



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:31 PM GMT

PDB ID : 1U0T  
Title : Crystal structure of Mycobacterium tuberculosis NAD kinase  
Authors : Garavaglia, S.; Raffaelli, N.; Finaurini, L.; Magni, G.; Rizzi, M.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2004-07-14  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

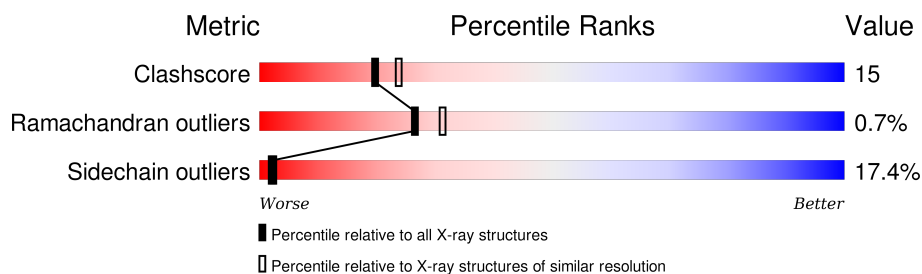
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	307	 56% 22% 8% • 13%
1	B	307	 66% 18% • • 10%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4364 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 Inorganic polyphosphate/ATP-NAD kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2010	1270	368	366	6			
1	B	276	Total	C	N	O	S	0	0	0
			2078	1308	380	384	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	122	Total	O	0	0
			122	122		
2	B	154	Total	O	0	0
			154	154		



## 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 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.76Å 145.66Å 68.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.30)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.226 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4364	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.84	2/2042 (0.1%)	1.06	15/2777 (0.5%)
1	B	0.90	1/2111 (0.0%)	1.05	13/2869 (0.5%)
All	All	0.87	3/4153 (0.1%)	1.06	28/5646 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	THR	CB-OG1	5.80	1.54	1.43
1	B	13	THR	CB-OG1	5.57	1.54	1.43
1	A	289	PHE	CE1-CZ	5.17	1.47	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	LEU	CA-CB-CG	8.41	134.65	115.30
1	A	139	LEU	CA-CB-CG	8.29	134.37	115.30
1	B	85	ASP	CB-CG-OD2	7.60	125.14	118.30
1	B	139	LEU	CA-CB-CG	7.50	132.56	115.30
1	A	269	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	A	16	ASP	CB-CG-OD2	7.13	124.71	118.30
1	A	263	LEU	CA-CB-CG	6.95	131.27	115.30
1	A	142	ASP	CB-CG-OD2	6.74	124.37	118.30
1	B	158	LEU	CA-CB-CG	6.59	130.46	115.30
1	A	189	ASP	CB-CG-OD2	6.48	124.13	118.30
1	B	158	LEU	CB-CG-CD2	-6.31	100.28	111.00
1	A	178	ILE	C-N-CA	-6.16	106.30	121.70
1	A	235	THR	N-CA-CB	-6.13	98.66	110.30
1	B	169	LEU	CA-CB-CG	6.11	129.34	115.30
1	B	138	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	B	248	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	31	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	291	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	270	LEU	CA-CB-CG	5.67	128.34	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	284	LEU	CB-CG-CD1	5.66	120.62	111.00
1	A	137	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	285	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	214	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	85	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	192	LEU	CA-CB-CG	5.38	127.68	115.30
1	B	285	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	81	VAL	CB-CA-C	-5.25	101.42	111.40
1	A	132	ASP	CB-CG-OD2	5.14	122.93	118.30

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	2010	0	2056	61	0
1	B	2078	0	2113	71	0
2	A	122	0	0	8	0
2	B	154	0	0	15	0
All	All	4364	0	4169	123	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 15.

All (123) 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:B:165:LYS:HA	1:B:172:LEU:CD1	1.46	1.44
1:B:165:LYS:CA	1:B:172:LEU:HD11	1.74	1.16
1:A:177:GLU:OE1	1:A:242:ALA:HB3	1.49	1.10
1:B:263:LEU:HB3	2:B:376:HOH:O	1.54	1.06
1:B:165:LYS:CA	1:B:172:LEU:CD1	2.34	1.03
1:B:160:GLU:HG2	2:B:321:HOH:O	1.58	1.02
1:B:172:LEU:CD2	2:B:375:HOH:O	2.09	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:TRP:HZ3	2:B:337:HOH:O	1.44	1.00
1:B:165:LYS:HB3	1:B:172:LEU:HG	1.48	0.94
1:B:254:VAL:HG12	1:B:264:ILE:HD11	1.53	0.90
1:A:177:GLU:OE1	1:A:242:ALA:CB	2.19	0.90
1:A:188:CYS:SG	2:A:423:HOH:O	1.98	0.90
1:B:254:VAL:CG1	1:B:264:ILE:HD11	2.02	0.89
1:B:165:LYS:CB	1:B:172:LEU:HG	2.03	0.88
1:A:19:THR:HB	2:A:388:HOH:O	1.72	0.88
1:B:200:THR:HG23	2:B:342:HOH:O	1.73	0.88
1:A:254:VAL:CG1	1:A:264:ILE:HD11	2.03	0.88
1:B:165:LYS:HA	1:B:172:LEU:HD12	1.53	0.88
1:B:178:ILE:O	1:B:240:THR:O	1.91	0.87
1:B:165:LYS:HA	1:B:172:LEU:HD11	0.88	0.87
1:B:200:THR:CG2	2:B:342:HOH:O	2.27	0.83
1:A:160:GLU:HG2	2:A:309:HOH:O	1.78	0.83
1:B:172:LEU:HD21	2:B:375:HOH:O	1.70	0.82
1:A:96:ARG:HD2	2:A:349:HOH:O	1.88	0.74
1:A:13:THR:HG22	1:A:16:ASP:OD2	1.91	0.71
1:A:301:VAL:O	1:A:301:VAL:HG12	1.90	0.70
1:B:165:LYS:CB	1:B:172:LEU:CG	2.71	0.69
1:B:235:THR:CG2	1:B:239:ALA:HB3	2.22	0.69
1:B:298:ARG:HA	1:B:298:ARG:HH11	1.57	0.68
1:A:301:VAL:CG1	1:A:301:VAL:O	2.41	0.67
1:A:254:VAL:HG11	1:A:264:ILE:HD11	1.75	0.66
1:B:19:THR:HG22	1:B:22:ALA:H	1.61	0.66
1:A:172:LEU:HB3	2:A:423:HOH:O	1.95	0.66
1:A:254:VAL:HG12	1:A:264:ILE:CG1	2.25	0.65
1:A:301:VAL:HG13	1:B:182:PRO:HB2	1.77	0.65
1:A:143:VAL:CG2	1:A:270:LEU:HD22	2.26	0.65
1:B:254:VAL:HG11	1:B:264:ILE:HD11	1.80	0.64
1:A:244:GLU:OE1	1:B:304:TRP:O	2.15	0.63
1:A:122:ASP:O	1:A:126:GLU:HG3	1.97	0.63
1:B:235:THR:HG23	1:B:239:ALA:CB	2.27	0.63
1:B:19:THR:HG23	2:B:404:HOH:O	2.00	0.62
1:A:163:LEU:HD21	1:A:245:ILE:HD11	1.83	0.61
1:B:306:GLY:O	1:B:307:LYS:HB2	2.00	0.61
1:A:182:PRO:HB2	1:B:301:VAL:HG22	1.83	0.61
1:B:235:THR:HG23	1:B:239:ALA:HB3	1.84	0.60
1:A:9:LEU:HD13	1:A:25:VAL:HG11	1.83	0.59
1:A:178:ILE:O	1:A:240:THR:O	2.20	0.59
1:B:143:VAL:CG2	1:B:270:LEU:HD22	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:VAL:HG12	1:B:264:ILE:CD1	2.31	0.59
1:A:141:LEU:O	1:A:156:TRP:HA	2.02	0.58
1:B:172:LEU:N	1:B:172:LEU:HD23	2.19	0.57
1:A:9:LEU:CD1	1:A:25:VAL:HG11	2.35	0.57
1:B:298:ARG:NH1	1:B:298:ARG:HA	2.17	0.57
1:A:143:VAL:HG23	1:A:270:LEU:HD22	1.86	0.56
1:A:236:SER:HB2	1:A:237:PRO:HD2	1.86	0.56
1:A:265:PRO:O	1:A:268:SER:OG	2.24	0.56
1:A:294:VAL:HA	1:A:299:LEU:HB2	1.87	0.56
1:B:69:ASP:HB2	1:B:72:ALA:HB2	1.88	0.55
1:A:90:ARG:O	1:A:93:GLU:HB3	2.06	0.55
1:A:110:ILE:HD13	1:A:295:ARG:HG2	1.88	0.55
1:A:301:VAL:CG1	1:B:182:PRO:HB2	2.36	0.54
1:B:165:LYS:CB	1:B:172:LEU:CD1	2.85	0.54
1:B:110:ILE:HD11	1:B:295:ARG:HH21	1.72	0.54
1:A:218:ILE:HB	1:A:235:THR:HG22	1.89	0.54
1:A:103:LEU:HB2	1:A:282:ALA:HB3	1.90	0.54
1:B:235:THR:CG2	1:B:239:ALA:CB	2.86	0.54
1:A:235:THR:HG23	1:A:239:ALA:HB3	1.90	0.54
1:B:259:ARG:CD	2:B:343:HOH:O	2.56	0.53
1:A:103:LEU:HD11	1:A:284:LEU:HD22	1.89	0.53
1:A:171:VAL:HG22	1:A:188:CYS:N	2.24	0.53
1:B:235:THR:HG21	1:B:239:ALA:HB3	1.91	0.52
1:A:254:VAL:CG1	1:A:264:ILE:CD1	2.83	0.52
1:A:167:PRO:HD2	2:A:417:HOH:O	2.10	0.52
1:B:301:VAL:HG13	2:B:325:HOH:O	2.11	0.51
1:A:165:LYS:NZ	2:A:404:HOH:O	2.38	0.51
1:B:304:TRP:O	1:B:306:GLY:N	2.44	0.51
1:B:259:ARG:HD3	2:B:343:HOH:O	2.10	0.50
1:A:124:VAL:O	1:A:128:VAL:HG23	2.11	0.50
1:B:165:LYS:HB2	1:B:172:LEU:CG	2.41	0.50
1:B:171:VAL:HG22	1:B:188:CYS:N	2.27	0.50
1:B:171:VAL:C	1:B:172:LEU:HD23	2.33	0.49
1:A:175:VAL:HG11	1:B:304:TRP:HA	1.95	0.49
1:B:263:LEU:HD12	2:B:376:HOH:O	2.13	0.48
1:B:196:PRO:HG2	1:B:215:LEU:O	2.14	0.48
1:A:13:THR:HG23	1:A:14:GLY:N	2.29	0.48
1:B:10:VAL:HB	1:B:81:VAL:HG13	1.95	0.48
1:A:162:SER:O	1:A:254:VAL:HA	2.13	0.47
1:A:110:ILE:HG13	1:A:110:ILE:H	1.51	0.47
1:A:138:ARG:HB3	1:A:281:TRP:NE1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:VAL:HG22	1:A:188:CYS:H	1.81	0.46
1:B:218:ILE:HB	1:B:235:THR:HG22	1.96	0.46
1:A:235:THR:HG21	1:A:241:ILE:HD11	1.97	0.46
1:A:269:ARG:HD3	1:A:271:GLU:OE2	2.16	0.46
1:A:235:THR:HG23	1:A:236:SER:O	2.16	0.46
1:B:12:HIS:HB3	1:B:16:ASP:OD2	2.17	0.45
1:A:82:LEU:HD23	1:A:105:VAL:HB	1.98	0.45
1:A:6:SER:HB3	1:A:35:ALA:HB3	1.99	0.44
1:A:267:GLY:O	1:B:307:LYS:HB3	2.17	0.44
1:B:117:GLU:OE2	1:B:295:ARG:NH2	2.50	0.44
1:B:235:THR:HG23	1:B:239:ALA:HB2	2.00	0.44
1:A:143:VAL:CG2	1:A:270:LEU:CD2	2.94	0.44
1:B:259:ARG:HD2	2:B:343:HOH:O	2.18	0.43
1:B:13:THR:O	1:B:16:ASP:HB2	2.19	0.43
1:A:254:VAL:HG12	1:A:264:ILE:HG13	1.98	0.43
1:A:37:ARG:HG2	1:A:37:ARG:H	1.68	0.43
1:B:39:LEU:C	1:B:39:LEU:HD12	2.39	0.43
1:B:103:LEU:HD11	1:B:284:LEU:HD22	2.01	0.42
1:A:172:LEU:HD21	1:A:245:ILE:HD12	2.01	0.42
1:B:294:VAL:HA	1:B:299:LEU:HB2	2.01	0.42
1:B:93:GLU:HG3	1:B:156:TRP:HZ2	1.83	0.42
1:A:160:GLU:CG	2:A:309:HOH:O	2.53	0.42
1:B:165:LYS:CB	1:B:172:LEU:HD11	2.44	0.41
1:B:9:LEU:HD11	1:B:82:LEU:HG	2.01	0.41
1:A:223:ASN:HD22	1:A:223:ASN:C	2.23	0.41
1:A:244:GLU:HG2	1:B:307:LYS:HA	2.02	0.41
1:B:259:ARG:HD2	2:B:387:HOH:O	2.19	0.41
1:A:158:LEU:HD13	1:A:281:TRP:HZ2	1.86	0.41
1:B:139:LEU:HD12	1:B:139:LEU:C	2.42	0.40
1:A:177:GLU:HG2	1:B:304:TRP:HE1	1.85	0.40
1:A:301:VAL:HG11	1:B:182:PRO:CG	2.51	0.40
1:B:235:THR:CG2	1:B:236:SER:O	2.69	0.40
1:B:208:GLY:HA3	2:B:315:HOH:O	2.21	0.40
1:B:248:ASP:C	1:B:248:ASP:OD2	2.59	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	263/307 (86%)	249 (95%)	12 (5%)	2 (1%)	24	27
1	B	272/307 (89%)	254 (93%)	16 (6%)	2 (1%)	26	31
All	All	535/614 (87%)	503 (94%)	28 (5%)	4 (1%)	26	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	B	304	TRP
1	A	31	ASP
1	B	169	LEU

### 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	210/242 (87%)	169 (80%)	41 (20%)	2	1
1	B	216/242 (89%)	183 (85%)	33 (15%)	3	3
All	All	426/484 (88%)	352 (83%)	74 (17%)	2	2

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	6	SER

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Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	THR
1	A	19	THR
1	A	24	ARG
1	A	27	LYS
1	A	37	ARG
1	A	39	LEU
1	A	40	SER
1	A	99	SER
1	A	100	ILE
1	A	102	VAL
1	A	110	ILE
1	A	134	ARG
1	A	139	LEU
1	A	158	LEU
1	A	159	ASN
1	A	160	GLU
1	A	169	LEU
1	A	171	VAL
1	A	172	LEU
1	A	174	VAL
1	A	177	GLU
1	A	186	PHE
1	A	192	LEU
1	A	223	ASN
1	A	228	LEU
1	A	235	THR
1	A	238	GLU
1	A	254	VAL
1	A	259	ARG
1	A	263	LEU
1	A	268	SER
1	A	270	LEU
1	A	274	ARG
1	A	284	LEU
1	A	285	ASP
1	A	293	LEU
1	A	298	ARG
1	A	299	LEU
1	B	15	ARG
1	B	19	THR
1	B	33	LYS

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Mol	Chain	Res	Type
1	B	39	LEU
1	B	70	GLN
1	B	81	VAL
1	B	106	ASN
1	B	139	LEU
1	B	142	ASP
1	B	144	VAL
1	B	150	ARG
1	B	154	ARG
1	B	160	GLU
1	B	169	LEU
1	B	192	LEU
1	B	200	THR
1	B	223	ASN
1	B	228	LEU
1	B	235	THR
1	B	236	SER
1	B	246	GLU
1	B	248	ASP
1	B	263	LEU
1	B	269	ARG
1	B	270	LEU
1	B	274	ARG
1	B	284	LEU
1	B	293	LEU
1	B	296	LYS
1	B	298	ARG
1	B	299	LEU
1	B	301	VAL
1	B	305	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	B	223	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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](#)

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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