



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 03:14 am GMT

PDB ID : 3K5R
Title : Crystal Structure of mouse T-cadherin EC1 EC2
Authors : Shapiro, L.; Ciatto, C.
Deposited on : 2009-10-07
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

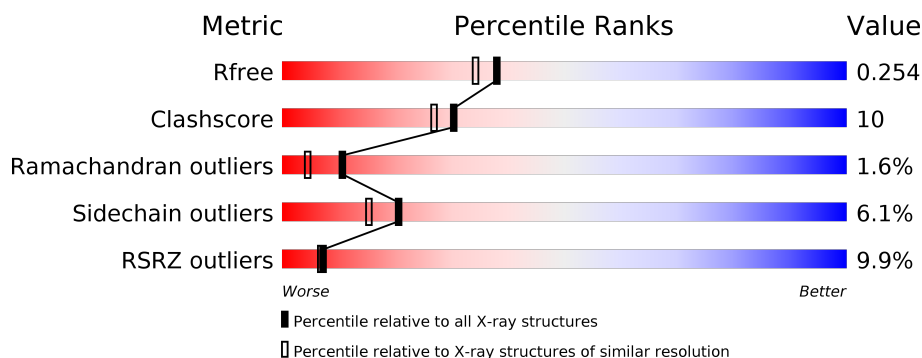
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	218	<div> <div>10%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>•</div> </div> </div>
1	B	218	<div> <div>10%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3550 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 Cadherin 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1678	1045	284	344	5			
1	B	218	Total	C	N	O	S	0	0	0
			1678	1045	284	344	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q8VDK4
A	1	GLY	-	EXPRESSION TAG	UNP Q8VDK4
B	0	SER	-	EXPRESSION TAG	UNP Q8VDK4
B	1	GLY	-	EXPRESSION TAG	UNP Q8VDK4

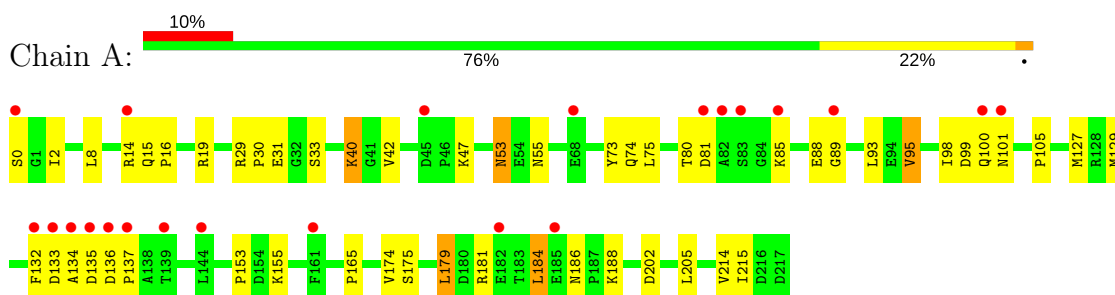
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total	O	0	0
			90	90		
2	B	104	Total	O	0	0
			104	104		

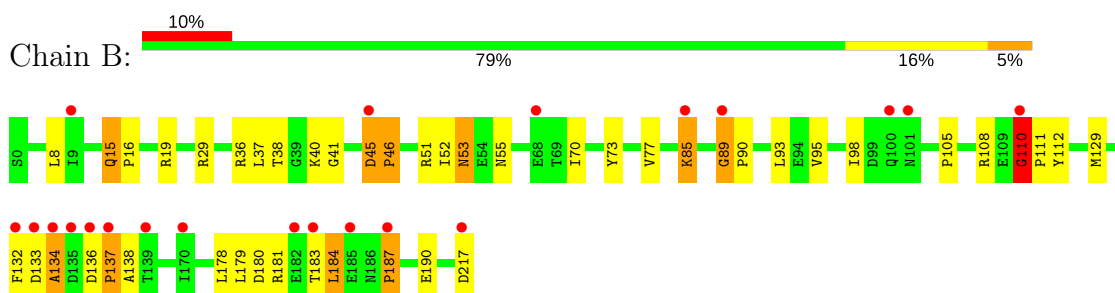
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Cadherin 13



• Molecule 1: Cadherin 13



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	107.72Å 107.72Å 226.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.00) 100.0 (19.66-2.00)	Depositor EDS
R_{merge}	0.67	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.91 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.213 , 0.259 0.208 , 0.254	Depositor DCC
R_{free} test set	1733 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3550	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 10.00% 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	A	0.88	2/1708 (0.1%)	0.92	3/2328 (0.1%)
1	B	0.93	0/1708	1.04	5/2328 (0.2%)
All	All	0.90	2/3416 (0.1%)	0.98	8/4656 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	LYS	CD-CE	6.42	1.67	1.51
1	A	47	LYS	CG-CD	6.37	1.74	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	ASP	C-N-CD	-10.23	98.09	120.60
1	B	29	ARG	NE-CZ-NH1	-8.92	115.84	120.30
1	B	29	ARG	NE-CZ-NH2	8.33	124.47	120.30
1	B	45	ASP	C-N-CA	6.88	150.91	122.00
1	B	184	LEU	CA-CB-CG	6.78	130.89	115.30
1	A	129	MET	CG-SD-CE	5.54	109.07	100.20
1	A	47	LYS	CG-CD-CE	-5.33	95.90	111.90
1	A	127	MET	CG-SD-CE	-5.09	92.06	100.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	PRO	Peptide
1	B	110	GLY	Peptide
1	B	137	PRO	Peptide
1	B	45	ASP	Peptide

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	1678	0	1658	35	0
1	B	1678	0	1658	32	0
2	A	90	0	0	3	1
2	B	104	0	0	5	0
All	All	3550	0	3316	67	1

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 10.

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:15:GLN:HE21	1:B:16:PRO:HA	1.27	0.97
1:B:85:LYS:HB2	2:B:312:HOH:O	1.67	0.93
1:B:181:ARG:HD3	1:B:217:ASP:OD2	1.79	0.83
1:A:40:LYS:HD2	1:A:73:TYR:HA	1.60	0.82
1:B:178:LEU:O	1:B:184:LEU:HD11	1.79	0.81
1:A:181:ARG:CZ	2:A:286:HOH:O	2.30	0.78
1:A:188:LYS:HG2	1:A:214:VAL:HG22	1.67	0.77
1:A:40:LYS:HE2	1:A:74:GLN:H	1.52	0.74
1:A:132:PHE:HA	2:A:299:HOH:O	1.92	0.69
1:A:134:ALA:O	1:A:135:ASP:HB2	1.92	0.68
1:B:180:ASP:H	1:B:184:LEU:HD13	1.61	0.65
1:B:178:LEU:O	1:B:184:LEU:CD1	2.45	0.64
1:A:73:TYR:HB2	1:A:95:VAL:HG13	1.80	0.64
1:A:105:PRO:HA	1:A:132:PHE:CZ	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:PRO:O	1:A:33:SER:HB2	1.99	0.62
1:B:133:ASP:O	1:B:134:ALA:HB3	2.01	0.60
1:A:15:GLN:HG3	1:A:16:PRO:HA	1.84	0.59
1:B:110:GLY:HA3	1:B:111:PRO:C	2.23	0.59
1:A:40:LYS:CE	1:A:74:GLN:H	2.16	0.58
1:A:8:LEU:HG	1:A:98:ILE:HD11	1.86	0.58
1:A:53:ASN:HD22	1:A:55:ASN:H	1.53	0.57
1:A:105:PRO:HA	1:A:132:PHE:CE2	2.39	0.56
1:B:53:ASN:HD22	1:B:55:ASN:H	1.53	0.56
1:B:36:ARG:NH1	1:B:38:THR:HG21	2.21	0.55
1:B:187:PRO:HA	2:B:269:HOH:O	2.08	0.53
1:A:29:ARG:HG2	1:A:33:SER:OG	2.10	0.52
1:B:180:ASP:H	1:B:184:LEU:CD1	2.23	0.52
1:B:133:ASP:O	1:B:134:ALA:CB	2.57	0.51
1:A:202:ASP:HB3	1:A:205:LEU:HD12	1.91	0.51
1:B:110:GLY:CA	1:B:111:PRO:O	2.60	0.50
1:B:105:PRO:HA	1:B:132:PHE:CZ	2.47	0.49
1:B:89:GLY:HA3	2:B:306:HOH:O	2.13	0.48
1:B:110:GLY:HA3	1:B:111:PRO:O	2.14	0.48
1:A:53:ASN:HD22	1:A:53:ASN:C	2.17	0.48
1:A:53:ASN:ND2	1:A:55:ASN:H	2.12	0.47
1:A:153:PRO:HG3	1:A:186:ASN:HB3	1.96	0.46
1:B:187:PRO:CA	2:B:269:HOH:O	2.64	0.46
1:B:40:LYS:HE2	1:B:73:TYR:HA	1.98	0.46
1:A:0:SER:O	1:A:0:SER:OG	2.32	0.46
1:A:133:ASP:O	1:A:134:ALA:HB3	2.16	0.46
1:A:181:ARG:NE	2:A:286:HOH:O	2.45	0.46
1:B:41:GLY:HA2	1:B:46:PRO:O	2.15	0.45
1:A:30:PRO:O	1:A:33:SER:CB	2.65	0.45
1:B:89:GLY:CA	2:B:306:HOH:O	2.64	0.45
1:B:15:GLN:NE2	1:B:16:PRO:HA	2.12	0.44
1:A:40:LYS:CD	1:A:74:GLN:H	2.31	0.44
1:A:133:ASP:HB3	1:A:136:ASP:CG	2.37	0.44
1:B:112:TYR:CD1	1:B:129:MET:HG2	2.53	0.44
1:A:40:LYS:HE2	1:A:74:GLN:N	2.25	0.43
1:B:40:LYS:HE3	1:B:70:ILE:HG21	1.99	0.43
1:A:133:ASP:HB3	1:A:136:ASP:HB3	1.99	0.43
1:A:184:LEU:HD21	1:A:215:ILE:HG12	2.01	0.43
1:A:14:ARG:HB2	1:A:14:ARG:CZ	2.47	0.43
1:A:80:THR:HA	1:A:85:LYS:O	2.19	0.43
1:A:2:ILE:HD11	1:A:88:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASP:OD1	1:A:101:ASN:HB2	2.20	0.42
1:B:37:LEU:HD22	1:B:52:ILE:HB	2.02	0.42
1:B:53:ASN:ND2	1:B:55:ASN:H	2.17	0.41
1:A:174:VAL:CG2	1:A:179:LEU:HD13	2.50	0.41
1:B:8:LEU:HG	1:B:98:ILE:HD11	2.02	0.41
1:B:93:LEU:C	1:B:93:LEU:HD23	2.40	0.41
1:A:40:LYS:HE2	1:A:74:GLN:CB	2.51	0.41
1:B:136:ASP:O	1:B:138:ALA:HA	2.20	0.40
1:B:110:GLY:CA	1:B:111:PRO:C	2.90	0.40
1:B:77:VAL:O	1:B:90:PRO:HA	2.22	0.40
1:B:133:ASP:HB3	1:B:136:ASP:HB3	2.03	0.40
1:A:42:VAL:HG23	1:A:75:LEU:HD22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:265:HOH:O	2:A:265:HOH:O[10_545]	1.28	0.92

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	216/218 (99%)	201 (93%)	13 (6%)	2 (1%)	19	12
1	B	216/218 (99%)	198 (92%)	13 (6%)	5 (2%)	7	2
All	All	432/436 (99%)	399 (92%)	26 (6%)	7 (2%)	11	4

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	PRO

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Mol	Chain	Res	Type
1	A	89	GLY
1	B	89	GLY
1	B	110	GLY
1	A	81	ASP
1	B	134	ALA
1	B	137	PRO

5.3.2 Protein sidechains ⓘ

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	190/190 (100%)	178 (94%)	12 (6%)	20	14
1	B	190/190 (100%)	179 (94%)	11 (6%)	22	17
All	All	380/380 (100%)	357 (94%)	23 (6%)	20	15

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	31	GLU
1	A	40	LYS
1	A	53	ASN
1	A	93	LEU
1	A	95	VAL
1	A	100	GLN
1	A	155	LYS
1	A	165	PRO
1	A	175	SER
1	A	179	LEU
1	A	184	LEU
1	B	15	GLN
1	B	19	ARG
1	B	51	ARG
1	B	53	ASN
1	B	85	LYS

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Mol	Chain	Res	Type
1	B	95	VAL
1	B	108	ARG
1	B	179	LEU
1	B	183	THR
1	B	187	PRO
1	B	190	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	53	ASN
1	A	100	GLN
1	B	12	ASN
1	B	15	GLN
1	B	53	ASN
1	B	100	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	218/218 (100%)	0.64	22 (10%) 7 6	19, 28, 41, 62	0
1	B	218/218 (100%)	0.55	21 (9%) 8 7	18, 28, 43, 59	0
All	All	436/436 (100%)	0.60	43 (9%) 7 7	18, 28, 42, 62	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	137	PRO	9.6
1	A	134	ALA	9.5
1	A	137	PRO	7.1
1	A	0	SER	7.0
1	A	135	ASP	6.8
1	A	136	ASP	6.1
1	B	135	ASP	5.4
1	A	133	ASP	5.3
1	B	183	THR	5.2
1	A	83	SER	4.8
1	B	89	GLY	4.4
1	B	134	ALA	4.2
1	B	182	GLU	4.1
1	A	132	PHE	3.9
1	B	136	ASP	3.9
1	B	185	GLU	3.9
1	A	139	THR	3.6
1	B	133	ASP	3.6
1	B	217	ASP	3.2
1	A	89	GLY	3.0
1	B	187	PRO	2.8
1	A	81	ASP	2.7
1	A	82	ALA	2.7
1	B	45	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	68	GLU	2.6
1	A	182	GLU	2.6
1	A	161	PHE	2.6
1	A	45	ASP	2.5
1	B	139	THR	2.5
1	A	185	GLU	2.4
1	B	9	ILE	2.4
1	A	144	LEU	2.3
1	B	101	ASN	2.3
1	A	14	ARG	2.3
1	B	110	GLY	2.3
1	A	101	ASN	2.2
1	B	100	GLN	2.2
1	A	68	GLU	2.1
1	A	100	GLN	2.1
1	B	170	ILE	2.1
1	A	85	LYS	2.1
1	B	85	LYS	2.1
1	B	132	PHE	2.1

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 carbohydrates 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.