



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:28 PM UTC

PDB ID : 1RYZ / pdb_00001ryz
Title : Uridine Phosphorylase from Salmonella typhimurium. Crystal Structure at 2.9 Å Resolution
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Deposited on : 2003-12-23
Resolution : 2.90 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)	:	2.49

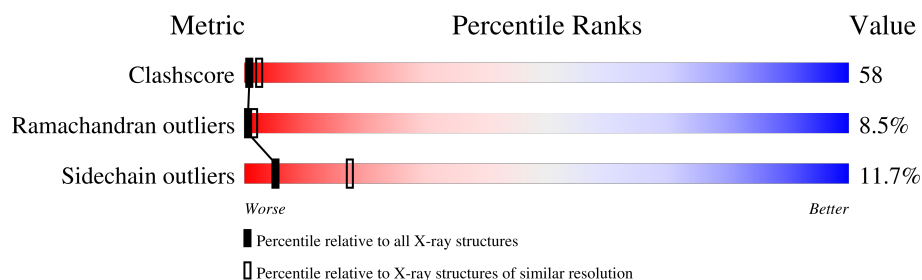
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	253	29% 54% 13% ..
1	B	253	26% 58% 13% ..
1	C	253	27% 56% 15% ..
1	D	253	30% 53% 15% ..
1	E	253	26% 57% 13% ..
1	F	253	26% 54% 16% ..

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACY	B	254	-	-	X	-

2 Entry composition [i](#)

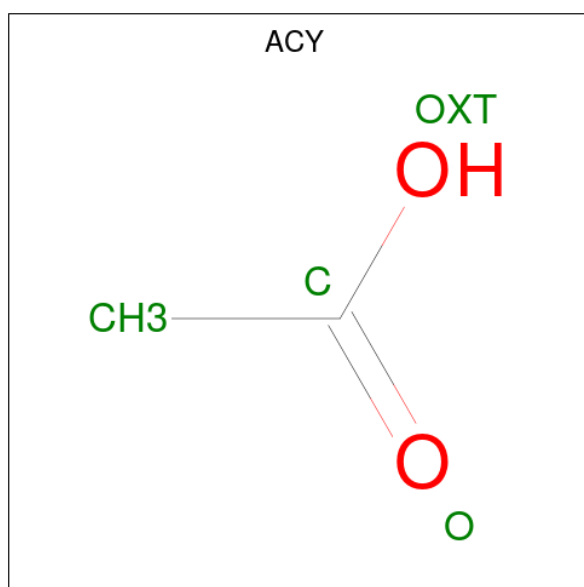
There are 2 unique types of molecules in this entry. The entry contains 11270 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	B	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	C	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	D	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	E	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	F	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			

- Molecule 2 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



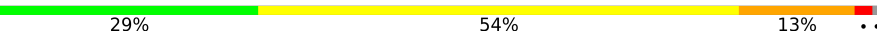
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

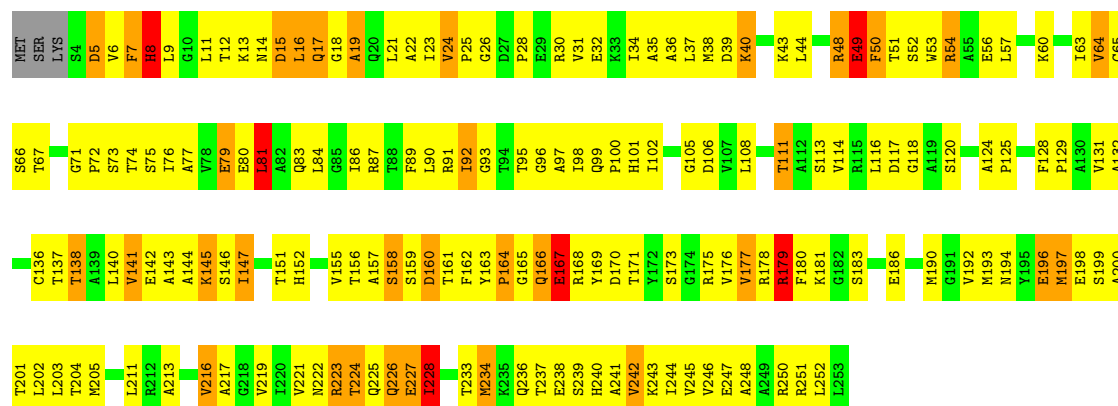
3 Residue-property plots

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.

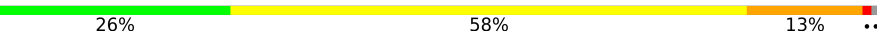
Note EDS was not executed.

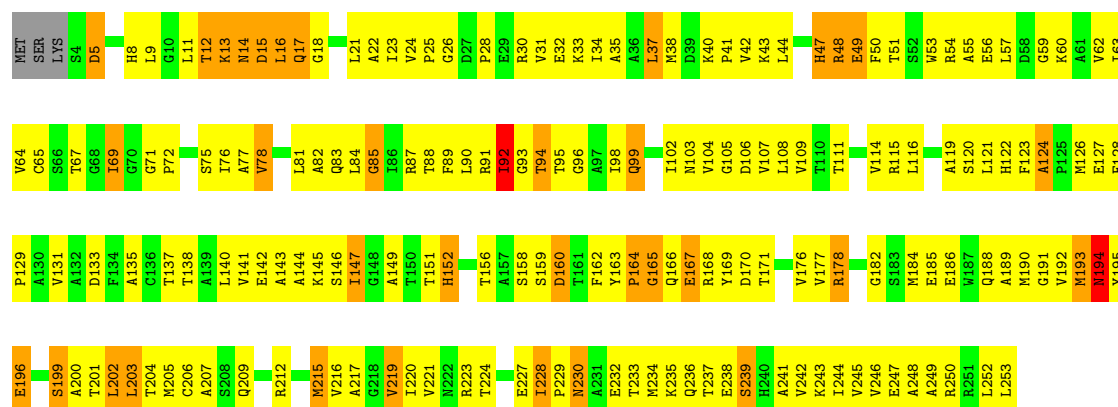
• Molecule 1: Uridine phosphorylase

Chain A: 

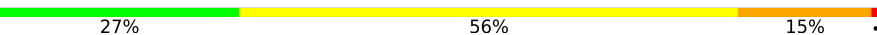


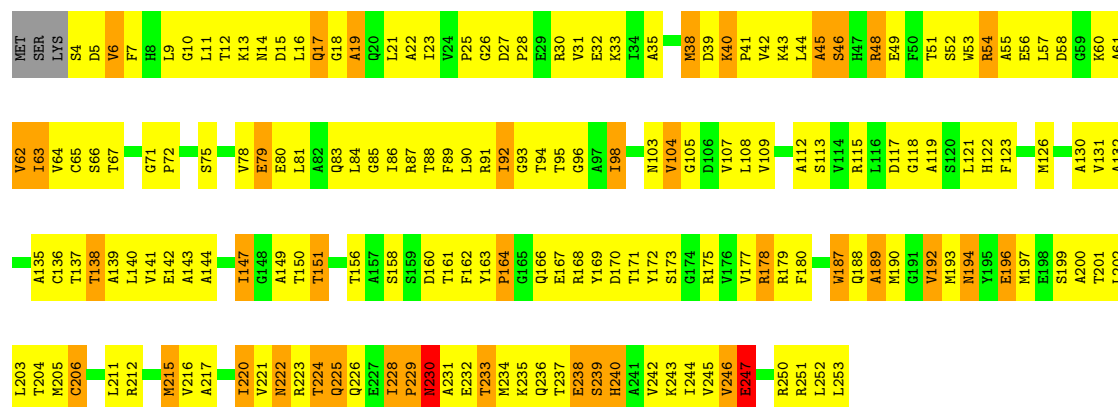
• Molecule 1: Uridine phosphorylase

Chain B: 



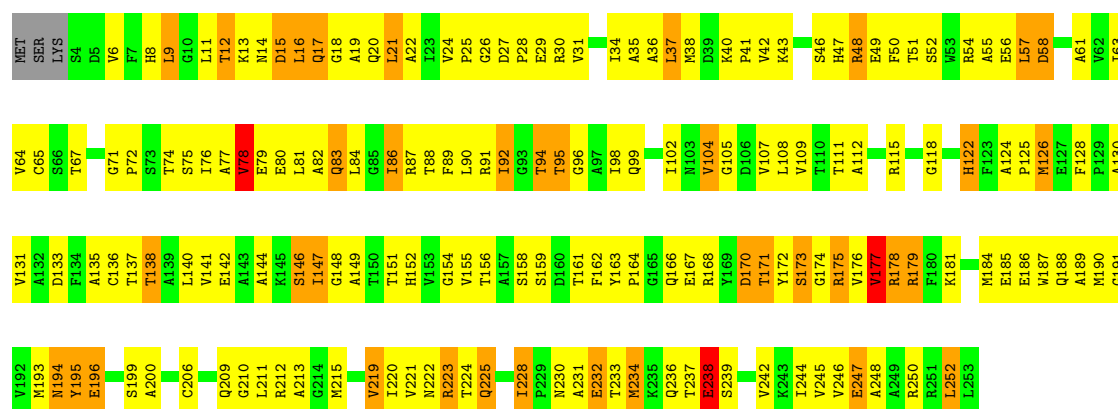
• Molecule 1: Uridine phosphorylase

Chain C: 



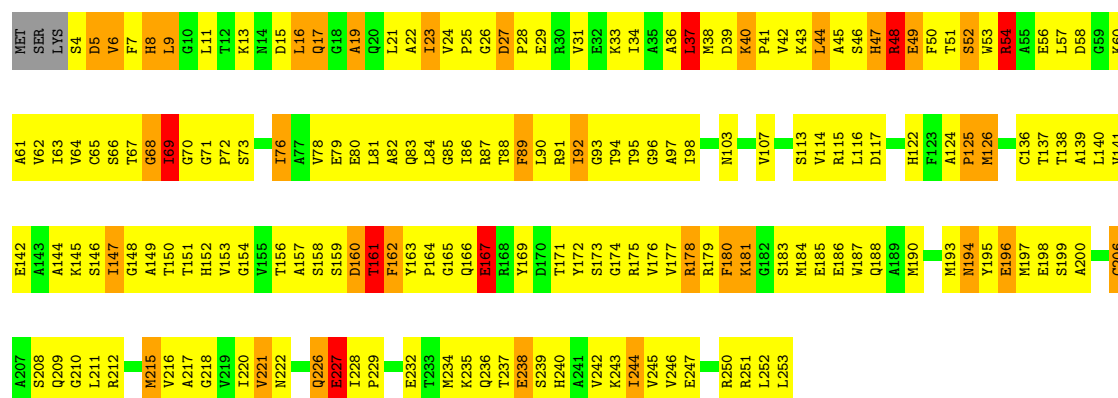
• Molecule 1: Uridine phosphorylase

Chain D: 30% 53% 15% ..



• Molecule 1: Uridine phosphorylase

Chain E: 26% 57% 13% ..



• Molecule 1: Uridine phosphorylase

Chain F: 26% 54% 16% ..

E198	A132	G71	MET
A200	D133	P72	SER
A199	T138	G71	LVS
T201	T139	S75	S4
L202	L140	T76	D5
L203	V141	A77	V6
T204	E142	T78	F7
M205	A143	E79	H8
C206	A144	E80	L9
S207	K145	L81	G10
S208	S146	L81	L11
Q209	T147	A82	T12
R212	G148	G83	K13
M215	A149	L84	M14
V216	T150	G85	D15
A217	T151	L86	L16
G218	H152	R87	Q17
V219	V153	T88	
L220	G154	F89	L21
T221	E155	L90	A22
L222	T156	R91	L92
N222	T157	T92	I23
R223	A157	G93	V24
E227	S158	T94	P25
L228	D160	T95	G26
P229	T161	G96	D27
N300	F162	A97	P28
N301	V163	T98	E29
A301	T164	G99	R30
E302	G165	P100	V81
T303	Q166	H101	E32
M304	E167	I102	K33
K305	R168	M103	I34
Q306	V169	V104	A35
T307	D170	G105	A36
E308	T171	D106	L37
H400	S172	L108	K38
A401	G174	V109	D39
V402	R175	T110	
K403	T176	T111	L44
L404	V177	A112	H47
E407	R178	S113	R48
A408	T179	V114	E49
E409	F180	L115	F50
R250	S183	L116	T51
R251	M184	D117	S52
L252	E185	G118	V53
L253	L187	A119	R54
	Q188	S120	A55
		F123	E56
		A124	L57
		P125	D58
		M126	G59
		T127	K60
		F128	A61
		P129	V62
		A130	I63
		V131	V64
			C65
			S66

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	92.26 Å 92.26 Å 267.46 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.46 – 2.90	Depositor
% Data completeness (in resolution range)	93.9 (29.46-2.90)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	0.18	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11270	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: ACY

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	0.53	0/1907	1.13	16/2584 (0.6%)
1	B	0.51	0/1907	1.07	14/2584 (0.5%)
1	C	0.50	0/1907	1.07	14/2584 (0.5%)
1	D	0.51	0/1907	1.05	10/2584 (0.4%)
1	E	0.54	0/1907	1.11	15/2584 (0.6%)
1	F	0.52	0/1907	1.11	14/2584 (0.5%)
All	All	0.52	0/11442	1.09	83/15504 (0.5%)

There are no bond length outliers.

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	6	VAL	N-CA-C	-9.13	94.29	108.44
1	F	98	ILE	N-CA-C	-8.94	104.66	111.90
1	F	227	GLU	N-CA-C	8.64	122.28	109.24
1	E	47	HIS	N-CA-C	7.81	124.98	114.12
1	F	49	GLU	N-CA-C	-7.64	101.63	113.02

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	1877	0	1887	192	0
1	B	1877	0	1887	241	0
1	C	1877	0	1887	204	0
1	D	1877	0	1887	212	0
1	E	1877	0	1887	263	0
1	F	1877	0	1887	252	0
2	B	8	0	6	5	0
All	All	11270	0	11328	1300	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 58.

The worst 5 of 1300 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:232:GLU:HG2	1:B:236:GLN:HB2	1.27	1.16
1:E:167:GLU:HG3	1:E:183:SER:H	1.15	1.10
1:C:201:THR:HG22	1:C:205:MET:HE2	1.34	1.08
1:C:228:ILE:HB	1:C:229:PRO:HD2	1.37	1.06
1:C:104:VAL:HG11	1:C:229:PRO:HB3	1.34	1.06

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	248/253 (98%)	172 (69%)	53 (21%)	23 (9%)	0	1
1	B	248/253 (98%)	174 (70%)	55 (22%)	19 (8%)	1	2
1	C	248/253 (98%)	186 (75%)	40 (16%)	22 (9%)	0	1
1	D	248/253 (98%)	174 (70%)	58 (23%)	16 (6%)	1	3
1	E	248/253 (98%)	166 (67%)	57 (23%)	25 (10%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	248/253 (98%)	168 (68%)	59 (24%)	21 (8%)	0	1
All	All	1488/1518 (98%)	1040 (70%)	322 (22%)	126 (8%)	0	1

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	17	GLN
1	A	26	GLY
1	A	167	GLU
1	A	223	ARG

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	199/202 (98%)	176 (88%)	23 (12%)	5	18
1	B	199/202 (98%)	183 (92%)	16 (8%)	11	34
1	C	199/202 (98%)	180 (90%)	19 (10%)	8	26
1	D	199/202 (98%)	168 (84%)	31 (16%)	2	9
1	E	199/202 (98%)	176 (88%)	23 (12%)	5	18
1	F	199/202 (98%)	171 (86%)	28 (14%)	3	11
All	All	1194/1212 (98%)	1054 (88%)	140 (12%)	5	17

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	38	MET
1	F	98	ILE
1	F	185	GLU
1	C	108	LEU
1	C	104	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	225	GLN
1	E	209	GLN
1	D	226	GLN
1	E	47	HIS
1	E	240	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	ACY	B	255	-	3,3,3	1.65	0	3,3,3	1.29	0
2	ACY	B	254	-	3,3,3	1.49	0	3,3,3	1.37	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	254	ACY	5	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 [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.