



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2025 – 10:18 PM JST

PDB ID : 9J1I
Title : Apo structure of the F2Y224-FtmOx1 mutant with metal Iron
Authors : Wang, X.Y.; Wang, J.; Yan, W.P.
Deposited on : 2024-08-05
Resolution : 2.11 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

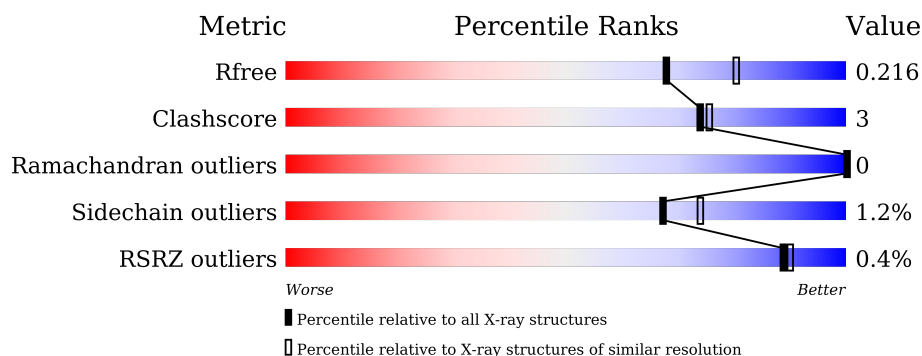
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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}	164625	7689 (2.14-2.10)
Clashscore	180529	8431 (2.14-2.10)
Ramachandran outliers	177936	8366 (2.14-2.10)
Sidechain outliers	177891	8367 (2.14-2.10)
RSRZ outliers	164620	7689 (2.14-2.10)

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	312	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 82%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 82%; width: 9%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 91%; width: 9%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> 82% 9% 9% </div> </div>
1	B	312	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 85%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 85%; width: 7%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 92%; width: 9%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> 85% 7% 9% </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4726 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 Verruculogen synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	F	N	O	S	0	0	0
			2249	1427	2	394	413	13			
1	B	285	Total	C	F	N	O	S	0	0	0
			2252	1429	2	394	414	13			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	LEU	-	expression tag	UNP Q4WAW9
A	293	GLU	-	expression tag	UNP Q4WAW9
A	294	VAL	-	expression tag	UNP Q4WAW9
A	295	ASP	-	expression tag	UNP Q4WAW9
A	296	LEU	-	expression tag	UNP Q4WAW9
A	297	GLN	-	expression tag	UNP Q4WAW9
A	298	GLY	-	expression tag	UNP Q4WAW9
A	299	ASP	-	expression tag	UNP Q4WAW9
A	300	HIS	-	expression tag	UNP Q4WAW9
A	301	GLY	-	expression tag	UNP Q4WAW9
A	302	LEU	-	expression tag	UNP Q4WAW9
A	303	SER	-	expression tag	UNP Q4WAW9
A	304	ALA	-	expression tag	UNP Q4WAW9
A	305	TRP	-	expression tag	UNP Q4WAW9
A	306	SER	-	expression tag	UNP Q4WAW9
A	307	HIS	-	expression tag	UNP Q4WAW9
A	308	PRO	-	expression tag	UNP Q4WAW9
A	309	GLN	-	expression tag	UNP Q4WAW9
A	310	PHE	-	expression tag	UNP Q4WAW9
A	311	GLU	-	expression tag	UNP Q4WAW9
A	312	LYS	-	expression tag	UNP Q4WAW9
B	292	LEU	-	expression tag	UNP Q4WAW9
B	293	GLU	-	expression tag	UNP Q4WAW9
B	294	VAL	-	expression tag	UNP Q4WAW9
B	295	ASP	-	expression tag	UNP Q4WAW9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	296	LEU	-	expression tag	UNP Q4WAW9
B	297	GLN	-	expression tag	UNP Q4WAW9
B	298	GLY	-	expression tag	UNP Q4WAW9
B	299	ASP	-	expression tag	UNP Q4WAW9
B	300	HIS	-	expression tag	UNP Q4WAW9
B	301	GLY	-	expression tag	UNP Q4WAW9
B	302	LEU	-	expression tag	UNP Q4WAW9
B	303	SER	-	expression tag	UNP Q4WAW9
B	304	ALA	-	expression tag	UNP Q4WAW9
B	305	TRP	-	expression tag	UNP Q4WAW9
B	306	SER	-	expression tag	UNP Q4WAW9
B	307	HIS	-	expression tag	UNP Q4WAW9
B	308	PRO	-	expression tag	UNP Q4WAW9
B	309	GLN	-	expression tag	UNP Q4WAW9
B	310	PHE	-	expression tag	UNP Q4WAW9
B	311	GLU	-	expression tag	UNP Q4WAW9
B	312	LYS	-	expression tag	UNP Q4WAW9

- 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	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

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

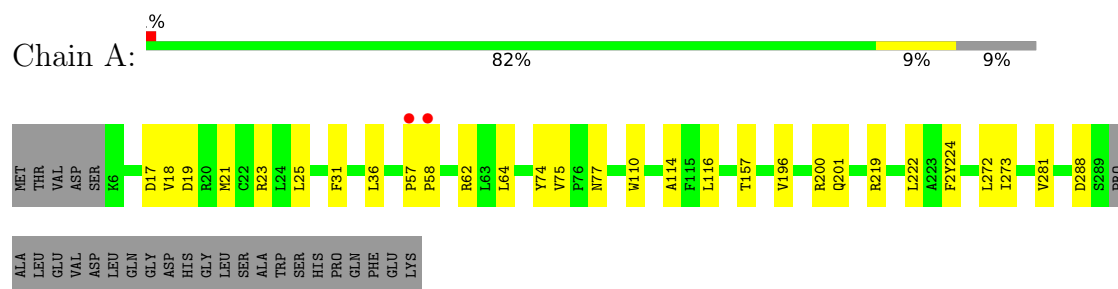
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	103	Total O 103 103	0	0
4	B	119	Total O 119 119	0	0

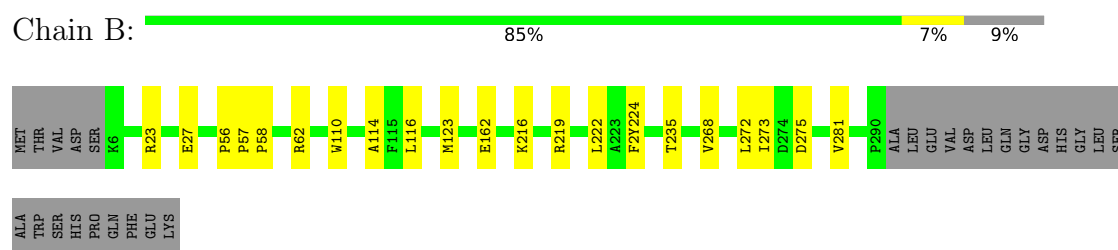
3 Residue-property plots [i](#)

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: Verruculogen synthase



• Molecule 1: Verruculogen synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.44Å 45.61Å 105.15Å 90.00° 100.02° 90.00°	Depositor
Resolution (Å)	36.08 – 2.11 36.08 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.2 (36.08-2.11) 99.2 (36.08-2.11)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.172 , 0.216 0.172 , 0.216	Depositor DCC
R_{free} test set	1876 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4726	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO, F2Y, 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	0.40	0/2288	0.65	0/3114
1	B	0.43	0/2292	0.66	0/3122
All	All	0.41	0/4580	0.65	0/6236

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	2249	0	2236	18	0
1	B	2252	0	2232	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
4	A	103	0	0	0	0
4	B	119	0	0	0	0
All	All	4726	0	4468	27	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 (27) 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:116:LEU:HD11	1:A:219:ARG:HG3	1.76	0.68
1:B:116:LEU:HD21	1:B:219:ARG:HG3	1.81	0.61
1:A:19:ASP:O	1:A:23:ARG:HG2	2.05	0.56
1:A:75:VAL:HB	1:A:116:LEU:HB3	1.87	0.55
1:A:17:ASP:OD2	1:A:19:ASP:HB2	2.07	0.55
1:A:64:LEU:HD23	1:A:74:TYR:CZ	2.43	0.54
1:A:273:ILE:HD13	1:B:235:THR:O	2.10	0.52
1:A:18:VAL:HG23	1:A:21:MET:HE3	1.93	0.51
1:A:64:LEU:HD13	1:B:268:VAL:HG21	1.91	0.51
1:B:116:LEU:HD21	1:B:219:ARG:CG	2.41	0.49
1:B:273:ILE:HG23	1:B:281:VAL:HG21	1.96	0.48
1:B:23:ARG:O	1:B:27:GLU:HG3	2.15	0.47
1:A:36:LEU:HD23	1:A:196:VAL:HG21	1.97	0.47
1:B:58:PRO:HD2	1:B:62:ARG:HD2	1.97	0.46
1:B:216:LYS:HE2	1:B:216:LYS:HB3	1.84	0.45
1:A:62:ARG:HD3	1:B:275:ASP:HB3	2.00	0.44
1:A:21:MET:HB3	1:A:31:PHE:CZ	2.53	0.43
1:A:57:PRO:HA	1:A:58:PRO:HD3	1.82	0.43
1:A:273:ILE:HG23	1:A:281:VAL:HG21	2.00	0.42
1:A:114:ALA:HA	1:A:222:LEU:O	2.19	0.42
1:A:25:LEU:HD23	1:A:25:LEU:HA	1.86	0.42
1:A:200:ARG:HG2	1:A:201:GLN:N	2.35	0.42
1:A:288:ASP:OD1	1:A:288:ASP:N	2.52	0.41
1:B:162:GLU:H	1:B:162:GLU:CD	2.22	0.41
1:B:56:PRO:HA	1:B:57:PRO:HD3	1.93	0.41
1:A:157:THR:HG23	1:A:219:ARG:HB3	2.02	0.41
1:B:114:ALA:HA	1:B:222:LEU:O	2.21	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	281/312 (90%)	276 (98%)	5 (2%)	0	100	100
1	B	282/312 (90%)	278 (99%)	4 (1%)	0	100	100
All	All	563/624 (90%)	554 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	245/269 (91%)	242 (99%)	3 (1%)	67	74
1	B	245/269 (91%)	242 (99%)	3 (1%)	67	74
All	All	490/538 (91%)	484 (99%)	6 (1%)	67	74

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	110	TRP
1	A	272	LEU
1	B	110	TRP
1	B	123	MET
1	B	272	LEU

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	F2Y	A	224	1	13,14,15	1.40	3 (23%)	16,19,21	1.88	5 (31%)
1	F2Y	B	224	1	13,14,15	1.17	0	16,19,21	2.15	4 (25%)

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	F2Y	A	224	1	-	2/5/6/8	0/1/1/1
1	F2Y	B	224	1	-	2/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	F2Y	CD2-CE2	2.46	1.41	1.37
1	A	224	F2Y	CD1-CE1	2.24	1.41	1.37
1	A	224	F2Y	CZ-CE1	2.14	1.41	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	F2Y	CD1-CE1-CZ	-5.08	119.81	123.79
1	A	224	F2Y	CD2-CE2-CZ	-3.96	120.69	123.79
1	A	224	F2Y	CD1-CE1-CZ	-3.88	120.75	123.79
1	B	224	F2Y	CD2-CE2-CZ	-3.59	120.98	123.79
1	B	224	F2Y	F2-CE2-CZ	3.58	119.78	117.13
1	B	224	F2Y	CG-CD1-CE1	3.02	121.33	119.37
1	A	224	F2Y	CG-CD2-CE2	2.52	121.00	119.37
1	A	224	F2Y	F2-CE2-CZ	2.46	118.96	117.13
1	A	224	F2Y	CG-CD1-CE1	2.25	120.83	119.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	224	F2Y	CA-CB-CG-CD2
1	A	224	F2Y	CA-CB-CG-CD1
1	B	224	F2Y	CA-CB-CG-CD2
1	B	224	F2Y	CA-CB-CG-CD1

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 [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	283/312 (90%)	-0.17	2 (0%) 84 85	23, 41, 74, 100	0
1	B	284/312 (91%)	-0.31	0 100 100	24, 36, 56, 82	0
All	All	567/624 (90%)	-0.24	2 (0%) 89 90	23, 39, 67, 100	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	PRO	2.7
1	A	58	PRO	2.1

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	F2Y	B	224	14/15	0.92	0.08	26,35,42,43	2
1	F2Y	A	224	14/15	0.96	0.06	28,38,43,45	2

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,

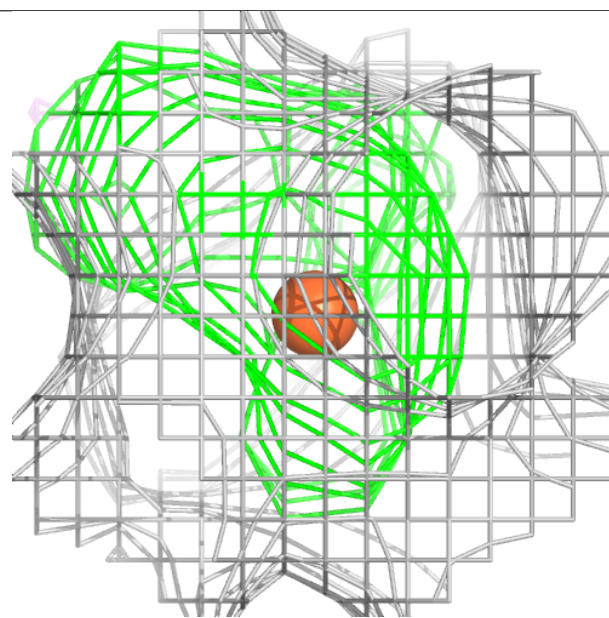
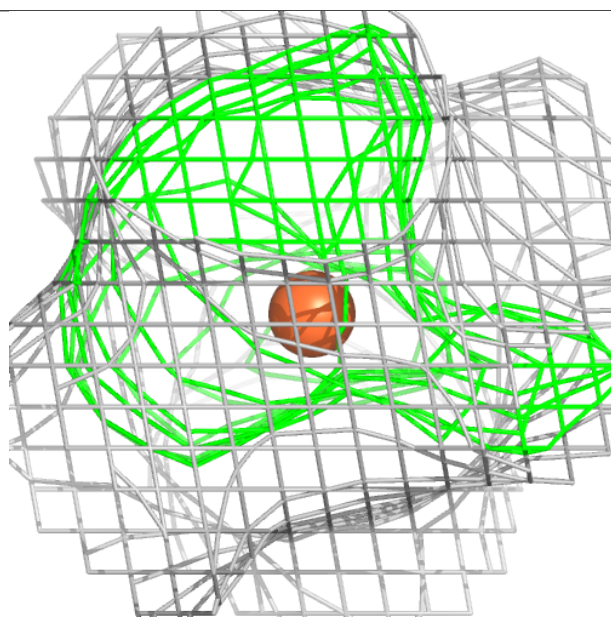
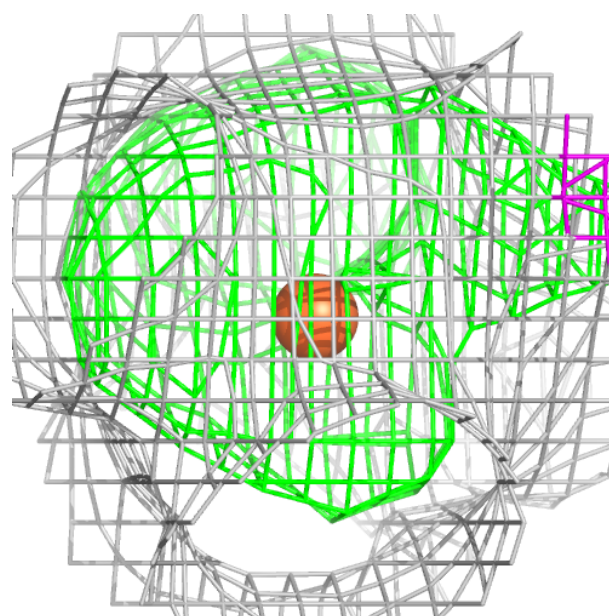
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FE2	A	401	1/1	0.99	0.11	44,44,44,44	0
3	CO	A	402	1/1	0.99	0.02	39,39,39,39	0
2	FE2	B	501	1/1	1.00	0.07	37,37,37,37	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.

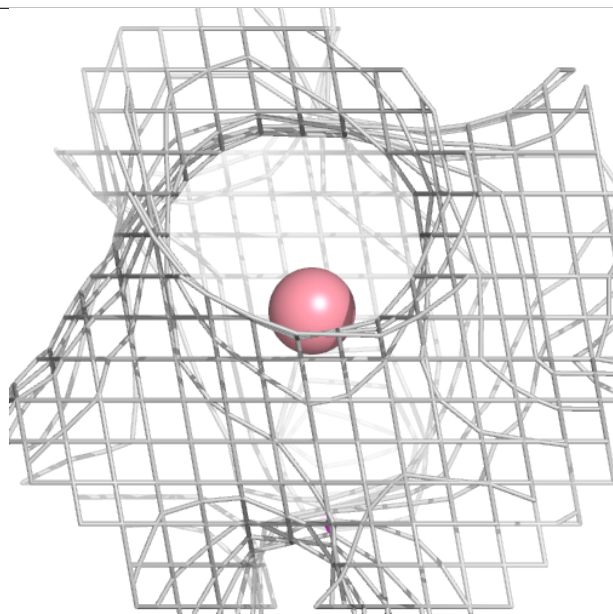
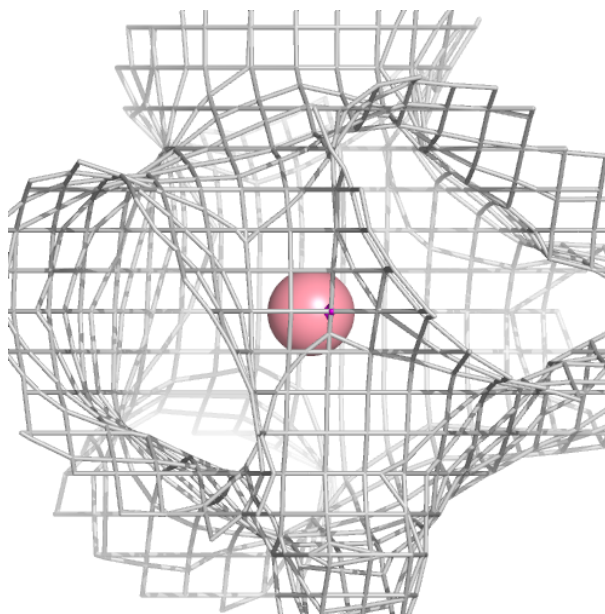
Electron density around FE2 A 401:

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



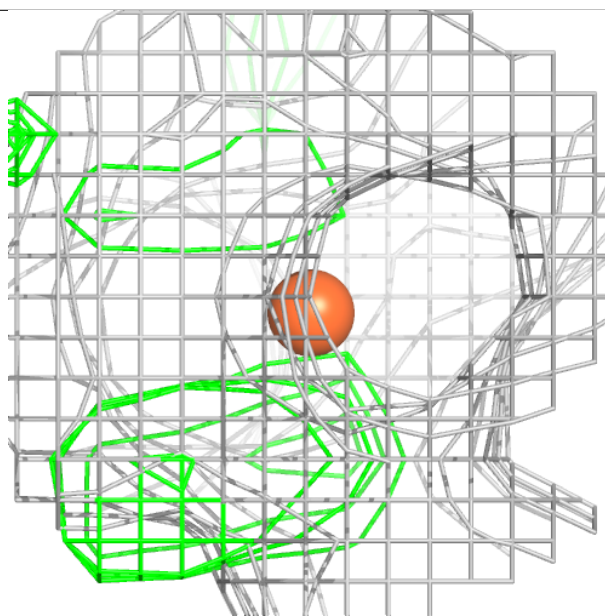
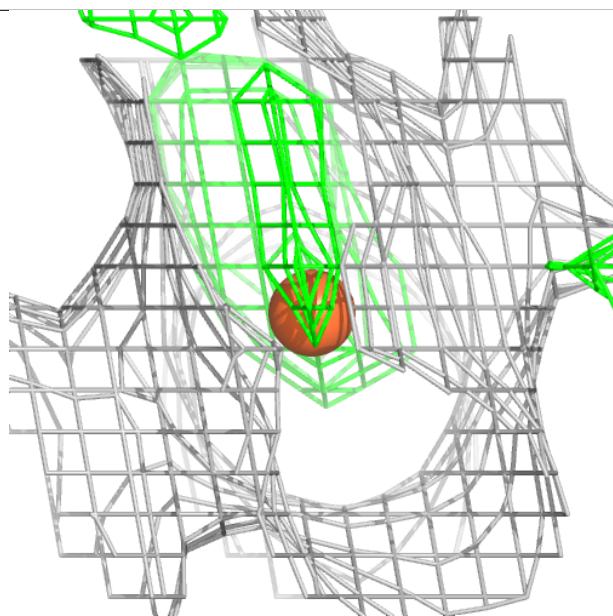
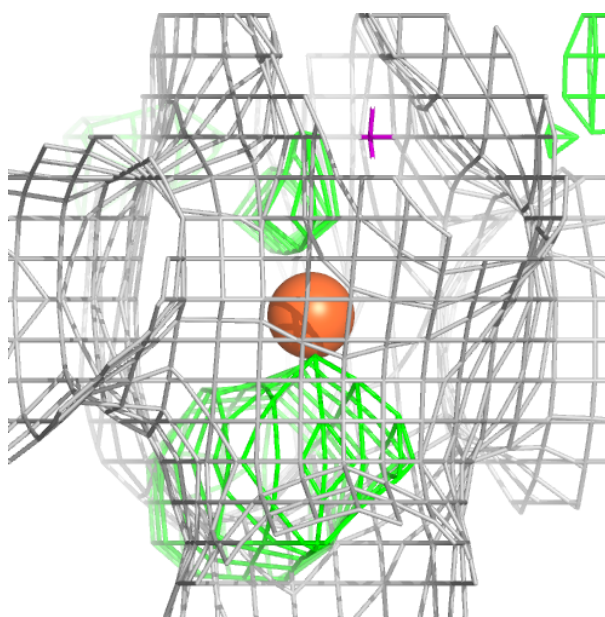
Electron density around CO A 402:

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



Electron density around FE2 B 501:

$2mF_o-DF_c$ (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.