



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:06 AM UTC

PDB ID : 4R2J / pdb_00004r2j
Title : Crystal structure of YdaA (Universal Stress Protein E) from *Salmonella typhimurium*
Authors : Bangera, M.; Murthy, M.R.N.
Deposited on : 2014-08-12
Resolution : 2.36 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

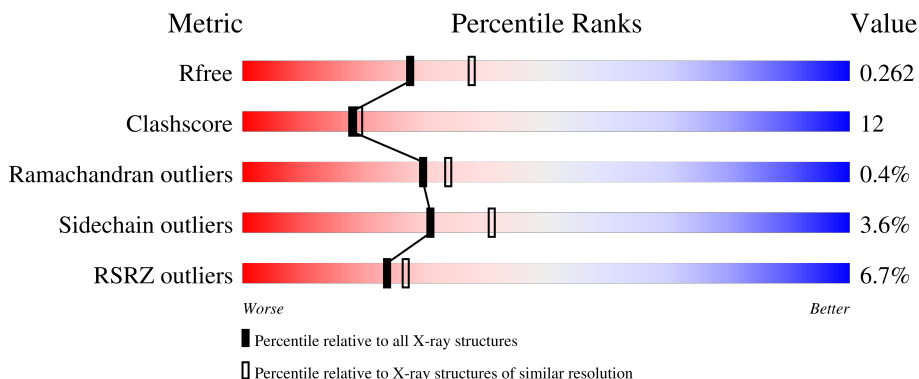
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	329	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2183 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 Universal stress protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2115	1365	366	377	7			

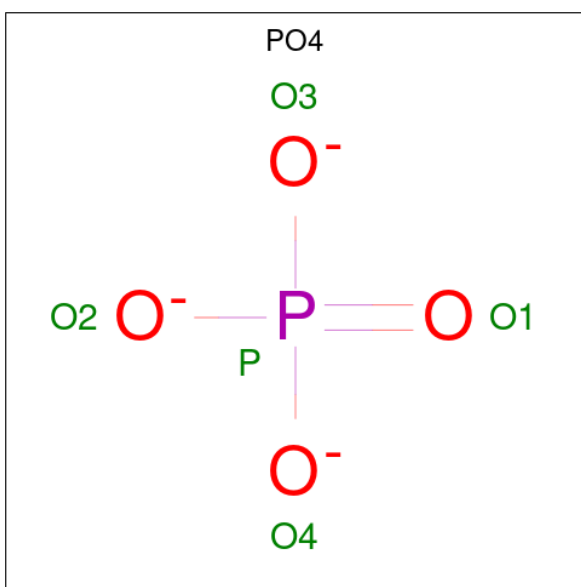
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q8ZP84
A	-12	ARG	-	expression tag	UNP Q8ZP84
A	-11	GLY	-	expression tag	UNP Q8ZP84
A	-10	SER	-	expression tag	UNP Q8ZP84
A	-9	HIS	-	expression tag	UNP Q8ZP84
A	-8	HIS	-	expression tag	UNP Q8ZP84
A	-7	HIS	-	expression tag	UNP Q8ZP84
A	-6	HIS	-	expression tag	UNP Q8ZP84
A	-5	HIS	-	expression tag	UNP Q8ZP84
A	-4	HIS	-	expression tag	UNP Q8ZP84
A	-3	GLY	-	expression tag	UNP Q8ZP84
A	-2	MET	-	expression tag	UNP Q8ZP84
A	-1	ALA	-	expression tag	UNP Q8ZP84
A	0	SER	-	expression tag	UNP Q8ZP84

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

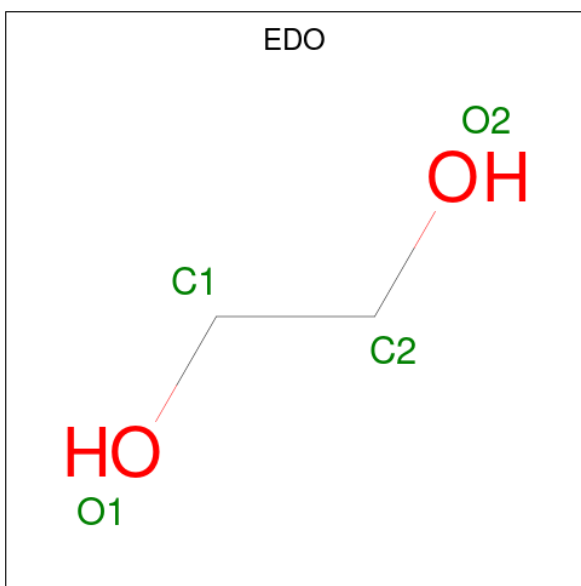
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



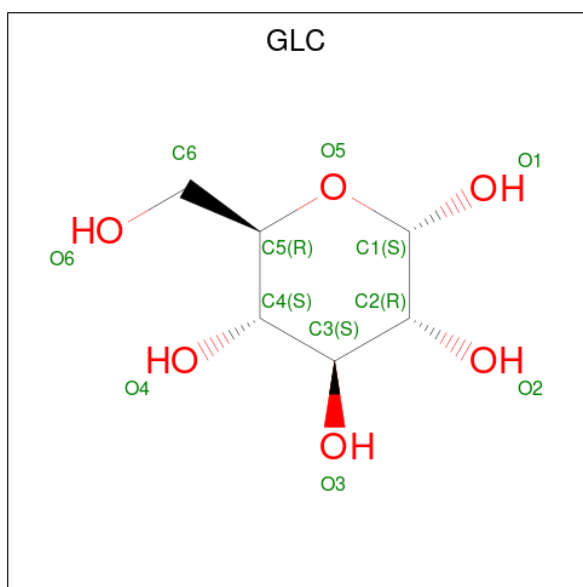
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is alpha-D-glucopyranose (CCD ID: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	6	6		
5	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	34	Total	O	0	0
			34	34		

i

- Molecule 1: Universal stress protein E



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	85.77Å 85.77Å 74.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.14 – 2.36 37.14 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.14-2.36) 99.9 (37.14-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.212 , 0.262 0.214 , 0.262	Depositor DCC
R_{free} test set	667 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2183	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.84% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO, PO4, GLC

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	0.87	0/2161	1.13	3/2959 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	TYR	N-CA-C	-8.03	102.28	114.16
1	A	282	GLY	N-CA-C	-5.93	105.31	112.48
1	A	41	ILE	CB-CA-C	-5.27	103.22	110.91

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	2115	0	1989	51	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	4	0	6	0	0
5	A	24	0	24	5	0
6	A	34	0	0	1	0
All	All	2183	0	2019	51	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 12.

All (51) 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:181:LEU:HD11	1:A:238:ILE:HD11	1.50	0.91
1:A:136:ARG:HH22	5:A:405:GLC:H61	1.42	0.82
1:A:136:ARG:HH22	5:A:405:GLC:C6	1.94	0.80
1:A:3:MET:CB	1:A:186:GLN:HE22	2.06	0.69
1:A:283:ASN:ND2	1:A:283:ASN:H	1.88	0.69
1:A:41:ILE:CD1	1:A:64:VAL:HG12	2.23	0.69
1:A:61:ARG:HH12	1:A:62:GLN:HE21	1.46	0.64
1:A:129:PRO:HA	5:A:405:GLC:O1	1.98	0.64
1:A:182:GLN:O	1:A:186:GLN:HG2	1.98	0.63
1:A:115:MET:HE3	1:A:116:ALA:C	2.25	0.62
1:A:233:ARG:HG3	1:A:238:ILE:HB	1.82	0.60
1:A:240:GLU:O	1:A:243:THR:HG22	2.04	0.57
1:A:61:ARG:O	1:A:65:ILE:HG12	2.06	0.56
1:A:233:ARG:HD2	1:A:240:GLU:HA	1.88	0.54
1:A:249:LEU:O	1:A:252:GLU:HB2	2.06	0.54
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.72	0.54
1:A:3:MET:CB	1:A:186:GLN:NE2	2.71	0.53
1:A:249:LEU:HB2	1:A:252:GLU:HG2	1.90	0.52
1:A:11:ILE:HD11	1:A:37:ALA:HB1	1.90	0.52
1:A:265:ILE:HD11	1:A:297:LEU:HB2	1.91	0.52
1:A:146:LYS:HD3	1:A:294:CYS:HA	1.92	0.52
1:A:41:ILE:HD13	1:A:64:VAL:HG12	1.93	0.51
1:A:23:ARG:NH1	1:A:295:ASP:OD2	2.38	0.51
1:A:233:ARG:HD3	1:A:243:THR:HG21	1.93	0.51
1:A:44:PHE:C	1:A:46:TYR:N	2.69	0.50
1:A:136:ARG:NH2	5:A:405:GLC:H61	2.20	0.50
1:A:96:PRO:O	1:A:100:ILE:HG13	2.11	0.50
1:A:11:ILE:HB	1:A:39:LEU:HB2	1.94	0.50
1:A:44:PHE:C	1:A:46:TYR:H	2.18	0.50
1:A:25:VAL:HG21	1:A:79:TYR:CD2	2.47	0.49
1:A:303:GLU:OE1	1:A:303:GLU:HA	2.12	0.49
1:A:61:ARG:HG3	1:A:92:TRP:CD2	2.49	0.48
1:A:115:MET:HE3	1:A:117:HIS:N	2.29	0.47
1:A:110:ASP:O	1:A:141:PRO:HD2	2.14	0.47
1:A:41:ILE:CD1	1:A:64:VAL:CG1	2.93	0.46
1:A:8:LEU:HD12	1:A:36:LYS:HB3	1.97	0.46
1:A:252:GLU:OE2	1:A:252:GLU:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:PRO:HG2	1:A:154:GLY:HA3	1.97	0.45
1:A:181:LEU:HD23	1:A:192:VAL:HG21	1.98	0.45
1:A:291:HIS:NE2	6:A:519:HOH:O	2.36	0.45
1:A:154:GLY:HA2	1:A:262:GLN:O	2.17	0.45
1:A:132:TRP:CD1	5:A:405:GLC:H5	2.52	0.44
1:A:269:GLY:HA2	1:A:299:ILE:O	2.16	0.44
1:A:8:LEU:CD1	1:A:36:LYS:HD2	2.47	0.44
1:A:60:MET:O	1:A:64:VAL:HG23	2.18	0.44
1:A:184:ALA:HB1	1:A:190:THR:O	2.19	0.43
1:A:203:ILE:O	1:A:206:ALA:HB3	2.19	0.43
1:A:233:ARG:HH11	1:A:233:ARG:HG2	1.85	0.41
1:A:232:LEU:O	1:A:233:ARG:C	2.64	0.41
1:A:120:ASP:OD2	1:A:122:LEU:HB2	2.21	0.41
1:A:226:LEU:HD23	1:A:245:VAL:HG21	2.02	0.41

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	275/329 (84%)	259 (94%)	15 (6%)	1 (0%)	30 34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	SER

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	197/284 (69%)	190 (96%)	7 (4%)	31	41

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	41	ILE
1	A	243	THR
1	A	271	VAL
1	A	283	ASN
1	A	293	ARG
1	A	303	GLU

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	62	GLN
1	A	186	GLN
1	A	262	GLN
1	A	283	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

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
5	GLC	A	404	2	12,12,12	0.96	1 (8%)	17,17,17	1.97	4 (23%)
4	EDO	A	403	-	3,3,3	0.44	0	2,2,2	0.60	0
3	PO4	A	402	-	4,4,4	1.45	1 (25%)	6,6,6	0.88	0
5	GLC	A	405	-	12,12,12	0.81	0	17,17,17	1.77	3 (17%)

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
5	GLC	A	404	2	-	2/2/22/22	0/1/1/1
4	EDO	A	403	-	-	1/1/1/1	-
5	GLC	A	405	-	-	1/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	PO4	P-O1	2.84	1.57	1.50
5	A	404	GLC	O3-C3	2.07	1.48	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	405	GLC	O5-C1-C2	4.67	118.52	110.30
5	A	404	GLC	C1-O5-C5	4.05	121.49	113.65
5	A	404	GLC	C3-C4-C5	3.78	117.09	110.23
5	A	405	GLC	C1-C2-C3	3.75	118.00	110.36
5	A	404	GLC	C4-C3-C2	-3.19	105.22	110.83
5	A	404	GLC	O5-C5-C4	3.16	115.40	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	405	GLC	C1-O5-C5	2.58	118.64	113.65

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	GLC	O5-C5-C6-O6
5	A	404	GLC	C4-C5-C6-O6
5	A	405	GLC	O5-C5-C6-O6
4	A	403	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	GLC	5	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	285/329 (86%)	0.33	19 (6%) 24 27	39, 62, 101, 117	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	PRO	4.4
1	A	50	THR	4.2
1	A	168	TYR	4.1
1	A	215	SER	4.1
1	A	214	PRO	3.9
1	A	221	ILE	3.7
1	A	271	VAL	3.2
1	A	204	ASN	3.2
1	A	207	ILE	3.0
1	A	92	TRP	2.9
1	A	279	ALA	2.9
1	A	4	TYR	2.8
1	A	48	MET	2.8
1	A	53	SER	2.4
1	A	45	SER	2.3
1	A	206	ALA	2.2
1	A	208	GLU	2.2
1	A	205	ILE	2.1
1	A	216	VAL	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
4	EDO	A	403	4/4	0.77	0.13	72,76,78,78	0
3	PO4	A	402	5/5	0.79	0.12	66,69,84,97	0
5	GLC	A	404	12/12	0.79	0.12	50,77,87,87	0
5	GLC	A	405	12/12	0.81	0.12	62,71,76,78	12
2	ZN	A	401	1/1	0.99	0.02	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.