



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 09:35 PM UTC

PDB ID : 9O4T / pdb_00009o4t
Title : RT XFEL structure of Soybean Lipxygenase-1 in large unit-cell
Authors : Wolff, A.M.; Thompson, M.C.
Deposited on : 2025-04-08
Resolution : 1.95 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
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

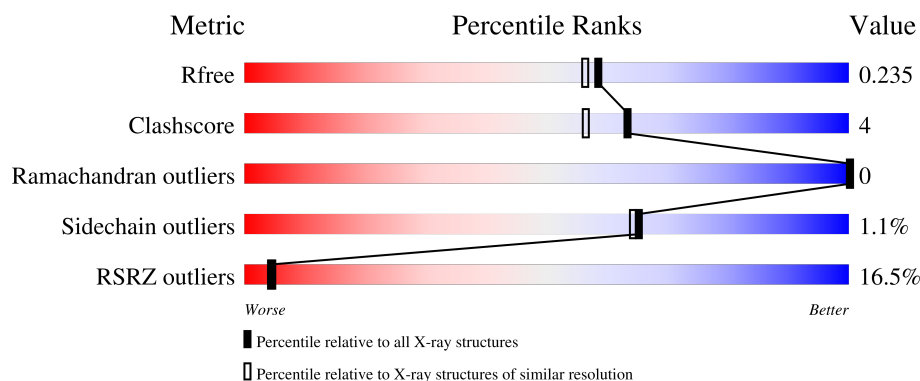
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	839	<div> <div>16%</div> <div>87%</div> <div>8%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12887 atoms, of which 6187 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 Seed linoleate 13S-lipoxygenase-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	802	Total	C	H	N	O	S	0	37	0
			12616	4114	6187	1082	1214	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	GLU	SER	conflict	UNP P08170

- 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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	270	Total	O	0	4
			270	270		

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: Seed linoleate 13S-lipoxygenase-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.03Å 94.54Å 50.53Å 90.00° 91.18° 90.00°	Depositor
Resolution (Å)	19.59 – 1.95 19.59 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.59-1.95) 95.5 (19.59-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.66 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.212 , 0.235 0.212 , 0.235	Depositor DCC
R_{free} test set	2012 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 78.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.057 for k,h,-l 0.058 for -k,-h,-l 0.065 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12887	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 4.54% 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: 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	0.17	2/6744 (0.0%)	0.30	0/9194

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	666[A]	TRP	N-CA	5.97	1.52	1.45
1	A	666[B]	TRP	N-CA	5.97	1.52	1.45

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	665[B]	TRP	Mainchain

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	6429	6187	6041	51	0
2	A	1	0	0	0	0
3	A	270	0	0	17	0
All	All	6700	6187	6041	51	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 (51) 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:A:217:ARG:O	3:A:1001:HOH:O	1.91	0.89
1:A:233:LYS:O	3:A:1002:HOH:O	1.93	0.86
1:A:142:ILE:O	3:A:1003:HOH:O	2.00	0.78
1:A:659:ASP:O	3:A:1004:HOH:O	2.01	0.78
1:A:255:LEU:N	3:A:1009:HOH:O	2.24	0.71
1:A:524:ILE:HD12	1:A:645:LEU:HD13	1.72	0.71
1:A:209:SER:OG	3:A:1005:HOH:O	2.09	0.69
1:A:187:ASP:N	3:A:1001:HOH:O	2.27	0.67
1:A:757:HIS:ND1	3:A:1017:HOH:O	2.28	0.65
1:A:284:HIS:NE2	3:A:1019:HOH:O	2.30	0.65
1:A:418:ARG:NH1	3:A:1020:HOH:O	2.30	0.64
1:A:219:ARG:NH2	3:A:1015:HOH:O	2.27	0.64
1:A:314:LYS:NZ	1:A:315:GLU:OE2	2.31	0.63
1:A:524:ILE:CD1	1:A:645:LEU:HD13	2.29	0.62
1:A:301:ARG:NH1	1:A:322:GLN:OE1	2.32	0.62
1:A:425:SER:OG	3:A:1006:HOH:O	2.17	0.58
1:A:91:MET:HA	1:A:91:MET:HE2	1.89	0.54
1:A:88:ASP:OD1	1:A:89:GLY:N	2.38	0.53
1:A:165:GLU:OE2	1:A:182:ARG:NH2	2.42	0.53
1:A:671:THR:HG23	1:A:674:ASP:H	1.74	0.53
1:A:188:VAL:HG23	1:A:190[B]:ASN:OD1	2.10	0.51
1:A:50:ALA:HB2	1:A:157:PRO:HG3	1.93	0.51
1:A:645:LEU:HD12	1:A:648:TRP:HE3	1.75	0.51
1:A:237:VAL:O	3:A:1007:HOH:O	2.19	0.50
1:A:649[B]:TRP:CZ2	1:A:667:PRO:O	2.65	0.50
1:A:406[B]:MET:HE3	1:A:408:ASP:HB2	1.94	0.49
1:A:645:LEU:HD12	1:A:648:TRP:CE3	2.48	0.48
1:A:98:TYR:CD1	1:A:140:VAL:HG13	2.49	0.48
1:A:183:ILE:HG22	3:A:1230:HOH:O	2.14	0.47
1:A:649[B]:TRP:CZ2	1:A:653:VAL:HG21	2.50	0.47
1:A:188:VAL:HG23	1:A:190[B]:ASN:CG	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:THR:OG1	1:A:162:ARG:NH1	2.48	0.47
1:A:818:THR:HG22	1:A:821:TYR:CZ	2.51	0.46
1:A:755:SER:O	1:A:828:LEU:HD12	2.17	0.45
1:A:455:SER:O	1:A:458:ASP:N	2.49	0.44
1:A:184:TYR:HB3	1:A:512:ILE:HG23	2.00	0.43
1:A:678:VAL:HG23	1:A:679:CYS:N	2.34	0.43
1:A:302:ASP:OD1	1:A:302:ASP:N	2.48	0.43
1:A:74:LEU:HD11	1:A:80:ALA:HB2	2.01	0.43
1:A:14:LEU:C	1:A:14:LEU:HD12	2.44	0.42
1:A:91:MET:HE3	3:A:1235:HOH:O	2.19	0.41
1:A:101:ASN:O	1:A:134:THR:HG22	2.19	0.41
1:A:742:LEU:HB3	1:A:743[B]:PRO:HD3	2.01	0.41
1:A:114:LEU:O	1:A:122:THR:HG23	2.21	0.41
1:A:360[B]:ARG:NH2	3:A:1037:HOH:O	2.45	0.41
1:A:308:ILE:N	1:A:309:PRO:CD	2.83	0.40
1:A:340:TRP:CZ2	1:A:341:MET:HG3	2.57	0.40
1:A:199:GLU:N	3:A:1051:HOH:O	2.51	0.40
1:A:755:SER:HB2	1:A:828:LEU:HD11	2.03	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	825/839 (98%)	800 (97%)	25 (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	699/730 (96%)	691 (99%)	8 (1%)	65	64

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	302	ASP
1	A	382	LYS
1	A	419	GLN
1	A	524	ILE
1	A	669	LEU
1	A	769[A]	ASN
1	A	769[B]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	HIS
1	A	495	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 1 ligands modelled in this entry, 1 is 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, 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	802/839 (95%)	0.71	132 (16%) 4 4	17, 68, 123, 180	22 (2%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	LEU	5.9
1	A	161	TYR	5.2
1	A	221	GLY	4.8
1	A	521	LEU	4.6
1	A	246	LEU	4.4
1	A	649[A]	TRP	4.3
1	A	669	LEU	4.2
1	A	11	THR	4.2
1	A	512	ILE	4.1
1	A	50	ALA	4.0
1	A	639	VAL	3.9
1	A	665[A]	TRP	3.9
1	A	239	TYR	3.8
1	A	155	PRO	3.7
1	A	374	ALA	3.6
1	A	645	LEU	3.6
1	A	183	ILE	3.6
1	A	633	TYR	3.5
1	A	220	THR	3.5
1	A	631	LEU	3.5
1	A	781	ALA	3.5
1	A	144	PHE	3.4
1	A	134	THR	3.4
1	A	520	VAL	3.4
1	A	660	LEU	3.4
1	A	459	LEU	3.3
1	A	513	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	143	PHE	3.3
1	A	205[A]	VAL	3.2
1	A	72	PRO	3.2
1	A	225	THR	3.1
1	A	131	VAL	3.1
1	A	661	LYS	3.1
1	A	156	ALA	3.1
1	A	523	PRO	3.1
1	A	142	ILE	3.1
1	A	44	LEU	3.1
1	A	226	VAL	3.1
1	A	61	ASP	3.0
1	A	648	TRP	3.0
1	A	157	PRO	3.0
1	A	186	TYR	2.9
1	A	656	GLY	2.9
1	A	764[A]	LEU	2.9
1	A	140	VAL	2.9
1	A	107	PHE	2.9
1	A	87	TRP	2.9
1	A	99	ILE	2.9
1	A	643	SER	2.9
1	A	775[A]	ASP	2.9
1	A	672	LEU	2.9
1	A	169	LEU	2.8
1	A	666[A]	TRP	2.8
1	A	642	ASP	2.8
1	A	73	THR	2.8
1	A	98	TYR	2.7
1	A	652	ALA	2.7
1	A	147	HIS	2.7
1	A	67	ILE	2.7
1	A	130	TRP	2.7
1	A	12	VAL	2.7
1	A	632	TYR	2.7
1	A	152	SER	2.7
1	A	517	HIS	2.7
1	A	8	ILE	2.6
1	A	16	PRO	2.6
1	A	522	HIS	2.6
1	A	123	ILE	2.6
1	A	634	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	667	PRO	2.6
1	A	658	GLY	2.6
1	A	96	ALA	2.6
1	A	647	HIS	2.5
1	A	637	ASP	2.5
1	A	624	TRP	2.5
1	A	125	PHE	2.5
1	A	166	LEU	2.5
1	A	779	LEU	2.5
1	A	45	ILE	2.5
1	A	524	ILE	2.5
1	A	94	PRO	2.4
1	A	518	LEU	2.4
1	A	195	PRO	2.4
1	A	653	VAL	2.4
1	A	10	GLY	2.4
1	A	89	GLY	2.4
1	A	207	GLY	2.4
1	A	41	SER	2.4
1	A	233	LYS	2.4
1	A	180	TYR	2.4
1	A	81	PHE	2.4
1	A	778	ALA	2.4
1	A	20	LEU	2.3
1	A	132	TYR	2.3
1	A	97	PHE	2.3
1	A	114	LEU	2.3
1	A	675	LEU	2.3
1	A	121	GLY	2.3
1	A	69	THR	2.3
1	A	173	GLY	2.3
1	A	14	LEU	2.3
1	A	219	ARG	2.2
1	A	181	ASP	2.2
1	A	187	ASP	2.2
1	A	105	VAL	2.2
1	A	511	VAL	2.2
1	A	149	TYR	2.2
1	A	184	TYR	2.2
1	A	218	GLY	2.2
1	A	241	PRO	2.2
1	A	85	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	83	ILE	2.1
1	A	237	VAL	2.1
1	A	129	SER	2.1
1	A	641	ASN	2.1
1	A	227	THR	2.1
1	A	150	VAL	2.1
1	A	463	VAL	2.1
1	A	525	TYR	2.1
1	A	457	GLY	2.1
1	A	630	PRO	2.1
1	A	770	PRO	2.1
1	A	516	ARG	2.1
1	A	308	ILE	2.0
1	A	151	PRO	2.0
1	A	206	LEU	2.0
1	A	7	LYS	2.0
1	A	655	LYS	2.0
1	A	139	SER	2.0
1	A	379	GLN	2.0
1	A	670	GLN	2.0
1	A	628	TYR	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](#)

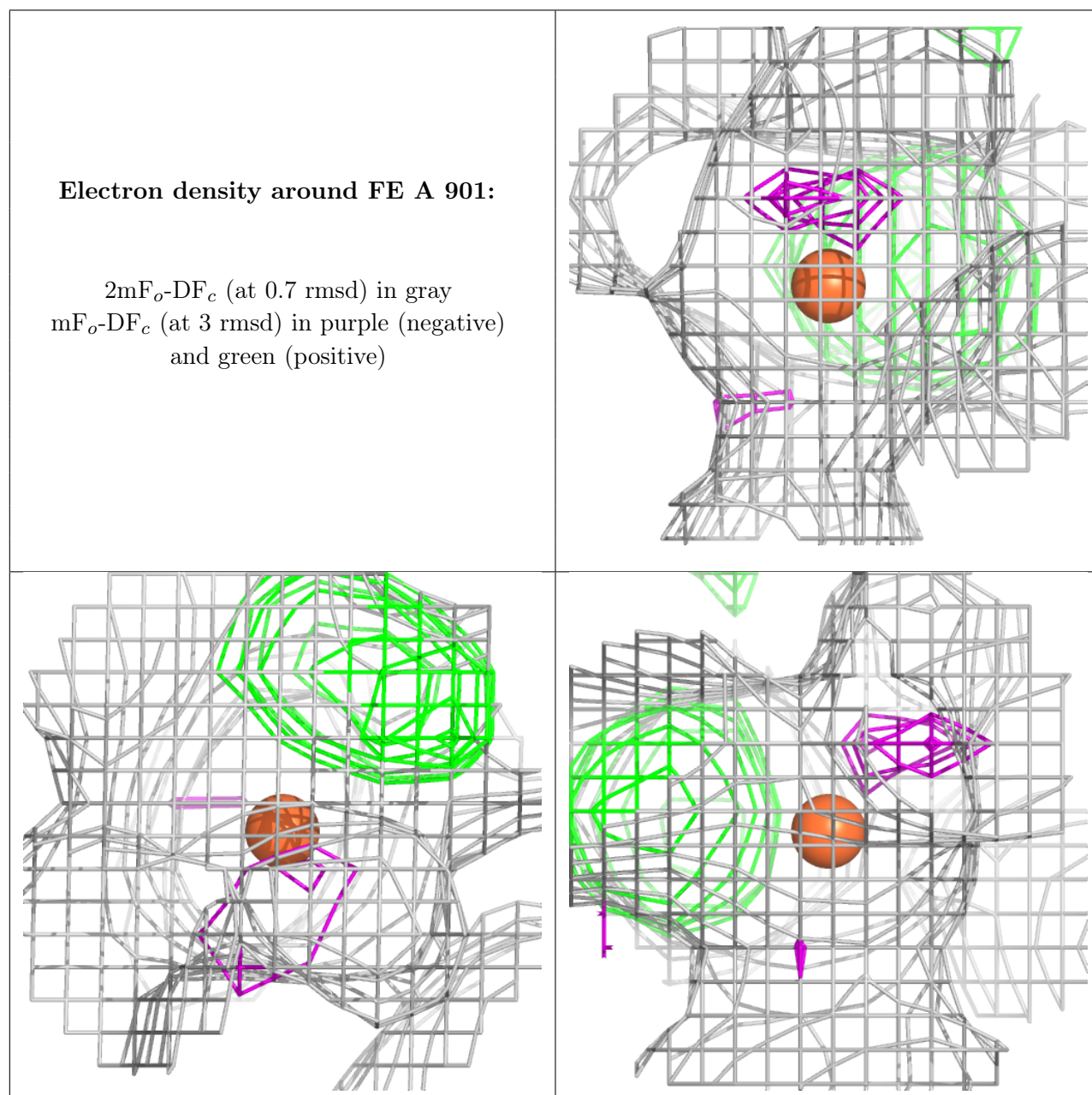
There are no oligosaccharides in this entry.

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(\AA^2)	Q<0.9
2	FE	A	901	1/1	0.96	0.05	38,38,38,38	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.