
3	B	1	Total Fe 1 1	0	0
3	C	1	Total Fe 1 1	0	0
3	D	1	Total Fe 1 1	0	0

- Molecule 4 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 14 5 4 5	0	0
4	B	1	Total C H O 14 5 4 5	0	0
4	C	1	Total C H O 14 5 4 5	0	0
4	D	1	Total C H O 14 5 4 5	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 7 2 3 2	0	0
5	A	1	Total C H O 7 2 3 2	0	0
5	B	1	Total C H O 7 2 3 2	0	0
5	C	1	Total C H O 7 2 3 2	0	0
5	C	1	Total C H O 7 2 3 2	0	0
5	D	1	Total C H O 7 2 3 2	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Na 1 1	0	0
6	C	1	Total Na 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	284	Total O 284 284	0	0

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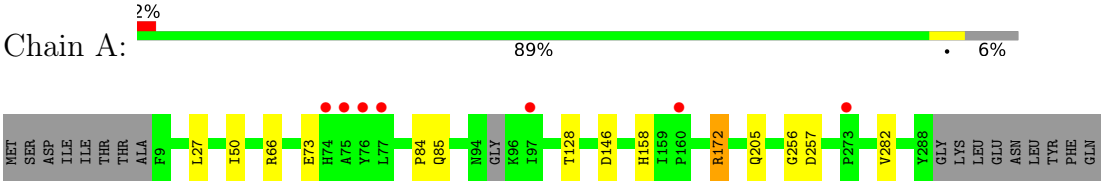
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	258	Total O 258 258	0	0
7	C	259	Total O 259 259	0	0
7	D	259	Total O 259 259	0	0

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.

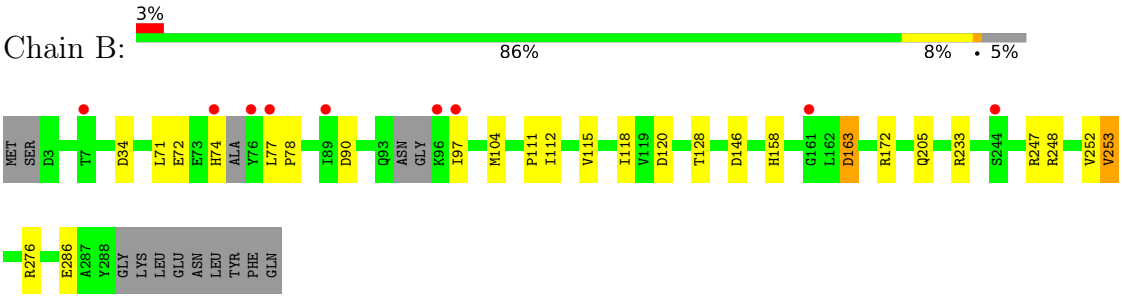
- Molecule 1: PlaO1

Chain A:



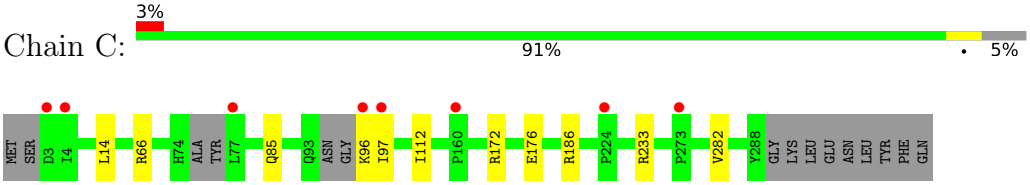
- Molecule 1: PlaO1

Chain B:



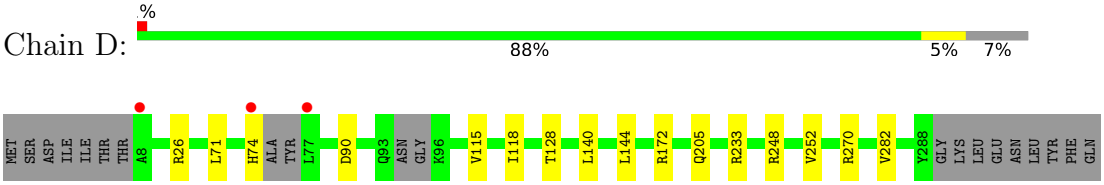
- Molecule 1: PlaO1

Chain C:



- Molecule 1: PlaO1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.12Å 108.22Å 116.41Å 90.00° 94.75° 90.00°	Depositor
Resolution (Å)	63.90 – 1.75 79.13 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.90-1.75) 99.9 (79.13-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.20-4459	Depositor
R, R_{free}	0.141 , 0.165 0.141 , 0.164	Depositor DCC
R_{free} test set	7717 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	19738	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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 38.21 % 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 3.8153e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ACT, FE2, MLI, AKG

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	0.49	0/2511	0.70	0/3421
1	B	0.49	0/2474	0.69	0/3376
1	C	0.49	0/2529	0.68	0/3449
1	D	0.49	0/2415	0.69	0/3294
All	All	0.49	0/9929	0.69	0/13540

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	2369	2309	2238	11	0
1	B	2354	2297	2250	22	0
1	C	2377	2321	2241	14	0
1	D	2300	2229	2178	9	0
2	A	7	2	2	0	0
2	C	7	2	2	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	10	4	4	1	0
4	B	10	4	4	1	0
4	C	10	4	4	0	0
4	D	10	4	4	1	0
5	A	8	6	6	0	0
5	B	4	3	3	0	0
5	C	8	6	6	0	0
5	D	4	3	3	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	284	0	0	3	0
7	B	258	0	0	8	0
7	C	259	0	0	8	0
7	D	259	0	0	2	0
All	All	10544	9194	8945	52	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 3.

All (52) 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:146[B]:ASP:OD2	7:B:401:HOH:O	1.95	0.84
1:A:172[A]:ARG:NH2	1:A:257:ASP:OD2	2.16	0.78
1:B:286[B]:GLU:OE1	7:B:402:HOH:O	2.06	0.73
1:B:233[B]:ARG:NH2	7:B:407:HOH:O	2.24	0.70
1:C:14[B]:LEU:HD21	7:C:450:HOH:O	1.91	0.69
1:B:34:ASP:OD2	7:B:404:HOH:O	2.12	0.68
1:B:118:ILE:O	7:B:403:HOH:O	2.12	0.67
1:B:97:ILE:N	7:B:405:HOH:O	2.22	0.66
1:C:233[B]:ARG:NH2	7:C:401:HOH:O	2.20	0.66
1:A:205[A]:GLN:OE1	1:D:282:VAL:HG23	1.97	0.65
1:A:146[A]:ASP:OD2	7:A:401:HOH:O	2.16	0.61
1:D:233[A]:ARG:NH2	7:D:404:HOH:O	2.36	0.58
1:A:66:ARG:NH2	1:A:85[B]:GLN:OE1	2.36	0.58
1:C:233[B]:ARG:NH2	7:C:406:HOH:O	2.36	0.57
1:B:128:THR:OG1	4:B:302:AKG:O3	2.22	0.55
1:D:128:THR:OG1	4:D:302:AKG:O4	2.24	0.55
1:A:282:VAL:HG23	1:D:205:GLN:OE1	2.07	0.55
1:B:90:ASP:OD2	1:B:248:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLU:HB3	1:B:253[A]:VAL:HG23	1.91	0.52
1:D:118:ILE:O	7:D:401:HOH:O	2.19	0.52
1:B:115:VAL:HB	1:B:252[A]:VAL:HG22	1.93	0.51
1:D:115:VAL:HB	1:D:252[B]:VAL:HG22	1.93	0.50
1:C:97[A]:ILE:O	1:C:97[A]:ILE:HG23	2.11	0.49
1:B:71:LEU:HD22	1:B:252[B]:VAL:CG1	2.42	0.49
1:A:256:GLY:O	7:A:402:HOH:O	2.19	0.49
1:B:158:HIS:ND1	1:B:163:ASP:OD1	2.46	0.47
1:C:176:GLU:OE1	7:C:401:HOH:O	2.20	0.47
1:A:73:GLU:OE2	1:A:85[B]:GLN:NE2	2.47	0.47
1:C:66:ARG:NH2	1:C:85[B]:GLN:OE1	2.45	0.47
1:B:112[B]:ILE:HG23	1:B:233[B]:ARG:CZ	2.45	0.46
1:B:205:GLN:OE1	1:C:282:VAL:HG23	2.16	0.46
1:C:186[B]:ARG:CZ	7:C:427:HOH:O	2.64	0.45
1:D:90:ASP:OD2	1:D:248:ARG:NH1	2.49	0.45
1:A:158:HIS:CD2	7:A:550:HOH:O	2.69	0.45
1:B:104:MET:HE2	1:B:111:PRO:HG3	1.99	0.45
1:A:128:THR:OG1	4:A:303:AKG:O3	2.27	0.45
1:A:73:GLU:HG2	1:A:84:PRO:HB2	2.00	0.44
1:D:71:LEU:HD22	1:D:252[A]:VAL:CG1	2.48	0.44
1:B:104:MET:HE3	7:B:604:HOH:O	2.18	0.43
1:D:140:LEU:HD22	1:D:144[A]:LEU:HD23	2.00	0.42
1:C:112[B]:ILE:HG23	1:C:233[B]:ARG:CZ	2.49	0.42
1:C:186[B]:ARG:NH2	7:C:408:HOH:O	2.39	0.42
1:C:186[B]:ARG:NE	7:C:407:HOH:O	2.36	0.42
1:B:77:LEU:HD23	1:B:78:PRO:N	2.34	0.42
1:B:120:ASP:O	1:B:247:ARG:HA	2.20	0.42
1:A:27:LEU:HD21	1:A:50[B]:ILE:HD13	2.01	0.41
1:B:158:HIS:CD2	7:B:447:HOH:O	2.73	0.41
1:B:115:VAL:HB	1:B:252[A]:VAL:CG2	2.50	0.41
1:C:14[B]:LEU:HD23	1:C:14[B]:LEU:HA	1.97	0.41
1:B:276:ARG:HG3	1:C:97[B]:ILE:HB	2.03	0.41
1:B:77:LEU:HD23	1:B:78:PRO:O	2.21	0.40
1:C:186[B]:ARG:HD3	7:C:427:HOH:O	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	297/297 (100%)	288 (97%)	9 (3%)	0	100	100
1	B	295/297 (99%)	285 (97%)	10 (3%)	0	100	100
1	C	299/297 (101%)	290 (97%)	9 (3%)	0	100	100
1	D	286/297 (96%)	276 (96%)	10 (4%)	0	100	100
All	All	1177/1188 (99%)	1139 (97%)	38 (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	260/254 (102%)	258 (99%)	2 (1%)	81	72
1	B	255/254 (100%)	250 (98%)	5 (2%)	55	34
1	C	264/254 (104%)	261 (99%)	3 (1%)	73	60
1	D	248/254 (98%)	244 (98%)	4 (2%)	62	45
All	All	1027/1016 (101%)	1013 (99%)	14 (1%)	71	52

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

Mol	Chain	Res	Type
1	A	172[A]	ARG
1	A	172[B]	ARG

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Mol	Chain	Res	Type
1	B	74	HIS
1	B	163	ASP
1	B	172	ARG
1	B	253[A]	VAL
1	B	253[B]	VAL
1	C	96[A]	LYS
1	C	96[B]	LYS
1	C	172	ARG
1	D	26	ARG
1	D	74	HIS
1	D	172	ARG
1	D	270	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	$\#\|Z\|>2$
5	ACT	B	303	-	3,3,3	1.31	0	3,3,3	1.53	0
2	MLI	C	306	-	6,6,6	1.14	0	7,7,7	1.55	2 (28%)
4	AKG	A	303	3	9,9,9	0.48	0	11,11,11	0.54	0
4	AKG	B	302	3	9,9,9	1.13	1 (11%)	11,11,11	0.83	1 (9%)
5	ACT	A	305	-	3,3,3	1.54	1 (33%)	3,3,3	1.31	0
2	MLI	A	301	-	6,6,6	1.49	0	7,7,7	0.70	0
4	AKG	D	302	3	9,9,9	1.01	1 (11%)	11,11,11	0.70	0
5	ACT	D	303	-	3,3,3	1.31	0	3,3,3	1.41	0
5	ACT	C	303	-	3,3,3	1.40	0	3,3,3	1.43	0
5	ACT	A	304	-	3,3,3	1.37	0	3,3,3	1.51	0
4	AKG	C	302	3	9,9,9	0.56	0	11,11,11	0.61	0
5	ACT	C	304	-	3,3,3	1.31	0	3,3,3	1.34	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	MLI	C	306	-	-	0/4/4/4	-
4	AKG	A	303	3	-	1/9/9/9	-
4	AKG	B	302	3	-	3/9/9/9	-
2	MLI	A	301	-	-	0/4/4/4	-
4	AKG	D	302	3	-	1/9/9/9	-
4	AKG	C	302	3	-	1/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	AKG	C2-C1	2.89	1.57	1.53
4	D	302	AKG	C2-C1	2.80	1.57	1.53
5	A	305	ACT	CH3-C	2.37	1.59	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	302	AKG	O5-C2-C1	2.43	122.95	119.43
2	C	306	MLI	O7-C2-C1	2.21	121.60	114.54
2	C	306	MLI	O9-C3-C1	2.17	121.47	114.54

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	302	AKG	C1-C2-C3-C4
4	C	302	AKG	C1-C2-C3-C4
4	D	302	AKG	C1-C2-C3-C4
4	A	303	AKG	C1-C2-C3-C4
4	B	302	AKG	C3-C4-C5-O4
4	B	302	AKG	C3-C4-C5-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	AKG	1	0
4	B	302	AKG	1	0
4	D	302	AKG	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	279/297 (93%)	-0.00	7 (2%)	57	63	14, 21, 53, 84	0
1	B	283/297 (95%)	0.07	9 (3%)	47	54	12, 21, 56, 86	0
1	C	282/297 (94%)	0.02	8 (2%)	53	58	13, 21, 51, 87	0
1	D	277/297 (93%)	-0.04	3 (1%)	80	86	13, 22, 55, 83	0
All	All	1121/1188 (94%)	0.01	27 (2%)	59	65	12, 21, 55, 87	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	76	TYR	4.0
1	A	76	TYR	3.9
1	C	97[A]	ILE	3.7
1	C	160	PRO	3.7
1	B	244	SER	3.5
1	D	8	ALA	3.5
1	C	3	ASP	3.4
1	A	160	PRO	3.3
1	B	74	HIS	3.0
1	B	161	GLY	2.8
1	C	96[A]	LYS	2.8
1	C	4	ILE	2.8
1	B	97	ILE	2.6
1	D	77	LEU	2.6
1	A	97[A]	ILE	2.4
1	D	74	HIS	2.4
1	B	77	LEU	2.3
1	B	7	THR	2.3
1	C	224	PRO	2.3
1	B	96	LYS	2.3
1	A	74	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	75	ALA	2.2
1	C	273	PRO	2.1
1	A	77	LEU	2.1
1	C	77	LEU	2.1
1	B	89	ILE	2.1
1	A	273	PRO	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
5	ACT	A	305	4/4	0.70	0.23	47,61,62,72	0
5	ACT	D	303	4/4	0.80	0.17	52,62,77,77	0
5	ACT	C	303	4/4	0.84	0.23	46,56,82,82	0
5	ACT	C	304	4/4	0.85	0.18	56,62,68,68	0
5	ACT	B	303	4/4	0.86	0.23	36,46,60,60	7
5	ACT	A	304	4/4	0.88	0.15	52,64,78,78	0
4	AKG	D	302	10/10	0.90	0.12	22,47,62,62	14
4	AKG	B	302	10/10	0.92	0.10	20,40,51,51	14
4	AKG	C	302	10/10	0.94	0.10	22,29,38,38	14
4	AKG	A	303	10/10	0.95	0.10	20,29,45,45	14
6	NA	C	305	1/1	0.95	0.33	49,49,49,49	0
6	NA	B	304	1/1	0.96	0.25	49,49,49,49	0
2	MLI	C	306	7/7	0.98	0.09	15,16,19,22	0
2	MLI	A	301	7/7	0.99	0.08	14,15,17,17	0
3	FE2	C	301	1/1	0.99	0.11	19,19,19,19	1
3	FE2	B	301	1/1	1.00	0.10	18,18,18,18	1
3	FE2	A	302	1/1	1.00	0.11	18,18,18,18	1

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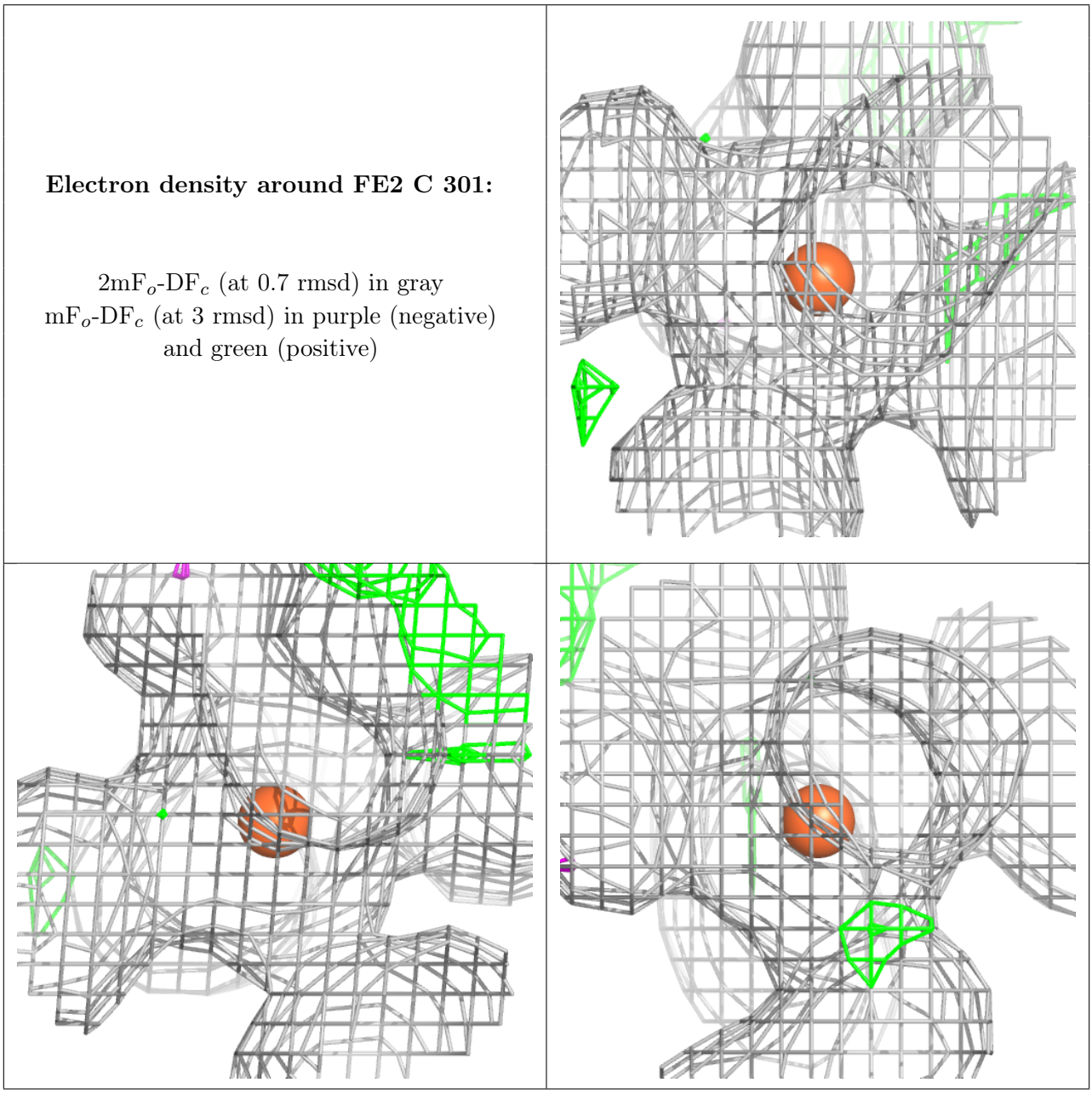
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FE2	D	301	1/1	1.00	0.12	18,18,18,18	1

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.

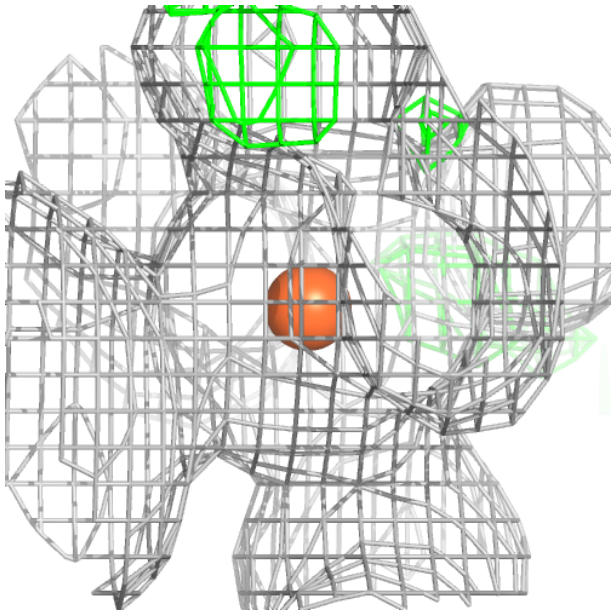
Electron density around FE2 C 301:

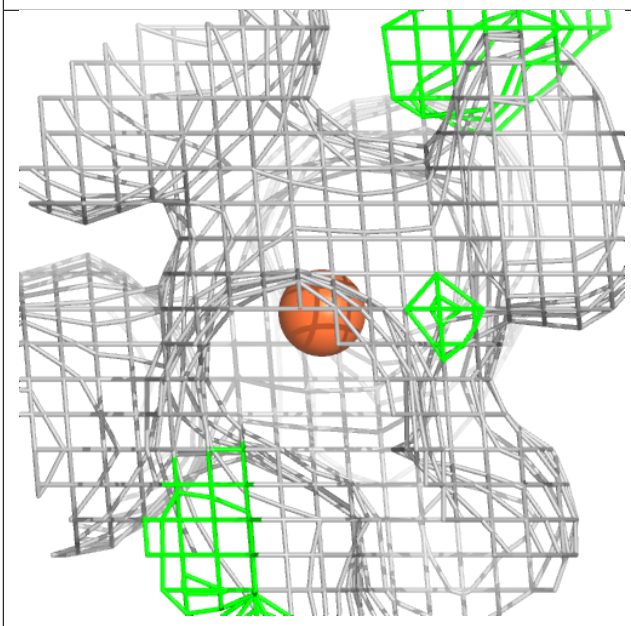
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

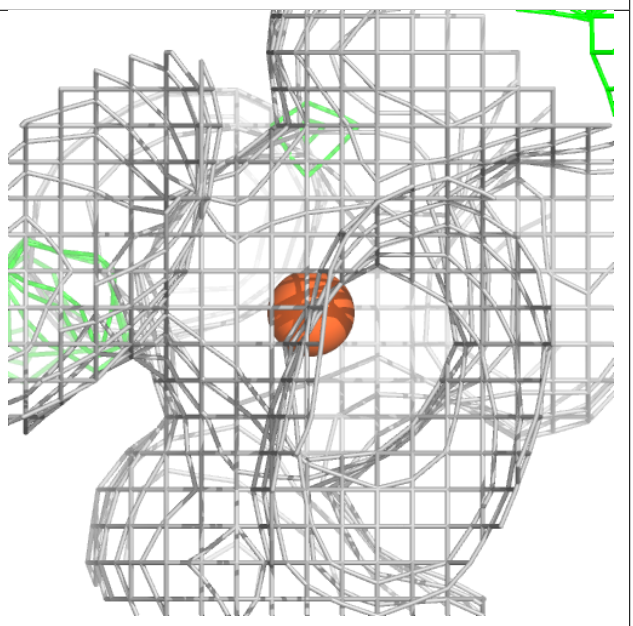


Electron density around FE2 B 301:

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

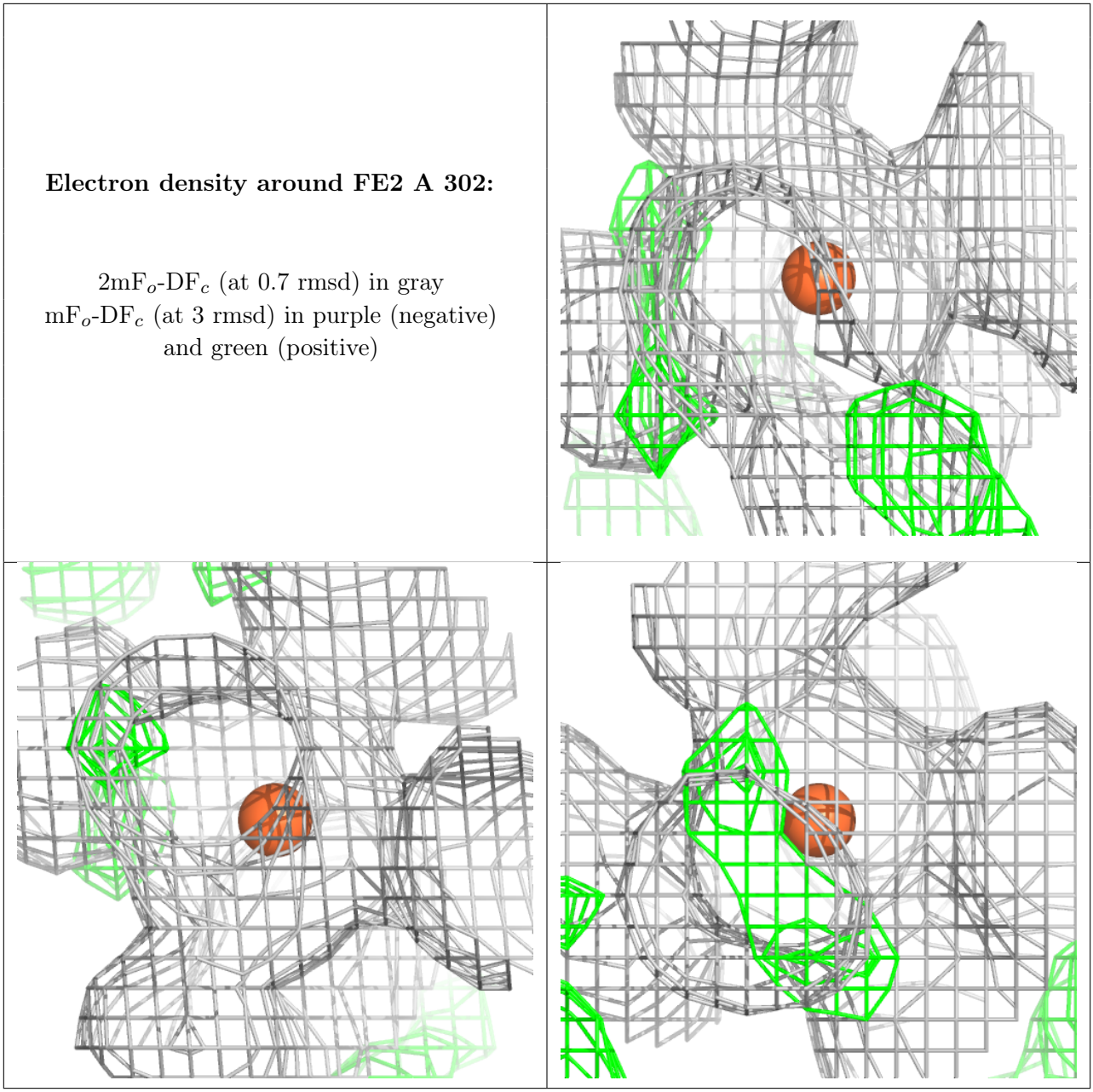






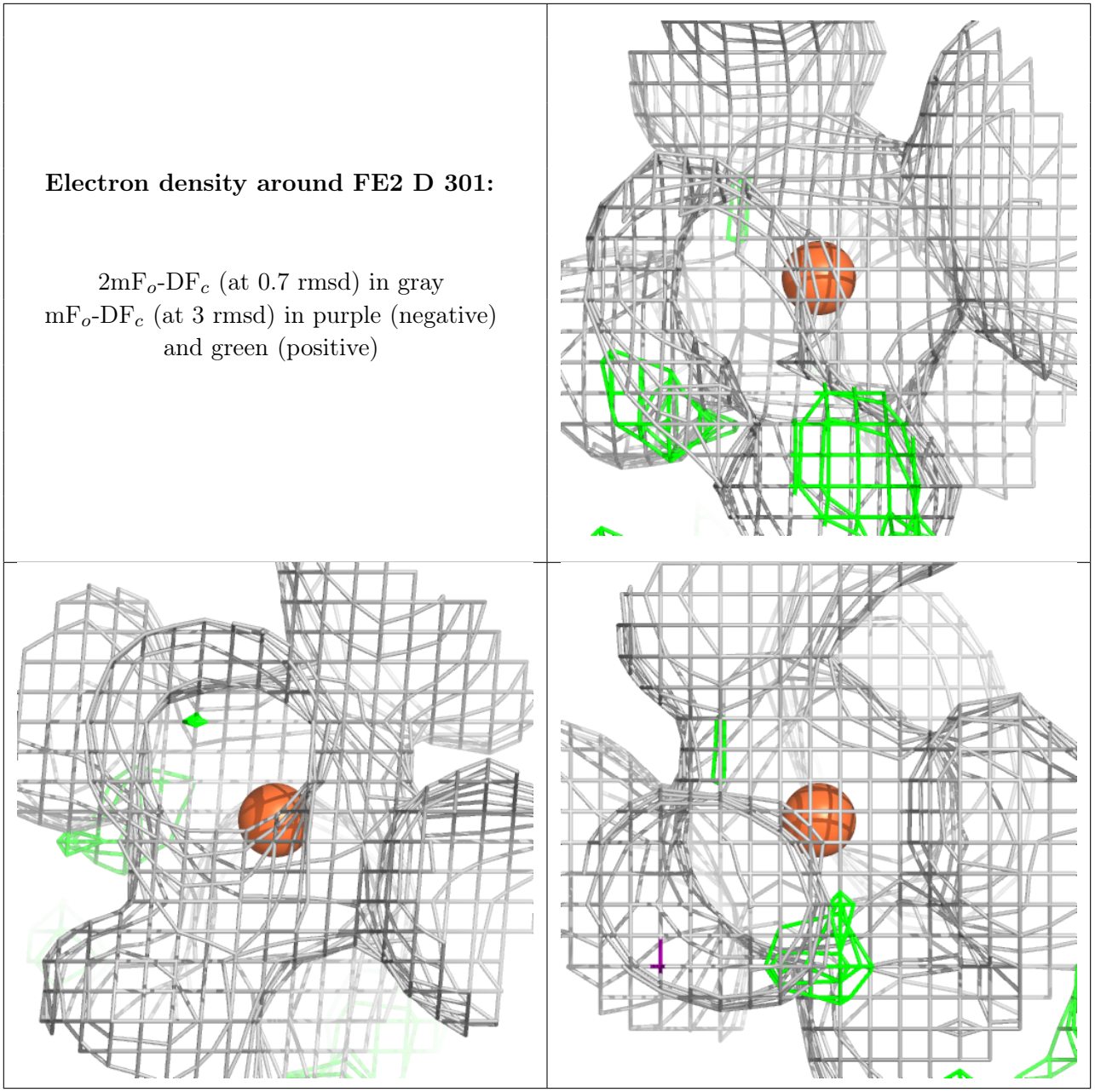
Electron density around FE2 A 302:

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



Electron density around FE2 D 301:

$2mF_o$-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.