



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 02:01 AM UTC

PDB ID : 9L52 / pdb_00009L52
Title : The ring expansion oxygenase SpoC in complex with Fe and stipitaldehyde
Authors : Liu, M.; He, X.
Deposited on : 2024-12-23
Resolution : 1.80 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
Mogul : 2022.3.0, CSD as543be (2022)
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

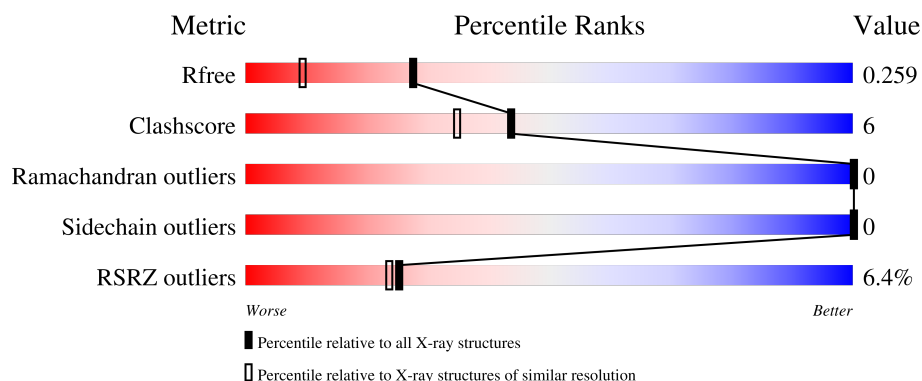
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	374	5% 75% 9% 16%
1	B	374	6% 72% 12% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	402	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5899 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 ring expansion oxygenase SpoC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	3	0
			2510	1609	424	463	14			
1	B	315	Total	C	N	O	S	0	1	0
			2499	1600	424	461	14			

- 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		
2	B	1	Total	Fe	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

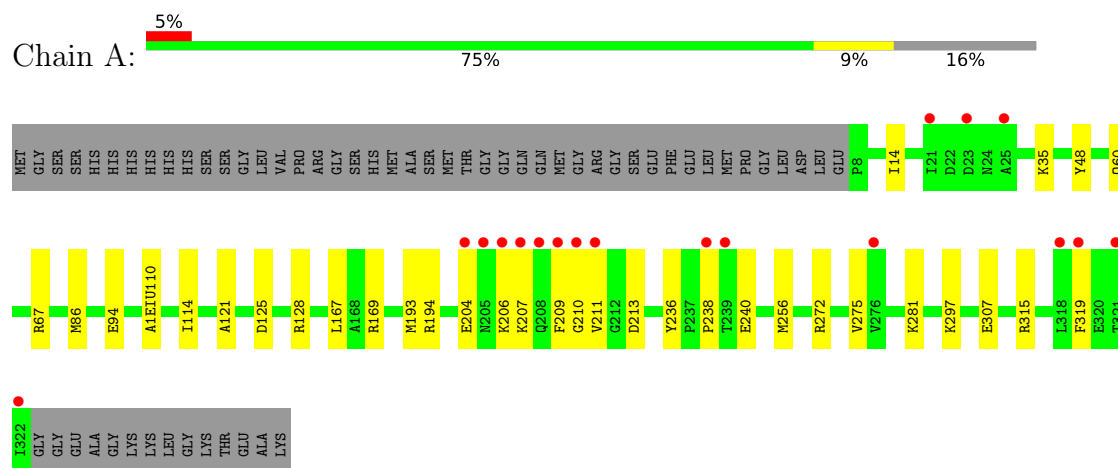
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	436	Total	O	0	0
			436	436		
4	B	451	Total	O	0	0
			451	451		

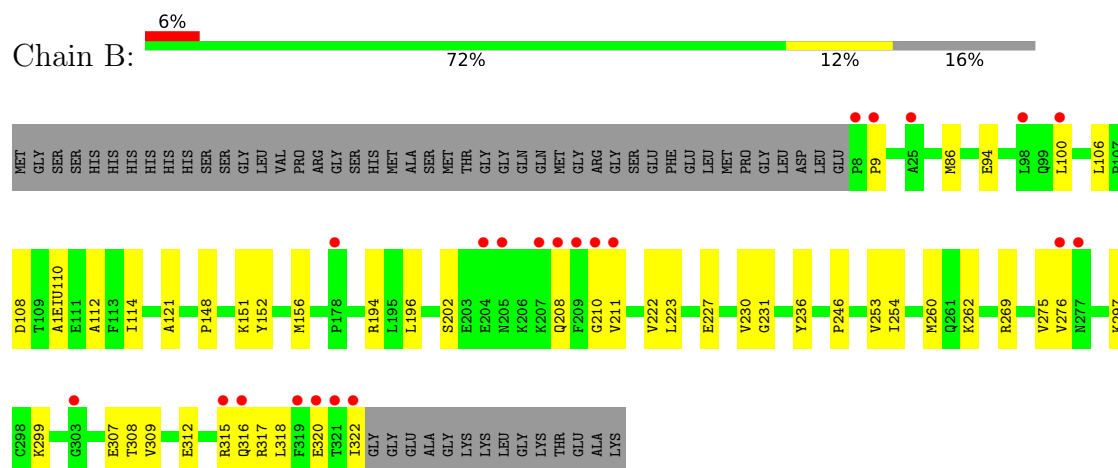
3 Residue-property plots [i](#)

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: ring expansion oxygenase SpoC



• Molecule 1: ring expansion oxygenase SpoC



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.58Å 85.24Å 104.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.98 – 1.80 43.98 – 1.80	Depositor EDS
% Data completeness (in resolution range)	90.9 (43.98-1.80) 90.9 (43.98-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.213 , 0.257 0.215 , 0.259	Depositor DCC
R_{free} test set	3080 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5899	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 23.61 % 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 4.5041e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, CL, A1EIU

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	0.13	0/2565	0.35	0/3482
1	B	0.12	0/2548	0.34	0/3458
All	All	0.13	0/5113	0.35	0/6940

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 [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	2510	0	2457	23	0
1	B	2499	0	2440	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	2	0
4	A	436	0	0	9	0
4	B	451	0	0	4	0
All	All	5899	0	4897	60	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 6.

All (60) 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:94[A]:GLU:OE1	1:A:194[A]:ARG:NH1	2.25	0.70
3:A:402:CL:CL	4:A:780:HOH:O	2.48	0.68
3:A:402:CL:CL	4:A:551:HOH:O	2.48	0.68
1:B:315:ARG:NH2	4:B:502:HOH:O	2.26	0.67
1:A:60:GLN:NE2	4:A:506:HOH:O	2.31	0.64
1:A:204:GLU:HG2	1:A:206:LYS:H	1.63	0.63
1:B:262:LYS:NZ	1:B:308:THR:OG1	2.31	0.63
1:B:94:GLU:OE2	1:B:114:ILE:HD11	1.98	0.63
1:A:125:ASP:HA	1:A:128:ARG:HD3	1.82	0.61
1:A:297:LYS:HE3	1:A:307:GLU:HG2	1.81	0.61
1:B:297:LYS:HG2	1:B:307:GLU:HG2	1.83	0.60
1:B:269:ARG:NH1	4:B:509:HOH:O	2.34	0.59
1:B:202:SER:OG	1:B:208:GLN:NE2	2.24	0.59
1:B:9:PRO:HG3	1:B:236:TYR:CD2	2.38	0.59
1:A:169:ARG:NH1	4:A:515:HOH:O	2.35	0.58
1:B:94:GLU:OE2	1:B:194[B]:ARG:NH1	2.36	0.58
1:B:309:VAL:HB	1:B:312:GLU:HG3	1.85	0.58
1:B:148:PRO:HA	1:B:151:LYS:HE3	1.86	0.57
1:A:194[A]:ARG:NH1	4:A:519:HOH:O	2.38	0.57
1:B:210:GLY:N	1:B:275:VAL:O	2.40	0.55
1:A:167:LEU:HD11	1:A:256:MET:HE1	1.88	0.54
1:A:67:ARG:NH1	4:A:523:HOH:O	2.40	0.52
1:B:299:LYS:NZ	4:B:510:HOH:O	2.40	0.52
1:A:35:LYS:NZ	4:A:517:HOH:O	2.38	0.52
1:A:213:ASP:OD1	1:A:272:ARG:NE	2.43	0.51
1:B:317:ARG:NH1	1:B:320:GLU:OE1	2.38	0.50
1:B:227:GLU:H	1:B:227:GLU:CD	2.21	0.49
1:B:100:LEU:HD23	1:B:106:LEU:HD11	1.94	0.48
1:A:315:ARG:HB3	1:A:319:PHE:HE2	1.80	0.47
1:A:86:MET:HE1	1:A:121:ALA:O	2.15	0.47
1:B:86:MET:HE1	1:B:121:ALA:HB1	1.96	0.46
1:B:230:VAL:HG22	1:B:246:PRO:HB3	1.98	0.46
1:B:151:LYS:HD2	1:B:152:TYR:N	2.29	0.46
1:B:108:ASP:OD2	1:B:208:GLN:NE2	2.48	0.46
1:A:210:GLY:N	1:A:275:VAL:O	2.49	0.45
1:B:260:MET:HE2	1:B:260:MET:HB2	1.93	0.45
1:A:238:PRO:C	1:A:240:GLU:H	2.25	0.44
1:B:152:TYR:CZ	1:B:156:MET:HE3	2.52	0.44
1:B:316:GLN:O	1:B:320:GLU:HG3	2.18	0.44
1:B:148:PRO:CA	1:B:151:LYS:HE3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:VAL:HG22	1:B:254:ILE:HD12	1.99	0.43
1:A:207:LYS:NZ	4:A:537:HOH:O	2.51	0.43
1:B:231:GLY:O	1:B:276:VAL:N	2.46	0.43
1:B:223:LEU:HB3	1:B:253:VAL:HB	2.01	0.43
1:A:14[A]:ILE:HG12	1:A:48:TYR:HB2	2.01	0.43
1:B:148:PRO:HA	1:B:151:LYS:HG3	2.00	0.43
1:B:112:ALA:HB2	1:B:196:LEU:HD23	2.01	0.42
1:B:318:LEU:HD23	1:B:322:ILE:HD13	2.01	0.42
1:A:213:ASP:OD1	1:A:213:ASP:C	2.62	0.42
1:B:202:SER:HG	1:B:208:GLN:HE22	1.56	0.42
1:A:207:LYS:HE3	1:A:209:PHE:CZ	2.54	0.42
1:B:151:LYS:HD2	1:B:151:LYS:C	2.46	0.41
1:A:211:VAL:HG12	1:A:275:VAL:HB	2.02	0.41
1:B:211:VAL:HG12	1:B:275:VAL:HB	2.01	0.41
1:B:151:LYS:HE2	4:B:799:HOH:O	2.20	0.41
1:B:297:LYS:CG	1:B:307:GLU:HG2	2.50	0.40
1:A:281:LYS:NZ	4:A:543:HOH:O	2.54	0.40
1:A:114:ILE:HA	1:A:193:MET:O	2.22	0.40
1:A:236:TYR:CZ	1:A:238:PRO:HG2	2.56	0.40
1:B:86:MET:HE3	1:B:86:MET:HB2	1.91	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	315/374 (84%)	305 (97%)	10 (3%)	0	100	100
1	B	313/374 (84%)	306 (98%)	7 (2%)	0	100	100
All	All	628/748 (84%)	611 (97%)	17 (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	274/315 (87%)	274 (100%)	0	100	100
1	B	272/315 (86%)	272 (100%)	0	100	100
All	All	546/630 (87%)	546 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	201	GLN
1	A	219	ASN
1	B	28	GLN
1	B	39	HIS
1	B	61	GLN
1	B	101	HIS
1	B	219	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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	A1EIU	B	110	2,1	18,21,22	3.32	8 (44%)	14,27,29	1.15	1 (7%)
1	A1EIU	A	110	2,1	18,21,22	3.30	8 (44%)	14,27,29	2.65	1 (7%)

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
1	A1EIU	B	110	2,1	-	0/8/11/13	0/1/1/1
1	A1EIU	A	110	2,1	-	0/8/11/13	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	110	A1EIU	C11-NZ	10.25	1.43	1.27
1	A	110	A1EIU	C11-NZ	10.16	1.43	1.27
1	B	110	A1EIU	C05-C04	5.19	1.53	1.36
1	A	110	A1EIU	C05-C04	5.19	1.53	1.36
1	A	110	A1EIU	C11-C03	4.13	1.53	1.45
1	B	110	A1EIU	C11-C03	4.10	1.53	1.45
1	B	110	A1EIU	C01-C07	3.85	1.53	1.37
1	A	110	A1EIU	C01-C07	3.85	1.53	1.37
1	B	110	A1EIU	C05-C06	2.84	1.52	1.44
1	A	110	A1EIU	C05-C06	2.82	1.52	1.44
1	A	110	A1EIU	O08-C07	2.55	1.40	1.33
1	B	110	A1EIU	O13-C02	2.55	1.40	1.33
1	B	110	A1EIU	O08-C07	2.54	1.40	1.33
1	A	110	A1EIU	O13-C02	2.52	1.40	1.33
1	B	110	A1EIU	O09-C06	-2.15	1.18	1.24
1	A	110	A1EIU	O09-C06	-2.14	1.18	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	A1EIU	CE-NZ-C11	-9.46	103.78	117.47
1	B	110	A1EIU	CE-NZ-C11	3.31	122.25	117.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	314/374 (83%)	0.29	18 (5%) 29 28	9, 19, 42, 91	3 (0%)
1	B	314/374 (83%)	0.44	22 (7%) 22 21	10, 21, 42, 92	1 (0%)
All	All	628/748 (83%)	0.37	40 (6%) 25 24	9, 20, 42, 92	4 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	319	PHE	9.0
1	A	319	PHE	8.1
1	B	322	ILE	7.3
1	B	211	VAL	5.9
1	B	209	PHE	5.7
1	A	322	ILE	4.9
1	B	208	GLN	4.8
1	A	210	GLY	4.3
1	B	321	THR	4.2
1	B	210	GLY	4.1
1	A	209	PHE	4.0
1	A	211	VAL	4.0
1	B	8	PRO	4.0
1	A	208	GLN	3.8
1	B	315	ARG	3.7
1	B	276	VAL	3.6
1	A	321	THR	3.4
1	A	276	VAL	3.4
1	A	238	PRO	3.1
1	B	100	LEU	3.1
1	B	303	GLY	3.1
1	B	204	GLU	3.0
1	A	23	ASP	3.0
1	B	205	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	318	LEU	2.9
1	A	205	ASN	2.8
1	A	239	THR	2.8
1	B	25	ALA	2.6
1	A	206	LYS	2.5
1	A	21	ILE	2.5
1	B	98	LEU	2.4
1	B	207	LYS	2.4
1	A	207	LYS	2.3
1	B	178	PRO	2.2
1	A	25	ALA	2.2
1	B	277	ASN	2.1
1	B	9	PRO	2.1
1	B	316	GLN	2.1
1	A	204	GLU	2.0
1	B	320	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	A1EIU	B	110	21/22	0.92	0.10	12,17,25,27	0
1	A1EIU	A	110	21/22	0.93	0.09	12,19,23,28	0

6.3 Carbohydrates [i](#)

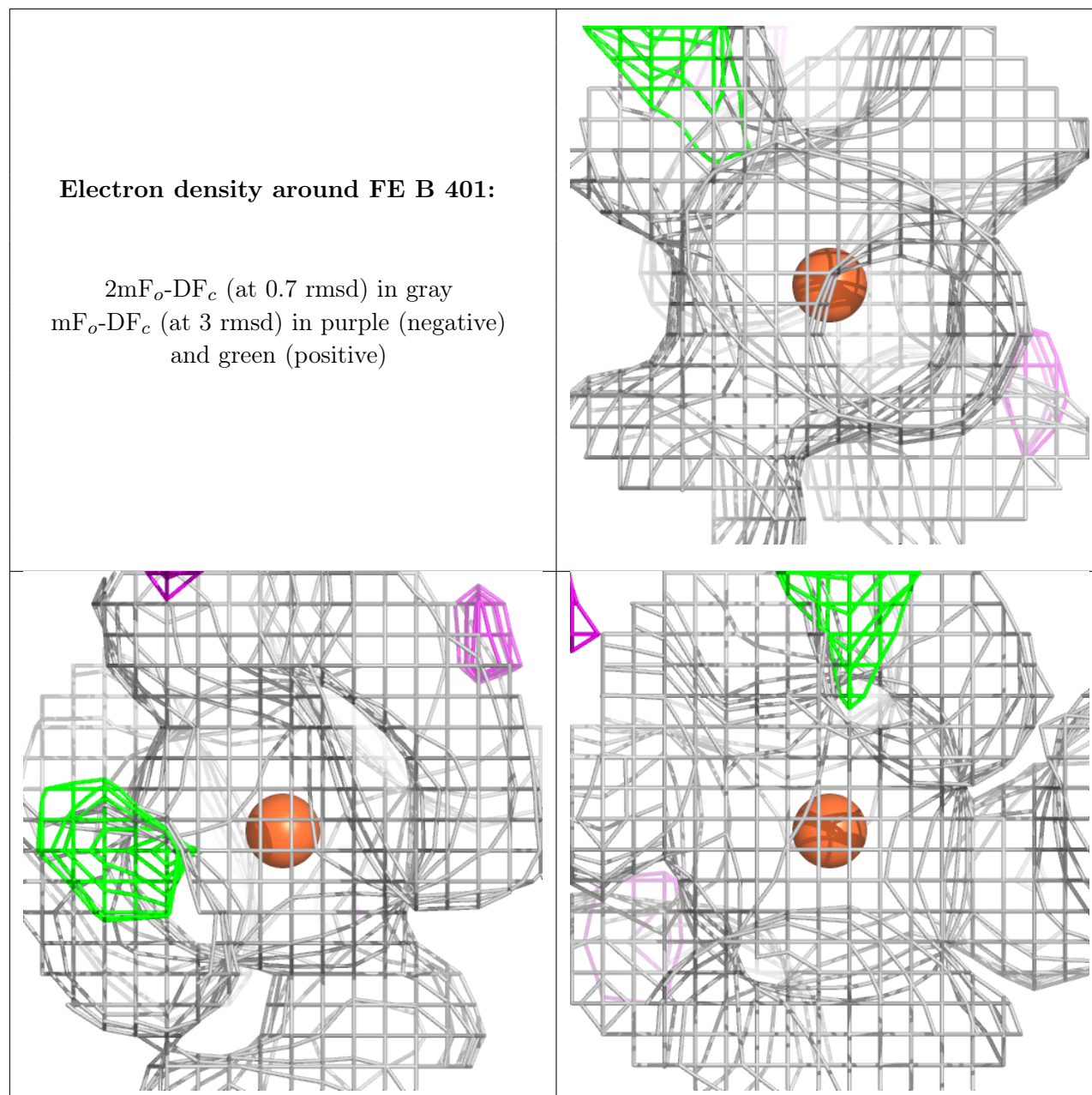
There are no oligosaccharides in this entry.

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.

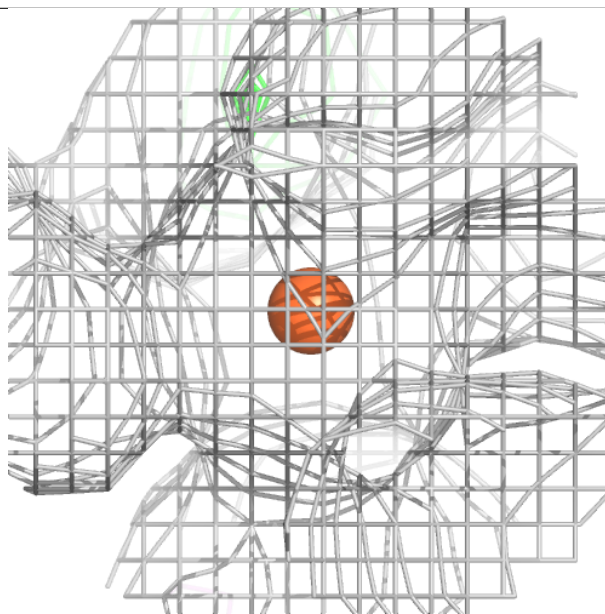
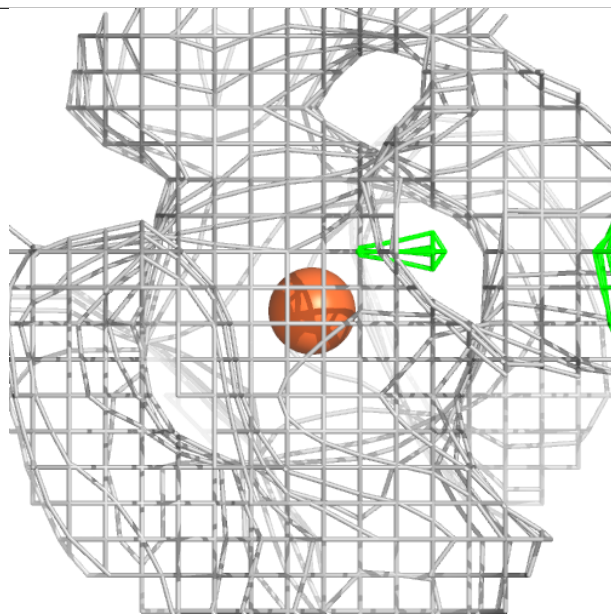
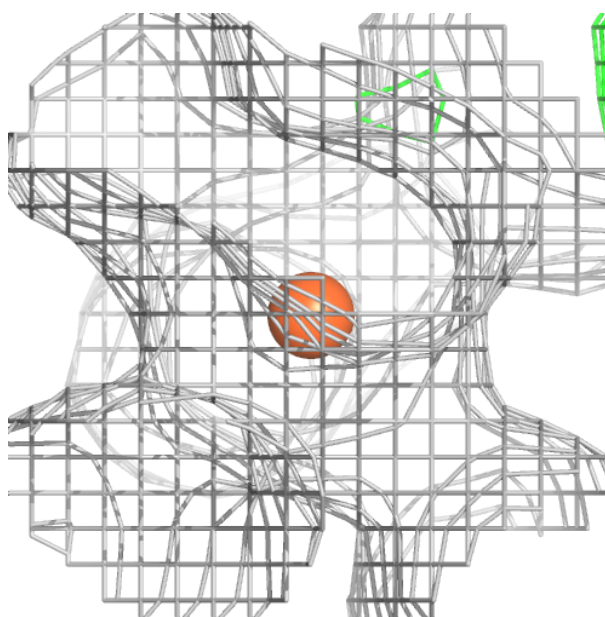
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	A	402	1/1	0.88	0.13	54,54,54,54	0
2	FE	B	401	1/1	1.00	0.02	11,11,11,11	0
2	FE	A	401	1/1	1.00	0.01	12,12,12,12	0

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 401:

$2mF_o-DF_c$ (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.