



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 11, 2025 – 06:18 PM EDT

PDB ID : 9N0I / pdb_00009n0i
Title : Crystal structure of KABLE double mutant (Lys14Pro, Leu20Trp)
Authors : Correy, G.J.; Fraser, J.S.
Deposited on : 2025-01-24
Resolution : 2.15 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 Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

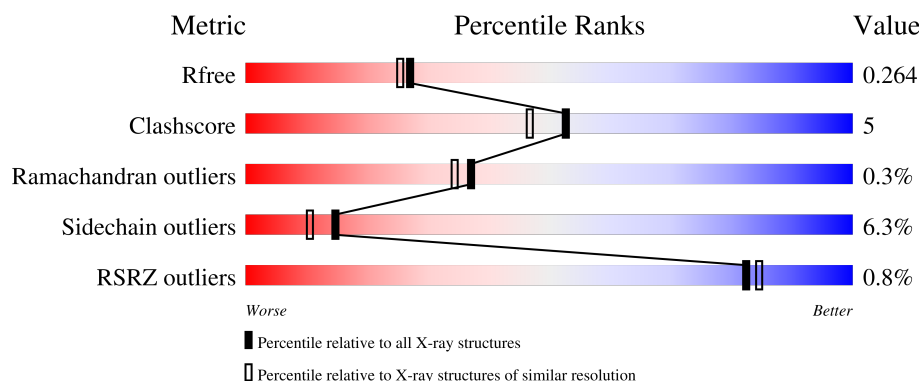
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 78%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 78% 10% •• 10% </div> </div>
1	B	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 78%, yellow 11%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 78% 11% • 10% </div> </div>
1	C	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 78%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 78% 11% • 10% </div> </div>
1	D	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 75%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 75% 14% • 10% </div> </div>
1	E	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 80%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 80% 14% • 5% </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	140	<div><div><div>%</div><div><div></div></div><div>82%</div><div><div>6%</div><div>•</div><div>10%</div></div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11972 atoms, of which 6019 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 De novo designed KABLE protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	126	Total	C	H	N	O	S	0	0	0
			1953	614	993	165	179	2			
1	B	126	Total	C	H	N	O	S	0	2	0
			1968	618	1000	167	181	2			
1	C	126	Total	C	H	N	O	S	0	0	0
			1953	614	993	165	179	2			
1	D	126	Total	C	H	N	O	S	0	0	0
			1953	614	993	165	179	2			
1	E	133	Total	C	H	N	O	S	0	0	0
			2070	655	1047	174	192	2			
1	F	126	Total	C	H	N	O	S	0	0	0
			1953	614	993	165	179	2			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		
3	B	19	Total	O	0	0
			19	19		
3	C	26	Total	O	0	0
			26	26		
3	D	22	Total	O	0	0
			22	22		
3	E	18	Total	O	0	0
			18	18		

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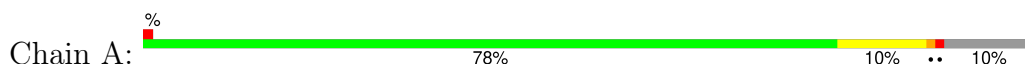
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	13	Total	O	0	0
			13	13		

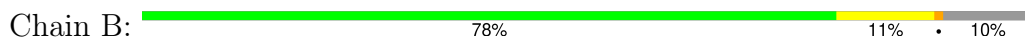
3 Residue-property plots [i](#)

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.

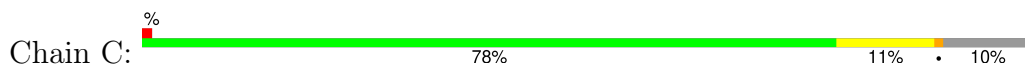
- Molecule 1: De novo designed KABLE protein



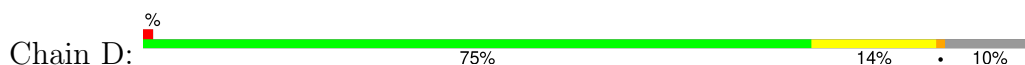
- Molecule 1: De novo designed KABLE protein



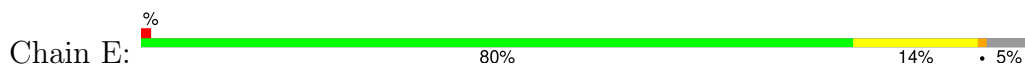
- Molecule 1: De novo designed KABLE protein



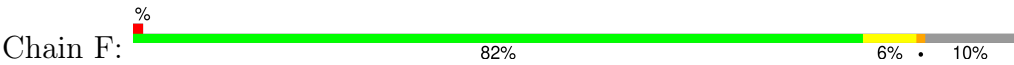
- Molecule 1: De novo designed KABLE protein



- Molecule 1: De novo designed KABLE protein



- Molecule 1: De novo designed KABLE protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.90Å 90.29Å 89.57Å 90.00° 100.93° 90.00°	Depositor
Resolution (Å)	48.98 – 2.15 48.98 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.98-2.15) 99.6 (48.98-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.200 , 0.264 0.200 , 0.264	Depositor DCC
R_{free} test set	2271 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11972	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% 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:
CL

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	0.69	1/970 (0.1%)	0.66	0/1303
1	B	0.57	0/987	0.65	0/1326
1	C	0.59	0/970	0.70	0/1303
1	D	0.61	0/970	0.70	0/1303
1	E	0.55	0/1035	0.61	0/1391
1	F	0.55	0/970	0.62	0/1303
All	All	0.59	1/5902 (0.0%)	0.66	0/7929

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	ILE	CG1-CD1	8.18	1.83	1.51

There are no bond angle outliers.

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	960	993	995	12	0
1	B	968	1000	995	10	0
1	C	960	993	995	9	0
1	D	960	993	995	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1023	1047	1049	11	0
1	F	960	993	995	4	0
2	D	1	0	0	0	0
3	A	23	0	0	0	0
3	B	19	0	0	0	0
3	C	26	0	0	1	0
3	D	22	0	0	0	0
3	E	18	0	0	1	0
3	F	13	0	0	0	0
All	All	5953	6019	6024	58	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 5.

All (58) 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:12:ILE:CD1	1:A:12:ILE:CG1	1.83	1.53
1:C:16:ILE:HG13	1:C:45:LEU:HD13	1.66	0.77
1:A:85:MET:HE2	1:A:108:ILE:HG13	1.74	0.67
1:C:75:GLN:NE2	1:C:119:VAL:HG22	2.12	0.65
1:D:24:ARG:HH11	1:D:24:ARG:HG2	1.62	0.64
1:B:85:MET:HE2	1:B:108:ILE:HG13	1.81	0.63
1:A:85:MET:HE2	1:A:108:ILE:CG1	2.30	0.61
1:F:24:ARG:HB2	1:F:105:LEU:HD12	1.82	0.61
1:B:74:GLU:O	1:B:78:ARG:HG2	2.02	0.60
1:D:120:GLU:OE2	1:D:123:LYS:NZ	2.36	0.59
1:E:2:LEU:HD21	1:E:126:ILE:HB	1.85	0.59
1:A:85:MET:HE1	1:A:107:ALA:C	2.28	0.59
1:D:117:PRO:O	1:D:120:GLU:N	2.34	0.58
1:D:3:LYS:HG2	1:D:126:ILE:HD12	1.87	0.56
1:C:75:GLN:HE22	1:C:119:VAL:HG22	1.70	0.55
1:D:15:ARG:HG2	1:D:45:LEU:HD11	1.89	0.54
1:D:6:PHE:CE1	1:D:122:ILE:HG22	2.43	0.53
1:C:115:LEU:O	1:C:119:VAL:HG23	2.09	0.52
1:A:39:LEU:O	1:A:43:LYS:HG2	2.09	0.52
1:F:74:GLU:O	1:F:78:ARG:HG2	2.10	0.51
1:E:74:GLU:O	1:E:78:ARG:HG2	2.11	0.50
1:B:85:MET:HE1	1:B:107:ALA:C	2.36	0.50
1:B:8:GLU:O	1:B:12:ILE:HG13	2.12	0.50
1:F:21:GLN:OE1	1:F:24:ARG:NH2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ILE:HD12	1:B:52:LEU:HD12	1.92	0.49
1:C:74:GLU:OE2	1:C:78:ARG:NH1	2.46	0.49
1:A:9:TYR:HH	1:A:75:GLN:CD	2.18	0.48
1:F:85:MET:CE	1:F:107:ALA:HB1	2.43	0.48
1:C:85:MET:HE2	1:C:108:ILE:HG13	1.96	0.48
1:A:75:GLN:NE2	1:A:118:LEU:HB2	2.31	0.46
1:E:20:TRP:CE2	1:E:108:ILE:HG21	2.50	0.46
1:E:12:ILE:HG23	1:E:45:LEU:HD22	1.97	0.46
1:B:9:TYR:CE1	1:B:49:ASP:OD1	2.69	0.46
1:E:85:MET:CE	1:E:107:ALA:HB1	2.46	0.45
1:D:85:MET:HE1	1:D:107:ALA:C	2.42	0.45
1:E:85:MET:HE3	1:E:107:ALA:HB1	1.99	0.45
1:D:116:LEU:N	1:D:117:PRO:HD2	2.32	0.45
1:E:85:MET:HE1	1:E:107:ALA:C	2.42	0.45
1:A:85:MET:HE1	1:A:107:ALA:O	2.17	0.44
1:A:6:PHE:CD1	1:A:6:PHE:C	2.95	0.44
1:A:75:GLN:HE22	1:A:118:LEU:HB2	1.83	0.43
1:B:6:PHE:O	1:B:7:ALA:C	2.61	0.43
1:C:118:LEU:HD12	1:C:121:ALA:HB3	2.00	0.43
1:E:111:GLU:HG3	3:E:212:HOH:O	2.19	0.43
1:C:85:MET:HE1	1:C:107:ALA:C	2.44	0.42
1:D:24:ARG:HH11	1:D:24:ARG:CG	2.31	0.42
1:D:56:MET:HE3	1:D:72:LEU:CD2	2.48	0.42
1:A:75:GLN:HG3	1:A:115:LEU:HD22	2.02	0.42
1:A:31:ASP:O	1:A:35:VAL:HG23	2.19	0.42
1:B:102:GLY:O	1:B:106:GLU:HG2	2.20	0.41
1:E:2:LEU:HB2	1:E:59:GLU:OE1	2.20	0.41
1:E:19:LEU:HB2	1:E:42:LEU:HD21	2.02	0.41
1:E:85:MET:CE	1:E:107:ALA:CB	2.98	0.41
1:C:80:LYS:NZ	3:C:205:HOH:O	2.54	0.41
1:D:52:LEU:O	1:D:56:MET:HG3	2.20	0.41
1:B:19:LEU:HD23	1:B:19:LEU:HA	1.93	0.40
1:B:115:LEU:HD23	1:B:115:LEU:HA	1.86	0.40
1:D:34:ARG:HH11	1:D:34:ARG:HG3	1.86	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	124/140 (89%)	123 (99%)	1 (1%)	0	100	100
1	B	126/140 (90%)	125 (99%)	1 (1%)	0	100	100
1	C	124/140 (89%)	122 (98%)	2 (2%)	0	100	100
1	D	124/140 (89%)	122 (98%)	1 (1%)	1 (1%)	16	11
1	E	131/140 (94%)	129 (98%)	2 (2%)	0	100	100
1	F	124/140 (89%)	121 (98%)	2 (2%)	1 (1%)	16	11
All	All	753/840 (90%)	742 (98%)	9 (1%)	2 (0%)	37	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	65	ASN
1	D	117	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	89/103 (86%)	82 (92%)	7 (8%)	10	6
1	B	91/103 (88%)	88 (97%)	3 (3%)	33	33
1	C	89/103 (86%)	84 (94%)	5 (6%)	17	14
1	D	89/103 (86%)	84 (94%)	5 (6%)	17	14
1	E	96/103 (93%)	87 (91%)	9 (9%)	7	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	89/103 (86%)	84 (94%)	5 (6%)	17	14
All	All	543/618 (88%)	509 (94%)	34 (6%)	15	10

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	43	LYS
1	A	44	GLU
1	A	67	GLU
1	A	74	GLU
1	A	75	GLN
1	A	124	GLU
1	B	44	GLU
1	B	74	GLU
1	B	78	ARG
1	C	44	GLU
1	C	45	LEU
1	C	50	LEU
1	C	59	GLU
1	C	62	GLU
1	D	17	LEU
1	D	24	ARG
1	D	50	LEU
1	D	62	GLU
1	D	105	LEU
1	E	-6	GLU
1	E	-4	LEU
1	E	0	SER
1	E	59	GLU
1	E	62	GLU
1	E	74	GLU
1	E	75	GLN
1	E	80	LYS
1	E	105	LEU
1	F	17	LEU
1	F	21	GLN
1	F	66	LYS
1	F	69	VAL
1	F	105	LEU

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

sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	54	ASN

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	126/140 (90%)	-0.22	1 (0%) 82 84	31, 50, 77, 91	0
1	B	126/140 (90%)	-0.06	0 100 100	21, 55, 88, 102	1 (0%)
1	C	126/140 (90%)	-0.12	1 (0%) 82 84	35, 51, 79, 89	0
1	D	126/140 (90%)	-0.03	2 (1%) 70 73	32, 50, 85, 110	0
1	E	133/140 (95%)	0.07	1 (0%) 82 84	36, 59, 95, 116	0
1	F	126/140 (90%)	0.19	1 (0%) 82 84	39, 63, 86, 100	0
All	All	763/840 (90%)	-0.03	6 (0%) 82 84	21, 54, 86, 116	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	118	LEU	3.1
1	D	115	LEU	3.1
1	E	118	LEU	2.5
1	C	118	LEU	2.2
1	A	12	ILE	2.1
1	F	125	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	D	201	1/1	0.98	0.11	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.