

Full wwPDB X-ray Structure Validation Report (i)

Nov 28, 2023 – 02:09 pm GMT

:	80N1
:	NI,FE-CODH -600mV state : 4 h Dioxygen Exposure
:	Basak, Y.; Jeoung, JH.; Dobbek, H.
	2023-03-31
:	1.37 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 (i) 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 (1)) were used in the production of this report:

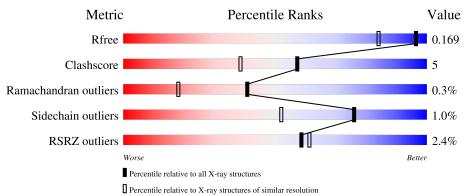
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 1.37 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2907 (1.40-1.36)
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)
RSRZ outliers	127900	2846 (1.40-1.36)

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	Х	636	^{2%} 93%	6%				



80N1

2 Entry composition (i)

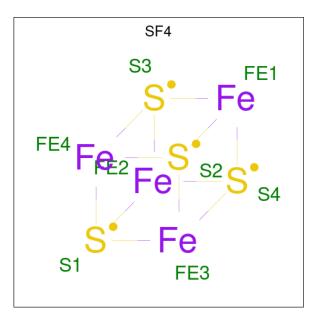
There are 6 unique types of molecules in this entry. The entry contains 10367 atoms, of which 4961 are hydrogens and 0 are deuteriums.

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 Carbon monoxide dehydrogenase 2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	X	633	Total 9755	C 3013	Н 4961	N 844	O 895	S 42	0	28	0

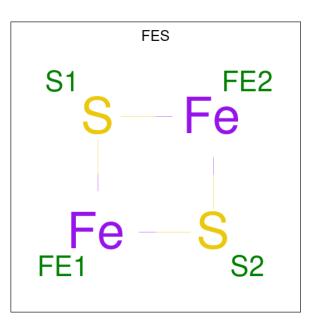
• Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Ate	\mathbf{oms}		ZeroOcc	AltConf
2	Х	1	Total 8	Fe 4	${ m S}$ 4	0	0

• Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).





Mol	Chain	Residues	Ate	\mathbf{oms}		ZeroOcc	AltConf
3	Х	1	Total 4	Fe 2	${ m S} { m 2}$	0	0

• Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Х	6	Total Fe 6 6	0	0

• Molecule 5 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Х	1	Total Fe 2 2	0	1

• Molecule 6 is water.

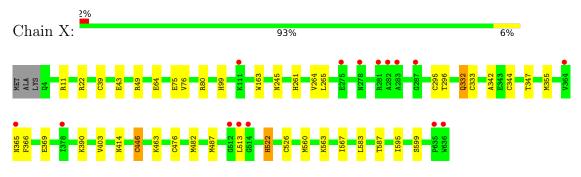
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Х	592	Total O 592 592	0	0



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: Carbon monoxide dehydrogenase 2





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	112.41Å 75.36Å 71.35Å	Depositor
a, b, c, α , β , γ	90.00° 111.44° 90.00°	Depositor
Resolution (Å)	35.30 - 1.37	Depositor
Resolution (A)	40.85 - 1.37	EDS
% Data completeness	97.9 (35.30-1.37)	Depositor
(in resolution range)	97.9(40.85 - 1.37)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.40 (at 1.37 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
B B.	0.126 , 0.168	Depositor
R, R_{free}	0.126 , 0.169	DCC
R_{free} test set	2000 reflections $(1.75%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	15.5	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35 , 47.5	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	0.98	EDS
Total number of atoms	10367	wwPDB-VP
Average B, all atoms $(Å^2)$	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.20% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: FES, FE2, SF4, FE, CSO

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	Boi	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Х	0.71	1/4935~(0.0%)	0.87	0/6699	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Х	22	ARG	CB-CG	-5.24	1.38	1.52

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	Х	4794	4961	4959	48	0
2	Х	8	0	0	0	0
3	Х	4	0	0	0	0
4	Х	6	0	0	0	0
5	Х	2	0	0	0	0
6	Х	592	0	0	27	2
All	All	5406	4961	4959	48	2

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 5.



	• · · · ·	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:261[B]:HIS:CE1	6:X:1102:HOH:O	2.05	1.08
1:X:75[A]:GLU:OE2	6:X:1101:HOH:O	1.84	0.95
1:X:463:LYS:HE2	6:X:1589:HOH:O	1.82	0.79
1:X:261[B]:HIS:NE2	6:X:1103:HOH:O	2.10	0.73
1:X:265:LEU:HD13	1:X:366:PHE:CD2	2.23	0.72
1:X:587:THR:HG22	6:X:1307:HOH:O	1.89	0.72
1:X:583[A]:LEU:HD21	6:X:1671:HOH:O	1.89	0.70
1:X:99[A]:HIS:CE1	1:X:264:VAL:HG11	2.30	0.66
1:X:513:LEU:HD11	6:X:1677:HOH:O	1.96	0.65
1:X:563:LYS:NZ	6:X:1102:HOH:O	2.33	0.61
1:X:265:LEU:HD13	1:X:366:PHE:HD2	1.66	0.60
1:X:261[B]:HIS:NE2	6:X:1102:HOH:O	2.24	0.60
1:X:261[B]:HIS:CD2	6:X:1492:HOH:O	2.54	0.59
1:X:476:CYS:SG	6:X:1516:HOH:O	2.58	0.58
1:X:39:CYS:O	1:X:43:GLU:HG3	2.04	0.58
1:X:403:VAL:HG11	1:X:482[B]:MET:SD	2.46	0.56
1:X:583[B]:LEU:HD11	1:X:587:THR:CG2	2.37	0.54
1:X:526[B]:CYS:SG	1:X:567:ILE:HD11	2.48	0.52
1:X:482[B]:MET:CG	1:X:487[B]:MET:SD	2.98	0.51
1:X:482[B]:MET:HG3	1:X:487[B]:MET:SD	2.52	0.50
1:X:261[A]:HIS:ND1	1:X:332:GLN:HB2	2.26	0.50
1:X:295[A]:CYS:SG	6:X:1548:HOH:O	2.60	0.50
1:X:583[B]:LEU:HD11	1:X:587:THR:HG21	1.93	0.50
1:X:261[B]:HIS:CE1	6:X:1458:HOH:O	2.65	0.49
1:X:261[B]:HIS:HE1	6:X:1458:HOH:O	1.96	0.49
1:X:296:THR:HG21	6:X:1107:HOH:O	2.12	0.49
1:X:560:MET:HE1	6:X:1650:HOH:O	2.11	0.48
1:X:261[A]:HIS:HE1	1:X:333:CYS:HB2	1.78	0.48
1:X:64[A]:GLU:HG3	6:X:1155:HOH:O	2.13	0.48
1:X:587:THR:HA	6:X:1307:HOH:O	2.14	0.48
1:X:526[B]:CYS:SG	6:X:1507:HOH:O	2.07	0.47
1:X:11[A]:ARG:HD3	6:X:1191:HOH:O	2.14	0.47
1:X:482[B]:MET:HG2	1:X:487[B]:MET:SD	2.55	0.47
1:X:526[B]:CYS:SG	1:X:567:ILE:CD1	3.03	0.47
1:X:369:GLU:OE2	6:X:1105:HOH:O	2.21	0.46
1:X:261[B]:HIS:HD2	6:X:1492:HOH:O	1.95	0.46
1:X:414:ASN:HB2	6:X:1547:HOH:O	2.15	0.46
1:X:265:LEU:HD13	1:X:366:PHE:CE2	2.51	0.46
1:X:513:LEU:HD23	6:X:1454:HOH:O	2.17	0.43
1:X:342:ALA:HB1	1:X:347:THR:O	2.18	0.43

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:344:CYS:SG	6:X:1656:HOH:O	2.62	0.43
1:X:487[B]:MET:SD	1:X:522:HIS:HB2	2.59	0.43
1:X:49:ARG:NH2	6:X:1128:HOH:O	2.53	0.41
1:X:446:CYS:HA	1:X:476:CYS:HB2	2.02	0.41
1:X:76:VAL:O	1:X:80:ARG:HG3	2.21	0.41
1:X:265:LEU:HB3	6:X:1149:HOH:O	2.20	0.41
1:X:365:ASN:OD1	1:X:365:ASN:C	2.60	0.40
1:X:595:ILE:HA	1:X:599[A]:SER:OG	2.21	0.40

Continued from previous page...

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:1451:HOH:O	6:X:1644:HOH:O[4_747]	1.99	0.21
6:X:1346:HOH:O	6:X:1369:HOH:O[4_747]	2.18	0.02

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	Х	657/636~(103%)	635~(97%)	20 (3%)	2(0%)	41 18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Х	245	ASN
1	Х	332	GLN



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Х	522/497~(105%)	517~(99%)	5(1%)	76 52	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Х	163	TRP
1	Х	355	MET
1	Х	390	LYS
1	Х	446	CYS
1	Х	522	HIS

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)

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	Turne	Chain	Res Link		B	ond leng	gths	В	ond ang	gles
	Type	Unam	Res		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
1	CSO	Х	294[A]	4	3,6,7	1.04	0	$0,\!6,\!8$	-	-
1	CSO	Х	294[B]	4	$3,\!5,\!7$	1.01	0	$0,\!5,\!8$	-	-



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	CSO	Х	294[A]	4	-	0/1/5/7	-
1	CSO	Х	294[B]	4	-	1/1/4/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Х	294[B]	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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 Ty	Type	Chain	Dec	Link	B	ond leng	$_{ m gths}$	Bond angles		
	Type		Res		Counts	RMSZ	# Z > 2	Counts	RMSZ # Z > 2	
2	SF4	Х	1001	1	0,12,12	-	-	-		
3	FES	Х	1002	1	0,4,4	-	-	-		

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
2	SF4	Х	1001	1	-	-	0/6/5/5
3	FES	Х	1002	1	-	-	0/1/1/1

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, 95^{th} 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		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9	
1	Х	632/636~(99%)	-0.25	15 (2%)	59	61	12, 20, 42, 67	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Х	514	GLY	4.0
1	Х	513	LEU	3.5
1	Х	512	GLY	3.3
1	Х	111	LYS	3.1
1	Х	364	VAL	2.7
1	Х	635	PRO	2.5
1	Х	365	ASN	2.5
1	Х	278	ASN	2.4
1	Х	636	TRP	2.3
1	Х	275	GLU	2.3
1	Х	283	ALA	2.2
1	Х	282	ALA	2.1
1	Х	281	ARG	2.1
1	Х	378	ILE	2.1
1	Х	287	GLY	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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
1	CSO	Х	294[A]	7/8	0.97	0.09	17,18,22,23	7
1	CSO	Х	294[B]	6/8	0.97	0.09	17,20,28,28	6



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

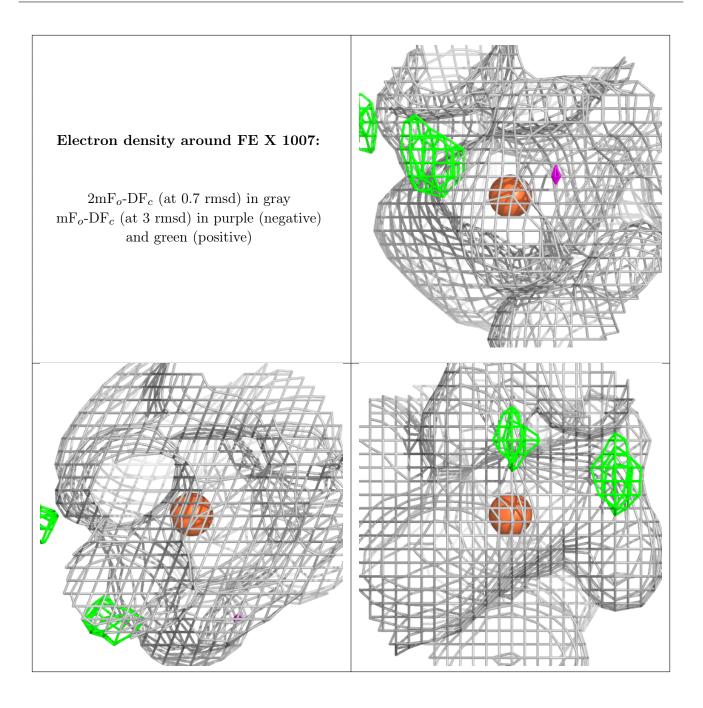
6.4 Ligands (i)

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, 95^{th} 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.

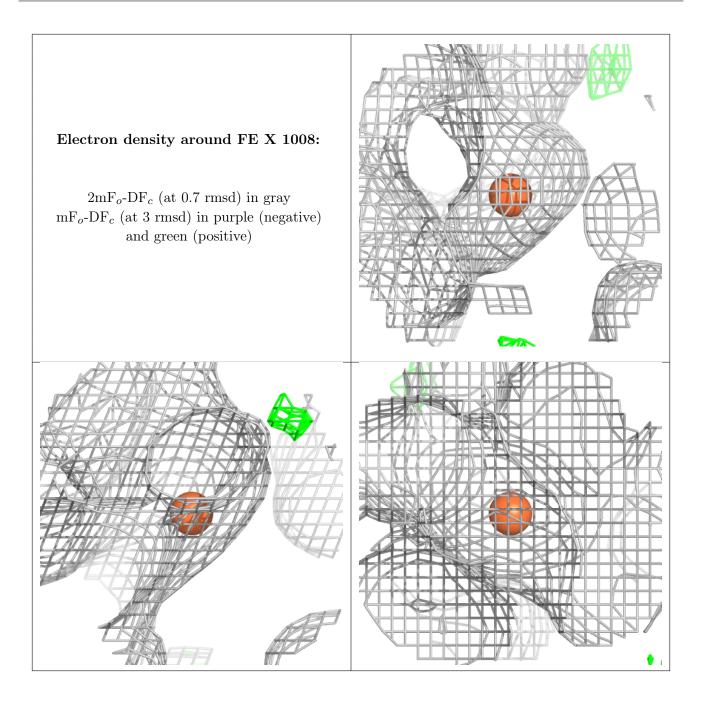
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q < 0.9
4	FE	Х	1007	1/1	0.93	0.10	48,48,48,48	1
4	FE	Х	1008	1/1	0.95	0.16	62,62,62,62	1
4	FE	Х	1003	1/1	0.97	0.16	42,42,42,42	1
4	FE	Х	1006	1/1	0.97	0.10	44,44,44,44	1
4	FE	Х	1005	1/1	0.98	0.08	59,59,59,59	1
4	FE	Х	1004	1/1	0.98	0.13	47,47,47,47	1
3	FES	Х	1002	4/4	0.99	0.04	16,17,17,17	4
5	FE2	Х	1009[A]	1/1	0.99	0.03	33,33,33,33	1
5	FE2	Х	1009[B]	1/1	0.99	0.03	43,43,43,43	1
2	SF4	Х	1001	8/8	1.00	0.07	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.

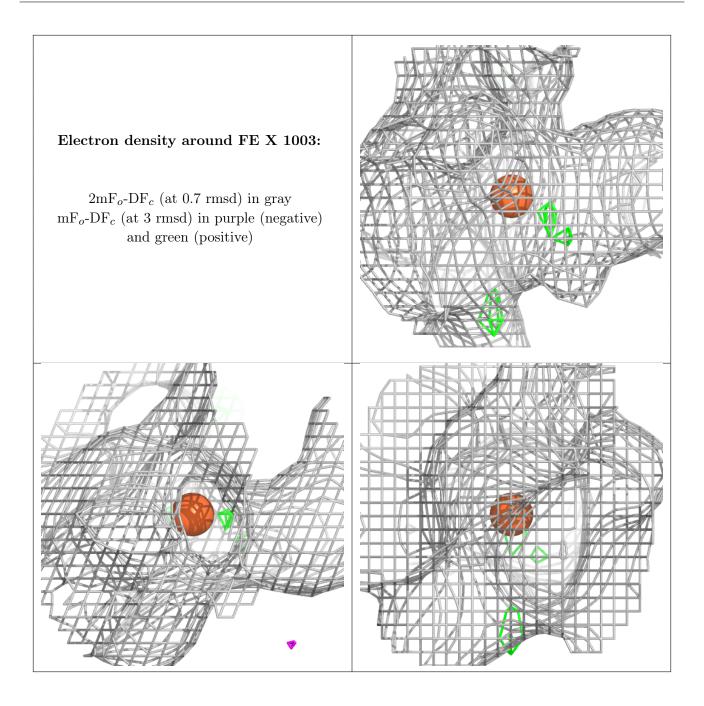




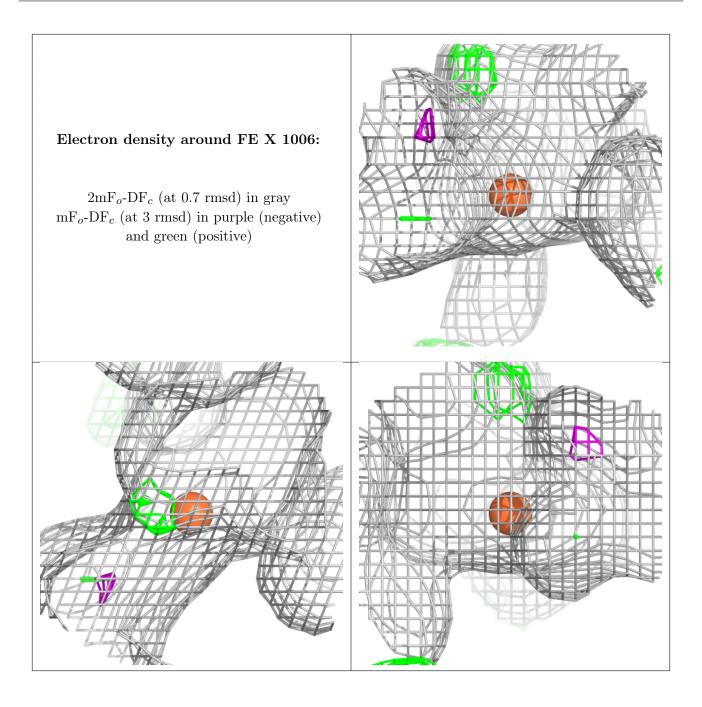




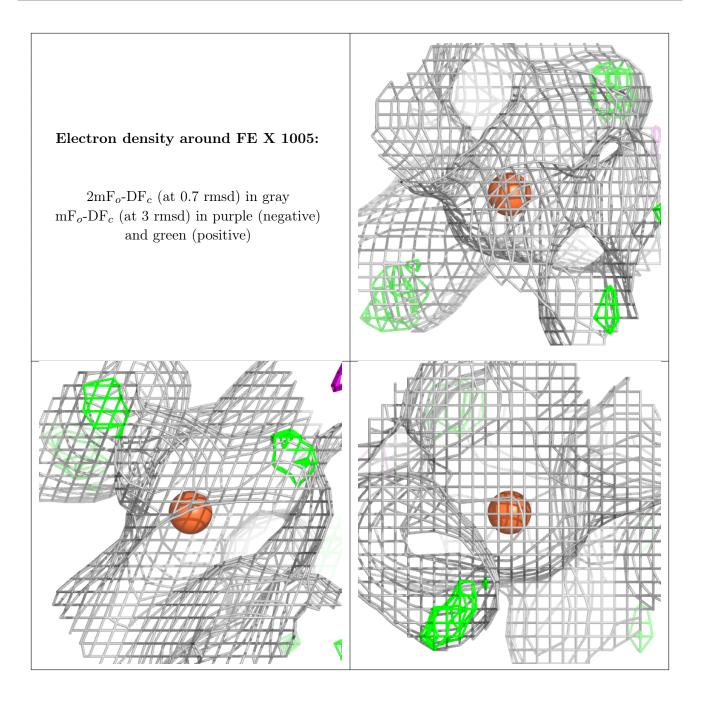




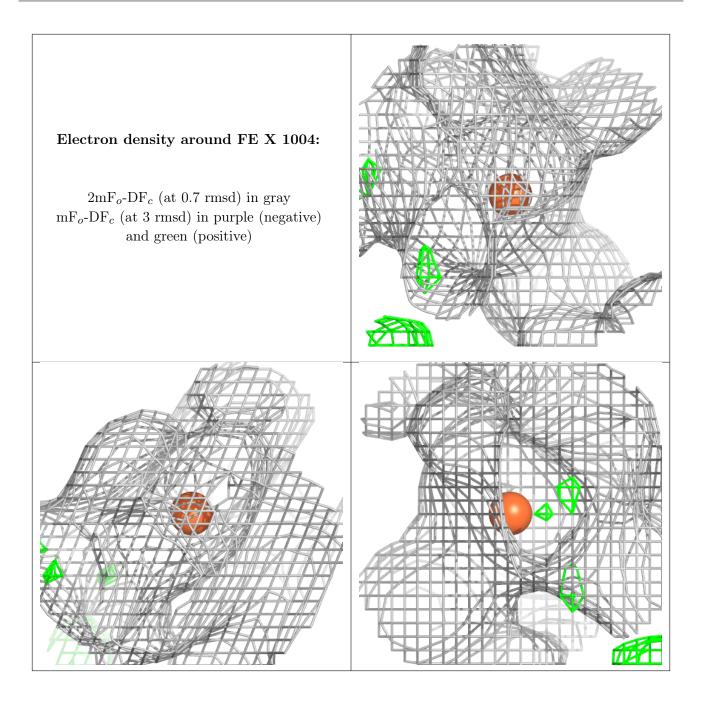




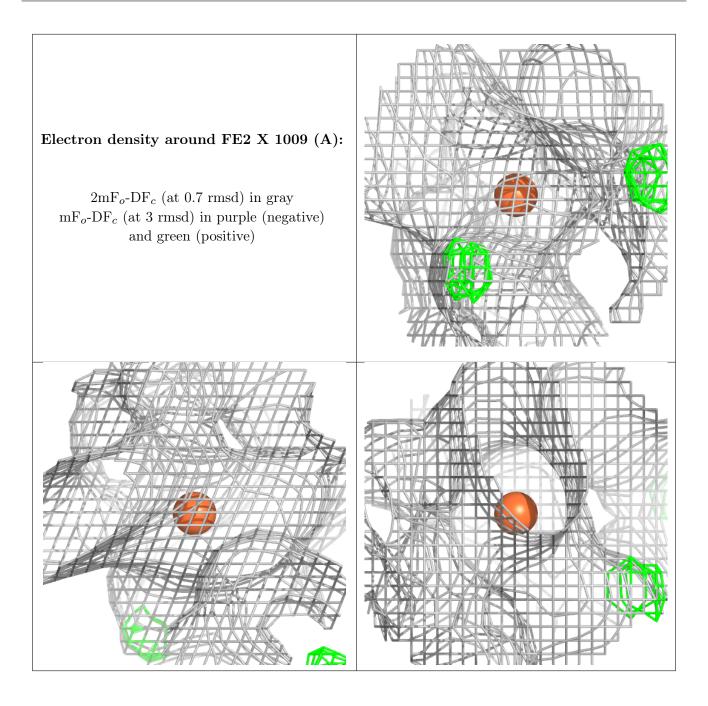




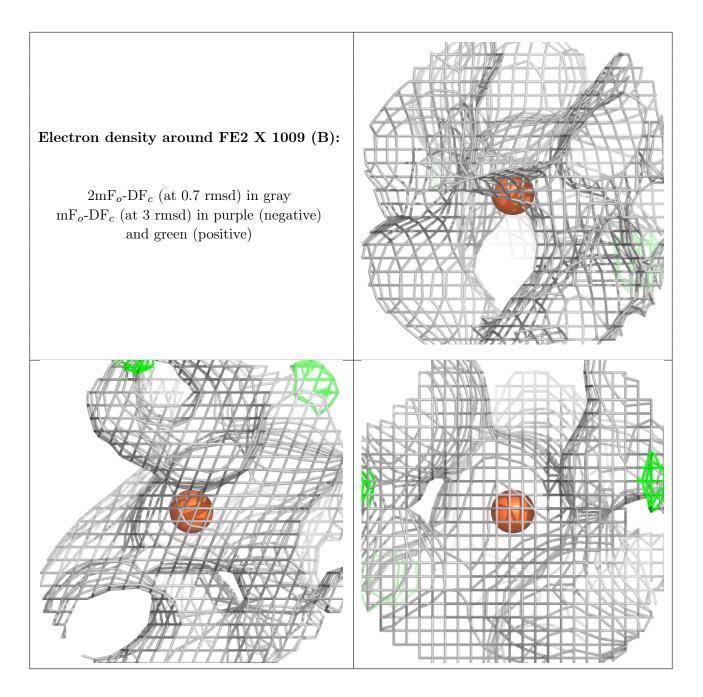












6.5 Other polymers (i)

There are no such residues in this entry.

