



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 08:53 AM EDT

PDB ID : 5BJ4
Title : THERMUS THERMOPHILUS ASPARTATE AMINOTRANSFERASE
TETRA MUTANT 2
Authors : Ura, H.; Nakai, T.; Kawaguchi, S.I.; Miyahara, I.; Hirotsu, K.; Kuramitsu, S.
Deposited on : 1999-01-11
Resolution : 2.00 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

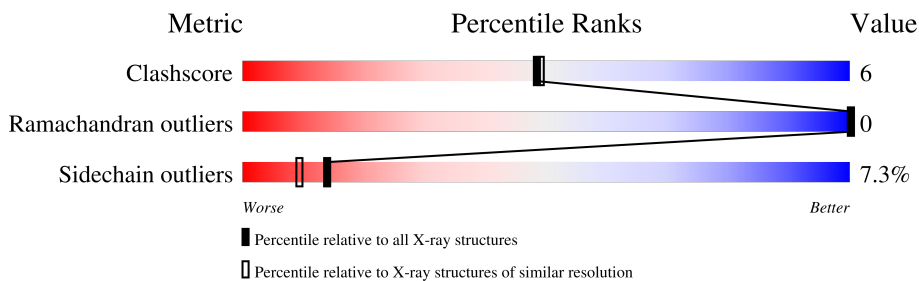
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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	385	 77% 16% • 5%
1	B	385	 82% 12% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5952 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 PROTEIN (ASPARTATE AMINOTRANSFERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2826	1791	498	529	8			
1	B	366	Total	C	N	O	S	0	0	0
			2826	1791	498	529	8			

There are 8 discrepancies between the modelled and reference sequences:

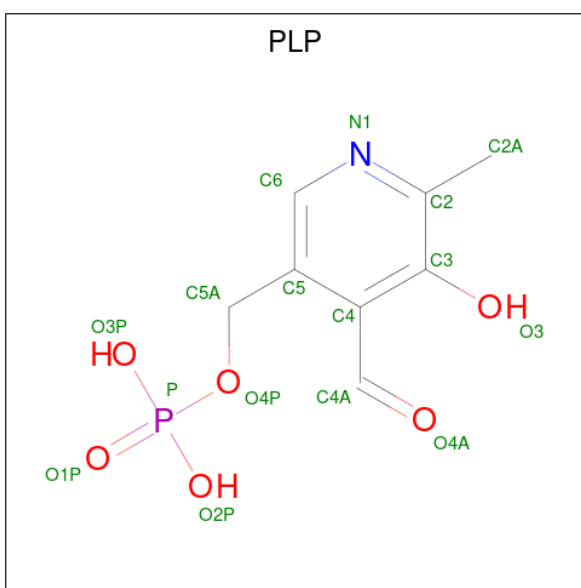
Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ASP	SER	engineered mutation	UNP Q56232
A	16	VAL	THR	engineered mutation	UNP Q56232
A	101	SER	LYS	engineered mutation	UNP Q56232
A	261	ARG	SER	engineered mutation	UNP Q56232
B	14	ASP	SER	engineered mutation	UNP Q56232
B	16	VAL	THR	engineered mutation	UNP Q56232
B	101	SER	LYS	engineered mutation	UNP Q56232
B	261	ARG	SER	engineered mutation	UNP Q56232

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	P		0	0
			5	4	1			
2	B	1	Total	O	P		0	0
			5	4	1			

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	115	Total 115	O 115	0	0
4	B	145	Total 145	O 145	0	0

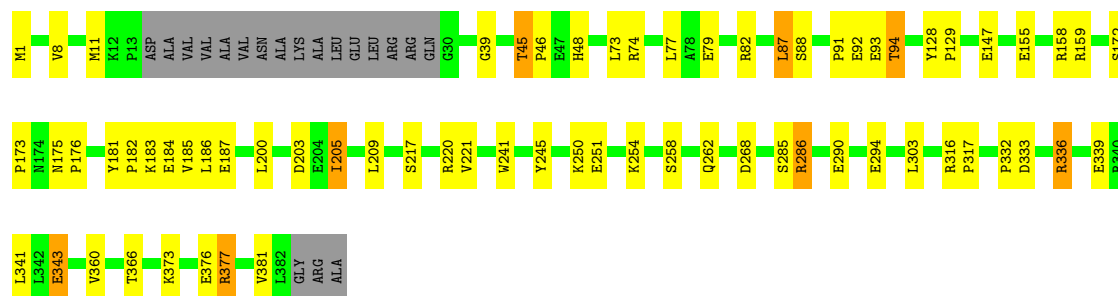
3 Residue-property plots

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.

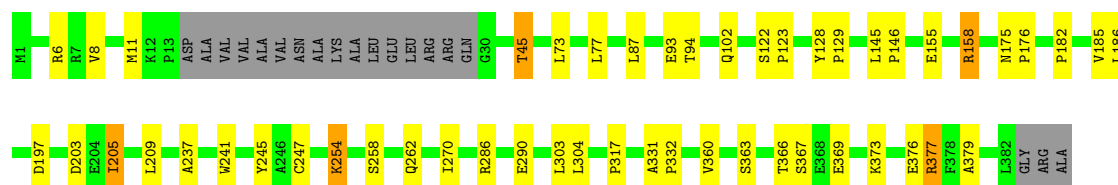
• Molecule 1: PROTEIN (ASPARTATE AMINOTRANSFERASE)

Chain A: 



• Molecule 1: PROTEIN (ASPARTATE AMINOTRANSFERASE)

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.78Å 113.52Å 124.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	82.8 (8.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.185 , 0.214	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5952	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: PLP, PO4

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	0.38	0/2886	0.68	1/3924 (0.0%)
1	B	0.40	0/2886	0.70	1/3924 (0.0%)
All	All	0.39	0/5772	0.69	2/7848 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ASN	N-CA-C	-5.62	95.84	111.00
1	A	175	ASN	N-CA-C	-5.34	96.57	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2826	0	2830	43	0
1	B	2826	0	2830	31	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
4	A	115	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	145	0	0	1	0
All	All	5952	0	5674	68	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 6.

All (68) 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:A:45:THR:HG21	1:A:241:TRP:HE1	1.34	0.92
1:B:45:THR:HG21	1:B:241:TRP:HE1	1.34	0.91
1:B:286:ARG:O	1:B:290:GLU:HG2	1.89	0.71
1:A:217:SER:O	1:A:220:ARG:HG3	1.92	0.69
1:B:373:LYS:O	1:B:377:ARG:HG2	1.94	0.68
1:A:332:PRO:HG2	1:A:336:ARG:NH2	2.09	0.67
1:A:251:GLU:HA	1:A:254:LYS:HE3	1.75	0.66
1:A:155:GLU:O	1:A:159:ARG:HG3	1.98	0.64
1:A:45:THR:HG21	1:A:241:TRP:NE1	2.11	0.63
1:B:45:THR:HG21	1:B:241:TRP:NE1	2.09	0.63
1:A:373:LYS:O	1:A:377:ARG:HG2	2.00	0.61
1:A:339:GLU:O	1:A:343:GLU:HG2	2.02	0.59
1:A:11:MET:CE	1:B:258:SER:HB3	2.33	0.58
1:B:128:TYR:HB2	1:B:129:PRO:HD3	1.87	0.56
1:A:258:SER:HB3	1:B:11:MET:CE	2.36	0.56
1:B:203:ASP:OD1	1:B:205:ILE:HG13	2.06	0.56
1:B:262:GLN:NE2	1:B:262:GLN:HA	2.22	0.55
1:A:79:GLU:HG2	1:A:82:ARG:HH21	1.72	0.55
1:A:373:LYS:HB2	1:A:373:LYS:NZ	2.21	0.55
1:A:262:GLN:NE2	1:A:262:GLN:HA	2.22	0.54
1:A:258:SER:HB3	1:B:11:MET:HE2	1.89	0.53
1:A:333:ASP:OD1	1:A:336:ARG:HG3	2.09	0.52
1:A:184:GLU:H	1:A:184:GLU:CD	2.13	0.52
1:A:203:ASP:OD1	1:A:205:ILE:HG13	2.09	0.52
1:A:93:GLU:CG	1:A:250:LYS:HD2	2.40	0.52
1:A:183:LYS:O	1:A:187:GLU:HG3	2.10	0.51
1:A:11:MET:HE2	1:B:258:SER:HB3	1.91	0.51
1:A:286:ARG:O	1:A:290:GLU:HG2	2.12	0.50
1:A:366:THR:HG21	4:A:603:HOH:O	2.10	0.50
1:A:79:GLU:HG2	1:A:82:ARG:NH2	2.25	0.50
1:A:82:ARG:HA	1:A:87:LEU:O	2.12	0.49
1:B:270:ILE:HD12	1:B:270:ILE:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:THR:HG22	1:B:237:ALA:O	2.14	0.48
1:B:158:ARG:O	1:B:158:ARG:NE	2.47	0.48
1:B:376:GLU:O	1:B:379:ALA:HB3	2.14	0.48
1:B:182:PRO:HG2	1:B:185:VAL:HG23	1.96	0.47
1:A:48:HIS:HE1	1:A:285:SER:OG	1.98	0.47
1:B:304:LEU:HD11	1:B:317:PRO:HD2	1.96	0.47
1:B:254:LYS:HB3	1:B:254:LYS:HE3	1.51	0.46
1:A:39:GLY:HA3	2:A:414:PO4:O2	2.14	0.46
1:A:1:MET:HA	1:B:197:ASP:O	2.16	0.46
1:B:254:LYS:HD2	4:B:826:HOH:O	2.16	0.46
1:A:91:PRO:O	1:A:94:THR:HB	2.16	0.46
1:B:262:GLN:HA	1:B:262:GLN:HE21	1.80	0.46
1:B:369:GLU:H	1:B:369:GLU:CD	2.20	0.45
1:A:74:ARG:HA	1:A:94:THR:HG21	1.99	0.44
1:A:46:PRO:HB2	1:A:48:HIS:CD2	2.52	0.44
1:B:93:GLU:O	1:B:247:CYS:HA	2.17	0.44
1:A:92:GLU:HB2	1:A:250:LYS:HE3	1.99	0.44
1:B:377:ARG:HG2	1:B:377:ARG:H	1.57	0.44
1:A:268:ASP:OD1	1:B:241:TRP:HA	2.18	0.43
1:A:341:LEU:HD23	1:A:381:VAL:HG21	2.00	0.43
1:B:182:PRO:HG2	1:B:185:VAL:CG2	2.47	0.43
1:A:182:PRO:HG2	1:A:185:VAL:HG23	2.00	0.43
1:B:102:GLN:O	1:B:102:GLN:HG2	2.16	0.43
1:B:367:SER:HB2	1:B:369:GLU:OE1	2.18	0.43
1:A:155:GLU:OE2	1:A:158:ARG:HD2	2.19	0.43
1:A:172:SER:HA	1:A:173:PRO:C	2.40	0.43
1:B:331:ALA:HB1	1:B:332:PRO:HD2	2.01	0.43
1:A:182:PRO:HB2	1:A:184:GLU:OE1	2.20	0.42
1:A:262:GLN:HA	1:A:262:GLN:HE21	1.85	0.42
1:A:128:TYR:HB2	1:A:129:PRO:CD	2.50	0.41
1:B:122:SER:HA	1:B:123:PRO:C	2.41	0.41
1:A:93:GLU:HG2	1:A:250:LYS:HD2	2.01	0.41
1:A:82:ARG:HG3	4:A:600:HOH:O	2.19	0.41
1:A:316:ARG:HA	1:A:317:PRO:HD2	1.97	0.40
1:B:145:LEU:HA	1:B:146:PRO:HD3	1.90	0.40
1:A:181:TYR:N	1:A:181:TYR:CD1	2.89	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	362/385 (94%)	353 (98%)	9 (2%)	0	100	100
1	B	362/385 (94%)	353 (98%)	9 (2%)	0	100	100
All	All	724/770 (94%)	706 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	293/306 (96%)	270 (92%)	23 (8%)	12	8
1	B	293/306 (96%)	273 (93%)	20 (7%)	16	11
All	All	586/612 (96%)	543 (93%)	43 (7%)	14	9

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	45	THR
1	A	73	LEU
1	A	77	LEU
1	A	87	LEU
1	A	88	SER
1	A	94	THR
1	A	147	GLU

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Mol	Chain	Res	Type
1	A	176	PRO
1	A	186	LEU
1	A	200	LEU
1	A	205	ILE
1	A	209	LEU
1	A	221	VAL
1	A	245	TYR
1	A	286	ARG
1	A	294	GLU
1	A	303	LEU
1	A	336	ARG
1	A	343	GLU
1	A	360	VAL
1	A	376	GLU
1	A	377	ARG
1	B	6	ARG
1	B	8	VAL
1	B	45	THR
1	B	73	LEU
1	B	77	LEU
1	B	87	LEU
1	B	94	THR
1	B	155	GLU
1	B	158	ARG
1	B	176	PRO
1	B	186	LEU
1	B	205	ILE
1	B	209	LEU
1	B	245	TYR
1	B	254	LYS
1	B	303	LEU
1	B	360	VAL
1	B	363	SER
1	B	366	THR
1	B	377	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	208	HIS
1	A	262	GLN

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Mol	Chain	Res	Type
1	A	370	ASN
1	B	48	HIS
1	B	59	GLN
1	B	106	ASN
1	B	208	HIS
1	B	262	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	PLP	B	2413	1	15,15,16	2.08	4 (26%)	20,22,23	1.65	4 (20%)
2	PO4	B	415	-	4,4,4	0.90	0	6,6,6	0.78	0
2	PO4	A	414	-	4,4,4	0.89	0	6,6,6	0.75	0
3	PLP	A	1413	1	15,15,16	1.45	1 (6%)	20,22,23	1.93	4 (20%)

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	PLP	B	2413	1	-	2/6/6/8	0/1/1/1
3	PLP	A	1413	1	-	2/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2413	PLP	C5-C4	5.06	1.46	1.40
3	A	1413	PLP	C3-C2	-3.61	1.37	1.40
3	B	2413	PLP	C3-C2	-3.39	1.37	1.40
3	B	2413	PLP	C2A-C2	2.93	1.55	1.50
3	B	2413	PLP	P-O1P	-2.05	1.43	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1413	PLP	O4P-C5A-C5	5.96	120.70	109.35
3	B	2413	PLP	O4P-C5A-C5	4.92	118.73	109.35
3	A	1413	PLP	O2P-P-O4P	-2.92	98.97	106.73
3	B	2413	PLP	C5A-C5-C6	-2.49	115.27	119.37
3	B	2413	PLP	C5-C6-N1	-2.49	119.68	123.82
3	A	1413	PLP	C4A-C4-C5	2.33	123.33	120.94
3	B	2413	PLP	O2P-P-O4P	-2.05	101.27	106.73
3	A	1413	PLP	C5A-C5-C6	-2.04	116.02	119.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1413	PLP	C4-C5-C5A-O4P
3	A	1413	PLP	C6-C5-C5A-O4P
3	B	2413	PLP	C4-C5-C5A-O4P
3	B	2413	PLP	C6-C5-C5A-O4P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	414	PO4	1	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.