



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 11:23 PM UTC

PDB ID : 24QJ / pdb\_000024qj  
Title : Crystal structure of a tailspike depolymerase (Solidus\_gp83) from Acinetobacter phage Solidus  
Authors : Matyuta, I.O.; Shneider, M.M.; Timoshina, O.Y.; Popov, V.O.; Boyko, K.M.  
Deposited on : 2026-03-16  
Resolution : 2.49 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)

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<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>.

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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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

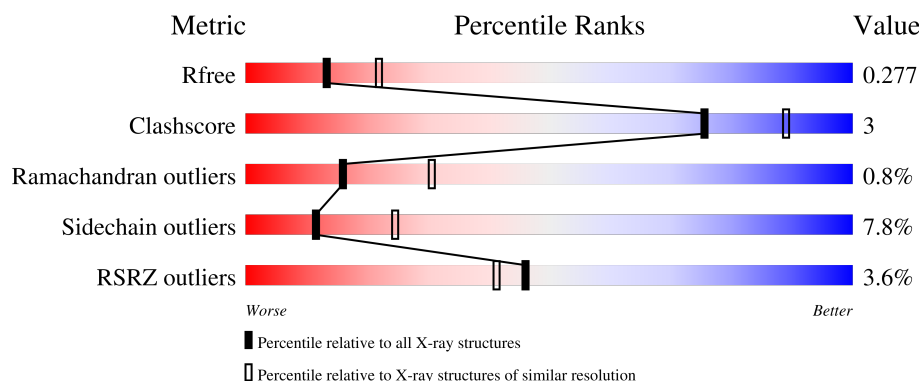
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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  $\leq 5\%$ . 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	486	<div> <div>3%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

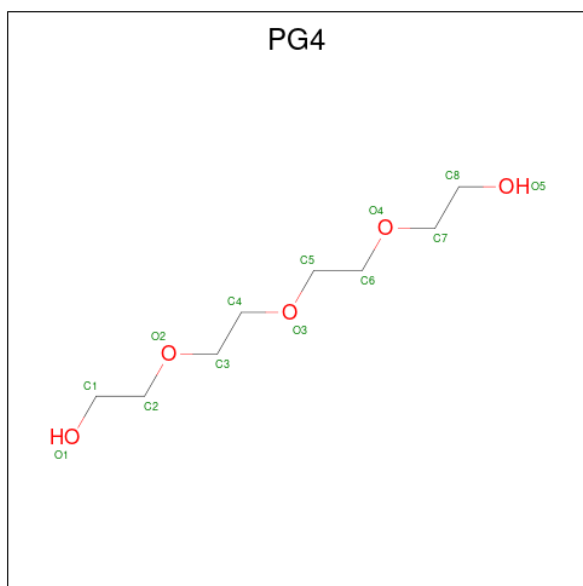
There are 4 unique types of molecules in this entry. The entry contains 3642 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tailspike depolymerase.

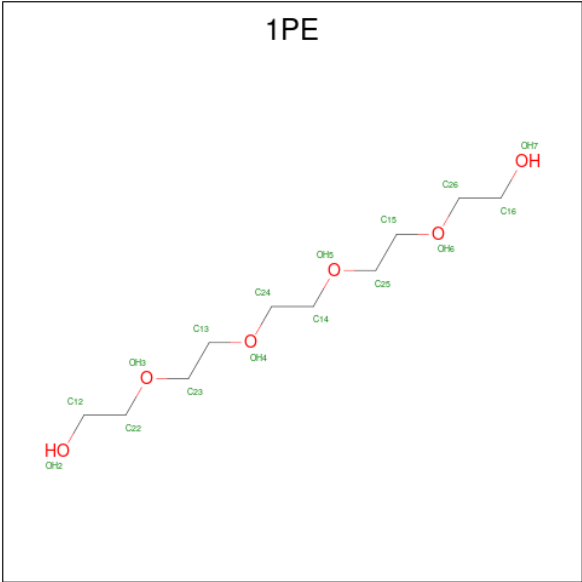
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	475	3592	2257	609	716	10	0	0	0

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	8	5	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		

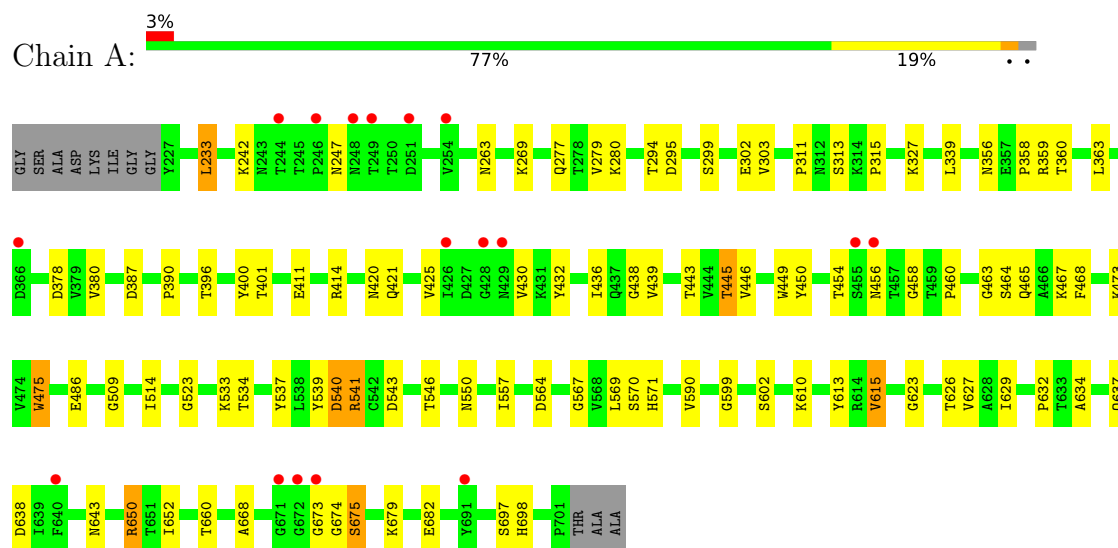
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		

### 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 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: Tailspike depolymerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.22Å 84.22Å 529.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.17 – 2.49 40.17 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.17-2.49) 99.0 (40.17-2.49)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.207 , 0.277 0.212 , 0.277	Depositor DCC
$R_{free}$ test set	1325 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 36.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3642	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, PG4

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	1.32	14/3675 (0.4%)	1.66	32/5019 (0.6%)

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
1	A	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	438	GLY	C-O	7.32	1.30	1.23
1	A	557	ILE	C-O	-6.44	1.16	1.24
1	A	509	GLY	C-O	-6.39	1.17	1.24
1	A	567	GLY	C-O	6.39	1.32	1.23
1	A	473	LYS	C-O	6.31	1.31	1.23
1	A	468	PHE	C-O	6.27	1.31	1.24
1	A	315	PRO	C-O	-6.24	1.16	1.23
1	A	414	ARG	C-O	-5.83	1.17	1.24
1	A	311	PRO	C-O	-5.64	1.16	1.24
1	A	570	SER	C-O	-5.61	1.17	1.24
1	A	380	VAL	C-O	-5.58	1.18	1.24
1	A	698	HIS	CE1-NE2	5.55	1.38	1.32
1	A	443	THR	C-O	5.39	1.30	1.24
1	A	537	TYR	C-O	-5.01	1.18	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	THR	CB-CA-C	9.12	124.79	109.75
1	A	626	THR	CA-CB-OG1	-7.06	99.02	109.60
1	A	263	ASN	CA-CB-CG	7.02	119.62	112.60
1	A	550	ASN	CB-CA-C	6.93	117.23	110.71
1	A	590	VAL	CA-C-O	-6.54	115.16	121.63
1	A	571	HIS	CA-C-N	6.54	131.41	122.19
1	A	571	HIS	C-N-CA	6.54	131.41	122.19
1	A	643	ASN	CB-CA-C	6.46	117.74	109.80
1	A	450	TYR	CA-C-O	-6.12	114.07	121.05
1	A	460	PRO	N-CA-CB	6.12	106.62	103.19
1	A	279	VAL	CA-C-O	-6.09	114.29	121.05
1	A	546	THR	CA-CB-OG1	6.04	118.66	109.60
1	A	401	THR	CA-CB-OG1	-5.86	100.81	109.60
1	A	610	LYS	CA-C-N	5.83	131.22	123.00
1	A	610	LYS	C-N-CA	5.83	131.22	123.00
1	A	378	ASP	CA-C-O	-5.59	114.59	120.80
1	A	295	ASP	CA-C-N	5.56	128.05	120.54
1	A	295	ASP	C-N-CA	5.56	128.05	120.54
1	A	294	THR	CA-CB-OG1	-5.56	101.27	109.60
1	A	599	GLY	CA-C-O	-5.55	116.16	121.49
1	A	571	HIS	CA-C-O	-5.34	114.58	120.30
1	A	467	LYS	CA-C-N	5.33	129.71	122.19
1	A	467	LYS	C-N-CA	5.33	129.71	122.19
1	A	534	THR	CA-CB-OG1	-5.31	101.64	109.60
1	A	277	GLN	N-CA-C	-5.29	105.43	111.14
1	A	557	ILE	CA-C-O	-5.28	114.92	120.57
1	A	356	ASN	CB-CA-C	-5.26	98.75	109.65
1	A	380	VAL	CA-C-O	-5.21	114.91	120.39
1	A	668	ALA	CA-C-O	-5.16	116.12	122.36
1	A	543	ASP	CB-CA-C	5.14	119.42	110.79
1	A	387	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	615	VAL	CB-CA-C	5.06	116.87	111.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	420	ASN	Peptide



## 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	3592	0	3433	21	0
2	A	13	0	18	0	0
3	A	16	0	22	0	0
4	A	21	0	0	0	0
All	All	3642	0	3473	21	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 3.

All (21) 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:396:THR:O	1:A:463:GLY:HA2	1.92	0.69
1:A:299:SER:O	1:A:303:VAL:HG23	1.99	0.62
1:A:539:TYR:O	1:A:540:ASP:O	2.24	0.54
1:A:569:LEU:HD23	1:A:569:LEU:C	2.34	0.52
1:A:613:TYR:HA	1:A:627:VAL:O	2.13	0.49
1:A:673:GLY:O	1:A:675:SER:N	2.46	0.48
1:A:339:LEU:HA	1:A:360:THR:O	2.14	0.47
1:A:446:VAL:HG21	1:A:449:TRP:CE2	2.49	0.47
1:A:400:TYR:OH	1:A:464:SER:O	2.30	0.46
1:A:313:SER:O	1:A:327:LYS:HE3	2.15	0.46
1:A:421:GLN:HB2	1:A:436:ILE:HD12	1.99	0.45
1:A:475:TRP:CD1	1:A:475:TRP:N	2.85	0.45
1:A:634:ALA:O	1:A:637:GLN:HG3	2.17	0.45
1:A:632:PRO:HA	1:A:637:GLN:OE1	2.17	0.44
1:A:446:VAL:HG21	1:A:449:TRP:CZ2	2.52	0.44
1:A:233:LEU:HD12	1:A:233:LEU:HA	1.90	0.44
1:A:425:VAL:HA	1:A:465:GLN:O	2.19	0.43
1:A:449:TRP:HB2	1:A:458:GLY:O	2.19	0.42
1:A:623:GLY:O	1:A:650:ARG:NH2	2.42	0.42
1:A:615:VAL:HA	1:A:629:ILE:O	2.19	0.41
1:A:679:LYS:HB2	1:A:682:GLU:CD	2.46	0.40

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	473/486 (97%)	440 (93%)	29 (6%)	4 (1%)	16	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	541	ARG
1	A	674	GLY
1	A	540	ASP
1	A	523	GLY

### 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	386/399 (97%)	356 (92%)	30 (8%)	11	24

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	LEU
1	A	242	LYS
1	A	247	ASN
1	A	269	LYS
1	A	280	LYS
1	A	302	GLU
1	A	358	PRO

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Mol	Chain	Res	Type
1	A	359	ARG
1	A	363	LEU
1	A	390	PRO
1	A	411	GLU
1	A	430	VAL
1	A	432	TYR
1	A	439	VAL
1	A	445	THR
1	A	454	THR
1	A	456	ASN
1	A	475	TRP
1	A	486	GLU
1	A	514	ILE
1	A	533	LYS
1	A	541	ARG
1	A	564	ASP
1	A	602	SER
1	A	638	ASP
1	A	650	ARG
1	A	652	ILE
1	A	660	THR
1	A	675	SER
1	A	697	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	ASN
1	A	373	ASN
1	A	456	ASN
1	A	480	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 [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	PG4	A	801	-	12,12,12	0.82	0	11,11,11	0.52	0
3	1PE	A	802	-	15,15,15	0.43	0	14,14,14	0.36	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
2	PG4	A	801	-	-	5/10/10/10	-
3	1PE	A	802	-	-	6/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	1PE	OH4-C13-C23-OH3
2	A	801	PG4	O3-C5-C6-O4
3	A	802	1PE	OH7-C16-C26-OH6
2	A	801	PG4	O2-C3-C4-O3
3	A	802	1PE	OH2-C12-C22-OH3
2	A	801	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
2	A	801	PG4	C5-C6-O4-C7
3	A	802	1PE	C13-C23-OH3-C22
3	A	802	1PE	C15-C25-OH5-C14
2	A	801	PG4	C1-C2-O2-C3
3	A	802	1PE	C12-C22-OH3-C23

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	475/486 (97%)	0.17	17 (3%) 46 41	24, 42, 68, 93	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	429	ASN	4.4
1	A	366	ASP	3.9
1	A	254	VAL	3.4
1	A	426	ILE	3.3
1	A	455	SER	3.3
1	A	671	GLY	3.2
1	A	246	PRO	3.0
1	A	672	GLY	2.5
1	A	428	GLY	2.4
1	A	456	ASN	2.4
1	A	244	THR	2.3
1	A	248	ASN	2.2
1	A	691	TYR	2.2
1	A	249	THR	2.2
1	A	673	GLY	2.2
1	A	640	PHE	2.2
1	A	251	ASP	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 oligosaccharides 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
2	PG4	A	801	13/13	0.88	0.18	54,67,79,81	0
3	1PE	A	802	16/16	0.88	0.19	51,67,77,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.