



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:55 AM UTC

PDB ID : 8HFW / pdb_00008hfw
Title : The crystal structure of alpha/beta fold hydrolase
Authors : Lu, H.; Xu, Y.
Deposited on : 2022-11-12
Resolution : 1.66 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

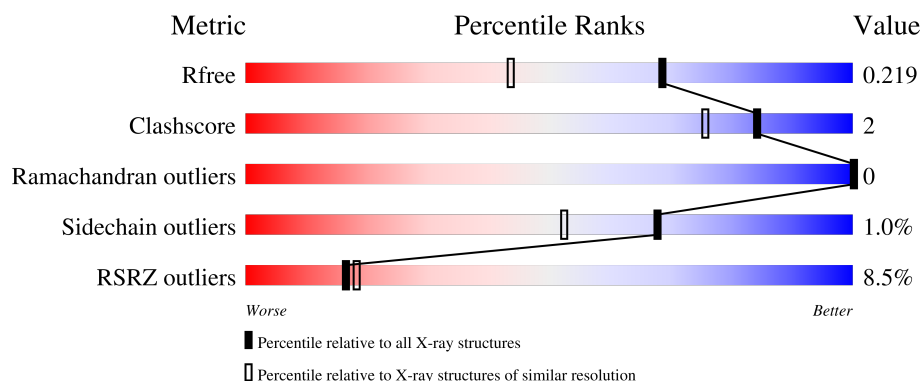
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	304	2% 88% 6% 6%
1	B	304	10% 85% 6% 8%
1	C	304	12% 88% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6318 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 Alpha/beta fold hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	2	1
			2077	1322	366	379	10			
1	B	280	Total	C	N	O	S	0	2	1
			1975	1257	341	367	10			
1	C	281	Total	C	N	O	S	0	1	0
			1937	1228	342	358	9			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	VAL	ILE	conflict	UNP A0A4V2WUI0
A	8	ALA	PRO	conflict	UNP A0A4V2WUI0
A	9	ALA	GLN	conflict	UNP A0A4V2WUI0
A	10	PRO	GLN	conflict	UNP A0A4V2WUI0
A	11	SER	ALA	conflict	UNP A0A4V2WUI0
A	38	GLU	ALA	conflict	UNP A0A4V2WUI0
A	92	GLU	GLN	conflict	UNP A0A4V2WUI0
A	102	HIS	ARG	conflict	UNP A0A4V2WUI0
A	160	ALA	GLY	conflict	UNP A0A4V2WUI0
A	161	PRO	ALA	conflict	UNP A0A4V2WUI0
A	186	ALA	ASP	conflict	UNP A0A4V2WUI0
A	187	LEU	THR	conflict	UNP A0A4V2WUI0
A	188	ALA	MET	conflict	UNP A0A4V2WUI0
A	197	ALA	PRO	conflict	UNP A0A4V2WUI0
A	204	MET	VAL	conflict	UNP A0A4V2WUI0
A	208	MET	LEU	conflict	UNP A0A4V2WUI0
A	219	THR	SER	conflict	UNP A0A4V2WUI0
A	226	ALA	VAL	conflict	UNP A0A4V2WUI0
A	240	ALA	GLN	conflict	UNP A0A4V2WUI0
A	260	VAL	ALA	conflict	UNP A0A4V2WUI0
A	280	GLN	GLU	conflict	UNP A0A4V2WUI0
A	281	PRO	ALA	conflict	UNP A0A4V2WUI0
A	282	GLY	ALA	conflict	UNP A0A4V2WUI0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	289	VAL	ALA	conflict	UNP A0A4V2WUI0
A	295	ILE	-	expression tag	UNP A0A4V2WUI0
A	296	ALA	-	expression tag	UNP A0A4V2WUI0
A	297	LEU	-	expression tag	UNP A0A4V2WUI0
A	298	GLU	-	expression tag	UNP A0A4V2WUI0
A	299	HIS	-	expression tag	UNP A0A4V2WUI0
A	300	HIS	-	expression tag	UNP A0A4V2WUI0
A	301	HIS	-	expression tag	UNP A0A4V2WUI0
A	302	HIS	-	expression tag	UNP A0A4V2WUI0
A	303	HIS	-	expression tag	UNP A0A4V2WUI0
A	304	HIS	-	expression tag	UNP A0A4V2WUI0
B	5	VAL	ILE	conflict	UNP A0A4V2WUI0
B	8	ALA	PRO	conflict	UNP A0A4V2WUI0
B	9	ALA	GLN	conflict	UNP A0A4V2WUI0
B	10	PRO	GLN	conflict	UNP A0A4V2WUI0
B	11	SER	ALA	conflict	UNP A0A4V2WUI0
B	38	GLU	ALA	conflict	UNP A0A4V2WUI0
B	92	GLU	GLN	conflict	UNP A0A4V2WUI0
B	102	HIS	ARG	conflict	UNP A0A4V2WUI0
B	160	ALA	GLY	conflict	UNP A0A4V2WUI0
B	161	PRO	ALA	conflict	UNP A0A4V2WUI0
B	186	ALA	ASP	conflict	UNP A0A4V2WUI0
B	187	LEU	THR	conflict	UNP A0A4V2WUI0
B	188	ALA	MET	conflict	UNP A0A4V2WUI0
B	197	ALA	PRO	conflict	UNP A0A4V2WUI0
B	204	MET	VAL	conflict	UNP A0A4V2WUI0
B	208	MET	LEU	conflict	UNP A0A4V2WUI0
B	219	THR	SER	conflict	UNP A0A4V2WUI0
B	226	ALA	VAL	conflict	UNP A0A4V2WUI0
B	240	ALA	GLN	conflict	UNP A0A4V2WUI0
B	260	VAL	ALA	conflict	UNP A0A4V2WUI0
B	280	GLN	GLU	conflict	UNP A0A4V2WUI0
B	281	PRO	ALA	conflict	UNP A0A4V2WUI0
B	282	GLY	ALA	conflict	UNP A0A4V2WUI0
B	289	VAL	ALA	conflict	UNP A0A4V2WUI0
B	295	ILE	-	expression tag	UNP A0A4V2WUI0
B	296	ALA	-	expression tag	UNP A0A4V2WUI0
B	297	LEU	-	expression tag	UNP A0A4V2WUI0
B	298	GLU	-	expression tag	UNP A0A4V2WUI0
B	299	HIS	-	expression tag	UNP A0A4V2WUI0
B	300	HIS	-	expression tag	UNP A0A4V2WUI0
B	301	HIS	-	expression tag	UNP A0A4V2WUI0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	302	HIS	-	expression tag	UNP A0A4V2WUI0
B	303	HIS	-	expression tag	UNP A0A4V2WUI0
B	304	HIS	-	expression tag	UNP A0A4V2WUI0
C	5	VAL	ILE	conflict	UNP A0A4V2WUI0
C	8	ALA	PRO	conflict	UNP A0A4V2WUI0
C	9	ALA	GLN	conflict	UNP A0A4V2WUI0
C	10	PRO	GLN	conflict	UNP A0A4V2WUI0
C	11	SER	ALA	conflict	UNP A0A4V2WUI0
C	38	GLU	ALA	conflict	UNP A0A4V2WUI0
C	92	GLU	GLN	conflict	UNP A0A4V2WUI0
C	102	HIS	ARG	conflict	UNP A0A4V2WUI0
C	160	ALA	GLY	conflict	UNP A0A4V2WUI0
C	161	PRO	ALA	conflict	UNP A0A4V2WUI0
C	186	ALA	ASP	conflict	UNP A0A4V2WUI0
C	187	LEU	THR	conflict	UNP A0A4V2WUI0
C	188	ALA	MET	conflict	UNP A0A4V2WUI0
C	197	ALA	PRO	conflict	UNP A0A4V2WUI0
C	204	MET	VAL	conflict	UNP A0A4V2WUI0
C	208	MET	LEU	conflict	UNP A0A4V2WUI0
C	219	THR	SER	conflict	UNP A0A4V2WUI0
C	226	ALA	VAL	conflict	UNP A0A4V2WUI0
C	240	ALA	GLN	conflict	UNP A0A4V2WUI0
C	260	VAL	ALA	conflict	UNP A0A4V2WUI0
C	280	GLN	GLU	conflict	UNP A0A4V2WUI0
C	281	PRO	ALA	conflict	UNP A0A4V2WUI0
C	282	GLY	ALA	conflict	UNP A0A4V2WUI0
C	289	VAL	ALA	conflict	UNP A0A4V2WUI0
C	295	ILE	-	expression tag	UNP A0A4V2WUI0
C	296	ALA	-	expression tag	UNP A0A4V2WUI0
C	297	LEU	-	expression tag	UNP A0A4V2WUI0
C	298	GLU	-	expression tag	UNP A0A4V2WUI0
C	299	HIS	-	expression tag	UNP A0A4V2WUI0
C	300	HIS	-	expression tag	UNP A0A4V2WUI0
C	301	HIS	-	expression tag	UNP A0A4V2WUI0
C	302	HIS	-	expression tag	UNP A0A4V2WUI0
C	303	HIS	-	expression tag	UNP A0A4V2WUI0
C	304	HIS	-	expression tag	UNP A0A4V2WUI0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	167	Total O 167 167	0	0

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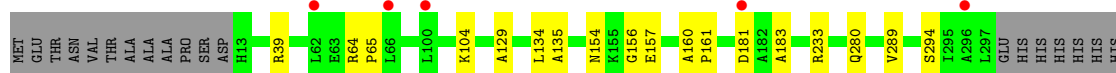
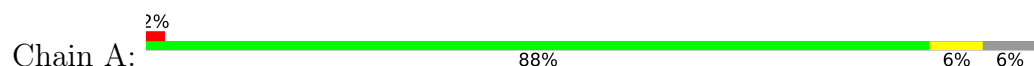
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	80	Total	O	0	0
			80	80		
2	C	82	Total	O	0	0
			82	82		

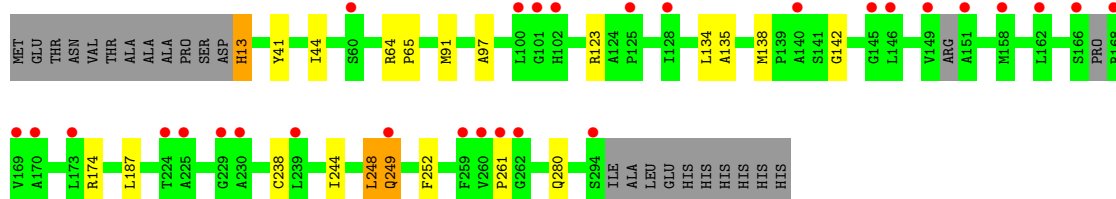
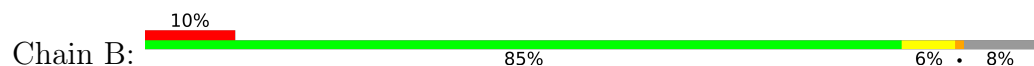
3 Residue-property plots [i](#)

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.

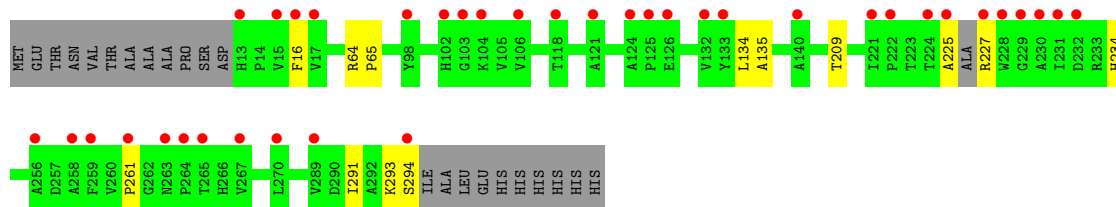
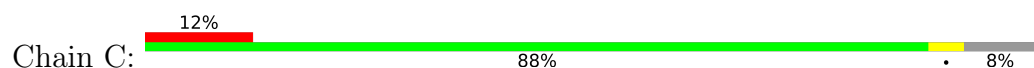
- Molecule 1: Alpha/beta fold hydrolase



- Molecule 1: Alpha/beta fold hydrolase



- Molecule 1: Alpha/beta fold hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.96Å 68.41Å 75.34Å 90.00° 93.58° 90.00°	Depositor
Resolution (Å)	57.64 – 1.66 57.64 – 1.66	Depositor EDS
% Data completeness (in resolution range)	98.4 (57.64-1.66) 98.4 (57.64-1.66)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.194 , 0.229 (Not available) , 0.219	Depositor DCC
R_{free} test set	4917 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.5	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	0.95	EDS
Total number of atoms	6318	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.66% 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	0.79	2/2140 (0.1%)	1.00	3/2925 (0.1%)
1	B	0.76	0/2029	1.10	5/2761 (0.2%)
1	C	0.73	0/1986	1.06	1/2699 (0.0%)
All	All	0.76	2/6155 (0.0%)	1.06	9/8385 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	294	SER	C-N	6.12	1.41	1.33
1	A	233	ARG	CD-NE	-5.14	1.39	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	GLN	O-C-N	7.93	130.34	122.09
1	B	248	LEU	O-C-N	-7.02	114.15	122.15
1	A	154	ASN	CA-CB-CG	6.68	119.28	112.60
1	A	181[A]	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	181[B]	ASP	CA-CB-CG	5.79	118.39	112.60

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	2077	0	1979	7	0
1	B	1975	0	1789	10	0
1	C	1937	0	1708	9	0
2	A	167	0	0	0	0
2	B	80	0	0	0	0
2	C	82	0	0	2	0
All	All	6318	0	5476	26	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 2.

The worst 5 of 26 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:C:16:PHE:CE1	1:C:16:PHE:CG	2.41	1.01
1:B:238:CYS:H	1:B:249:GLN:HE22	1.37	0.71
1:B:244:ILE:HG23	1:B:248:LEU:HD23	1.74	0.67
1:B:138:MET:O	1:B:252:PHE:HD1	1.90	0.54
1:B:138:MET:O	1:B:252:PHE:CD1	2.62	0.52

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	285/304 (94%)	280 (98%)	5 (2%)	0	100	100
1	B	275/304 (90%)	269 (98%)	6 (2%)	0	100	100
1	C	278/304 (91%)	273 (98%)	5 (2%)	0	100	100
All	All	838/912 (92%)	822 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	193/226 (85%)	192 (100%)	1 (0%)	81	72
1	B	170/226 (75%)	166 (98%)	4 (2%)	43	20
1	C	153/226 (68%)	153 (100%)	0	100	100
All	All	516/678 (76%)	511 (99%)	5 (1%)	68	52

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	GLN
1	B	13	HIS
1	B	174	ARG
1	B	187	LEU
1	B	280	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	198	GLN
1	B	249	GLN
1	B	268	HIS
1	B	24	HIS
1	A	13	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	285/304 (93%)	-0.12	5 (1%) 67 73	13, 22, 36, 45	2 (0%)
1	B	280/304 (92%)	0.78	29 (10%) 11 12	19, 34, 52, 63	2 (0%)
1	C	281/304 (92%)	0.85	38 (13%) 7 7	21, 37, 62, 76	1 (0%)
All	All	846/912 (92%)	0.50	72 (8%) 16 18	13, 30, 56, 76	5 (0%)

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	LEU	5.1
1	B	168	ARG	4.6
1	C	121	ALA	4.6
1	B	151	ALA	4.5
1	C	225	ALA	4.4

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.