



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:16 PM GMT

PDB ID : 3WO1  
Title : Crystal structure of Trp332Ala mutant YwfE, an L-amino acid ligase, with bound ADP-Mg-Ala  
Authors : Tsuda, T.; Kojima, S.  
Deposited on : 2013-12-19  
Resolution : 2.30 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  
<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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

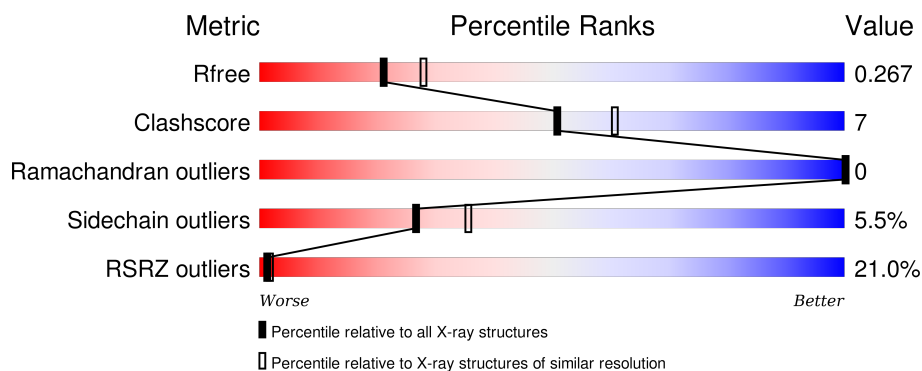
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	470	<div> <div>21%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3745 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.

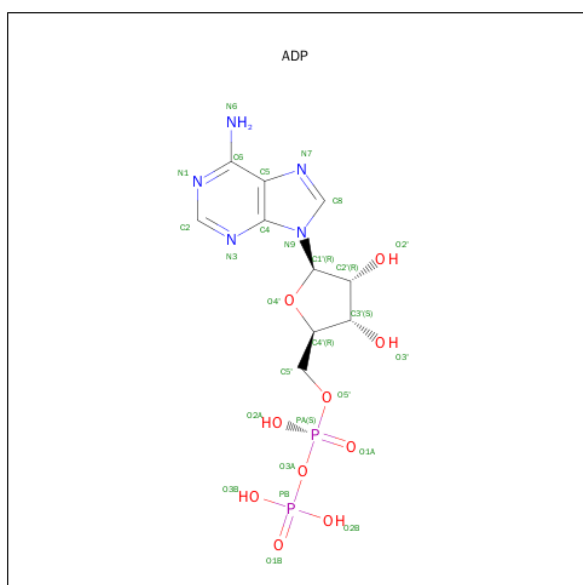
- Molecule 1 is a protein called Alanine-anticapsin ligase BacD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	466	3623	2309	592	709	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P39641
A	0	PRO	-	EXPRESSION TAG	UNP P39641
A	1	LEU	-	EXPRESSION TAG	UNP P39641
A	2	GLY	-	EXPRESSION TAG	UNP P39641
A	3	SER	-	EXPRESSION TAG	UNP P39641
A	332	ALA	TRP	ENGINEERED MUTATION	UNP P39641

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

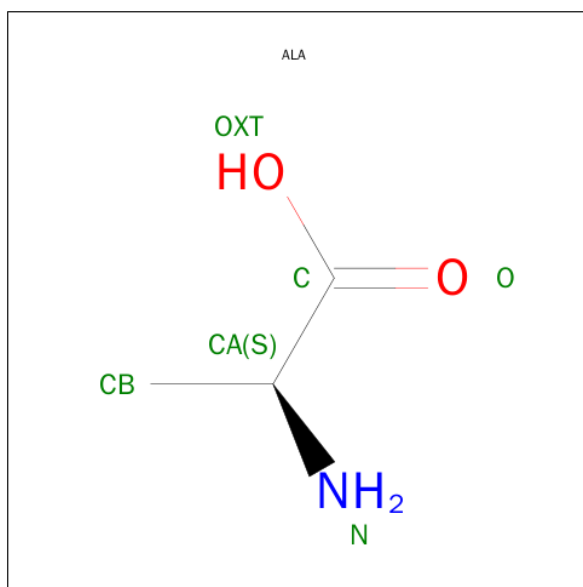


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ALANINE (three-letter code: ALA) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			6	3	1	2		

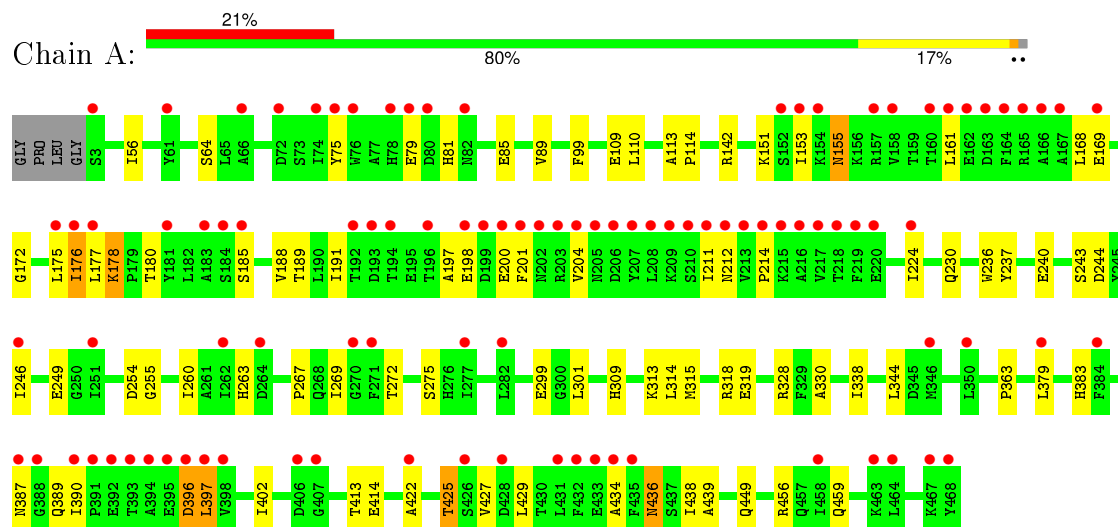
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total	O	0	0
			87	87		

### 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 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 ( $\text{RSRZ} > 2$ ). 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: Alanine-anticapsin ligase BacD



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.13 Å 91.13 Å 258.76 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.74 – 2.30 19.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.74-2.30) 97.9 (19.73-2.30)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.18 (at 2.30 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.221 , 0.261 0.228 , 0.267	Depositor DCC
$R_{free}$ test set	1480 reflections (5.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 28564 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3745	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: MG, ADP

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	0.57	0/3698	0.64	0/5010

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 [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	3623	0	3571	48	1
2	A	27	0	12	3	0
3	A	2	0	0	0	0
4	A	6	0	4	0	0
5	A	87	0	0	1	0
All	All	3745	0	3587	50	1

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 7.

All (50) 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:185:SER:N	2:A:501:ADP:O1B	2.05	0.89
1:A:267:PRO:O	5:A:1045:HOH:O	2.08	0.70
1:A:113:ALA:HB3	1:A:114:PRO:HD3	1.78	0.65
1:A:178:LYS:HB2	1:A:188:VAL:HG22	1.84	0.60
1:A:396:ASP:N	1:A:396:ASP:OD1	2.35	0.59
1:A:178:LYS:CB	1:A:188:VAL:HG22	2.35	0.56
1:A:197:ALA:O	1:A:201:PHE:N	2.40	0.55
1:A:81:HIS:HB3	1:A:214:PRO:HA	1.89	0.54
1:A:79:GLU:O	1:A:212:ASN:ND2	2.41	0.53
1:A:113:ALA:HB3	1:A:114:PRO:CD	2.37	0.53
1:A:249:GLU:OE2	1:A:309:HIS:HD2	1.92	0.53
1:A:309:HIS:CD2	1:A:330:ALA:HB2	2.43	0.53
1:A:269:ILE:HD11	1:A:383:HIS:NE2	2.24	0.53
1:A:379:LEU:HB2	1:A:439:ALA:HB3	1.91	0.52
1:A:189:THR:HG21	1:A:204:VAL:HG11	1.91	0.52
1:A:456:ARG:HA	1:A:459:GLN:OE1	2.11	0.51
1:A:390:ILE:HG21	1:A:429:LEU:CD1	2.40	0.51
1:A:161:LEU:O	1:A:161:LEU:HD23	2.11	0.51
1:A:260:ILE:HD13	1:A:363:PRO:HG2	1.94	0.50
2:A:501:ADP:H8	2:A:501:ADP:O5'	1.95	0.50
1:A:110:LEU:HD13	1:A:214:PRO:CD	2.42	0.49
1:A:85:GLU:O	1:A:89:VAL:HG23	2.14	0.48
1:A:237:TYR:HE2	1:A:243:SER:O	1.99	0.46
1:A:402:ILE:HD11	1:A:438:ILE:HD12	1.97	0.46
1:A:389:GLN:OE1	1:A:389:GLN:HA	2.16	0.46
1:A:198:GLU:C	1:A:200:GLU:H	2.19	0.46
1:A:56:ILE:HD11	1:A:99:PHE:HE2	1.81	0.45
1:A:236:TRP:CZ2	1:A:318:ARG:HA	2.52	0.45
1:A:110:LEU:HD13	1:A:214:PRO:HD2	1.99	0.45
1:A:413:THR:HG22	1:A:414:GLU:N	2.32	0.45
1:A:272:THR:HG23	1:A:434:ALA:HB2	1.98	0.45
1:A:211:ILE:HG22	1:A:212:ASN:N	2.32	0.44
1:A:397:LEU:HD22	1:A:429:LEU:HD11	1.99	0.44
1:A:236:TRP:CD1	1:A:314:LEU:HB3	2.53	0.44
1:A:176:ILE:HD13	1:A:189:THR:O	2.18	0.43
1:A:260:ILE:CD1	1:A:363:PRO:HG2	2.49	0.43
1:A:244:ASP:O	1:A:313:LYS:HD2	2.19	0.43
1:A:263:HIS:HE1	1:A:338:ILE:HD11	1.84	0.43
1:A:255:GLY:O	1:A:299:GLU:HG2	2.19	0.43
1:A:422:ALA:HB3	1:A:425:THR:HG23	2.00	0.42
1:A:142:ARG:CZ	1:A:153:ILE:HD11	2.49	0.42
1:A:269:ILE:HD11	1:A:383:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ILE:HD12	1:A:246:ILE:C	2.41	0.42
1:A:230:GLN:O	1:A:315:MET:HG2	2.20	0.41
2:A:501:ADP:C8	2:A:501:ADP:O5'	2.74	0.41
1:A:155:ASN:HB2	1:A:224:ILE:HD11	2.03	0.41
1:A:427:VAL:HG13	1:A:436:ASN:HD21	1.86	0.41
1:A:175:LEU:HB3	1:A:191:ILE:HB	2.04	0.40
1:A:172:GLY:O	1:A:175:LEU:HB2	2.22	0.40
1:A:109:GLU:HG3	1:A:328:ARG:HE	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:GLN:OE1	1:A:449:GLN:OE1[10_665]	2.05	0.15

## 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	464/470 (99%)	434 (94%)	30 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	385/387 (100%)	364 (94%)	21 (6%)	27	36

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	SER
1	A	75	TYR
1	A	151	LYS
1	A	155	ASN
1	A	168	LEU
1	A	169	GLU
1	A	176	ILE
1	A	177	LEU
1	A	178	LYS
1	A	180	THR
1	A	240	GLU
1	A	254	ASP
1	A	275	SER
1	A	301	LEU
1	A	319	GLU
1	A	344	LEU
1	A	387	ASN
1	A	396	ASP
1	A	397	LEU
1	A	425	THR
1	A	436	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	108	ASN
1	A	146	ASN
1	A	155	ASN
1	A	212	ASN
1	A	309	HIS
1	A	337	ASN
1	A	382	GLN
1	A	436	ASN
1	A	461	HIS

### 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	$\# Z  > 2$
2	ADP	A	501	3	22,29,29	1.04	2 (9%)	27,45,45	2.20	6 (22%)
4	ALA	A	504	-	2,5,5	0.51	0	0,6,6	0.00	-

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
2	ADP	A	501	3	-	0/12/32/32	0/3/3/3
4	ALA	A	504	-	-	0/0/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ADP	O4'-C1'	2.15	1.43	1.41
2	A	501	ADP	C5-C4	2.96	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ADP	N3-C2-N1	-7.08	123.47	128.89
2	A	501	ADP	C2'-C1'-N9	-5.48	105.92	114.29
2	A	501	ADP	C4-C5-N7	-3.65	106.12	109.48
2	A	501	ADP	PA-O3A-PB	-2.74	123.46	132.67
2	A	501	ADP	O3B-PB-O2B	2.19	115.72	107.38
2	A	501	ADP	O4'-C1'-N9	2.27	112.85	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ADP	3	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

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	466/470 (99%)	1.11	98 (21%) <b>1</b> <b>2</b>	37, 60, 146, 170	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	VAL	13.9
1	A	468	TYR	11.5
1	A	208	LEU	10.4
1	A	219	PHE	9.7
1	A	207	TYR	8.8
1	A	75	TYR	8.0
1	A	210	SER	8.0
1	A	76	TRP	7.7
1	A	393	THR	7.4
1	A	199	ASP	7.0
1	A	216	ALA	6.4
1	A	211	ILE	6.4
1	A	201	PHE	6.4
1	A	432	PHE	6.2
1	A	82	ASN	6.2
1	A	218	THR	5.9
1	A	206	ASP	5.8
1	A	166	ALA	5.6
1	A	213	VAL	5.6
1	A	78	HIS	5.4
1	A	395	GLU	5.2
1	A	388	GLY	5.1
1	A	183	ALA	5.1
1	A	434	ALA	5.0
1	A	192	THR	4.9
1	A	79	GLU	4.8
1	A	220	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	202	ASN	4.6
1	A	193	ASP	4.5
1	A	204	VAL	4.5
1	A	435	PHE	4.2
1	A	391	PRO	4.2
1	A	80	ASP	4.2
1	A	209	LYS	4.2
1	A	277	ILE	4.1
1	A	160	THR	4.0
1	A	169	GLU	4.0
1	A	184	SER	4.0
1	A	212	ASN	4.0
1	A	165	ARG	3.9
1	A	396	ASP	3.9
1	A	467	LYS	3.8
1	A	162	GLU	3.7
1	A	406	ASP	3.7
1	A	431	LEU	3.6
1	A	205	ASN	3.6
1	A	214	PRO	3.6
1	A	428	ASP	3.5
1	A	161	LEU	3.5
1	A	185	SER	3.5
1	A	200	GLU	3.4
1	A	397	LEU	3.3
1	A	394	ALA	3.3
1	A	215	LYS	3.2
1	A	196	THR	3.2
1	A	463	LYS	3.1
1	A	176	ILE	3.1
1	A	464	LEU	3.1
1	A	203	ARG	3.0
1	A	164	PHE	2.9
1	A	246	ILE	2.9
1	A	390	ILE	2.9
1	A	426	SER	2.9
1	A	398	VAL	2.9
1	A	224	ILE	2.9
1	A	177	LEU	2.8
1	A	379	LEU	2.8
1	A	181	TYR	2.8
1	A	198	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	194	THR	2.7
1	A	270	GLY	2.6
1	A	251	ILE	2.6
1	A	74	ILE	2.5
1	A	392	GLU	2.5
1	A	433	GLU	2.4
1	A	152	SER	2.4
1	A	282	LEU	2.4
1	A	72	ASP	2.4
1	A	163	ASP	2.4
1	A	158	VAL	2.3
1	A	262	ILE	2.3
1	A	66	ALA	2.3
1	A	271	PHE	2.3
1	A	175	LEU	2.2
1	A	422	ALA	2.2
1	A	384	PHE	2.1
1	A	157	ARG	2.1
1	A	350	LEU	2.1
1	A	346	MET	2.1
1	A	167	ALA	2.1
1	A	61	TYR	2.1
1	A	3	SER	2.1
1	A	153	ILE	2.1
1	A	387	ASN	2.0
1	A	458	ILE	2.0
1	A	264	ASP	2.0
1	A	407	GLY	2.0
1	A	154	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	ALA	A	504	6/6	0.95	0.15	0.57	43,50,55,62	0
3	MG	A	503	1/1	0.65	0.18	-0.50	86,86,86,86	0
2	ADP	A	501	27/27	0.82	0.18	-0.52	84,99,123,132	0
3	MG	A	502	1/1	0.96	0.30	-	89,89,89,89	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.