



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:24 pm BST

PDB ID : 6AEF  
Title : PapA2 acyl transferase  
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Deposited on : 2018-08-04  
Resolution : 2.16 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

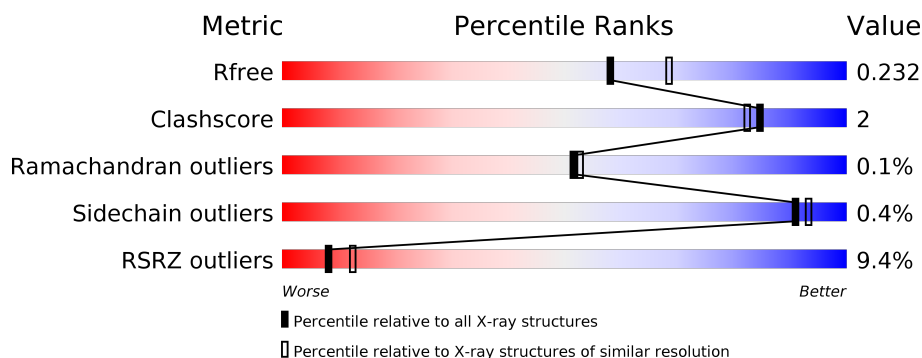
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	468	<div> <div>14%</div> <div> <div></div> <div>93%</div> <div>5% •</div> </div> </div>
1	B	468	<div> <div>4%</div> <div> <div></div> <div>94%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14660 atoms, of which 6968 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 Polyketide synthase associated protein PapA2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	458	Total	C	H	N	O	S	0	0	0
			7076	2278	3473	638	668	19			
1	A	458	Total	C	H	N	O	S	0	0	0
			7083	2278	3480	638	668	19			

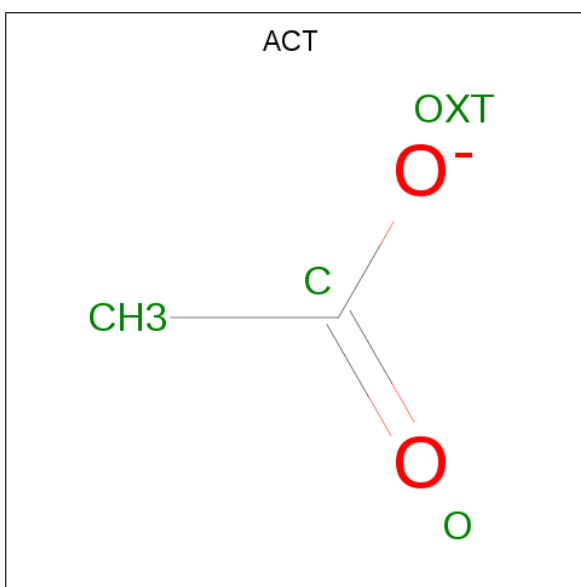
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	VAL	-	expression tag	UNP R4MC47
A	1	VAL	-	expression tag	UNP R4MC47

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

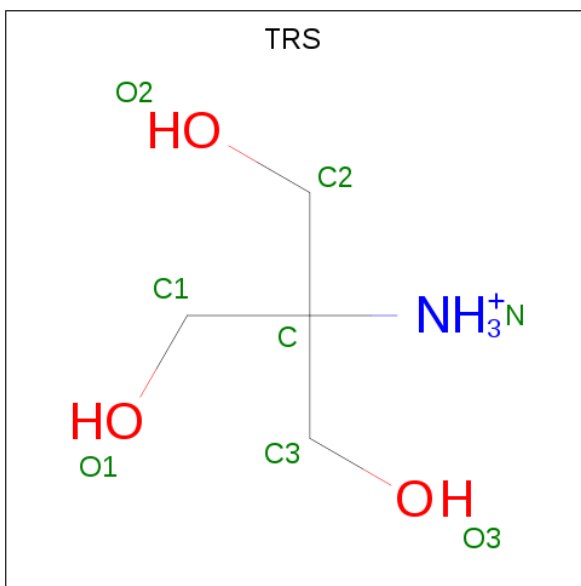
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

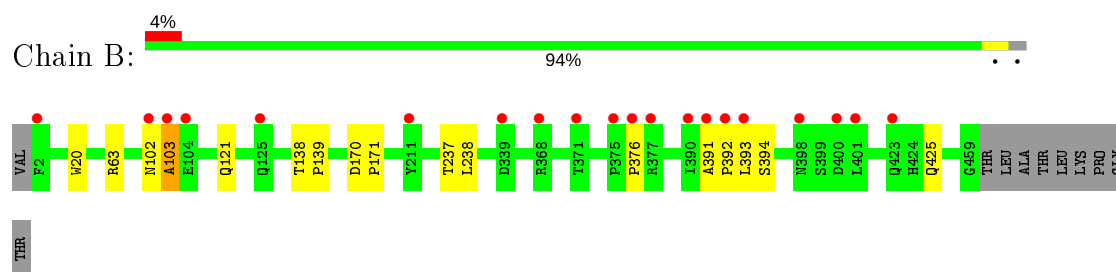
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	259	Total 259	O 259	0	0
5	A	213	Total 213	O 213	0	0

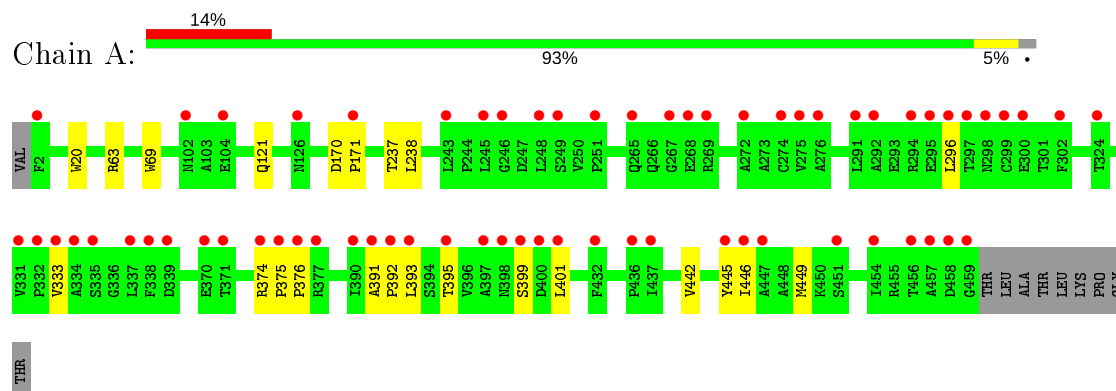
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 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.

- Molecule 1: Polyketide synthase associated protein PapA2



- Molecule 1: Polyketide synthase associated protein PapA2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.71Å 100.67Å 128.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.71 – 2.16 39.71 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.4 (39.71-2.16) 98.7 (39.71-2.16)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575)	Depositor
R, $R_{free}$	0.198 , 0.232 0.202 , 0.232	Depositor DCC
$R_{free}$ test set	2642 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 36.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14660	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, TRS, ACT

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	0.43	0/3702	0.60	0/5056
1	B	0.40	0/3702	0.54	0/5056
All	All	0.41	0/7404	0.57	0/10112

There are no bond length outliers.

There are no bond angle outliers.

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	3603	3480	3479	17	0
1	B	3603	3473	3479	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	3	3	0	0
4	A	8	12	12	0	0
5	A	213	0	0	0	0
5	B	259	0	0	0	0
All	All	7692	6968	6973	32	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 2.



All (32) 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:391:ALA:HB1	1:B:392:PRO:HD2	1.75	0.69
1:A:69:TRP:CD1	1:A:401:LEU:HD23	2.28	0.68
1:B:237:THR:OG1	1:B:376:PRO:HD3	1.98	0.64
1:B:237:THR:OG1	1:B:376:PRO:CD	2.49	0.61
1:A:237:THR:HG23	1:A:238:LEU:O	2.04	0.58
1:A:395:THR:O	1:A:399:SER:HB2	2.07	0.55
1:A:391:ALA:C	1:A:393:LEU:N	2.61	0.53
1:B:391:ALA:HB1	1:B:392:PRO:CD	2.36	0.53
1:A:296:LEU:CD1	1:A:445:TYR:HA	2.39	0.53
1:B:102:ASN:O	1:B:103:ALA:HB3	2.10	0.51
1:B:391:ALA:C	1:B:393:LEU:N	2.63	0.51
1:B:237:THR:HG23	1:B:238:LEU:N	2.25	0.51
1:A:237:THR:HG23	1:A:238:LEU:N	2.26	0.49
1:A:237:THR:OG1	1:A:376:PRO:HB3	2.13	0.48
1:A:333:VAL:HG13	1:A:333:VAL:O	2.12	0.48
1:A:296:LEU:HD11	1:A:445:TYR:HA	1.95	0.47
1:B:102:ASN:O	1:B:103:ALA:CB	2.61	0.47
1:A:170:ASP:HB2	1:A:171:PRO:CD	2.44	0.47
1:B:138:THR:N	1:B:139:PRO:CD	2.77	0.46
1:B:170:ASP:HB2	1:B:171:PRO:CD	2.45	0.46
1:B:238:LEU:H	1:B:376:PRO:HG3	1.79	0.46
1:A:392:PRO:O	1:A:393:LEU:C	2.54	0.45
1:A:170:ASP:HB2	1:A:171:PRO:HD2	1.99	0.44
1:A:391:ALA:C	1:A:393:LEU:H	2.20	0.44
1:B:391:ALA:O	1:B:394:SER:N	2.48	0.44
1:B:237:THR:HG23	1:B:238:LEU:O	2.18	0.44
1:B:237:THR:HG1	1:B:376:PRO:HD3	1.81	0.44
1:A:445:TYR:CE1	1:A:449:MET:HE2	2.53	0.44
1:B:20:TRP:CE2	1:B:121:GLN:HB3	2.53	0.43
1:A:442:VAL:O	1:A:446:ILE:HG13	2.18	0.43
1:A:374:ARG:HB2	1:A:375:PRO:HD2	2.02	0.42
1:A:20:TRP:CE2	1:A:121:GLN:HB3	2.56	0.41

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	456/468 (97%)	441 (97%)	15 (3%)	0	100	100
1	B	456/468 (97%)	442 (97%)	13 (3%)	1 (0%)	47	46
All	All	912/936 (97%)	883 (97%)	28 (3%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	103	ALA

### 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	386/394 (98%)	385 (100%)	1 (0%)	92	95
1	B	386/394 (98%)	384 (100%)	2 (0%)	88	92
All	All	772/788 (98%)	769 (100%)	3 (0%)	91	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	63	ARG
1	B	425	GLN
1	A	63	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	ACT	A	501	-	1,3,3	0.90	0	0,3,3	0.00	-
4	TRS	A	502	-	7,7,7	0.33	0	9,9,9	0.56	0

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
4	TRS	A	502	-	-	2/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	TRS	C1-C-C3-O3
4	A	502	TRS	N-C-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	458/468 (97%)	0.87	66 (14%) 2 3	22, 42, 93, 130	0
1	B	458/468 (97%)	0.38	20 (4%) 34 43	21, 34, 60, 124	0
All	All	916/936 (97%)	0.62	86 (9%) 8 12	21, 37, 82, 130	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	ALA	7.5
1	A	457	ALA	6.4
1	B	391	ALA	6.0
1	A	454	ILE	5.9
1	A	390	ILE	5.5
1	A	335	SER	5.3
1	A	299	CYS	5.0
1	A	276	ALA	4.9
1	B	390	ILE	4.7
1	A	296	LEU	4.6
1	A	456	THR	4.6
1	B	103	ALA	4.5
1	A	272	ALA	4.5
1	A	295	GLU	4.5
1	A	338	PHE	4.1
1	A	333	VAL	4.1
1	A	102	ASN	4.0
1	A	371	THR	3.9
1	A	339	ASP	3.9
1	A	248	LEU	3.8
1	A	392	PRO	3.8
1	A	265	GLN	3.8
1	B	376	PRO	3.7
1	A	269	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	125	GLN	3.6
1	B	368	ARG	3.6
1	A	104	GLU	3.6
1	A	375	PRO	3.5
1	A	297	THR	3.5
1	A	446	ILE	3.5
1	B	102	ASN	3.4
1	A	249	SER	3.3
1	A	298	ASN	3.3
1	A	243	LEU	3.3
1	A	398	ASN	3.2
1	A	267	GLY	3.2
1	A	377	ARG	3.1
1	A	291	LEU	3.1
1	A	445	TYR	3.1
1	A	458	ASP	3.1
1	A	294	ARG	3.1
1	A	401	LEU	3.1
1	B	400	ASP	3.1
1	A	397	ALA	3.0
1	B	392	PRO	3.0
1	A	251	PRO	3.0
1	A	2	PHE	3.0
1	B	401	LEU	3.0
1	A	245	LEU	2.9
1	A	292	ALA	2.8
1	B	398	ASN	2.8
1	A	332	PRO	2.8
1	A	376	PRO	2.8
1	A	370	GLU	2.7
1	A	268	GLU	2.7
1	A	334	ALA	2.7
1	A	337	LEU	2.7
1	A	246	GLY	2.7
1	A	300	GLU	2.7
1	B	371	THR	2.7
1	B	377	ARG	2.7
1	A	400	ASP	2.7
1	A	331	VAL	2.6
1	A	451	SER	2.6
1	B	375	PRO	2.6
1	B	2	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	459	GLY	2.5
1	A	399	SER	2.5
1	B	393	LEU	2.4
1	A	437	ILE	2.4
1	A	171	PRO	2.4
1	A	374	ARG	2.4
1	A	436	PRO	2.3
1	B	339	ASP	2.3
1	A	126	ASN	2.3
1	A	274	CYS	2.3
1	A	302	PHE	2.3
1	A	275	VAL	2.3
1	A	393	LEU	2.2
1	A	324	THR	2.2
1	B	423	GLN	2.1
1	B	104	GLU	2.1
1	A	447	ALA	2.1
1	A	432	PHE	2.1
1	B	211	TYR	2.0
1	A	395	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	TRS	A	502	8/8	0.70	0.27	66,79,84,84	0
3	ACT	A	501	4/4	0.94	0.15	39,40,47,47	0
2	ZN	B	501	1/1	0.99	0.07	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	503	1/1	0.99	0.17	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.