



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 04:26 am BST

PDB ID : 4AK8
Title : Structure of F241L mutant of langerin carbohydrate recognition domain.
Authors : Chabrol, E.; Thepaut, M.; Dezutter-Dambuyant, C.; Vives, C.; Marcoux, J.; Kahn, R.; Valadeau-Guilemond, J.; Vachette, P.; Durand, D.; Fieschi, F.
Deposited on : 2012-02-22
Resolution : 1.40 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 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	:	2.11
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)	:	2.11

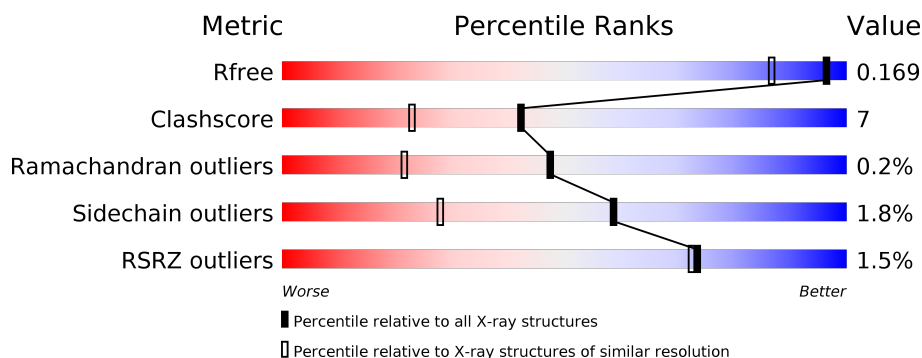
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 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	155	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>23%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	155	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>19%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	155	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>25%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	155	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>22%</div> <div>•</div> <div>14%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5148 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 C-TYPE LECTIN DOMAIN FAMILY 4 MEMBER K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	2	0
			1069	692	175	197	5			
1	B	128	Total	C	N	O	S	0	6	0
			1075	703	176	191	5			
1	C	130	Total	C	N	O	S	0	5	0
			1083	705	176	197	5			
1	D	133	Total	C	N	O	S	0	5	0
			1105	718	179	203	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	174	MET	-	expression tag	UNP Q9UJ71
A	175	TRP	-	expression tag	UNP Q9UJ71
A	176	SER	-	expression tag	UNP Q9UJ71
A	177	HIS	-	expression tag	UNP Q9UJ71
A	178	PRO	-	expression tag	UNP Q9UJ71
A	179	GLN	-	expression tag	UNP Q9UJ71
A	180	PHE	-	expression tag	UNP Q9UJ71
A	181	GLU	-	expression tag	UNP Q9UJ71
A	182	LYS	-	expression tag	UNP Q9UJ71
A	183	ILE	-	expression tag	UNP Q9UJ71
A	184	GLU	-	expression tag	UNP Q9UJ71
A	185	GLY	-	expression tag	UNP Q9UJ71
A	186	ARG	-	expression tag	UNP Q9UJ71
A	187	MET	-	expression tag	UNP Q9UJ71
A	241	LEU	PHE	engineered mutation	UNP Q9UJ71
A	278	ALA	VAL	variant	UNP Q9UJ71
B	174	MET	-	expression tag	UNP Q9UJ71
B	175	TRP	-	expression tag	UNP Q9UJ71
B	176	SER	-	expression tag	UNP Q9UJ71
B	177	HIS	-	expression tag	UNP Q9UJ71
B	178	PRO	-	expression tag	UNP Q9UJ71

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Chain	Residue	Modelled	Actual	Comment	Reference
B	179	GLN	-	expression tag	UNP Q9UJ71
B	180	PHE	-	expression tag	UNP Q9UJ71
B	181	GLU	-	expression tag	UNP Q9UJ71
B	182	LYS	-	expression tag	UNP Q9UJ71
B	183	ILE	-	expression tag	UNP Q9UJ71
B	184	GLU	-	expression tag	UNP Q9UJ71
B	185	GLY	-	expression tag	UNP Q9UJ71
B	186	ARG	-	expression tag	UNP Q9UJ71
B	187	MET	-	expression tag	UNP Q9UJ71
B	241	LEU	PHE	engineered mutation	UNP Q9UJ71
B	278	ALA	VAL	variant	UNP Q9UJ71
C	174	MET	-	expression tag	UNP Q9UJ71
C	175	TRP	-	expression tag	UNP Q9UJ71
C	176	SER	-	expression tag	UNP Q9UJ71
C	177	HIS	-	expression tag	UNP Q9UJ71
C	178	PRO	-	expression tag	UNP Q9UJ71
C	179	GLN	-	expression tag	UNP Q9UJ71
C	180	PHE	-	expression tag	UNP Q9UJ71
C	181	GLU	-	expression tag	UNP Q9UJ71
C	182	LYS	-	expression tag	UNP Q9UJ71
C	183	ILE	-	expression tag	UNP Q9UJ71
C	184	GLU	-	expression tag	UNP Q9UJ71
C	185	GLY	-	expression tag	UNP Q9UJ71
C	186	ARG	-	expression tag	UNP Q9UJ71
C	187	MET	-	expression tag	UNP Q9UJ71
C	241	LEU	PHE	engineered mutation	UNP Q9UJ71
C	278	ALA	VAL	variant	UNP Q9UJ71
D	174	MET	-	expression tag	UNP Q9UJ71
D	175	TRP	-	expression tag	UNP Q9UJ71
D	176	SER	-	expression tag	UNP Q9UJ71
D	177	HIS	-	expression tag	UNP Q9UJ71
D	178	PRO	-	expression tag	UNP Q9UJ71
D	179	GLN	-	expression tag	UNP Q9UJ71
D	180	PHE	-	expression tag	UNP Q9UJ71
D	181	GLU	-	expression tag	UNP Q9UJ71
D	182	LYS	-	expression tag	UNP Q9UJ71
D	183	ILE	-	expression tag	UNP Q9UJ71
D	184	GLU	-	expression tag	UNP Q9UJ71
D	185	GLY	-	expression tag	UNP Q9UJ71
D	186	ARG	-	expression tag	UNP Q9UJ71
D	187	MET	-	expression tag	UNP Q9UJ71
D	241	LEU	PHE	engineered mutation	UNP Q9UJ71

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Chain	Residue	Modelled	Actual	Comment	Reference
D	278	ALA	VAL	variant	UNP Q9UJ71

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	225	Total O 225 225	0	0
5	B	209	Total O 209 209	0	0
5	C	174	Total O 174 174	0	0

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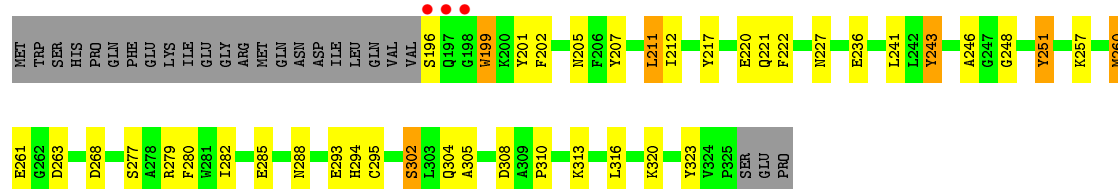
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	199	Total 199	O 199	0	0

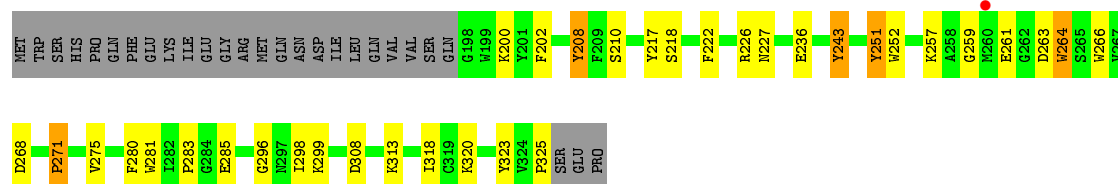
3 Residue-property plots

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.

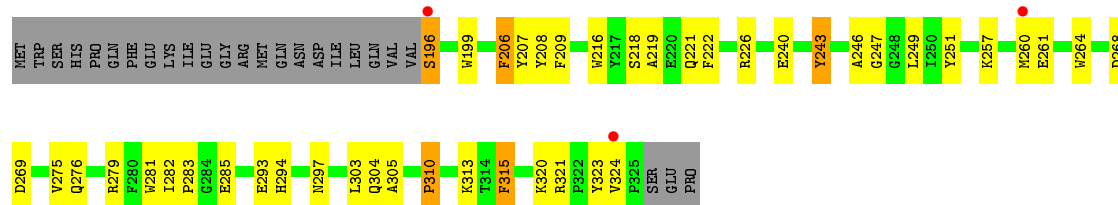
• Molecule 1: C-TYPE LECTIN DOMAIN FAMILY 4 MEMBER K



• Molecule 1: C-TYPE LECTIN DOMAIN FAMILY 4 MEMBER K



• Molecule 1: C-TYPE LECTIN DOMAIN FAMILY 4 MEMBER K



• Molecule 1: C-TYPE LECTIN DOMAIN FAMILY 4 MEMBER K





4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	79.96Å 79.96Å 90.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.52 – 1.40 19.39 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.52-1.40) 99.2 (19.39-1.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.175 , 0.219 0.177 , 0.169	Depositor DCC
R_{free} test set	5599 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.104 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5148	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MG, 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	2.02	22/1110 (2.0%)	1.68	18/1511 (1.2%)
1	B	1.93	22/1128 (2.0%)	1.64	13/1534 (0.8%)
1	C	1.90	21/1136 (1.8%)	1.68	19/1545 (1.2%)
1	D	1.83	14/1159 (1.2%)	1.58	20/1575 (1.3%)
All	All	1.92	79/4533 (1.7%)	1.64	70/6165 (1.1%)

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	TYR	CG-CD1	11.23	1.53	1.39
1	D	206	PHE	CD1-CE1	10.44	1.60	1.39
1	B	280	PHE	CE1-CZ	8.98	1.54	1.37
1	D	247	GLY	N-CA	8.45	1.58	1.46
1	B	323	TYR	CE1-CZ	-8.19	1.27	1.38

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	ASP	CB-CG-OD2	-9.90	109.39	118.30
1	D	268	ASP	CB-CG-OD2	-8.94	110.26	118.30
1	D	268	ASP	CB-CG-OD1	8.78	126.20	118.30
1	C	249	LEU	CB-CG-CD1	-8.63	96.33	111.00
1	B	268	ASP	CB-CG-OD2	-8.53	110.63	118.30

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	1069	0	997	18	0
1	B	1075	0	1036	16	0
1	C	1083	0	1030	20	0
1	D	1105	0	1051	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	D	1	0	0	0	0
5	A	225	0	0	4	0
5	B	209	0	0	6	0
5	C	174	0	0	1	0
5	D	199	0	0	3	0
All	All	5148	0	4114	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 7.

The worst 5 of 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:227:ASN:HB2	1:C:260:MET:CE	1.68	1.22
1:A:227:ASN:CB	1:C:260:MET:HE2	1.83	1.06
1:B:227:ASN:HB2	1:D:260:MET:SD	2.02	0.99
1:B:251:TYR:HB2	1:B:298[B]:ILE:HD11	1.52	0.92
1:C:276:GLN:O	1:C:279:ARG:NH1	2.07	0.86

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	130/155 (84%)	128 (98%)	2 (2%)	0	100	100
1	B	132/155 (85%)	125 (95%)	6 (4%)	1 (1%)	19	4
1	C	133/155 (86%)	132 (99%)	1 (1%)	0	100	100
1	D	136/155 (88%)	131 (96%)	5 (4%)	0	100	100
All	All	531/620 (86%)	516 (97%)	14 (3%)	1 (0%)	47	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	GLY

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	114/136 (84%)	112 (98%)	2 (2%)	59	28
1	B	116/136 (85%)	114 (98%)	2 (2%)	60	31
1	C	117/136 (86%)	114 (97%)	3 (3%)	46	13
1	D	120/136 (88%)	119 (99%)	1 (1%)	81	62
All	All	467/544 (86%)	459 (98%)	8 (2%)	59	31

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	271	PRO
1	D	243	TYR
1	C	243	TYR
1	B	261	GLU
1	C	196	SER

Some 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	294	HIS
1	D	294	HIS
1	C	294	HIS
1	B	227	ASN
1	D	221	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are 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	130/155 (83%)	-0.49	3 (2%) 60 60	9, 13, 26, 50	0
1	B	128/155 (82%)	-0.40	1 (0%) 86 84	7, 14, 30, 42	0
1	C	130/155 (83%)	-0.40	3 (2%) 60 60	8, 15, 29, 44	0
1	D	133/155 (85%)	-0.52	1 (0%) 86 84	7, 14, 27, 43	0
All	All	521/620 (84%)	-0.45	8 (1%) 73 72	7, 15, 29, 50	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	GLN	3.7
1	A	198	GLY	3.5
1	D	260	MET	3.3
1	C	196	SER	3.1
1	C	260	MET	3.0

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 carbohydrates 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(\AA^2)	Q<0.9
4	CL	D	1329	1/1	0.97	0.04	31,31,31,31	0
3	MG	C	1327	1/1	1.00	0.07	21,21,21,21	0
2	CA	C	1326	1/1	1.00	0.04	19,19,19,19	0
2	CA	D	1330	1/1	1.00	0.04	16,16,16,16	0
3	MG	D	1331	1/1	1.00	0.08	13,13,13,13	0
2	CA	A	1326	1/1	1.00	0.06	16,16,16,16	0
2	CA	B	1326	1/1	1.00	0.04	19,19,19,19	0
3	MG	A	1327	1/1	1.00	0.08	20,20,20,20	0
3	MG	B	1327	1/1	1.00	0.07	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.