wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2020 – 09:39 AM BST

PDB ID	:	4DX9
Title	:	ICAP1 in complex with integrin beta 1 cytoplasmic tail
Authors	:	Liu, W.; Draheim, K.; Zhang, R.; Calderwood, D.A.; Boggon, T.J.
Deposited on	:	2012-02-27
Resolution	:	2.99 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 following versions of software and data (see references (1)) were used in the production of this report:

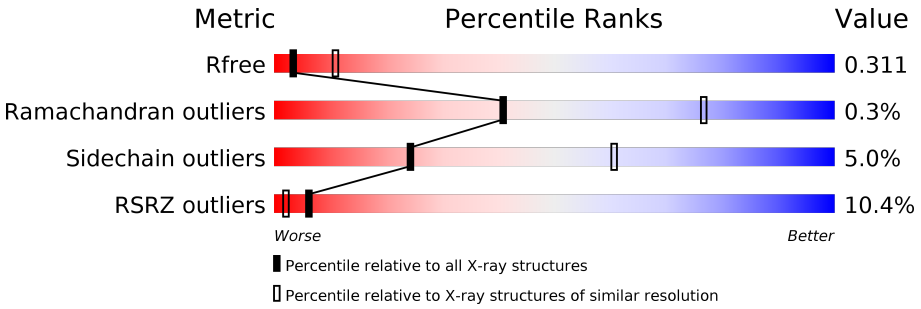
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.3.dev2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.3.dev2

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 2.99 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	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	0	157	3% 68% 30%
1	1	157	74% 25%
1	2	157	5% 55% 42%
1	3	157	8% 64% 34%
1	4	157	4% 80% 18%
1	5	157	76% 18%
1	A	157	3% 64% 32%

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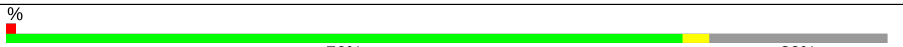
Mol	Chain	Length	Quality of chain
1	C	157	
1	E	157	
1	G	157	
1	I	157	
1	K	157	
1	M	157	
1	O	157	
1	Q	157	
1	S	157	
1	U	157	
1	W	157	
1	Y	157	
1	a	157	
1	c	157	
1	e	157	
1	g	157	
1	i	157	
1	k	157	
1	m	157	
1	o	157	
1	q	157	
1	s	157	
1	u	157	
1	w	157	
1	y	157	

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Mol	Chain	Length	Quality of chain
2	6	15	73% 27%
2	7	15	73% 27%
2	8	15	7% 47% 7% 47%
2	9	15	53% 47%
2	B	15	7% 60% 7% 33%
2	D	15	73% 27%
2	F	15	67% 7% 27%
2	H	15	67% 7% 27%
2	J	15	7% 73% 27%
2	L	15	73% 27%
2	N	15	60% 13% 27%
2	P	15	60% 13% 27%
2	R	15	7% 67% 7% 27%
2	T	15	73% 27%
2	V	15	60% 7% 33%
2	X	15	73% 7% 20%
2	Z	15	73% 27%
2	b	15	67% 33%
2	d	15	73% 27%
2	f	15	7% 67% 7% 27%
2	h	15	7% 60% 7% 33%
2	j	15	27% 73%
2	l	15	47% 53%
2	n	15	13% 73% 27%
2	p	15	13% 33% 67%

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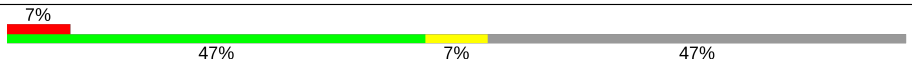
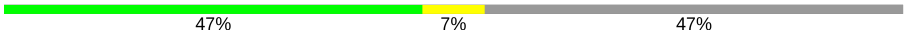
Mol	Chain	Length	Quality of chain
2	r	15	
2	t	15	
2	v	15	
2	x	15	
2	z	15	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 29306 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 Integrin beta-1-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	Se	0	0	0
			844	547	134	157	4	2			
1	0	110	Total	C	N	O	S	Se	0	0	0
			858	558	138	156	4	2			
1	k	105	Total	C	N	O	S	Se	0	0	0
			827	535	133	153	4	2			
1	m	127	Total	C	N	O	S	Se	0	0	0
			991	635	158	192	4	2			
1	1	118	Total	C	N	O	S	Se	0	0	0
			919	591	147	175	4	2			
1	C	127	Total	C	N	O	S	Se	0	0	0
			997	640	158	193	4	2			
1	2	91	Total	C	N	O	S	Se	0	0	0
			716	465	117	128	4	2			
1	E	113	Total	C	N	O	S	Se	0	0	0
			875	565	140	164	4	2			
1	3	104	Total	C	N	O	S	Se	0	0	0
			810	523	132	149	4	2			
1	G	127	Total	C	N	O	S	Se	0	0	0
			995	639	157	193	4	2			
1	o	63	Total	C	N	O	S	Se	0	0	0
			489	319	73	92	3	2			
1	q	47	Total	C	N	O	S	Se	0	0	0
			359	234	57	62	4	2			
1	I	125	Total	C	N	O	S	Se	0	0	0
			979	627	155	191	4	2			
1	4	129	Total	C	N	O	S	Se	0	0	0
			1000	641	158	195	4	2			
1	K	116	Total	C	N	O	S	Se	0	0	0
			905	584	144	171	4	2			
1	5	128	Total	C	N	O	S	Se	0	0	0
			1000	642	158	194	4	2			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	M	124	Total	C	N	O	S	Se	0	0	0
			970	623	154	187	4	2			
1	O	102	Total	C	N	O	S	Se	0	0	0
			812	528	127	151	4	2			
1	a	99	Total	C	N	O	S	Se	0	0	0
			777	507	124	140	4	2			
1	s	102	Total	C	N	O	S	Se	0	0	0
			813	529	130	148	4	2			
1	u	106	Total	C	N	O	S	Se	0	0	0
			831	536	135	154	4	2			
1	c	120	Total	C	N	O	S	Se	0	0	0
			934	603	149	176	4	2			
1	e	126	Total	C	N	O	S	Se	0	0	0
			987	633	156	192	4	2			
1	g	127	Total	C	N	O	S	Se	0	0	0
			994	636	157	195	4	2			
1	i	101	Total	C	N	O	S	Se	0	0	0
			779	506	126	141	4	2			
1	Q	122	Total	C	N	O	S	Se	0	0	0
			945	606	150	183	4	2			
1	S	126	Total	C	N	O	S	Se	0	0	0
			987	633	156	192	4	2			
1	U	101	Total	C	N	O	S	Se	0	0	0
			811	528	129	148	4	2			
1	W	128	Total	C	N	O	S	Se	0	0	0
			1005	647	159	193	4	2			
1	w	49	Total	C	N	O	S	Se	0	0	0
			378	248	59	66	3	2			
1	Y	129	Total	C	N	O	S	Se	0	0	0
			1013	651	161	195	4	2			
1	y	93	Total	C	N	O	S	Se	0	0	0
			738	488	111	133	4	2			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLY	-	expression tag	UNP O14713
A	45	PRO	-	expression tag	UNP O14713
A	46	LEU	-	expression tag	UNP O14713
A	47	GLY	-	expression tag	UNP O14713
A	48	SER	-	expression tag	UNP O14713
0	44	GLY	-	expression tag	UNP O14713
0	45	PRO	-	expression tag	UNP O14713

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Chain	Residue	Modelled	Actual	Comment	Reference
0	46	LEU	-	expression tag	UNP O14713
0	47	GLY	-	expression tag	UNP O14713
0	48	SER	-	expression tag	UNP O14713
k	44	GLY	-	expression tag	UNP O14713
k	45	PRO	-	expression tag	UNP O14713
k	46	LEU	-	expression tag	UNP O14713
k	47	GLY	-	expression tag	UNP O14713
k	48	SER	-	expression tag	UNP O14713
m	44	GLY	-	expression tag	UNP O14713
m	45	PRO	-	expression tag	UNP O14713
m	46	LEU	-	expression tag	UNP O14713
m	47	GLY	-	expression tag	UNP O14713
m	48	SER	-	expression tag	UNP O14713
1	44	GLY	-	expression tag	UNP O14713
1	45	PRO	-	expression tag	UNP O14713
1	46	LEU	-	expression tag	UNP O14713
1	47	GLY	-	expression tag	UNP O14713
1	48	SER	-	expression tag	UNP O14713
C	44	GLY	-	expression tag	UNP O14713
C	45	PRO	-	expression tag	UNP O14713
C	46	LEU	-	expression tag	UNP O14713
C	47	GLY	-	expression tag	UNP O14713
C	48	SER	-	expression tag	UNP O14713
2	44	GLY	-	expression tag	UNP O14713
2	45	PRO	-	expression tag	UNP O14713
2	46	LEU	-	expression tag	UNP O14713
2	47	GLY	-	expression tag	UNP O14713
2	48	SER	-	expression tag	UNP O14713
E	44	GLY	-	expression tag	UNP O14713
E	45	PRO	-	expression tag	UNP O14713
E	46	LEU	-	expression tag	UNP O14713
E	47	GLY	-	expression tag	UNP O14713
E	48	SER	-	expression tag	UNP O14713
3	44	GLY	-	expression tag	UNP O14713
3	45	PRO	-	expression tag	UNP O14713
3	46	LEU	-	expression tag	UNP O14713
3	47	GLY	-	expression tag	UNP O14713
3	48	SER	-	expression tag	UNP O14713
G	44	GLY	-	expression tag	UNP O14713
G	45	PRO	-	expression tag	UNP O14713
G	46	LEU	-	expression tag	UNP O14713
G	47	GLY	-	expression tag	UNP O14713

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Chain	Residue	Modelled	Actual	Comment	Reference
G	48	SER	-	expression tag	UNP O14713
o	44	GLY	-	expression tag	UNP O14713
o	45	PRO	-	expression tag	UNP O14713
o	46	LEU	-	expression tag	UNP O14713
o	47	GLY	-	expression tag	UNP O14713
o	48	SER	-	expression tag	UNP O14713
q	44	GLY	-	expression tag	UNP O14713
q	45	PRO	-	expression tag	UNP O14713
q	46	LEU	-	expression tag	UNP O14713
q	47	GLY	-	expression tag	UNP O14713
q	48	SER	-	expression tag	UNP O14713
I	44	GLY	-	expression tag	UNP O14713
I	45	PRO	-	expression tag	UNP O14713
I	46	LEU	-	expression tag	UNP O14713
I	47	GLY	-	expression tag	UNP O14713
I	48	SER	-	expression tag	UNP O14713
4	44	GLY	-	expression tag	UNP O14713
4	45	PRO	-	expression tag	UNP O14713
4	46	LEU	-	expression tag	UNP O14713
4	47	GLY	-	expression tag	UNP O14713
4	48	SER	-	expression tag	UNP O14713
K	44	GLY	-	expression tag	UNP O14713
K	45	PRO	-	expression tag	UNP O14713
K	46	LEU	-	expression tag	UNP O14713
K	47	GLY	-	expression tag	UNP O14713
K	48	SER	-	expression tag	UNP O14713
5	44	GLY	-	expression tag	UNP O14713
5	45	PRO	-	expression tag	UNP O14713
5	46	LEU	-	expression tag	UNP O14713
5	47	GLY	-	expression tag	UNP O14713
5	48	SER	-	expression tag	UNP O14713
M	44	GLY	-	expression tag	UNP O14713
M	45	PRO	-	expression tag	UNP O14713
M	46	LEU	-	expression tag	UNP O14713
M	47	GLY	-	expression tag	UNP O14713
M	48	SER	-	expression tag	UNP O14713
O	44	GLY	-	expression tag	UNP O14713
O	45	PRO	-	expression tag	UNP O14713
O	46	LEU	-	expression tag	UNP O14713
O	47	GLY	-	expression tag	UNP O14713
O	48	SER	-	expression tag	UNP O14713
a	44	GLY	-	expression tag	UNP O14713

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Chain	Residue	Modelled	Actual	Comment	Reference
a	45	PRO	-	expression tag	UNP O14713
a	46	LEU	-	expression tag	UNP O14713
a	47	GLY	-	expression tag	UNP O14713
a	48	SER	-	expression tag	UNP O14713
s	44	GLY	-	expression tag	UNP O14713
s	45	PRO	-	expression tag	UNP O14713
s	46	LEU	-	expression tag	UNP O14713
s	47	GLY	-	expression tag	UNP O14713
s	48	SER	-	expression tag	UNP O14713
u	44	GLY	-	expression tag	UNP O14713
u	45	PRO	-	expression tag	UNP O14713
u	46	LEU	-	expression tag	UNP O14713
u	47	GLY	-	expression tag	UNP O14713
u	48	SER	-	expression tag	UNP O14713
c	44	GLY	-	expression tag	UNP O14713
c	45	PRO	-	expression tag	UNP O14713
c	46	LEU	-	expression tag	UNP O14713
c	47	GLY	-	expression tag	UNP O14713
c	48	SER	-	expression tag	UNP O14713
e	44	GLY	-	expression tag	UNP O14713
e	45	PRO	-	expression tag	UNP O14713
e	46	LEU	-	expression tag	UNP O14713
e	47	GLY	-	expression tag	UNP O14713
e	48	SER	-	expression tag	UNP O14713
g	44	GLY	-	expression tag	UNP O14713
g	45	PRO	-	expression tag	UNP O14713
g	46	LEU	-	expression tag	UNP O14713
g	47	GLY	-	expression tag	UNP O14713
g	48	SER	-	expression tag	UNP O14713
i	44	GLY	-	expression tag	UNP O14713
i	45	PRO	-	expression tag	UNP O14713
i	46	LEU	-	expression tag	UNP O14713
i	47	GLY	-	expression tag	UNP O14713
i	48	SER	-	expression tag	UNP O14713
Q	44	GLY	-	expression tag	UNP O14713
Q	45	PRO	-	expression tag	UNP O14713
Q	46	LEU	-	expression tag	UNP O14713
Q	47	GLY	-	expression tag	UNP O14713
Q	48	SER	-	expression tag	UNP O14713
S	44	GLY	-	expression tag	UNP O14713
S	45	PRO	-	expression tag	UNP O14713
S	46	LEU	-	expression tag	UNP O14713

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Chain	Residue	Modelled	Actual	Comment	Reference
S	47	GLY	-	expression tag	UNP O14713
S	48	SER	-	expression tag	UNP O14713
U	44	GLY	-	expression tag	UNP O14713
U	45	PRO	-	expression tag	UNP O14713
U	46	LEU	-	expression tag	UNP O14713
U	47	GLY	-	expression tag	UNP O14713
U	48	SER	-	expression tag	UNP O14713
W	44	GLY	-	expression tag	UNP O14713
W	45	PRO	-	expression tag	UNP O14713
W	46	LEU	-	expression tag	UNP O14713
W	47	GLY	-	expression tag	UNP O14713
W	48	SER	-	expression tag	UNP O14713
w	44	GLY	-	expression tag	UNP O14713
w	45	PRO	-	expression tag	UNP O14713
w	46	LEU	-	expression tag	UNP O14713
w	47	GLY	-	expression tag	UNP O14713
w	48	SER	-	expression tag	UNP O14713
Y	44	GLY	-	expression tag	UNP O14713
Y	45	PRO	-	expression tag	UNP O14713
Y	46	LEU	-	expression tag	UNP O14713
Y	47	GLY	-	expression tag	UNP O14713
Y	48	SER	-	expression tag	UNP O14713
y	44	GLY	-	expression tag	UNP O14713
y	45	PRO	-	expression tag	UNP O14713
y	46	LEU	-	expression tag	UNP O14713
y	47	GLY	-	expression tag	UNP O14713
y	48	SER	-	expression tag	UNP O14713

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	l	7	Total	C	N	O	0	0	0
			49	31	9	9			
2	n	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	x	4	Total	C	N	O	0	0	0
			25	15	4	6			
2	D	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	8	8	Total	C	N	O	0	0	0
			55	35	9	11			
2	H	11	Total	C	N	O	0	0	0
			79	50	14	15			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	p	5	Total C N O 38 25 7 6	0	0	0
2	B	10	Total C N O 70 44 12 14	0	0	0
2	9	8	Total C N O 54 33 9 12	0	0	0
2	F	11	Total C N O 79 50 14 15	0	0	0
2	r	2	Total C N O 15 9 3 3	0	0	0
2	J	11	Total C N O 79 50 14 15	0	0	0
2	7	11	Total C N O 79 50 14 15	0	0	0
2	L	11	Total C N O 79 50 14 15	0	0	0
2	6	11	Total C N O 79 50 14 15	0	0	0
2	N	11	Total C N O 79 50 14 15	0	0	0
2	P	11	Total C N O 79 50 14 15	0	0	0
2	t	8	Total C N O 58 37 11 10	0	0	0
2	v	8	Total C N O 55 35 9 11	0	0	0
2	b	10	Total C N O 70 44 12 14	0	0	0
2	d	11	Total C N O 79 50 14 15	0	0	0
2	f	11	Total C N O 79 50 14 15	0	0	0
2	h	10	Total C N O 70 44 12 14	0	0	0
2	j	4	Total C N O 27 17 5 5	0	0	0
2	R	11	Total C N O 79 50 14 15	0	0	0
2	T	11	Total C N O 79 50 14 15	0	0	0
2	V	10	Total C N O 70 44 12 14	0	0	0

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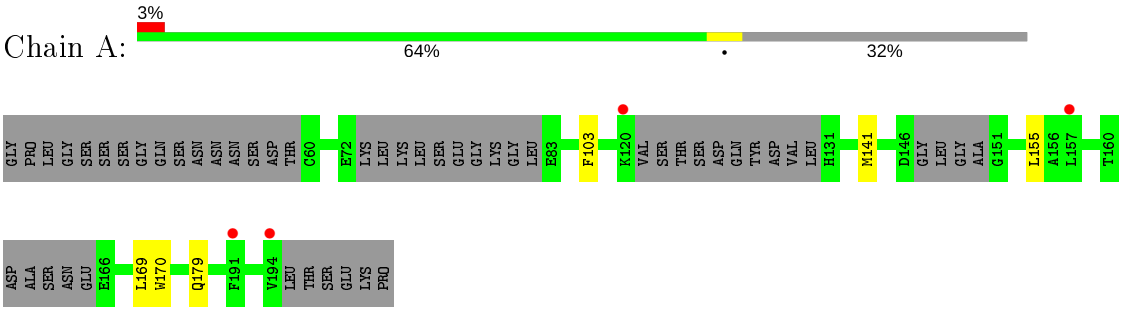
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	X	12	Total	C	N	O	0	0	0
			91	59	15	17			
2	Z	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	z	5	Total	C	N	O	0	0	0
			36	23	6	7			

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.

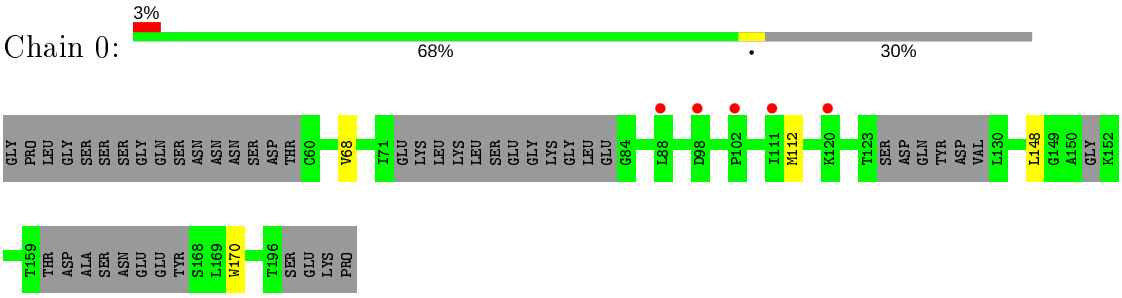
- Molecule 1: Integrin beta-1-binding protein 1

Chain A:



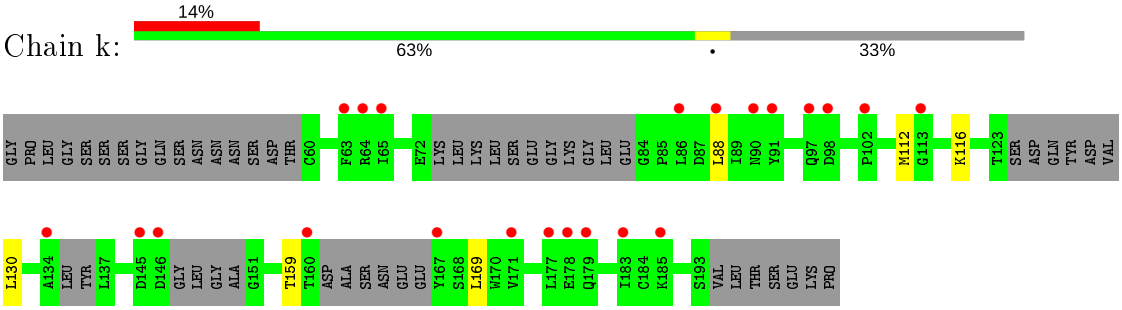
- Molecule 1: Integrin beta-1-binding protein 1

Chain 0:



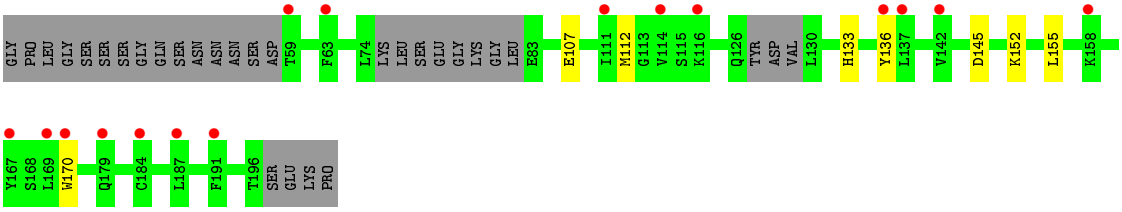
- Molecule 1: Integrin beta-1-binding protein 1

Chain k:



- Molecule 1: Integrin beta-1-binding protein 1

Chain m:



• Molecule 1: Integrin beta-1-binding protein 1

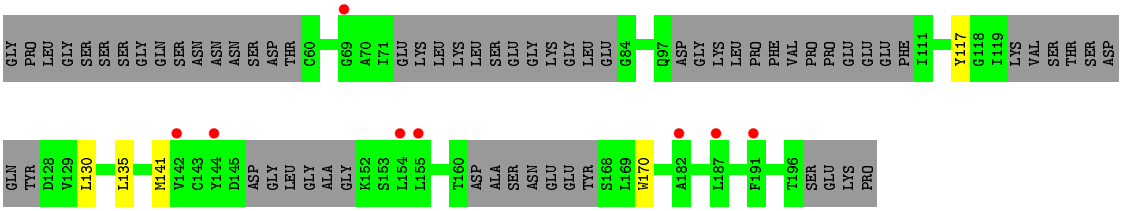
Chain 1:

• Molecule 1: Integrin beta-1-binding protein 1

Chain C:

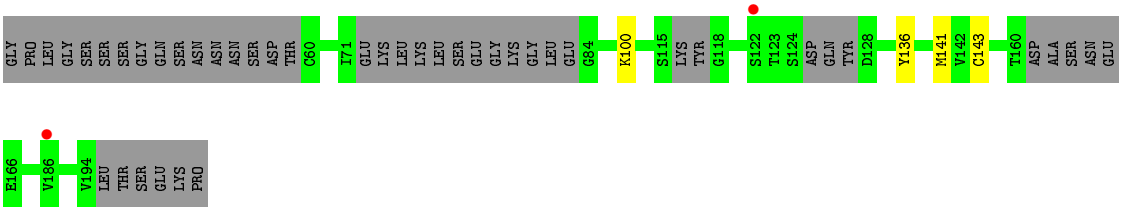
• Molecule 1: Integrin beta-1-binding protein 1

Chain 2:



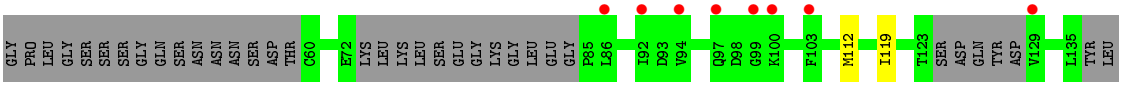
• Molecule 1: Integrin beta-1-binding protein 1

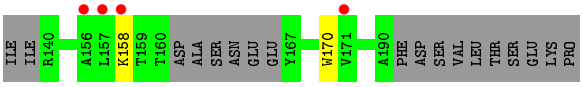
Chain E:



• Molecule 1: Integrin beta-1-binding protein 1

Chain 3:



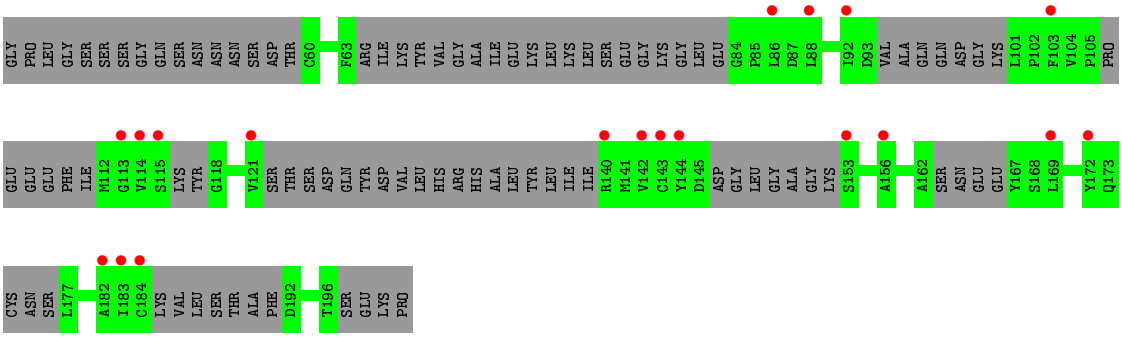


• Molecule 1: Integrin beta-1-binding protein 1

Chain G:

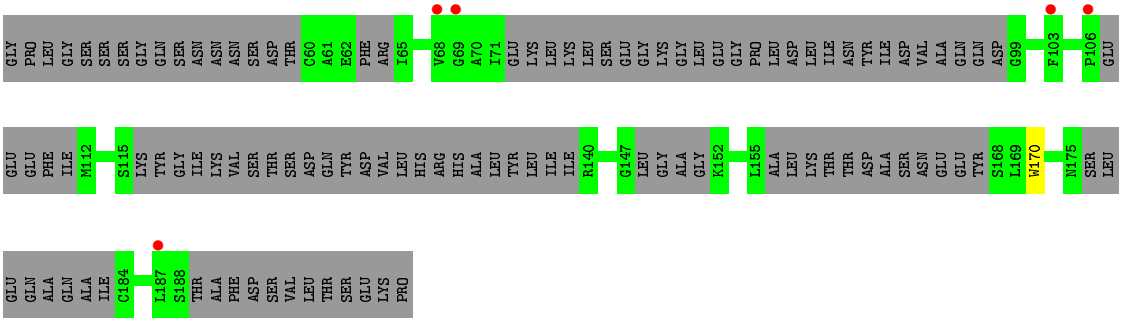
• Molecule 1: Integrin beta-1-binding protein 1

Chain o:



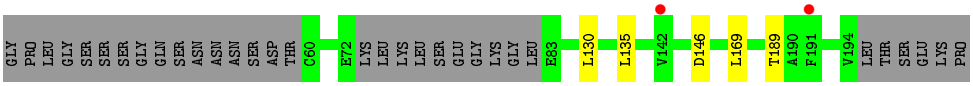
• Molecule 1: Integrin beta-1-binding protein 1

Chain q:



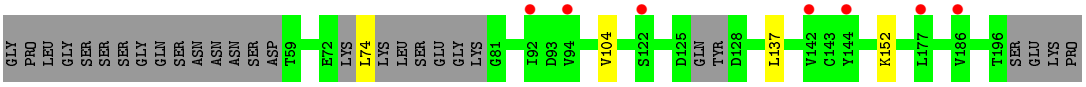
• Molecule 1: Integrin beta-1-binding protein 1

Chain I:



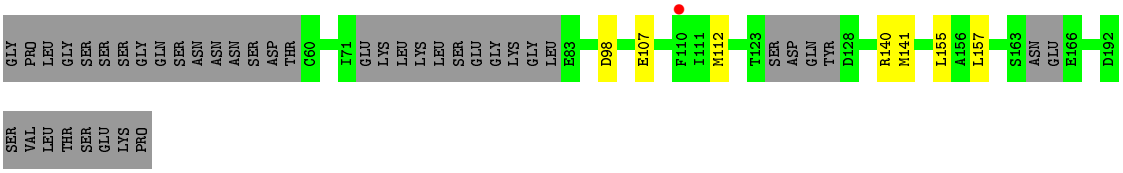
• Molecule 1: Integrin beta-1-binding protein 1

Chain 4:



• Molecule 1: Integrin beta-1-binding protein 1

Chain K:

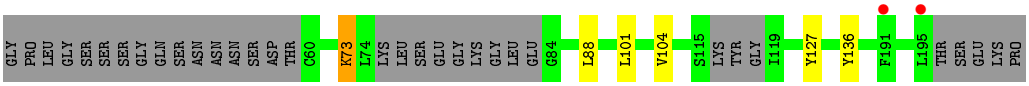


• Molecule 1: Integrin beta-1-binding protein 1

Chain 5:

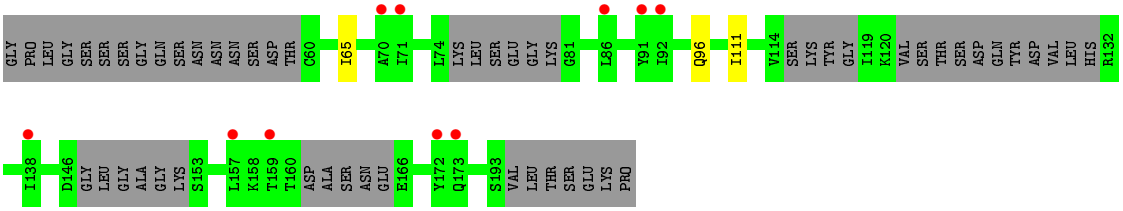
• Molecule 1: Integrin beta-1-binding protein 1

Chain M:



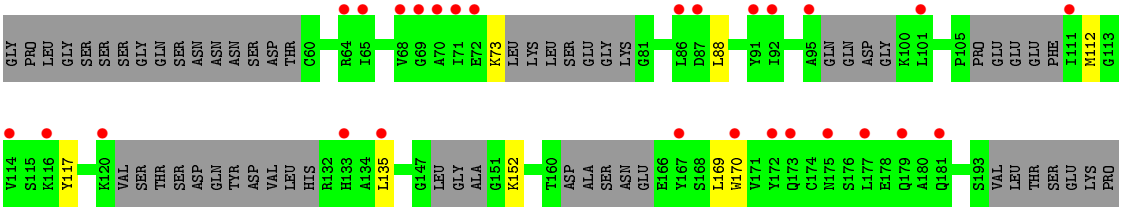
• Molecule 1: Integrin beta-1-binding protein 1

Chain O:



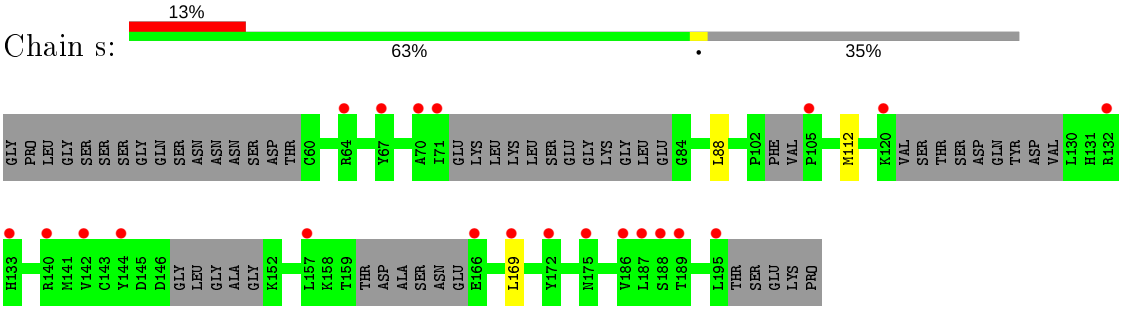
• Molecule 1: Integrin beta-1-binding protein 1

Chain a:



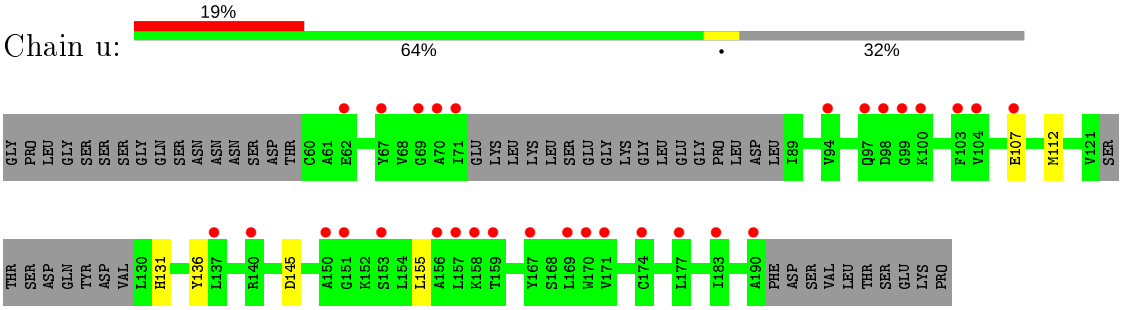
• Molecule 1: Integrin beta-1-binding protein 1

Chain s:



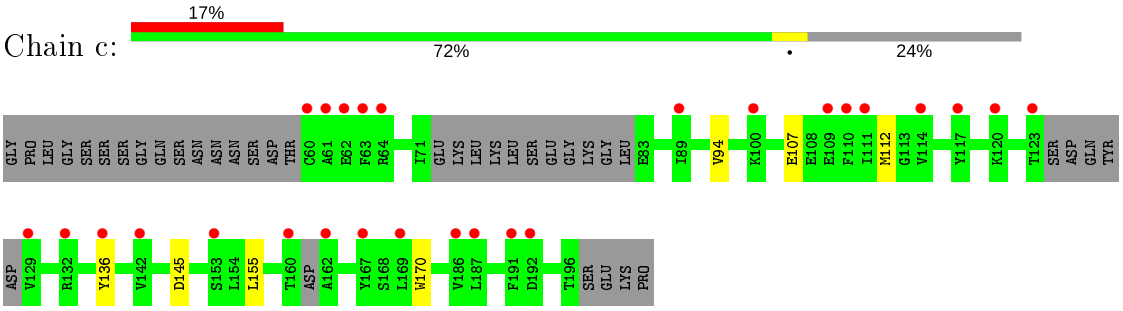
• Molecule 1: Integrin beta-1-binding protein 1

Chain u:



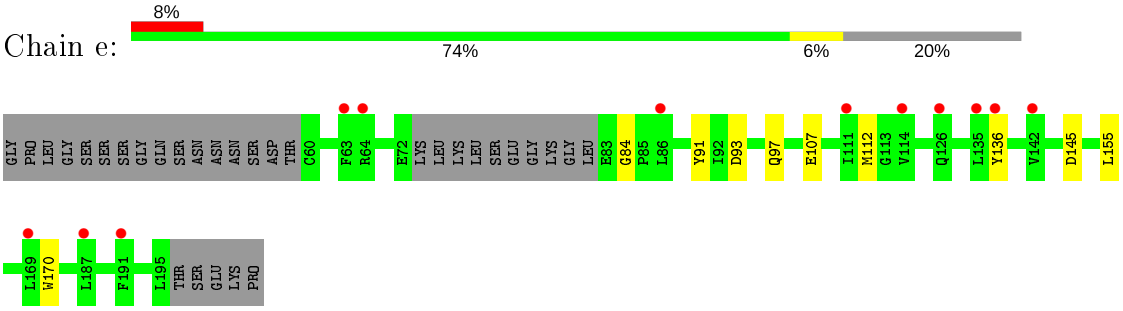
• Molecule 1: Integrin beta-1-binding protein 1

Chain c:



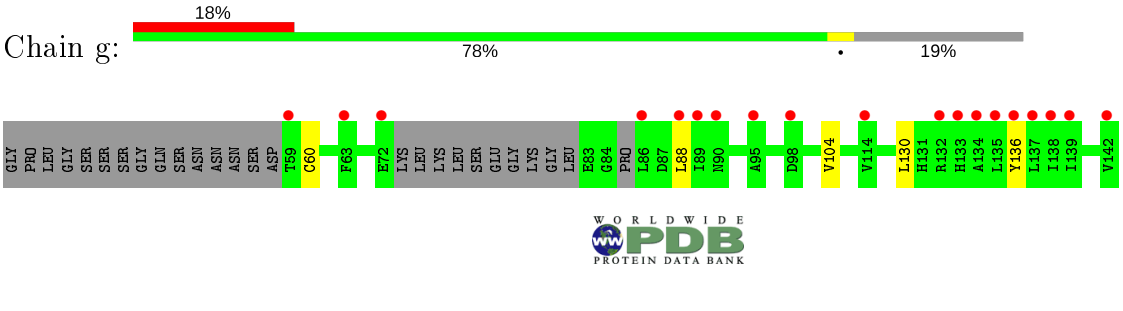
• Molecule 1: Integrin beta-1-binding protein 1

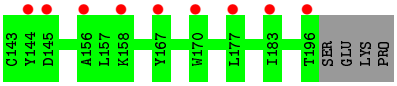
Chain e:



• Molecule 1: Integrin beta-1-binding protein 1

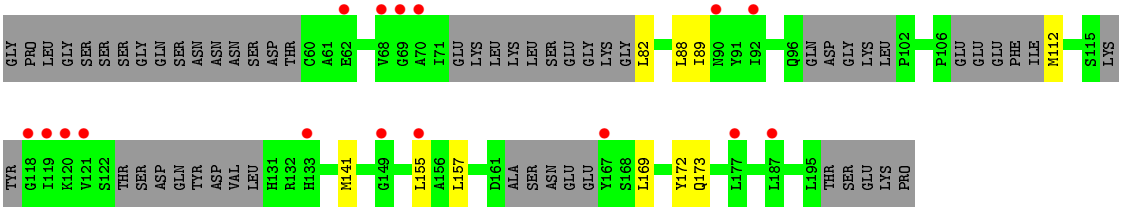
Chain g:





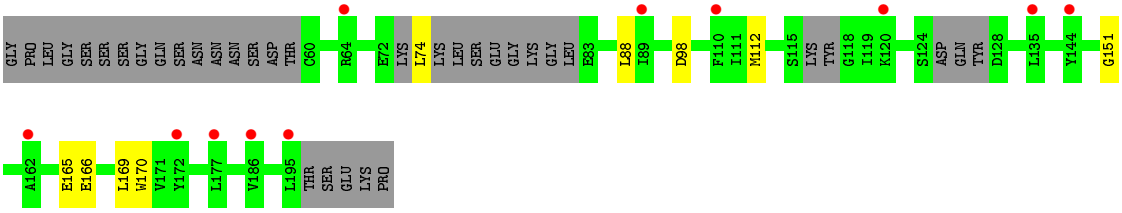
• Molecule 1: Integrin beta-1-binding protein 1

Chain i:



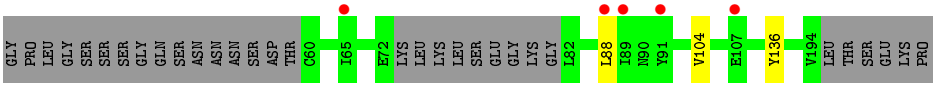
• Molecule 1: Integrin beta-1-binding protein 1

Chain Q:



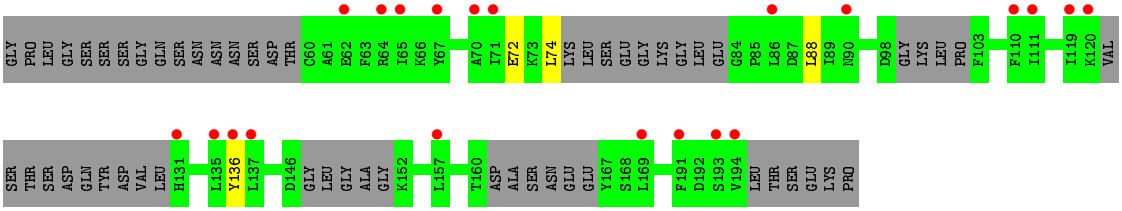
• Molecule 1: Integrin beta-1-binding protein 1

Chain S:



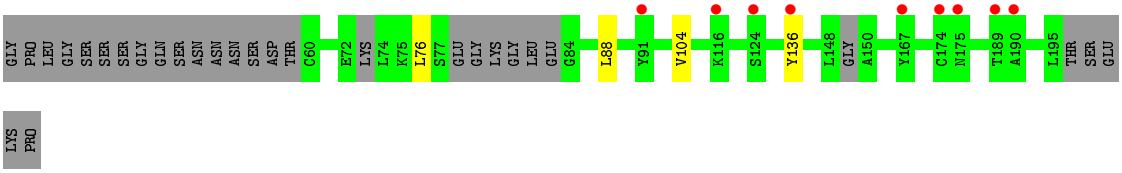
• Molecule 1: Integrin beta-1-binding protein 1

Chain U:

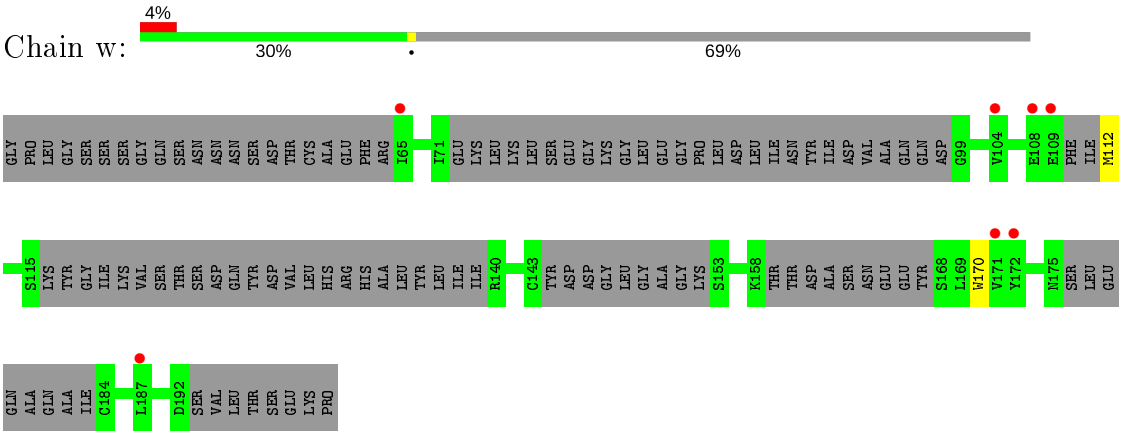


• Molecule 1: Integrin beta-1-binding protein 1

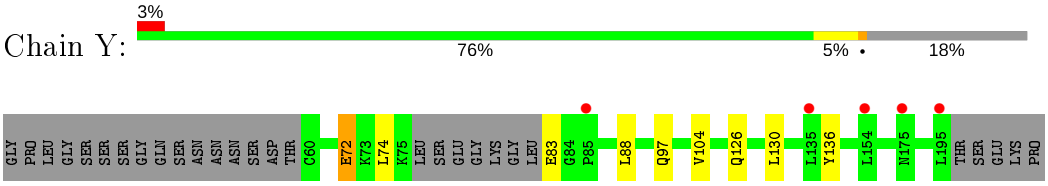
Chain W:



• Molecule 1: Integrin beta-1-binding protein 1

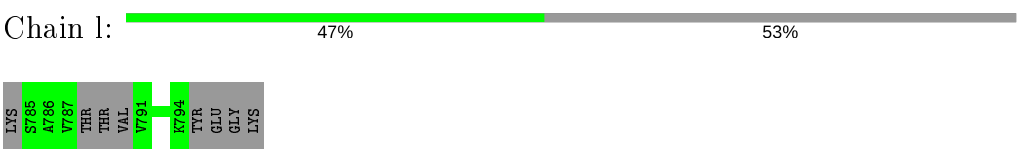


• Molecule 1: Integrin beta-1-binding protein 1



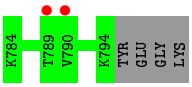
• Molecule 1: Integrin beta-1-binding protein 1

• Molecule 2: Integrin beta-1



• Molecule 2: Integrin beta-1

Chain n:

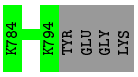


• Molecule 2: Integrin beta-1

Chain x:

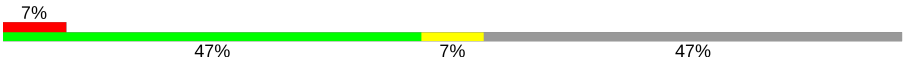
• Molecule 2: Integrin beta-1

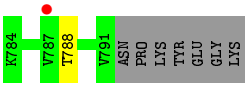
Chain D:



• Molecule 2: Integrin beta-1

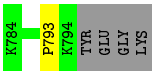
Chain 8:





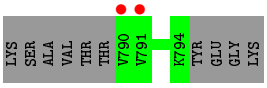
• Molecule 2: Integrin beta-1

Chain H:



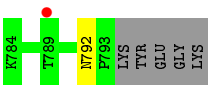
• Molecule 2: Integrin beta-1

Chain p:



• Molecule 2: Integrin beta-1

Chain B:

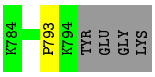


• Molecule 2: Integrin beta-1

Chain 9:

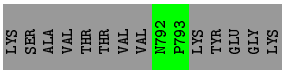
- Molecule 2: Integrin beta-1

Chain F:



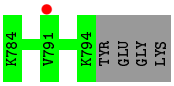
- Molecule 2: Integrin beta-1

Chain r:



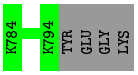
- Molecule 2: Integrin beta-1

Chain J:



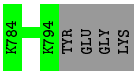
- Molecule 2: Integrin beta-1

Chain 7:



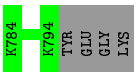
- Molecule 2: Integrin beta-1

Chain L:



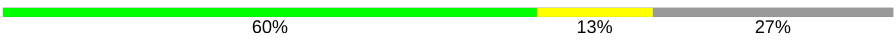
- Molecule 2: Integrin beta-1

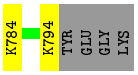
Chain 6:



- Molecule 2: Integrin beta-1

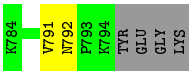
Chain N:





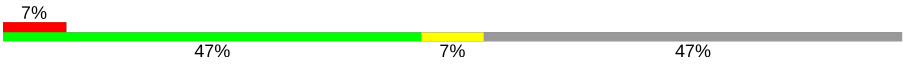
- Molecule 2: Integrin beta-1

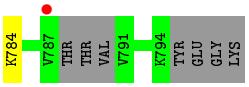
Chain P:



- Molecule 2: Integrin beta-1

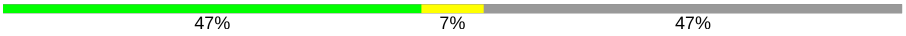
Chain t:

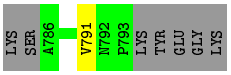




- Molecule 2: Integrin beta-1

Chain v:



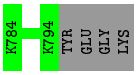


- Molecule 2: Integrin beta-1

Chain b:

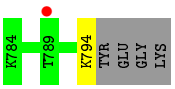
- Molecule 2: Integrin beta-1

Chain d:



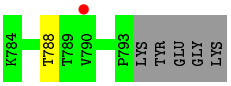
- Molecule 2: Integrin beta-1

Chain f:



- Molecule 2: Integrin beta-1

Chain h:

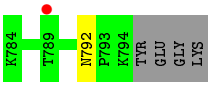


• Molecule 2: Integrin beta-1

Chain j:

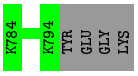
• Molecule 2: Integrin beta-1

Chain R:



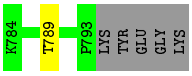
• Molecule 2: Integrin beta-1

Chain T:



• Molecule 2: Integrin beta-1

Chain V:

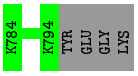


• Molecule 2: Integrin beta-1

Chain X:

• Molecule 2: Integrin beta-1

Chain Z:



• Molecule 2: Integrin beta-1

Chain z:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	75.62Å 122.21Å 135.27Å 89.97° 89.99° 108.11°	Depositor
Resolution (Å)	50.01 – 2.99 49.28 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.01-2.99) 97.1 (49.28-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.251 , 0.312 0.251 , 0.311	Depositor DCC
R_{free} test set	5828 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å^2)	67.0	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.458 for h,-h-k,-l 0.458 for -h,-k,l 0.458 for -h,h+k,-l	Xtriage
Reported twinning fraction	0.273 for H, K, L 0.239 for -h,-k,l 0.248 for h,-h-k,-l 0.239 for -H, H+K, -L	Depositor
Outliers	0 of 111606 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	29306	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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	0	0.40	1/869 (0.1%)	0.48	0/1168
1	1	0.39	0/933	0.47	0/1258
1	2	0.41	1/721 (0.1%)	0.45	0/966
1	3	0.40	1/820 (0.1%)	0.46	0/1100
1	4	0.38	0/1013	0.50	0/1366
1	5	0.39	0/1015	0.50	0/1371
1	A	0.40	1/856 (0.1%)	0.44	0/1149
1	C	0.42	1/1011 (0.1%)	0.54	0/1362
1	E	0.39	0/886	0.47	0/1192
1	G	0.38	0/1011	0.47	0/1366
1	I	0.40	0/995	0.50	0/1344
1	K	0.39	0/918	0.47	0/1236
1	M	0.40	0/984	0.50	1/1328 (0.1%)
1	O	0.38	0/821	0.51	0/1101
1	Q	0.38	1/956 (0.1%)	0.48	0/1287
1	S	0.37	0/1003	0.45	0/1355
1	U	0.55	1/821 (0.1%)	0.47	0/1100
1	W	0.38	0/1019	0.45	0/1373
1	Y	1.06	2/1029 (0.2%)	0.59	4/1388 (0.3%)
1	a	0.38	1/784 (0.1%)	0.46	0/1046
1	c	0.40	1/947 (0.1%)	0.46	0/1276
1	e	0.38	1/1003 (0.1%)	0.45	0/1355
1	g	0.38	0/1008	0.46	0/1360
1	i	0.40	0/788	0.49	0/1058
1	k	0.39	0/837	0.47	0/1122
1	m	0.38	1/1005 (0.1%)	0.47	0/1355
1	o	0.40	0/489	0.45	0/651
1	q	0.45	1/359 (0.3%)	0.46	0/472
1	s	0.39	0/823	0.45	0/1102
1	u	0.39	0/843	0.45	0/1134
1	w	0.45	1/379 (0.3%)	0.47	0/501
1	y	0.53	2/746 (0.3%)	0.45	0/1001
2	6	0.33	0/79	0.47	0/107
2	7	0.35	0/79	0.50	0/107

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	8	0.35	0/54	0.50	0/73
2	9	0.36	0/53	0.45	0/73
2	B	0.37	0/70	0.53	0/96
2	D	0.35	0/79	0.45	0/107
2	F	0.34	0/79	0.52	0/107
2	H	0.32	0/79	0.52	0/107
2	J	0.31	0/79	0.52	0/107
2	L	0.36	0/79	0.55	0/107
2	N	0.32	0/79	0.44	0/107
2	P	0.32	0/79	0.53	0/107
2	R	0.34	0/79	0.49	0/107
2	T	0.32	0/79	0.46	0/107
2	V	0.31	0/70	0.48	0/96
2	X	0.33	0/92	0.50	0/125
2	Z	0.32	0/79	0.45	0/107
2	b	0.33	0/70	0.43	0/96
2	d	0.31	0/79	0.50	0/107
2	f	0.32	0/79	0.47	0/107
2	h	0.35	0/70	0.46	0/96
2	j	0.38	0/26	0.37	0/33
2	l	0.32	0/48	0.40	0/63
2	n	0.31	0/79	0.48	0/107
2	p	0.37	0/38	0.44	0/51
2	r	0.48	0/15	0.40	0/20
2	t	0.36	0/57	0.54	0/74
2	v	0.34	0/55	0.48	0/77
2	x	0.48	0/24	0.45	0/32
2	z	0.42	0/36	0.41	0/50
All	All	0.44	17/29655 (0.1%)	0.48	5/39903 (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	Y	0	1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	72	GLU	CD-OE2	30.35	1.59	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	72	GLU	CD-OE1	10.66	1.37	1.25
1	Y	72	GLU	C-O	-8.52	1.07	1.23
1	y	173	GLN	CD-NE2	-7.73	1.13	1.32
1	y	173	GLN	CD-OE1	-7.25	1.07	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	72	GLU	OE1-CD-OE2	-6.96	114.95	123.30
1	Y	72	GLU	CA-C-N	6.70	131.94	117.20
1	Y	72	GLU	O-C-N	-6.16	112.84	122.70
1	Y	72	GLU	C-N-CA	-6.00	106.69	121.70
1	M	73	LYS	N-CA-C	5.61	126.14	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Y	72	GLU	Sidechain

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	0	100/157 (64%)	92 (92%)	7 (7%)	1 (1%)	15 53
1	1	112/157 (71%)	105 (94%)	7 (6%)	0	100 100
1	2	79/157 (50%)	74 (94%)	5 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	94/157 (60%)	88 (94%)	6 (6%)	0	100	100
1	4	122/157 (78%)	107 (88%)	15 (12%)	0	100	100
1	5	123/157 (78%)	115 (94%)	7 (6%)	1 (1%)	19	57
1	A	96/157 (61%)	88 (92%)	7 (7%)	1 (1%)	15	53
1	C	121/157 (77%)	103 (85%)	18 (15%)	0	100	100
1	E	103/157 (66%)	98 (95%)	5 (5%)	0	100	100
1	G	123/157 (78%)	115 (94%)	8 (6%)	0	100	100
1	I	121/157 (77%)	110 (91%)	11 (9%)	0	100	100
1	K	108/157 (69%)	95 (88%)	12 (11%)	1 (1%)	17	55
1	M	118/157 (75%)	113 (96%)	5 (4%)	0	100	100
1	O	90/157 (57%)	84 (93%)	6 (7%)	0	100	100
1	Q	113/157 (72%)	105 (93%)	6 (5%)	2 (2%)	8	37
1	S	122/157 (78%)	119 (98%)	3 (2%)	0	100	100
1	U	89/157 (57%)	88 (99%)	1 (1%)	0	100	100
1	W	120/157 (76%)	116 (97%)	4 (3%)	0	100	100
1	Y	125/157 (80%)	120 (96%)	4 (3%)	1 (1%)	19	57
1	a	85/157 (54%)	85 (100%)	0	0	100	100
1	c	112/157 (71%)	105 (94%)	7 (6%)	0	100	100
1	e	122/157 (78%)	114 (93%)	7 (6%)	1 (1%)	19	57
1	g	121/157 (77%)	117 (97%)	4 (3%)	0	100	100
1	i	87/157 (55%)	77 (88%)	10 (12%)	0	100	100
1	k	93/157 (59%)	92 (99%)	1 (1%)	0	100	100
1	m	121/157 (77%)	110 (91%)	11 (9%)	0	100	100
1	o	43/157 (27%)	41 (95%)	2 (5%)	0	100	100
1	q	31/157 (20%)	29 (94%)	2 (6%)	0	100	100
1	s	90/157 (57%)	86 (96%)	4 (4%)	0	100	100
1	u	100/157 (64%)	93 (93%)	7 (7%)	0	100	100
1	w	35/157 (22%)	31 (89%)	4 (11%)	0	100	100
1	y	81/157 (52%)	79 (98%)	2 (2%)	0	100	100
2	6	9/15 (60%)	9 (100%)	0	0	100	100
2	7	9/15 (60%)	7 (78%)	2 (22%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	8	6/15 (40%)	6 (100%)	0	0	100	100
2	9	6/15 (40%)	5 (83%)	1 (17%)	0	100	100
2	B	8/15 (53%)	7 (88%)	1 (12%)	0	100	100
2	D	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	F	9/15 (60%)	8 (89%)	0	1 (11%)	0	2
2	H	9/15 (60%)	7 (78%)	1 (11%)	1 (11%)	0	2
2	J	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	L	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	N	9/15 (60%)	9 (100%)	0	0	100	100
2	P	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	R	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	T	9/15 (60%)	7 (78%)	2 (22%)	0	100	100
2	V	8/15 (53%)	8 (100%)	0	0	100	100
2	X	10/15 (67%)	9 (90%)	1 (10%)	0	100	100
2	Z	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	b	8/15 (53%)	8 (100%)	0	0	100	100
2	d	9/15 (60%)	7 (78%)	2 (22%)	0	100	100
2	f	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	h	8/15 (53%)	8 (100%)	0	0	100	100
2	j	2/15 (13%)	2 (100%)	0	0	100	100
2	l	3/15 (20%)	3 (100%)	0	0	100	100
2	n	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	p	3/15 (20%)	3 (100%)	0	0	100	100
2	t	4/15 (27%)	3 (75%)	1 (25%)	0	100	100
2	v	6/15 (40%)	6 (100%)	0	0	100	100
2	x	2/15 (13%)	1 (50%)	1 (50%)	0	100	100
2	z	3/15 (20%)	2 (67%)	1 (33%)	0	100	100
All	All	3412/5459 (62%)	3183 (93%)	219 (6%)	10 (0%)	41	76

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	151	GLY

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Mol	Chain	Res	Type
1	K	107	GLU
1	5	116	LYS
1	Y	126	GLN
1	A	103	PHE

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	0	94/132 (71%)	92 (98%)	2 (2%)	53	82
1	1	100/132 (76%)	98 (98%)	2 (2%)	55	83
1	2	79/132 (60%)	75 (95%)	4 (5%)	24	60
1	3	88/132 (67%)	85 (97%)	3 (3%)	37	72
1	4	110/132 (83%)	106 (96%)	4 (4%)	35	70
1	5	110/132 (83%)	103 (94%)	7 (6%)	17	51
1	A	92/132 (70%)	88 (96%)	4 (4%)	29	66
1	C	109/132 (83%)	101 (93%)	8 (7%)	14	44
1	E	96/132 (73%)	92 (96%)	4 (4%)	30	66
1	G	109/132 (83%)	106 (97%)	3 (3%)	43	77
1	I	107/132 (81%)	102 (95%)	5 (5%)	26	63
1	K	98/132 (74%)	92 (94%)	6 (6%)	18	53
1	M	107/132 (81%)	101 (94%)	6 (6%)	21	56
1	O	89/132 (67%)	86 (97%)	3 (3%)	37	72
1	Q	104/132 (79%)	98 (94%)	6 (6%)	20	55
1	S	108/132 (82%)	105 (97%)	3 (3%)	43	77
1	U	89/132 (67%)	86 (97%)	3 (3%)	37	72
1	W	111/132 (84%)	107 (96%)	4 (4%)	35	70
1	Y	111/132 (84%)	105 (95%)	6 (5%)	22	57
1	a	84/132 (64%)	77 (92%)	7 (8%)	11	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	c	102/132 (77%)	96 (94%)	6 (6%)	19 54
1	e	108/132 (82%)	100 (93%)	8 (7%)	13 44
1	g	109/132 (83%)	104 (95%)	5 (5%)	27 64
1	i	85/132 (64%)	75 (88%)	10 (12%)	5 22
1	k	91/132 (69%)	85 (93%)	6 (7%)	16 49
1	m	109/132 (83%)	102 (94%)	7 (6%)	17 51
1	o	55/132 (42%)	55 (100%)	0	100 100
1	q	41/132 (31%)	41 (100%)	0	100 100
1	s	89/132 (67%)	86 (97%)	3 (3%)	37 72
1	u	89/132 (67%)	83 (93%)	6 (7%)	16 49
1	w	43/132 (33%)	42 (98%)	1 (2%)	50 80
1	y	83/132 (63%)	77 (93%)	6 (7%)	14 45
2	6	10/13 (77%)	10 (100%)	0	100 100
2	7	10/13 (77%)	10 (100%)	0	100 100
2	8	7/13 (54%)	6 (86%)	1 (14%)	3 15
2	9	7/13 (54%)	7 (100%)	0	100 100
2	B	9/13 (69%)	8 (89%)	1 (11%)	6 25
2	D	10/13 (77%)	10 (100%)	0	100 100
2	F	10/13 (77%)	10 (100%)	0	100 100
2	H	10/13 (77%)	10 (100%)	0	100 100
2	J	10/13 (77%)	10 (100%)	0	100 100
2	L	10/13 (77%)	10 (100%)	0	100 100
2	N	10/13 (77%)	8 (80%)	2 (20%)	1 7
2	P	10/13 (77%)	8 (80%)	2 (20%)	1 7
2	R	10/13 (77%)	9 (90%)	1 (10%)	7 29
2	T	10/13 (77%)	10 (100%)	0	100 100
2	V	9/13 (69%)	8 (89%)	1 (11%)	6 25
2	X	11/13 (85%)	10 (91%)	1 (9%)	9 34
2	Z	10/13 (77%)	10 (100%)	0	100 100
2	b	9/13 (69%)	9 (100%)	0	100 100
2	d	10/13 (77%)	10 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	f	10/13 (77%)	9 (90%)	1 (10%)	7 29
2	h	9/13 (69%)	8 (89%)	1 (11%)	6 25
2	j	3/13 (23%)	3 (100%)	0	100 100
2	l	6/13 (46%)	6 (100%)	0	100 100
2	n	10/13 (77%)	10 (100%)	0	100 100
2	p	5/13 (38%)	5 (100%)	0	100 100
2	r	2/13 (15%)	2 (100%)	0	100 100
2	t	7/13 (54%)	6 (86%)	1 (14%)	3 15
2	v	7/13 (54%)	6 (86%)	1 (14%)	3 15
2	x	3/13 (23%)	3 (100%)	0	100 100
2	z	5/13 (38%)	5 (100%)	0	100 100
All	All	3248/4614 (70%)	3087 (95%)	161 (5%)	24 60

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	136	TYR
2	t	784	LYS
2	X	784	LYS
2	N	794	LYS
1	a	88	LEU

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	C	90	ASN
1	Y	181	GLN
1	4	173	GLN
1	A	133	HIS
1	U	181	GLN

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

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	0	108/157 (68%)	0.26	5 (4%) 32 12	65, 77, 88, 97	0
1	1	116/157 (73%)	0.20	0 100 100	66, 72, 83, 91	0
1	2	89/157 (56%)	0.69	8 (8%) 9 3	76, 85, 94, 97	0
1	3	102/157 (64%)	0.58	12 (11%) 4 1	75, 91, 105, 110	0
1	4	127/157 (80%)	0.50	7 (5%) 25 9	58, 76, 87, 90	0
1	5	126/157 (80%)	0.29	0 100 100	55, 72, 82, 86	0
1	A	104/157 (66%)	0.26	4 (3%) 40 16	64, 77, 85, 90	0
1	C	125/157 (79%)	-0.07	0 100 100	46, 50, 56, 67	0
1	E	111/157 (70%)	0.18	2 (1%) 68 40	60, 73, 86, 95	0
1	G	125/157 (79%)	0.11	0 100 100	58, 67, 79, 91	0
1	I	123/157 (78%)	0.05	2 (1%) 72 44	49, 57, 66, 77	0
1	K	114/157 (72%)	0.11	1 (0%) 84 63	55, 70, 82, 85	0
1	M	122/157 (77%)	0.44	2 (1%) 72 44	64, 78, 92, 105	0
1	O	100/157 (63%)	0.66	10 (10%) 7 2	73, 97, 116, 124	0
1	Q	120/157 (76%)	0.56	11 (9%) 9 3	72, 94, 106, 113	0
1	S	124/157 (78%)	0.46	5 (4%) 38 15	71, 87, 101, 110	0
1	U	99/157 (63%)	1.21	21 (21%) 0 0	82, 116, 134, 149	0
1	W	126/157 (80%)	0.76	9 (7%) 16 5	67, 89, 106, 115	0
1	Y	127/157 (80%)	0.62	5 (3%) 39 15	67, 85, 107, 123	0
1	a	97/157 (61%)	1.36	27 (27%) 0 0	101, 119, 153, 158	0
1	c	118/157 (75%)	1.55	27 (22%) 0 0	91, 116, 149, 159	0
1	e	124/157 (78%)	0.72	12 (9%) 7 2	68, 92, 108, 116	0
1	g	125/157 (79%)	1.13	28 (22%) 0 0	87, 106, 120, 134	0
1	i	99/157 (63%)	0.73	16 (16%) 1 0	79, 105, 118, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	k	103/157 (65%)	1.07	22 (21%) 0 0	90, 110, 125, 131	0
1	m	125/157 (79%)	0.80	16 (12%) 3 1	75, 98, 110, 120	0
1	o	61/157 (38%)	1.58	19 (31%) 0 0	64, 112, 132, 147	0
1	q	45/157 (28%)	0.83	5 (11%) 5 1	73, 107, 121, 127	0
1	s	100/157 (63%)	1.26	21 (21%) 1 0	89, 112, 129, 134	0
1	u	104/157 (66%)	1.32	30 (28%) 0 0	88, 116, 139, 147	0
1	w	47/157 (29%)	0.91	7 (14%) 2 1	77, 107, 133, 139	0
1	y	91/157 (57%)	2.14	41 (45%) 0 0	106, 134, 155, 168	0
2	6	11/15 (73%)	0.03	0 100 100	72, 77, 82, 90	0
2	7	11/15 (73%)	-0.28	0 100 100	66, 72, 75, 75	0
2	8	8/15 (53%)	0.31	1 (12%) 3 1	68, 73, 79, 80	0
2	9	8/15 (53%)	0.04	0 100 100	64, 70, 78, 79	0
2	B	10/15 (66%)	0.63	1 (10%) 7 2	54, 69, 74, 75	0
2	D	11/15 (73%)	0.02	0 100 100	36, 38, 64, 71	0
2	F	11/15 (73%)	0.28	0 100 100	44, 65, 79, 80	0
2	H	11/15 (73%)	0.02	0 100 100	46, 54, 63, 63	0
2	J	11/15 (73%)	0.69	1 (9%) 9 3	78, 83, 104, 112	0
2	L	11/15 (73%)	-0.04	0 100 100	59, 64, 70, 72	0
2	N	11/15 (73%)	0.40	0 100 100	61, 66, 75, 80	0
2	P	11/15 (73%)	0.22	0 100 100	45, 70, 90, 92	0
2	R	11/15 (73%)	0.70	1 (9%) 9 3	75, 85, 102, 104	0
2	T	11/15 (73%)	0.13	0 100 100	80, 84, 87, 87	0
2	V	10/15 (66%)	0.47	0 100 100	67, 71, 92, 93	0
2	X	12/15 (80%)	0.33	0 100 100	64, 73, 80, 81	0
2	Z	11/15 (73%)	0.78	0 100 100	87, 90, 92, 93	0
2	b	10/15 (66%)	0.57	0 100 100	88, 100, 116, 117	0
2	d	11/15 (73%)	0.46	0 100 100	65, 90, 99, 101	0
2	f	11/15 (73%)	0.44	1 (9%) 9 3	73, 78, 81, 83	0
2	h	10/15 (66%)	0.80	1 (10%) 7 2	78, 88, 93, 94	0
2	j	4/15 (26%)	-0.01	0 100 100	90, 92, 92, 95	0
2	l	7/15 (46%)	0.03	0 100 100	72, 80, 99, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	n	11/15 (73%)	0.65	2 (18%) 1 0	89, 92, 94, 95	0
2	p	5/15 (33%)	1.11	2 (40%) 0 0	111, 117, 118, 121	0
2	r	2/15 (13%)	-0.09	0 100 100	76, 76, 76, 82	0
2	t	8/15 (53%)	0.04	1 (12%) 3 1	53, 57, 92, 94	0
2	v	8/15 (53%)	0.46	0 100 100	80, 88, 104, 104	0
2	x	4/15 (26%)	0.46	0 100 100	74, 78, 80, 83	0
2	z	5/15 (33%)	0.58	0 100 100	99, 102, 108, 109	0
All	All	3703/5474 (67%)	0.66	386 (10%) 6 2	36, 87, 129, 168	0

The worst 5 of 386 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	c	60	CYS	22.8
1	a	70	ALA	12.6
1	y	70	ALA	11.6
1	y	169	LEU	11.3
1	c	109	GLU	9.5

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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.