



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 10:07 AM EDT

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 Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
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) : 2.37.1

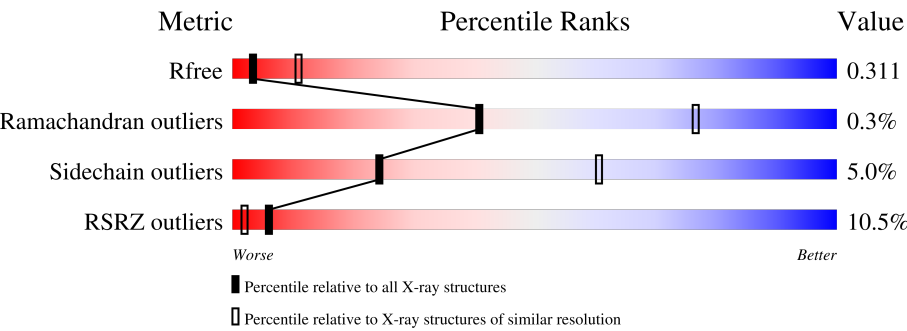
# 1 Overall quality at a glance i

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.











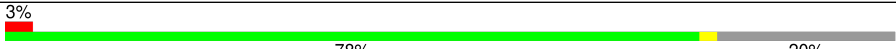

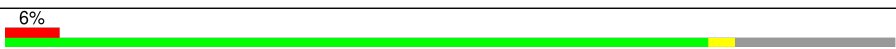




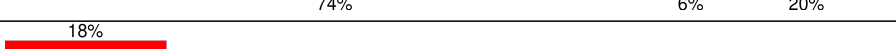
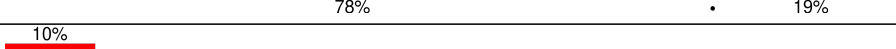

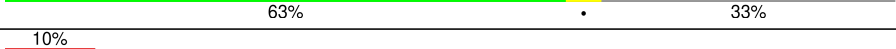




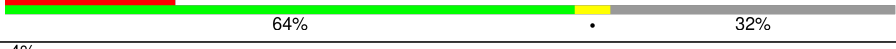

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	0	157	
1	1	157	
1	2	157	
1	3	157	
1	4	157	
1	5	157	
1	A	157	



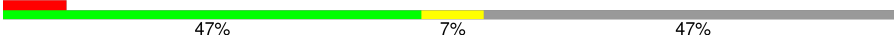






















Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	6	15	
2	7	15	
2	8	15	
2	9	15	
2	B	15	
2	D	15	
2	F	15	
2	H	15	
2	J	15	
2	L	15	
2	N	15	
2	P	15	
2	R	15	
2	T	15	
2	V	15	
2	X	15	
2	Z	15	
2	b	15	
2	d	15	
2	f	15	
2	h	15	
2	j	15	
2	l	15	
2	n	15	
2	p	15	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	r	15	<div><div></div><div>13%87%</div></div>
2	t	15	<div><div></div><div>7%47%7%47%</div></div>
2	v	15	<div><div></div><div>47%7%47%</div></div>
2	x	15	<div><div></div><div>27%73%</div></div>
2	z	15	<div><div></div><div>33%67%</div></div>

## 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			

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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			

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

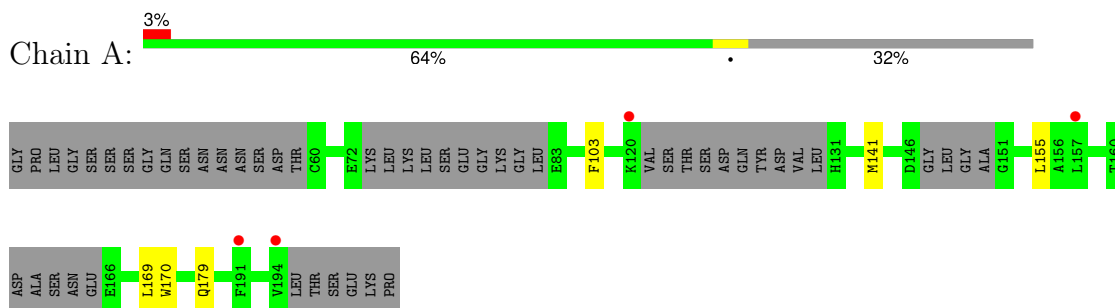
*Continued from previous page...*

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			

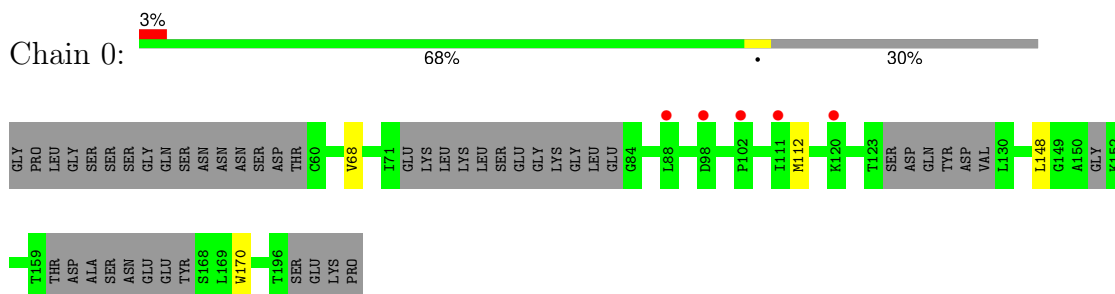
### 3 Residue-property plots [i](#)

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.

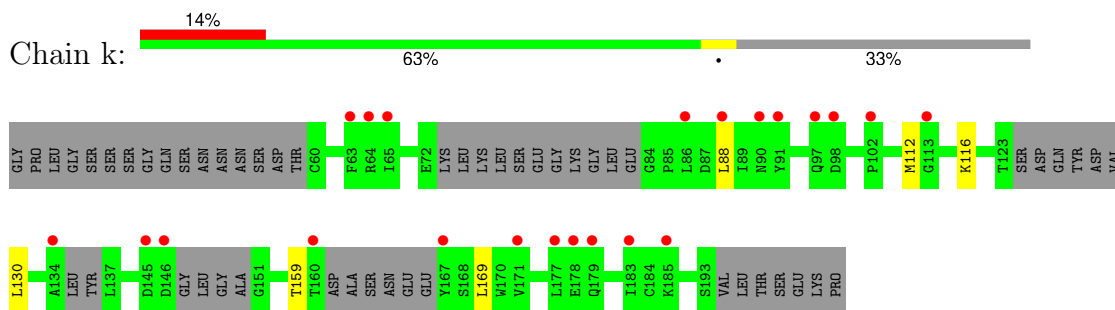
- Molecule 1: Integrin beta-1-binding protein 1



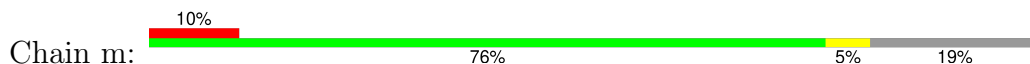
- Molecule 1: Integrin beta-1-binding protein 1

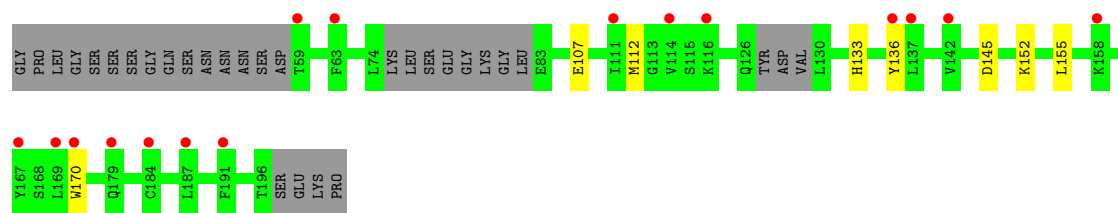


- Molecule 1: Integrin beta-1-binding protein 1



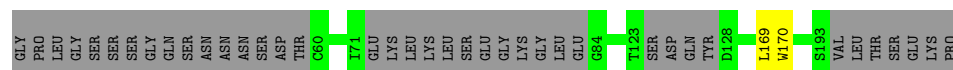
- Molecule 1: Integrin beta-1-binding protein 1





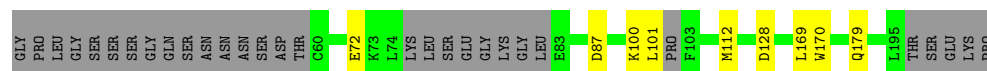
- Molecule 1: Integrin beta-1-binding protein 1

Chain 1: 74% 25%



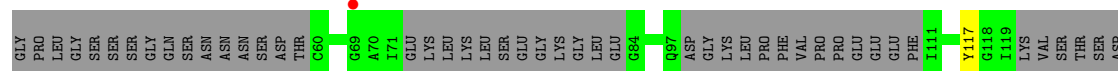
- Molecule 1: Integrin beta-1-binding protein 1

Chain C: 75% 6% 19%



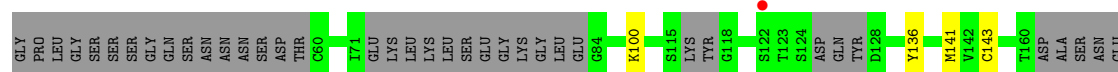
- Molecule 1: Integrin beta-1-binding protein 1

Chain 2: 5% 55% 42%



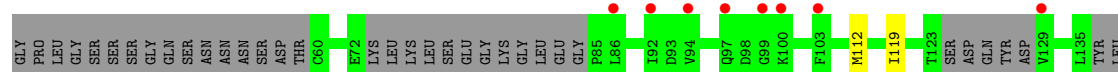
- Molecule 1: Integrin beta-1-binding protein 1

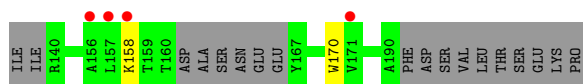
Chain E: 69% 28%



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

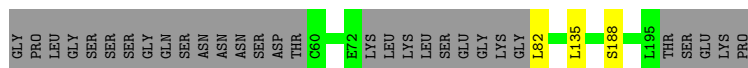
Chain 3: 8% 64% 34%





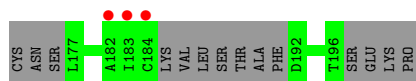
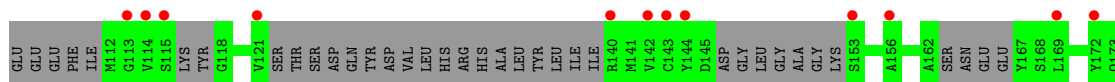
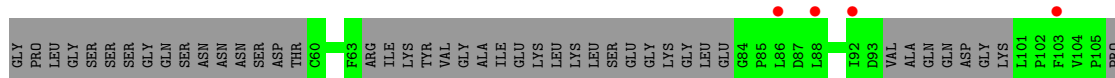
- Molecule 1: Integrin beta-1-binding protein 1

Chain G: 79% 19%



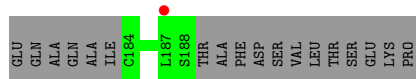
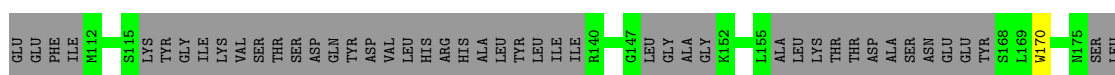
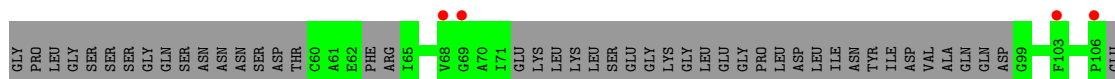
- Molecule 1: Integrin beta-1-binding protein 1

Chain o: 12% 40% 60%



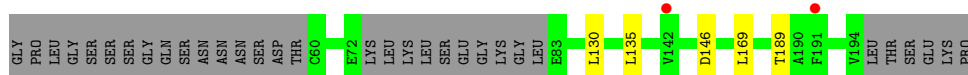
- Molecule 1: Integrin beta-1-binding protein 1

Chain q: 3% 29% 70%



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

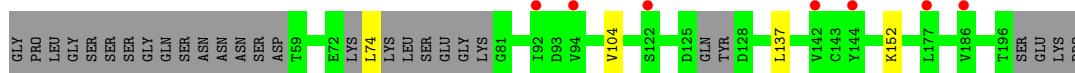
Chain I: 76% 20%



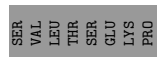
- Molecule 1: Integrin beta-1-binding protein 1

Chain 4: 4% 80% 18%

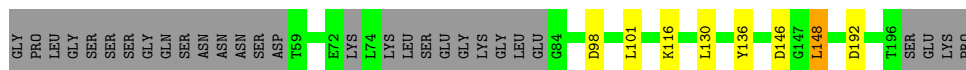




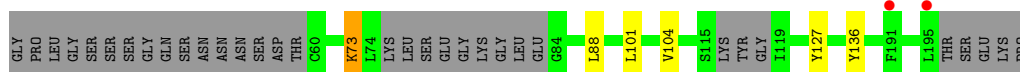
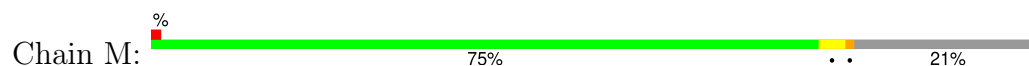
- Molecule 1: Integrin beta-1-binding protein 1



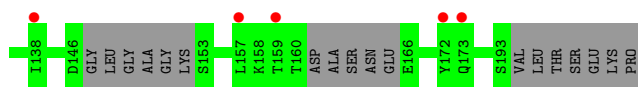
- Molecule 1: Integrin beta-1-binding protein 1



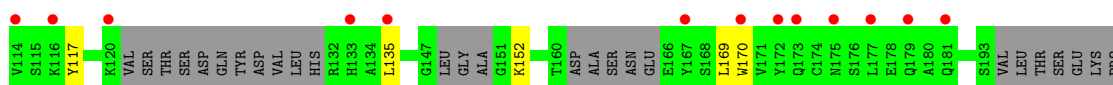
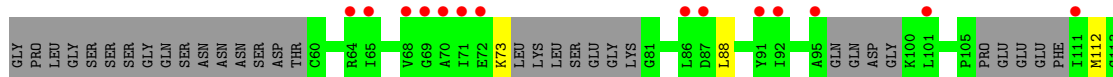
- Molecule 1: Integrin beta-1-binding protein 1



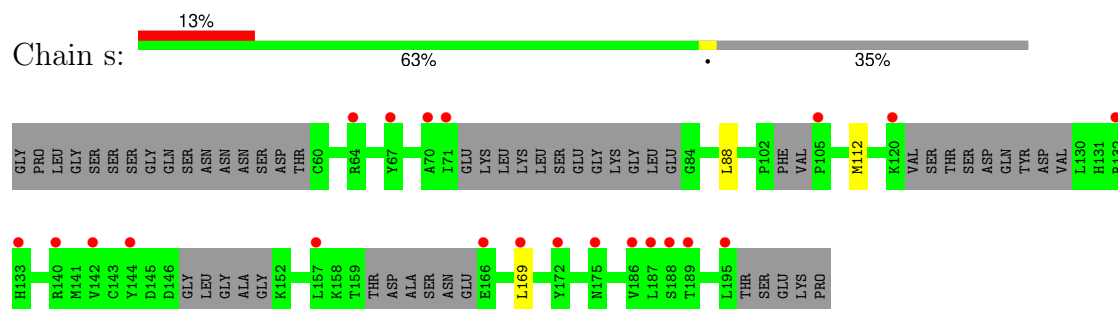
- Molecule 1: Integrin beta-1-binding protein 1



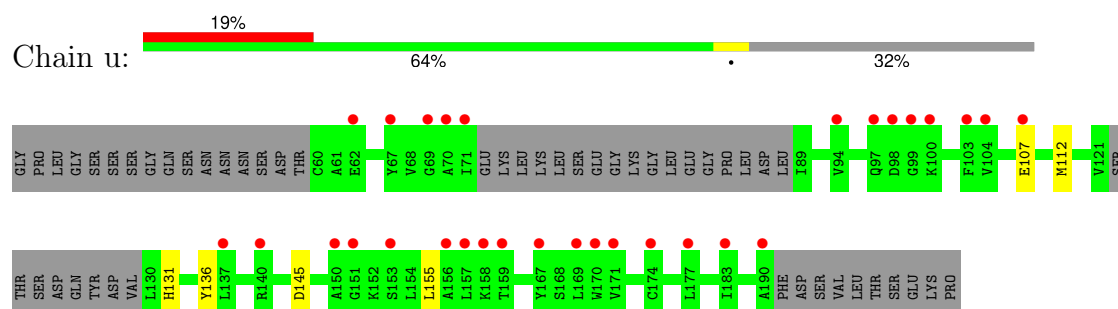
- Molecule 1: Integrin beta-1-binding protein 1



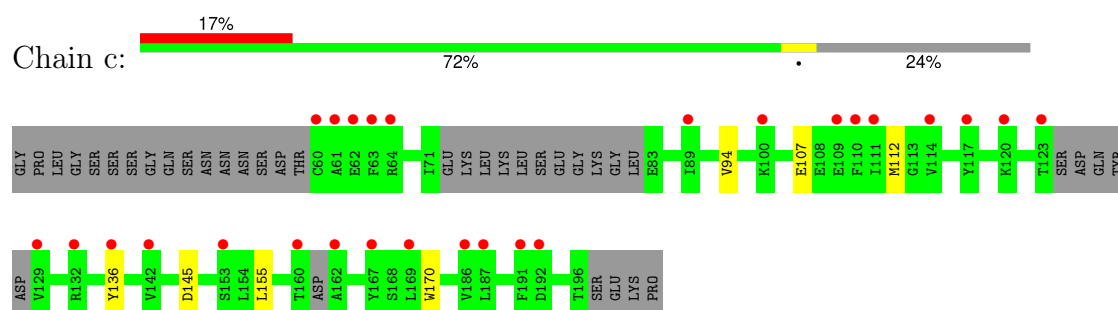
- Molecule 1: Integrin beta-1-binding protein 1



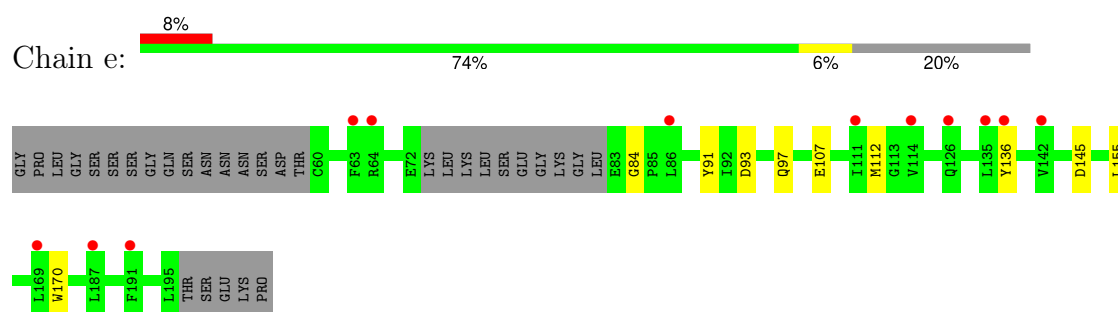
- Molecule 1: Integrin beta-1-binding protein 1



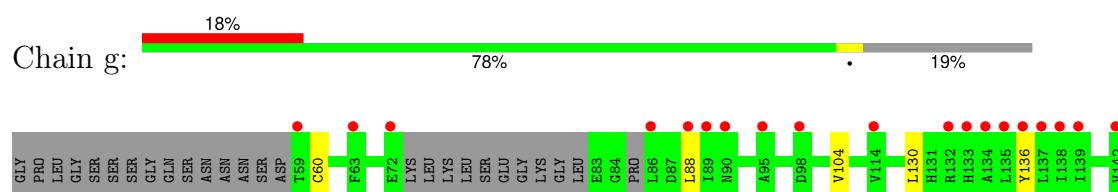
- Molecule 1: Integrin beta-1-binding protein 1

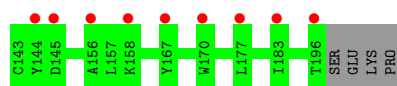


- Molecule 1: Integrin beta-1-binding protein 1

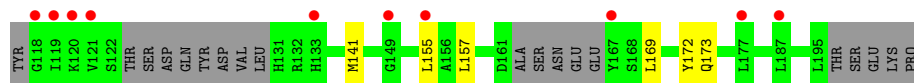
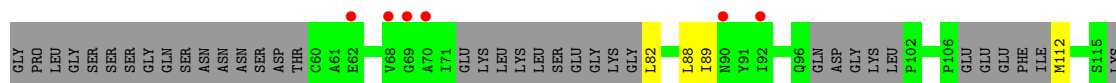


- Molecule 1: Integrin beta-1-binding protein 1

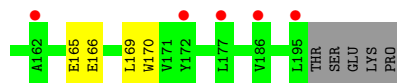
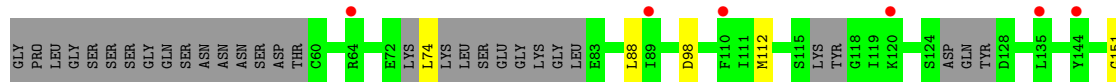
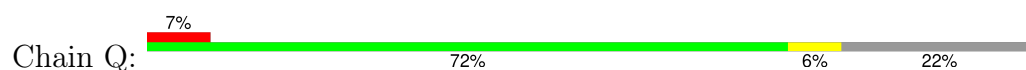




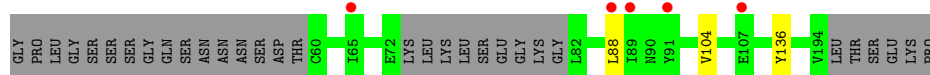
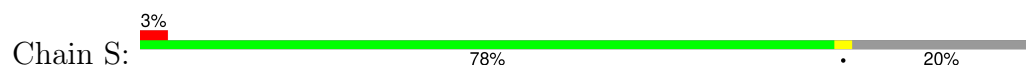
• Molecule 1: Integrin beta-1-binding protein 1



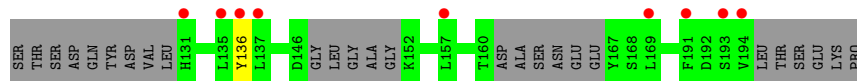
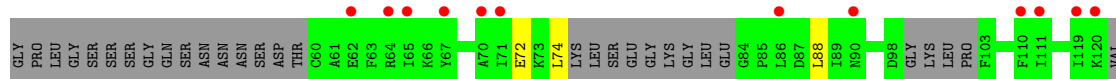
• Molecule 1: Integrin beta-1-binding protein 1



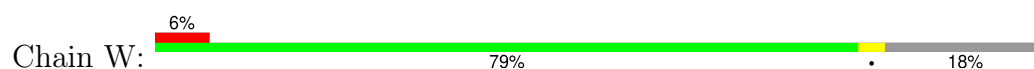
• Molecule 1: Integrin beta-1-binding protein 1

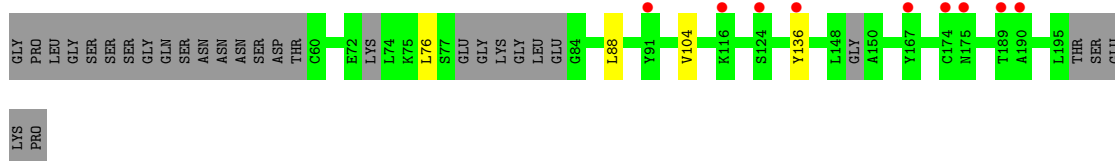


• Molecule 1: Integrin beta-1-binding protein 1



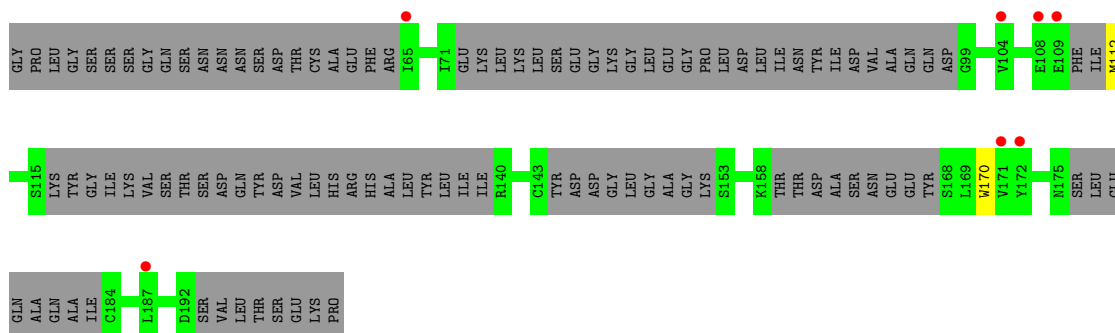
• Molecule 1: Integrin beta-1-binding protein 1





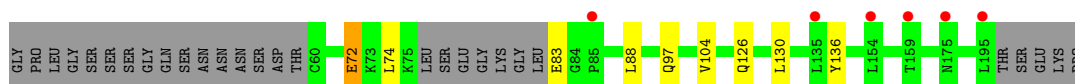
- Molecule 1: Integrin beta-1-binding protein 1

Chain w: 4% 30% 69%



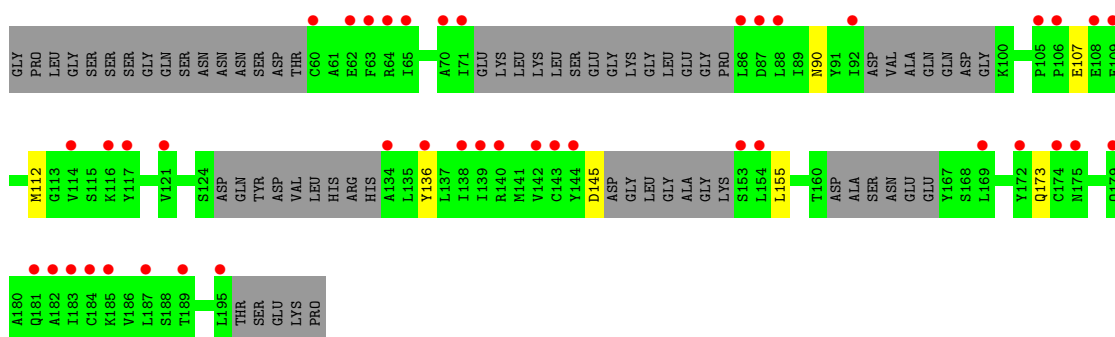
- Molecule 1: Integrin beta-1-binding protein 1

Chain Y: 4% 76% 5% 18%



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

Chain y: 27% 55% 41%

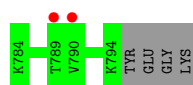
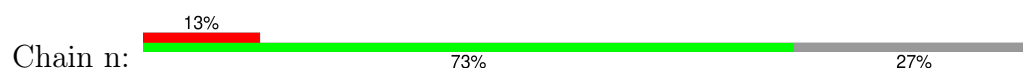


- Molecule 2: Integrin beta-1

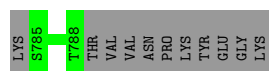
Chain l: 47% 53%



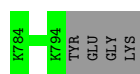
- Molecule 2: Integrin beta-1



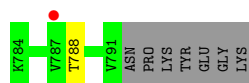
- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1



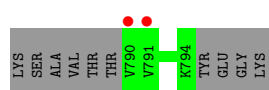
- Molecule 2: Integrin beta-1



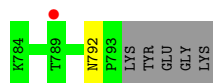
- Molecule 2: Integrin beta-1




- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1

Chain 9:  53% 47%



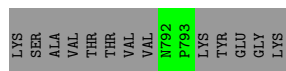
• Molecule 2: Integrin beta-1

Chain F:  67% 7% 27%



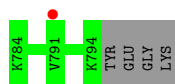
• Molecule 2: Integrin beta-1

Chain r:  13% 87%



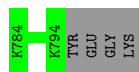
• Molecule 2: Integrin beta-1

Chain J:  7% 73% 27%



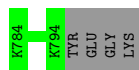
• Molecule 2: Integrin beta-1

Chain 7:  73% 27%



• Molecule 2: Integrin beta-1

Chain L:  73% 27%



• Molecule 2: Integrin beta-1

Chain 6:  73% 27%



• Molecule 2: Integrin beta-1

Chain N:  60% 13% 27%



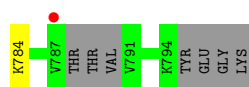
• Molecule 2: Integrin beta-1

Chain P:  60% 13% 27%



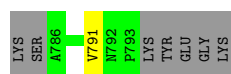
• Molecule 2: Integrin beta-1

Chain t:  7% 47% 7% 47%



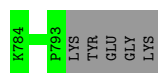
• Molecule 2: Integrin beta-1

Chain v:  47% 7% 47%



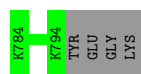
• Molecule 2: Integrin beta-1

Chain b:  67% 33%



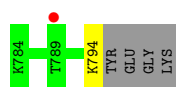
• Molecule 2: Integrin beta-1

Chain d:  73% 27%

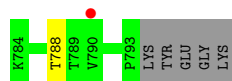


• Molecule 2: Integrin beta-1

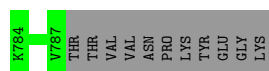
Chain f:  7% 67% 7% 27%



• Molecule 2: Integrin beta-1



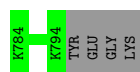
- Molecule 2: Integrin beta-1



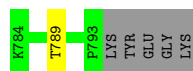
- Molecule 2: Integrin beta-1



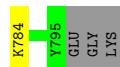
- Molecule 2: Integrin beta-1



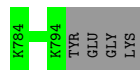
- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1





LYS	LYS
SER	LYS
ALA	TYR
VAL	GLU
THR	GLY
T789	LYS
T793	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	67.0	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	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 <sup>2</sup> )	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.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

All (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

*Continued on next page...*

*Continued from previous page...*

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
1	C	170	TRP	CD2-CE2	5.08	1.47	1.41
1	q	170	TRP	CD2-CE2	5.06	1.47	1.41
1	a	170	TRP	CD2-CE2	5.06	1.47	1.41
1	A	170	TRP	CD2-CE2	5.05	1.47	1.41
1	3	170	TRP	CD2-CE2	5.05	1.47	1.41
1	Q	170	TRP	CD2-CE2	5.02	1.47	1.41
1	m	170	TRP	CD2-CE2	5.02	1.47	1.41
1	2	170	TRP	CD2-CE2	5.02	1.47	1.41
1	w	170	TRP	CD2-CE2	5.02	1.47	1.41
1	0	170	TRP	CD2-CE2	5.01	1.47	1.41
1	c	170	TRP	CD2-CE2	5.01	1.47	1.41
1	e	170	TRP	CD2-CE2	5.01	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 [i](#)

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
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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	151	GLY
1	K	107	GLU
1	5	116	LYS
1	Y	126	GLN
1	A	103	PHE
1	0	68	VAL
1	Q	98	ASP
2	H	793	PRO
1	e	84	GLY
2	F	793	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	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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	MSE
1	A	155	LEU
1	A	169	LEU
1	A	179	GLN
1	0	112	MSE

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	0	148	LEU
1	k	88	LEU
1	k	112	MSE
1	k	116	LYS
1	k	130	LEU
1	k	159	THR
1	k	169	LEU
1	m	107	GLU
1	m	112	MSE
1	m	133	HIS
1	m	136	TYR
1	m	145	ASP
1	m	152	LYS
1	m	155	LEU
1	1	169	LEU
1	1	170	TRP
1	C	72	GLU
1	C	87	ASP
1	C	100	LYS
1	C	101	LEU
1	C	112	MSE
1	C	128	ASP
1	C	169	LEU
1	C	179	GLN
1	2	117	TYR
1	2	130	LEU
1	2	135	LEU
1	2	141	MSE
1	E	100	LYS
1	E	136	TYR
1	E	141	MSE
1	E	143	CYS
1	3	112	MSE
1	3	119	ILE
1	3	158	LYS
1	G	82	LEU
1	G	135	LEU
1	G	188	SER
2	8	788	THR
2	B	792	ASN
1	I	130	LEU
1	I	135	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	I	146	ASP
1	I	169	LEU
1	I	189	THR
1	4	74	LEU
1	4	104	VAL
1	4	137	LEU
1	4	152	LYS
1	K	98	ASP
1	K	112	MSE
1	K	140	ARG
1	K	141	MSE
1	K	155	LEU
1	K	157	LEU
1	5	98	ASP
1	5	101	LEU
1	5	130	LEU
1	5	136	TYR
1	5	146	ASP
1	5	148	LEU
1	5	192	ASP
1	M	73	LYS
1	M	88	LEU
1	M	101	LEU
1	M	104	VAL
1	M	127	TYR
1	M	136	TYR
2	N	784	LYS
2	N	794	LYS
1	O	65	ILE
1	O	96	GLN
1	O	111	ILE
2	P	791	VAL
2	P	792	ASN
1	a	73	LYS
1	a	88	LEU
1	a	112	MSE
1	a	117	TYR
1	a	135	LEU
1	a	152	LYS
1	a	169	LEU
1	s	88	LEU
1	s	112	MSE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	s	169	LEU
2	t	784	LYS
1	u	107	GLU
1	u	112	MSE
1	u	131	HIS
1	u	136	TYR
1	u	145	ASP
1	u	155	LEU
2	v	791	VAL
1	c	94	VAL
1	c	107	GLU
1	c	112	MSE
1	c	136	TYR
1	c	145	ASP
1	c	155	LEU
1	e	91	TYR
1	e	93	ASP
1	e	97	GLN
1	e	107	GLU
1	e	112	MSE
1	e	136	TYR
1	e	145	ASP
1	e	155	LEU
2	f	794	LYS
1	g	60	CYS
1	g	88	LEU
1	g	104	VAL
1	g	130	LEU
1	g	136	TYR
2	h	788	THR
1	i	82	LEU
1	i	88	LEU
1	i	89	ILE
1	i	112	MSE
1	i	141	MSE
1	i	155	LEU
1	i	157	LEU
1	i	169	LEU
1	i	172	TYR
1	i	173	GLN
1	Q	74	LEU
1	Q	88	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	Q	112	MSE
1	Q	165	GLU
1	Q	166	GLU
1	Q	169	LEU
2	R	792	ASN
1	S	88	LEU
1	S	104	VAL
1	S	136	TYR
1	U	74	LEU
1	U	88	LEU
1	U	136	TYR
2	V	789	THR
1	W	76	LEU
1	W	88	LEU
1	W	104	VAL
1	W	136	TYR
1	w	112	MSE
2	X	784	LYS
1	Y	74	LEU
1	Y	83	GLU
1	Y	88	LEU
1	Y	104	VAL
1	Y	130	LEU
1	Y	136	TYR
1	y	90	ASN
1	y	107	GLU
1	y	112	MSE
1	y	136	TYR
1	y	145	ASP
1	y	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	133	HIS
1	C	90	ASN
1	4	173	GLN
1	U	181	GLN
1	Y	181	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	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%)	0.70	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%)	1.22	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	6 (4%) 31 11	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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	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	42 (46%) 0 0	106, 134, 155, 168	0
2	6	11/15 (73%)	0.02	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%)	0.64	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%)	0.79	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%)	0.45	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

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	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	388 (10%) 6 2	36, 87, 129, 168	0

All (388) 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
1	c	110	PHE	8.8
1	u	70	ALA	8.5
1	U	194	VAL	8.5
1	o	142	VAL	8.5
1	c	132	ARG	8.3
1	y	92	ILE	7.8
1	k	178	GLU	7.3
1	o	121	VAL	7.1
1	4	142	VAL	7.1
1	M	195	LEU	7.0
1	u	100	LYS	6.8
1	k	91	TYR	6.7
1	U	70	ALA	6.4
1	m	142	VAL	6.4
1	W	167	TYR	6.3
1	c	117	TYR	6.0
1	y	62	GLU	5.9
1	g	139	ILE	5.9
1	y	142	VAL	5.9
1	s	187	LEU	5.8
1	i	69	GLY	5.7
1	s	188	SER	5.7
1	Y	195	LEU	5.7

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	s	70	ALA	5.6
1	u	170	TRP	5.6
1	y	105	PRO	5.6
1	a	86	LEU	5.6
1	W	136	TYR	5.6
1	y	88	LEU	5.4
1	m	167	TYR	5.4
1	g	138	ILE	5.4
1	U	120	LYS	5.3
1	q	68	VAL	5.3
1	w	187	LEU	5.2
1	c	111	ILE	5.2
1	W	91	TYR	5.1
1	o	144	TYR	5.1
1	u	103	PHE	5.1
1	c	61	ALA	5.0
1	w	104	VAL	5.0
1	o	114	VAL	5.0
1	a	175	ASN	4.9
1	a	111	ILE	4.8
1	o	140	ARG	4.8
1	i	120	LYS	4.8
1	s	133	HIS	4.8
1	a	65	ILE	4.7
1	k	64	ARG	4.7
1	y	136	TYR	4.7
1	0	111	ILE	4.7
1	3	100	LYS	4.6
1	u	157	LEU	4.6
1	g	144	TYR	4.6
1	3	99	GLY	4.6
1	s	142	VAL	4.6
1	g	134	ALA	4.6
1	c	64	ARG	4.6
1	2	69	GLY	4.6
1	W	174	CYS	4.5
1	2	142	VAL	4.5
1	k	179	GLN	4.5
1	o	184	CYS	4.5
1	a	92	ILE	4.4
1	2	191	PHE	4.4
1	s	195	LEU	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	W	124	SER	4.3
1	i	177	LEU	4.3
1	y	71	ILE	4.3
1	w	109	GLU	4.3
1	o	92	ILE	4.3
1	o	143	CYS	4.2
1	y	64	ARG	4.2
1	y	106	PRO	4.2
1	g	135	LEU	4.2
1	g	167	TYR	4.2
1	a	167	TYR	4.1
1	u	177	LEU	4.1
1	u	69	GLY	4.1
2	R	789	THR	4.1
1	o	183	ILE	4.1
1	u	158	LYS	4.1
1	u	153	SER	4.0
1	i	149	GLY	4.0
1	2	187	LEU	4.0
1	Q	135	LEU	4.0
1	g	59	THR	4.0
1	U	193	SER	4.0
1	g	89	ILE	3.9
1	a	71	ILE	3.9
1	a	72	GLU	3.9
1	m	137	LEU	3.9
1	y	154	LEU	3.9
1	g	158	LYS	3.9
1	g	133	HIS	3.9
1	i	133	HIS	3.9
1	u	97	GLN	3.9
1	k	134	ALA	3.9
1	y	108	GLU	3.9
1	k	167	TYR	3.8
1	a	91	TYR	3.8
1	o	169	LEU	3.8
1	O	159	THR	3.8
1	y	187	LEU	3.8
1	O	172	TYR	3.8
1	a	120	LYS	3.8
2	B	789	THR	3.7
1	Q	89	ILE	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	y	139	ILE	3.7
1	g	170	TRP	3.7
1	c	191	PHE	3.7
1	U	65	ILE	3.7
1	m	116	LYS	3.6
1	u	171	VAL	3.6
1	e	136	TYR	3.6
1	k	63	PHE	3.6
1	y	116	LYS	3.6
1	u	62	GLU	3.6
1	2	155	LEU	3.6
1	u	151	GLY	3.6
1	s	67	TYR	3.6
1	3	156	ALA	3.6
1	k	113	GLY	3.6
1	c	136	TYR	3.6
1	a	173	GLN	3.5
1	s	71	ILE	3.5
1	s	132	ARG	3.5
1	O	138	ILE	3.5
1	w	108	GLU	3.5
1	O	92	ILE	3.5
1	e	111	ILE	3.5
1	g	142	VAL	3.5
1	y	63	PHE	3.5
1	k	65	ILE	3.5
1	i	70	ALA	3.5
1	Q	162	ALA	3.5
1	o	172	TYR	3.4
1	U	135	LEU	3.4
1	c	63	PHE	3.4
1	W	175	ASN	3.4
1	y	140	ARG	3.4
1	a	133	HIS	3.4
1	i	121	VAL	3.4
1	y	134	ALA	3.4
1	c	129	VAL	3.4
1	u	67	TYR	3.4
1	a	68	VAL	3.3
1	s	64	ARG	3.3
1	g	196	THR	3.3
1	y	189	THR	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	a	95	ALA	3.3
1	u	104	VAL	3.3
1	m	136	TYR	3.3
1	U	136	TYR	3.3
1	y	153	SER	3.3
1	Q	195	LEU	3.3
1	y	172	TYR	3.3
1	y	174	CYS	3.3
1	y	65	ILE	3.3
1	U	67	TYR	3.2
1	2	182	ALA	3.2
1	s	144	TYR	3.2
1	e	63	PHE	3.2
1	4	94	VAL	3.2
1	g	136	TYR	3.2
1	u	174	CYS	3.1
1	i	155	LEU	3.1
1	m	111	ILE	3.1
1	y	121	VAL	3.1
1	k	160	THR	3.1
1	c	167	TYR	3.1
1	c	120	LYS	3.1
1	g	183	ILE	3.1
1	c	162	ALA	3.1
1	4	177	LEU	3.1
1	m	114	VAL	3.1
1	y	143	CYS	3.1
1	g	63	PHE	3.1
1	O	71	ILE	3.1
1	m	63	PHE	3.1
1	3	92	ILE	3.1
1	i	119	ILE	3.0
1	y	86	LEU	3.0
1	a	170	TRP	3.0
1	g	137	LEU	3.0
1	U	71	ILE	3.0
1	Q	172	TYR	3.0
1	3	129	VAL	3.0
1	g	114	VAL	3.0
1	a	101	LEU	3.0
1	w	65	ILE	3.0
1	k	88	LEU	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	o	86	LEU	2.9
1	m	59	THR	2.9
1	a	177	LEU	2.9
1	e	187	LEU	2.9
1	U	119	ILE	2.9
1	a	114	VAL	2.9
1	c	123	THR	2.9
1	e	114	VAL	2.9
1	o	88	LEU	2.9
1	O	86	LEU	2.9
1	4	92	ILE	2.9
1	w	171	VAL	2.9
1	o	115	SER	2.9
1	Y	85	PRO	2.8
1	3	94	VAL	2.8
1	s	186	VAL	2.8
1	q	106	PRO	2.8
1	O	173	GLN	2.8
1	U	131	HIS	2.8
1	u	137	LEU	2.8
1	S	91	TYR	2.8
1	m	179	GLN	2.8
1	g	132	ARG	2.8
1	a	172	TYR	2.8
2	p	791	VAL	2.8
1	s	120	LYS	2.8
1	e	191	PHE	2.8
1	U	191	PHE	2.8
1	q	69	GLY	2.7
1	O	70	ALA	2.7
1	g	156	ALA	2.7
1	g	90	ASN	2.7
1	u	156	ALA	2.7
1	m	184	CYS	2.7
1	s	157	LEU	2.7
1	o	153	SER	2.7
1	3	97	GLN	2.7
1	S	107	GLU	2.6
1	e	86	LEU	2.6
1	Q	120	LYS	2.6
1	c	114	VAL	2.6
1	c	62	GLU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	62	GLU	2.6
1	i	167	TYR	2.6
1	e	142	VAL	2.6
1	e	126	GLN	2.6
1	S	89	ILE	2.6
1	Q	64	ARG	2.6
1	c	192	ASP	2.6
1	g	98	ASP	2.6
1	E	122	SER	2.6
2	n	790	VAL	2.6
2	p	790	VAL	2.6
1	Q	110	PHE	2.6
1	u	169	LEU	2.6
1	c	187	LEU	2.6
1	S	88	LEU	2.6
1	A	157	LEU	2.6
1	m	169	LEU	2.6
1	u	94	VAL	2.6
1	2	144	TYR	2.6
1	a	64	ARG	2.6
1	u	159	THR	2.5
1	U	137	LEU	2.5
1	a	116	LYS	2.5
1	k	86	LEU	2.5
1	A	120	LYS	2.5
2	J	791	VAL	2.5
1	c	153	SER	2.5
1	a	179	GLN	2.5
1	S	65	ILE	2.5
1	U	90	ASN	2.5
1	g	86	LEU	2.5
1	c	160	THR	2.5
1	k	185	LYS	2.5
1	y	182	ALA	2.5
1	a	69	GLY	2.5
1	q	187	LEU	2.5
1	u	98	ASP	2.5
1	c	89	ILE	2.5
1	m	158	LYS	2.5
1	i	118	GLY	2.5
1	u	71	ILE	2.5
1	c	100	LYS	2.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	y	185	LYS	2.5
1	M	191	PHE	2.5
1	o	113	GLY	2.5
1	o	182	ALA	2.5
1	k	146	ASP	2.5
1	y	87	ASP	2.5
1	E	186	VAL	2.4
1	I	191	PHE	2.4
1	A	194	VAL	2.4
1	y	60	CYS	2.4
1	W	190	ALA	2.4
1	U	86	LEU	2.4
1	U	111	ILE	2.4
1	3	103	PHE	2.4
1	I	142	VAL	2.4
1	s	175	ASN	2.4
1	s	169	LEU	2.4
1	k	97	GLN	2.4
1	o	156	ALA	2.4
1	m	187	LEU	2.4
1	U	169	LEU	2.4
1	Y	154	LEU	2.4
1	i	62	GLU	2.4
1	s	166	GLU	2.3
1	y	181	GLN	2.3
1	i	187	LEU	2.3
1	q	103	PHE	2.3
1	U	110	PHE	2.3
1	c	186	VAL	2.3
1	O	157	LEU	2.3
1	Q	177	LEU	2.3
2	n	789	THR	2.3
1	k	98	ASP	2.3
2	h	790	VAL	2.3
1	0	120	LYS	2.3
1	y	138	ILE	2.3
1	u	150	ALA	2.3
1	y	144	TYR	2.3
1	U	64	ARG	2.3
1	Q	186	VAL	2.3
1	s	172	TYR	2.3
1	k	171	VAL	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	Y	175	ASN	2.3
1	3	86	LEU	2.3
1	c	169	LEU	2.3
1	g	88	LEU	2.3
1	k	183	ILE	2.3
1	3	158	LYS	2.2
1	u	183	ILE	2.2
1	Q	144	TYR	2.2
1	y	183	ILE	2.2
1	m	170	TRP	2.2
1	0	98	ASP	2.2
1	k	145	ASP	2.2
1	a	181	GLN	2.2
1	4	186	VAL	2.2
1	a	87	ASP	2.2
1	4	122	SER	2.2
1	y	179	GLN	2.2
2	f	789	THR	2.2
2	8	787	VAL	2.2
1	K	110	PHE	2.2
1	y	175	ASN	2.2
1	i	92	ILE	2.2
1	y	117	TYR	2.2
1	3	157	LEU	2.2
1	i	68	VAL	2.2
1	k	90	ASN	2.1
1	e	64	ARG	2.1
1	m	191	PHE	2.1
1	e	169	LEU	2.1
1	s	140	ARG	2.1
1	0	102	PRO	2.1
1	0	88	LEU	2.1
1	O	91	TYR	2.1
1	u	190	ALA	2.1
1	c	142	VAL	2.1
1	g	177	LEU	2.1
1	y	195	LEU	2.1
1	a	135	LEU	2.1
1	U	157	LEU	2.1
2	t	787	VAL	2.1
1	A	191	PHE	2.1
1	2	154	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	u	167	TYR	2.1
1	g	145	ASP	2.1
1	s	189	THR	2.1
1	W	189	THR	2.1
1	u	107	GLU	2.1
1	k	177	LEU	2.0
1	Y	135	LEU	2.0
1	u	99	GLY	2.0
1	y	184	CYS	2.0
1	3	171	VAL	2.0
1	s	105	PRO	2.0
1	4	144	TYR	2.0
1	o	103	PHE	2.0
1	w	172	TYR	2.0
1	y	114	VAL	2.0
1	k	102	PRO	2.0
1	e	135	LEU	2.0
1	g	72	GLU	2.0
1	y	109	GLU	2.0
1	g	95	ALA	2.0
1	u	140	ARG	2.0
1	Y	159	THR	2.0
1	W	116	LYS	2.0
1	i	90	ASN	2.0

## 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 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.