



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6KQW / pdb_00006kqw
Title : Crystal structure of Yijc from B. subtilis
Authors : Hu, Y.M.; Dai, L.H.; Huang, J.W.; Liu, W.D.; Chen, C.C.; Guo, R.T.
Deposited on : 2019-08-20
Resolution : 2.18 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

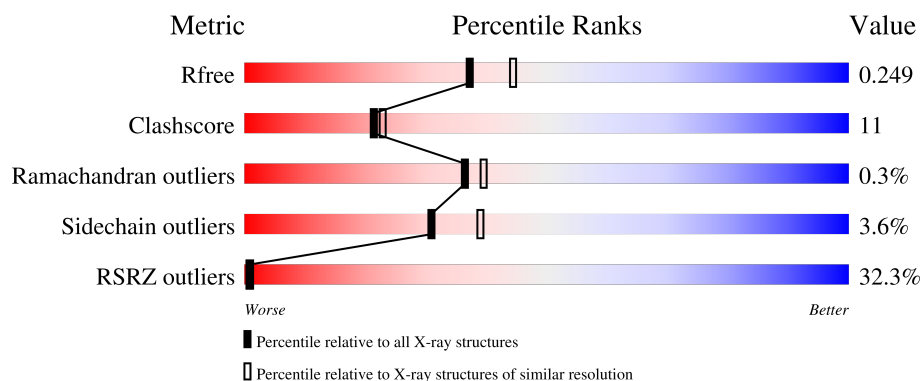
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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 $\leq 5\%$. 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	387	27% 68% 13% • 17%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2629 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 Uncharacterized UDP-glucosyltransferase YjiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2510	1603	405	487	15			

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	0
			13	6	7		

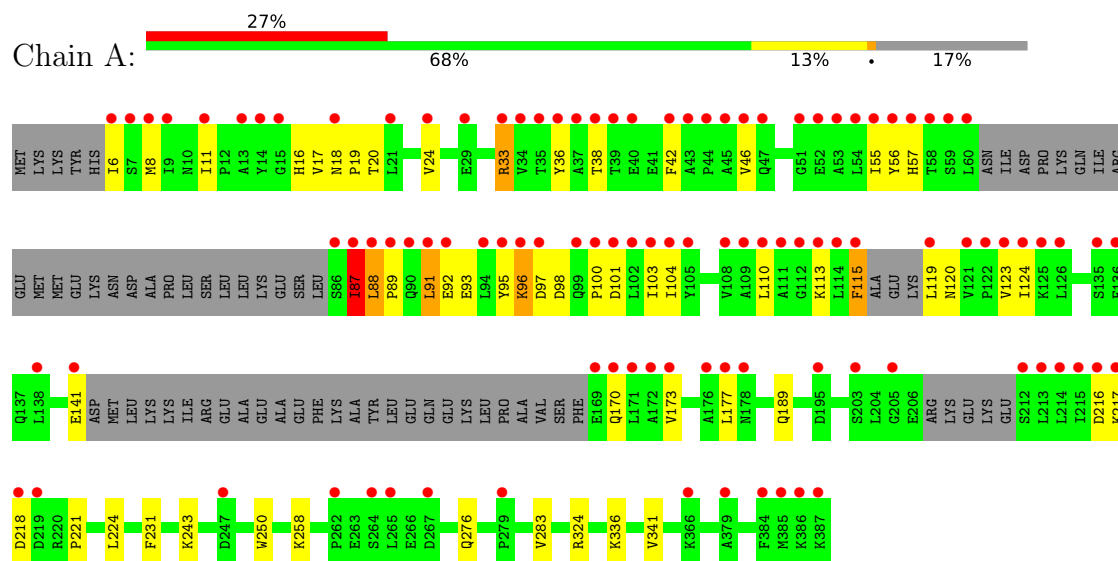
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	93	Total	O	0	0
			93	93		

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: Uncharacterized UDP-glucosyltransferase YjiC



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	51.82Å 116.84Å 187.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.81 – 2.18 23.81 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.9 (23.81-2.18) 99.7 (23.81-2.18)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.17Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.223 , 0.250 0.226 , 0.249	Depositor DCC
R_{free} test set	1524 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2629	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIT

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	0.31	0/2555	0.49	0/3458

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

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	2510	0	2493	55	0
2	A	26	0	10	3	0
3	A	93	0	0	0	0
All	All	2629	0	2503	55	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 11.

All (55) 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:103:ILE:HG22	1:A:123:VAL:HG23	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:CG2	1:A:123:VAL:HG23	1.94	0.96
1:A:88:LEU:HD22	1:A:88:LEU:H	1.41	0.84
1:A:113:LYS:O	1:A:113:LYS:HD2	1.82	0.79
1:A:93:GLU:O	1:A:96:LYS:HG3	1.86	0.75
1:A:88:LEU:HD22	1:A:88:LEU:N	2.02	0.75
1:A:103:ILE:HG22	1:A:123:VAL:CG2	2.17	0.74
1:A:33:ARG:HH22	1:A:100:PRO:HB3	1.54	0.72
1:A:189:GLN:N	2:A:402:CIT:O2	2.28	0.67
1:A:38:THR:HA	1:A:56:TYR:HE1	1.61	0.65
1:A:324:ARG:NH1	2:A:402:CIT:O1	2.32	0.63
1:A:89:PRO:HB2	1:A:115:PHE:HZ	1.66	0.61
1:A:57:HIS:H	1:A:91:LEU:HD12	1.70	0.56
1:A:89:PRO:HB2	1:A:115:PHE:CZ	2.42	0.54
1:A:33:ARG:HH22	1:A:100:PRO:CB	2.21	0.54
1:A:124:ILE:HD13	1:A:177:LEU:HD23	1.89	0.53
1:A:95:TYR:HE1	1:A:98:ASP:HB3	1.73	0.53
1:A:93:GLU:O	1:A:96:LYS:CG	2.58	0.52
1:A:91:LEU:HD23	1:A:91:LEU:N	2.24	0.52
1:A:243:LYS:HD3	1:A:341:VAL:HG21	1.91	0.51
1:A:119:LEU:N	1:A:119:LEU:CD1	2.73	0.51
1:A:95:TYR:HD1	1:A:95:TYR:O	1.93	0.51
1:A:8:MET:SD	1:A:24:VAL:HG12	2.54	0.48
1:A:324:ARG:NH2	2:A:402:CIT:O6	2.40	0.48
1:A:33:ARG:NH2	1:A:100:PRO:HB3	2.24	0.47
1:A:95:TYR:CE1	1:A:98:ASP:HB3	2.48	0.47
1:A:6:ILE:N	1:A:101:ASP:OD1	2.47	0.47
1:A:87:ILE:HG22	1:A:88:LEU:HD13	1.97	0.46
1:A:170:GLN:OE1	1:A:173:VAL:HB	2.15	0.46
1:A:88:LEU:N	1:A:88:LEU:CD2	2.73	0.46
1:A:38:THR:O	1:A:55:ILE:HA	2.16	0.46
1:A:96:LYS:HB3	1:A:96:LYS:HE3	1.54	0.46
1:A:231:PHE:CE1	1:A:336:LYS:HG3	2.51	0.46
1:A:103:ILE:HG21	1:A:123:VAL:HG23	1.90	0.45
1:A:93:GLU:HA	1:A:96:LYS:HG3	1.99	0.44
1:A:92:GLU:CD	1:A:92:GLU:C	2.86	0.44
1:A:17:VAL:O	1:A:20:THR:OG1	2.30	0.44
1:A:38:THR:OG1	1:A:42:PHE:HB2	2.17	0.44
1:A:93:GLU:O	1:A:96:LYS:HB2	2.18	0.43
1:A:38:THR:HA	1:A:56:TYR:CE1	2.48	0.43
1:A:87:ILE:HG22	1:A:88:LEU:CD1	2.49	0.43
1:A:216:ASP:O	1:A:217:LYS:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PRO:HB2	1:A:250:TRP:CZ3	2.53	0.43
1:A:95:TYR:O	1:A:95:TYR:CD1	2.71	0.43
1:A:224:LEU:HD13	1:A:283:VAL:HG11	2.01	0.43
1:A:36:TYR:HB3	1:A:46:VAL:HG11	2.00	0.42
1:A:258:LYS:HE3	1:A:276:GLN:CD	2.44	0.42
1:A:217:LYS:HG3	1:A:218:ASP:O	2.19	0.42
1:A:93:GLU:O	1:A:96:LYS:CB	2.68	0.42
1:A:119:LEU:N	1:A:119:LEU:HD12	2.34	0.41
1:A:11:ILE:HD11	1:A:16:HIS:CD2	2.55	0.41
1:A:104:ILE:HG12	1:A:124:ILE:HB	2.03	0.41
1:A:8:MET:HE2	1:A:8:MET:HB3	1.98	0.41
1:A:20:THR:O	1:A:24:VAL:HG13	2.21	0.41
1:A:18:ASN:N	1:A:19:PRO:HD2	2.36	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	312/387 (81%)	297 (95%)	14 (4%)	1 (0%)	36	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ILE

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	277/336 (82%)	267 (96%)	10 (4%)	31	39

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	87	ILE
1	A	88	LEU
1	A	91	LEU
1	A	96	LYS
1	A	97	ASP
1	A	110	LEU
1	A	115	PHE
1	A	120	ASN
1	A	141	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	297	ASN

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 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	CIT	A	402	-	12,12,12	1.10	0	17,17,17	1.48	2 (11%)
2	CIT	A	401	-	12,12,12	1.08	0	17,17,17	1.41	2 (11%)

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	CIT	A	402	-	-	10/16/16/16	-
2	CIT	A	401	-	-	2/16/16/16	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	CIT	O6-C6-C3	4.00	120.82	113.14
2	A	401	CIT	O6-C6-C3	3.62	120.09	113.14
2	A	402	CIT	O4-C5-C4	2.17	121.22	114.35
2	A	401	CIT	O4-C5-C4	2.10	121.00	114.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	CIT	C2-C3-C4-C5
2	A	402	CIT	O7-C3-C6-O5
2	A	401	CIT	C3-C4-C5-O4
2	A	401	CIT	C3-C4-C5-O3
2	A	402	CIT	C6-C3-C4-C5
2	A	402	CIT	C2-C3-C6-O5
2	A	402	CIT	C2-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	402	CIT	C4-C3-C6-O5
2	A	402	CIT	C4-C3-C6-O6
2	A	402	CIT	O7-C3-C6-O6
2	A	402	CIT	C3-C4-C5-O4
2	A	402	CIT	C3-C4-C5-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	CIT	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, 95th 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	A	322/387 (83%)	1.40	104 (32%) ⓘ ⓘ	30, 63, 124, 137	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	PHE	8.9
1	A	94	LEU	8.3
1	A	119	LEU	8.0
1	A	60	LEU	6.6
1	A	95	TYR	6.1
1	A	88	LEU	6.0
1	A	87	ILE	5.8
1	A	214	LEU	5.5
1	A	33	ARG	5.5
1	A	86	SER	5.2
1	A	111	ALA	5.0
1	A	122	PRO	4.9
1	A	170	GLN	4.7
1	A	213	LEU	4.5
1	A	96	LYS	4.5
1	A	172	ALA	4.4
1	A	110	LEU	4.4
1	A	14	TYR	4.4
1	A	89	PRO	4.3
1	A	171	LEU	4.3
1	A	91	LEU	4.2
1	A	121	VAL	4.2
1	A	9	ILE	4.0
1	A	101	ASP	4.0
1	A	247	ASP	4.0
1	A	92	GLU	3.9
1	A	112	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	55	ILE	3.8
1	A	53	ALA	3.7
1	A	42	PHE	3.7
1	A	173	VAL	3.7
1	A	102	LEU	3.7
1	A	215	ILE	3.7
1	A	385	MET	3.6
1	A	386	LYS	3.5
1	A	103	ILE	3.2
1	A	51	GLY	3.2
1	A	100	PRO	3.2
1	A	387	LYS	3.1
1	A	114	LEU	3.1
1	A	58	THR	3.0
1	A	216	ASP	3.0
1	A	212	SER	3.0
1	A	90	GLN	3.0
1	A	136	PHE	3.0
1	A	34	VAL	3.0
1	A	54	LEU	3.0
1	A	6	ILE	3.0
1	A	218	ASP	2.9
1	A	195	ASP	2.8
1	A	178	ASN	2.8
1	A	57	HIS	2.8
1	A	384	PHE	2.8
1	A	141	GLU	2.8
1	A	56	TYR	2.7
1	A	15	GLY	2.7
1	A	217	LYS	2.7
1	A	123	VAL	2.7
1	A	13	ALA	2.7
1	A	37	ALA	2.7
1	A	138	LEU	2.7
1	A	176	ALA	2.6
1	A	11	ILE	2.6
1	A	205	GLY	2.5
1	A	35	THR	2.5
1	A	40	GLU	2.5
1	A	45	ALA	2.5
1	A	113	LYS	2.5
1	A	104	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	18	ASN	2.5
1	A	47	GLN	2.5
1	A	7	SER	2.4
1	A	109	ALA	2.4
1	A	379	ALA	2.4
1	A	125	LYS	2.4
1	A	46	VAL	2.4
1	A	279	PRO	2.4
1	A	264	SER	2.4
1	A	262	PRO	2.4
1	A	105	TYR	2.3
1	A	52	GLU	2.3
1	A	265	LEU	2.3
1	A	124	ILE	2.3
1	A	169	GLU	2.3
1	A	24	VAL	2.3
1	A	108	VAL	2.3
1	A	21	LEU	2.3
1	A	126	LEU	2.3
1	A	39	THR	2.3
1	A	36	TYR	2.3
1	A	43	ALA	2.2
1	A	177	LEU	2.2
1	A	38	THR	2.2
1	A	97	ASP	2.2
1	A	29	GLU	2.2
1	A	203	SER	2.1
1	A	366	LYS	2.1
1	A	135	SER	2.1
1	A	219	ASP	2.1
1	A	59	SER	2.1
1	A	267	ASP	2.1
1	A	8	MET	2.0
1	A	99	GLN	2.0
1	A	44	PRO	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 [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, 95th 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	CIT	A	402	13/13	0.79	0.15	47,58,88,94	0
2	CIT	A	401	13/13	0.80	0.13	54,71,87,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.