



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 02:11 PM EDT

PDB ID : 1FP4 / pdb_00001fp4
Title : CRYSTAL STRUCTURE OF THE ALPHA-H195Q MUTANT OF NITRO-GENASE
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Deposited on : 2000-08-30
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

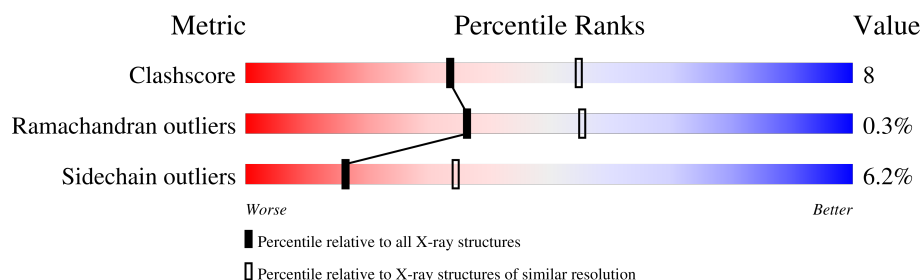
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	492	
1	C	492	
2	B	523	
2	D	523	

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
4	CFM	A	496	-	-	X	-
4	CFM	C	497	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16295 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 NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3708	2360	629	695	24			
1	C	468	Total	C	N	O	S	0	0	0
			3712	2363	630	695	24			

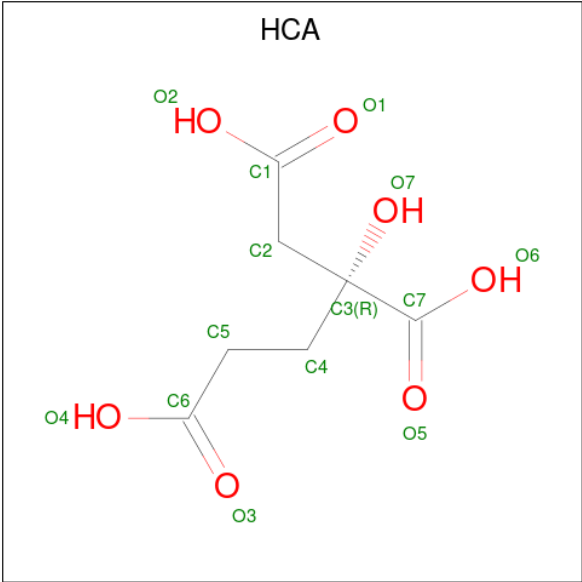
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	GLN	HIS	engineered mutation	UNP P07328
C	195	GLN	HIS	engineered mutation	UNP P07328

- Molecule 2 is a protein called NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN.

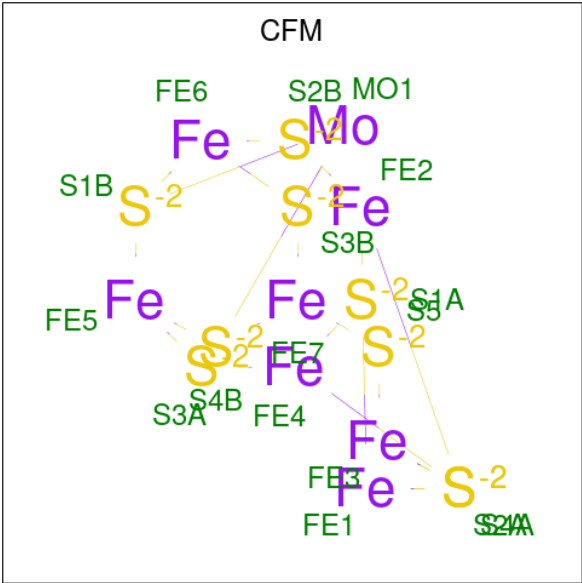
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$).



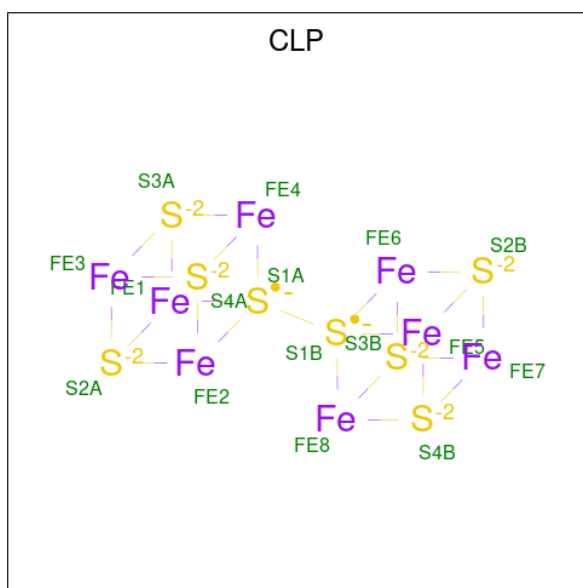
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	7	7		
3	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 4 is FE-MO-S CLUSTER (CCD ID: CFM) (formula: Fe₇MoS₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
4	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 5 is FE-S CLUSTER (CCD ID: CLP) (formula: Fe_8S_8).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			15	8	7		
5	C	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

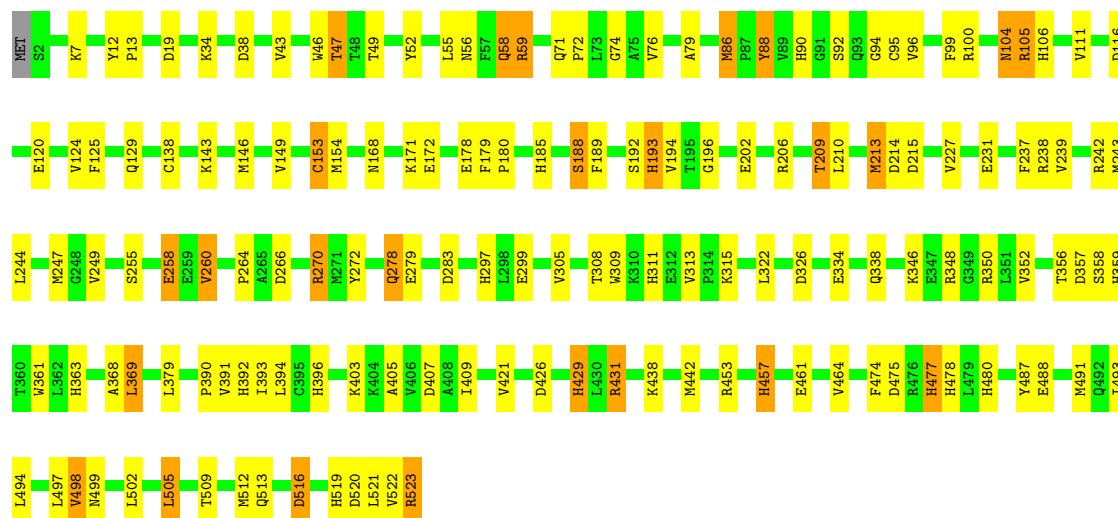
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	102	Total	O	0	0
			102	102		
7	B	114	Total	O	0	0
			114	114		
7	C	74	Total	O	0	0
			74	74		
7	D	143	Total	O	0	0
			143	143		

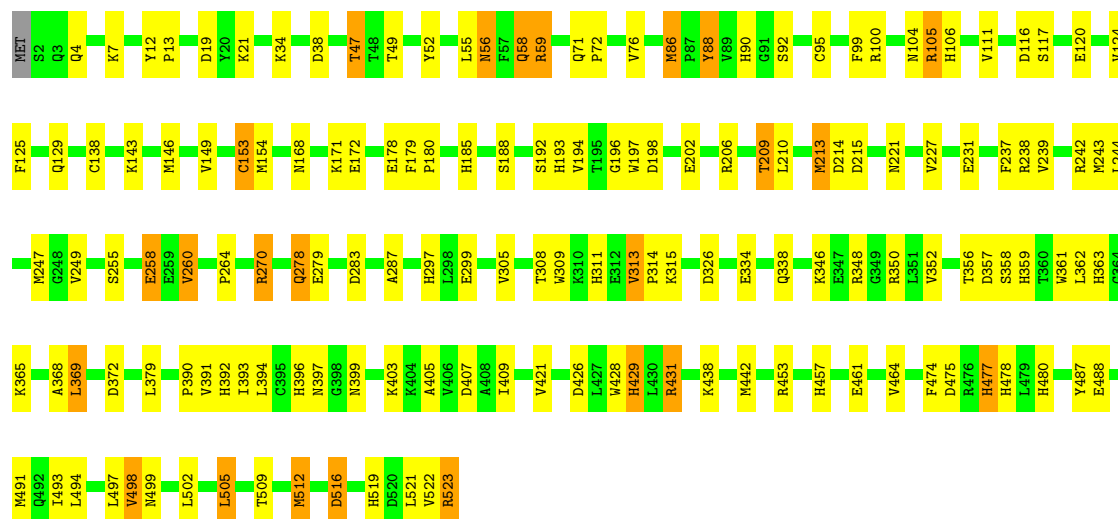
• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

Chain B: 



• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

Chain D: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.20Å 130.20Å 80.40Å 90.00° 111.20° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.184 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16295	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

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: CFM, CLP, CA, HCA

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	0.91	18/3793 (0.5%)	1.68	58/5114 (1.1%)
1	C	0.99	18/3797 (0.5%)	1.71	73/5120 (1.4%)
2	B	0.89	18/4280 (0.4%)	1.57	63/5786 (1.1%)
2	D	0.89	19/4280 (0.4%)	1.57	66/5786 (1.1%)
All	All	0.92	73/16150 (0.5%)	1.63	260/21806 (1.2%)

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	418	PRO	N-CD	-26.90	1.10	1.47
1	A	70	VAL	CA-CB	8.54	1.64	1.55
2	D	297	HIS	CD2-NE2	-7.60	1.29	1.37
2	B	297	HIS	CD2-NE2	-7.51	1.29	1.37
2	B	457	HIS	CD2-NE2	-7.14	1.29	1.37

The worst 5 of 260 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	51	LYS	N-CA-C	17.52	133.02	110.24
1	A	49	ASN	CB-CA-C	-14.36	81.84	110.42
1	C	49	ASN	CB-CA-C	-14.01	82.54	110.42
1	C	418	PRO	CA-N-CD	13.44	130.82	112.00
1	A	51	LYS	N-CA-C	12.20	126.94	110.35

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	3708	0	3638	72	0
1	C	3712	0	3640	63	0
2	B	4174	0	4087	70	0
2	D	4174	0	4087	62	0
3	A	14	0	6	0	0
3	C	14	0	6	0	0
4	A	17	0	0	5	0
4	C	17	0	0	6	0
5	A	15	0	0	3	0
5	C	15	0	0	2	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	102	0	0	7	0
7	B	114	0	0	2	0
7	C	74	0	0	2	0
7	D	143	0	0	2	0
All	All	16295	0	15464	242	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 8.

The worst 5 of 242 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)
2:B:146:MET:HG3	2:B:180:PRO:HB2	1.62	0.82
2:D:390:PRO:HB2	2:D:393:ILE:HD11	1.63	0.81
2:B:390:PRO:HB2	2:B:393:ILE:HD11	1.64	0.80
1:C:350:ARG:NH1	1:C:416:ILE:O	2.17	0.77
2:D:146:MET:HG3	2:D:180:PRO:HB2	1.66	0.77

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	463/492 (94%)	433 (94%)	28 (6%)	2 (0%)	30	49
1	C	464/492 (94%)	437 (94%)	26 (6%)	1 (0%)	43	63
2	B	520/523 (99%)	508 (98%)	11 (2%)	1 (0%)	43	63
2	D	520/523 (99%)	507 (98%)	12 (2%)	1 (0%)	43	63
All	All	1967/2030 (97%)	1885 (96%)	77 (4%)	5 (0%)	36	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
2	B	255	SER
2	D	255	SER
1	A	355	ILE
1	C	355	ILE

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	397/415 (96%)	373 (94%)	24 (6%)	17	36
1	C	396/415 (95%)	373 (94%)	23 (6%)	18	38
2	B	454/455 (100%)	425 (94%)	29 (6%)	16	33
2	D	454/455 (100%)	425 (94%)	29 (6%)	16	33
All	All	1701/1740 (98%)	1596 (94%)	105 (6%)	16	34

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	70	VAL
1	C	404	VAL
2	D	369	LEU
1	C	98	ASN
1	C	264	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	457	HIS
2	D	278	GLN
1	C	53	GLN
2	D	499	ASN
2	D	136	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
3	HCA	C	495	4	13,13,13	2.34	4 (30%)	15,18,18	2.00	5 (33%)
3	HCA	A	494	4	13,13,13	2.33	4 (30%)	15,18,18	2.05	6 (40%)
4	CFM	C	497	3,1	0,24,24	-	-	-		
4	CFM	A	496	3,1	0,24,24	-	-	-		
5	CLP	A	498	1,2	0,21,25	-	-	-		
5	CLP	C	499	1,2	0,21,25	-	-	-		

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
3	HCA	C	495	4	-	5/17/17/17	-
5	CLP	A	498	1,2	-	-	0/10/9/10
3	HCA	A	494	4	-	5/17/17/17	-
5	CLP	C	499	1,2	-	-	0/10/9/10

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	495	HCA	O5-C7	6.80	1.43	1.22
3	A	494	HCA	O5-C7	6.65	1.42	1.22
3	C	495	HCA	O1-C1	2.90	1.31	1.22
3	A	494	HCA	O1-C1	2.81	1.31	1.22
3	C	495	HCA	O6-C7	-2.57	1.21	1.30

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	495	HCA	O6-C7-C3	4.65	122.07	113.14
3	A	494	HCA	O6-C7-C3	4.62	121.99	113.14
3	A	494	HCA	O2-C1-O1	-2.50	116.90	123.33
3	A	494	HCA	O4-C6-C5	2.48	121.82	114.00
3	C	495	HCA	O2-C1-O1	-2.43	117.09	123.33

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	494	HCA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	494	HCA	C7-C3-C4-C5
3	A	494	HCA	O7-C3-C4-C5
3	C	495	HCA	C2-C3-C4-C5
3	C	495	HCA	C7-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	497	CFM	6	0
4	A	496	CFM	5	0
5	A	498	CLP	3	0
5	C	499	CLP	2	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.