W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 10:38 AM EDT

PDB ID	:	7SOI
Title	:	Structure of I552A Soybean Lipoxygenase at 277K
Authors	:	Gee, C.L.; Offenbacher, A.R.; Hu, S.
Deposited on	:	2021-10-31
Resolution	:	2.00 Å(reported)

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

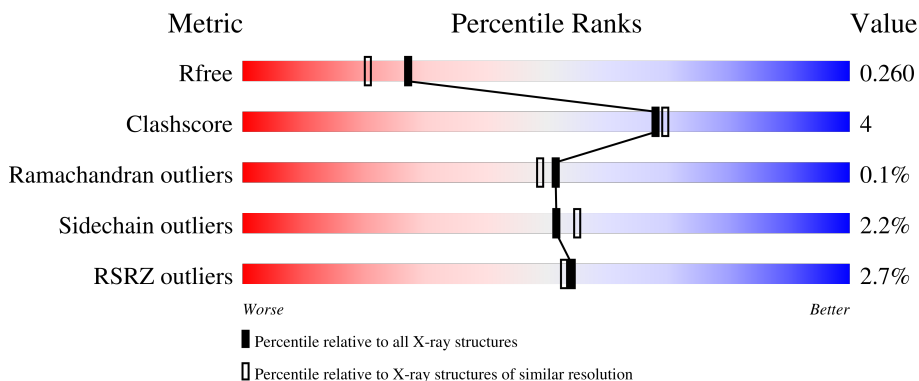|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.260
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		2.2%
RSRZ outliers		2.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

◫ Percentile relative to X-ray structures of similar resolution

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	839	3% / 84% / 13% / • •
1	B	839	2% / 89% / 8% / •

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 27364 atoms, of which 13398 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 Lipoxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	818	Total	C	H	N	O	S	0	57	0
			13419	4294	6701	1142	1263	19			
1	B	819	Total	C	H	N	O	S	0	56	0
			13424	4301	6697	1137	1270	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	ALA	ILE	engineered mutation	UNP B3TDK4
B	552	ALA	ILE	engineered mutation	UNP B3TDK4

- Molecule 2 is FE (III) ION (three-letter code: 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		
2	B	1	Total	Fe	0	1
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	275	Total	O	0	0
			275	275		

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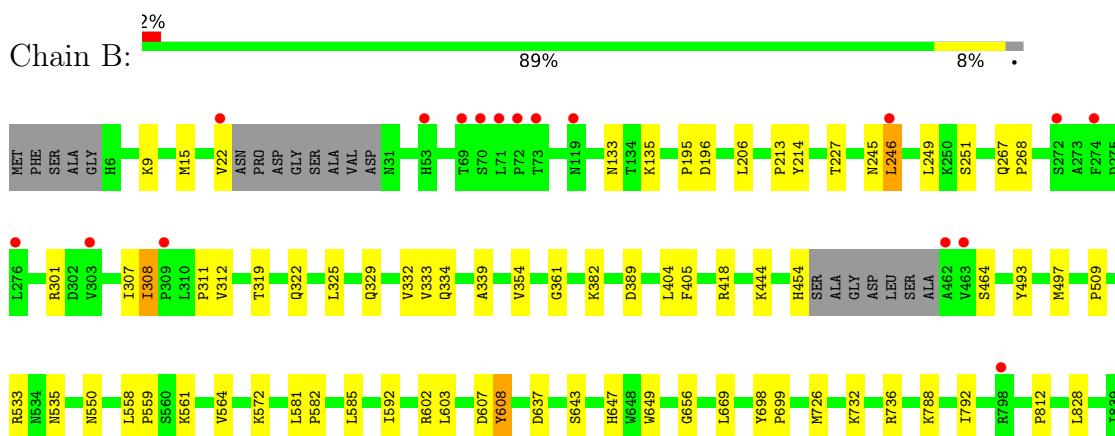| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	243	Total O 243 243		0	0

3 Residue-property plots ⓘ

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: Lipoxygenase

• Molecule 1: Lipoxygenase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.53Å 92.76Å 99.84Å 90.00° 93.56° 90.00°	Depositor
Resolution (Å)	46.38 – 2.00 46.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.2 (46.38-2.00) 95.2 (46.38-2.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.198 , 0.259 0.198 , 0.260	Depositor DCC
R_{free} test set	5185 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	27364	wwPDB-VP
Average B, all atoms (Å^2)	51.0	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 84.37 % 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 1.6937e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: FE, NA

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	0.59	0/7113	0.74	2/9658 (0.0%)
1	B	0.58	0/7122	0.72	0/9679
All	All	0.58	0/14235	0.73	2/19337 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	497	MET	CG-SD-CE	5.83	109.52	100.20
1	A	636	ASP	CB-CG-OD1	5.66	123.39	118.30

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	6718	6701	6453	66	0
1	B	6727	6697	6458	36	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	1	0	0	0	0
4	A	275	0	0	4	0
4	B	243	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13966	13398	12911	102	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 (102) 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:308:ILE:HD11	1:B:319[A]:THR:HG21	1.48	0.93
1:B:319[B]:THR:HG22	1:B:325:LEU:HD23	1.64	0.80
1:B:196:ASP:OD1	1:B:227:THR:HG23	1.82	0.79
1:A:253:ASP:OD2	1:A:759:SER:OG	2.02	0.78
1:B:301:ARG:NH1	1:B:322[A]:GLN:OE1	2.26	0.69
1:A:304:ILE:HG22	1:A:308:ILE:HD13	1.75	0.68
1:A:299:LEU:HB2	1:A:304:ILE:HD11	1.73	0.68
1:B:319[B]:THR:CG2	1:B:325:LEU:HD23	2.24	0.68
1:A:300:PRO:O	1:A:304:ILE:HD12	1.94	0.67
1:A:775[A]:ASP:OD2	4:A:1001:HOH:O	2.14	0.66
1:A:818:THR:HG22	1:A:821:TYR:CZ	2.34	0.63
1:B:245[B]:ASN:ND2	4:B:1004:HOH:O	2.31	0.60
1:A:803:PRO:HA	1:A:806[B]:GLN:HG2	1.83	0.60
1:B:339:ALA:HB1	1:B:812:PRO:HB2	1.83	0.59
1:A:157:PRO:O	4:A:1002:HOH:O	2.16	0.59
1:B:206:LEU:CD1	1:B:564:VAL:HG12	2.34	0.57
1:A:793:GLU:O	1:A:797:VAL:HG23	2.06	0.56
1:A:607:ASP:O	1:A:609:PRO:HD3	2.06	0.55
1:A:222:ARG:O	1:A:233:LYS:HD3	2.08	0.54
1:A:214:TYR:CG	1:A:215:PRO:HD2	2.43	0.54
1:A:424:ASN:OD1	1:A:424:ASN:N	2.40	0.53
1:A:307:ILE:C	1:A:309:PRO:HD2	2.28	0.53
1:B:267:GLN:HB3	1:B:268:PRO:HD3	1.91	0.53
1:A:262:LEU:HD13	1:A:313:ILE:HD12	1.89	0.53
1:A:163[B]:GLU:HG3	1:A:167:LYS:HE3	1.89	0.53
1:A:320:ASP:OD2	1:A:323[B]:HIS:ND1	2.41	0.53
1:B:592:ILE:HD11	1:B:602:ARG:HH21	1.75	0.52
1:B:361:GLY:HA2	1:B:405:PHE:CD2	2.44	0.52
1:B:389:ASP:O	1:B:444:LYS:NZ	2.40	0.52
1:B:607:ASP:O	1:B:607:ASP:OD1	2.28	0.52
1:A:410:HIS:CE1	1:A:414:MET:CE	2.94	0.51
1:A:493:TYR:O	1:A:497:MET:HB2	2.09	0.51
1:B:15:MET:HE1	1:B:249:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ASN:OD1	1:A:427:LYS:HA	2.12	0.49
1:B:213:PRO:HG3	1:B:572:LYS:HG2	1.95	0.49
1:B:246[B]:LEU:HD11	1:B:533:ARG:HG2	1.94	0.49
1:A:198:SER:OG	1:A:200:LYS:HG2	2.12	0.49
1:A:242:ARG:NH1	1:A:245[B]:ASN:O	2.46	0.49
1:B:329[B]:GLN:OE1	1:B:334:GLN:HG2	2.13	0.49
1:A:486:VAL:O	1:A:489:ASN:HB2	2.13	0.49
1:B:354[A]:VAL:HG23	4:B:1148:HOH:O	2.13	0.48
1:A:243:ASP:OD2	4:A:1003:HOH:O	2.20	0.48
1:B:311:PRO:O	1:B:312:VAL:HB	2.13	0.48
1:B:22:VAL:HG13	1:B:251:SER:HB2	1.94	0.48
1:B:133:ASN:OD1	1:B:135:LYS:HB2	2.14	0.47
1:A:529:THR:N	1:A:530:PRO:CD	2.77	0.47
1:A:340:TRP:CZ2	1:A:341:MET:HG3	2.50	0.47
1:B:732:LYS:HE3	1:B:736:ARG:HH11	1.79	0.46
1:B:581:LEU:HB3	1:B:582:PRO:HD3	1.97	0.46
1:B:649:TRP:HB2	1:B:669:LEU:HD22	1.98	0.46
1:A:320:ASP:OD2	1:A:323[B]:HIS:CE1	2.68	0.46
1:A:793:GLU:OE2	1:A:831:ARG:NH2	2.48	0.46
1:A:117[B]:ILE:HG23	1:A:118[B]:SER:N	2.31	0.46
1:A:414:MET:HE2	1:A:430:ALA:HB3	1.98	0.46
1:A:768:ASP:OD1	1:A:769:ASN:N	2.49	0.46
1:A:802:ASP:OD1	1:A:804:SER:OG	2.30	0.46
1:B:643:SER:O	1:B:647:HIS:ND1	2.48	0.46
1:A:265:ILE:HG21	1:A:310:LEU:HD11	1.98	0.45
1:A:643[A]:SER:O	1:A:647:HIS:ND1	2.49	0.45
1:B:726:MET:O	4:B:1001:HOH:O	2.21	0.44
1:A:308:ILE:N	1:A:309:PRO:CD	2.80	0.44
1:A:322:GLN:HB2	1:A:323[B]:HIS:CE1	2.53	0.44
1:B:558:LEU:HB3	1:B:559:PRO:HD3	1.99	0.44
1:A:298:LYS:HG3	1:A:324:ILE:HD13	2.00	0.44
1:B:332:VAL:HG13	1:B:333:VAL:HG13	2.00	0.44
1:A:679:CYS:O	1:A:683:ILE:HG13	2.17	0.43
1:B:493:TYR:O	1:B:497:MET:HB2	2.17	0.43
1:A:803:PRO:HA	1:A:806[B]:GLN:CG	2.47	0.43
1:A:453:PRO:O	1:A:454:HIS:CB	2.66	0.43
1:A:333:VAL:CG1	1:A:703:LEU:HD22	2.48	0.43
1:B:592:ILE:HD11	1:B:602:ARG:HE	1.84	0.43
1:A:636:ASP:O	1:A:640[B]:LYS:HG3	2.19	0.43
1:A:626:GLN:O	1:A:630:PRO:CD	2.67	0.42
1:A:249:LEU:HD23	1:A:249:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLU:HG3	4:A:1023:HOH:O	2.19	0.42
1:A:254:ALA:O	1:A:257:ILE:HG12	2.18	0.42
1:A:649:TRP:HB2	1:A:669:LEU:HD22	2.00	0.42
1:B:698:TYR:HB3	1:B:699:PRO:HD3	2.01	0.42
1:A:311:PRO:O	1:A:312:VAL:HB	2.20	0.42
1:B:585:LEU:HD13	1:B:603:LEU:HD21	2.01	0.42
1:A:304:ILE:O	1:A:308:ILE:HG12	2.20	0.42
1:A:451:SER:HA	1:A:464:SER:HB3	2.02	0.42
1:A:698:TYR:N	1:A:699:PRO:CD	2.83	0.42
1:A:352:ALA:HB2	1:A:609:PRO:HG2	2.02	0.41
1:A:410:HIS:CE1	1:A:414:MET:HE1	2.55	0.41
1:A:410:HIS:HA	1:A:430:ALA:HB1	2.02	0.41
1:A:22:VAL:HG13	1:A:251:SER:HB2	2.01	0.41
1:B:788:LYS:O	1:B:792:ILE:HG13	2.20	0.41
1:A:669:LEU:HD12	1:A:669:LEU:HA	1.91	0.41
1:A:38:ARG:HA	1:A:63:PHE:CD1	2.54	0.41
1:A:195:PRO:HA	1:A:198:SER:O	2.20	0.41
1:A:404:LEU:HD12	1:A:404:LEU:HA	1.86	0.41
1:B:195:PRO:HB2	1:B:227:THR:OG1	2.21	0.41
1:B:509:PRO:HB3	1:B:656:GLY:HA3	2.03	0.41
1:A:645:LEU:HD21	1:A:675:LEU:HD13	2.03	0.40
1:B:307:ILE:HD12	1:B:325:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	868/839 (104%)	824 (95%)	42 (5%)	2 (0%)	47	44
1	B	866/839 (103%)	831 (96%)	34 (4%)	1 (0%)	51	49
All	All	1734/1678 (103%)	1655 (95%)	76 (4%)	3 (0%)	51	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116[A]	ALA
1	A	116[B]	ALA
1	B	608	TYR

5.3.2 Protein sidechains ⓘ

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	760/729 (104%)	743 (98%)	17 (2%)	52	55
1	B	764/729 (105%)	748 (98%)	16 (2%)	53	57
All	All	1524/1458 (104%)	1491 (98%)	33 (2%)	52	55

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	GLU
1	A	250	LYS
1	A	281	ILE
1	A	424	ASN
1	A	425	SER
1	A	435	LEU
1	A	438	ARG
1	A	463	VAL
1	A	465	GLN
1	A	489	ASN
1	A	535	ASN
1	A	550	ASN
1	A	561	LYS
1	A	593	LYS
1	A	608	TYR
1	A	668	LYS
1	A	828	LEU
1	B	9	LYS
1	B	214	TYR
1	B	246[A]	LEU

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Mol	Chain	Res	Type
1	B	246[B]	LEU
1	B	308	ILE
1	B	382	LYS
1	B	404	LEU
1	B	418	ARG
1	B	454	HIS
1	B	464	SER
1	B	535	ASN
1	B	550	ASN
1	B	561	LYS
1	B	608	TYR
1	B	637	ASP
1	B	828	LEU

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	410	HIS
1	A	419	GLN
1	B	104	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	818/839 (97%)	0.05	28 (3%)	45	44	24, 41, 79, 108	0
1	B	819/839 (97%)	-0.02	17 (2%)	63	62	25, 43, 79, 106	0
All	All	1637/1678 (97%)	0.01	45 (2%)	54	53	24, 42, 79, 108	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117[A]	ILE	6.8
1	A	119[A]	ASN	5.9
1	B	462	ALA	4.6
1	A	276	LEU	4.6
1	A	463	VAL	4.5
1	B	70	SER	4.3
1	B	72	PRO	4.1
1	B	463	VAL	4.1
1	A	118[A]	SER	3.9
1	A	299	LEU	3.7
1	A	324	ILE	3.6
1	A	325	LEU	3.5
1	A	274	PHE	3.3
1	A	116[A]	ALA	3.3
1	A	69	THR	3.3
1	A	307	ILE	3.2
1	A	72	PRO	3.1
1	A	6	HIS	3.1
1	B	276[A]	LEU	3.1
1	A	303[A]	VAL	3.1
1	A	598	PRO	3.1
1	B	73	THR	3.1
1	A	279	THR	3.1
1	A	120[A]	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	71	LEU	3.0
1	A	22	VAL	2.9
1	A	73	THR	2.7
1	A	306	THR	2.5
1	B	303	VAL	2.5
1	A	322	GLN	2.5
1	B	119	ASN	2.4
1	A	297	ILE	2.3
1	A	281	ILE	2.3
1	B	71	LEU	2.2
1	B	246[A]	LEU	2.2
1	B	53	HIS	2.2
1	B	274	PHE	2.2
1	B	798	ARG	2.2
1	B	69[A]	THR	2.2
1	A	31	ASN	2.1
1	B	22	VAL	2.1
1	A	720	THR	2.1
1	A	323[A]	HIS	2.1
1	B	309[A]	PRO	2.0
1	B	272	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.
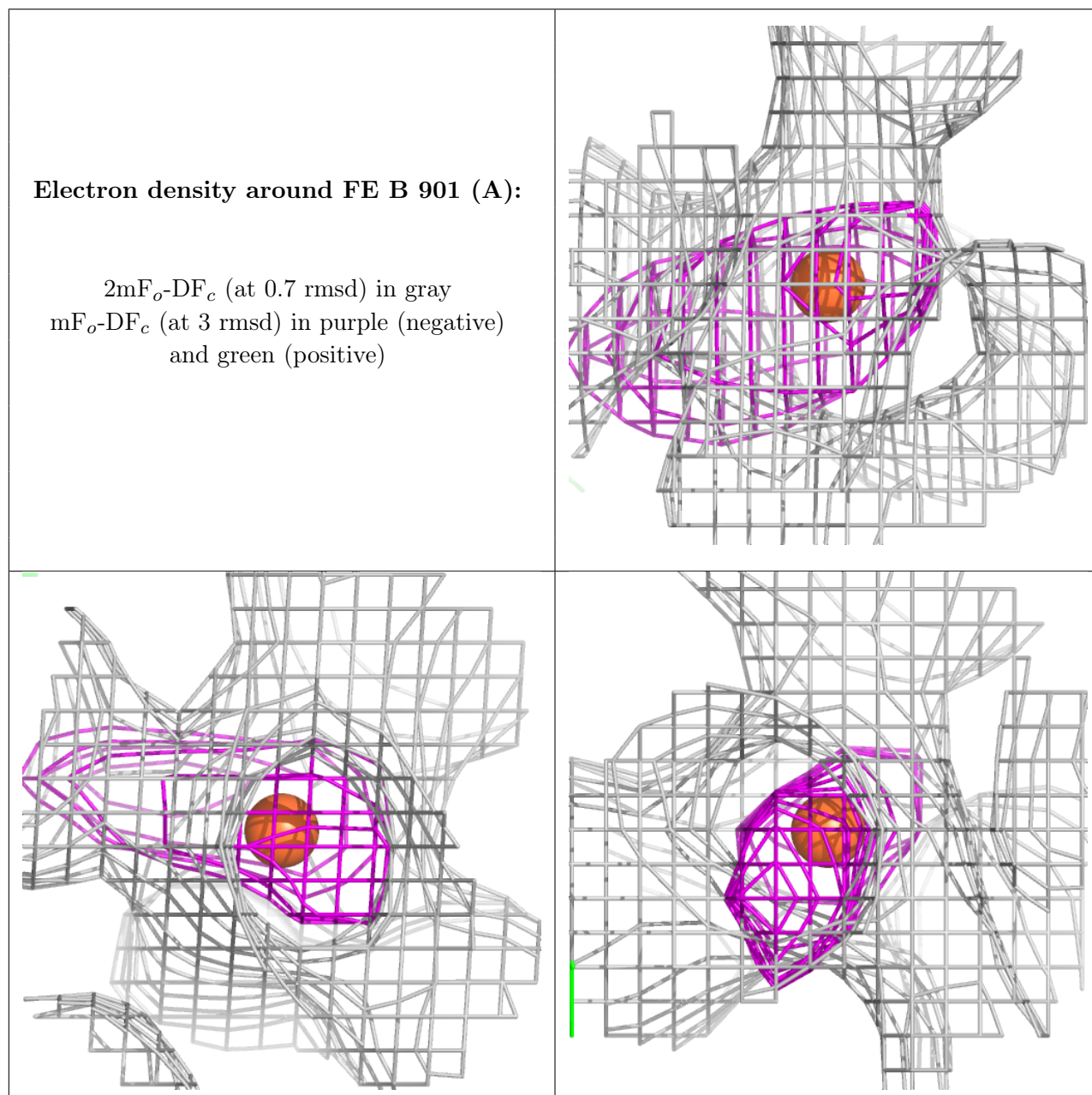
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	NA	B	902	1/1	0.76	0.17	76,76,76,76	0
2	FE	B	901[A]	1/1	0.97	0.06	55,55,55,55	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	A	901	1/1	0.98	0.09	63,63,63,63	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 FE B 901 (A):

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around FE A 901:

$2mF_o$-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.