



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 10, 2014 – 01:25 PM EDT

PDB ID : 1UBU  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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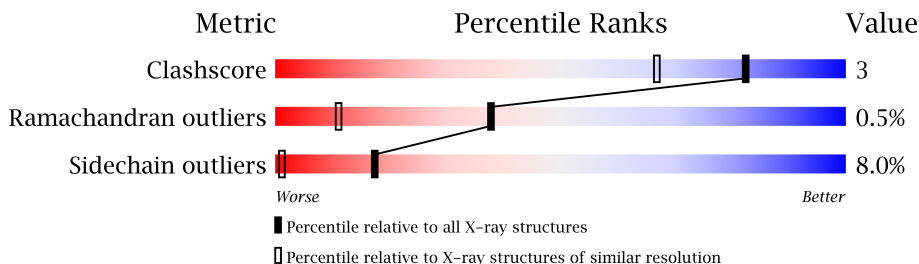
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : **FAILED**  
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) : stable22978

# 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  $\geq 3$ , 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 (i)

There are 7 unique types of molecules in this entry. The entry contains 7157 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			

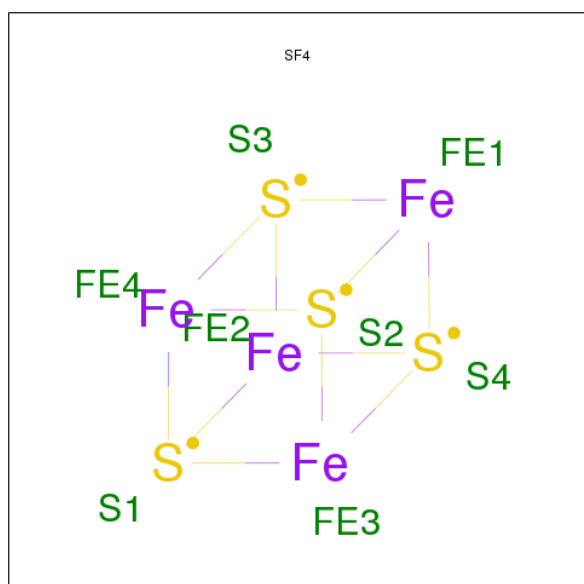
- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase Large subunit.

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:

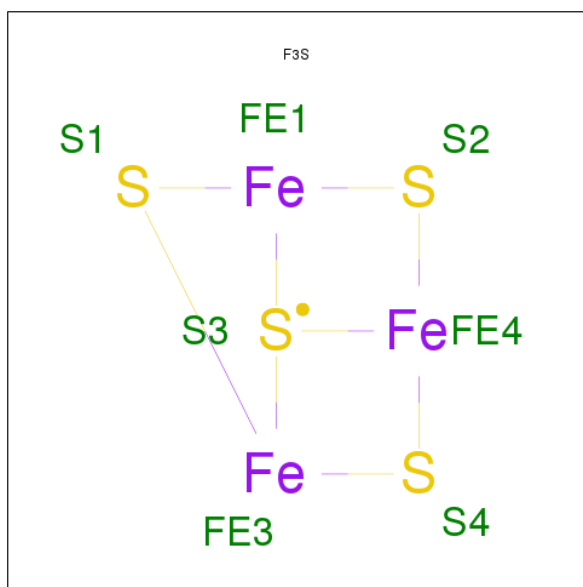
Chain	Residue	Modelled	Actual	Comment	Reference
L	514	LYS	ASN	SEE REMARK 999	UNP P21852
L	515	LEU	VAL	SEE REMARK 999	UNP P21852

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).

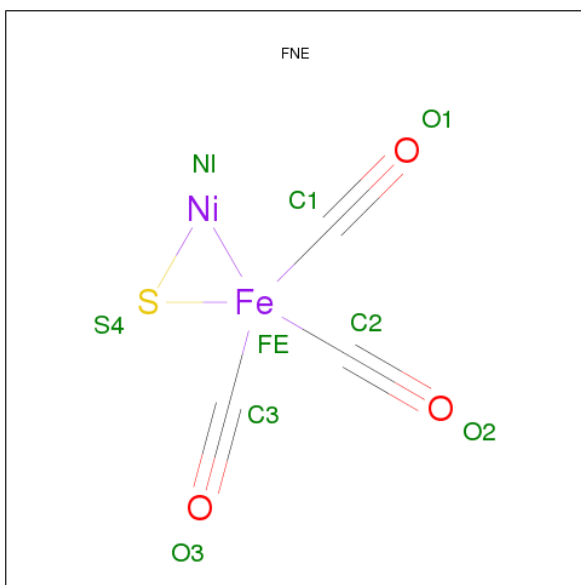


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- 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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	S	317	Total O 317 317	0	0
7	L	612	Total O 612 612	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.

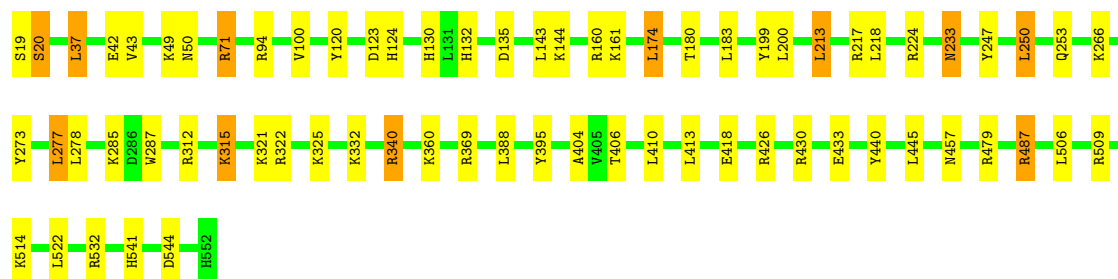
- Molecule 1: Periplasmic [NiFe] hydrogenase Small subunit

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, $\alpha$ , $\beta$ , $\gamma$	98.01Å 126.02Å 66.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.35	Depositor
% Data completeness (in resolution range)	91.9 (10.00-1.35)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.121 , 0.186	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	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: 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	0.68	1/2075 (0.0%)	1.47	21/2830 (0.7%)
2	L	0.62	0/4288	1.33	45/5831 (0.8%)
All	All	0.64	1/6363 (0.0%)	1.38	66/8661 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	267	ASN	C-O	6.93	1.36	1.23

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	6	ARG	CD-NE-CZ	27.92	162.69	123.60
1	S	100	ARG	NE-CZ-NH1	14.17	127.38	120.30
1	S	5	ARG	NE-CZ-NH1	-12.47	114.06	120.30
2	L	217	ARG	NE-CZ-NH1	-11.59	114.50	120.30
2	L	273	TYR	CB-CG-CD1	10.67	127.40	121.00
2	L	506	LEU	CA-CB-CG	10.67	139.84	115.30
1	S	2	MET	CA-CB-CG	10.62	131.36	113.30
2	L	340	ARG	NE-CZ-NH2	-10.53	115.03	120.30
2	L	160	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	S	233	LYS	CD-CE-NZ	8.58	131.44	111.70
2	L	430	ARG	NE-CZ-NH2	-8.56	116.02	120.30
2	L	426	ARG	NE-CZ-NH1	8.48	124.54	120.30
2	L	487	ARG	CB-CG-CD	8.46	133.61	111.60
1	S	26	ARG	NE-CZ-NH2	-8.43	116.08	120.30
2	L	273	TYR	CG-CD1-CE1	8.11	127.79	121.30
1	S	197	PHE	CB-CG-CD2	-7.88	115.28	120.80
2	L	120	TYR	CB-CG-CD2	-7.84	116.30	121.00
2	L	532	ARG	NE-CZ-NH2	-7.80	116.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	71	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	S	218	TYR	CB-CG-CD1	7.56	125.54	121.00
2	L	218	LEU	CA-CB-CG	-7.47	98.12	115.30
2	L	71	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	S	1	LEU	O-C-N	7.01	133.91	122.70
2	L	287	TRP	CA-CB-CG	-6.99	100.41	113.70
2	L	479	ARG	NE-CZ-NH1	6.66	123.63	120.30
2	L	174	LEU	CA-CB-CG	6.61	130.50	115.30
1	S	218	TYR	CB-CG-CD2	-6.51	117.09	121.00
2	L	213	LEU	CA-CB-CG	6.38	129.98	115.30
1	S	26	ARG	CG-CD-NE	-6.29	98.60	111.80
1	S	233	LYS	CA-CB-CG	6.21	127.06	113.40
1	S	26	ARG	NE-CZ-NH1	6.13	123.36	120.30
2	L	509	ARG	NE-CZ-NH2	6.12	123.36	120.30
2	L	247	TYR	CB-CG-CD2	-6.10	117.34	121.00
2	L	224	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	S	100	ARG	CD-NE-CZ	6.10	132.14	123.60
2	L	277	LEU	CA-CB-CG	6.08	129.28	115.30
2	L	430	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	L	100	VAL	CA-CB-CG2	-5.97	101.95	110.90
2	L	273	TYR	CB-CG-CD2	-5.96	117.42	121.00
1	S	243	VAL	CA-CB-CG1	5.89	119.74	110.90
2	L	340	ARG	NH1-CZ-NH2	5.87	125.86	119.40
2	L	250	LEU	CA-CB-CG	5.85	128.76	115.30
1	S	85	ILE	CA-CB-CG1	-5.78	100.02	111.00
2	L	123	ASP	CB-CG-OD2	-5.67	113.19	118.30
2	L	369	ARG	NE-CZ-NH1	5.59	123.10	120.30
2	L	160	ARG	NH1-CZ-NH2	5.57	125.52	119.40
2	L	42	GLU	OE1-CD-OE2	5.52	129.93	123.30
2	L	322	ARG	NE-CZ-NH2	5.47	123.03	120.30
2	L	440	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	S	187	VAL	CA-CB-CG1	5.44	119.06	110.90
2	L	544	ASP	CB-CG-OD1	-5.44	113.41	118.30
2	L	180	THR	CA-CB-CG2	-5.44	104.79	112.40
2	L	487	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	L	199	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	S	5	ARG	CA-C-N	5.21	128.66	117.20
2	L	37	LEU	CA-CB-CG	5.19	127.25	115.30
2	L	120	TYR	CA-CB-CG	5.19	123.26	113.40
1	S	86	TYR	CB-CG-CD1	-5.17	117.90	121.00
2	L	404	ALA	C-N-CA	-5.15	108.83	121.70
1	S	164	TYR	CB-CG-CD2	-5.15	117.91	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	395	TYR	CB-CG-CD2	5.14	124.09	121.00
2	L	94	ARG	NE-CZ-NH2	5.14	122.87	120.30
2	L	426	ARG	NE-CZ-NH2	-5.13	117.73	120.30
2	L	273	TYR	CD1-CE1-CZ	-5.07	115.23	119.80
1	S	1	LEU	CA-C-N	-5.04	106.11	117.20
2	L	130	HIS	CA-CB-CG	-5.01	105.08	113.60

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	8	0
2	L	4177	0	0	12	0
3	S	16	0	0	0	0
4	S	7	0	0	0	0
5	L	1	0	0	0	0
6	L	8	0	0	0	0
7	L	612	0	0	8	0
7	S	317	0	0	5	0
All	All	7157	0	0	19	0

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:6:ARG:NH2	7:S:3175:HOH:O	2.46	0.49
1:S:6:ARG:NE	7:S:3175:HOH:O	2.49	0.46
1:S:91:ASN:ND2	7:L:3537:HOH:O	2.49	0.46
2:L:312:ARG:O	2:L:315:LYS:NZ	2.49	0.45
2:L:332:LYS:NZ	7:L:3867:HOH:O	2.49	0.45
2:L:124:HIS:NE2	2:L:433:GLU:OE1	2.49	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:332:LYS:NZ	7:L:3618:HOH:O	2.50	0.45
1:S:166:LYS:NZ	7:S:3502:HOH:O	2.49	0.45
2:L:285:LYS:NZ	2:L:413:LEU:O	2.50	0.45
2:L:487:ARG:NH2	7:L:3311:HOH:O	2.49	0.45
1:S:233:LYS:NZ	7:S:3243:HOH:O	2.50	0.44
2:L:71:ARG:NH1	7:L:3888:HOH:O	2.49	0.44
2:L:266:LYS:NZ	7:L:3874:HOH:O	2.51	0.44
2:L:285:LYS:NZ	7:L:3674:HOH:O	2.50	0.43
2:L:135:ASP:OD2	2:L:541:HIS:ND1	2.53	0.42
1:S:13:HIS:CD2	7:S:3020:HOH:O	2.73	0.41
1:S:26:ARG:NH2	2:L:233:ASN:ND2	2.69	0.40
2:L:514:LYS:NZ	7:L:3883:HOH:O	2.55	0.40
1:S:230:ASN:ND2	1:S:230:ASN:N	2.69	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	S	265/267 (99%)	257 (97%)	5 (2%)	3 (1%)	21	3
2	L	532/534 (100%)	518 (97%)	13 (2%)	1 (0%)	56	24
All	All	797/801 (100%)	775 (97%)	18 (2%)	4 (0%)	38	11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	4	PRO
2	L	20	SER
1	S	5	ARG
1	S	3	GLY

### 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%)	192 (90%)	21 (10%)	11	0
2	L	438/438 (100%)	407 (93%)	31 (7%)	21	1
All	All	651/651 (100%)	599 (92%)	52 (8%)	17	1

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	1	LEU
1	S	2	MET
1	S	4	PRO
1	S	5	ARG
1	S	35	LEU
1	S	37	LEU
1	S	40	LEU
1	S	61	GLU
1	S	79	PRO
1	S	85	ILE
1	S	91	ASN
1	S	95	LEU
1	S	126	ASN
1	S	168	LYS
1	S	173	LEU
1	S	176	LEU
1	S	187	VAL
1	S	220	LEU
1	S	229	ASN
1	S	230	ASN
1	S	243	VAL
2	L	19	SER
2	L	20	SER
2	L	37	LEU
2	L	43	VAL
2	L	49	LYS
2	L	50	ASN
2	L	132	HIS
2	L	143	LEU

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Mol	Chain	Res	Type
2	L	144	LYS
2	L	161	LYS
2	L	174	LEU
2	L	183	LEU
2	L	200	LEU
2	L	213	LEU
2	L	233	ASN
2	L	250	LEU
2	L	253	GLN
2	L	277	LEU
2	L	278	LEU
2	L	315	LYS
2	L	321	LYS
2	L	325	LYS
2	L	340	ARG
2	L	360	LYS
2	L	388	LEU
2	L	406	THR
2	L	410	LEU
2	L	418	GLU
2	L	445	LEU
2	L	457	ASN
2	L	522	LEU

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 ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 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.