



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:06 AM UTC

PDB ID : 3ME1 / pdb_00003me1
Title : Crystal Structure of the Desulfovibrio vulgaris Urea Transporter in the P3(1) Space Group at 3.86
Authors : Levin, E.J.; Zhou, M.; New York Consortium on Membrane Protein Structure (NYCOMPS)
Deposited on : 2010-03-31
Resolution : 3.86 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

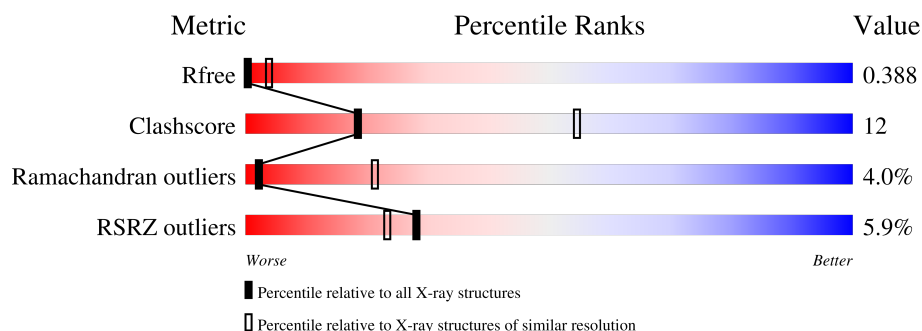
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.86 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	1165 (4.02-3.70)
Clashscore	190562	1207 (4.02-3.70)
Ramachandran outliers	187476	1149 (4.02-3.70)
RSRZ outliers	180081	1164 (4.02-3.70)

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 $\leq 5\%$. 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	335	7% 81% 13% . .
1	B	335	5% 82% 12% . .
1	C	335	5% 82% 10% . 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4673 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.

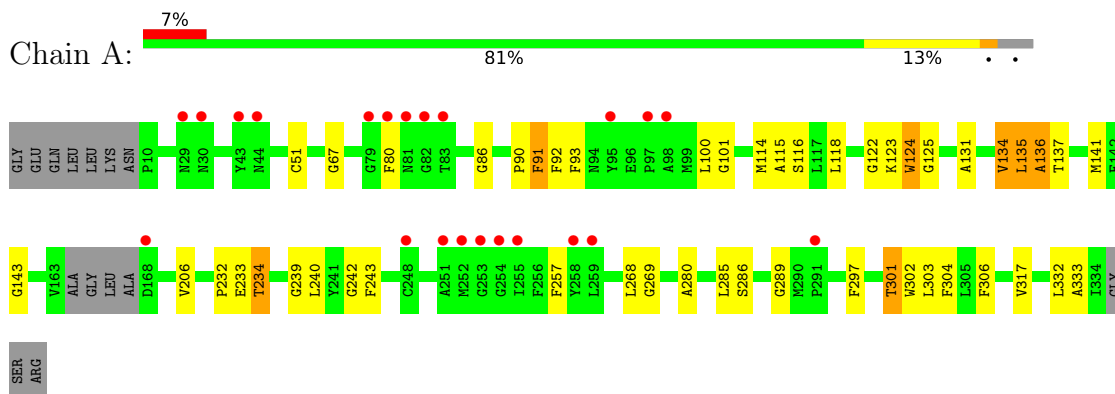
- Molecule 1 is a protein called Urea transporter.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	0	0	0
			1569	927	321	321			
1	B	323	Total	C	N	O	0	0	0
			1579	933	323	323			
1	C	312	Total	C	N	O	0	0	0
			1525	901	312	312			

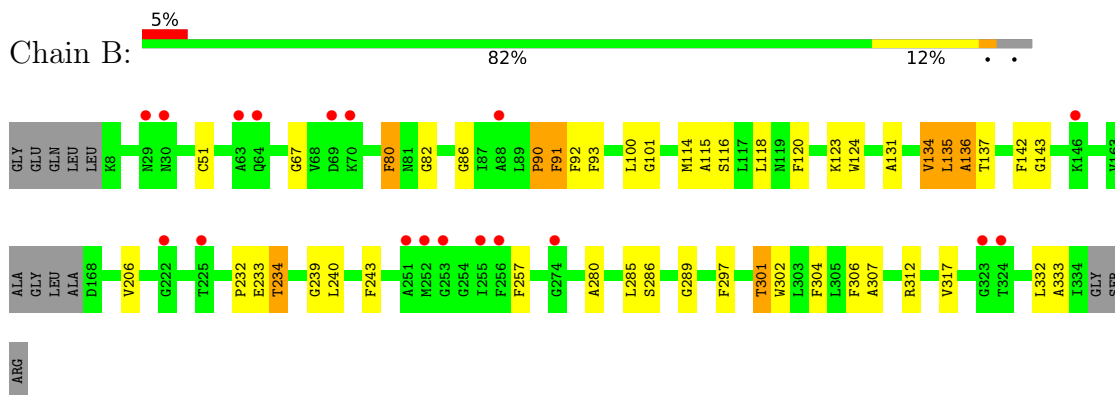
3 Residue-property plots [i](#)

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.

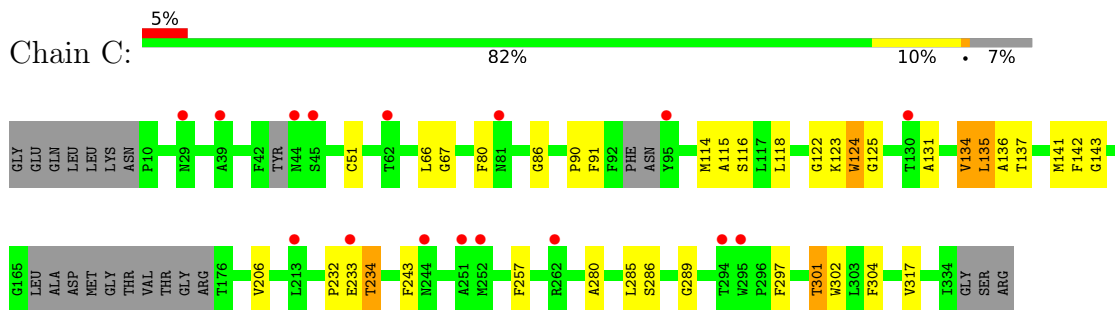
• Molecule 1: Urea transporter



• Molecule 1: Urea transporter



• Molecule 1: Urea transporter



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	103.20Å 103.20Å 141.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.81 – 3.86 34.81 – 3.86	Depositor EDS
% Data completeness (in resolution range)	97.4 (34.81-3.86) 97.6 (34.81-3.86)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.321 , 0.387 0.317 , 0.388	Depositor DCC
R_{free} test set	774 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	174.8	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l 0.125 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4673	wwPDB-VP
Average B, all atoms (Å ²)	251.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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

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	0.48	0/1567	0.98	5/2169 (0.2%)
1	B	0.49	0/1577	1.01	5/2183 (0.2%)
1	C	0.40	0/1521	0.94	5/2102 (0.2%)
All	All	0.46	0/4665	0.98	15/6454 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	ALA	CA-C-N	-9.73	108.24	118.85
1	B	131	ALA	C-N-CA	-9.73	108.24	118.85
1	A	131	ALA	CA-C-N	-9.64	108.34	118.85
1	A	131	ALA	C-N-CA	-9.64	108.34	118.85
1	C	131	ALA	CA-C-N	-8.77	109.29	118.85
1	C	131	ALA	C-N-CA	-8.77	109.29	118.85
1	B	234	THR	CA-C-N	6.83	127.11	119.32
1	B	234	THR	C-N-CA	6.83	127.11	119.32
1	A	124	TRP	N-CA-C	-6.20	104.99	114.16
1	C	124	TRP	N-CA-C	-5.88	105.46	114.16
1	B	124	TRP	N-CA-C	-5.83	105.53	114.16
1	C	234	THR	CA-C-N	5.76	126.15	119.47
1	C	234	THR	C-N-CA	5.76	126.15	119.47
1	A	234	THR	CA-C-N	5.41	125.75	119.47
1	A	234	THR	C-N-CA	5.41	125.75	119.47

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	1569	0	757	34	0
1	B	1579	0	760	34	0
1	C	1525	0	739	25	0
All	All	4673	0	2256	83	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 (83) 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:280:ALA:HB1	1:B:142:PHE:CB	2.25	0.66
1:B:280:ALA:HB1	1:C:142:PHE:CB	2.30	0.61
1:C:134:VAL:O	1:C:136:ALA:N	2.35	0.59
1:A:134:VAL:O	1:A:136:ALA:N	2.36	0.59
1:B:134:VAL:O	1:B:136:ALA:N	2.36	0.58
1:A:91:PHE:C	1:A:93:PHE:H	2.11	0.58
1:A:91:PHE:O	1:A:93:PHE:N	2.37	0.57
1:B:91:PHE:O	1:B:93:PHE:N	2.34	0.55
1:B:91:PHE:C	1:B:93:PHE:H	2.16	0.54
1:A:232:PRO:O	1:A:234:THR:N	2.40	0.54
1:C:285:LEU:O	1:C:289:GLY:N	2.41	0.54
1:B:280:ALA:HA	1:C:143:GLY:N	2.24	0.53
1:B:114:MET:O	1:B:118:LEU:N	2.39	0.53
1:B:232:PRO:O	1:B:234:THR:N	2.42	0.52
1:C:232:PRO:O	1:C:234:THR:N	2.43	0.51
1:B:136:ALA:O	1:B:137:THR:C	2.52	0.51
1:B:312:ARG:N	1:C:66:LEU:O	2.43	0.51
1:B:285:LEU:O	1:B:289:GLY:N	2.45	0.50
1:A:134:VAL:O	1:A:135:LEU:C	2.55	0.50
1:A:301:THR:O	1:A:304:PHE:N	2.44	0.50
1:B:232:PRO:C	1:B:234:THR:H	2.20	0.50
1:C:232:PRO:C	1:C:234:THR:H	2.21	0.49
1:A:280:ALA:HA	1:B:143:GLY:N	2.27	0.49
1:A:114:MET:O	1:A:118:LEU:N	2.43	0.49
1:A:285:LEU:O	1:A:289:GLY:N	2.46	0.48
1:C:134:VAL:O	1:C:135:LEU:C	2.57	0.48
1:A:232:PRO:C	1:A:234:THR:H	2.22	0.48
1:A:286:SER:C	1:A:289:GLY:H	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ALA:O	1:B:118:LEU:N	2.47	0.47
1:B:134:VAL:O	1:B:135:LEU:C	2.58	0.47
1:C:257:PHE:HA	1:C:317:VAL:H	1.81	0.46
1:A:301:THR:O	1:A:302:TRP:C	2.58	0.46
1:A:257:PHE:HA	1:A:317:VAL:H	1.80	0.46
1:B:286:SER:C	1:B:289:GLY:H	2.24	0.45
1:A:297:PHE:O	1:A:301:THR:CB	2.64	0.44
1:C:114:MET:O	1:C:118:LEU:N	2.42	0.44
1:A:122:GLY:O	1:A:125:GLY:N	2.48	0.44
1:C:137:THR:O	1:C:141:MET:N	2.51	0.44
1:A:136:ALA:O	1:A:137:THR:C	2.61	0.44
1:B:297:PHE:O	1:B:301:THR:CB	2.66	0.44
1:B:115:ALA:O	1:B:116:SER:C	2.61	0.44
1:C:134:VAL:O	1:C:137:THR:N	2.51	0.44
1:B:307:ALA:HA	1:C:115:ALA:HB1	1.99	0.44
1:C:297:PHE:O	1:C:301:THR:CB	2.66	0.44
1:A:115:ALA:O	1:A:118:LEU:N	2.51	0.43
1:A:280:ALA:CB	1:B:142:PHE:CB	2.95	0.43
1:B:306:PHE:CB	1:C:116:SER:HA	2.47	0.43
1:B:51:CYS:O	1:B:86:GLY:HA3	2.19	0.43
1:B:134:VAL:O	1:B:137:THR:N	2.52	0.43
1:B:80:PHE:C	1:B:82:GLY:N	2.76	0.43
1:C:134:VAL:C	1:C:136:ALA:N	2.77	0.43
1:A:301:THR:O	1:A:303:LEU:N	2.53	0.42
1:C:301:THR:O	1:C:302:TRP:C	2.63	0.42
1:A:134:VAL:O	1:A:137:THR:N	2.52	0.42
1:A:134:VAL:C	1:A:136:ALA:N	2.78	0.42
1:B:257:PHE:HA	1:B:317:VAL:H	1.85	0.42
1:B:100:LEU:O	1:B:101:GLY:C	2.62	0.42
1:B:301:THR:O	1:B:302:TRP:C	2.63	0.42
1:A:115:ALA:O	1:A:116:SER:C	2.63	0.41
1:B:134:VAL:C	1:B:136:ALA:N	2.78	0.41
1:C:122:GLY:C	1:C:124:TRP:H	2.28	0.41
1:A:306:PHE:C	1:B:116:SER:HA	2.45	0.41
1:B:301:THR:O	1:B:304:PHE:N	2.52	0.41
1:B:332:LEU:O	1:B:333:ALA:C	2.64	0.41
1:A:91:PHE:C	1:A:93:PHE:N	2.77	0.41
1:A:122:GLY:C	1:A:124:TRP:H	2.27	0.41
1:C:122:GLY:O	1:C:125:GLY:N	2.50	0.41
1:A:137:THR:O	1:A:141:MET:N	2.54	0.41
1:C:115:ALA:O	1:C:118:LEU:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:SER:C	1:C:289:GLY:H	2.28	0.41
1:A:239:GLY:O	1:A:242:GLY:N	2.53	0.41
1:A:239:GLY:O	1:A:240:LEU:C	2.62	0.41
1:C:51:CYS:O	1:C:86:GLY:HA3	2.20	0.41
1:A:100:LEU:O	1:A:101:GLY:C	2.64	0.41
1:A:143:GLY:N	1:C:280:ALA:HA	2.36	0.41
1:A:332:LEU:O	1:A:333:ALA:C	2.64	0.41
1:C:301:THR:O	1:C:304:PHE:N	2.52	0.41
1:A:51:CYS:O	1:A:86:GLY:HA3	2.21	0.40
1:B:80:PHE:C	1:B:82:GLY:H	2.29	0.40
1:B:90:PRO:O	1:B:93:PHE:O	2.39	0.40
1:A:268:LEU:O	1:A:269:GLY:C	2.65	0.40
1:B:239:GLY:O	1:B:240:LEU:C	2.65	0.40
1:C:115:ALA:O	1:C:116:SER:C	2.64	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	317/335 (95%)	261 (82%)	43 (14%)	13 (4%)	2	21
1	B	319/335 (95%)	259 (81%)	46 (14%)	14 (4%)	2	20
1	C	304/335 (91%)	248 (82%)	45 (15%)	11 (4%)	2	23
All	All	940/1005 (94%)	768 (82%)	134 (14%)	38 (4%)	2	21

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	GLU
1	B	233	GLU
1	A	91	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	92	PHE
1	A	134	VAL
1	A	135	LEU
1	B	91	PHE
1	B	92	PHE
1	B	134	VAL
1	B	135	LEU
1	C	91	PHE
1	C	134	VAL
1	C	135	LEU
1	C	233	GLU
1	A	301	THR
1	B	301	THR
1	C	123	LYS
1	C	301	THR
1	A	80	PHE
1	A	243	PHE
1	B	80	PHE
1	B	243	PHE
1	C	80	PHE
1	C	243	PHE
1	A	123	LYS
1	A	136	ALA
1	B	120	PHE
1	B	123	LYS
1	B	136	ALA
1	B	67	GLY
1	A	67	GLY
1	A	206	VAL
1	B	206	VAL
1	C	206	VAL
1	A	90	PRO
1	C	90	PRO
1	B	90	PRO
1	C	67	GLY

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

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	321/335 (95%)	0.01	22 (6%) 23 20	78, 198, 350, 453	0
1	B	323/335 (96%)	-0.02	18 (5%) 30 24	53, 206, 375, 478	0
1	C	312/335 (93%)	0.07	16 (5%) 33 26	141, 316, 463, 556	0
All	All	956/1005 (95%)	0.02	56 (5%) 28 23	53, 235, 431, 556	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	29	ASN	5.7
1	A	168	ASP	5.6
1	C	44	ASN	5.5
1	A	30	ASN	5.4
1	A	81	ASN	5.1
1	B	222	GLY	5.0
1	A	291	PRO	4.9
1	A	29	ASN	4.5
1	A	44	ASN	4.5
1	C	244	ASN	4.2
1	B	251	ALA	3.9
1	B	64	GLN	3.7
1	B	30	ASN	3.4
1	A	43	TYR	3.3
1	B	323	GLY	3.2
1	C	295	TRP	3.2
1	B	253	GLY	3.1
1	B	255	ILE	3.0
1	B	324	THR	2.9
1	A	80	PHE	2.9
1	A	258	TYR	2.9
1	B	256	PHE	2.8
1	A	98	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	45	SER	2.8
1	B	29	ASN	2.8
1	A	251	ALA	2.7
1	C	233	GLU	2.7
1	A	248	CYS	2.6
1	C	81	ASN	2.6
1	C	95	TYR	2.6
1	B	146	LYS	2.5
1	C	252	MET	2.5
1	A	253	GLY	2.5
1	C	262	ARG	2.5
1	B	225	THR	2.5
1	A	252	MET	2.4
1	A	83	THR	2.4
1	A	97	PRO	2.3
1	A	79	GLY	2.3
1	C	39	ALA	2.3
1	A	255	ILE	2.3
1	C	294	THR	2.3
1	A	259	LEU	2.3
1	B	63	ALA	2.3
1	B	69	ASP	2.3
1	C	62	THR	2.2
1	B	70	LYS	2.2
1	B	88	ALA	2.2
1	B	252	MET	2.2
1	C	251	ALA	2.2
1	A	95	TYR	2.1
1	C	130	THR	2.1
1	A	254	GLY	2.1
1	C	213	LEU	2.1
1	B	274	GLY	2.0
1	A	82	GLY	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.