



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 11:06 PM UTC

PDB ID : 1TOC / pdb\_00001toc  
Title : STRUCTURE OF SERINE PROTEINASE  
Authors : Van De Locht, A.; Huber, R.; Bode, W.  
Deposited on : 1996-07-20  
Resolution : 3.10 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

<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  
Xtrriage (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) : 2.49

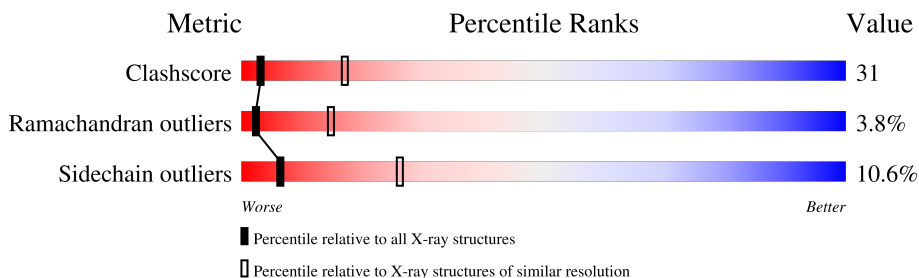
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)




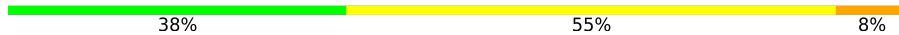
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	49	24% (green), 29% (yellow), 43% (grey), 6% (orange), 0% (red)
1	C	49	22% (green), 22% (yellow), 43% (grey), 12% (orange), 0% (red)
1	E	49	31% (green), 20% (yellow), 43% (grey), 6% (orange), 0% (red)
1	G	49	22% (green), 29% (yellow), 43% (grey), 6% (orange), 0% (red)
2	B	259	51% (green), 42% (yellow), 5% (orange), 0% (red)
2	D	259	49% (green), 43% (yellow), 8% (orange), 0% (red)
2	F	259	48% (green), 45% (yellow), 6% (orange), 0% (red)
2	H	259	46% (green), 49% (yellow), 5% (orange), 0% (red)

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	R	120	 39% 48% 11% •
3	S	120	 42% 45% 10% •
3	T	120	 42% 48% 11%
3	U	120	 38% 55% 8%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13467 atoms, of which 608 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 THROMBIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	28	244	148	10	37	48	1	10	0	0
1	C	28	244	148	10	37	48	1	10	0	0
1	E	28	244	148	10	37	48	1	10	0	0
1	G	28	244	148	10	37	48	1	21	0	0

- Molecule 2 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	259	2206	1337	112	376	369	12	147	0	0
2	D	259	2206	1337	112	376	369	12	160	0	0
2	F	259	2206	1337	112	376	369	12	135	0	0
2	H	259	2206	1337	112	376	369	12	145	0	0

- Molecule 3 is a protein called ORNITHODORIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	R	120	909	521	30	147	197	14	53	0	0
3	S	120	909	521	30	147	197	14	50	0	0
3	T	120	909	521	30	147	197	14	51	0	0
3	U	120	909	521	30	147	197	14	47	0	0

- Molecule 4 is water.

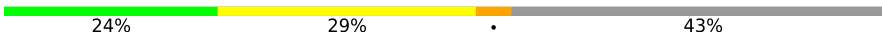
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	B	8	Total O 8 8	0	0
4	D	7	Total O 7 7	0	0
4	F	8	Total O 8 8	0	0
4	H	8	Total O 8 8	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

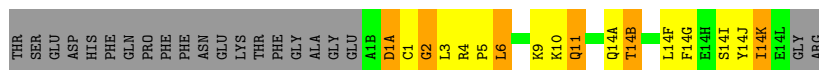
- Molecule 1: THROMBIN

Chain A: 




- Molecule 1: THROMBIN

Chain C: 



- Molecule 1: THROMBIN

Chain E: 



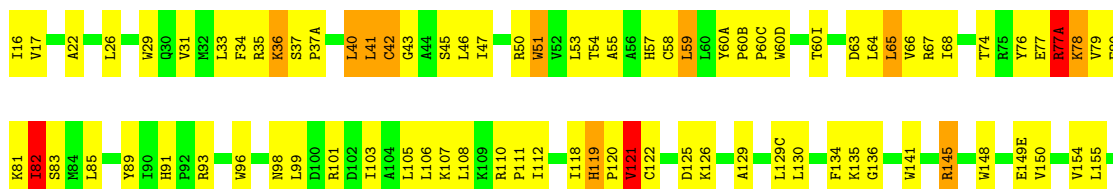
- Molecule 1: THROMBIN

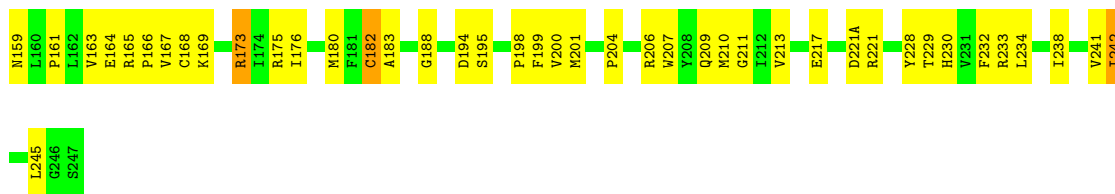
Chain G: 



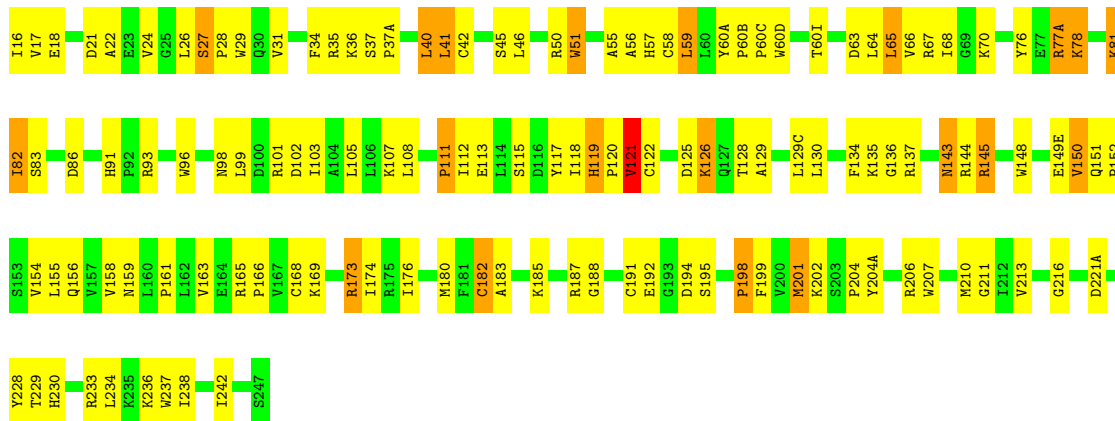
- Molecule 2: THROMBIN

Chain B: 

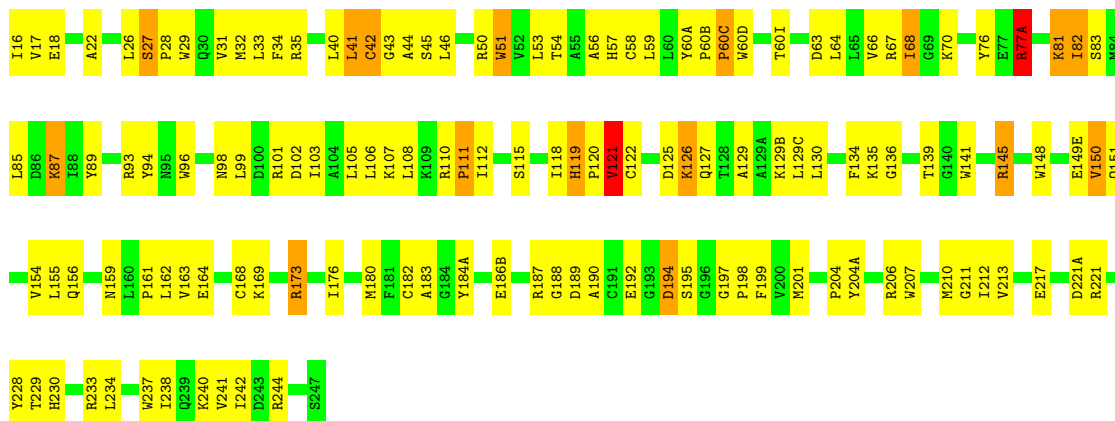




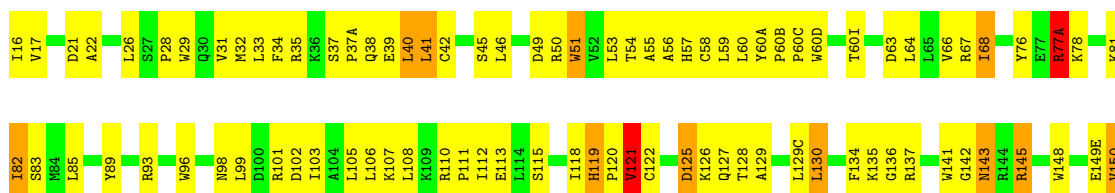
• Molecule 2: THROMBIN

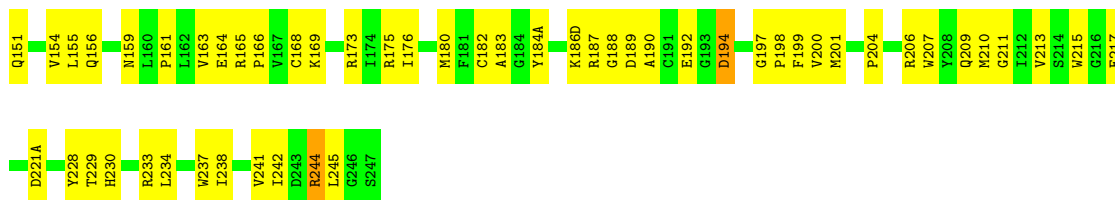


• Molecule 2: THROMBIN

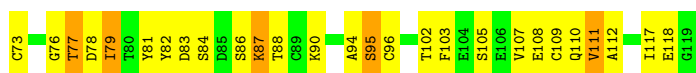
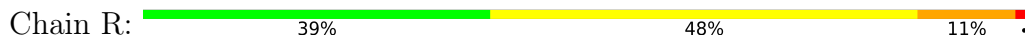


• Molecule 2: THROMBIN

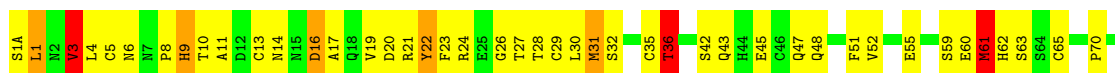




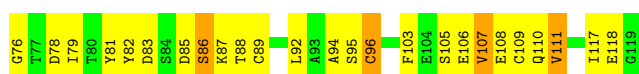
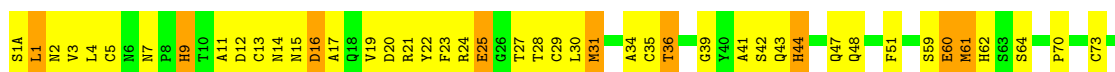
• Molecule 3: ORNITHODORIN



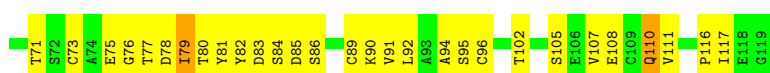
• Molecule 3: ORNITHODORIN



• Molecule 3: ORNITHODORIN



• Molecule 3: ORNITHODORIN



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	125.30Å 89.90Å 101.40Å 90.00° 108.40° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.10)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.230 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13467	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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	0.58	0/237	0.87	0/316
1	C	0.55	0/237	0.88	0/316
1	E	0.60	0/237	0.88	0/316
1	G	0.59	0/237	0.84	1/316 (0.3%)
2	B	0.72	0/2148	1.11	8/2905 (0.3%)
2	D	0.72	1/2148 (0.0%)	1.09	11/2905 (0.4%)
2	F	0.68	0/2148	1.11	10/2905 (0.3%)
2	H	0.70	1/2148 (0.0%)	1.14	12/2905 (0.4%)
3	R	0.71	1/895 (0.1%)	1.07	4/1215 (0.3%)
3	S	0.76	0/895	1.14	4/1215 (0.3%)
3	T	0.72	1/895 (0.1%)	1.08	2/1215 (0.2%)
3	U	0.70	1/895 (0.1%)	1.04	2/1215 (0.2%)
All	All	0.70	5/13120 (0.0%)	1.09	54/17744 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	S	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	MET	SD-CE	-7.22	1.61	1.79
3	U	48	GLN	CD-OE1	5.75	1.34	1.23
3	T	48	GLN	CD-OE1	5.53	1.34	1.23
3	R	48	GLN	CD-OE1	5.45	1.33	1.23
2	H	32	MET	SD-CE	5.38	1.93	1.79

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	51	TRP	N-CA-C	8.00	122.36	110.52
3	S	3	VAL	CB-CA-C	-7.84	98.43	111.29
2	F	51	TRP	N-CA-C	7.62	122.43	110.17
2	F	151	GLN	CA-C-N	7.17	127.17	119.78
2	F	151	GLN	C-N-CA	7.17	127.17	119.78

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	S	22	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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	234	10	227	14	0
1	C	234	10	227	20	0
1	E	234	10	227	10	0
1	G	234	10	227	16	0
2	B	2094	112	2097	121	0
2	D	2094	112	2097	144	0
2	F	2094	112	2097	136	0
2	H	2094	112	2097	141	0
3	R	879	30	768	73	0
3	S	879	30	768	65	0
3	T	879	30	768	68	0
3	U	879	30	768	62	0
4	B	8	0	0	1	0
4	D	7	0	0	1	0
4	F	8	0	0	2	0
4	H	8	0	0	2	0
All	All	12859	608	12368	766	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 31.

The worst 5 of 766 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:H:81:LYS:HE3	2:H:113:GLU:HB3	1.33	1.08
2:D:99:LEU:HD11	3:S:1:LEU:HD13	1.42	0.98
2:B:217:GLU:HB3	3:R:4:LEU:HD21	1.48	0.95
3:S:107:VAL:HA	3:S:110:GLN:HE21	1.30	0.93
3:S:28:THR:HG23	3:S:30:LEU:HD21	1.48	0.93

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	26/49 (53%)	16 (62%)	6 (23%)	4 (15%)	0	0
1	C	26/49 (53%)	16 (62%)	5 (19%)	5 (19%)	0	0
1	E	26/49 (53%)	16 (62%)	6 (23%)	4 (15%)	0	0
1	G	26/49 (53%)	16 (62%)	5 (19%)	5 (19%)	0	0
2	B	257/259 (99%)	218 (85%)	34 (13%)	5 (2%)	6	27
2	D	257/259 (99%)	217 (84%)	35 (14%)	5 (2%)	6	27
2	F	257/259 (99%)	216 (84%)	35 (14%)	6 (2%)	5	23
2	H	257/259 (99%)	217 (84%)	35 (14%)	5 (2%)	6	27
3	R	118/120 (98%)	93 (79%)	20 (17%)	5 (4%)	2	13
3	S	118/120 (98%)	91 (77%)	21 (18%)	6 (5%)	1	10
3	T	118/120 (98%)	91 (77%)	21 (18%)	6 (5%)	1	10
3	U	118/120 (98%)	91 (77%)	22 (19%)	5 (4%)	2	13
All	All	1604/1712 (94%)	1298 (81%)	245 (15%)	61 (4%)	2	15

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	77(A)	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	149(E)	GLU
1	C	2	GLY
2	D	77(A)	ARG
2	D	149(E)	GLU

### 5.3.2 Protein sidechains [i](#)

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	26/43 (60%)	23 (88%)	3 (12%)	5	23
1	C	26/43 (60%)	23 (88%)	3 (12%)	5	23
1	E	26/43 (60%)	23 (88%)	3 (12%)	5	23
1	G	26/43 (60%)	23 (88%)	3 (12%)	5	23
2	B	226/226 (100%)	209 (92%)	17 (8%)	12	39
2	D	226/226 (100%)	210 (93%)	16 (7%)	13	41
2	F	226/226 (100%)	213 (94%)	13 (6%)	18	48
2	H	226/226 (100%)	214 (95%)	12 (5%)	20	51
3	R	101/101 (100%)	81 (80%)	20 (20%)	1	6
3	S	101/101 (100%)	78 (77%)	23 (23%)	1	4
3	T	101/101 (100%)	84 (83%)	17 (17%)	2	10
3	U	101/101 (100%)	81 (80%)	20 (20%)	1	6
All	All	1412/1480 (95%)	1262 (89%)	150 (11%)	6	26

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	3	LEU
3	U	73	CYS
2	H	41	LEU
3	U	1(A)	SER
2	D	78	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
3	S	14	ASN
2	F	57	HIS
3	U	43	GLN
3	S	62	HIS
3	T	15	ASN

### 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](#)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.