



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 11:44 PM EST

PDB ID : 5WO9  
Title : Crystal Structure of Transient Receptor Potential (TRP) channel TRPV6\* in the presence of Calcium  
Authors : Singh, A.K.; Saotome, K.; Sobolevsky, A.I.  
Deposited on : 2017-08-01  
Resolution : 3.70 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.

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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

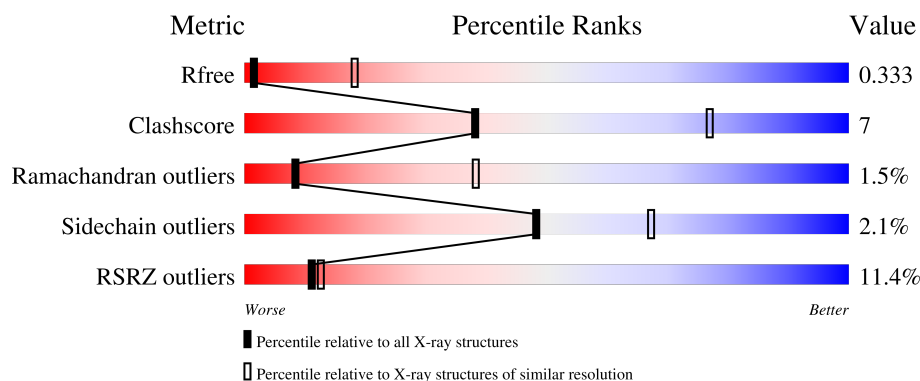
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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))
$R_{free}$	164625	1017 (3.80-3.60)
Clashscore	180529	1074 (3.80-3.60)
Ramachandran outliers	177936	1055 (3.80-3.60)
Sidechain outliers	177891	1052 (3.80-3.60)
RSRZ outliers	164620	1017 (3.80-3.60)

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	672	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	A	703	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	A	704	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4773 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.

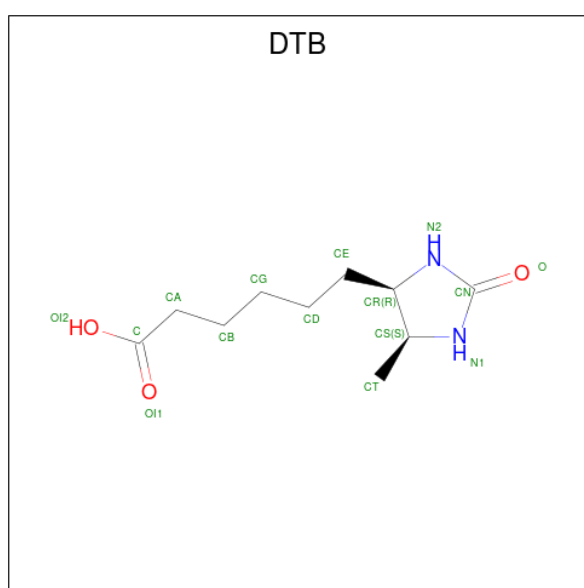
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4755	3079	797	845	34			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	TYR	ILE	engineered mutation	UNP Q9R186
A	92	ASN	LEU	engineered mutation	UNP Q9R186
A	96	GLN	MET	engineered mutation	UNP Q9R186
A	670	VAL	-	expression tag	UNP Q9R186
A	671	PRO	-	expression tag	UNP Q9R186
A	672	ARG	-	expression tag	UNP Q9R186

- Molecule 2 is 6-(5-METHYL-2-OXO-IMIDAZOLIDIN-4-YL)-HEXANOIC ACID (three-letter code: DTB) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	10	2	3		

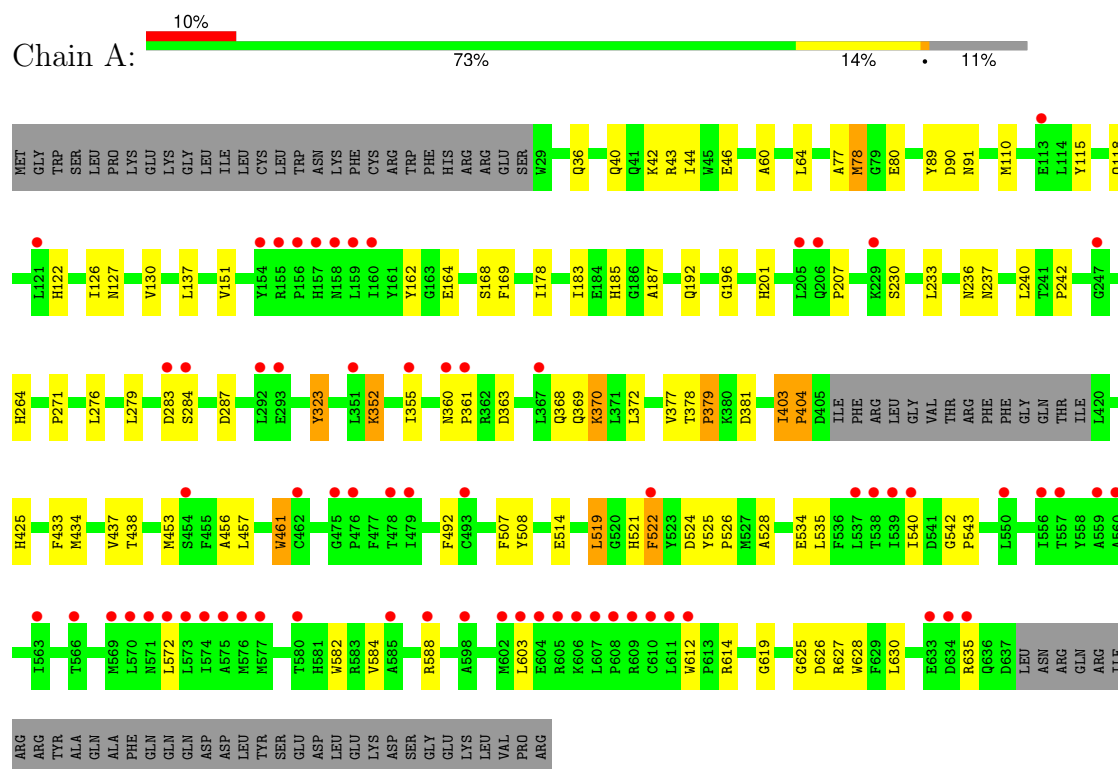
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		

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

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: Transient receptor potential cation channel subfamily V member 6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.48Å 145.48Å 110.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.66 – 3.70 46.66 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.66-3.70) 99.9 (46.66-3.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 3.66Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.272 , 0.316 0.284 , 0.333	Depositor DCC
$R_{free}$ test set	662 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	156.9	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 83.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	4773	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: DTB, CA

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	0.25	0/4865	0.45	1/6608 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	TYR	CB-CA-C	-5.12	100.16	110.40

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	4755	0	4791	63	0
2	A	15	0	16	6	0
3	A	3	0	0	0	0
All	All	4773	0	4807	65	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 7.

All (65) 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:372:LEU:O	1:A:372:LEU:HD23	1.72	0.90
1:A:377:VAL:HG13	1:A:379:PRO:HD3	1.72	0.70
1:A:379:PRO:HD2	1:A:381:ASP:H	1.62	0.65
1:A:434:MET:O	1:A:438:THR:OG1	2.20	0.59
1:A:130:VAL:HG22	1:A:178:ILE:HD11	1.89	0.55
1:A:535:LEU:HD23	1:A:540:ILE:HB	1.88	0.54
1:A:183:ILE:HA	1:A:187:ALA:HB3	1.90	0.53
1:A:137:LEU:HD21	1:A:185:HIS:CG	2.43	0.53
1:A:323:TYR:O	1:A:612:TRP:CE3	2.62	0.53
1:A:434:MET:HB3	1:A:456:ALA:HB2	1.91	0.53
1:A:80:GLU:HA	1:A:110:MET:HG2	1.91	0.53
1:A:535:LEU:HD22	1:A:542:GLY:HA2	1.91	0.52
2:A:701:DTB:HCT2	2:A:701:DTB:HCD1	1.89	0.52
1:A:115:TYR:CE2	2:A:701:DTB:N2	2.67	0.52
1:A:137:LEU:HD11	1:A:185:HIS:CE1	2.45	0.51
1:A:433:PHE:O	1:A:437:VAL:HG23	2.10	0.51
1:A:403:ILE:HG22	1:A:404:PRO:HD3	1.94	0.50
1:A:115:TYR:CE1	2:A:701:DTB:HCE1	2.47	0.49
1:A:369:GLN:HG3	1:A:370:LYS:HG3	1.94	0.49
1:A:151:VAL:O	2:A:701:DTB:OI1	2.31	0.49
1:A:625:GLY:O	1:A:626:ASP:C	2.51	0.49
1:A:323:TYR:O	1:A:612:TRP:CZ3	2.66	0.48
1:A:507:PHE:HB3	1:A:522:PHE:CE2	2.48	0.48
1:A:118:GLN:HG3	1:A:122:HIS:HB2	1.96	0.47
1:A:192:GLN:HB3	1:A:196:GLY:HA2	1.96	0.47
1:A:461:TRP:CE3	1:A:461:TRP:HA	2.50	0.47
1:A:619:GLY:N	1:A:627:ARG:O	2.48	0.47
1:A:521:HIS:CE1	1:A:543:PRO:HA	2.49	0.47
1:A:264:HIS:O	1:A:276:LEU:N	2.40	0.46
1:A:162:TYR:O	1:A:168:SER:OG	2.21	0.46
1:A:89:TYR:O	1:A:91:ASN:N	2.49	0.46
1:A:137:LEU:HD11	1:A:185:HIS:NE2	2.30	0.46
1:A:614:ARG:HD3	1:A:628:TRP:CE2	2.51	0.46
1:A:457:LEU:O	1:A:461:TRP:HB2	2.15	0.46
1:A:279:LEU:HD11	1:A:630:LEU:HB2	1.98	0.45
1:A:36:GLN:HB3	1:A:78:MET:HE1	1.97	0.45
1:A:230:SER:HB3	1:A:233:LEU:HD23	1.97	0.45
1:A:360:ASN:HB3	1:A:361:PRO:HD3	1.96	0.45
1:A:352:LYS:HD2	1:A:368:GLN:O	2.16	0.45
1:A:372:LEU:O	1:A:372:LEU:CD2	2.53	0.45
1:A:522:PHE:HB3	1:A:528:ALA:HA	1.99	0.45
1:A:584:VAL:O	1:A:588:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LYS:HB2	1:A:368:GLN:O	2.17	0.44
1:A:514:GLU:HG2	1:A:519:LEU:HD11	1.99	0.44
2:A:701:DTB:HCT2	2:A:701:DTB:CD	2.47	0.44
1:A:492:PHE:CE1	1:A:572:LEU:HD22	2.53	0.44
1:A:126:ILE:HB	1:A:169:PHE:HD2	1.83	0.43
1:A:60:ALA:O	1:A:64:LEU:HG	2.19	0.43
1:A:236:ASN:OD1	1:A:237:ASN:N	2.52	0.42
1:A:115:TYR:CE1	2:A:701:DTB:CE	2.95	0.42
1:A:378:THR:N	1:A:379:PRO:HD3	2.34	0.42
1:A:43:ARG:HG3	1:A:77:ALA:HB2	2.02	0.42
1:A:271:PRO:HB2	1:A:635:ARG:HG3	2.01	0.42
1:A:438:THR:HG21	1:A:453:MET:HG3	2.01	0.42
1:A:626:ASP:O	1:A:627:ARG:HG3	2.19	0.42
1:A:42:LYS:HE3	1:A:46:GLU:OE2	2.20	0.41
1:A:40:GLN:O	1:A:44:ILE:HG12	2.19	0.41
1:A:534:GLU:HB3	1:A:540:ILE:HG12	2.02	0.41
1:A:514:GLU:CG	1:A:519:LEU:HD11	2.51	0.41
1:A:287:ASP:OD1	1:A:287:ASP:N	2.53	0.41
1:A:201:HIS:NE2	1:A:242:PRO:HD3	2.35	0.41
1:A:525:TYR:N	1:A:526:PRO:HD2	2.36	0.41
1:A:115:TYR:CE1	1:A:151:VAL:HG21	2.56	0.40
1:A:508:TYR:HE1	1:A:524:ASP:HA	1.85	0.40
1:A:240:LEU:HD12	1:A:240:LEU:HA	1.94	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	591/672 (88%)	545 (92%)	37 (6%)	9 (2%)	<b>8</b> 38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	PRO
1	A	90	ASP
1	A	284	SER
1	A	363	ASP
1	A	370	LYS
1	A	519	LEU
1	A	404	PRO
1	A	207	PRO
1	A	355	ILE

### 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	513/584 (88%)	502 (98%)	11 (2%)	48 67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	MET
1	A	127	ASN
1	A	164	GLU
1	A	283	ASP
1	A	352	LYS
1	A	403	ILE
1	A	425	HIS
1	A	461	TRP
1	A	522	PHE
1	A	582	TRP
1	A	603	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

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](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	DTB	A	701	-	15,15,15	0.65	0	16,19,19	1.18	1 (6%)

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	DTB	A	701	-	-	5/8/20/20	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	DTB	OI2-C-CA	2.30	121.26	114.00

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	DTB	CE-CD-CG-CB
2	A	701	DTB	CD-CE-CR-N2
2	A	701	DTB	OI2-C-CA-CB
2	A	701	DTB	OI1-C-CA-CB
2	A	701	DTB	CG-CD-CE-CR

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	DTB	6	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	595/672 (88%)	0.49	68 (11%)	<b>11</b> <b>12</b>	110, 143, 203, 241	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	LEU	11.7
1	A	569	MET	8.5
1	A	570	LEU	7.9
1	A	573	LEU	7.7
1	A	577	MET	7.2
1	A	605	ARG	7.0
1	A	572	LEU	6.6
1	A	574	ILE	6.5
1	A	607	LEU	6.0
1	A	603	LEU	5.8
1	A	293	GLU	5.7
1	A	556	ILE	5.6
1	A	155	ARG	5.3
1	A	608	PRO	5.3
1	A	154	TYR	5.2
1	A	355	ILE	5.0
1	A	610	CYS	5.0
1	A	360	ASN	4.8
1	A	602	MET	4.6
1	A	158	ASN	4.5
1	A	560	ALA	4.3
1	A	454	SER	4.1
1	A	157	HIS	4.1
1	A	292	LEU	3.9
1	A	283	ASP	3.8
1	A	478	THR	3.7
1	A	611	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	571	ASN	3.6
1	A	598	ALA	3.6
1	A	156	PRO	3.5
1	A	633	GLU	3.3
1	A	540	ILE	3.2
1	A	604	GLU	3.2
1	A	635	ARG	3.2
1	A	462	CYS	3.2
1	A	538	THR	3.1
1	A	361	PRO	3.0
1	A	205	LEU	3.0
1	A	606	LYS	3.0
1	A	563	ILE	2.9
1	A	559	ALA	2.9
1	A	493	CYS	2.9
1	A	284	SER	2.9
1	A	634	ASP	2.8
1	A	550	LEU	2.8
1	A	580	THR	2.8
1	A	612	TRP	2.7
1	A	585	ALA	2.7
1	A	609	ARG	2.7
1	A	566	THR	2.7
1	A	113	GLU	2.6
1	A	476	PRO	2.6
1	A	522	PHE	2.6
1	A	121	LEU	2.6
1	A	351	LEU	2.6
1	A	206	GLN	2.5
1	A	576	MET	2.5
1	A	160	ILE	2.4
1	A	367	LEU	2.3
1	A	588	ARG	2.2
1	A	247	GLY	2.2
1	A	475	GLY	2.2
1	A	575	ALA	2.1
1	A	537	LEU	2.1
1	A	479	ILE	2.0
1	A	539	ILE	2.0
1	A	557	THR	2.0
1	A	229	LYS	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 monosaccharides 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
3	CA	A	703	1/1	-0.50	0.50	160,160,160,160	1
3	CA	A	704	1/1	0.25	1.71	190,190,190,190	1
2	DTB	A	701	15/15	0.83	0.17	92,103,113,122	0
3	CA	A	702	1/1	0.95	0.06	170,170,170,170	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.