wwPDB X-ray Structure Validation Summary Report (i)

Mar 7, 2024 – 12:56 pm GMT

PDB ID	:	8OZ3
Title	:	Crystal structure of scFv ATOR 1017 bound to human 4-1BB
Authors	:	Hakansson, M.; Von Schantz, L.; Rose, N.
Deposited on	:	2023-05-08
Resolution	:	3.10 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 (i) 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 (1)) were used in the production of this report:

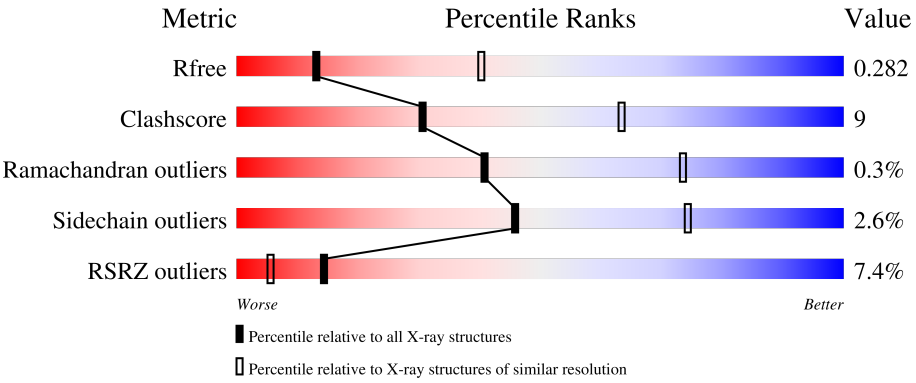
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 <=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	230	8% 45% 6% 49%
1	H	230	4% 46% 5% 49%
2	B	216	4% 41% 10% 50%
2	L	216	4% 36% 14% 50%
3	C	141	4% 74% 21%

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Mol	Chain	Length	Quality of chain
3	D	141	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10655 atoms, of which 5182 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 Single chain Fv.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	117	Total	C	H	N	O	S	37	0	0
			1745	561	853	152	175	4			
1	H	118	Total	C	H	N	O	S	37	0	0
			1762	566	861	153	178	4			

- Molecule 2 is a protein called Single chain Fv.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	109	Total	C	H	N	O	S	35	0	0
			1643	527	810	136	167	3			
2	L	109	Total	C	H	N	O	S	35	0	0
			1643	527	810	136	167	3			

- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	136	Total	C	H	N	O	S	23	0	0
			1926	592	924	187	202	21			
3	D	136	Total	C	H	N	O	S	23	0	0
			1926	592	924	187	202	21			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	121	SER	CYS	conflict	UNP Q07011
C	138	ASP	ASN	conflict	UNP Q07011
C	149	GLN	ASN	conflict	UNP Q07011
C	161	GLY	-	expression tag	UNP Q07011
C	162	SER	-	expression tag	UNP Q07011
C	163	LEU	-	expression tag	UNP Q07011
C	164	GLY	-	expression tag	UNP Q07011
D	121	SER	CYS	conflict	UNP Q07011

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Chain	Residue	Modelled	Actual	Comment	Reference
D	138	ASP	ASN	conflict	UNP Q07011
D	149	GLN	ASN	conflict	UNP Q07011
D	161	GLY	-	expression tag	UNP Q07011
D	162	SER	-	expression tag	UNP Q07011
D	163	LEU	-	expression tag	UNP Q07011
D	164	GLY	-	expression tag	UNP Q07011

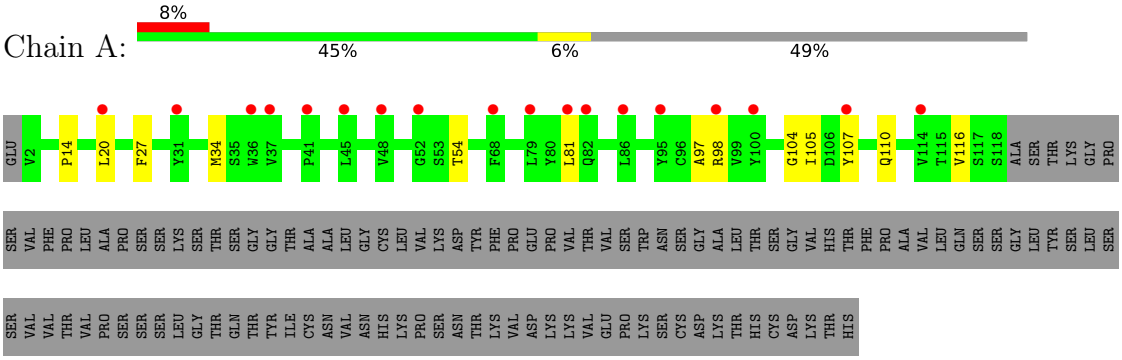
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	C	2	Total O 2 2	0	0
4	D	3	Total O 3 3	0	0
4	H	3	Total O 3 3	0	0
4	L	1	Total O 1 1	0	0

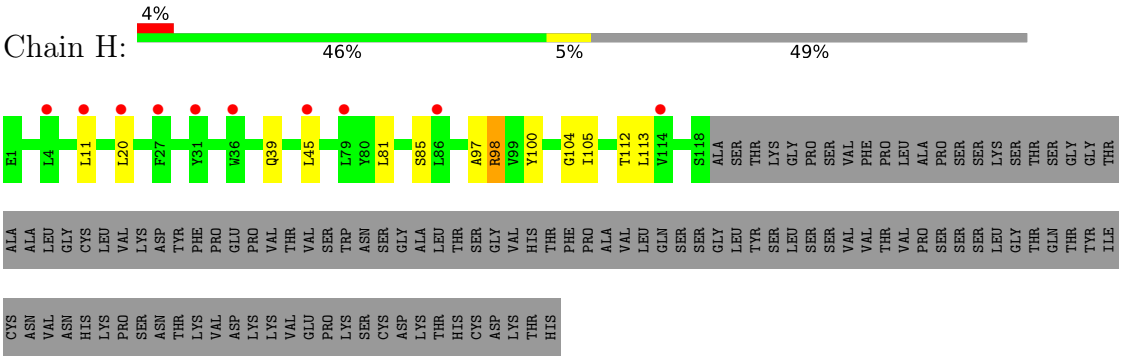
3 Residue-property plots (i)

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.

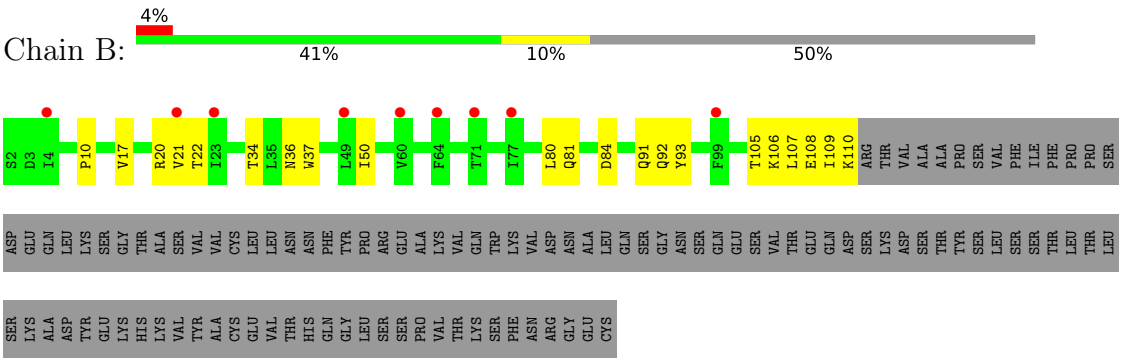
• Molecule 1: Single chain Fv



• Molecule 1: Single chain Fv

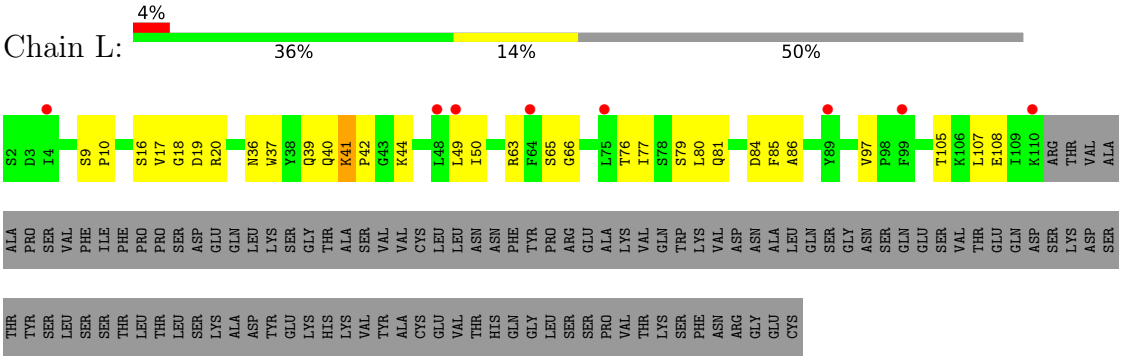


• Molecule 2: Single chain Fv



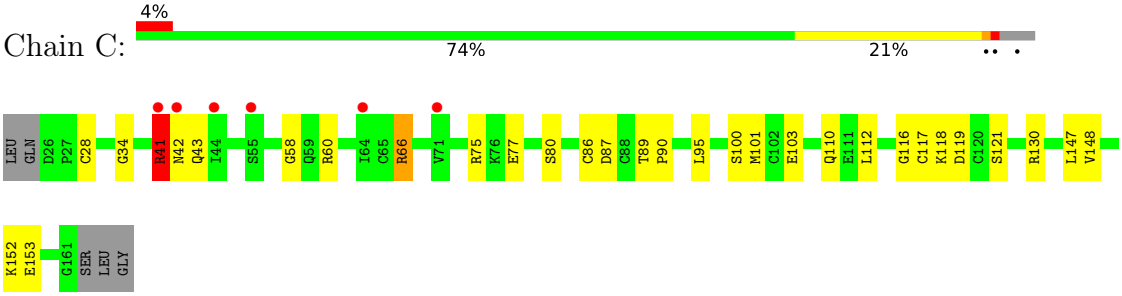
• Molecule 2: Single chain Fv

Chain L:



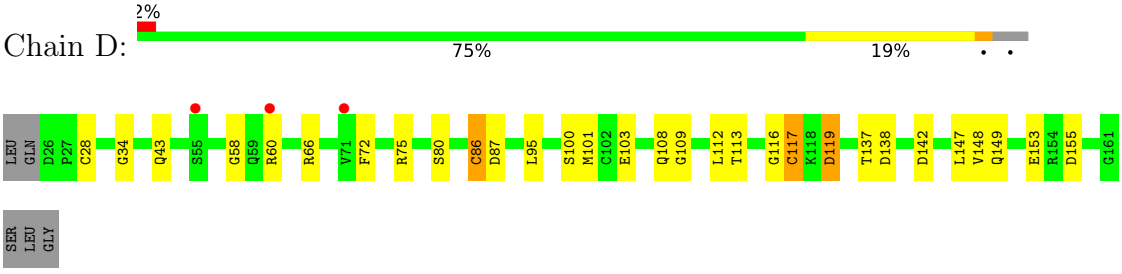
• Molecule 3: Tumor necrosis factor receptor superfamily member 9

Chain C:



• Molecule 3: Tumor necrosis factor receptor superfamily member 9

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.92Å 125.21Å 128.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.78 – 3.10 89.78 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (89.78-3.10) 99.9 (89.78-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.205 , 0.271 0.216 , 0.282	Depositor DCC
R_{free} test set	915 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	105.2	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 102.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.033 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10655	wwPDB-VP
Average B, all atoms (Å^2)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.41	0/913	0.64	0/1238
1	H	0.41	0/922	0.70	0/1250
2	B	0.39	0/853	0.72	0/1158
2	L	0.39	0/853	0.71	0/1158
3	C	0.40	0/1018	0.77	1/1367 (0.1%)
3	D	0.39	0/1018	0.73	0/1367
All	All	0.40	0/5577	0.71	1/7538 (0.0%)

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	H	0	1
2	B	0	1
3	C	0	3
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	66	ARG	NE-CZ-NH1	-6.38	117.11	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	20	ARG	Sidechain
3	C	41	ARG	Sidechain
3	C	60	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	C	66	ARG	Sidechain
1	H	98	ARG	Sidechain

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	892	853	851	10	0
1	H	901	861	860	10	0
2	B	833	810	807	14	0
2	L	833	810	807	29	0
3	C	1002	924	922	18	0
3	D	1002	924	922	23	0
4	A	1	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
4	H	3	0	0	0	0
4	L	1	0	0	0	0
All	All	5473	5182	5169	98	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 9.

The worst 5 of 98 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:L:80:LEU:HD13	2:L:81:GLN:N	1.79	0.95
1:A:97:ALA:HB1	1:A:105:ILE:HG21	1.60	0.81
3:D:113:THR:OG1	3:D:116:GLY:O	1.99	0.80
2:L:17:VAL:HA	2:L:80:LEU:HD12	1.61	0.80
1:H:97:ALA:HB1	1:H:105:ILE:HG21	1.65	0.79

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	115/230 (50%)	110 (96%)	5 (4%)	0	100 100
1	H	116/230 (50%)	112 (97%)	4 (3%)	0	100 100
2	B	107/216 (50%)	100 (94%)	7 (6%)	0	100 100
2	L	107/216 (50%)	97 (91%)	8 (8%)	2 (2%)	8 33
3	C	134/141 (95%)	125 (93%)	9 (7%)	0	100 100
3	D	134/141 (95%)	123 (92%)	11 (8%)	0	100 100
All	All	713/1174 (61%)	667 (94%)	44 (6%)	2 (0%)	41 73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	79	SER
2	L	42	PRO

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	96/195 (49%)	94 (98%)	2 (2%)	53 79
1	H	97/195 (50%)	96 (99%)	1 (1%)	76 90
2	B	94/190 (50%)	92 (98%)	2 (2%)	53 79
2	L	94/190 (50%)	93 (99%)	1 (1%)	73 89
3	C	117/121 (97%)	111 (95%)	6 (5%)	24 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D	117/121 (97%)	113 (97%)	4 (3%)	37 69
All	All	615/1012 (61%)	599 (97%)	16 (3%)	46 74

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	85	SER
3	D	119	ASP
3	C	119	ASP
3	D	117	CYS
3	C	86	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	110	GLN
1	H	77	ASN

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 monosaccharides 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 (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, 95^{th} 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	117/230 (50%)	0.90	18 (15%) 2 1	102, 140, 180, 206	0
1	H	118/230 (51%)	0.81	10 (8%) 10 4	90, 118, 153, 172	0
2	B	109/216 (50%)	0.72	9 (8%) 11 4	96, 140, 175, 197	0
2	L	109/216 (50%)	0.66	8 (7%) 15 6	94, 129, 172, 198	0
3	C	136/141 (96%)	0.56	6 (4%) 34 17	95, 123, 164, 177	0
3	D	136/141 (96%)	0.51	3 (2%) 62 41	89, 126, 166, 202	0
All	All	725/1174 (61%)	0.69	54 (7%) 14 5	89, 129, 172, 206	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	64	PHE	6.1
1	A	86	LEU	3.8
3	C	55	SER	3.6
1	A	79	LEU	3.5
1	A	20	LEU	3.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.