



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:10 AM UTC

PDB ID : 6GJE / pdb_00006gje
Title : Structure of the Amnionless(20-357)-Cubilin(36-135) complex
Authors : Larsen, C.; Etzerodt, A.; Madsen, M.; Skjoedt, K.; Moestrup, S.K.; Andersen, C.B.F.
Deposited on : 2018-05-16
Resolution : 2.30 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

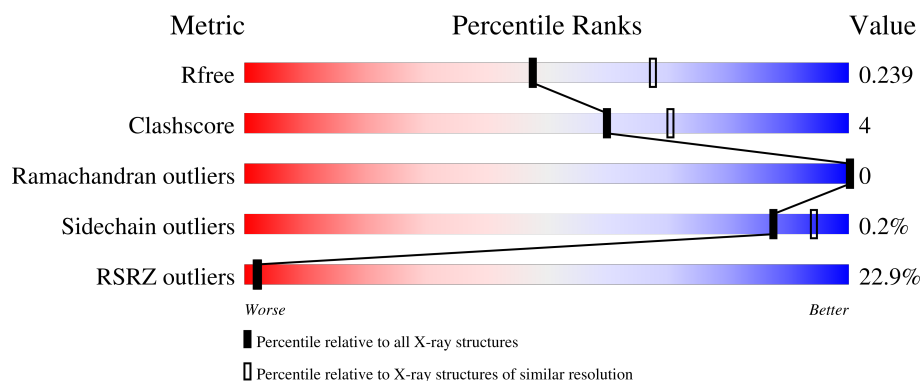
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	338	21% 93% 7%
2	B	110	20% 60% 14% • 25%
2	C	110	19% 67% 8% 25%
2	D	110	19% 66% 8% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4551 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 Protein amnionless.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	1	0
			2521	1573	461	472	15			

- Molecule 2 is a protein called Cubilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total	C	N	O	S	0	0	0
			642	398	113	129	2			
2	C	83	Total	C	N	O	S	0	0	0
			649	403	115	129	2			
2	D	82	Total	C	N	O	S	0	0	0
			641	397	114	128	2			

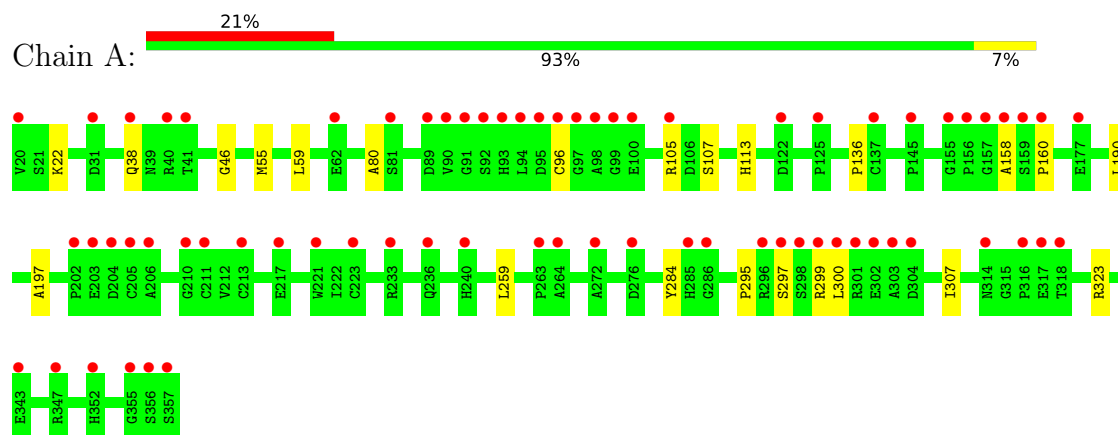
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total	O	0	0
			57	57		
3	B	17	Total	O	0	0
			17	17		
3	C	16	Total	O	0	0
			16	16		
3	D	8	Total	O	0	0
			8	8		

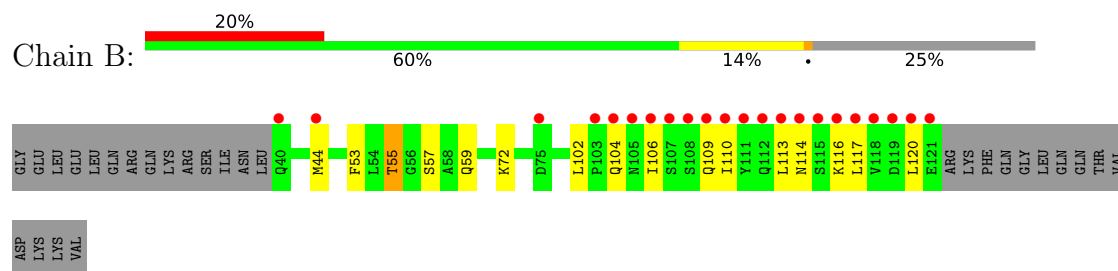
3 Residue-property plots [i](#)

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.

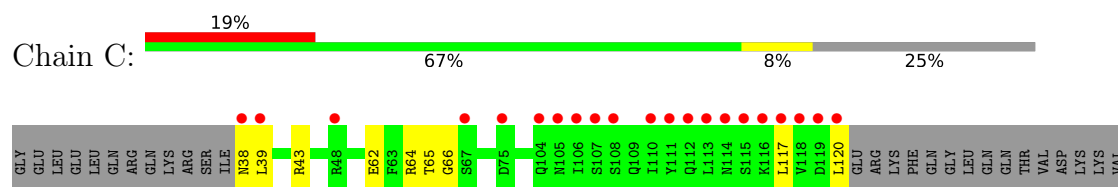
- Molecule 1: Protein amnionless



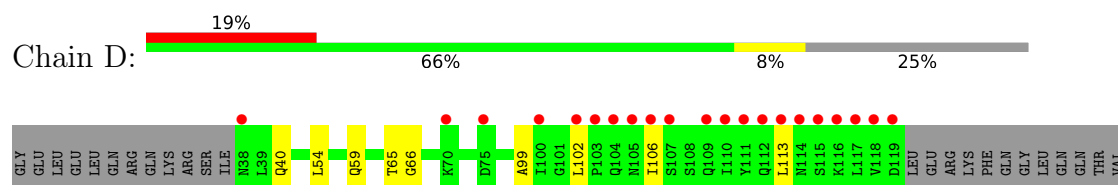
- Molecule 2: Cubilin



- Molecule 2: Cubilin



- Molecule 2: Cubilin



ASP
LYS
LYS
VAL

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	70.28Å 158.84Å 237.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.51 – 2.30 47.51 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.51-2.30) 99.9 (47.51-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.211 , 0.230 0.220 , 0.239	Depositor DCC
R_{free} test set	2562 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 71.0	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	0.95	EDS
Total number of atoms	4551	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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	0.20	0/2585	0.45	0/3519
2	B	0.14	0/647	0.37	0/868
2	C	0.20	0/654	0.37	0/878
2	D	0.17	0/646	0.42	0/867
All	All	0.19	0/4532	0.43	0/6132

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	2521	0	2427	13	0
2	B	642	0	652	16	0
2	C	649	0	663	10	0
2	D	641	0	652	9	0
3	A	57	0	0	1	0
3	B	17	0	0	0	0
3	C	16	0	0	2	0
3	D	8	0	0	1	0
All	All	4551	0	4394	38	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 4.

All (38) 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:107:SER:OG	3:A:501:HOH:O	1.97	0.82
2:B:113:LEU:HD13	2:D:113:LEU:HD11	1.72	0.70
2:B:114:ASN:HA	2:B:117:LEU:HG	1.74	0.68
1:A:297:SER:HB3	1:A:299:ARG:HG3	1.75	0.66
2:B:102:LEU:HD13	2:D:99:ALA:HB3	1.78	0.65
2:B:116:LYS:HD2	2:C:117:LEU:HD13	1.84	0.60
2:B:120:LEU:HD21	2:C:120:LEU:HD13	1.85	0.58
2:B:104:GLN:OE1	2:B:109:GLN:NE2	2.37	0.57
2:B:55:THR:HG22	2:D:65:THR:HA	1.85	0.57
1:A:160:PRO:HB3	1:A:197:ALA:HB3	1.87	0.56
1:A:259:LEU:HB2	1:A:307:ILE:HB	1.87	0.56
2:C:38:ASN:O	3:C:3701:HOH:O	2.18	0.55
2:C:117:LEU:HD23	2:C:120:LEU:HD12	1.88	0.54
2:C:65:THR:OG1	2:D:59:GLN:O	2.25	0.54
2:C:38:ASN:ND2	3:C:3703:HOH:O	2.39	0.53
2:D:102:LEU:HD12	2:D:106:ILE:HD11	1.91	0.53
2:C:39:LEU:O	2:C:43:ARG:NH1	2.44	0.51
2:B:72:LYS:HB2	2:C:62:GLU:HG2	1.94	0.50
2:C:64:ARG:HB2	2:D:54:LEU:HD23	1.94	0.49
2:B:106:ILE:O	2:B:110:ILE:HG13	2.13	0.47
2:B:106:ILE:HD12	2:B:109:GLN:HB2	1.97	0.47
2:D:40:GLN:NE2	3:D:3701:HOH:O	2.25	0.47
1:A:284:TYR:HE1	1:A:323:ARG:HG2	1.80	0.46
2:C:65:THR:HG23	2:C:66:GLY:O	2.16	0.46
2:B:57:SER:HA	2:D:66:GLY:HA3	1.97	0.45
1:A:113:HIS:NE2	1:A:158:ALA:HB1	2.32	0.45
1:A:59:LEU:HD11	1:A:80:ALA:HB2	1.99	0.45
1:A:38:GLN:HA	1:A:105[B]:ARG:HH22	1.82	0.45
2:B:55:THR:HG23	2:B:59:GLN:HB2	2.00	0.44
2:B:104:GLN:H	2:B:104:GLN:CD	2.25	0.44
2:B:44:MET:HE2	2:B:53:PHE:HE1	1.82	0.44
2:B:113:LEU:HD22	2:D:113:LEU:HD13	2.00	0.44
1:A:46:GLY:HA3	1:A:96:CYS:SG	2.59	0.43
2:B:110:ILE:HA	2:B:113:LEU:CD1	2.50	0.41
1:A:22:LYS:HG3	1:A:136:PRO:HA	2.03	0.41
1:A:295:PRO:C	1:A:297:SER:H	2.28	0.41
1:A:55:MET:HG2	1:A:190:LEU:HD23	2.02	0.40
1:A:300:LEU:O	1:A:300:LEU:HD13	2.21	0.40

There are no symmetry-related clashes.

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	337/338 (100%)	321 (95%)	16 (5%)	0	100	100
2	B	80/110 (73%)	77 (96%)	3 (4%)	0	100	100
2	C	81/110 (74%)	80 (99%)	1 (1%)	0	100	100
2	D	80/110 (73%)	79 (99%)	1 (1%)	0	100	100
All	All	578/668 (86%)	557 (96%)	21 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	262/261 (100%)	262 (100%)	0	100	100
2	B	73/99 (74%)	72 (99%)	1 (1%)	59	76
2	C	74/99 (75%)	74 (100%)	0	100	100
2	D	73/99 (74%)	73 (100%)	0	100	100
All	All	482/558 (86%)	481 (100%)	1 (0%)	87	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	55	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	HIS
1	A	285	HIS
2	B	84	GLN
2	D	83	HIS

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	338/338 (100%)	1.15	70 (20%)	2	3	31, 69, 153, 243	1 (0%)
2	B	82/110 (74%)	1.26	22 (26%)	1	1	48, 66, 182, 223	0
2	C	83/110 (75%)	1.40	21 (25%)	1	2	49, 64, 195, 263	0
2	D	82/110 (74%)	1.48	21 (25%)	1	2	47, 71, 185, 214	0
All	All	585/668 (87%)	1.25	134 (22%)	2	2	31, 68, 177, 263	1 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	LEU	9.7
2	C	120	LEU	9.6
1	A	94	LEU	9.1
1	A	90	VAL	8.3
2	B	120	LEU	8.1
1	A	303	ALA	7.8
1	A	156	PRO	7.6
1	A	158	ALA	7.6
2	D	118	VAL	7.4
2	D	103	PRO	7.2
2	B	118	VAL	7.0
2	B	117	LEU	6.8
1	A	92	SER	6.5
2	C	118	VAL	6.4
2	B	110	ILE	6.3
1	A	316	PRO	6.2
2	D	102	LEU	6.2
1	A	99	GLY	6.1
1	A	38	GLN	5.8
2	C	117	LEU	5.6
2	D	117	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
2	C	116	LYS	5.6
1	A	20	VAL	5.5
1	A	318	THR	5.5
1	A	155	GLY	5.4
1	A	301	ARG	5.3
1	A	233	ARG	5.2
2	D	106	ILE	5.1
2	C	111	TYR	5.0
2	C	105	ASN	4.9
1	A	98	ALA	4.8
2	D	110	ILE	4.8
2	D	111	TYR	4.7
2	C	107	SER	4.5
2	D	38	ASN	4.5
2	B	113	LEU	4.4
2	B	106	ILE	4.4
2	B	111	TYR	4.3
2	C	113	LEU	4.3
2	D	116	LYS	4.3
1	A	264	ALA	4.2
1	A	93	HIS	4.1
2	D	119	ASP	4.1
1	A	91	GLY	4.1
2	D	107	SER	4.1
1	A	213	CYS	4.1
1	A	276	ASP	4.0
1	A	89	ASP	4.0
2	D	100	ILE	4.0
1	A	160	PRO	4.0
1	A	263	PRO	3.9
1	A	40	ARG	3.9
2	C	119	ASP	3.9
2	D	105	ASN	3.9
1	A	304	ASP	3.9
1	A	159	SER	3.9
1	A	298	SER	3.9
2	C	106	ILE	3.9
1	A	205	CYS	3.8
1	A	202	PRO	3.8
2	C	38	ASN	3.8
2	D	114	ASN	3.8
2	D	104	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	356	SER	3.7
2	C	112	GLN	3.7
2	C	104	GLN	3.6
1	A	95	ASP	3.6
1	A	105[A]	ARG	3.6
2	C	114	ASN	3.6
1	A	299	ARG	3.6
2	C	39	LEU	3.6
2	C	115	SER	3.5
1	A	204	ASP	3.5
1	A	157	GLY	3.5
1	A	357	SER	3.4
2	B	121	GLU	3.4
1	A	41	THR	3.4
2	D	109	GLN	3.3
2	B	105	ASN	3.3
2	B	107	SER	3.3
2	D	75	ASP	3.3
2	C	110	ILE	3.3
2	B	104	GLN	3.2
1	A	355	GLY	3.1
1	A	31	ASP	3.1
1	A	302	GLU	3.1
2	B	114	ASN	3.0
1	A	81	SER	2.9
1	A	217	GLU	2.9
1	A	297	SER	2.9
2	C	67	SER	2.9
2	B	112	GLN	2.9
1	A	210	GLY	2.9
2	B	40	GLN	2.8
1	A	317	GLU	2.8
1	A	240	HIS	2.8
1	A	203	GLU	2.8
1	A	97	GLY	2.7
1	A	206	ALA	2.7
2	D	70	LYS	2.7
2	D	115	SER	2.7
2	C	48	ARG	2.7
1	A	100	GLU	2.6
1	A	177	GLU	2.6
1	A	314	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	211	CYS	2.5
2	C	75	ASP	2.5
1	A	62	GLU	2.4
1	A	96	CYS	2.4
2	D	113	LEU	2.4
2	B	108	SER	2.4
2	C	108	SER	2.4
2	B	116	LYS	2.4
1	A	285	HIS	2.4
1	A	343	GLU	2.4
2	B	44	MET	2.4
2	B	119	ASP	2.3
2	B	115	SER	2.3
2	D	112	GLN	2.3
1	A	223	CYS	2.2
1	A	286	GLY	2.2
2	B	109	GLN	2.2
1	A	221	TRP	2.2
1	A	236	GLN	2.2
1	A	296	ARG	2.2
1	A	137	CYS	2.1
2	B	103	PRO	2.1
1	A	272	ALA	2.0
1	A	352	HIS	2.0
1	A	122	ASP	2.0
2	B	75	ASP	2.0
1	A	145	PRO	2.0
1	A	347	ARG	2.0
1	A	125	PRO	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.