



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:49 PM UTC

PDB ID : 3TDU / pdb_00003tdu
Title : N-terminal acetylation acts as an avidity enhancer within an interconnected multiprotein complex: Structure of a human Cul1WHB-Dcn1P-acetylated Ubc12N complex
Authors : Scott, D.C.; Monda, J.K.; Bennett, E.J.; Harper, J.W.; Schulman, B.A.
Deposited on : 2011-08-11
Resolution : 1.50 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

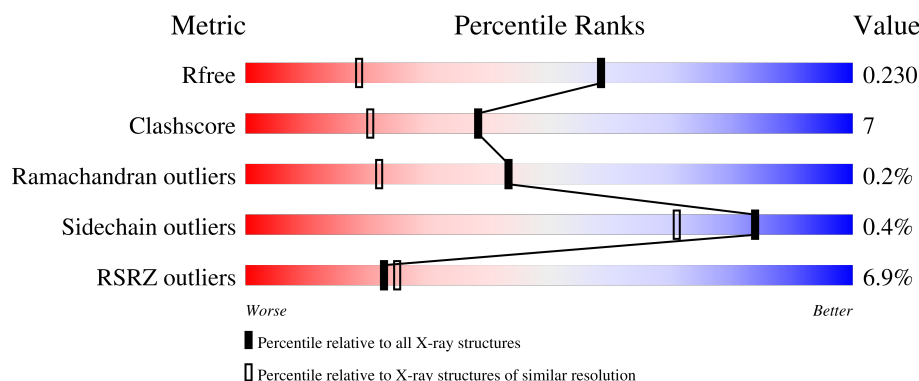
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	200	4% 84% 12% .
1	B	200	5% 84% 11% ..
2	C	77	9% 90% 8% .
2	D	77	17% 86% 13% .
3	E	16	6% 69% 31%

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Mol	Chain	Length	Quality of chain
3	F	16	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5371 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 DCN1-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	1	5	0
			1615	1043	263	300	9			
1	B	194	Total	C	N	O	S	2	7	0
			1632	1056	270	297	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLY	-	expression tag	UNP Q96GG9
A	61	SER	-	expression tag	UNP Q96GG9
B	60	GLY	-	expression tag	UNP Q96GG9
B	61	SER	-	expression tag	UNP Q96GG9

- Molecule 2 is a protein called Cullin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	75	Total	C	N	O	S	0	0	0
			618	397	108	110	3			
2	D	76	Total	C	N	O	S	0	4	0
			651	419	113	115	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	700	GLY	-	expression tag	UNP Q13616
C	701	SER	-	expression tag	UNP Q13616
D	700	GLY	-	expression tag	UNP Q13616
D	701	SER	-	expression tag	UNP Q13616

- Molecule 3 is a protein called NEDD8-conjugating enzyme Ubc12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	16	Total 133	C 86	N 21	O 25	S 1	0	0	0
3	F	16	Total 133	C 86	N 21	O 25	S 1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	ACE	-	acetylation	UNP P61081
E	2	MET	-	initiating methionine	UNP P61081
F	1	ACE	-	acetylation	UNP P61081
F	2	MET	-	initiating methionine	UNP P61081

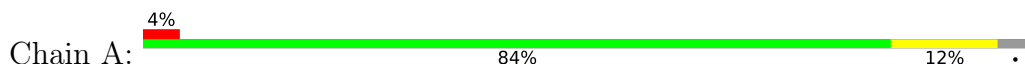
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	228	Total 228	O 228	0	0
4	B	238	Total 238	O 238	0	0
4	C	47	Total 47	O 47	0	0
4	D	54	Total 54	O 54	0	0
4	E	12	Total 12	O 12	0	0
4	F	10	Total 10	O 10	0	0

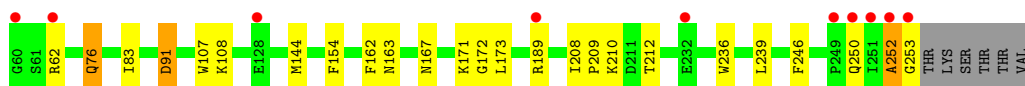
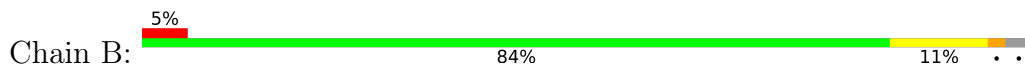
3 Residue-property plots [i](#)

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: DCN1-like protein 1



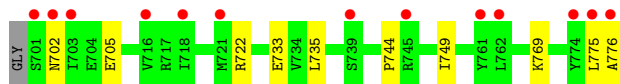
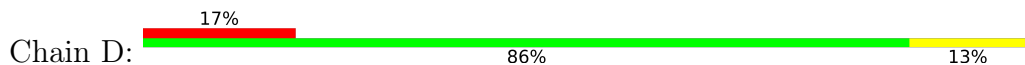
- Molecule 1: DCN1-like protein 1



- Molecule 2: Cullin-1



- Molecule 2: Cullin-1



- Molecule 3: NEDD8-conjugating enzyme Ubc12



- Molecule 3: NEDD8-conjugating enzyme Ubc12

Chain F:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.43Å 65.45Å 64.18Å 90.00° 104.73° 90.00°	Depositor
Resolution (Å)	50.00 – 1.50 50.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.00-1.50) 96.1 (50.00-1.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.206 , 0.232 0.203 , 0.230	Depositor DCC
R_{free} test set	4150 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5371	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.38% 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: ACE

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	0.73	2/1671 (0.1%)	0.76	2/2250 (0.1%)
1	B	0.80	3/1691 (0.2%)	0.80	4/2276 (0.2%)
2	C	0.38	0/624	0.69	0/833
2	D	0.39	0/669	0.72	0/892
3	E	0.43	0/131	0.65	0/170
3	F	0.36	0/131	0.69	0/170
All	All	0.67	5/4917 (0.1%)	0.75	6/6591 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	ASP	CA-CB	23.26	1.90	1.53
1	A	140	GLN	CD-NE2	21.06	1.77	1.33
1	B	76	GLN	CB-CG	13.27	1.92	1.52
1	A	140	GLN	CD-OE1	11.70	1.45	1.23
1	B	91	ASP	CA-C	8.52	1.64	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ASP	CA-CB-CG	-11.09	101.51	112.60
1	A	140	GLN	OE1-CD-NE2	-10.32	112.28	122.60
1	B	76	GLN	CB-CG-CD	-7.96	99.07	112.60
1	B	91	ASP	N-CA-C	6.56	119.27	111.33
1	B	252	ALA	N-CA-C	6.17	118.81	111.71
1	A	140	GLN	CG-CD-NE2	5.76	125.04	116.40

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	1615	0	1590	25	0
1	B	1632	0	1616	26	0
2	C	618	0	668	7	0
2	D	651	0	716	9	0
3	E	133	0	145	4	0
3	F	133	0	145	0	0
4	A	228	0	0	9	0
4	B	238	0	0	9	0
4	C	47	0	0	1	0
4	D	54	0	0	1	0
4	E	12	0	0	0	0
4	F	10	0	0	0	0
All	All	5371	0	4880	67	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 7.

All (67) 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:108[A]:LYS:HG3	1:B:144:MET:SD	1.89	1.11
1:A:108[A]:LYS:HG3	1:A:144:MET:SD	1.92	1.10
2:D:722[B]:ARG:CZ	2:D:733[B]:GLU:OE1	2.05	1.03
1:A:109:PHE:HB2	4:A:355:HOH:O	1.62	1.00
1:B:208:ILE:O	4:B:511:HOH:O	1.81	0.96
1:A:111:ALA:HB2	4:A:355:HOH:O	1.70	0.90
1:B:162:PHE:CZ	4:B:511:HOH:O	2.29	0.85
2:D:722[B]:ARG:NH2	2:D:733[B]:GLU:OE1	2.10	0.83
1:A:221[A]:THR:HG22	4:A:591:HOH:O	1.86	0.75
2:C:745:ARG:HH12	2:C:748:VAL:HG23	1.58	0.69
1:B:172:GLY:HA2	4:B:511:HOH:O	1.93	0.68
2:D:722[B]:ARG:NH1	2:D:733[B]:GLU:OE1	2.29	0.65
1:B:162:PHE:HZ	4:B:511:HOH:O	1.72	0.65
1:B:83:ILE:HD11	3:E:12:LYS:HE3	1.79	0.64
1:B:167[B]:ASN:OD1	4:B:541:HOH:O	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:HG2	4:A:595:HOH:O	1.98	0.62
1:A:108[B]:LYS:HD2	1:A:128:GLU:OE1	1.98	0.62
1:B:212:THR:HG21	1:B:239:LEU:HD23	1.81	0.61
1:B:173:LEU:N	4:B:511:HOH:O	2.33	0.60
1:B:162:PHE:CE1	4:B:511:HOH:O	2.49	0.60
1:A:198:LYS:HE2	1:A:202:GLU:HG3	1.84	0.59
1:B:83:ILE:HD12	3:E:9:LYS:HG2	1.83	0.58
1:B:252:ALA:N	1:B:253:GLY:HA2	2.18	0.58
1:B:91:ASP:CB	1:B:91:ASP:C	2.77	0.58
2:C:705:GLU:HA	2:C:708:LYS:HE3	1.84	0.58
1:A:183:ASN:O	1:A:187:ASN:HB2	2.04	0.58
1:A:135[B]:GLU:HG3	4:A:301:HOH:O	2.05	0.55
1:A:108[A]:LYS:CG	1:A:144:MET:SD	2.82	0.55
2:D:702:ASN:HB3	2:D:705:GLU:HB2	1.89	0.55
1:B:108[A]:LYS:CG	1:B:144:MET:SD	2.81	0.54
2:D:735:LEU:HD23	2:D:744:PRO:HD2	1.90	0.54
2:C:745:ARG:HB2	2:C:745:ARG:NH1	2.22	0.54
1:B:154:PHE:CE1	1:B:189[B]:ARG:NH1	2.78	0.52
1:A:109:PHE:CB	4:A:355:HOH:O	2.38	0.52
1:A:198:LYS:CE	1:A:202:GLU:HG3	2.40	0.52
1:A:212:THR:HG21	1:A:239:LEU:HD23	1.92	0.51
2:C:745:ARG:HH12	2:C:748:VAL:CG2	2.23	0.51
1:B:62[B]:ARG:NH2	4:B:317:HOH:O	2.43	0.51
1:B:163:ASN:HD21	1:B:210:LYS:HE2	1.76	0.51
1:A:250:GLN:C	1:A:252:ALA:H	2.20	0.49
1:B:83:ILE:HD11	3:E:12:LYS:CE	2.43	0.49
1:A:198:LYS:HE2	1:A:202:GLU:CG	2.43	0.48
1:B:76:GLN:CG	1:B:76:GLN:CA	2.92	0.47
2:C:745:ARG:NH1	2:C:748:VAL:HG23	2.26	0.47
1:A:221[A]:THR:HG21	4:A:592:HOH:O	2.14	0.47
1:A:218:ASP:O	1:A:221[B]:THR:HG22	2.14	0.46
1:A:198:LYS:HE2	1:A:202:GLU:CD	2.40	0.46
1:B:209:PRO:HB3	4:D:526:HOH:O	2.14	0.46
2:D:775:LEU:O	2:D:776:ALA:HB3	2.16	0.46
1:B:236:TRP:CE2	2:D:769:LYS:HE3	2.51	0.46
1:A:221[B]:THR:HG21	4:A:592:HOH:O	2.15	0.45
1:B:107:TRP:CZ3	1:B:108[A]:LYS:HD3	2.52	0.44
2:D:722[B]:ARG:NH2	2:D:733[B]:GLU:CD	2.74	0.44
1:A:143:LYS:HB3	1:A:143:LYS:HE3	1.65	0.44
1:A:135[B]:GLU:CG	4:A:301:HOH:O	2.63	0.44
1:A:108[A]:LYS:HA	1:A:108[A]:LYS:HD2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ALA:N	1:B:253:GLY:CA	2.79	0.44
3:E:4:LYS:HE3	3:E:8:LEU:HD21	2.00	0.43
1:B:246:PHE:CE1	1:B:250:GLN:NE2	2.86	0.43
2:D:744:PRO:HB2	2:D:749:ILE:HD11	2.00	0.43
2:C:750:LYS:NZ	4:C:58:HOH:O	2.52	0.42
1:A:108[B]:LYS:HG2	1:A:129:LEU:HD21	2.01	0.41
1:B:154:PHE:CZ	1:B:189[B]:ARG:NH1	2.89	0.41
1:A:222:MET:HE2	1:A:223:ILE:HA	2.03	0.40
1:A:233:GLU:O	2:C:727:HIS:HE1	2.04	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	196/200 (98%)	195 (100%)	0	1 (0%)	24	8
1	B	199/200 (100%)	197 (99%)	2 (1%)	0	100	100
2	C	73/77 (95%)	70 (96%)	3 (4%)	0	100	100
2	D	78/77 (101%)	75 (96%)	3 (4%)	0	100	100
3	E	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	F	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
All	All	574/586 (98%)	563 (98%)	10 (2%)	1 (0%)	43	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	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	175/176 (99%)	174 (99%)	1 (1%)	78	62
1	B	175/176 (99%)	175 (100%)	0	100	100
2	C	69/71 (97%)	69 (100%)	0	100	100
2	D	75/71 (106%)	75 (100%)	0	100	100
3	E	15/15 (100%)	14 (93%)	1 (7%)	15	1
3	F	15/15 (100%)	15 (100%)	0	100	100
All	All	524/524 (100%)	522 (100%)	2 (0%)	84	71

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	MET
3	E	13	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	204	HIS
1	B	88	GLN
1	B	163	ASN
2	C	727	HIS
3	F	10	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	A	193/200 (96%)	0.16	8 (4%) 41 45	7, 13, 33, 48	9 (4%)
1	B	194/200 (97%)	0.26	10 (5%) 33 35	8, 16, 34, 48	9 (4%)
2	C	75/77 (97%)	0.81	7 (9%) 14 15	14, 26, 44, 61	0
2	D	76/77 (98%)	1.27	13 (17%) 4 4	14, 30, 53, 69	4 (5%)
3	E	15/16 (93%)	0.76	1 (6%) 24 26	14, 26, 51, 72	0
3	F	15/16 (93%)	0.91	0 100 100	13, 22, 46, 60	0
All	All	568/586 (96%)	0.46	39 (6%) 23 25	7, 18, 42, 72	22 (3%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	776	ALA	6.7
2	C	776	ALA	5.6
2	D	701	SER	5.1
1	A	251	ILE	4.9
2	D	762	LEU	4.8
1	A	252	ALA	4.3
2	D	702	ASN	4.0
2	C	762	LEU	3.5
2	C	702	ASN	3.4
2	D	761	TYR	3.3
1	B	253	GLY	3.2
2	D	721[A]	MET	3.2
1	B	249	PRO	3.1
2	D	774	TYR	3.1
2	D	718	ILE	3.1
2	D	775	LEU	3.0
2	C	775	LEU	2.9
1	B	251	ILE	2.8
2	D	716	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	249	PRO	2.8
1	B	252	ALA	2.7
1	A	168	PRO	2.7
1	B	250	GLN	2.7
1	A	232	GLU	2.5
1	B	62[A]	ARG	2.5
1	B	60	GLY	2.5
1	A	222	MET	2.5
2	C	774	TYR	2.4
1	A	250	GLN	2.4
1	B	232	GLU	2.4
2	C	761	TYR	2.4
2	D	703	ILE	2.3
2	C	703	ILE	2.2
1	A	221[A]	THR	2.1
2	D	745	ARG	2.1
3	E	16	GLU	2.1
1	B	189[A]	ARG	2.0
2	D	739	SER	2.0
1	B	128	GLU	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.