



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:30 am BST

PDB ID : 2VDD  
Title : Crystal Structure of the Open State of TolC Outer Membrane Component of Mutlidrug Efflux Pumps  
Authors : Bavro, V.N.; Pietras, Z.; Furnham, N.; Perez-Cano, L.; Fernandez-Recio, J.; Pei, X.Y.; Truer, R.; Misra, R.; Luisi, B.  
Deposited on : 2007-10-04  
Resolution : 3.30 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

<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
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

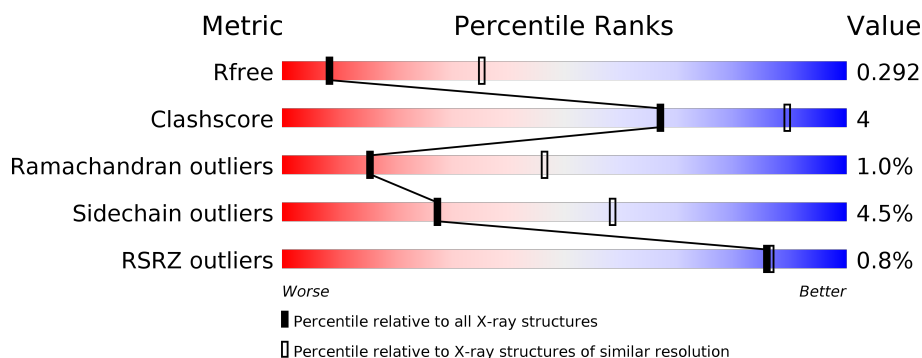
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	460	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	460	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>7%</div> </div> </div>
1	C	460	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>•</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9915 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 OUTER MEMBRANE PROTEIN TOLC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	12	0	1
			3303	2037	584	677	5			
1	B	429	Total	C	N	O	S	31	0	1
			3302	2036	584	677	5			
1	C	429	Total	C	N	O	S	5	0	1
			3303	2037	584	677	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ARG	LYS	conflict	UNP P02930
B	2	ARG	LYS	conflict	UNP P02930
C	2	ARG	LYS	conflict	UNP P02930
A	191	LEU	VAL	engineered mutation	UNP P02930
A	384	PHE	TYR	engineered mutation	UNP P02930
A	389	GLU	ARG	engineered mutation	UNP P02930
B	191	LEU	VAL	engineered mutation	UNP P02930
B	384	PHE	TYR	engineered mutation	UNP P02930
B	389	GLU	ARG	engineered mutation	UNP P02930
C	191	LEU	VAL	engineered mutation	UNP P02930
C	384	PHE	TYR	engineered mutation	UNP P02930
C	389	GLU	ARG	engineered mutation	UNP P02930

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	K	0	0
			2	2		
3	C	1	Total	K	0	0
			1	1		

- Molecule 4 is water.

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



M319	I356	N357	A358	S359	I360	S361	S362	V386	G387	L416	Q419	L441	S442	R443	P444	L451	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.48 Å   70.97 Å   219.95 Å 90.00°   100.61°   90.00°	Depositor
Resolution (Å)	29.80 – 3.30 29.80 – 3.28	Depositor EDS
% Data completeness (in resolution range)	97.2 (29.80-3.30) 96.7 (29.80-3.28)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 3.24 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.236 , 0.295 0.234 , 0.292	Depositor DCC
$R_{free}$ test set	1410 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.5	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , -3.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.427 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.429 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9915	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.18% 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: K, CL

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	0.55	0/3344	0.56	0/4543
1	B	0.54	1/3343 (0.0%)	0.58	3/4541 (0.1%)
1	C	0.57	0/3344	0.58	2/4543 (0.0%)
All	All	0.56	1/10031 (0.0%)	0.57	5/13627 (0.0%)

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	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	392	VAL	CA-CB	5.10	1.65	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	224	LYS	CB-CA-C	10.90	132.20	110.40
1	C	224	LYS	CA-CB-CG	6.97	128.74	113.40
1	B	393	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	392	VAL	CB-CA-C	-5.12	101.68	111.40
1	B	226	ASP	CA-CB-CG	-5.04	102.32	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	B	292	ALA	Peptide
1	B	79	ALA	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	3303	0	3246	29	0
1	B	3302	0	3242	22	0
1	C	3303	0	3246	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
4	C	1	0	0	0	0
All	All	9915	0	9734	76	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 4.

All (76) 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:C:205:ARG:HH21	1:C:211:TYR:HB2	1.43	0.84
1:A:104:ARG:HG3	1:A:264:ASP:OD2	1.88	0.72
1:C:104:ARG:HG3	1:C:264:ASP:OD2	1.93	0.69
1:C:26:MET:O	1:C:30:GLN:HG2	1.94	0.67
1:B:204:LEU:O	1:B:208:THR:HG22	1.95	0.67
1:C:261:GLN:HA	1:C:264:ASP:OD2	1.96	0.66
1:B:208:THR:HG23	1:B:210:ASN:H	1.59	0.66
1:B:281:THR:O	1:B:298:ASP:HB2	1.96	0.65
1:C:76:TYR:CD1	1:C:77:ARG:HG2	2.31	0.65
1:A:75:GLY:H	1:A:83:ASN:HB3	1.63	0.64
1:A:26:MET:O	1:A:30:GLN:HG2	1.97	0.63
1:C:97:ILE:HD11	1:C:272:LEU:HB2	1.81	0.62
1:C:55:GLU:O	1:C:58:SER:HB3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:TYR:HD1	1:C:77:ARG:HG2	1.64	0.59
1:A:82:ILE:HG22	1:A:288:THR:HB	1.86	0.57
1:A:194:ARG:HG3	1:A:449:PRO:HB3	1.86	0.57
1:A:86:ALA:HB2	1:A:281:THR:HG23	1.87	0.56
1:A:235:LEU:HD11	1:A:346:VAL:HG23	1.88	0.56
1:A:219:ASN:HD22	1:A:442:SER:HB2	1.71	0.55
1:A:77:ARG:CZ	1:A:77:ARG:HB3	2.37	0.55
1:C:152:LYS:HD3	1:C:190:GLU:OE1	2.07	0.54
1:B:168:VAL:HG13	1:B:170:LEU:HD23	1.89	0.54
1:C:441:LEU:O	1:C:442:SER:HB3	2.07	0.53
1:A:79:ALA:HB2	1:C:301:MET:HE2	1.91	0.53
1:A:58:SER:OG	1:C:319:MET:HB2	2.09	0.53
1:A:76:TYR:HA	1:A:80:ASN:HA	1.91	0.52
1:B:360:ILE:HG13	1:B:361:SER:N	2.25	0.52
1:C:223:PHE:HD2	1:C:225:THR:H	1.56	0.51
1:A:77:ARG:C	1:A:79:ALA:H	2.12	0.50
1:A:74:ASN:HA	1:A:83:ASN:HB2	1.93	0.50
1:C:199:ASN:O	1:C:203:GLN:HG2	2.11	0.50
1:C:356:ILE:HD11	1:C:419:GLN:HG2	1.92	0.50
1:A:55:GLU:O	1:A:58:SER:HB3	2.11	0.50
1:B:419:GLN:O	1:B:422:ILE:HG22	2.12	0.50
1:B:84:SER:HA	1:B:282:SER:O	2.12	0.49
1:B:388:THR:HG22	1:B:389:GLU:HG3	1.96	0.48
1:B:26:MET:O	1:B:30:GLN:HG2	2.14	0.48
1:A:82:ILE:O	1:A:82:ILE:HG13	2.13	0.48
1:C:183:TYR:O	1:C:186:VAL:HG12	2.13	0.48
1:C:46:ARG:HA	1:C:116:GLN:HG2	1.96	0.47
1:C:135:TYR:CE1	1:C:215:LEU:HD22	2.49	0.47
1:B:360:ILE:HG13	1:B:361:SER:H	1.78	0.47
1:C:358:ALA:O	1:C:362:SER:HB2	2.16	0.46
1:C:23:GLU:OE2	1:C:444:PRO:HB3	2.15	0.46
1:A:72:TYR:HD1	1:A:85:ASN:HB3	1.80	0.46
1:C:136:PHE:O	1:C:140:ASN:HB2	2.16	0.45
1:A:300:ASN:O	1:B:78:ASP:HB3	2.16	0.45
1:B:236:LYS:O	1:B:240:LYS:HE3	2.17	0.45
1:C:225:THR:HG23	1:C:360:ILE:HG12	1.98	0.45
1:B:151:GLN:O	1:B:155:ILE:HG12	2.16	0.44
1:C:441:LEU:O	1:C:442:SER:CB	2.65	0.44
1:B:246:LEU:O	1:B:250:LEU:HG	2.17	0.43
1:B:390:THR:HG22	1:B:392:VAL:H	1.84	0.43
1:C:84:SER:HA	1:C:282:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:TYR:O	1:A:186:VAL:HG12	2.18	0.43
1:A:205:ARG:NH1	1:A:211:TYR:HB2	2.34	0.43
1:A:328:GLN:O	1:A:332:VAL:HG23	2.19	0.43
1:A:448:ASN:C	1:A:450:GLU:H	2.21	0.43
1:C:111:LYS:HB3	1:C:254:LEU:HD23	2.00	0.43
1:A:59:PRO:HB2	1:A:102:LYS:HD3	1.99	0.43
1:C:205:ARG:NH2	1:C:211:TYR:HB2	2.24	0.42
1:B:373:ALA:HB1	1:B:401:LEU:HA	2.01	0.42
1:A:326:GLN:OE1	1:B:52:LYS:HD3	2.19	0.42
1:B:70:TYR:HA	1:B:86:ALA:O	2.18	0.42
1:A:77:ARG:O	1:A:79:ALA:N	2.44	0.42
1:B:61:LEU:HB3	1:B:62:PRO:CD	2.49	0.42
1:A:77:ARG:NH2	1:A:77:ARG:HB3	2.35	0.42
1:C:237:GLU:OE2	1:C:241:ARG:NH1	2.53	0.42
1:A:159:LEU:HD21	1:A:180:ARG:HH11	1.84	0.42
1:B:359:SER:HB3	1:B:415:TYR:HB2	2.03	0.41
1:A:419:GLN:O	1:A:422:ILE:HG22	2.20	0.41
1:A:81:GLY:HA3	1:A:287:LYS:H	1.86	0.41
1:C:24:ASN:HB3	1:C:27:GLN:HB2	2.03	0.41
1:B:36:ASN:HA	1:B:37:PRO:HD3	1.83	0.41
1:B:61:LEU:HB3	1:B:62:PRO:HD2	2.03	0.40
1:C:28:VAL:HG22	1:C:212:TYR:CE2	2.56	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	427/460 (93%)	397 (93%)	24 (6%)	6 (1%)	11	38
1	B	427/460 (93%)	414 (97%)	12 (3%)	1 (0%)	47	77
1	C	427/460 (93%)	395 (92%)	26 (6%)	6 (1%)	11	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1281/1380 (93%)	1206 (94%)	62 (5%)	13 (1%)	15	46

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ASP
1	C	289	ARG
1	C	386	VAL
1	C	442	SER
1	A	292	ALA
1	B	77	ARG
1	C	286	SER
1	A	391	ILE
1	A	450	GLU
1	A	442	SER
1	C	220	VAL
1	C	387	GLY
1	A	449	PRO

### 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	358/387 (92%)	340 (95%)	18 (5%)	24	55
1	B	358/387 (92%)	343 (96%)	15 (4%)	30	60
1	C	358/387 (92%)	343 (96%)	15 (4%)	30	60
All	All	1074/1161 (92%)	1026 (96%)	48 (4%)	27	58

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	66	LEU
1	A	77	ARG

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Mol	Chain	Res	Type
1	A	78	ASP
1	A	92	GLN
1	A	126	THR
1	A	210	ASN
1	A	281	THR
1	A	294	THR
1	A	298	ASP
1	A	337	GLN
1	A	346	VAL
1	A	362	SER
1	A	380	MET
1	A	388	THR
1	A	389	GLU
1	A	390	THR
1	A	391	ILE
1	B	23	GLU
1	B	73	SER
1	B	76	TYR
1	B	96	SER
1	B	100	MET
1	B	119	THR
1	B	126	THR
1	B	140	ASN
1	B	151	GLN
1	B	189	ASN
1	B	225	THR
1	B	378	ASP
1	B	386	VAL
1	B	400	THR
1	B	441	LEU
1	C	23	GLU
1	C	58	SER
1	C	126	THR
1	C	171	VAL
1	C	191	LEU
1	C	210	ASN
1	C	235	LEU
1	C	289	ARG
1	C	296	TYR
1	C	297	ASP
1	C	298	ASP
1	C	303	GLN

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Mol	Chain	Res	Type
1	C	311	SER
1	C	362	SER
1	C	416	LEU

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

Mol	Chain	Res	Type
1	B	266	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

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 ⓘ

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	429/460 (93%)	0.01	3 (0%) 87 88	20, 47, 85, 93	2 (0%)
1	B	428/460 (93%)	0.01	4 (0%) 84 84	18, 48, 81, 90	7 (1%)
1	C	429/460 (93%)	0.04	3 (0%) 87 88	18, 48, 85, 97	1 (0%)
All	All	1286/1380 (93%)	0.02	10 (0%) 86 86	18, 48, 84, 97	10 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	THR	5.4
1	A	379	ALA	4.1
1	B	293	GLY	3.9
1	B	294	THR	3.6
1	A	393	ASP	2.7
1	C	291	ALA	2.4
1	C	293	GLY	2.2
1	B	395	LEU	2.1
1	A	438	ASN	2.0
1	C	294	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
3	K	C	1455	1/1	0.94	0.17	79,79,79,79	0
3	K	A	1455	1/1	0.94	0.23	66,66,66,66	0
3	K	A	1456	1/1	0.96	0.16	68,68,68,68	0
2	CL	C	1454	1/1	0.96	0.18	42,42,42,42	0
2	CL	A	1454	1/1	0.97	0.20	51,51,51,51	0
2	CL	B	1454	1/1	0.99	0.13	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.