



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:37 PM GMT

PDB ID : 1L1F  
Title : Structure of human glutamate dehydrogenase-apo form  
Authors : Smith, T.J.; Schmidt, T.; Fang, J.; Wu, J.; Siuzdak, G.; Stanley, C.A.  
Deposited on : 2002-02-15  
Resolution : 2.70 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](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

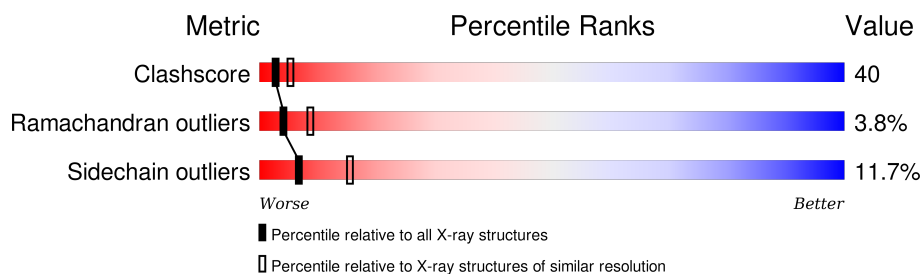
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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	505	 43% 46% 8% ..
1	B	505	 41% 48% 9% ..
1	C	505	 40% 49% 9% ..
1	D	505	 43% 46% 9% ..
1	E	505	 43% 45% 9% ..
1	F	505	 43% 46% 8% ..

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23244 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 Glutamate Dehydrogenase 1.

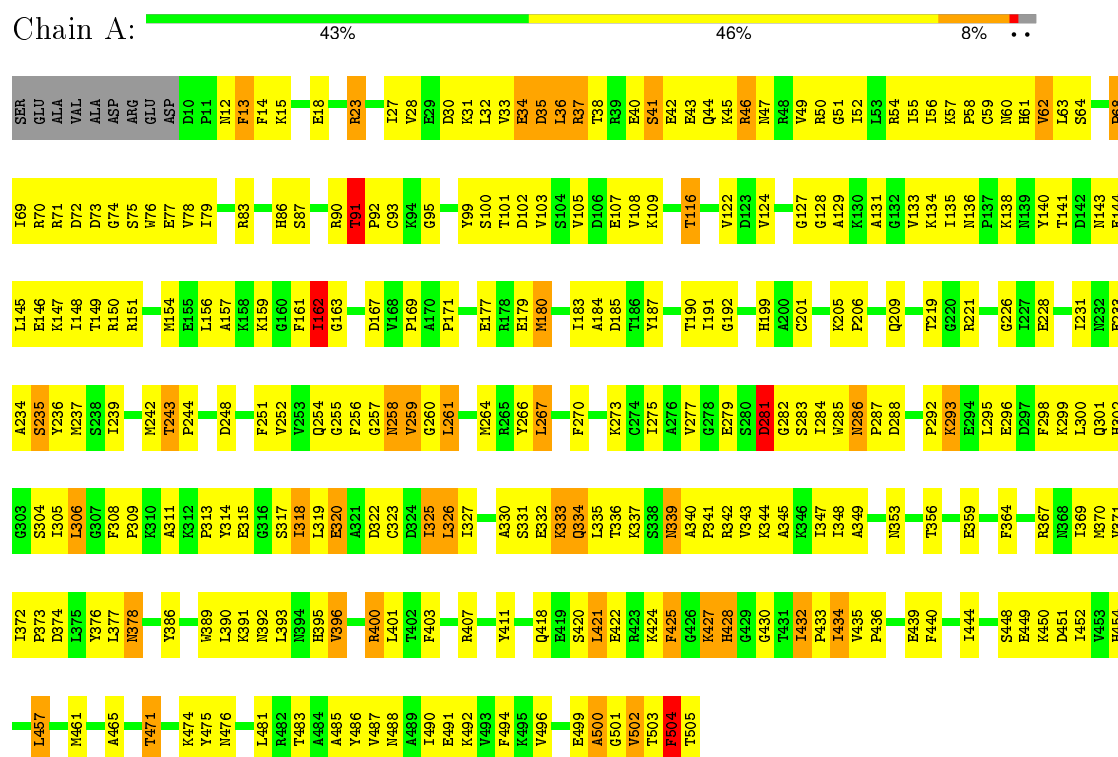
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	B	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	C	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	D	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	E	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	F	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			

### 3 Residue-property plots

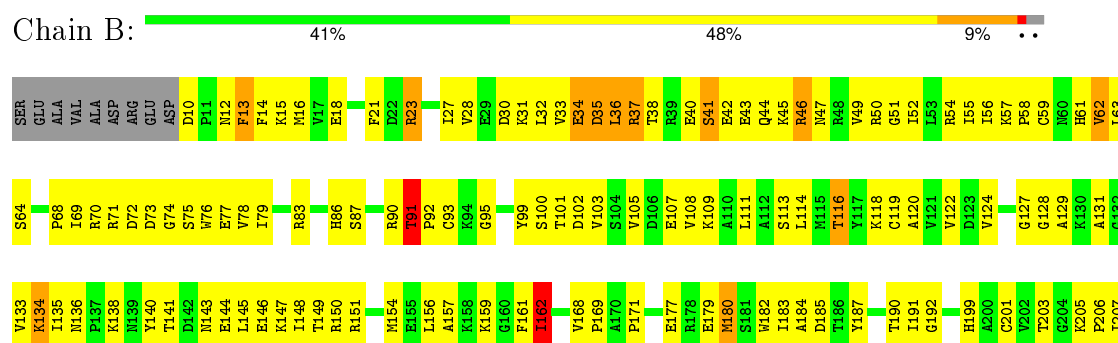
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

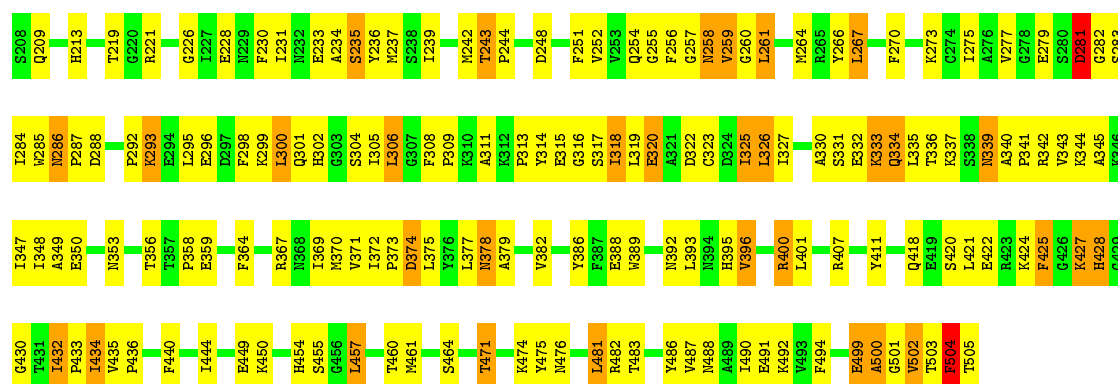
Note EDS was not executed.

#### • Molecule 1: Glutamate Dehydrogenase 1



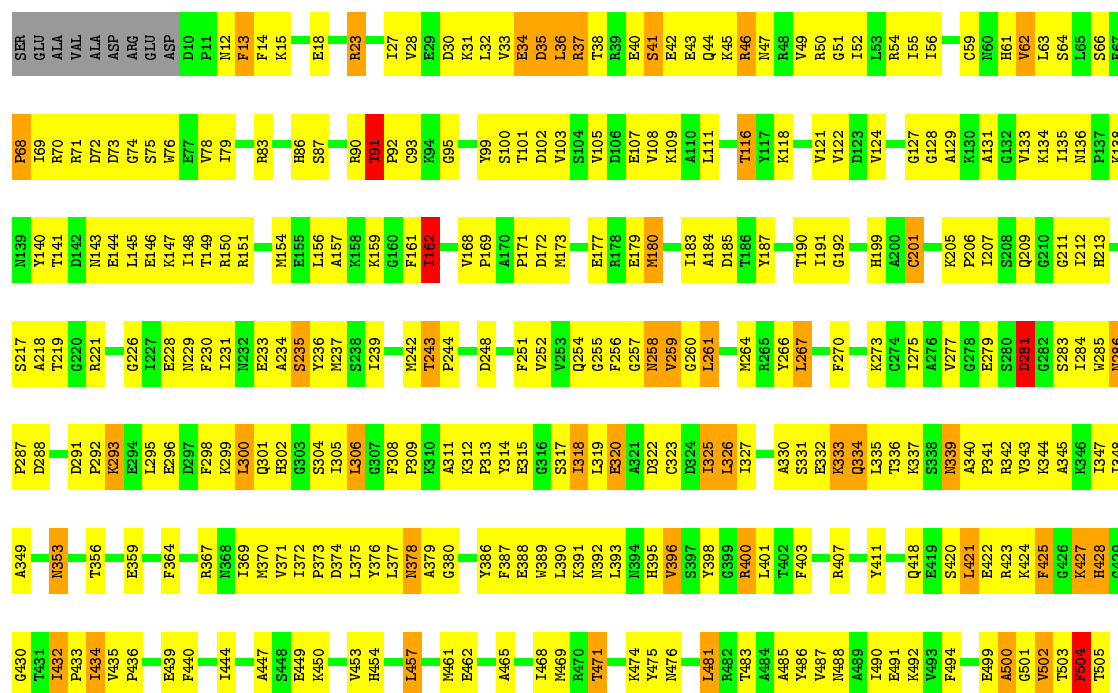
#### • Molecule 1: Glutamate Dehydrogenase 1





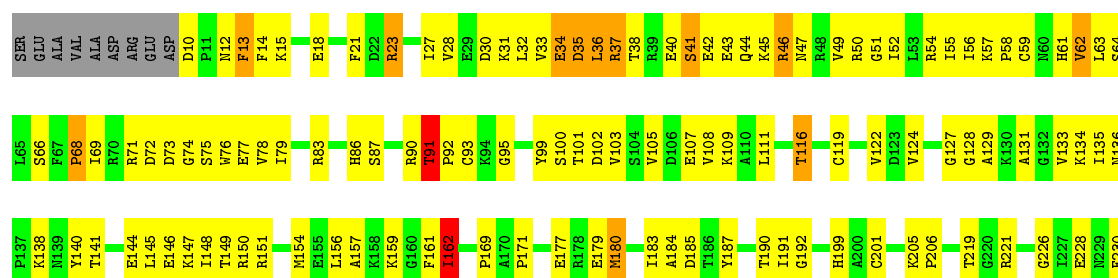
• Molecule 1: Glutamate Dehydrogenase 1

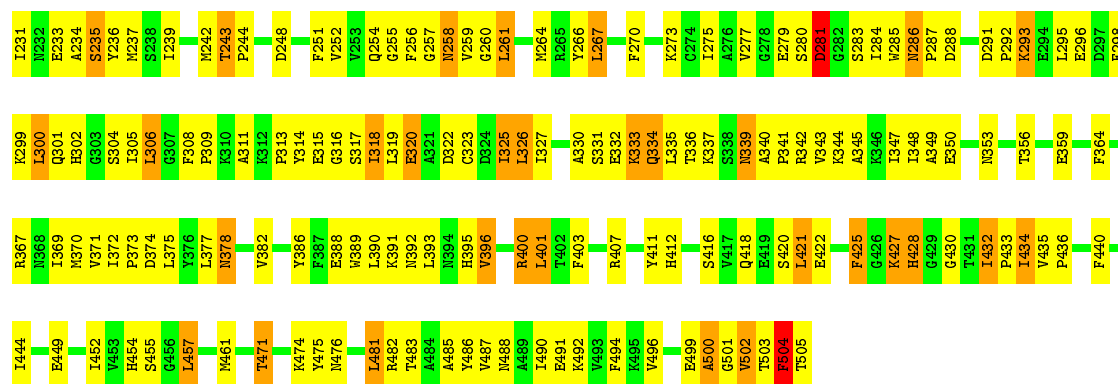
Chain C: 40% 49% 9% ..



• Molecule 1: Glutamate Dehydrogenase 1

Chain D: 43% 46% 9% ..





A234	G303	V371	H454
S235	S304	I372	I457
Y236	I305	D373	E462
M237	I306	D374	R463
G238	G307	L375	S464
I239	F308	Y376	A465
	P309	L377	T471
M242	K310	K378	K474
T243	A311	A379	Y475
P244	K312	Y386	M476
D248	P313		
	Y314	K389	
F251	E315	L390	
V252	G316	K391	
V253	S317	K392	L481
Q254	I318	L393	R482
G255	L319	K394	T483
F256	E320	K395	A484
G257	A321	V396	A485
M258	D322		Y486
G260	C323	R400	V487
L261	D324	L401	M488
	I325	T402	A489
	L326	F403	I490
	I327		E491
M264	P328	R407	K492
R265	A329	Y411	F494
Y266	A330		
L267	S331		E499
	E332		A500
		Q418	G501
F270	K333	E419	V502
	Q334	S420	T503
K273	L335	L421	F504
C274	T336	E422	T505
I275	K337	R423	
A276	S338	K424	
V277	M339	F425	
G278	A340	G426	
E279	P341	K427	
S280	R342	H428	
D281	V343	G429	
G282	K344	Q430	
S283	A345	T431	
I284	K346	I432	
M285	I347	P433	
I286	I348	T434	
P287	A349	V435	
D288		P436	
	M353		
		E439	
P292	T356	F440	
K293		I444	
E294	E359		
L295		A447	
E296	F364	S448	
D297		E449	
F298		K450	
K299	R367		
L300	M368		
Q301	I369		
H302	M370		

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.80 Å 98.80 Å 124.20 Å 86.26° 70.28° 60.34°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	O	Depositor
R, $R_{free}$	0.262 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	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	0.62	1/3958 (0.0%)	0.82	3/5340 (0.1%)
1	B	0.63	1/3958 (0.0%)	0.82	5/5340 (0.1%)
1	C	0.65	2/3958 (0.1%)	0.82	4/5340 (0.1%)
1	D	0.62	1/3958 (0.0%)	0.82	5/5340 (0.1%)
1	E	0.62	1/3958 (0.0%)	0.82	4/5340 (0.1%)
1	F	0.62	2/3958 (0.1%)	0.82	5/5340 (0.1%)
All	All	0.63	8/23748 (0.0%)	0.82	26/32040 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	59	CYS	CB-SG	8.91	1.97	1.82
1	C	59	CYS	CB-SG	8.33	1.96	1.82
1	A	59	CYS	CB-SG	7.79	1.95	1.82
1	B	59	CYS	CB-SG	7.48	1.95	1.82
1	F	201	CYS	CB-SG	-7.10	1.70	1.82

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	504	PHE	N-CA-C	-7.28	91.34	111.00
1	C	504	PHE	N-CA-C	-7.28	91.35	111.00
1	B	504	PHE	N-CA-C	-7.27	91.38	111.00
1	F	504	PHE	N-CA-C	-7.25	91.43	111.00
1	D	504	PHE	N-CA-C	-7.19	91.60	111.00

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	3874	0	3841	316	0
1	B	3874	0	3841	333	0
1	C	3874	0	3841	366	0
1	D	3874	0	3841	326	0
1	E	3874	0	3841	341	0
1	F	3874	0	3841	324	0
All	All	23244	0	23046	1865	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 40.

The worst 5 of 1865 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:C:285:TRP:HB2	1:C:314:TYR:HB2	1.31	1.13
1:E:285:TRP:HB2	1:E:314:TYR:HB2	1.30	1.12
1:F:285:TRP:HB2	1:F:314:TYR:HB2	1.29	1.09
1:A:285:TRP:HB2	1:A:314:TYR:HB2	1.30	1.08
1:B:285:TRP:HB2	1:B:314:TYR:HB2	1.29	1.08

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	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	<b>4</b> <b>9</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	4	9
1	C	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	4	9
1	D	494/505 (98%)	426 (86%)	49 (10%)	19 (4%)	4	9
1	E	494/505 (98%)	425 (86%)	50 (10%)	19 (4%)	4	9
1	F	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	4	9
All	All	2964/3030 (98%)	2563 (86%)	287 (10%)	114 (4%)	4	9

5 of 114 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	41	SER
1	A	91	THR
1	A	102	ASP
1	A	258	ASN

### 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	413/420 (98%)	365 (88%)	48 (12%)	7	16
1	B	413/420 (98%)	364 (88%)	49 (12%)	6	15
1	C	413/420 (98%)	365 (88%)	48 (12%)	7	16
1	D	413/420 (98%)	364 (88%)	49 (12%)	6	15
1	E	413/420 (98%)	365 (88%)	48 (12%)	7	16
1	F	413/420 (98%)	365 (88%)	48 (12%)	7	16
All	All	2478/2520 (98%)	2188 (88%)	290 (12%)	7	15

5 of 290 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	378	ASN

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Mol	Chain	Res	Type
1	D	235	SER
1	F	315	GLU
1	C	421	LEU
1	D	36	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	410	ASN
1	D	378	ASN
1	F	378	ASN
1	C	488	ASN
1	D	86	HIS

### 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 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.