

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	7TL5
Title	:	Crystal structure of putative hydrolase yjcS from Klebsiella pneumoniae.
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		nomics of Infectious Diseases (CSGID)
Deposited on	:	2022-01-18
Resolution	:	2.69 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) 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	:	2.26
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)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.69 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.



Motria	Whole archive	Similar resolution		
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R _{free}	130704	2808 (2.70-2.70)		
Clashscore	141614	3122 (2.70-2.70)		
Ramachandran outliers	138981	3069 (2.70-2.70)		
Sidechain outliers	138945	3069 (2.70-2.70)		
RSRZ outliers	127900	2737 (2.70-2.70)		

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 >=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 <=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	А	633	80%	18%	•
1	В	633	^{2%} 82%	17%	•



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9930 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 Lactamase_B domain-containing protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	632	Total	С	Ν	0	Se	0	Ο	0
		032	4918	3121	842	935	20	0	0	0
1	P	620	Total	С	Ν	0	Se	0	1	0
	I B	032	4933	3131	845	937	20	0	1	0

• Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atom	S	ZeroOcc	AltConf
2	В	1	Total C 4 2	O 2	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	30	Total O 30 30	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	45	$\begin{array}{cc} \text{Total} & \text{O} \\ 45 & 45 \end{array}$	0	0



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.







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	76.45Å 80.16 Å 243.82 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	41.66 - 2.69	Depositor
Resolution (A)	48.52 - 2.69	EDS
% Data completeness	75.0 (41.66-2.69)	Depositor
(in resolution range)	82.2 (48.52-2.69)	EDS
R _{merge}	0.06	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.47 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
P. P.	0.209 , 0.248	Depositor
n, n_{free}	0.213 , 0.252	DCC
R_{free} test set	1741 reflections $(4.97%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	42.8	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29, 22.6	EDS
L-test for $twinning^2$	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9930	wwPDB-VP
Average B, all atoms $(Å^2)$	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: EDO

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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.24	0/5013	0.46	0/6772	
1	В	0.25	0/5028	0.46	0/6791	
All	All	0.25	0/10041	0.46	0/13563	

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	А	4918	0	4812	72	0
1	В	4933	0	4837	58	0
2	В	4	0	6	0	0
3	А	30	0	0	0	0
3	В	45	0	0	0	0
All	All	9930	0	9655	119	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 6.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:303:GLU:HG2	1:B:303:GLU:H	1.44	0.81
1:A:87:LEU:HD13	1:A:96:TRP:HB3	1.69	0.75
1:A:433:HIS:HD2	1:A:528:TRP:HE1	1.38	0.71
1:A:548:THR:O	1:A:550:ASN:N	2.24	0.71
1:A:231:ASN:HB3	1:A:335:ARG:HB3	1.73	0.70
1:A:95:ILE:HD13	1:A:167:GLU:HG3	1.74	0.70
1:A:298:MSE:HE3	1:A:305:PRO:HB2	1.74	0.68
1:B:205:VAL:HG21	1:B:215:VAL:HG11	1.75	0.68
1:A:133:VAL:HB	1:A:137:VAL:HG23	1.77	0.67
1:A:299:ALA:HB2	1:A:307:GLU:HB2	1.78	0.66
1:A:153:GLY:HA3	1:A:290:ASP:HB3	1.78	0.66
1:B:387:MSE:HE2	1:B:391:ILE:HG13	1.78	0.65
1:A:417:SER:OG	1:B:602:ASN:OD1	2.15	0.65
1:A:551:THR:OG1	1:A:552:ALA:N	2.29	0.62
1:A:389:ARG:HD2	1:B:604:VAL:HG13	1.82	0.62
1:B:238:MSE:SE	1:B:336:GLY:HA3	2.51	0.61
1:A:475:ILE:HB	1:A:498:ILE:HD11	1.85	0.59
1:A:430:SER:HB3	1:A:433:HIS:CD2	2.38	0.59
1:B:135:ASP:O	1:B:315:LYS:NZ	2.32	0.58
1:A:323:ASP:OD1	1:A:340:ARG:NH1	2.36	0.57
1:A:490:TRP:CZ2	1:B:464:LYS:HB3	2.39	0.57
1:A:143:LEU:HD23	1:A:172:ALA:HB2	1.87	0.57
1:A:160:ILE:HD13	1:A:310:TRP:HZ2	1.70	0.56
1:B:286:GLN:OE1	1:B:313:LYS:NZ	2.38	0.56
1:B:191:THR:HG21	1:B:321:ALA:HB2	1.87	0.56
1:A:160:ILE:HG12	1:A:189:LEU:HD12	1.86	0.56
1:B:64:PRO:HG3	1:B:420:LYS:HD2	1.89	0.55
1:B:476:MSE:HE2	1:B:507:GLN:HG2	1.89	0.54
1:A:167:GLU:HG2	1:A:168:PRO:HD3	1.89	0.54
1:A:464:LYS:HB3	1:B:490:TRP:CE2	2.43	0.53
1:A:597:LYS:HG3	1:A:613:ALA:HB2	1.91	0.52
1:B:202:ARG:NH1	1:B:555:ASP:OD2	2.42	0.52
1:A:457:PRO:HG2	1:A:460:GLN:HB2	1.91	0.52
1:A:360:ALA:O	1:A:374:ASN:ND2	2.35	0.51
1:B:165:SER:HB2	1:B:168:PRO:HD2	1.91	0.51
1:A:205:VAL:HG21	1:A:215:VAL:HG11	1.93	0.51
1:B:565:PHE:CE1	1:B:631:ILE:HG12	2.46	0.51
1:B:536:ALA:HA	1:B:539:LEU:HD12	1.92	0.51
1:B:137:VAL:HG12	1:B:151:ILE:HG23	1.93	0.50
1:A:525:ALA:HB3	1:A:528:TRP:HB2	1.94	0.50
1:A:464:LYS:HB3	1:B:490:TRP:CZ2	2.47	0.50
1:B:180:ARG:HG3	1:B:181:PRO:HD2	1.92	0.50
		Continue	ed on next page



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:224:MSE:HE1	1:A:276:PRO:HD2	1.94	0.49
1:A:300:PRO:O	1:A:302:SER:N	2.45	0.49
1:B:320:ALA:HB1	1:B:324:VAL:HB	1.95	0.49
1:B:403:MSE:HE3	1:B:407:GLU:HG2	1.94	0.49
1:A:240:ARG:HG3	1:A:671:ILE:HD11	1.95	0.48
1:A:303:GLU:HG2	1:B:302:SER:HB2	1.96	0.48
1:B:425:ARG:HB2	1:B:427:TYR:CE2	2.49	0.47
1:B:509:ARG:HB3	1:B:539:LEU:HB3	1.97	0.46
1:B:627:LEU:O	1:B:631:ILE:HG13	2.16	0.46
1:A:433:HIS:CD2	1:A:528:TRP:HE1	2.25	0.46
1:A:579:GLY:HA3	1:B:415:PRO:HB3	1.96	0.46
1:B:256:GLY:HA2	1:B:533:LEU:HD13	1.98	0.46
1:A:299:ALA:O	1:A:301:GLY:N	2.49	0.46
1:B:297:MSE:HE3	1:B:355:ARG:HD2	1.97	0.46
1:A:573:ILE:HD13	1:A:662:MSE:HG3	1.98	0.46
1:B:587:ILE:HD13	1:B:620:ILE:HB	1.99	0.45
1:A:325:THR:O	1:A:384:GLN:NE2	2.49	0.45
1:A:535:GLY:O	1:A:539:LEU:HB2	2.16	0.45
1:B:480:LYS:O	1:B:484:GLN:HG2	2.17	0.45
1:A:560:MSE:O	1:A:624:ARG:NH2	2.32	0.45
1:B:275:PRO:HA	1:B:276:PRO:HD3	1.91	0.45
1:A:138:TYR:CZ	1:A:180:ARG:HD2	2.52	0.45
1:A:486:GLY:HA2	1:A:488:TYR:CZ	2.52	0.45
1:A:489:ARG:NH2	1:B:455:GLU:O	2.34	0.45
1:A:220:PRO:HB2	1:A:305:PRO:O	2.17	0.45
1:A:373:GLY:O	1:A:377:ILE:N	2.41	0.45
1:B:334:LEU:HD23	1:B:335:ARG:HG3	2.00	0.44
1:A:148:MSE:HG3	1:A:162:PRO:HA	2.00	0.44
1:B:330:ASN:HB2	1:B:428:TYR:CE2	2.53	0.44
1:A:43:ALA:HB3	1:A:540:ARG:HD3	2.00	0.44
1:B:298:MSE:HE3	1:B:305:PRO:HB2	2.00	0.44
1:B:672:VAL:HG13	1:B:673:THR:HG23	2.00	0.44
1:A:233:MSE:HB3	1:B:396:LEU:HD13	2.00	0.43
1:A:224:MSE:O	1:A:228:VAL:HG22	2.18	0.43
1:A:452:THR:HA	1:A:455:GLU:HG3	2.00	0.43
1:B:133:VAL:HB	1:B:137:VAL:HG23	2.01	0.43
1:B:164:LEU:HD12	1:B:195:VAL:HG12	2.01	0.43
1:B:638:LYS:HD3	1:B:638:LYS:HA	1.84	0.43
1:B:403:MSE:HE1	1:B:411:ASN:HB2	2.00	0.43
1:A:197:HIS:NE2	1:A:322:GLU:OE2	2.30	0.43
1:A:330:ASN:O	1:A:331:THR:OG1	2.27	0.43



A + a 1	A + amo 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:378:VAL:O	1:A:382:LYS:HB2	2.18	0.43
1:A:217:ILE:HB	1:A:276:PRO:HA	2.00	0.42
1:A:307:GLU:HG3	1:A:340:ARG:HH21	1.84	0.42
1:A:490:TRP:CE2	1:B:464:LYS:HB3	2.54	0.42
1:A:586:ASN:ND2	1:A:612:VAL:HG13	2.33	0.42
1:B:191:THR:HG21	1:B:321:ALA:CB	2.49	0.42
1:A:87:LEU:HD11	1:A:171:GLU:OE1	2.19	0.42
1:A:554:PRO:HA	1:A:632:LEU:HD21	2.01	0.42
1:A:189:LEU:HD23	1:A:218:TYR:HB2	2.01	0.42
1:A:425:ARG:HB2	1:A:427:TYR:CE2	2.55	0.42
1:B:322:GLU:HG2	1:B:367:HIS:CD2	2.54	0.42
1:B:56:ASN:HB3	1:B:116:PRO:HD3	2.01	0.42
1:A:88:LYS:HD3	1:A:92:GLY:HA2	2.01	0.42
1:B:149:THR:HB	1:B:160:ILE:HB	2.02	0.42
1:B:643:GLN:HB2	1:B:645:LYS:HE2	2.02	0.42
1:A:353:ILE:HD13	1:A:382:LYS:HD2	2.02	0.41
1:A:363:ILE:HG22	1:A:377:ILE:HG12	2.02	0.41
1:A:202:ARG:HA	1:A:205:VAL:O	2.20	0.41
1:B:160:ILE:HD13	1:B:310:TRP:HZ2	1.84	0.41
1:A:75:HIS:HE2	1:A:106:GLU:CD	2.23	0.41
1:A:149:THR:HB	1:A:160:ILE:HB	2.03	0.41
1:A:382:LYS:HG3	1:A:385:ARG:NH2	2.36	0.41
1:A:436:LYS:O	1:A:440:VAL:HG23	2.20	0.41
1:A:202:ARG:HE	1:A:202:ARG:HB3	1.63	0.41
1:B:134:THR:HG22	1:B:137:VAL:HG22	2.03	0.41
1:B:224:MSE:O	1:B:228:VAL:HG22	2.21	0.41
1:A:490:TRP:O	1:A:494:VAL:HG22	2.21	0.41
1:B:192:HIS:HB2	1:B:197:HIS:CD2	2.56	0.41
1:B:390:TYR:CZ	1:B:394:GLN:HG3	2.56	0.40
1:B:167:GLU:HB2	1:B:168:PRO:HD3	2.03	0.40
1:B:330:ASN:O	1:B:331:THR:OG1	2.33	0.40
1:A:390:TYR:CZ	1:A:415:PRO:HD3	2.57	0.40
1:A:439:TYR:CE2	1:A:443:LEU:HD12	2.56	0.40
1:B:156:GLY:HA2	1:B:183:LYS:HB3	2.03	0.40
1:B:232:ILE:HG12	1:B:233:MSE:HE2	2.03	0.40
1:B:363:ILE:HG22	1:B:377:ILE:HG12	2.04	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	Perce	entiles
1	А	630/633~(100%)	595~(94%)	32~(5%)	3 (0%)	29	54
1	В	631/633~(100%)	596~(94%)	33~(5%)	2(0%)	41	66
All	All	1261/1266~(100%)	1191 (94%)	65~(5%)	5 (0%)	34	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	301	GLY
1	А	549	PRO
1	В	547	PRO
1	А	300	PRO
1	В	550	ASN

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	А	507/489~(104%)	489 (96%)	18 (4%)	35	64
1	В	510/489~(104%)	489 (96%)	21 (4%)	30	59
All	All	1017/978~(104%)	978~(96%)	39 (4%)	33	62

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type				
1	А	54	GLU				



Mol	Chain	Res	Type
1	А	76	GLN
1	А	211	LYS
1	А	258	VAL
1	А	283	THR
1	А	290	ASP
1	А	314	GLU
1	А	384	GLN
1	А	387	MSE
1	А	516	LEU
1	А	539	LEU
1	А	551	THR
1	А	561	THR
1	А	569	LEU
1	А	621	SER
1	А	625	ASP
1	А	635	GLU
1	А	649	SER
1	В	47	ASP
1	В	189	LEU
1	В	202	ARG
1	В	204	VAL
1	В	205	VAL
1	В	292	LEU
1	В	315	LYS
1	В	334	LEU
1	В	433	HIS
1	В	494	VAL
1	В	516	LEU
1	В	541	ASN
1	В	543	VAL
1	В	548	THR
1	В	558	ARG
1	В	561	THR
1	В	569	LEU
1	В	600	LEU
1	В	612	VAL
1	В	625	ASP
1	В	664	THR

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



Mol	Chain	Res	Type
1	А	433	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	Dog	Tink	B	ond leng	gths	E	ond ang	gles
IVIOI			nes Li		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	EDO	В	701	-	3,3,3	0.46	0	$2,\!2,\!2$	0.35	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	EDO	В	701	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.



There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	701	EDO	O1-C1-C2-O2

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^{th} 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	$OWAB(Å^2)$	Q<0.9
1	А	612/633~(96%)	0.19	24 (3%) 39 38	24, 46, 83, 123	0
1	В	612/633~(96%)	-0.08	10 (1%) 72 74	20, 39, 67, 133	0
All	All	1224/1266~(96%)	0.05	34 (2%) 53 54	20, 42, 78, 133	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	В	547	PRO	4.9	
1	А	301	GLY	4.7	
1	В	546	LEU	4.0	
1	А	332	TYR	3.8	
1	А	545	LYS	3.7	
1	А	305	PRO	3.6	
1	А	218	TYR	3.3	
1	А	92	GLY	3.2	
1	В	620	ILE	3.2	
1	А	303	GLU	3.1	
1	А	330	ASN	2.9	
1	А	215	VAL	2.8	
1	А	210	VAL	2.7	
1	А	498	ILE	2.7	
1	В	303	GLU	2.7	
1	А	589	LEU	2.7	
1	А	189	LEU	2.6	
1	В	649	SER	2.6	
1	В	550	ASN	2.6	
1	А	188	VAL	2.5	
1	А	550	ASN	2.5	
1	А	331	THR	2.4	
1	A	302	SER	2.3	
1	A	211	LYS	2.3	



Mal	Chain	Dog	Tuno	DCD7	
IVIOI	Unam	nes	Type	nsnz	
1	А	551	THR	2.2	
1	А	359	GLU	2.2	
1	В	548	THR	2.1	
1	А	484	GLN	2.1	
1	А	335	ARG	2.1	
1	В	60	TYR	2.1	
1	В	44	LEU	2.0	
1	А	329	HIS	2.0	
1	В	565	PHE	2.0	
1	А	292	LEU	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^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	EDO	В	701	4/4	0.82	0.60	$38,\!41,\!42,\!43$	0

6.5 Other polymers (i)

There are no such residues in this entry.

