



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:19 PM GMT

PDB ID : 3TCX  
Title : Structure of Engineered Single Domain ICAM-1 D1 with High-Affinity aL Integrin I Domain of Native C-Terminal Helix Conformation  
Authors : Kang, S.; Kim, C.U.; Gu, X.; Owens, R.M.; van Rijn, S.J.; Boonyaleepun, V.; Mao, Y.; Springer, T.A.; Jin, M.M.  
Deposited on : 2011-08-09  
Resolution : 3.60 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

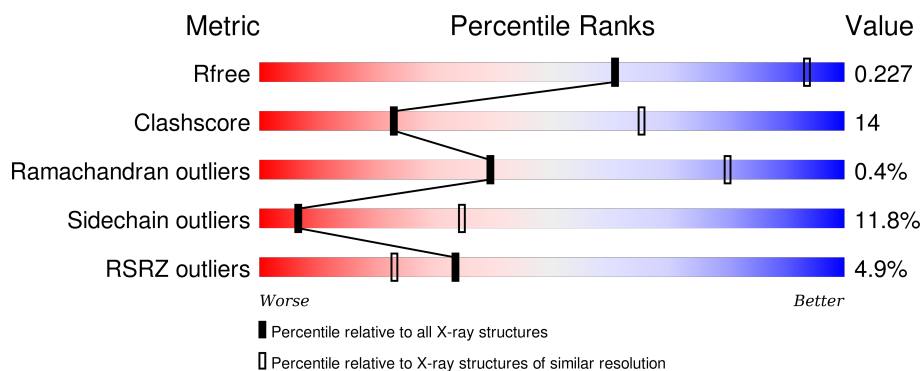
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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.






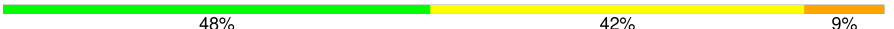


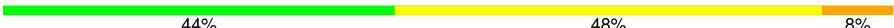
















Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	85	
1	C	85	
1	E	85	
1	G	85	
1	I	85	

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Mol	Chain	Length	Quality of chain
1	K	85	
1	M	85	
1	O	85	
1	Q	85	
1	S	85	
1	U	85	
1	W	85	
1	Y	85	
1	a	85	
2	B	180	
2	D	180	
2	F	180	
2	H	180	
2	J	180	
2	L	180	
2	N	180	
2	P	180	
2	R	180	
2	T	180	
2	V	180	
2	X	180	
2	Z	180	
2	b	180	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	L	901	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29330 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 Intercellular adhesion molecule 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	85	Total	C	N	O	S	0	0	0
			641	404	106	125	6			
1	C	85	Total	C	N	O	S	0	0	0
			641	404	106	125	6			
1	E	85	Total	C	N	O	S	0	0	0
			641	404	106	125	6			
1	G	85	Total	C	N	O	S	0	0	0
			641	404	106	125	6			
1	I	85	Total	C	N	O	S	0	0	0
			641	404	106	125	6			
1	K	85	Total	C	N	O	S	0	0	0
			641	404	106	125	6			
1	M	85	Total	C	N	O	S	0	0	0
			641	404	106	125	6			
1	O	85	Total	C	N	O	S	0	0	0
			641	404	106	125	6			
1	Q	85	Total	C	N	O	S	0	0	0
			641	404	106	125	6			
1	S	85	Total	C	N	O	S	0	0	0
			641	404	106	125	6			
1	U	85	Total	C	N	O	S	0	0	0
			641	404	106	125	6			
1	W	85	Total	C	N	O	S	0	0	0
			641	404	106	125	6			
1	Y	85	Total	C	N	O	S	0	0	0
			641	404	106	125	6			
1	a	85	Total	C	N	O	S	0	0	0
			641	404	106	125	6			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P05362

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	THR	ENGINEERED MUTATION	UNP P05362
A	10	THR	ILE	ENGINEERED MUTATION	UNP P05362
A	23	ALA	THR	ENGINEERED MUTATION	UNP P05362
A	38	VAL	PRO	ENGINEERED MUTATION	UNP P05362
A	63	VAL	PRO	ENGINEERED MUTATION	UNP P05362
A	67	ALA	SER	ENGINEERED MUTATION	UNP P05362
A	78	ALA	THR	ENGINEERED MUTATION	UNP P05362
C	1	MET	-	EXPRESSION TAG	UNP P05362
C	2	VAL	THR	ENGINEERED MUTATION	UNP P05362
C	10	THR	ILE	ENGINEERED MUTATION	UNP P05362
C	23	ALA	THR	ENGINEERED MUTATION	UNP P05362
C	38	VAL	PRO	ENGINEERED MUTATION	UNP P05362
C	63	VAL	PRO	ENGINEERED MUTATION	UNP P05362
C	67	ALA	SER	ENGINEERED MUTATION	UNP P05362
C	78	ALA	THR	ENGINEERED MUTATION	UNP P05362
E	1	MET	-	EXPRESSION TAG	UNP P05362
E	2	VAL	THR	ENGINEERED MUTATION	UNP P05362
E	10	THR	ILE	ENGINEERED MUTATION	UNP P05362
E	23	ALA	THR	ENGINEERED MUTATION	UNP P05362
E	38	VAL	PRO	ENGINEERED MUTATION	UNP P05362
E	63	VAL	PRO	ENGINEERED MUTATION	UNP P05362
E	67	ALA	SER	ENGINEERED MUTATION	UNP P05362
E	78	ALA	THR	ENGINEERED MUTATION	UNP P05362
G	1	MET	-	EXPRESSION TAG	UNP P05362
G	2	VAL	THR	ENGINEERED MUTATION	UNP P05362
G	10	THR	ILE	ENGINEERED MUTATION	UNP P05362
G	23	ALA	THR	ENGINEERED MUTATION	UNP P05362
G	38	VAL	PRO	ENGINEERED MUTATION	UNP P05362
G	63	VAL	PRO	ENGINEERED MUTATION	UNP P05362
G	67	ALA	SER	ENGINEERED MUTATION	UNP P05362
G	78	ALA	THR	ENGINEERED MUTATION	UNP P05362
I	1	MET	-	EXPRESSION TAG	UNP P05362
I	2	VAL	THR	ENGINEERED MUTATION	UNP P05362
I	10	THR	ILE	ENGINEERED MUTATION	UNP P05362
I	23	ALA	THR	ENGINEERED MUTATION	UNP P05362
I	38	VAL	PRO	ENGINEERED MUTATION	UNP P05362
I	63	VAL	PRO	ENGINEERED MUTATION	UNP P05362
I	67	ALA	SER	ENGINEERED MUTATION	UNP P05362
I	78	ALA	THR	ENGINEERED MUTATION	UNP P05362
K	1	MET	-	EXPRESSION TAG	UNP P05362
K	2	VAL	THR	ENGINEERED MUTATION	UNP P05362
K	10	THR	ILE	ENGINEERED MUTATION	UNP P05362

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Chain	Residue	Modelled	Actual	Comment	Reference
K	23	ALA	THR	ENGINEERED MUTATION	UNP P05362
K	38	VAL	PRO	ENGINEERED MUTATION	UNP P05362
K	63	VAL	PRO	ENGINEERED MUTATION	UNP P05362
K	67	ALA	SER	ENGINEERED MUTATION	UNP P05362
K	78	ALA	THR	ENGINEERED MUTATION	UNP P05362
M	1	MET	-	EXPRESSION TAG	UNP P05362
M	2	VAL	THR	ENGINEERED MUTATION	UNP P05362
M	10	THR	ILE	ENGINEERED MUTATION	UNP P05362
M	23	ALA	THR	ENGINEERED MUTATION	UNP P05362
M	38	VAL	PRO	ENGINEERED MUTATION	UNP P05362
M	63	VAL	PRO	ENGINEERED MUTATION	UNP P05362
M	67	ALA	SER	ENGINEERED MUTATION	UNP P05362
M	78	ALA	THR	ENGINEERED MUTATION	UNP P05362
O	1	MET	-	EXPRESSION TAG	UNP P05362
O	2	VAL	THR	ENGINEERED MUTATION	UNP P05362
O	10	THR	ILE	ENGINEERED MUTATION	UNP P05362
O	23	ALA	THR	ENGINEERED MUTATION	UNP P05362
O	38	VAL	PRO	ENGINEERED MUTATION	UNP P05362
O	63	VAL	PRO	ENGINEERED MUTATION	UNP P05362
O	67	ALA	SER	ENGINEERED MUTATION	UNP P05362
O	78	ALA	THR	ENGINEERED MUTATION	UNP P05362
Q	1	MET	-	EXPRESSION TAG	UNP P05362
Q	2	VAL	THR	ENGINEERED MUTATION	UNP P05362
Q	10	THR	ILE	ENGINEERED MUTATION	UNP P05362
Q	23	ALA	THR	ENGINEERED MUTATION	UNP P05362
Q	38	VAL	PRO	ENGINEERED MUTATION	UNP P05362
Q	63	VAL	PRO	ENGINEERED MUTATION	UNP P05362
Q	67	ALA	SER	ENGINEERED MUTATION	UNP P05362
Q	78	ALA	THR	ENGINEERED MUTATION	UNP P05362
S	1	MET	-	EXPRESSION TAG	UNP P05362
S	2	VAL	THR	ENGINEERED MUTATION	UNP P05362
S	10	THR	ILE	ENGINEERED MUTATION	UNP P05362
S	23	ALA	THR	ENGINEERED MUTATION	UNP P05362
S	38	VAL	PRO	ENGINEERED MUTATION	UNP P05362
S	63	VAL	PRO	ENGINEERED MUTATION	UNP P05362
S	67	ALA	SER	ENGINEERED MUTATION	UNP P05362
S	78	ALA	THR	ENGINEERED MUTATION	UNP P05362
U	1	MET	-	EXPRESSION TAG	UNP P05362
U	2	VAL	THR	ENGINEERED MUTATION	UNP P05362
U	10	THR	ILE	ENGINEERED MUTATION	UNP P05362
U	23	ALA	THR	ENGINEERED MUTATION	UNP P05362
U	38	VAL	PRO	ENGINEERED MUTATION	UNP P05362

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Chain	Residue	Modelled	Actual	Comment	Reference
U	63	VAL	PRO	ENGINEERED MUTATION	UNP P05362
U	67	ALA	SER	ENGINEERED MUTATION	UNP P05362
U	78	ALA	THR	ENGINEERED MUTATION	UNP P05362
W	1	MET	-	EXPRESSION TAG	UNP P05362
W	2	VAL	THR	ENGINEERED MUTATION	UNP P05362
W	10	THR	ILE	ENGINEERED MUTATION	UNP P05362
W	23	ALA	THR	ENGINEERED MUTATION	UNP P05362
W	38	VAL	PRO	ENGINEERED MUTATION	UNP P05362
W	63	VAL	PRO	ENGINEERED MUTATION	UNP P05362
W	67	ALA	SER	ENGINEERED MUTATION	UNP P05362
W	78	ALA	THR	ENGINEERED MUTATION	UNP P05362
Y	1	MET	-	EXPRESSION TAG	UNP P05362
Y	2	VAL	THR	ENGINEERED MUTATION	UNP P05362
Y	10	THR	ILE	ENGINEERED MUTATION	UNP P05362
Y	23	ALA	THR	ENGINEERED MUTATION	UNP P05362
Y	38	VAL	PRO	ENGINEERED MUTATION	UNP P05362
Y	63	VAL	PRO	ENGINEERED MUTATION	UNP P05362
Y	67	ALA	SER	ENGINEERED MUTATION	UNP P05362
Y	78	ALA	THR	ENGINEERED MUTATION	UNP P05362
a	1	MET	-	EXPRESSION TAG	UNP P05362
a	2	VAL	THR	ENGINEERED MUTATION	UNP P05362
a	10	THR	ILE	ENGINEERED MUTATION	UNP P05362
a	23	ALA	THR	ENGINEERED MUTATION	UNP P05362
a	38	VAL	PRO	ENGINEERED MUTATION	UNP P05362
a	63	VAL	PRO	ENGINEERED MUTATION	UNP P05362
a	67	ALA	SER	ENGINEERED MUTATION	UNP P05362
a	78	ALA	THR	ENGINEERED MUTATION	UNP P05362

- Molecule 2 is a protein called Integrin alpha-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	D	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	F	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	H	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	J	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	L	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	P	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	R	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	T	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	V	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	X	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	Z	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	b	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	128	MET	-	EXPRESSION TAG	UNP P20701
B	189	TRP	ARG	SEE REMARK 999	UNP P20701
B	265	SER	PHE	ENGINEERED MUTATION	UNP P20701
D	128	MET	-	EXPRESSION TAG	UNP P20701
D	189	TRP	ARG	SEE REMARK 999	UNP P20701
D	265	SER	PHE	ENGINEERED MUTATION	UNP P20701
F	128	MET	-	EXPRESSION TAG	UNP P20701
F	189	TRP	ARG	SEE REMARK 999	UNP P20701
F	265	SER	PHE	ENGINEERED MUTATION	UNP P20701
H	128	MET	-	EXPRESSION TAG	UNP P20701
H	189	TRP	ARG	SEE REMARK 999	UNP P20701
H	265	SER	PHE	ENGINEERED MUTATION	UNP P20701
J	128	MET	-	EXPRESSION TAG	UNP P20701
J	189	TRP	ARG	SEE REMARK 999	UNP P20701
J	265	SER	PHE	ENGINEERED MUTATION	UNP P20701
L	128	MET	-	EXPRESSION TAG	UNP P20701
L	189	TRP	ARG	SEE REMARK 999	UNP P20701
L	265	SER	PHE	ENGINEERED MUTATION	UNP P20701
N	128	MET	-	EXPRESSION TAG	UNP P20701
N	189	TRP	ARG	SEE REMARK 999	UNP P20701
N	265	SER	PHE	ENGINEERED MUTATION	UNP P20701
P	128	MET	-	EXPRESSION TAG	UNP P20701
P	189	TRP	ARG	SEE REMARK 999	UNP P20701

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Chain	Residue	Modelled	Actual	Comment	Reference
P	265	SER	PHE	ENGINEERED MUTATION	UNP P20701
R	128	MET	-	EXPRESSION TAG	UNP P20701
R	189	TRP	ARG	SEE REMARK 999	UNP P20701
R	265	SER	PHE	ENGINEERED MUTATION	UNP P20701
T	128	MET	-	EXPRESSION TAG	UNP P20701
T	189	TRP	ARG	SEE REMARK 999	UNP P20701
T	265	SER	PHE	ENGINEERED MUTATION	UNP P20701
V	128	MET	-	EXPRESSION TAG	UNP P20701
V	189	TRP	ARG	SEE REMARK 999	UNP P20701
V	265	SER	PHE	ENGINEERED MUTATION	UNP P20701
X	128	MET	-	EXPRESSION TAG	UNP P20701
X	189	TRP	ARG	SEE REMARK 999	UNP P20701
X	265	SER	PHE	ENGINEERED MUTATION	UNP P20701
Z	128	MET	-	EXPRESSION TAG	UNP P20701
Z	189	TRP	ARG	SEE REMARK 999	UNP P20701
Z	265	SER	PHE	ENGINEERED MUTATION	UNP P20701
b	128	MET	-	EXPRESSION TAG	UNP P20701
b	189	TRP	ARG	SEE REMARK 999	UNP P20701
b	265	SER	PHE	ENGINEERED MUTATION	UNP P20701

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Mg 1 1	0	0
3	J	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	V	1	Total Mg 1 1	0	0
3	Z	1	Total Mg 1 1	0	0
3	T	1	Total Mg 1 1	0	0
3	N	1	Total Mg 1 1	0	0
3	X	1	Total Mg 1 1	0	0

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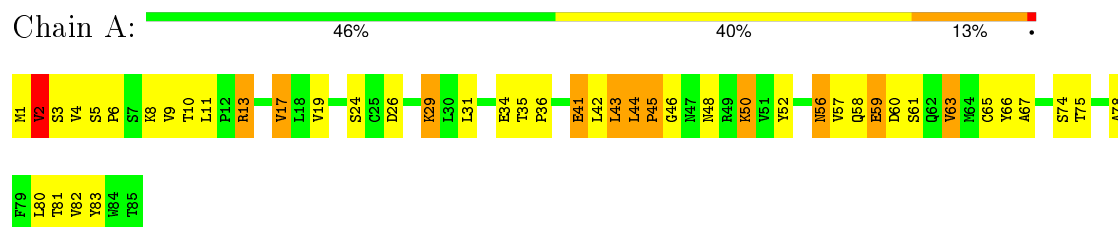
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	R	1	Total 1	Mg 1	0	0
3	L	1	Total 1	Mg 1	0	0
3	b	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0

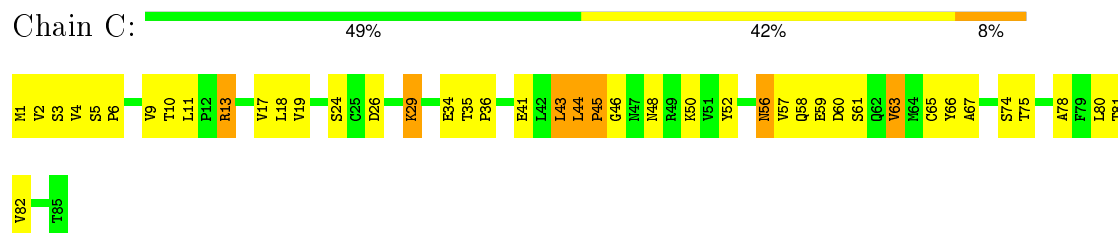
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

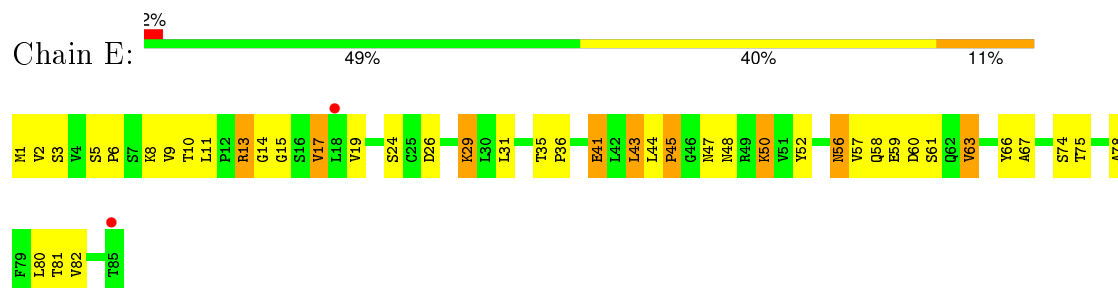
#### • Molecule 1: Intercellular adhesion molecule 1



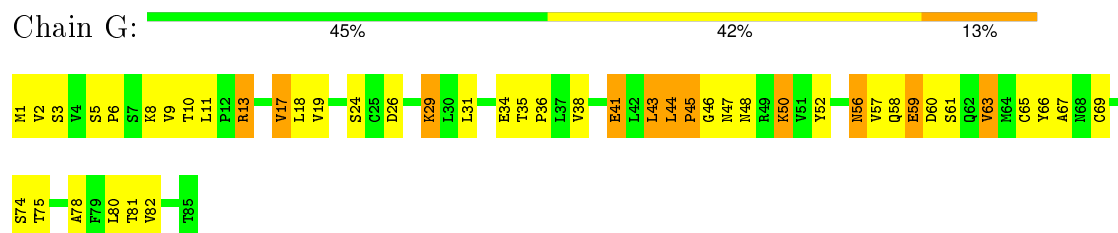
#### • Molecule 1: Intercellular adhesion molecule 1



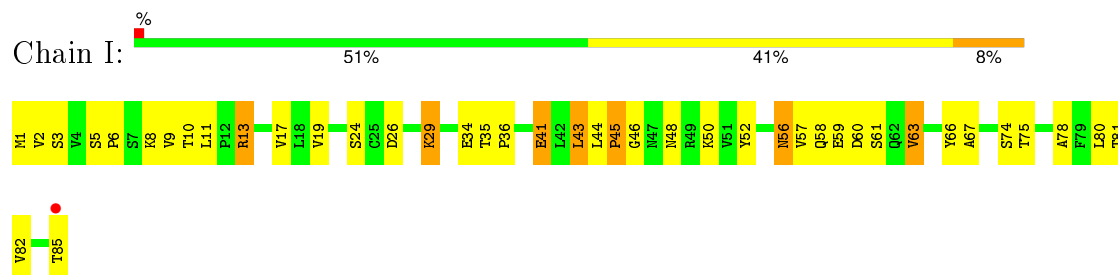
#### • Molecule 1: Intercellular adhesion molecule 1



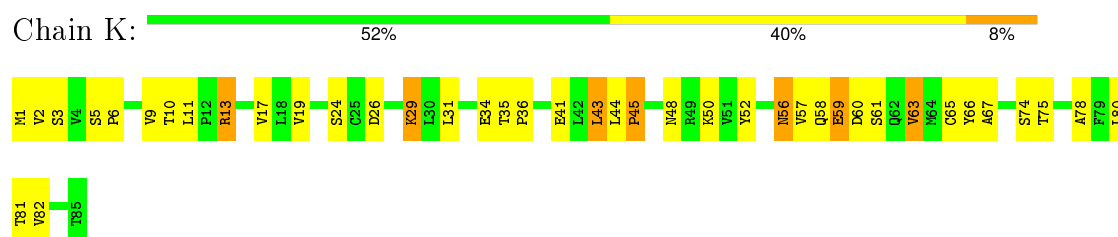
#### • Molecule 1: Intercellular adhesion molecule 1



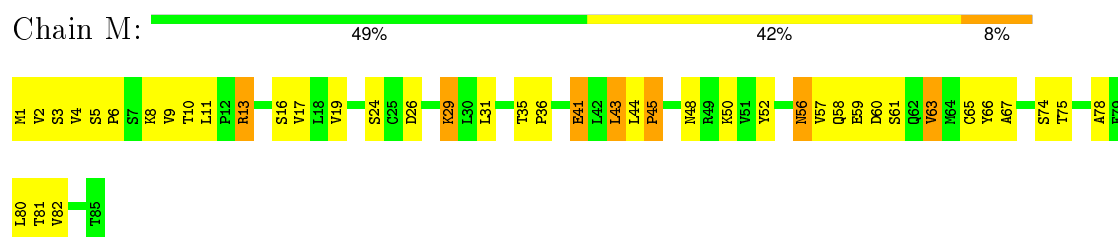
- Molecule 1: Intercellular adhesion molecule 1



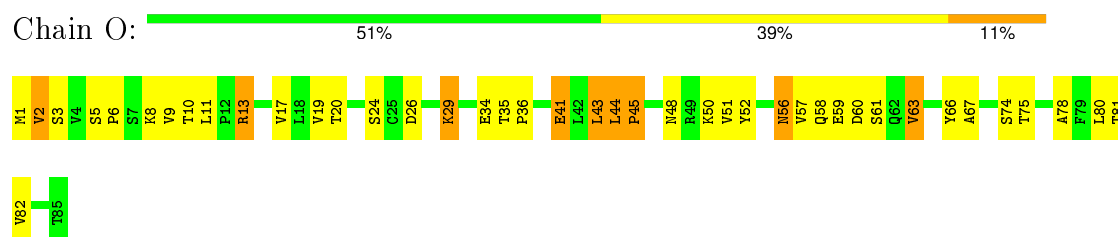
- Molecule 1: Intercellular adhesion molecule 1



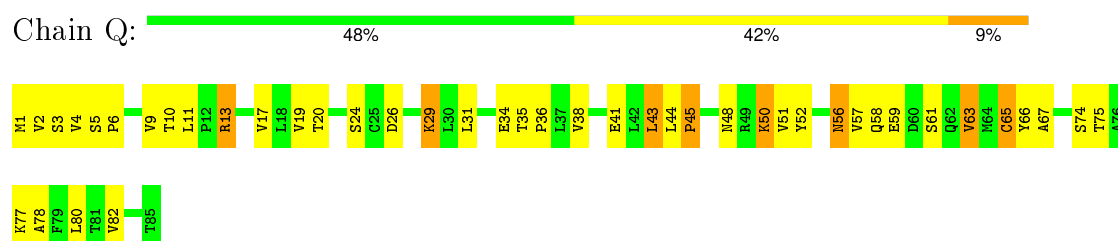
- Molecule 1: Intercellular adhesion molecule 1



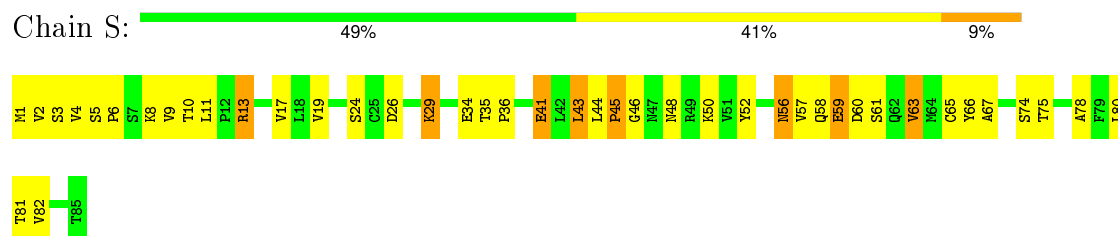
- Molecule 1: Intercellular adhesion molecule 1



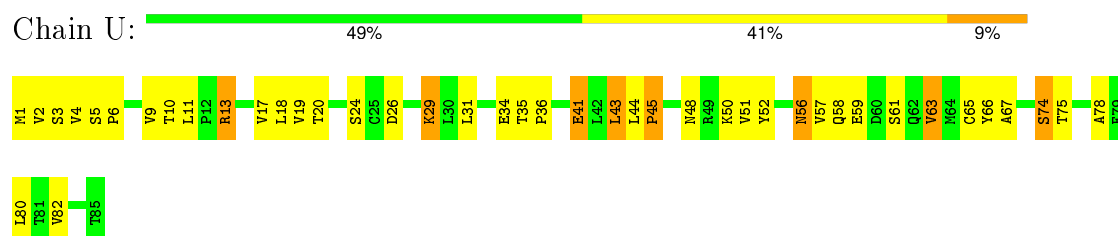
- Molecule 1: Intercellular adhesion molecule 1



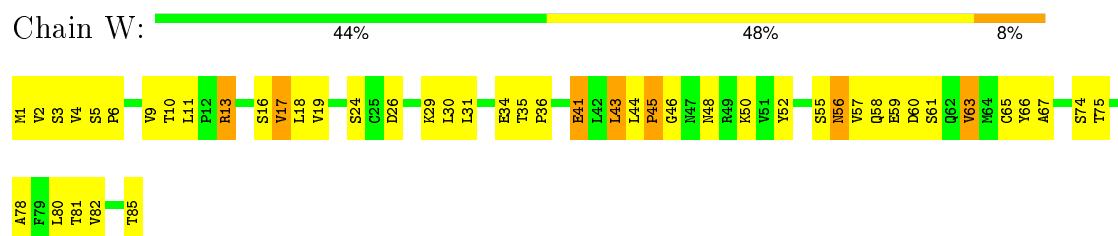
- Molecule 1: Intercellular adhesion molecule 1



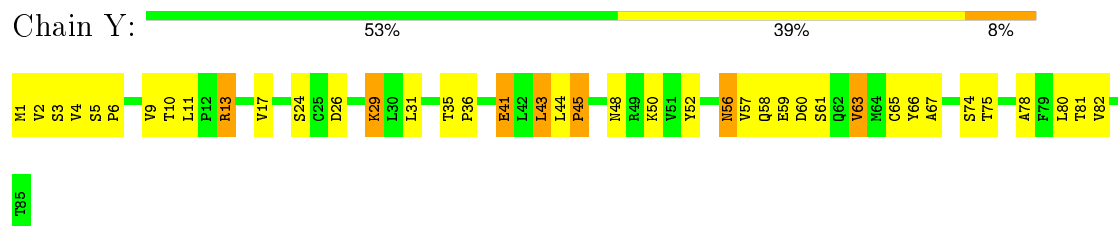
- Molecule 1: Intercellular adhesion molecule 1



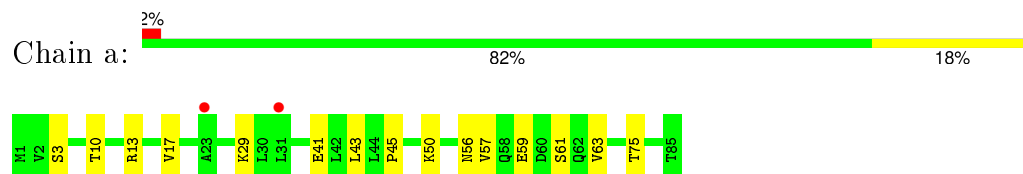
- Molecule 1: Intercellular adhesion molecule 1



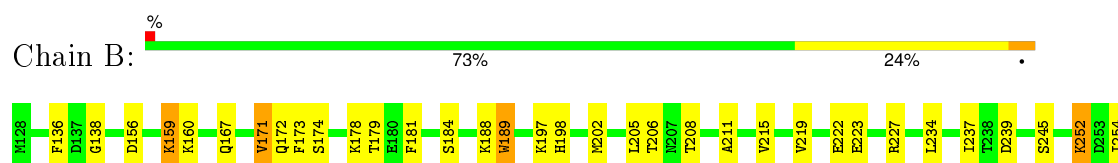
- Molecule 1: Intercellular adhesion molecule 1

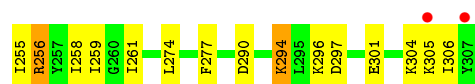


- Molecule 1: Intercellular adhesion molecule 1

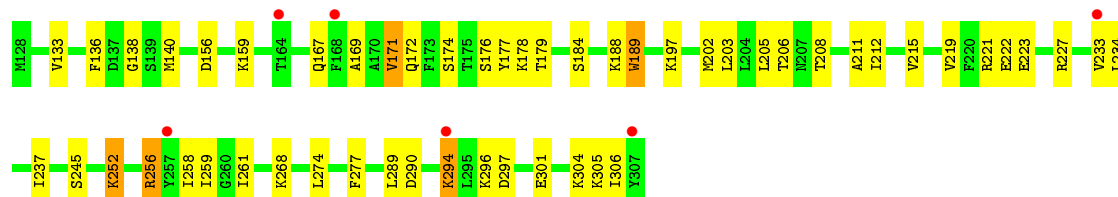


- Molecule 2: Integrin alpha-L

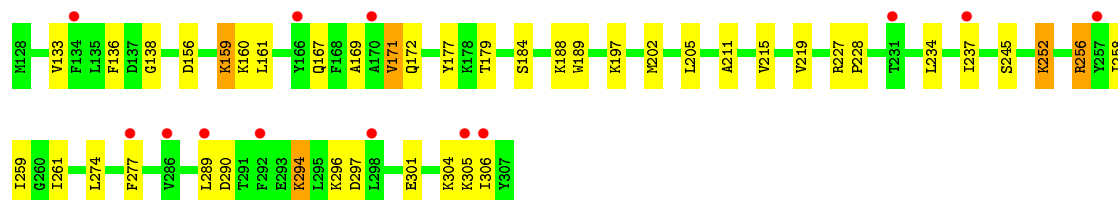
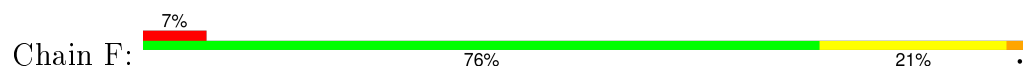




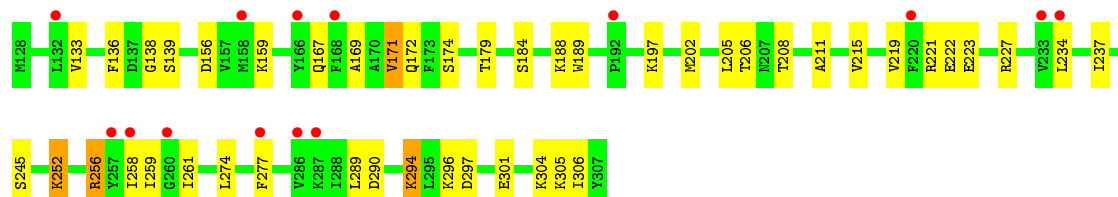
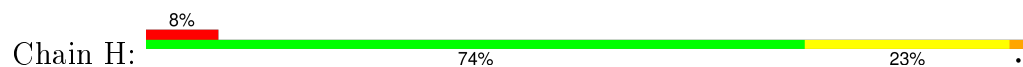
• Molecule 2: Integrin alpha-L



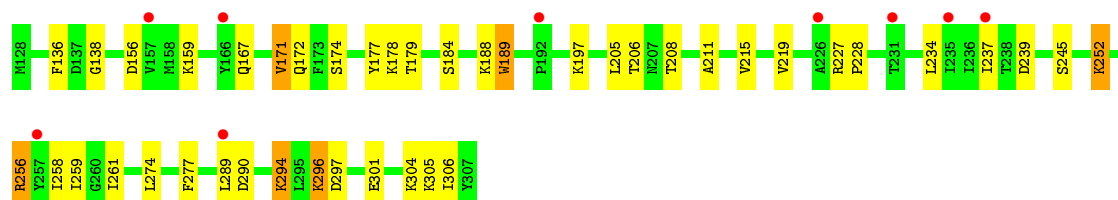
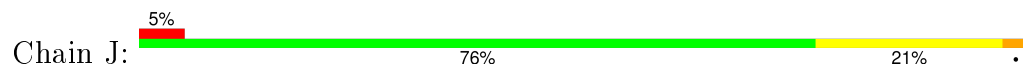
• Molecule 2: Integrin alpha-L



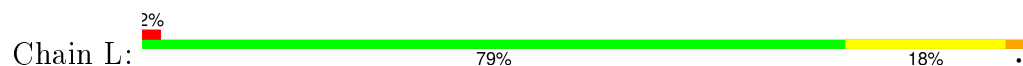
• Molecule 2: Integrin alpha-L



• Molecule 2: Integrin alpha-L

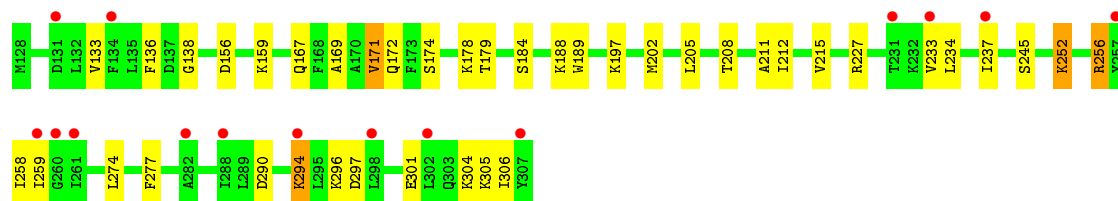
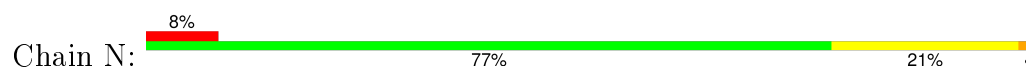


• Molecule 2: Integrin alpha-L

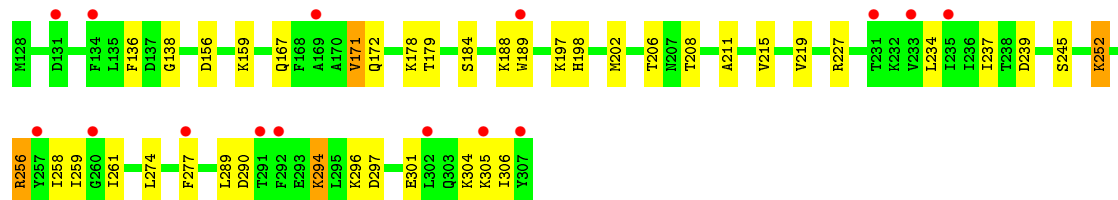
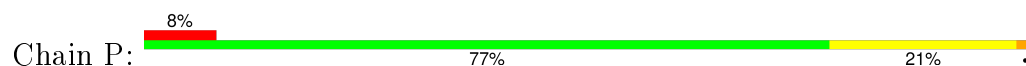




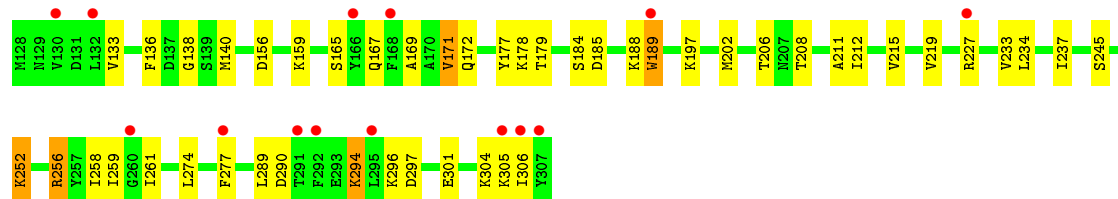
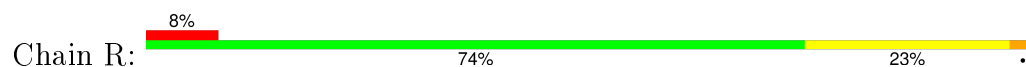
• Molecule 2: Integrin alpha-L



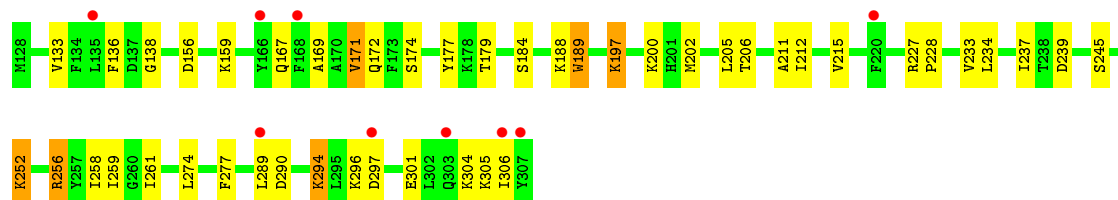
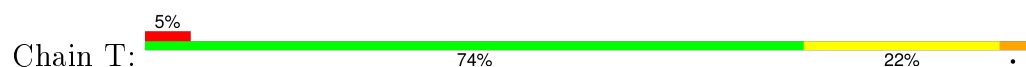
• Molecule 2: Integrin alpha-L



• Molecule 2: Integrin alpha-L

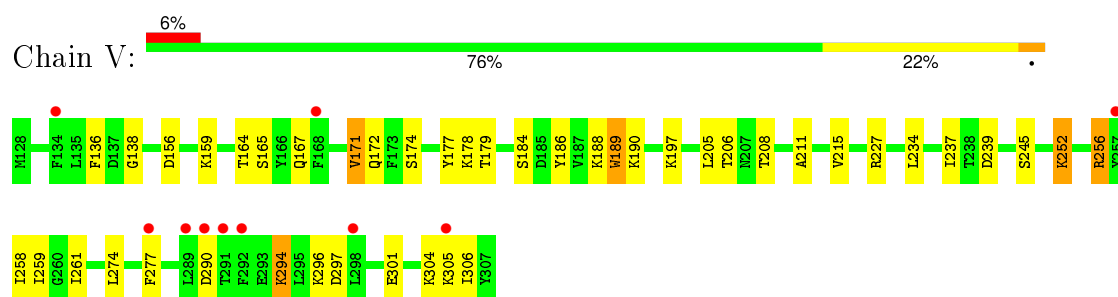


• Molecule 2: Integrin alpha-L

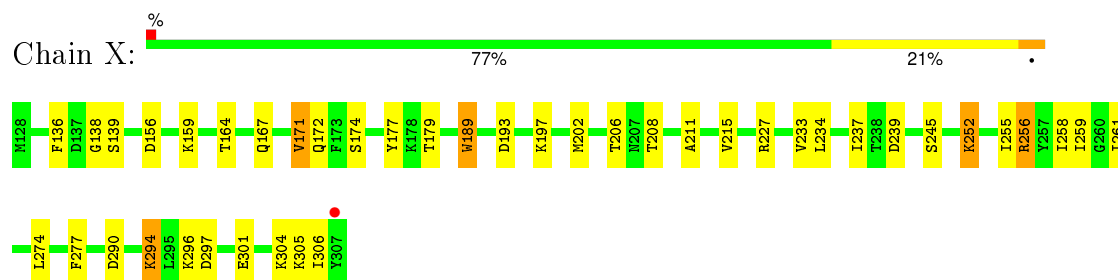


• Molecule 2: Integrin alpha-L

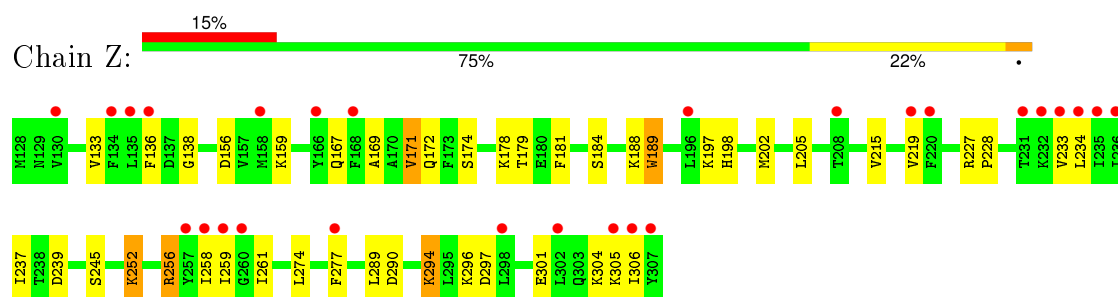




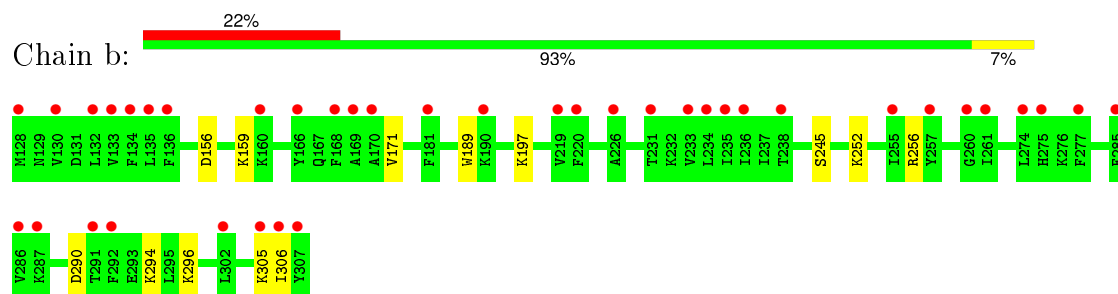
- Molecule 2: Integrin alpha-L



- Molecule 2: Integrin alpha-L



- Molecule 2: Integrin alpha-L



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.04Å 166.33Å 299.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.54 – 3.60 49.54 – 3.60	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.54-3.60) 95.9 (49.54-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.13 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.218 , 0.234 0.210 , 0.227	Depositor DCC
$R_{free}$ test set	2984 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	121.2	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 105.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 58807 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	29330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	165.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG

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	0.99	1/652 (0.2%)	0.93	1/887 (0.1%)
1	C	0.90	0/652	0.88	0/887
1	E	0.67	0/652	0.78	0/887
1	G	0.92	3/652 (0.5%)	0.84	0/887
1	I	0.71	0/652	0.80	0/887
1	K	0.96	2/652 (0.3%)	0.88	0/887
1	M	0.78	0/652	0.80	0/887
1	O	0.80	0/652	0.83	1/887 (0.1%)
1	Q	0.78	1/652 (0.2%)	0.77	0/887
1	S	0.79	1/652 (0.2%)	0.81	0/887
1	U	0.79	0/652	0.80	0/887
1	W	0.81	0/652	0.85	0/887
1	Y	0.66	0/652	0.76	0/887
1	a	0.71	0/652	0.76	0/887
2	B	0.65	0/1482	0.68	0/1994
2	D	0.58	0/1482	0.66	0/1994
2	F	0.47	0/1482	0.60	0/1994
2	H	0.50	0/1482	0.62	0/1994
2	J	0.50	0/1482	0.62	0/1994
2	L	0.72	0/1482	0.71	0/1994
2	N	0.50	0/1482	0.61	0/1994
2	P	0.50	0/1482	0.61	0/1994
2	R	0.51	0/1482	0.63	0/1994
2	T	0.52	0/1482	0.63	0/1994
2	V	0.59	1/1482 (0.1%)	0.64	0/1994
2	X	0.64	1/1482 (0.1%)	0.67	0/1994
2	Z	0.47	0/1482	0.60	0/1994
2	b	0.43	0/1482	0.59	0/1994
All	All	0.64	10/29876 (0.0%)	0.70	2/40334 (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	A	0	1
1	C	0	1
1	G	0	1
1	O	0	1
All	All	0	4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	65	CYS	CB-SG	-6.37	1.71	1.82
1	A	59	GLU	CG-CD	5.80	1.60	1.51
1	G	65	CYS	CB-SG	-5.78	1.72	1.81
2	X	189	TRP	CB-CG	5.74	1.60	1.50
1	K	59	GLU	CG-CD	5.54	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	VAL	CB-CA-C	-6.26	99.50	111.40
1	O	2	VAL	CB-CA-C	-5.15	101.62	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	LEU	Peptide
1	C	44	LEU	Peptide
1	G	44	LEU	Peptide
1	O	44	LEU	Peptide

## 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	641	0	653	38	0
1	C	641	0	653	38	0
1	E	641	0	653	45	0
1	G	641	0	653	40	4
1	I	641	0	653	37	0
1	K	641	0	653	32	0
1	M	641	0	653	34	0
1	O	641	0	653	32	0
1	Q	641	0	653	36	0
1	S	641	0	653	33	0
1	U	641	0	653	31	0
1	W	641	0	653	34	0
1	Y	641	0	653	25	0
1	a	641	0	653	0	0
2	B	1453	0	1455	55	0
2	D	1453	0	1455	51	0
2	F	1453	0	1455	33	0
2	H	1453	0	1455	42	0
2	J	1453	0	1455	33	0
2	L	1453	0	1455	25	0
2	N	1453	0	1455	23	0
2	P	1453	0	1455	26	0
2	R	1453	0	1455	32	0
2	T	1453	0	1455	33	0
2	V	1453	0	1455	26	4
2	X	1453	0	1455	34	0
2	Z	1453	0	1455	32	0
2	b	1453	0	1455	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
3	N	1	0	0	0	0
3	P	1	0	0	0	0
3	R	1	0	0	0	0
3	T	1	0	0	0	0
3	V	1	0	0	0	0
3	X	1	0	0	0	0
3	Z	1	0	0	0	0
3	b	1	0	0	0	0
All	All	29330	0	29512	795	4

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 14.

The worst 5 of 795 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:D:223:GLU:CG	2:H:223:GLU:HG3	1.73	1.18
1:C:29:LYS:HA	2:X:164:THR:OG1	1.47	1.13
1:E:15:GLY:HA2	1:I:85:THR:CG2	1.83	1.07
1:E:14:GLY:O	1:I:85:THR:HB	1.53	1.07
1:C:29:LYS:HE2	2:X:164:THR:H	1.19	1.06

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:ASN:OD1	2:V:164:THR:CG2[1_655]	1.93	0.27
1:G:46:GLY:N	2:V:164:THR:OG1[1_655]	1.98	0.22
1:G:46:GLY:CA	2:V:164:THR:OG1[1_655]	2.14	0.06
1:G:43:LEU:CD2	2:V:190:LYS:CD[1_655]	2.17	0.03

## 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	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	16	62
1	C	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	16	62
1	E	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	16	62
1	G	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	16	62
1	I	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	16	62
1	K	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	16	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	16	62
1	O	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	16	62
1	Q	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	16	62
1	S	83/85 (98%)	76 (92%)	6 (7%)	1 (1%)	16	62
1	U	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	16	62
1	W	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	16	62
1	Y	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	16	62
1	a	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	16	62
2	B	178/180 (99%)	155 (87%)	23 (13%)	0	100	100
2	D	178/180 (99%)	157 (88%)	21 (12%)	0	100	100
2	F	178/180 (99%)	160 (90%)	17 (10%)	1 (1%)	30	74
2	H	178/180 (99%)	158 (89%)	20 (11%)	0	100	100
2	J	178/180 (99%)	159 (89%)	19 (11%)	0	100	100
2	L	178/180 (99%)	162 (91%)	15 (8%)	1 (1%)	30	74
2	N	178/180 (99%)	161 (90%)	17 (10%)	0	100	100
2	P	178/180 (99%)	160 (90%)	18 (10%)	0	100	100
2	R	178/180 (99%)	159 (89%)	19 (11%)	0	100	100
2	T	178/180 (99%)	160 (90%)	18 (10%)	0	100	100
2	V	178/180 (99%)	158 (89%)	20 (11%)	0	100	100
2	X	178/180 (99%)	160 (90%)	18 (10%)	0	100	100
2	Z	178/180 (99%)	161 (90%)	17 (10%)	0	100	100
2	b	178/180 (99%)	159 (89%)	19 (11%)	0	100	100
All	All	3654/3710 (98%)	3311 (91%)	327 (9%)	16 (0%)	39	80

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	PRO
1	C	45	PRO
1	E	45	PRO
1	G	45	PRO
1	I	45	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	76/76 (100%)	60 (79%)	16 (21%)	1	10
1	C	76/76 (100%)	63 (83%)	13 (17%)	2	18
1	E	76/76 (100%)	62 (82%)	14 (18%)	2	14
1	G	76/76 (100%)	61 (80%)	15 (20%)	1	12
1	I	76/76 (100%)	62 (82%)	14 (18%)	2	14
1	K	76/76 (100%)	63 (83%)	13 (17%)	2	18
1	M	76/76 (100%)	62 (82%)	14 (18%)	2	14
1	O	76/76 (100%)	62 (82%)	14 (18%)	2	14
1	Q	76/76 (100%)	62 (82%)	14 (18%)	2	14
1	S	76/76 (100%)	62 (82%)	14 (18%)	2	14
1	U	76/76 (100%)	61 (80%)	15 (20%)	1	12
1	W	76/76 (100%)	61 (80%)	15 (20%)	1	12
1	Y	76/76 (100%)	62 (82%)	14 (18%)	2	14
1	a	76/76 (100%)	62 (82%)	14 (18%)	2	14
2	B	161/161 (100%)	147 (91%)	14 (9%)	13	51
2	D	161/161 (100%)	146 (91%)	15 (9%)	11	48
2	F	161/161 (100%)	148 (92%)	13 (8%)	15	54
2	H	161/161 (100%)	148 (92%)	13 (8%)	15	54
2	J	161/161 (100%)	148 (92%)	13 (8%)	15	54
2	L	161/161 (100%)	146 (91%)	15 (9%)	11	48
2	N	161/161 (100%)	147 (91%)	14 (9%)	13	51
2	P	161/161 (100%)	148 (92%)	13 (8%)	15	54
2	R	161/161 (100%)	146 (91%)	15 (9%)	11	48
2	T	161/161 (100%)	147 (91%)	14 (9%)	13	51
2	V	161/161 (100%)	148 (92%)	13 (8%)	15	54
2	X	161/161 (100%)	147 (91%)	14 (9%)	13	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	161/161 (100%)	148 (92%)	13 (8%)	15	54
2	b	161/161 (100%)	148 (92%)	13 (8%)	15	54
All	All	3318/3318 (100%)	2927 (88%)	391 (12%)	6	34

5 of 391 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	56	ASN
2	P	290	ASP
2	Z	296	LYS
2	N	156	ASP
1	O	13	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	58	GLN
2	P	213	ASN
2	Z	275	HIS
2	N	167	GLN
1	O	56	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	85/85 (100%)	-0.15	0 100 100	69, 88, 125, 143	0
1	C	85/85 (100%)	-0.19	0 100 100	71, 94, 134, 166	0
1	E	85/85 (100%)	0.05	2 (2%) 62 47	110, 139, 193, 230	0
1	G	85/85 (100%)	-0.13	0 100 100	79, 108, 166, 194	0
1	I	85/85 (100%)	0.04	1 (1%) 81 69	96, 141, 228, 320	0
1	K	85/85 (100%)	-0.26	0 100 100	77, 100, 142, 171	0
1	M	85/85 (100%)	-0.19	0 100 100	96, 116, 149, 163	0
1	O	85/85 (100%)	-0.18	0 100 100	78, 109, 160, 182	0
1	Q	85/85 (100%)	-0.18	0 100 100	90, 112, 161, 190	0
1	S	85/85 (100%)	-0.18	0 100 100	91, 109, 141, 168	0
1	U	85/85 (100%)	-0.18	0 100 100	87, 106, 141, 166	0
1	W	85/85 (100%)	-0.22	0 100 100	85, 104, 139, 169	0
1	Y	85/85 (100%)	-0.10	0 100 100	95, 122, 182, 209	0
1	a	85/85 (100%)	-0.03	2 (2%) 62 47	99, 132, 216, 231	0
2	B	180/180 (100%)	-0.06	2 (1%) 82 70	69, 124, 207, 256	0
2	D	180/180 (100%)	-0.00	6 (3%) 50 36	78, 146, 229, 289	0
2	F	180/180 (100%)	0.32	13 (7%) 18 12	129, 220, 367, 441	0
2	H	180/180 (100%)	0.31	14 (7%) 16 10	108, 189, 288, 366	0
2	J	180/180 (100%)	0.22	9 (5%) 32 22	97, 182, 314, 409	0
2	L	180/180 (100%)	-0.04	3 (1%) 73 59	72, 115, 189, 225	0
2	N	180/180 (100%)	0.42	15 (8%) 14 10	111, 172, 255, 306	0
2	P	180/180 (100%)	0.37	15 (8%) 14 10	116, 190, 295, 377	0
2	R	180/180 (100%)	0.43	14 (7%) 16 10	104, 187, 297, 390	0
2	T	180/180 (100%)	0.08	9 (5%) 32 22	96, 170, 266, 336	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	V	180/180 (100%)	0.18	10 (5%) 28 19	94, 150, 238, 293	0
2	X	180/180 (100%)	-0.08	1 (0%) 90 83	85, 126, 195, 239	0
2	Z	180/180 (100%)	0.63	27 (15%) 3 3	122, 211, 329, 418	0
2	b	180/180 (100%)	0.88	39 (21%) 1 1	137, 258, 398, 507	0
All	All	3710/3710 (100%)	0.13	182 (4%) 33 23	69, 146, 294, 507	0

The worst 5 of 182 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	307	TYR	10.8
2	N	307	TYR	7.3
2	Z	220	PHE	6.9
2	T	307	TYR	6.0
2	T	306	ILE	5.9

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	L	901	1/1	0.99	0.24	2.07	52,52,52,52	0
3	MG	Z	901	1/1	1.00	0.24	1.69	104,104,104,104	0
3	MG	H	901	1/1	0.99	0.20	0.66	88,88,88,88	0
3	MG	F	901	1/1	0.93	0.19	0.48	118,118,118,118	0
3	MG	b	901	1/1	0.94	0.20	0.03	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	D	901	1/1	0.99	0.17	-0.06	62,62,62,62	0
3	MG	P	901	1/1	0.99	0.20	-0.41	97,97,97,97	0
3	MG	N	901	1/1	0.99	0.16	-0.41	94,94,94,94	0
3	MG	R	901	1/1	0.99	0.18	-0.49	88,88,88,88	0
3	MG	T	901	1/1	0.98	0.14	-0.76	84,84,84,84	0
3	MG	X	901	1/1	0.98	0.17	-0.87	65,65,65,65	0
3	MG	B	901	1/1	1.00	0.17	-1.20	51,51,51,51	0
3	MG	V	901	1/1	0.98	0.11	-1.44	77,77,77,77	0
3	MG	J	901	1/1	0.99	0.11	-1.46	88,88,88,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.