



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:04 PM UTC

PDB ID : 3F1L / pdb_00003f1l
Title : The 0.95 Å structure of an oxidoreductase, yciK from E.coli
Authors : Vijayalakshmi, J.; Woodard, R.W.
Deposited on : 2008-10-28
Resolution : 0.95 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
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

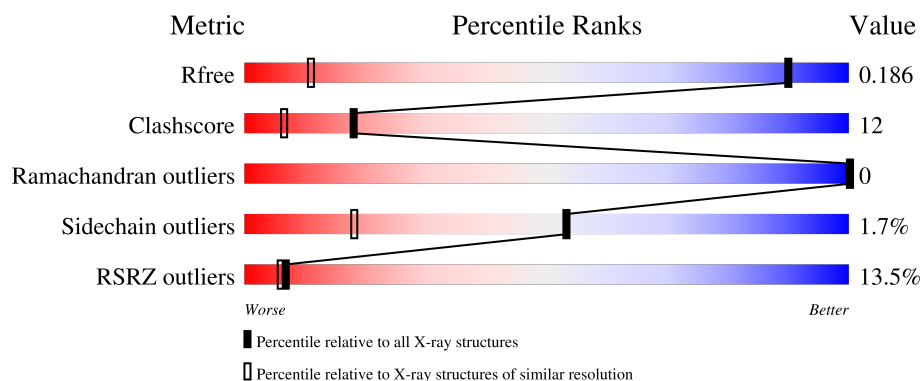
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.95 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	1045 (1.00-0.92)
Clashscore	190562	1090 (1.00-0.92)
Ramachandran outliers	187476	1032 (1.00-0.92)
Sidechain outliers	187428	1033 (1.00-0.92)
RSRZ outliers	180081	1043 (1.00-0.92)

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	252	13% 81% 15% ..
1	B	252	13% 79% 17% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8370 atoms, of which 3767 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 oxidoreductase yciK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	245	Total	C	H	N	O	S	24	5	0
			3807	1201	1885	345	361	15			
1	B	244	Total	C	H	N	O	S	0	5	0
			3800	1197	1882	342	363	16			

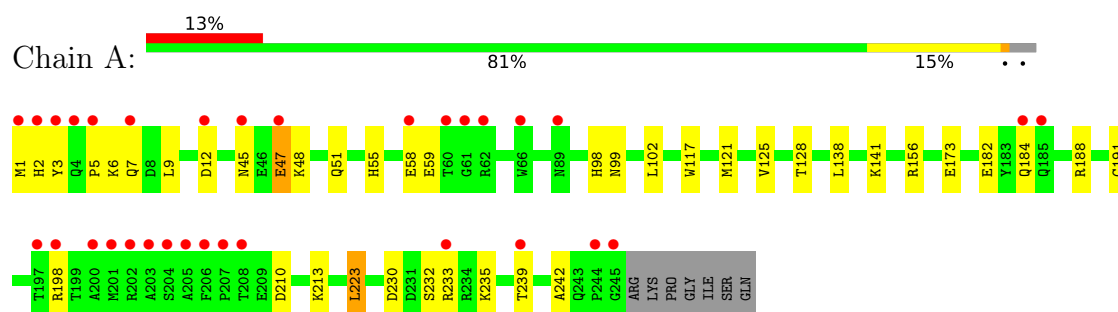
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	403	Total	O	0	0
			403	403		
2	B	360	Total	O	0	0
			360	360		

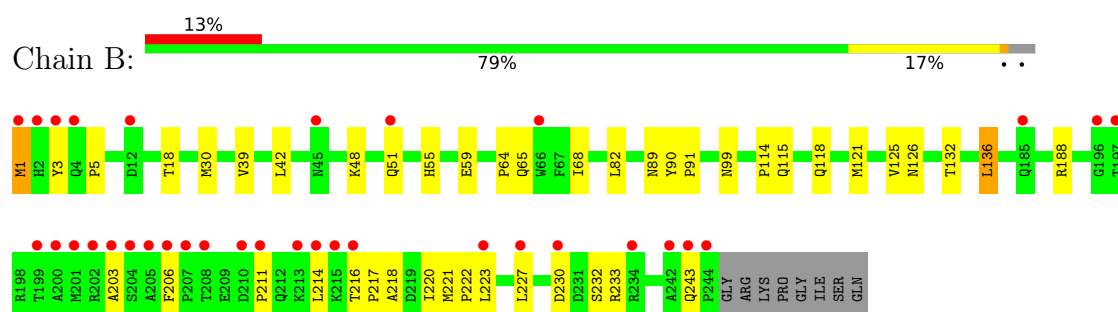
3 Residue-property plots [i](#)

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 oxidoreductase yciK



- Molecule 1: Uncharacterized oxidoreductase yciK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.87Å 66.80Å 65.05Å 90.00° 109.03° 90.00°	Depositor
Resolution (Å)	34.14 – 0.95 34.14 – 0.95	Depositor EDS
% Data completeness (in resolution range)	86.7 (34.14-0.95) 86.7 (34.14-0.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 0.90Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.171 , 0.192 0.166 , 0.186	Depositor DCC
R_{free} test set	2000 reflections (0.77%)	wwPDB-VP
Wilson B-factor (Å ²)	8.3	Xtrriage
Anisotropy	0.267	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8370	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4080e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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	0.51	0/1973	0.72	0/2673
1	B	0.47	0/1973	0.68	0/2674
All	All	0.49	0/3946	0.70	0/5347

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	A	1922	1885	1902	52	0
1	B	1918	1882	1901	47	0
2	A	403	0	0	19	0
2	B	360	0	0	11	0
All	All	4603	3767	3803	93	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 (93) 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:B:132:THR:O	1:B:136:LEU:HD13	1.51	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:HH21	1:A:239:THR:HG22	1.22	1.00
1:A:121:MET:HE2	1:B:121:MET:HE2	1.46	0.95
1:A:173:GLU:OE2	1:A:239:THR:HG21	1.75	0.87
1:A:191:CYS:HB2	1:A:239:THR:HG23	1.54	0.87
1:A:121:MET:CE	1:B:121:MET:HE2	2.05	0.87
1:A:121:MET:HE2	1:B:121:MET:CE	2.05	0.86
1:B:48:LYS:O	1:B:51:GLN:HG2	1.79	0.83
1:A:3:TYR:CE1	1:A:5:PRO:HG3	2.19	0.78
1:A:128:THR:O	2:A:700:HOH:O	2.01	0.77
1:A:182:GLU:HB3	2:A:724:HOH:O	1.85	0.76
1:A:230:ASP:O	1:A:233[A]:ARG:HG2	1.87	0.75
1:A:128:THR:HG23	2:A:700:HOH:O	1.87	0.74
1:A:184:GLN:HG3	2:A:356:HOH:O	1.88	0.72
1:B:211:PRO:HA	1:B:214:LEU:HD23	1.71	0.71
1:A:98:HIS:NE2	2:A:700:HOH:O	2.22	0.71
1:A:188:ARG:HD3	1:A:232:SER:O	1.90	0.71
1:B:1:MET:HE1	1:B:223:LEU:HD13	1.70	0.71
1:A:98:HIS:CE1	2:A:700:HOH:O	2.46	0.69
1:A:210:ASP:HB3	1:A:213:LYS:HE2	1.76	0.68
1:B:1:MET:CE	1:B:223:LEU:HD13	2.24	0.68
1:B:3:TYR:CE1	1:B:5:PRO:HG3	2.29	0.68
1:A:156:ARG:HH21	1:A:239:THR:CG2	2.03	0.65
1:B:216:THR:HG22	1:B:218:ALA:H	1.61	0.65
1:A:128:THR:CG2	2:A:700:HOH:O	2.44	0.64
1:B:42:LEU:HD21	1:B:82:LEU:HD21	1.80	0.63
1:B:114:PRO:O	1:B:118:GLN:HG3	1.98	0.63
1:A:121:MET:HE1	1:A:125:VAL:HG21	1.80	0.62
1:A:173:GLU:OE1	1:A:239:THR:OG1	2.18	0.61
1:A:233[A]:ARG:HG3	2:A:298:HOH:O	2.00	0.60
1:B:59:GLU:OE1	2:B:348:HOH:O	2.17	0.60
1:A:55:HIS:O	1:A:58:GLU:HG2	2.02	0.60
1:A:121:MET:CE	1:B:121:MET:CE	2.75	0.59
1:A:223:LEU:HD12	1:A:242:ALA:HA	1.84	0.59
1:A:156:ARG:NH2	1:A:239:THR:HG22	2.06	0.58
1:B:132:THR:HG22	1:B:136:LEU:HD11	1.85	0.58
1:B:216:THR:HG23	1:B:217:PRO:HD2	1.85	0.57
1:B:220:ILE:HG22	1:B:243:GLN:HG2	1.87	0.57
1:B:1:MET:SD	1:B:223:LEU:HA	2.44	0.57
1:B:206:PHE:CD2	2:B:755:HOH:O	2.53	0.55
1:B:99[B]:ASN:OD1	2:B:352:HOH:O	2.18	0.54
1:B:65:GLN:HE22	1:B:89:ASN:HD22	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102[B]:LEU:HD21	2:A:547:HOH:O	2.07	0.53
1:B:1:MET:HB2	1:B:3:TYR:HB2	1.89	0.53
1:A:3:TYR:CD1	1:A:5:PRO:HG3	2.43	0.53
1:A:7:GLN:O	1:A:7:GLN:HG3	2.08	0.53
1:B:1:MET:H3	1:B:1:MET:HE3	1.73	0.53
1:B:1:MET:N	2:B:762:HOH:O	2.42	0.53
1:B:55:HIS:CD2	2:B:664:HOH:O	2.62	0.53
1:B:1:MET:HE3	1:B:1:MET:N	2.24	0.52
1:A:121:MET:HG3	1:B:126:ASN:HD21	1.75	0.52
1:A:1:MET:HG3	1:A:3:TYR:HB2	1.91	0.51
1:B:121:MET:HE1	1:B:125:VAL:HG21	1.93	0.51
1:A:121:MET:CE	1:A:125:VAL:HG21	2.41	0.51
1:B:30[B]:MET:HB3	2:B:348:HOH:O	2.11	0.50
1:A:12:ASP:HB3	2:A:561:HOH:O	2.11	0.49
1:A:58:GLU:HB2	2:A:613:HOH:O	2.13	0.49
1:A:99:ASN:ND2	2:A:451:HOH:O	2.47	0.48
1:A:138:LEU:HD23	1:A:141[B]:LYS:CE	2.43	0.48
1:A:45:ASN:HB3	1:A:47[A]:GLU:OE1	2.14	0.48
1:A:117:TRP:HE1	1:B:126:ASN:HD22	1.62	0.47
2:A:434:HOH:O	1:B:114:PRO:HG3	2.15	0.47
1:B:1:MET:CE	1:B:1:MET:H3	2.27	0.47
1:A:138:LEU:HA	1:A:141[B]:LYS:NZ	2.30	0.47
1:A:98:HIS:HD2	2:A:300:HOH:O	1.97	0.47
1:B:1:MET:HE1	1:B:223:LEU:HB2	1.97	0.47
1:B:115:GLN:HG3	2:B:713:HOH:O	2.15	0.47
1:A:188:ARG:HG2	1:A:235:LYS:O	2.15	0.46
1:A:6:LYS:HE3	1:A:9:LEU:HA	1.98	0.46
1:B:132:THR:CG2	1:B:136:LEU:HD11	2.46	0.46
1:A:156:ARG:HE	1:A:239:THR:HG21	1.82	0.45
1:B:18:THR:O	1:B:99[B]:ASN:HB3	2.16	0.44
1:B:206:PHE:CE2	2:B:755:HOH:O	2.71	0.44
1:B:68:ILE:HD12	1:B:68:ILE:N	2.33	0.44
1:A:51:GLN:NE2	2:A:678:HOH:O	2.50	0.44
1:B:39:VAL:HG23	1:B:64:PRO:HB3	1.99	0.44
1:B:188:ARG:HD3	1:B:232:SER:O	2.18	0.44
1:B:121:MET:CE	1:B:125:VAL:HG21	2.49	0.42
1:A:223:LEU:HD12	1:A:242:ALA:CA	2.48	0.42
1:A:1:MET:HE3	1:A:1:MET:HA	2.01	0.42
1:A:48:LYS:HA	2:A:678:HOH:O	2.18	0.42
1:A:98:HIS:CD2	2:A:700:HOH:O	2.69	0.42
1:B:230:ASP:HA	1:B:233:ARG:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:HIS:O	1:A:59:GLU:HG2	2.20	0.41
1:B:230:ASP:HB3	2:B:527:HOH:O	2.20	0.41
1:B:221:MET:N	1:B:222:PRO:CD	2.84	0.41
1:B:90:TYR:HA	1:B:91:PRO:HD3	1.93	0.41
1:B:203:ALA:HB3	2:B:304:HOH:O	2.20	0.41
1:A:233[B]:ARG:HD3	2:A:410:HOH:O	2.20	0.40
1:A:58:GLU:CB	2:A:613:HOH:O	2.69	0.40
1:B:118:GLN:NE2	2:B:520:HOH:O	2.53	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	247/252 (98%)	240 (97%)	7 (3%)	0	100	100
1	B	247/252 (98%)	238 (96%)	9 (4%)	0	100	100
All	All	494/504 (98%)	478 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	207/209 (99%)	202 (98%)	5 (2%)	43	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	208/209 (100%)	205 (99%)	3 (1%)	59	21
All	All	415/418 (99%)	407 (98%)	8 (2%)	53	14

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	47[A]	GLU
1	A	47[B]	GLU
1	A	198	ARG
1	A	223	LEU
1	B	1	MET
1	B	136	LEU
1	B	227	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	7	GLN
1	A	45	ASN
1	A	51	GLN
1	A	81	GLN
1	A	84	GLN
1	A	98	HIS
1	A	99	ASN
1	A	161	ASN
1	A	185	GLN
1	A	243	GLN
1	B	57	ASN
1	B	89	ASN
1	B	112	GLN
1	B	126	ASN
1	B	133	GLN
1	B	161	ASN

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](#)

There are no ligands in this entry.

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	244/252 (96%)	0.48	32 (13%)	7 6	6, 11, 38, 65	4 (1%)
1	B	244/252 (96%)	0.75	34 (13%)	6 5	6, 12, 52, 77	5 (2%)
All	All	488/504 (96%)	0.62	66 (13%)	7 6	6, 11, 44, 77	9 (1%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	203	ALA	10.1
1	B	214	LEU	7.5
1	B	204	SER	6.9
1	B	244	PRO	5.9
1	B	1	MET	5.6
1	B	200	ALA	5.3
1	B	216	THR	5.2
1	B	208	THR	5.0
1	B	199	THR	4.9
1	A	2	HIS	4.9
1	A	201	MET	4.9
1	B	206	PHE	4.9
1	B	2	HIS	4.7
1	B	66	TRP	4.7
1	A	200	ALA	4.5
1	A	205	ALA	4.4
1	B	205	ALA	4.4
1	B	202	ARG	4.4
1	B	207	PRO	4.4
1	A	45	ASN	4.2
1	B	196	GLY	4.1
1	A	208	THR	4.1
1	A	203	ALA	4.0
1	B	51	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	206	PHE	3.8
1	A	233[A]	ARG	3.8
1	A	204	SER	3.8
1	A	7	GLN	3.7
1	A	207	PRO	3.6
1	B	234	ARG	3.6
1	A	61	GLY	3.6
1	A	4	GLN	3.6
1	B	210	ASP	3.5
1	B	4	GLN	3.5
1	B	242	ALA	3.5
1	A	1	MET	3.3
1	A	58	GLU	3.2
1	A	5	PRO	3.1
1	A	245	GLY	3.1
1	B	223	LEU	3.1
1	B	230	ASP	3.0
1	A	62	ARG	2.9
1	B	197	THR	2.8
1	B	243	GLN	2.8
1	B	201	MET	2.8
1	A	66	TRP	2.8
1	B	211	PRO	2.6
1	B	215	LYS	2.6
1	B	3	TYR	2.6
1	A	47[A]	GLU	2.5
1	A	89	ASN	2.4
1	B	227	LEU	2.3
1	A	3	TYR	2.3
1	A	244	PRO	2.2
1	B	185	GLN	2.2
1	B	12	ASP	2.2
1	A	184	GLN	2.2
1	A	185	GLN	2.2
1	A	202	ARG	2.1
1	A	239	THR	2.1
1	A	60	THR	2.1
1	B	213[A]	LYS	2.1
1	A	12	ASP	2.0
1	A	198	ARG	2.0
1	A	197	THR	2.0
1	B	45	ASN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.