



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 05:33 PM GMT

PDB ID : 1UBJ
Title : Three-dimensional Structure of The Carbon Monoxide Complex of [NiFe]hydrogenase From Desulfovibrio vulgaris Miyazaki F
Authors : Ogata, H.; Mizoguchi, Y.; Mizuno, N.; Miki, K.; Adachi, S.; Yasuoka, N.; Yagi, T.; Yamauchi, O.; Hirota, S.; Higuchi, Y.
Deposited on : 2003-04-04
Resolution : 1.35 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

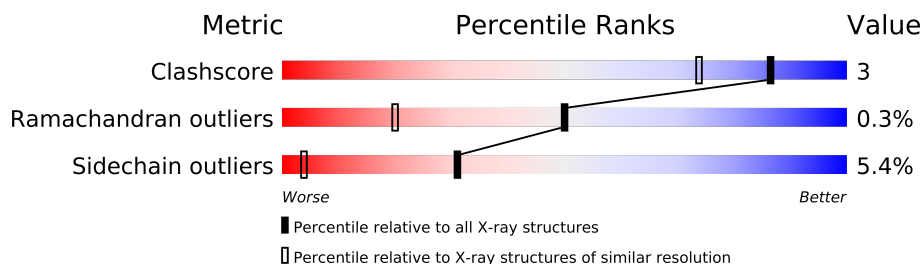
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.35 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))
Clashscore	79885	1707 (1.40-1.32)
Ramachandran outliers	78287	1662 (1.40-1.32)
Sidechain outliers	78261	1661 (1.40-1.32)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	S	267	
2	L	534	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7163 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Periplasmic [NiFe] hydrogenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	267	Total	C	N	O	S	0	0	0
			2019	1282	342	378	17			

- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	534	Total	C	N	O	S	0	0	0
			4177	2674	725	763	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	514	LYS	ASN	SEE REMARK 999	UNP P21852
L	515	LEU	VAL	SEE REMARK 999	UNP P21852

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

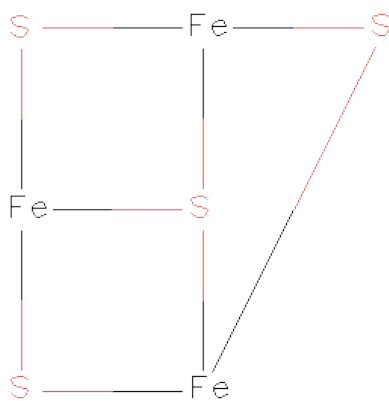
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	Mg	0	0
			1	1		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	Fe	S	0	0
			8	4	4		
4	S	1	Total	Fe	S	0	0
			8	4	4		

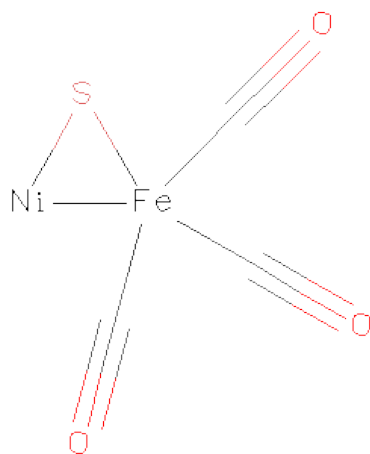
- Molecule 5 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	S	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 6 is (MU-SULPHIDO)-BIS(MU-CYS,S)-[TRICARBONYLIRON-DI-(CYS,S)NIC

KEL(II)](FE-NI) (three-letter code: FNE) (formula: $\text{C}_3\text{FeNiO}_3\text{S}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Fe	Ni	O	0	0
			8	3	1	1	3		

- Molecule 7 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			2	1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	607	Total 607	O 607	0	0
8	S	326	Total 326	O 326	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

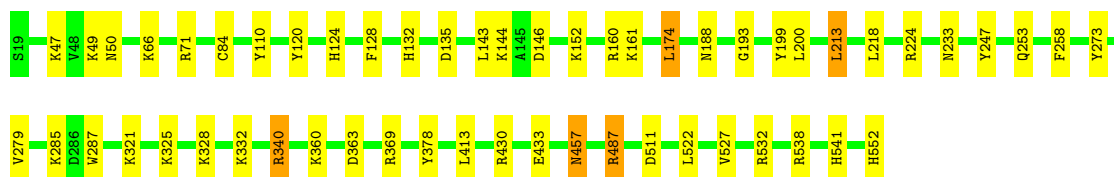
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain S: 



- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain L: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.74Å 125.86Å 66.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.35	Depositor
% Data completeness (in resolution range)	71.5 (20.00-1.35)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.121 , 0.183	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7163	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, MG, F3S, FNE, SF4

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	S	0.62	0/2075	1.26	21/2830 (0.7%)
2	L	0.60	1/4288 (0.0%)	1.34	33/5831 (0.6%)
All	All	0.60	1/6363 (0.0%)	1.32	54/8661 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	552	HIS	C-O	5.44	1.33	1.23

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	532	ARG	CD-NE-CZ	30.12	165.76	123.60
2	L	532	ARG	NE-CZ-NH2	-15.06	112.77	120.30
2	L	273	TYR	CB-CG-CD1	12.45	128.47	121.00
2	L	532	ARG	NE-CZ-NH1	12.13	126.37	120.30
2	L	160	ARG	NE-CZ-NH2	-9.37	115.62	120.30
2	L	71	ARG	NE-CZ-NH2	-9.21	115.69	120.30
2	L	224	ARG	NE-CZ-NH2	8.53	124.56	120.30
2	L	340	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	S	212	ARG	NE-CZ-NH2	7.81	124.20	120.30
2	L	340	ARG	NE-CZ-NH2	-7.62	116.49	120.30
2	L	174	LEU	CA-CB-CG	7.55	132.66	115.30
2	L	128	PHE	CB-CG-CD1	-7.37	115.64	120.80
2	L	199	TYR	CB-CG-CD2	-7.29	116.63	121.00
2	L	273	TYR	CB-CG-CD2	-7.25	116.65	121.00
1	S	256	ASP	CB-CG-OD1	7.23	124.81	118.30
1	S	218	TYR	CB-CG-CD1	7.21	125.32	121.00
1	S	163	TYR	CB-CG-CD2	-7.10	116.74	121.00
1	S	163	TYR	CB-CG-CD1	7.08	125.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	218	LEU	CA-CB-CG	-6.95	99.31	115.30
1	S	212	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	S	1	LEU	O-C-N	6.68	133.39	122.70
2	L	538	ARG	NE-CZ-NH1	6.56	123.58	120.30
2	L	369	ARG	NE-CZ-NH2	-6.54	117.03	120.30
2	L	146	ASP	CB-CG-OD2	-6.30	112.63	118.30
2	L	110	TYR	CB-CG-CD1	6.23	124.74	121.00
1	S	85	ILE	CA-CB-CG2	6.12	123.13	110.90
1	S	218	TYR	CB-CG-CD2	-6.08	117.35	121.00
2	L	538	ARG	NE-CZ-NH2	-6.01	117.29	120.30
2	L	363	ASP	CB-CG-OD2	5.92	123.63	118.30
1	S	33	ASP	CB-CG-OD1	5.88	123.59	118.30
1	S	164	TYR	CB-CG-CD1	-5.88	117.47	121.00
2	L	287	TRP	CA-CB-CG	-5.79	102.69	113.70
1	S	193	ARG	NE-CZ-NH1	5.73	123.16	120.30
2	L	430	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	L	146	ASP	CB-CG-OD1	5.62	123.36	118.30
2	L	120	TYR	CA-CB-CG	5.60	124.04	113.40
1	S	5	ARG	CA-C-N	5.60	129.52	117.20
1	S	233	LYS	CD-CE-NZ	5.60	124.57	111.70
2	L	247	TYR	CB-CG-CD1	5.58	124.35	121.00
2	L	160	ARG	NH1-CZ-NH2	5.57	125.52	119.40
2	L	273	TYR	CG-CD1-CE1	5.53	125.73	121.30
1	S	215	TRP	CH2-CZ2-CE2	-5.45	111.95	117.40
1	S	83	ASN	CA-CB-CG	-5.41	101.50	113.40
1	S	26	ARG	CG-CD-NE	-5.41	100.44	111.80
1	S	189	GLU	OE1-CD-OE2	-5.35	116.88	123.30
1	S	5	ARG	CA-C-O	-5.33	108.91	120.10
2	L	487	ARG	NE-CZ-NH1	5.29	122.95	120.30
2	L	213	LEU	CA-CB-CG	5.24	127.35	115.30
2	L	247	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	S	100	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	S	57	GLU	CA-CB-CG	5.09	124.60	113.40
2	L	378	TYR	CB-CG-CD2	-5.06	117.97	121.00
2	L	511	ASP	CB-CG-OD2	5.04	122.83	118.30
2	L	258	PHE	CB-CG-CD1	5.03	124.32	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	2019	0	0	3	0
2	L	4177	0	0	13	0
3	L	1	0	0	0	0
4	S	16	0	0	0	0
5	S	7	0	0	0	0
6	L	8	0	0	1	0
7	L	2	0	0	0	0
8	L	607	0	0	10	11
8	S	326	0	0	2	5
All	All	7163	0	0	16	11

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (16) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:124:HIS:NE2	2:L:433:GLU:OE1	2.49	0.45
1:S:91:ASN:ND2	8:L:3804:HOH:O	2.49	0.45
2:L:193:GLY:N	8:L:3800:HOH:O	2.49	0.45
2:L:66:LYS:NZ	8:L:3574:HOH:O	2.49	0.45
2:L:285:LYS:NZ	2:L:413:LEU:O	2.49	0.45
2:L:332:LYS:NZ	8:L:3459:HOH:O	2.49	0.45
2:L:135:ASP:OD2	2:L:541:HIS:ND1	2.50	0.45
2:L:487:ARG:NH2	8:L:3481:HOH:O	2.49	0.45
2:L:328:LYS:NZ	8:L:3675:HOH:O	2.49	0.45
2:L:328:LYS:NZ	8:L:3720:HOH:O	2.49	0.44
1:S:131:LYS:NZ	8:S:3487:HOH:O	2.50	0.44
2:L:188:ASN:ND2	8:L:3793:HOH:O	2.49	0.44
1:S:233:LYS:NZ	8:S:3602:HOH:O	2.49	0.43
2:L:47:LYS:NZ	8:L:3716:HOH:O	2.51	0.42
2:L:457:ASN:ND2	8:L:3203:HOH:O	2.51	0.42
2:L:84:CYS:CB	6:L:1004:FNE:C2	2.99	0.41

All (11) 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	Distance(Å)	Clash(Å)
8:L:3457:HOH:O	8:L:3715:HOH:O[3.647]	1.90	0.30
8:S:3811:HOH:O	8:L:3818:HOH:O[2.664]	1.93	0.27
8:L:3582:HOH:O	8:L:3700:HOH:O[2.664]	1.97	0.23
8:L:3270:HOH:O	8:L:3670:HOH:O[3.657]	2.01	0.19
8:S:3184:HOH:O	8:L:3740:HOH:O[2.664]	2.02	0.18
8:L:3670:HOH:O	8:L:3715:HOH:O[3.647]	2.06	0.14
8:L:3551:HOH:O	8:L:3921:HOH:O[2.664]	2.08	0.12
8:L:3700:HOH:O	8:L:3820:HOH:O[2.665]	2.09	0.11
8:S:3496:HOH:O	8:L:3419:HOH:O[2.664]	2.12	0.08
8:S:3483:HOH:O	8:L:3482:HOH:O[2.664]	2.13	0.07
8:S:3416:HOH:O	8:L:3779:HOH:O[2.664]	2.18	0.02

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	S	265/267 (99%)	256 (97%)	7 (3%)	2 (1%)	27	5
2	L	532/534 (100%)	519 (98%)	13 (2%)	0	100	100
All	All	797/801 (100%)	775 (97%)	20 (2%)	2 (0%)	50	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	5	ARG
1	S	4	PRO

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	S	213/213 (100%)	198 (93%)	15 (7%)	21	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	438/438 (100%)	418 (95%)	20 (5%)	37 5
All	All	651/651 (100%)	616 (95%)	35 (5%)	31 4

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	1	LEU
1	S	2	MET
1	S	5	ARG
1	S	25	LEU
1	S	35	LEU
1	S	37	LEU
1	S	85	ILE
1	S	91	ASN
1	S	95	LEU
1	S	124	LYS
1	S	126	ASN
1	S	143	LYS
1	S	166	LYS
1	S	229	ASN
1	S	230	ASN
2	L	49	LYS
2	L	50	ASN
2	L	132	HIS
2	L	143	LEU
2	L	144	LYS
2	L	152	LYS
2	L	161	LYS
2	L	174	LEU
2	L	200	LEU
2	L	213	LEU
2	L	233	ASN
2	L	253	GLN
2	L	279	VAL
2	L	321	LYS
2	L	325	LYS
2	L	340	ARG
2	L	360	LYS
2	L	457	ASN
2	L	522	LEU
2	L	527	VAL

Some 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 chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FNE	L	1004	2,7	6,7,9	7.76	3 (50%)	0,9,15	0.00	-
7	CMO	L	1006	6	0,1,1	0.00	-	0,0,0	0.00	-
4	SF4	S	1001	1	12,12,12	133.40	9 (75%)	0,24,24	0.00	-
4	SF4	S	1002	1	12,12,12	134.02	9 (75%)	0,24,24	0.00	-
5	F3S	S	1003	1	3,9,9	2.19	2 (66%)	0,15,15	0.00	-

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
6	FNE	L	1004	2,7	-	0/0/9/18	0/0/0/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CMO	L	1006	6	-	0/0/0/0	0/0/0/0
4	SF4	S	1001	1	-	0/0/48/48	0/0/5/5
4	SF4	S	1002	1	-	0/0/48/48	0/0/5/5
5	F3S	S	1003	1	-	0/0/24/24	0/0/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	1001	SF4	S2-FE4	242.71	3.96	2.33
4	S	1002	SF4	S2-FE4	240.73	3.95	2.33
4	S	1001	SF4	S4-FE1	232.31	3.89	2.33
4	S	1002	SF4	S3-FE2	231.25	3.88	2.33
4	S	1002	SF4	S1-FE3	230.98	3.88	2.33
4	S	1001	SF4	S1-FE3	229.41	3.87	2.33
4	S	1002	SF4	S4-FE1	224.43	3.84	2.33
4	S	1001	SF4	S3-FE2	218.46	3.80	2.33
6	L	1004	FNE	C1-FE	17.54	1.95	1.78
4	S	1002	SF4	S3-FE4	-13.76	2.24	2.33
4	S	1001	SF4	S2-FE1	-11.75	2.25	2.33
4	S	1002	SF4	S2-FE1	-9.04	2.27	2.33
4	S	1002	SF4	S4-FE3	-8.78	2.27	2.33
4	S	1001	SF4	S3-FE4	-8.78	2.27	2.33
4	S	1001	SF4	S1-FE2	-7.70	2.28	2.33
6	L	1004	FNE	C2-FE	6.28	1.84	1.78
4	S	1001	SF4	S3-FE1	-5.56	2.29	2.33
4	S	1002	SF4	S3-FE1	-3.41	2.31	2.33
6	L	1004	FNE	C3-FE	-3.22	1.75	1.78
4	S	1002	SF4	S1-FE2	-2.85	2.31	2.33
5	S	1003	F3S	S3-FE3	-2.74	2.31	2.33
5	S	1003	F3S	S3-FE4	-2.60	2.31	2.33
4	S	1001	SF4	S1-FE4	-2.53	2.31	2.33

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.