



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 04:50 PM EDT

PDB ID : 7TTJ
Title : Stable-5-LOX elongated Ha2
Authors : Gilbert, N.C.; Newcomer, M.E.
Deposited on : 2022-02-01
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

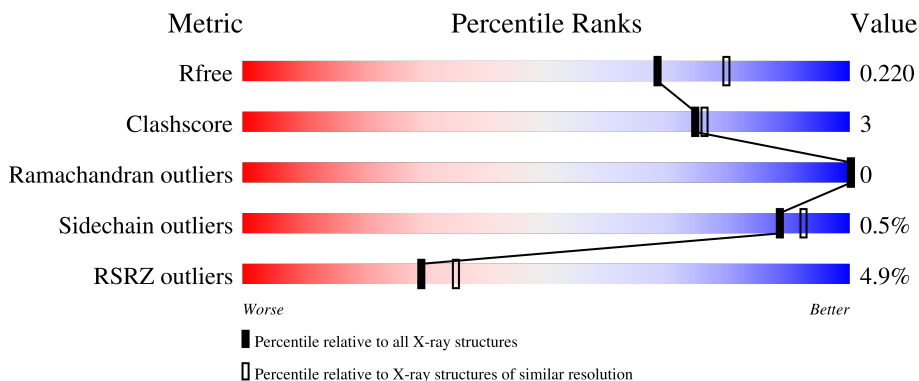
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	691	 5% 85% 8% 7%
1	B	691	 4% 80% 5% 15%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 20248 atoms, of which 9827 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 Arachidonate 5-lipoxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	B	590	9516	3084	4704	818	890	20	0	1	0
1	A	643	10371	3368	5123	887	970	23	0	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	MET	-	initiating methionine	UNP P09917
B	-13	GLY	-	expression tag	UNP P09917
B	-12	SER	-	expression tag	UNP P09917
B	-11	SER	-	expression tag	UNP P09917
B	-10	HIS	-	expression tag	UNP P09917
B	-9	HIS	-	expression tag	UNP P09917
B	-8	HIS	-	expression tag	UNP P09917
B	-7	HIS	-	expression tag	UNP P09917
B	-6	HIS	-	expression tag	UNP P09917
B	-6A	HIS	-	expression tag	UNP P09917
B	-6B	SER	-	expression tag	UNP P09917
B	-6C	SER	-	expression tag	UNP P09917
B	-6D	GLY	-	expression tag	UNP P09917
B	-6E	LEU	-	expression tag	UNP P09917
B	-6F	VAL	-	expression tag	UNP P09917
B	-6G	PRO	-	expression tag	UNP P09917
B	-6H	ARG	-	expression tag	UNP P09917
B	-6I	GLY	-	expression tag	UNP P09917
B	-6J	SER	-	expression tag	UNP P09917
B	-6K	HIS	-	expression tag	UNP P09917
B	16	GLU	TRP	conflict	UNP P09917
B	17	HIS	PHE	conflict	UNP P09917
B	?	-	PRO	deletion	UNP P09917
B	?	-	PHE	deletion	UNP P09917
B	?	-	TYR	deletion	UNP P09917

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Chain	Residue	Modelled	Actual	Comment	Reference
B	43	GLY	ASN	conflict	UNP P09917
B	44	SER	ASP	conflict	UNP P09917
B	75	GLY	TRP	conflict	UNP P09917
B	76	SER	LEU	conflict	UNP P09917
B	240	ALA	CYS	conflict	UNP P09917
B	561	ALA	CYS	conflict	UNP P09917
B	653	GLU	LYS	conflict	UNP P09917
B	654	ASN	LYS	conflict	UNP P09917
B	655	LEU	LYS	conflict	UNP P09917
A	-17	MET	-	initiating methionine	UNP P09917
A	-16	GLY	-	expression tag	UNP P09917
A	-15	SER	-	expression tag	UNP P09917
A	-14	SER	-	expression tag	UNP P09917
A	-13	HIS	-	expression tag	UNP P09917
A	-12	HIS	-	expression tag	UNP P09917
A	-11	HIS	-	expression tag	UNP P09917
A	-10	HIS	-	expression tag	UNP P09917
A	-9	HIS	-	expression tag	UNP P09917
A	-8	HIS	-	expression tag	UNP P09917
A	-7	SER	-	expression tag	UNP P09917
A	-6	SER	-	expression tag	UNP P09917
A	-5	GLY	-	expression tag	UNP P09917
A	-4	LEU	-	expression tag	UNP P09917
A	-3	VAL	-	expression tag	UNP P09917
A	-2	PRO	-	expression tag	UNP P09917
A	-1	ARG	-	expression tag	UNP P09917
A	0	GLY	-	expression tag	UNP P09917
A	1	SER	-	expression tag	UNP P09917
A	2	HIS	-	expression tag	UNP P09917
A	16	GLU	TRP	conflict	UNP P09917
A	17	HIS	PHE	conflict	UNP P09917
A	?	-	PRO	deletion	UNP P09917
A	?	-	PHE	deletion	UNP P09917
A	?	-	TYR	deletion	UNP P09917
A	43	GLY	ASN	conflict	UNP P09917
A	44	SER	ASP	conflict	UNP P09917
A	75	GLY	TRP	conflict	UNP P09917
A	76	SER	LEU	conflict	UNP P09917
A	240	ALA	CYS	conflict	UNP P09917
A	561	ALA	CYS	conflict	UNP P09917
A	653	GLU	LYS	conflict	UNP P09917
A	654	ASN	LYS	conflict	UNP P09917

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Chain	Residue	Modelled	Actual	Comment	Reference
A	655	LEU	LYS	conflict	UNP P09917

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	164	Total O 164 164	0	0
3	A	195	Total O 195 195	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.73Å 204.57Å 74.11Å 90.00° 107.65° 90.00°	Depositor
Resolution (Å)	50.25 – 2.10 51.14 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.25-2.10) 99.5 (51.14-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.184 , 0.224 0.183 , 0.220	Depositor DCC
R_{free} test set	4080 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtrriage
Anisotropy	0.684	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20248	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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: FE2

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	0.60	0/5380	0.69	1/7297 (0.0%)
1	B	0.61	0/4935	0.69	0/6696
All	All	0.60	0/10315	0.69	1/13993 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	665	ASP	CB-CG-OD2	5.52	123.27	118.30

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	5248	5123	5135	40	0
1	B	4812	4704	4706	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	195	0	0	12	0
3	B	164	0	0	9	0
All	All	10421	9827	9841	64	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.

The worst 5 of 64 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:223:MET:SD	3:B:961:HOH:O	2.12	1.07
1:B:159:CYS:SG	3:B:933:HOH:O	2.19	1.01
1:A:229:ASP:OD2	3:A:801:HOH:O	1.93	0.86
1:A:594:ARG:NH1	3:A:804:HOH:O	2.10	0.84
1:A:622:GLU:OE1	3:A:803:HOH:O	2.06	0.74

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	635/691 (92%)	620 (98%)	15 (2%)	0	100	100
1	B	577/691 (84%)	569 (99%)	8 (1%)	0	100	100
All	All	1212/1382 (88%)	1189 (98%)	23 (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	570/608 (94%)	568 (100%)	2 (0%)	91	94
1	B	523/608 (86%)	519 (99%)	4 (1%)	81	86
All	All	1093/1216 (90%)	1087 (100%)	6 (0%)	88	92

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	468	TYR
1	A	176	ASP
1	A	468	TYR
1	B	288	LEU
1	B	231	MET

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 2 ligands modelled in this entry, 2 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	643/691 (93%)	0.47	32 (4%) 28 34	33, 51, 92, 136	0
1	B	590/691 (85%)	0.38	29 (4%) 29 35	34, 52, 87, 116	0
All	All	1233/1382 (89%)	0.43	61 (4%) 29 35	33, 52, 91, 136	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	TRP	12.6
1	B	613	ASN	6.0
1	B	605	TRP	5.8
1	A	199	SER	5.6
1	A	74	TYR	5.0

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](#)

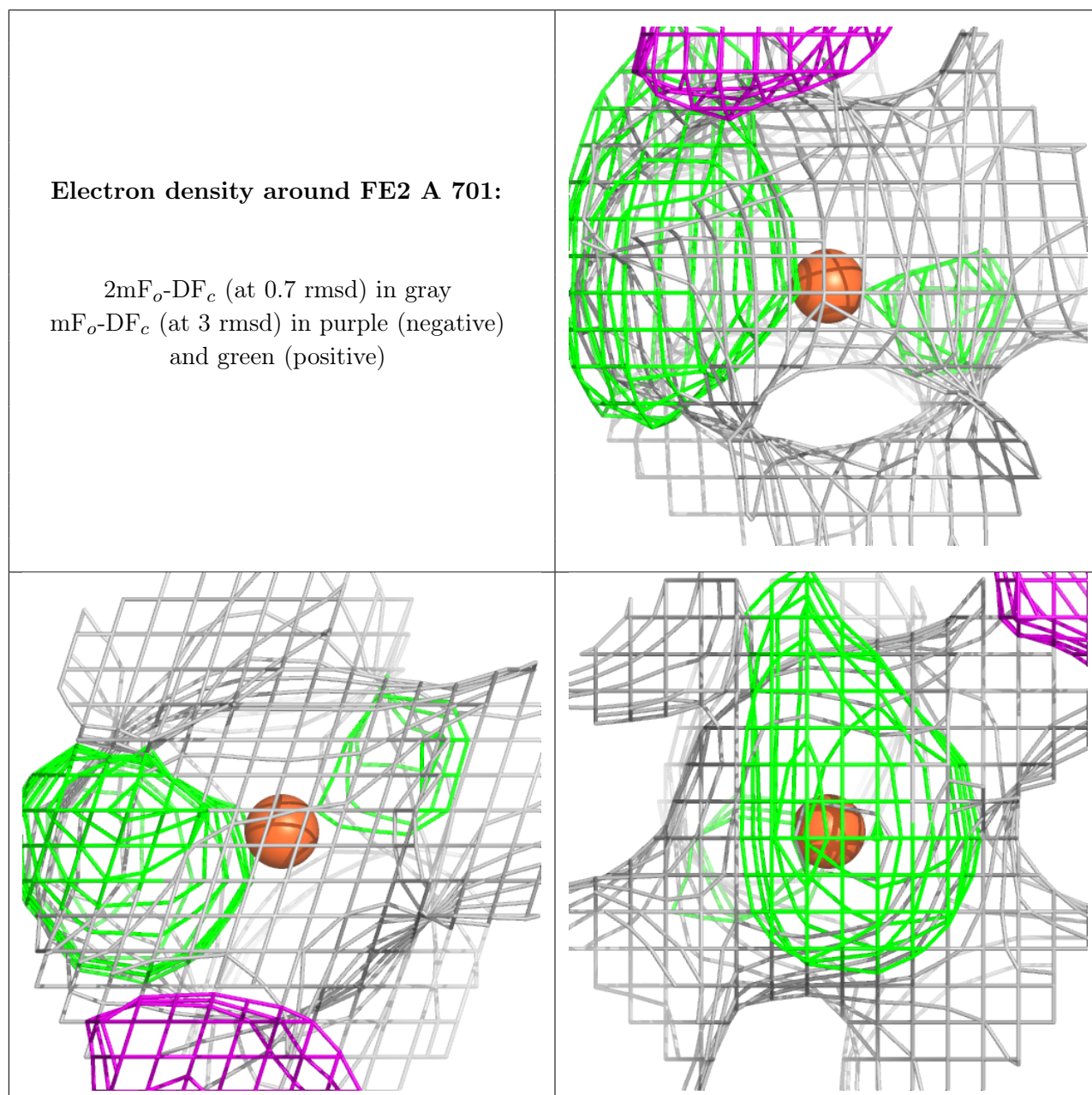
There are no monosaccharides in this entry.

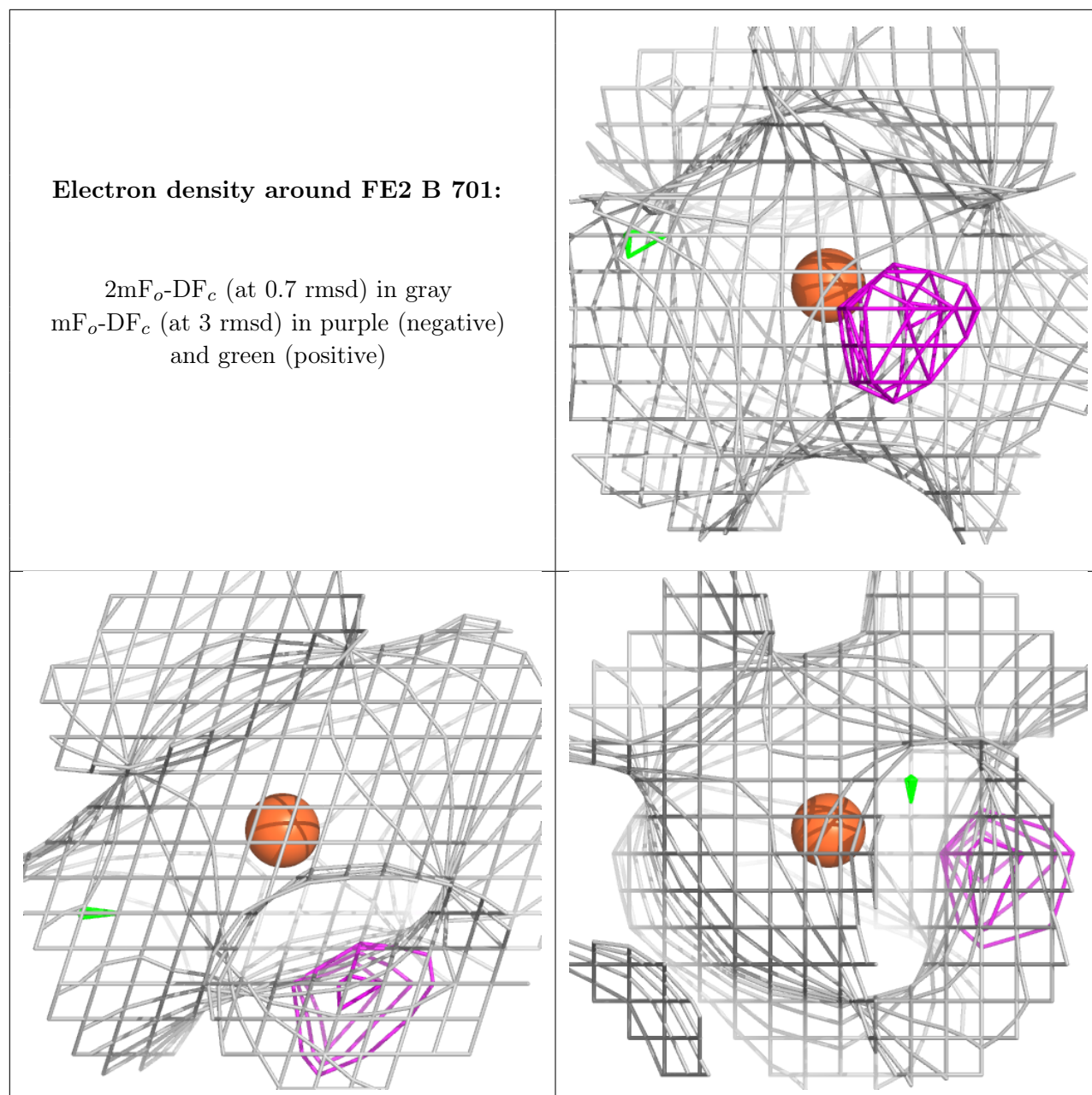
6.4 Ligands [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE2	A	701	1/1	0.97	0.21	43,43,43,43	0
2	FE2	B	701	1/1	0.98	0.14	52,52,52,52	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.