



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:06 AM UTC

PDB ID : 1P3Q / pdb_00001p3q
Title : Mechanism of Ubiquitin Recognition by the CUE Domain of VPS9
Authors : Prag, G.; Misra, S.; Jones, E.A.; Ghirlando, R.; Davies, B.A.; Horazdovsky, B.F.; Hurley, J.H.
Deposited on : 2003-04-18
Resolution : 1.70 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

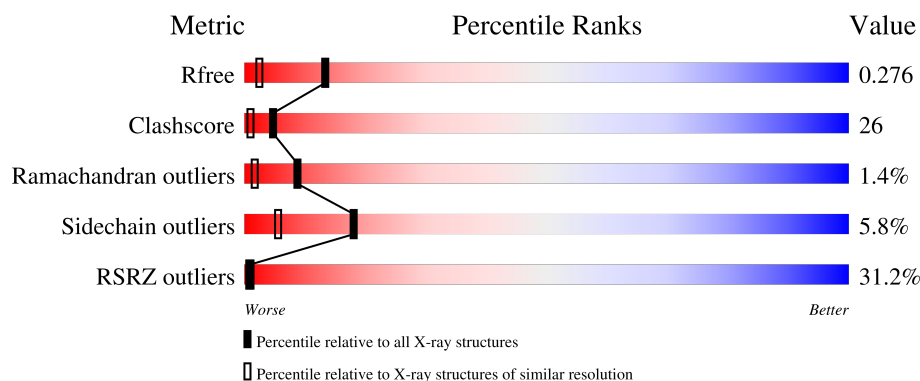
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	Q	54	43% 41% 37% 6% 17%
1	R	54	43% 24% 39% •• 33%
2	U	76	13% 76% 20% ••
2	V	76	18% 74% 18% ••

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1958 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 Vacuolar protein sorting-associated protein VPS9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	45	Total	C	N	O	S	Se	10	0	0
			342	210	55	73	2	2			
1	R	36	Total	C	N	O	S	Se	9	0	0
			265	165	41	55	2	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	435	ALA	LYS	engineered mutation	UNP P54787
Q	436	ALA	LYS	engineered mutation	UNP P54787
R	435	ALA	LYS	engineered mutation	UNP P54787
R	436	ALA	LYS	engineered mutation	UNP P54787

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	74	Total	C	N	O	S	0	0	0
			593	374	103	115	1			
2	V	73	Total	C	N	O	S	0	0	0
			582	368	99	114	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Q	19	Total	O	0	0
			19	19		
3	R	9	Total	O	0	0
			9	9		
3	U	83	Total	O	0	0
			83	83		
3	V	65	Total	O	0	0
			65	65		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.61Å 45.89Å 57.80Å 90.00° 96.53° 90.00°	Depositor
Resolution (Å)	28.71 – 1.70 28.71 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.6 (28.71-1.70) 94.7 (28.71-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.260 , 0.277 0.260 , 0.276	Depositor DCC
R_{free} test set	2777 reflections (9.59%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.1	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	0.91	EDS
Total number of atoms	1958	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.02% 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](#)

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	Q	0.48	0/342	1.02	2/457 (0.4%)
1	R	0.66	0/266	1.23	2/357 (0.6%)
2	U	0.64	0/599	1.00	0/806
2	V	0.64	0/588	0.99	0/792
All	All	0.61	0/1795	1.04	4/2412 (0.2%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	434	ALA	O-C-N	5.28	128.54	121.67
1	R	445	ALA	N-CA-C	-5.21	105.21	112.45
1	Q	440	GLY	CA-C-N	5.01	124.19	118.97
1	Q	440	GLY	C-N-CA	5.01	124.19	118.97

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	Q	342	0	336	28	0
1	R	265	0	261	37	0
2	U	593	0	623	22	0
2	V	582	0	610	18	0
3	Q	19	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	9	0	0	4	0
3	U	83	0	0	4	0
3	V	65	0	0	5	0
All	All	1958	0	1830	92	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 26.

All (92) 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)
2:V:51:GLU:HG3	3:V:96:HOH:O	1.50	1.10
1:Q:444:ASP:HA	3:Q:143:HOH:O	1.50	1.09
2:U:74:ARG:HB2	3:U:156:HOH:O	1.51	1.08
1:R:429:GLU:O	1:R:433:ILE:HD13	1.70	0.92
1:R:433:ILE:O	1:R:433:ILE:HG22	1.74	0.87
2:U:3:ILE:HD12	2:U:17:VAL:HG22	1.58	0.84
2:U:3:ILE:HD13	2:U:3:ILE:H	1.41	0.83
2:V:25:ASN:HB3	3:V:120:HOH:O	1.79	0.83
1:Q:437:SER:HB2	1:R:438:ARG:HD3	1.60	0.82
2:V:24:GLU:HG3	2:V:52:ASP:HB3	1.64	0.78
2:U:16:GLU:HG2	3:U:158:HOH:O	1.85	0.76
2:V:35:GLY:HA2	3:V:137:HOH:O	1.84	0.75
1:R:433:ILE:HD12	1:R:433:ILE:N	2.02	0.74
2:U:3:ILE:HD13	2:U:3:ILE:N	2.05	0.72
1:Q:441:PRO:HB2	1:R:435:ALA:HB1	1.70	0.71
2:U:3:ILE:HD13	2:U:15:LEU:O	1.90	0.71
1:R:448:SER:O	1:R:451:GLU:HG2	1.90	0.71
1:Q:403:LYS:O	1:Q:403:LYS:HD3	1.92	0.70
1:R:433:ILE:H	1:R:433:ILE:CD1	2.05	0.69
2:U:3:ILE:HD12	2:U:17:VAL:CG2	2.23	0.68
2:U:74:ARG:NH2	3:U:157:HOH:O	2.26	0.68
2:U:33:LYS:HG3	2:U:34:GLU:HG2	1.78	0.66
1:Q:408:GLU:HG3	1:Q:409:ARG:N	2.11	0.64
2:U:3:ILE:HD11	2:U:17:VAL:HG13	1.80	0.64
2:U:3:ILE:HD11	2:U:15:LEU:HB2	1.81	0.63
1:Q:437:SER:C	1:R:438:ARG:HB2	2.24	0.62
1:R:416:LEU:HD13	1:R:432:CYS:SG	2.38	0.62
1:R:432:CYS:C	1:R:434:ALA:H	2.07	0.62
1:R:438:ARG:HE	1:R:441:PRO:HG2	1.65	0.62
1:Q:413:LEU:O	1:Q:417:GLN:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:433:ILE:O	1:R:433:ILE:CG2	2.48	0.62
1:R:438:ARG:HG3	1:R:441:PRO:HG2	1.81	0.61
2:U:13:ILE:HG23	2:U:33:LYS:HD2	1.82	0.61
1:R:433:ILE:N	1:R:433:ILE:CD1	2.64	0.60
1:R:433:ILE:HD12	1:R:433:ILE:H	1.60	0.60
2:V:63:LYS:NZ	2:V:63:LYS:HB3	2.18	0.58
1:R:438:ARG:HG3	1:R:441:PRO:CG	2.33	0.58
1:R:416:LEU:CD1	1:R:432:CYS:SG	2.92	0.58
1:Q:410:LYS:HZ1	1:Q:414:ASN:CG	2.12	0.57
1:Q:441:PRO:O	1:Q:444:ASP:HB2	2.03	0.57
1:R:438:ARG:HG3	1:R:441:PRO:HD2	1.86	0.57
1:R:423:MSE:HG3	3:R:164:HOH:O	2.05	0.56
2:V:44:ILE:N	2:V:44:ILE:HD12	2.21	0.56
1:Q:418:ASN:ND2	2:U:62:GLN:OE1	2.33	0.55
1:Q:436:ALA:C	1:R:438:ARG:HG2	2.34	0.53
1:Q:410:LYS:HE2	1:Q:410:LYS:HA	1.90	0.53
1:Q:410:LYS:NZ	1:Q:414:ASN:CG	2.68	0.52
2:V:43:LEU:C	2:V:44:ILE:HD12	2.36	0.51
1:R:419:MSE:HE2	3:R:45:HOH:O	2.10	0.51
2:U:15:LEU:HD11	2:U:30:ILE:HD11	1.93	0.51
2:U:3:ILE:N	2:U:3:ILE:CD1	2.73	0.50
1:Q:410:LYS:NZ	1:Q:414:ASN:ND2	2.59	0.50
1:Q:443:VAL:O	1:Q:443:VAL:HG12	2.11	0.50
2:U:54:ARG:HD3	2:U:59:TYR:OH	2.12	0.50
2:V:63:LYS:HB3	2:V:63:LYS:HZ3	1.77	0.50
1:R:438:ARG:HG3	1:R:441:PRO:CD	2.41	0.49
1:Q:403:LYS:HD3	1:Q:403:LYS:C	2.36	0.49
2:V:33:LYS:NZ	2:V:33:LYS:HB3	2.27	0.49
2:U:13:ILE:CG2	2:U:33:LYS:HD2	2.43	0.49
1:Q:415:THR:CG2	1:Q:419:MSE:HE3	2.43	0.48
1:Q:418:ASN:HD22	2:V:68:HIS:HE1	1.60	0.48
1:R:432:CYS:C	1:R:434:ALA:N	2.68	0.48
1:R:430:ASP:HB3	2:V:8:LEU:HD12	1.96	0.48
1:Q:423:MSE:SE	1:R:446:LEU:HD22	2.64	0.47
1:R:427:LEU:HD23	3:R:164:HOH:O	2.14	0.47
1:Q:436:ALA:O	1:Q:437:SER:C	2.57	0.47
1:R:423:MSE:SE	3:R:164:HOH:O	2.83	0.47
1:R:432:CYS:O	1:R:434:ALA:N	2.45	0.47
2:V:63:LYS:HG2	2:V:64:GLU:HG3	1.96	0.47
2:U:6:LYS:HE3	3:U:144:HOH:O	2.15	0.47
2:V:8:LEU:HD11	2:V:36:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:444:ASP:OD1	2:V:42:ARG:NH1	2.47	0.46
2:V:24:GLU:CG	2:V:52:ASP:HB3	2.42	0.46
1:R:417:GLN:HE22	1:R:425:PRO:HG3	1.81	0.45
2:V:7:THR:HB	3:V:88:HOH:O	2.15	0.45
2:U:3:ILE:CD1	2:U:17:VAL:HG13	2.47	0.45
1:Q:441:PRO:HA	1:Q:444:ASP:OD2	2.16	0.45
2:U:3:ILE:HD11	2:U:17:VAL:CG1	2.46	0.45
1:Q:419:MSE:HE2	2:V:68:HIS:HB3	1.98	0.45
1:Q:442:CYS:SG	1:R:432:CYS:HA	2.58	0.43
1:R:427:LEU:O	1:R:431:VAL:HG23	2.18	0.43
2:U:44:ILE:HD13	2:U:49:GLN:HA	2.00	0.43
1:Q:443:VAL:HG13	1:R:419:MSE:SE	2.68	0.43
1:Q:403:LYS:HZ1	1:Q:406:GLU:CD	2.27	0.42
1:R:417:GLN:OE1	1:R:428:ILE:HD12	2.19	0.42
2:V:58:ASP:HA	3:V:133:HOH:O	2.20	0.42
1:R:438:ARG:HA	1:R:438:ARG:HD2	1.79	0.42
1:Q:403:LYS:NZ	1:Q:406:GLU:CD	2.79	0.41
1:Q:429:GLU:O	1:Q:433:ILE:HG13	2.20	0.41
1:Q:441:PRO:CB	1:R:435:ALA:HB1	2.46	0.41
1:R:438:ARG:NE	1:R:441:PRO:HG2	2.33	0.41
2:U:54:ARG:HD3	2:U:59:TYR:CZ	2.56	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	Q	41/54 (76%)	38 (93%)	2 (5%)	1 (2%)	4	1
1	R	34/54 (63%)	30 (88%)	2 (6%)	2 (6%)	1	0
2	U	72/76 (95%)	72 (100%)	0	0	100	100
2	V	71/76 (93%)	71 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	218/260 (84%)	211 (97%)	4 (2%)	3 (1%)	9 2

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	436	ALA
1	R	433	ILE
1	R	437	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	Q	41/47 (87%)	37 (90%)	4 (10%)	7 1
1	R	31/47 (66%)	29 (94%)	2 (6%)	15 4
2	U	68/68 (100%)	66 (97%)	2 (3%)	37 20
2	V	67/68 (98%)	63 (94%)	4 (6%)	17 5
All	All	207/230 (90%)	195 (94%)	12 (6%)	18 5

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	400	LEU
1	Q	402	LYS
1	Q	403	LYS
1	Q	410	LYS
1	R	433	ILE
1	R	439	ILE
2	U	3	ILE
2	U	19	PRO
2	V	15	LEU
2	V	33	LYS
2	V	51	GLU
2	V	63	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	417	GLN
1	Q	418	ASN
2	U	2	GLN
2	U	25	ASN
2	U	40	GLN
2	U	62	GLN
2	V	2	GLN
2	V	40	GLN
2	V	60	ASN
2	V	62	GLN

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	Q	43/54 (79%)	2.44	23 (53%) 0 0	17, 35, 55, 66	5 (11%)
1	R	34/54 (62%)	2.65	23 (67%) 0 0	15, 41, 54, 54	4 (11%)
2	U	74/76 (97%)	0.65	10 (13%) 7 6	7, 19, 28, 60	6 (8%)
2	V	73/76 (96%)	0.93	14 (19%) 3 3	15, 24, 37, 46	1 (1%)
All	All	224/260 (86%)	1.39	70 (31%) 1 1	7, 24, 50, 66	16 (7%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	U	14	THR	6.5
1	Q	436	ALA	6.5
2	V	73	LEU	6.3
1	R	436	ALA	6.0
1	R	430	ASP	5.7
1	R	433	ILE	5.3
1	Q	443	VAL	4.9
1	Q	437	SER	4.9
2	U	73	LEU	4.7
1	Q	440	GLY	4.7
1	Q	435	ALA	4.4
1	R	434	ALA	4.3
1	R	427	LEU	4.2
1	Q	441	PRO	4.2
2	V	10	GLY	4.0
1	R	438	ARG	3.9
2	U	62	GLN	3.9
1	Q	432	CYS	3.7
1	Q	442	CYS	3.7
1	Q	400	LEU	3.6
1	R	446	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	R	424	ASP	3.4
1	Q	401	ILE	3.4
1	Q	398	SER	3.4
2	U	9	THR	3.4
1	Q	407	ASN	3.3
1	Q	433	ILE	3.2
1	R	425	PRO	3.2
1	R	435	ALA	3.2
1	Q	399	SER	3.2
1	Q	404	ILE	3.1
1	R	426	SER	3.1
1	R	439	ILE	3.1
1	R	416	LEU	3.1
1	Q	422	ASP	3.0
2	V	39	ASP	3.0
1	Q	415	THR	3.0
1	Q	434	ALA	2.9
1	R	429	GLU	2.9
1	R	431	VAL	2.8
1	Q	405	GLU	2.7
1	R	428	ILE	2.7
2	U	10	GLY	2.7
2	V	35	GLY	2.7
2	V	8	LEU	2.6
1	Q	408	GLU	2.6
1	R	437	SER	2.5
1	Q	412	THR	2.5
2	V	7	THR	2.5
1	Q	444	ASP	2.4
1	R	432	CYS	2.4
2	U	48	LYS	2.4
1	R	445	ALA	2.4
2	V	28	ALA	2.4
1	Q	411	ASP	2.3
2	V	37	PRO	2.2
1	R	417	GLN	2.2
1	R	451	GLU	2.2
2	V	38	PRO	2.2
2	U	33	LYS	2.1
2	V	33	LYS	2.1
2	V	32	ASP	2.1
2	U	74	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	U	11	LYS	2.1
2	V	25	ASN	2.1
2	U	3	ILE	2.1
1	R	418	ASN	2.0
2	V	40	GLN	2.0
1	R	420	PHE	2.0
2	V	36	ILE	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.