Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:06 PM GMT

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
A user guide is available at
http://wwpdb.org/validation/2016/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:

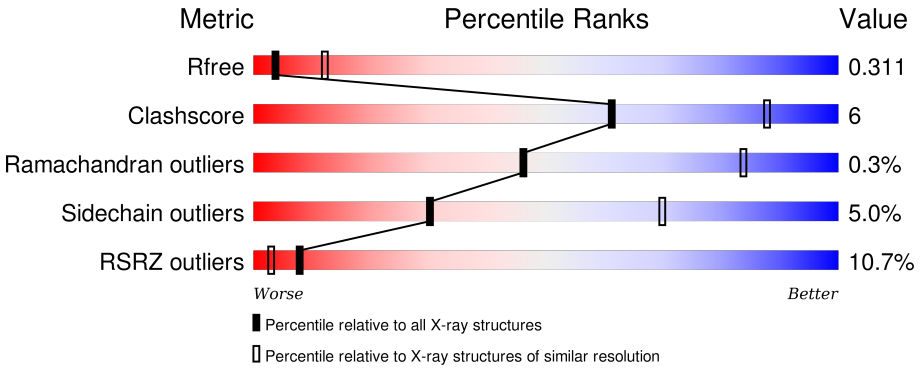
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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. 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% 61% 9% • 30%
1	1	157	61% 15% 25%
1	2	157	5% 54% • 42%
1	3	157	8% 57% 8% • 34%
1	4	157	4% 63% 18% • 18%

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Mol	Chain	Length	Quality of chain
1	5	157	69% 10% 18%
1	A	157	3% 56% 10% 32%
1	C	157	55% 25% 19%
1	E	157	% 54% 17% 28%
1	G	157	59% 22% 19%
1	I	157	% 59% 18% 20%
1	K	157	% 55% 17% 26%
1	M	157	% 61% 15% 21%
1	O	157	6% 50% 14% 35%
1	Q	157	8% 59% 18% 22%
1	S	157	3% 69% 11% 20%
1	U	157	13% 50% 13% 36%
1	W	157	6% 70% 10% 18%
1	Y	157	4% 68% 12% 18%
1	a	157	17% 58% 5% 37%
1	c	157	17% 72% 24%
1	e	157	8% 74% 6% 20%
1	g	157	18% 78% 19%
1	i	157	11% 58% 6% 36%
1	k	157	14% 63% 33%
1	m	157	11% 76% 5% 19%
1	o	157	13% 40% 60%
1	q	157	3% 29% 70%
1	s	157	14% 63% 35%
1	u	157	19% 64% 32%

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Mol	Chain	Length	Quality of chain
1	w	157	5% 30% 69%
1	y	157	27% 55% 41%
2	6	15	67% 7% 27%
2	7	15	60% 13% 27%
2	8	15	7% 47% 7% 47%
2	9	15	33% 20% 47%
2	B	15	7% 53% 13% 33%
2	D	15	60% 13% 27%
2	F	15	27% 47% 27%
2	H	15	20% 53% 27%
2	J	15	7% 40% 33% 27%
2	L	15	33% 40% 27%
2	N	15	53% 20% 27%
2	P	15	53% 13% 7% 27%
2	R	15	7% 53% 20% 27%
2	T	15	53% 20% 27%
2	V	15	33% 33% 33%
2	X	15	53% 27% 20%
2	Z	15	7% 60% 13% 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%

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Mol	Chain	Length	Quality of chain
2	n	15	13% 73% 27%
2	p	15	13% 33% 67%
2	r	15	13% 87%
2	t	15	7% 47% 7% 47%
2	v	15	47% 7% 47%
2	x	15	27% 73%
2	z	15	33% 67%

2 Entry composition

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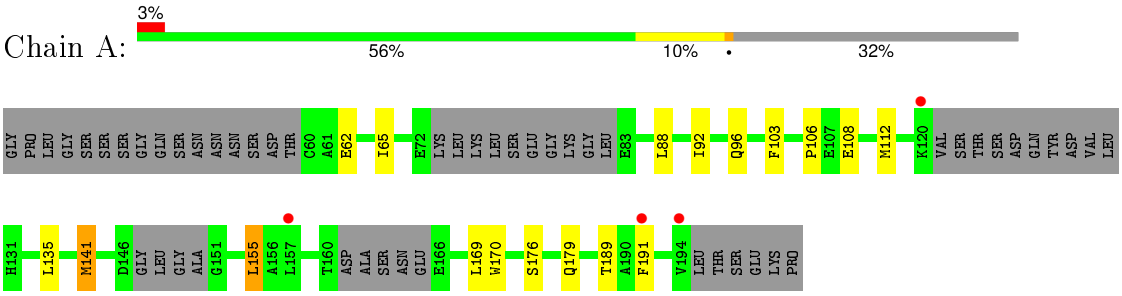
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	X	12	Total	C	N	O	0	0	0
			91	59	15	17			
2	Z	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	z	5	Total	C	N	O	0	0	0
			36	23	6	7			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

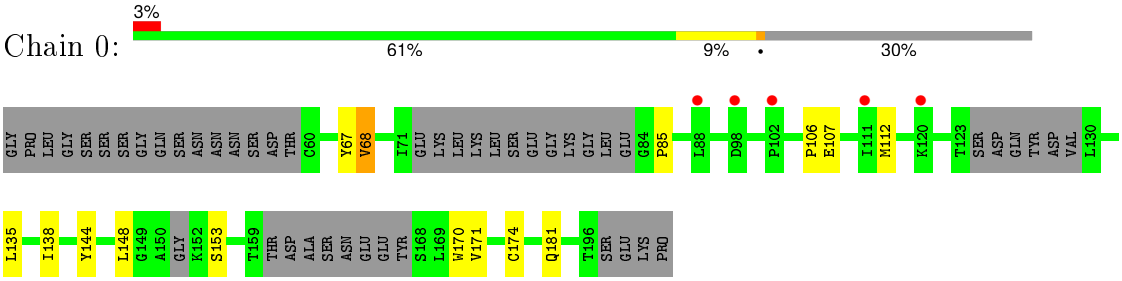
- Molecule 1: Integrin beta-1-binding protein 1

Chain A:



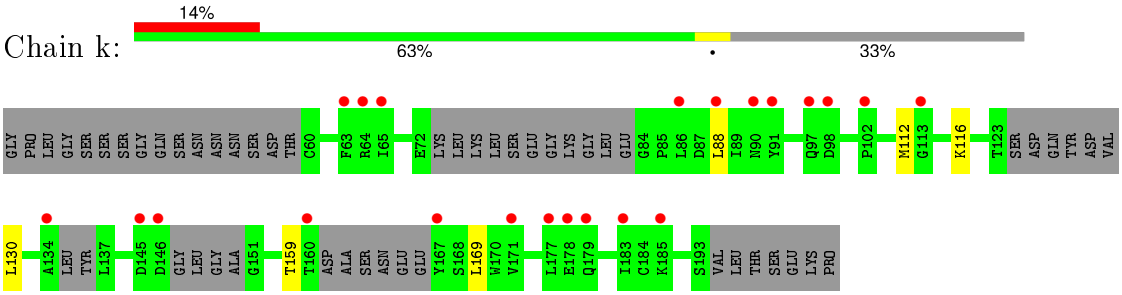
- Molecule 1: Integrin beta-1-binding protein 1

Chain 0:



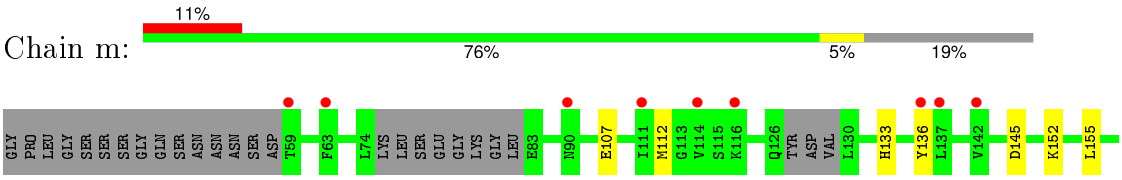
- Molecule 1: Integrin beta-1-binding protein 1

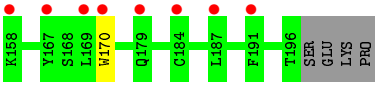
Chain k:



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

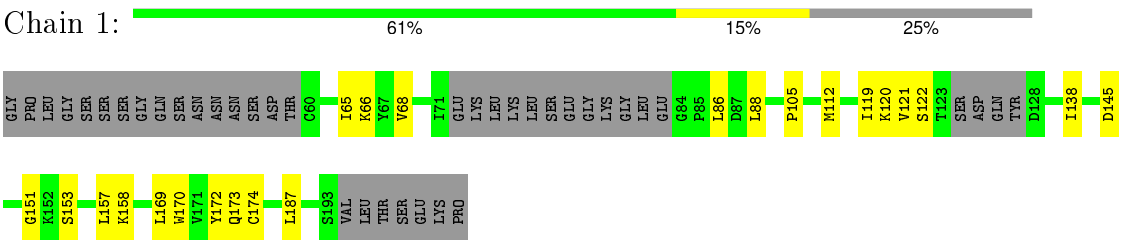
Chain m:





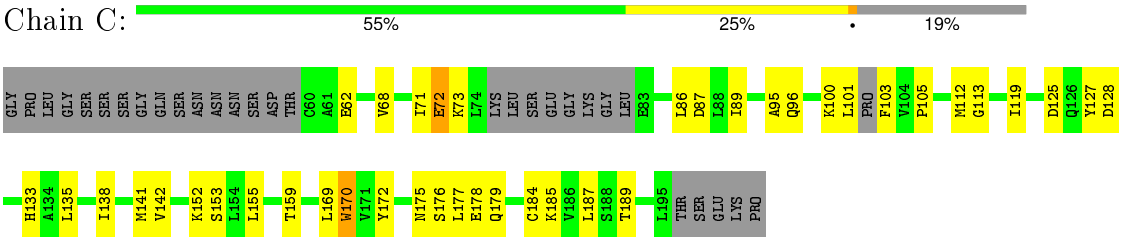
• Molecule 1: Integrin beta-1-binding protein 1

Chain 1:



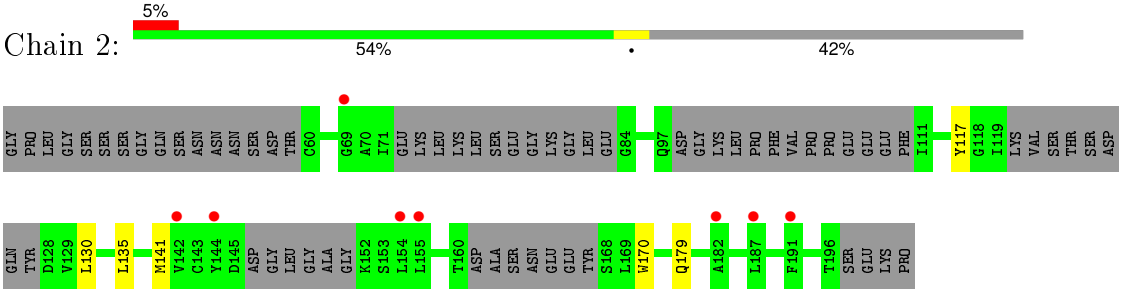
• Molecule 1: Integrin beta-1-binding protein 1

Chain C:



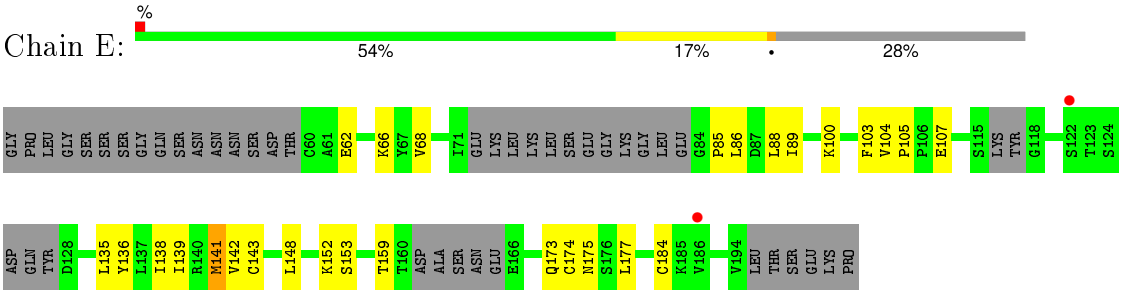
• Molecule 1: Integrin beta-1-binding protein 1

Chain 2:



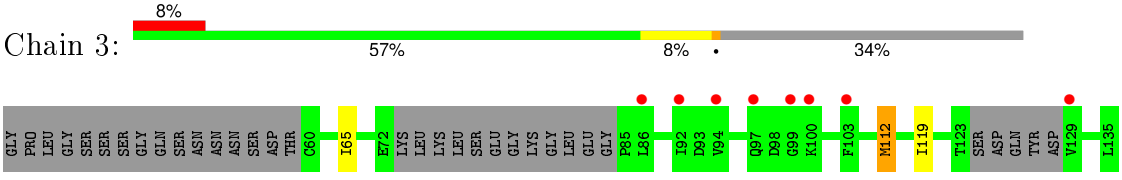
• Molecule 1: Integrin beta-1-binding protein 1

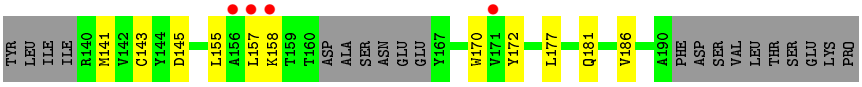
Chain E:



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

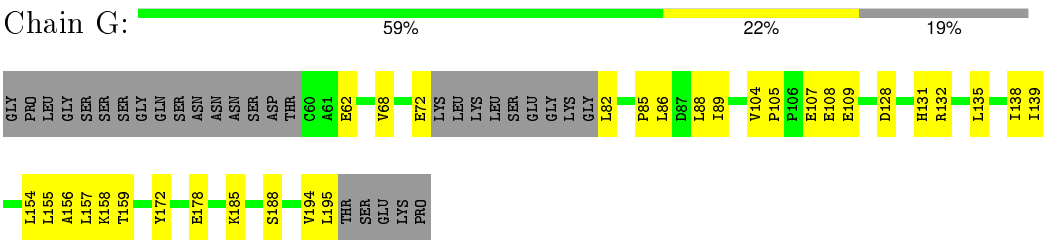
Chain 3:





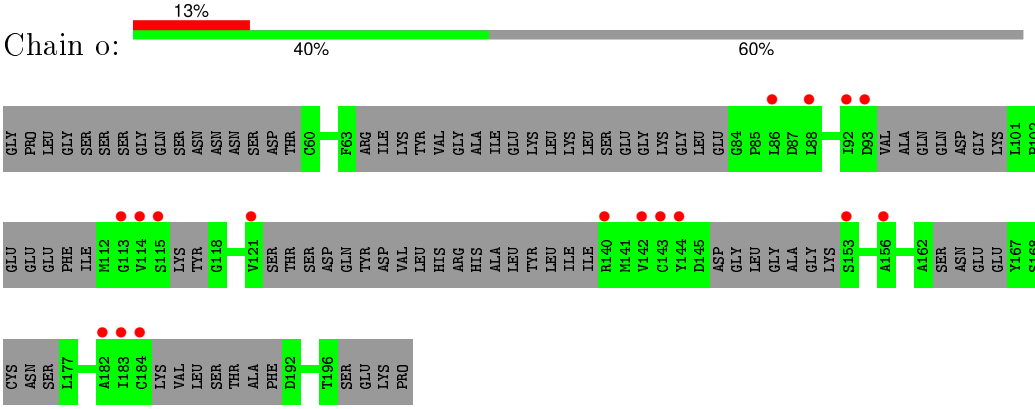
• Molecule 1: Integrin beta-1-binding protein 1

Chain G:



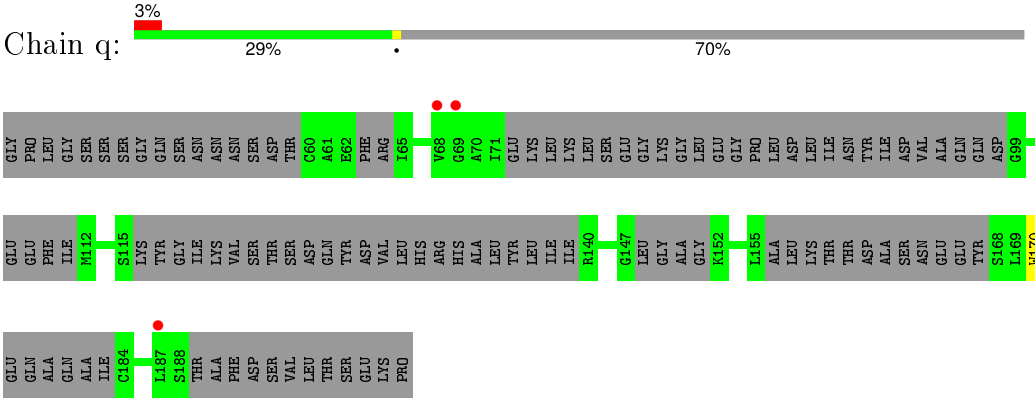
• Molecule 1: Integrin beta-1-binding protein 1

Chain o:



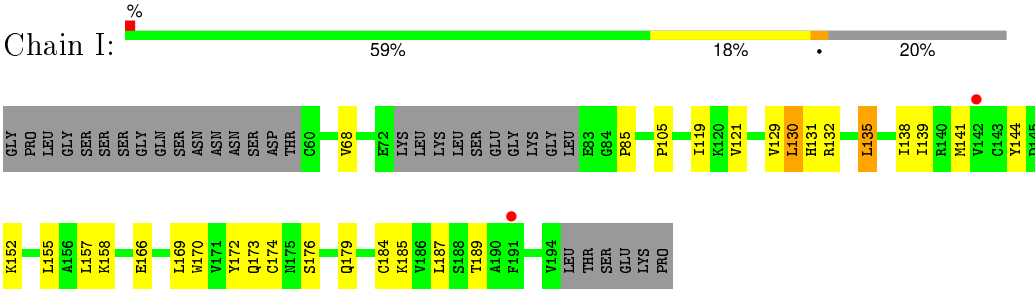
• Molecule 1: Integrin beta-1-binding protein 1

Chain q:



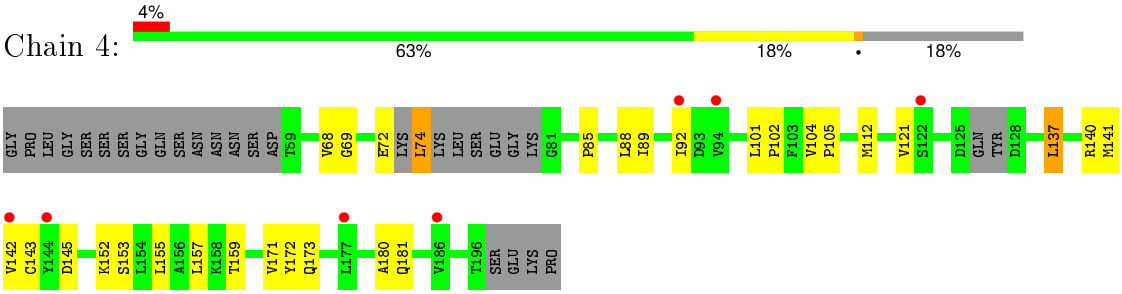
• Molecule 1: Integrin beta-1-binding protein 1

Chain I:



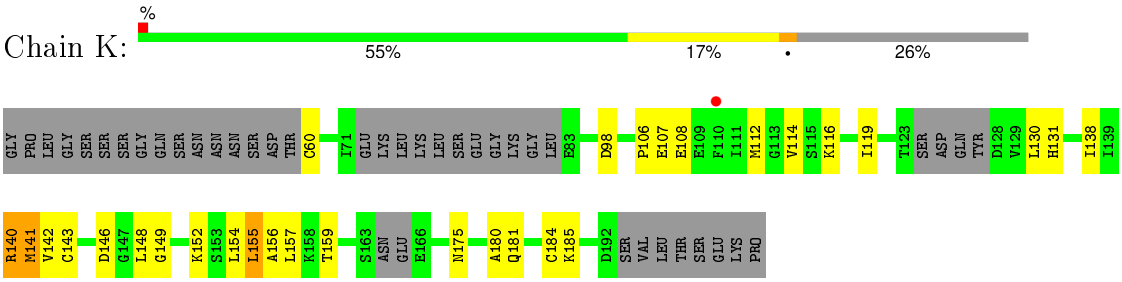
• Molecule 1: Integrin beta-1-binding protein 1

Chain 4:



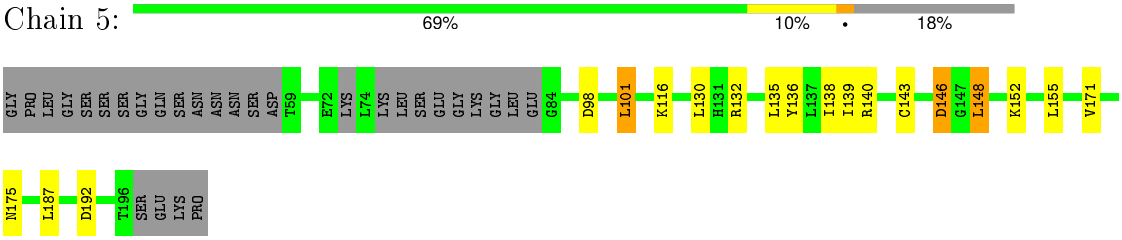
• Molecule 1: Integrin beta-1-binding protein 1

Chain K:



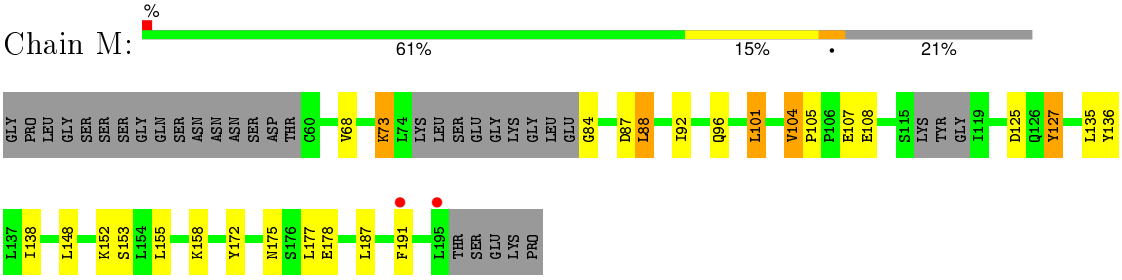
• Molecule 1: Integrin beta-1-binding protein 1

Chain 5:



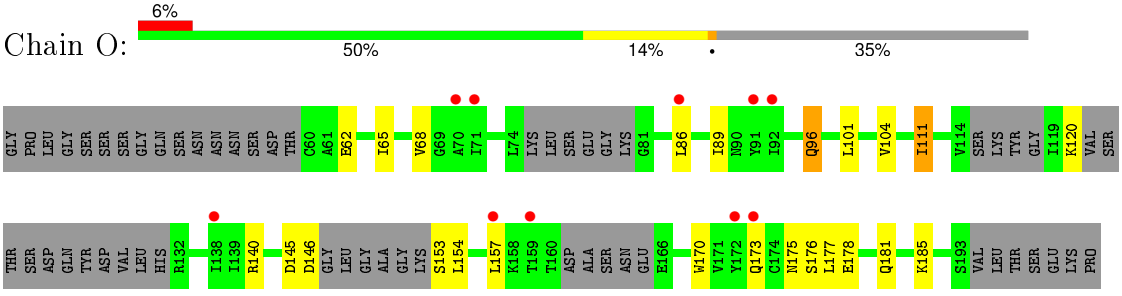
• Molecule 1: Integrin beta-1-binding protein 1

Chain M:



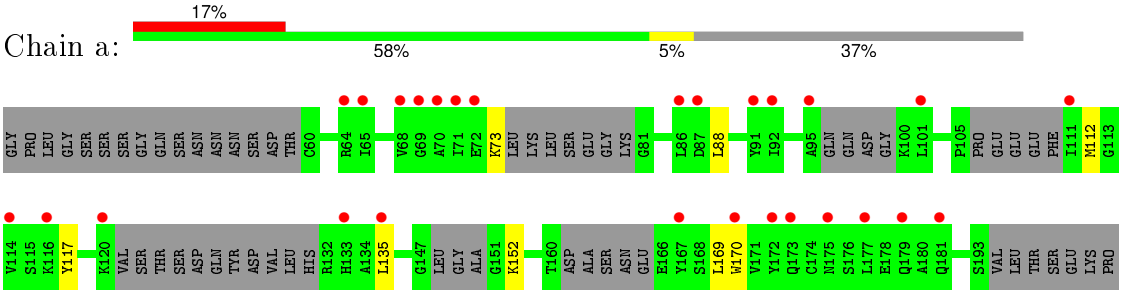
• Molecule 1: Integrin beta-1-binding protein 1

Chain O:



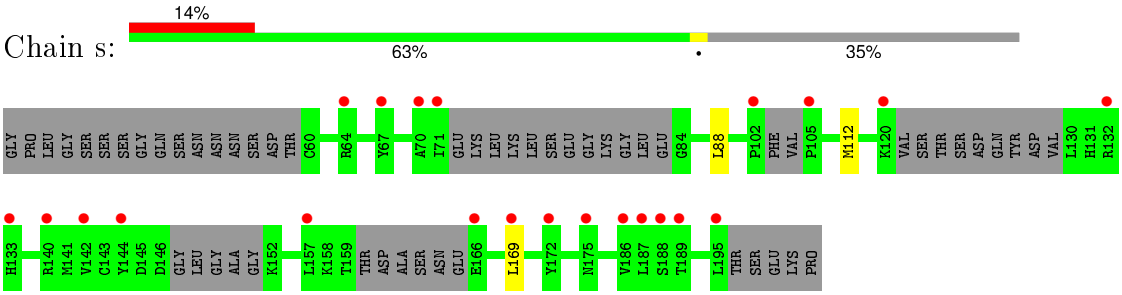
• Molecule 1: Integrin beta-1-binding protein 1

Chain a:



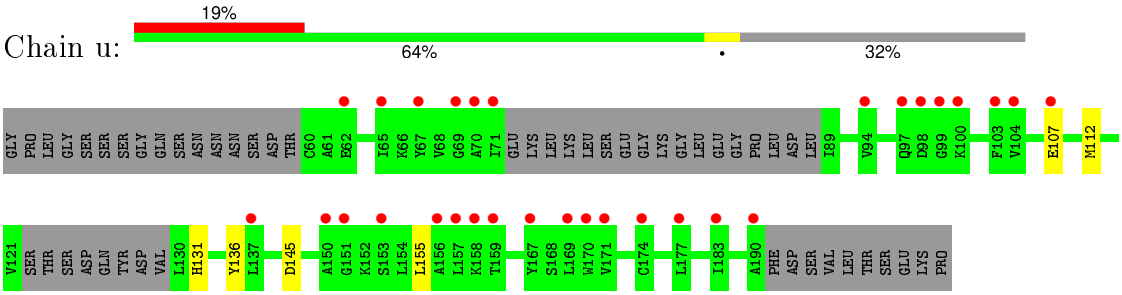
• Molecule 1: Integrin beta-1-binding protein 1

Chain s:



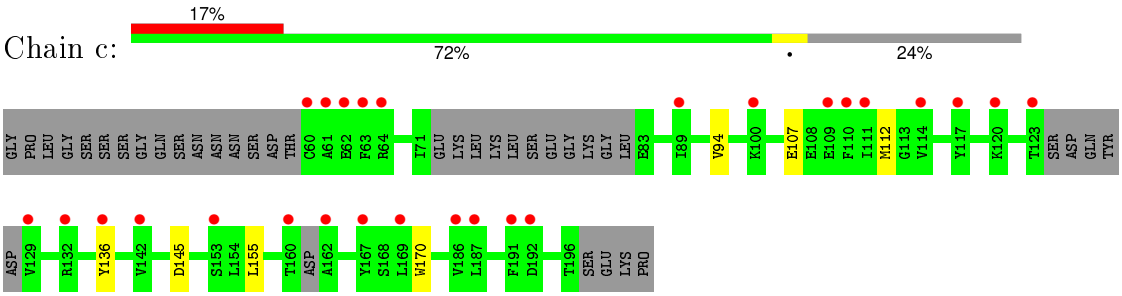
• Molecule 1: Integrin beta-1-binding protein 1

Chain u:



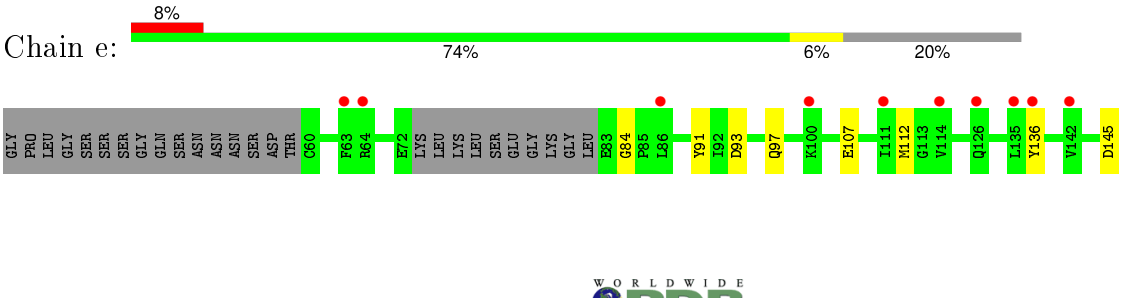
• Molecule 1: Integrin beta-1-binding protein 1

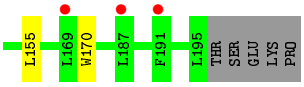
Chain c:



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

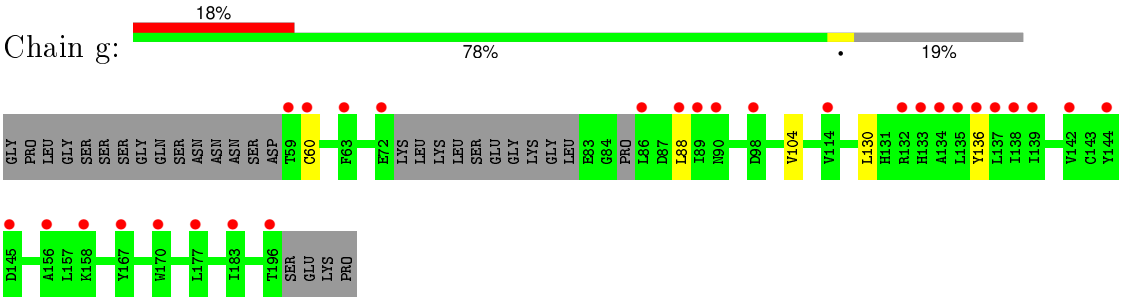
Chain e:





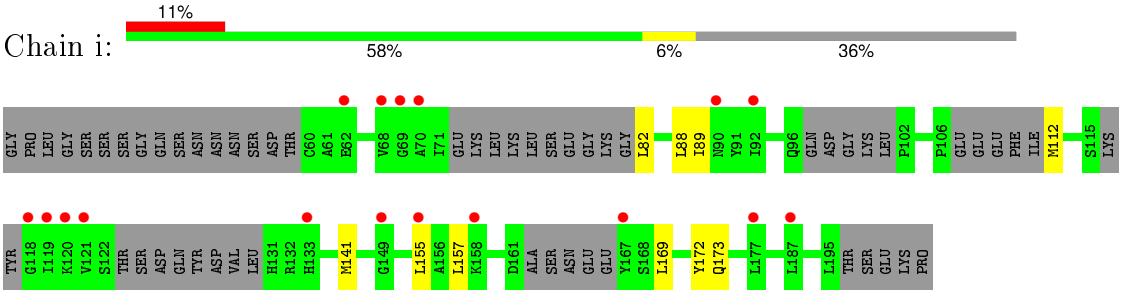
• Molecule 1: Integrin beta-1-binding protein 1

Chain g:



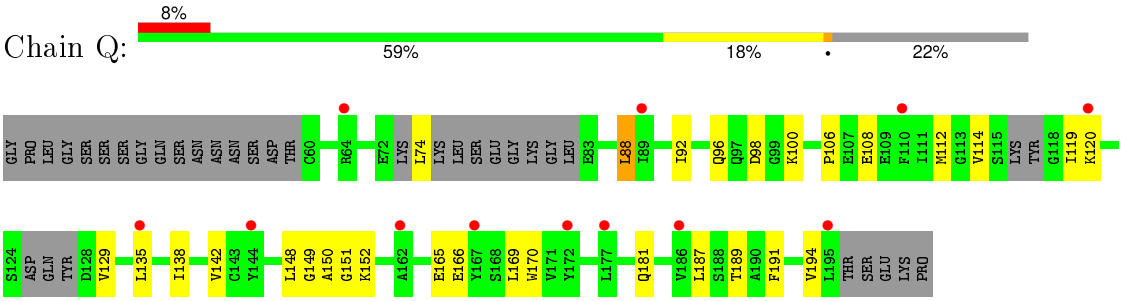
• Molecule 1: Integrin beta-1-binding protein 1

Chain i:



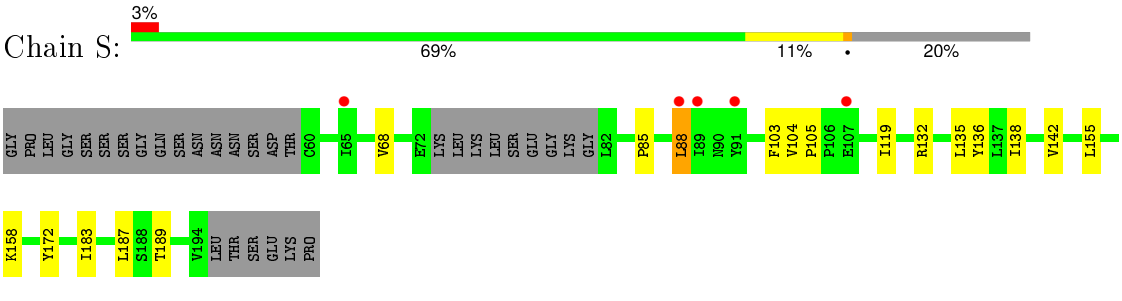
• Molecule 1: Integrin beta-1-binding protein 1

Chain Q:



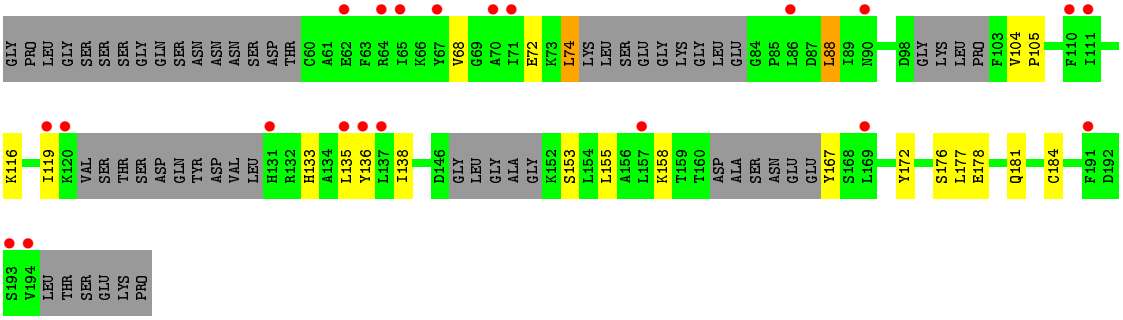
• Molecule 1: Integrin beta-1-binding protein 1

Chain S:



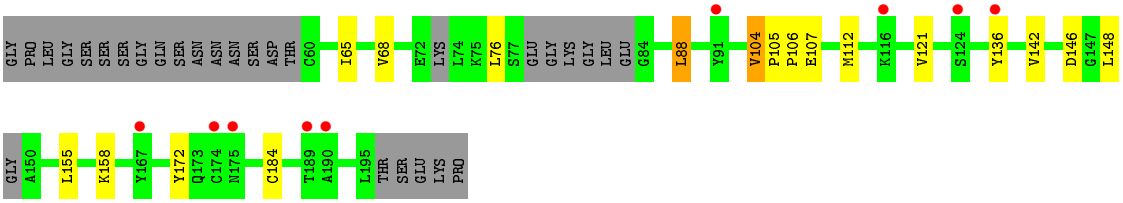
• Molecule 1: Integrin beta-1-binding protein 1

Chain U:



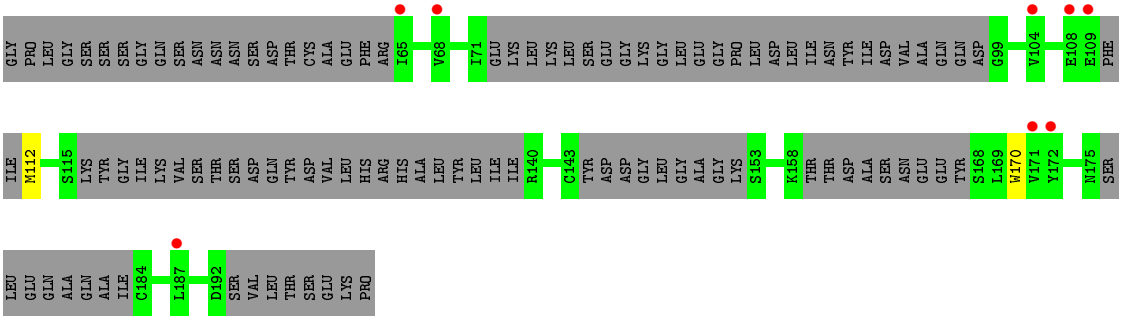
• Molecule 1: Integrin beta-1-binding protein 1

Chain W:



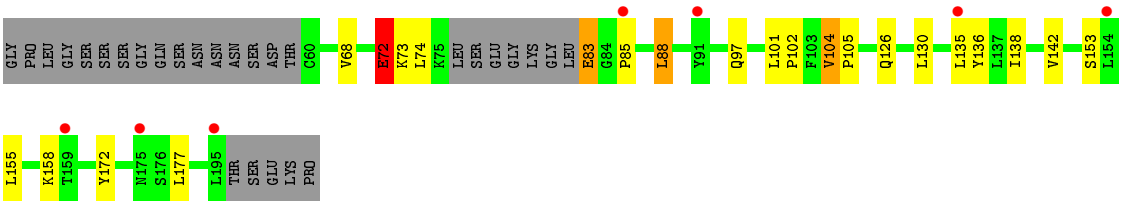
• Molecule 1: Integrin beta-1-binding protein 1

Chain w:



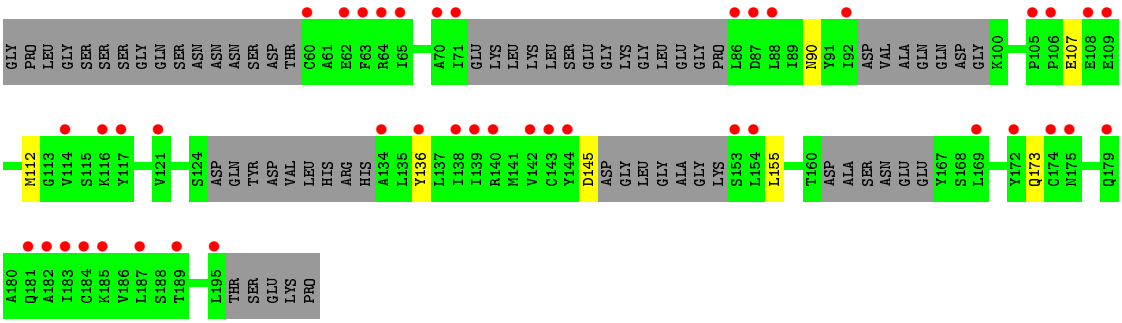
• Molecule 1: Integrin beta-1-binding protein 1

Chain Y:

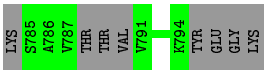


• Molecule 1: Integrin beta-1-binding protein 1

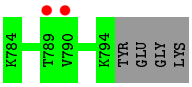
Chain y:



- Molecule 2: Integrin beta-1

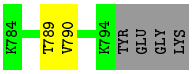


- Molecule 2: Integrin beta-1

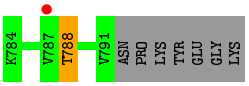


- Molecule 2: Integrin beta-1

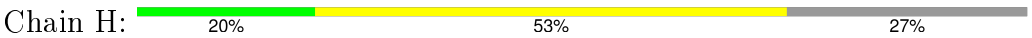
- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1

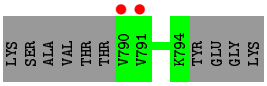


- Molecule 2: Integrin beta-1



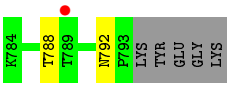
• Molecule 2: Integrin beta-1

Chain p:



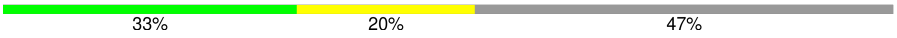
• Molecule 2: Integrin beta-1

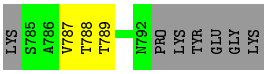
Chain B:



• Molecule 2: Integrin beta-1

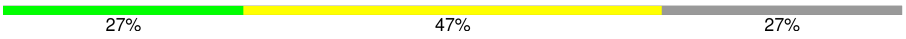
Chain 9:

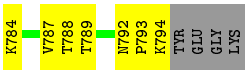




• Molecule 2: Integrin beta-1

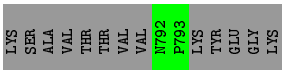
Chain F:





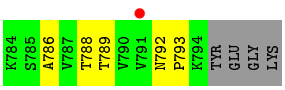
• Molecule 2: Integrin beta-1

Chain r:



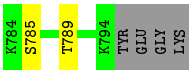
• Molecule 2: Integrin beta-1

Chain J:



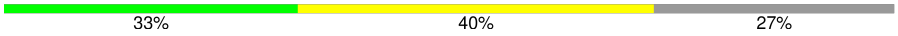
• Molecule 2: Integrin beta-1

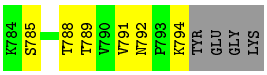
Chain 7:



• Molecule 2: Integrin beta-1

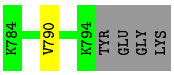
Chain L:





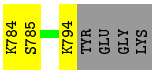
• Molecule 2: Integrin beta-1

Chain 6:



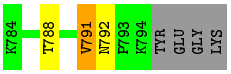
• Molecule 2: Integrin beta-1

Chain N:



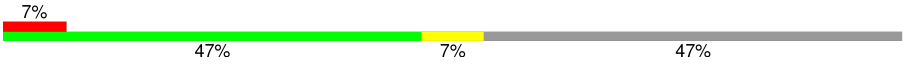
• Molecule 2: Integrin beta-1

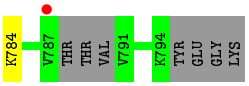
Chain P:



• Molecule 2: Integrin beta-1

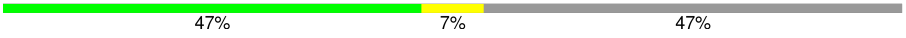
Chain t:

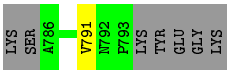




• Molecule 2: Integrin beta-1

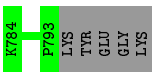
Chain v:





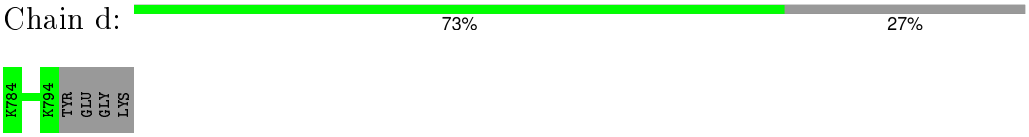
• Molecule 2: Integrin beta-1

Chain b:



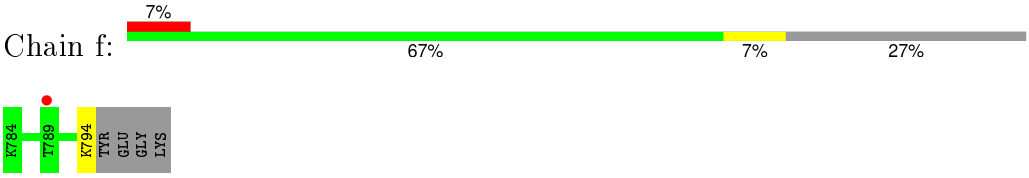
• Molecule 2: Integrin beta-1

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

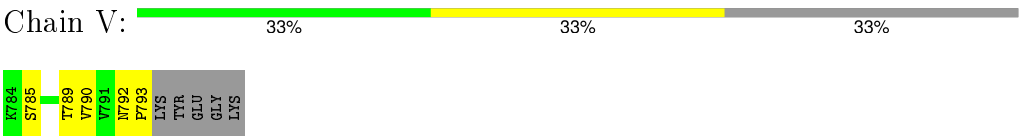
Chain R:

• 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	5105 reflections (5.87%)	DCC
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
Estimated 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 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
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
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, 0.375 respectively for untwinned datasets, and 0.333, 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

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

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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
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(^{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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	858	0	874	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	919	0	913	14	0
1	2	716	0	736	1	0
1	3	810	0	819	7	0
1	4	1000	0	992	23	0
1	5	1000	0	990	9	1
1	A	844	0	839	11	0
1	C	997	0	988	28	0
1	E	875	0	877	28	0
1	G	995	0	983	48	0
1	I	979	0	961	25	0
1	K	905	0	901	17	0
1	M	970	0	964	32	0
1	O	812	0	814	14	0
1	Q	945	0	937	24	0
1	S	987	0	972	13	0
1	U	811	0	813	17	0
1	W	1005	0	1001	22	0
1	Y	1013	0	1009	14	1
1	a	777	0	794	0	0
1	c	934	0	937	0	0
1	e	987	0	972	0	0
1	g	994	0	978	0	0
1	i	779	0	789	0	0
1	k	827	0	829	0	0
1	m	991	0	987	0	0
1	o	489	0	481	0	0
1	q	359	0	363	0	0
1	s	813	0	821	0	0
1	u	831	0	834	0	0
1	w	378	0	387	0	0
1	y	738	0	759	0	0
2	6	79	0	89	1	0
2	7	79	0	89	3	0
2	8	55	0	63	1	0
2	9	54	0	56	3	0
2	B	70	0	76	1	0
2	D	79	0	89	3	0
2	F	79	0	89	7	0
2	H	79	0	89	10	0
2	J	79	0	89	4	0
2	L	79	0	89	6	0
2	N	79	0	89	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	79	0	89	2	0
2	R	79	0	89	4	0
2	T	79	0	89	4	0
2	V	70	0	76	3	0
2	X	91	0	98	3	0
2	Z	79	0	89	3	0
2	b	70	0	76	0	0
2	d	79	0	89	0	0
2	f	79	0	89	0	0
2	h	70	0	76	0	0
2	j	27	0	31	0	0
2	l	49	0	52	0	0
2	n	79	0	89	0	0
2	p	38	0	43	0	0
2	r	15	0	12	0	0
2	t	58	0	65	0	0
2	v	55	0	58	0	0
2	x	25	0	25	0	0
2	z	36	0	37	0	0
All	All	29306	0	29493	320	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (320) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:105:PRO:O	1:M:107:GLU:CG	6.86	1.36
1:M:104:VAL:HG12	1:M:107:GLU:OE2	7.16	1.31
1:E:107:GLU:N	1:G:72:GLU:OE2	48.03	1.23
1:G:107:GLU:CD	1:W:105:PRO:O	95.77	1.16
1:G:107:GLU:OE2	1:W:105:PRO:O	96.42	1.15
1:4:105:PRO:HD2	1:4:173:GLN:NE2	1.65	1.11
1:M:104:VAL:HG12	1:M:107:GLU:CD	8.00	1.08
1:M:105:PRO:O	1:M:107:GLU:CD	7.25	1.04
1:C:127:TYR:HB3	1:Q:100:LYS:NZ	1.74	1.02
1:M:105:PRO:O	1:M:107:GLU:HG2	7.71	1.00
1:0:107:GLU:O	1:0:107:GLU:HG3	1.61	0.97
1:E:107:GLU:HB2	1:G:72:GLU:CD	48.17	0.95
1:E:107:GLU:HB2	1:G:72:GLU:OE2	48.89	0.94
1:4:105:PRO:CD	1:4:173:GLN:NE2	2.31	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:105:PRO:O	1:M:107:GLU:HG3	6.62	0.92
1:I:155:LEU:HB2	1:I:172:TYR:O	3.91	0.88
1:C:127:TYR:HB3	1:Q:100:LYS:HZ3	1.37	0.87
1:M:104:VAL:HB	1:M:107:GLU:OE1	10.14	0.87
1:4:105:PRO:HD2	1:4:173:GLN:HE22	1.39	0.84
1:U:181:GLN:NE2	2:V:785:SER:OG	2.12	0.82
1:E:103:PHE:CG	1:G:132:ARG:HD2	41.57	0.81
2:L:792:ASN:O	2:L:794:LYS:HA	1.81	0.81
1:G:104:VAL:CG2	1:W:148:LEU:HB3	96.70	0.79
1:M:104:VAL:CG1	1:M:107:GLU:OE2	7.81	0.79
1:S:189:THR:HG21	1:U:176:SER:HB2	30.68	0.78
1:0:107:GLU:HG2	1:U:116:LYS:HD2	97.37	0.77
1:K:181:GLN:HG2	2:L:788:THR:HG21	1.66	0.77
1:Y:72:GLU:O	1:Y:73:LYS:HG3	1.85	0.77
1:G:104:VAL:HG23	1:W:148:LEU:HB3	97.55	0.77
1:Y:72:GLU:O	1:Y:73:LYS:CG	2.32	0.76
1:E:103:PHE:HB2	1:G:132:ARG:HB2	40.83	0.76
1:E:104:VAL:HG21	1:G:131:HIS:HA	42.18	0.76
1:M:104:VAL:CB	1:M:107:GLU:OE1	10.57	0.75
1:Y:72:GLU:O	1:Y:73:LYS:CB	2.29	0.75
1:E:107:GLU:CB	1:G:72:GLU:OE2	49.35	0.74
1:C:127:TYR:HB3	1:Q:100:LYS:HZ1	1.48	0.74
1:M:104:VAL:CG1	1:M:107:GLU:CD	8.71	0.74
1:G:85:PRO:HB3	2:H:789:THR:HG21	1.68	0.73
1:Q:189:THR:HG23	1:U:178:GLU:HG3	1.70	0.72
1:C:187:LEU:HB3	2:D:790:VAL:HG11	3.06	0.72
1:I:173:GLN:HG3	1:I:174:CYS:N	4.37	0.72
1:I:141:MSE:HE2	1:I:187:LEU:HD22	1.72	0.71
1:5:101:LEU:HD11	1:5:171:VAL:HG21	1.71	0.71
1:E:107:GLU:CA	1:G:72:GLU:OE2	48.54	0.70
1:Q:189:THR:HG21	1:U:176:SER:HB2	1.73	0.70
1:G:86:LEU:HD11	1:I:144:TYR:HB2	67.36	0.70
1:I:141:MSE:HE3	1:I:184:CYS:HA	1.74	0.68
1:G:107:GLU:CD	1:W:105:PRO:C	95.52	0.67
1:0:107:GLU:CG	1:U:116:LYS:HD2	97.07	0.67
2:H:787:VAL:HB	2:F:787:VAL:HB	1.77	0.66
1:O:120:LYS:HE3	1:S:132:ARG:HH22	67.26	0.66
1:0:153:SER:HB3	1:0:174:CYS:HB2	1.78	0.66
1:M:104:VAL:CG1	1:M:107:GLU:OE1	9.65	0.65
1:4:112:MSE:HG3	1:4:121:VAL:HG22	1.78	0.64
1:M:104:VAL:HG13	1:M:104:VAL:HG22	2.50	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:GLU:OE2	1:W:105:PRO:C	96.16	0.64
1:4:141:MSE:HE2	1:4:155:LEU:HD21	1.80	0.63
1:W:142:VAL:HG22	2:X:789:THR:HG22	1.78	0.63
1:Q:114:VAL:HG22	1:Q:119:ILE:HG13	1.81	0.63
1:E:66:LYS:HB2	1:E:173:GLN:HB3	1.81	0.62
1:C:141:MSE:HE3	1:C:184:CYS:HA	1.81	0.62
1:C:142:VAL:HG22	2:D:789:THR:HG23	1.81	0.62
1:U:74:LEU:HD12	1:U:167:TYR:O	2.00	0.61
1:E:103:PHE:CG	1:G:132:ARG:CD	41.58	0.61
1:0:107:GLU:O	1:0:107:GLU:CG	2.43	0.61
1:K:148:LEU:HB3	1:Q:149:GLY:HA3	1.83	0.60
1:I:150:ALA:HB1	1:Y:104:VAL:HG22	40.11	0.60
1:E:103:PHE:CD2	1:G:132:ARG:HD3	41.99	0.60
1:4:89:ILE:HD11	1:4:142:VAL:HG11	1.85	0.59
1:I:152:LYS:HB3	1:I:173:GLN:OE1	3.63	0.59
1:G:107:GLU:CG	1:W:105:PRO:O	94.29	0.59
1:K:140:ARG:HG2	2:L:791:VAL:HG12	1.85	0.59
1:Q:189:THR:HG21	1:U:176:SER:CB	2.33	0.58
1:M:104:VAL:HG21	1:M:148:LEU:HD13	7.36	0.58
1:4:105:PRO:CD	1:4:173:GLN:HE21	2.13	0.58
1:Q:119:ILE:HD13	1:Q:138:ILE:HD13	1.86	0.58
1:4:137:LEU:HD12	1:4:159:THR:HB	1.86	0.58
2:R:788:THR:HA	2:T:786:ALA:H	1.70	0.57
1:G:141:MSE:HE3	1:G:157:LEU:HD13	1.87	0.57
1:K:185:LYS:HB3	1:O:178:GLU:O	2.05	0.57
1:S:85:PRO:HB3	2:T:789:THR:HG21	1.86	0.56
1:M:104:VAL:HG12	1:M:107:GLU:OE1	8.98	0.56
1:3:141:MSE:HG3	1:3:157:LEU:HG	1.88	0.56
1:G:68:VAL:HG22	1:G:105:PRO:HG3	1.88	0.56
1:G:107:GLU:OE2	1:W:104:VAL:HG12	94.58	0.55
1:C:185:LYS:HB3	1:G:178:GLU:HB3	1.87	0.55
1:C:125:ASP:C	1:C:127:TYR:H	2.10	0.55
1:1:145:ASP:HA	1:1:153:SER:HA	1.88	0.55
1:C:133:HIS:HD2	1:C:159:THR:HG21	4.89	0.55
1:G:107:GLU:OE2	1:W:105:PRO:N	94.54	0.54
1:E:138:ILE:HA	1:E:159:THR:HG22	1.88	0.54
1:4:85:PRO:HB3	2:7:789:THR:HG21	1.90	0.54
1:A:62:GLU:HB2	1:E:62:GLU:HB2	1.89	0.54
1:O:62:GLU:HG2	1:O:111:ILE:HG22	1.89	0.54
1:G:107:GLU:OE1	1:W:106:PRO:O	95.42	0.54
1:4:85:PRO:HG3	1:4:140:ARG:CZ	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:141:MSE:HE1	1:K:184:CYS:HA	1.89	0.53
1:S:119:ILE:HD11	1:S:187:LEU:HD21	3.43	0.53
1:Y:142:VAL:HG22	2:Z:789:THR:HG22	1.89	0.53
1:C:73:LYS:HE2	1:I:166:GLU:HG3	1.89	0.53
1:G:142:VAL:HG22	2:H:789:THR:HG22	1.90	0.52
1:I:85:PRO:HB3	2:J:789:THR:HG21	1.91	0.52
1:E:152:LYS:HD3	1:E:175:ASN:HA	3.43	0.52
1:E:142:VAL:HG22	2:F:789:THR:HG22	5.40	0.52
1:M:96:GLN:HA	1:M:101:LEU:O	2.09	0.52
1:G:143:CYS:HB3	1:G:155:LEU:HD23	1.89	0.52
2:F:792:ASN:O	2:F:794:LYS:N	2.42	0.52
2:H:792:ASN:O	2:H:794:LYS:N	2.40	0.52
1:E:86:LEU:HD11	1:G:89:ILE:HG21	1.92	0.52
1:A:176:SER:OG	1:C:189:THR:HG23	25.39	0.52
1:M:92:ILE:HG23	1:M:101:LEU:HD13	4.63	0.51
1:W:65:ILE:HG21	1:W:112:MSE:HE2	6.24	0.51
1:O:140:ARG:HG3	2:P:791:VAL:HG12	3.00	0.51
1:G:143:CYS:SG	2:H:788:THR:HG23	5.57	0.51
1:Q:142:VAL:HG22	2:R:789:THR:HG23	1.91	0.51
1:C:62:GLU:HB2	1:G:62:GLU:HB2	1.92	0.51
1:1:65:ILE:HD13	1:1:172:TYR:HD2	1.76	0.51
1:C:113:GLY:O	1:C:119:ILE:HA	2.11	0.51
1:E:86:LEU:HA	1:E:89:ILE:HD12	2.08	0.51
1:Q:135:LEU:HA	1:Q:138:ILE:HD12	1.93	0.50
1:W:112:MSE:HG3	1:W:121:VAL:HG22	1.93	0.50
1:4:88:LEU:O	1:4:92:ILE:HD12	2.11	0.50
1:C:71:ILE:HD11	1:C:95:ALA:CB	2.42	0.50
1:4:143:CYS:SG	1:4:180:ALA:HB3	2.51	0.50
1:W:184:CYS:O	2:X:790:VAL:HG21	2.12	0.50
1:1:66:LYS:HE2	1:1:105:PRO:HG2	1.93	0.50
1:M:104:VAL:CG1	1:M:104:VAL:HG22	2.66	0.50
1:5:132:ARG:HB3	1:S:103:PHE:HB2	1.94	0.50
1:G:138:ILE:HA	1:G:159:THR:HG22	1.93	0.50
1:4:68:VAL:HB	1:4:171:VAL:HG13	1.94	0.50
1:E:103:PHE:CD1	1:G:132:ARG:HD2	40.22	0.49
2:L:792:ASN:O	2:L:794:LYS:CA	2.56	0.49
1:0:85:PRO:HB3	2:9:789:THR:HG21	1.94	0.49
1:S:88:LEU:HD21	1:S:158:LYS:HB2	1.95	0.49
1:Q:106:PRO:HB2	1:Q:108:GLU:HG2	1.95	0.49
1:M:88:LEU:HD21	1:M:158:LYS:HB2	1.95	0.49
1:1:86:LEU:HD22	1:4:89:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:PHE:CD2	1:G:132:ARG:CD	42.11	0.48
1:Q:181:GLN:HG2	2:R:788:THR:HG21	1.93	0.48
1:0:67:TYR:O	1:0:106:PRO:HD2	2.13	0.48
1:K:114:VAL:HG22	1:K:119:ILE:HG12	2.05	0.48
1:W:88:LEU:HD21	1:W:158:LYS:HB2	1.95	0.48
1:C:86:LEU:HA	1:C:89:ILE:HD12	1.94	0.48
1:I:105:PRO:HG3	1:I:173:GLN:HE21	3.79	0.48
2:H:787:VAL:HG23	2:J:786:ALA:HB3	61.86	0.48
1:A:92:ILE:O	1:A:96:GLN:HB2	2.13	0.48
1:C:155:LEU:HB3	1:C:172:TYR:HB2	1.94	0.48
1:Y:88:LEU:HD21	1:Y:158:LYS:HB2	1.95	0.48
1:Q:187:LEU:O	1:Q:191:PHE:HB2	2.14	0.48
1:S:142:VAL:HG22	2:T:789:THR:HG22	1.96	0.48
1:C:152:LYS:HD2	1:C:175:ASN:HA	1.96	0.48
1:A:106:PRO:HB2	1:A:108:GLU:HG2	1.95	0.48
1:1:88:LEU:HD13	1:1:158:LYS:HE3	1.96	0.48
2:J:788:THR:HG22	2:L:785:SER:HA	1.95	0.48
1:K:138:ILE:HA	1:K:159:THR:HG22	1.94	0.47
1:4:105:PRO:HD2	1:4:173:GLN:HE21	1.66	0.47
1:G:88:LEU:HD21	1:G:158:LYS:HB2	2.23	0.47
1:A:112:MSE:HE1	1:A:155:LEU:HD22	1.95	0.47
1:M:152:LYS:HG3	1:M:175:ASN:HA	4.82	0.47
1:M:153:SER:OG	1:M:177:LEU:HA	2.83	0.47
1:4:142:VAL:HG22	2:7:789:THR:HG22	1.97	0.47
1:S:135:LEU:HA	1:S:138:ILE:HD12	2.14	0.47
1:M:107:GLU:OE1	1:M:108:GLU:HB3	9.21	0.47
1:I:170:TRP:HB2	1:I:172:TYR:HE1	2.52	0.47
1:G:194:VAL:HG23	1:G:195:LEU:HD12	5.39	0.47
1:U:88:LEU:HD21	1:U:158:LYS:HB2	1.95	0.47
1:Y:153:SER:OG	1:Y:177:LEU:HA	2.83	0.47
1:U:184:CYS:O	2:V:790:VAL:HG21	2.14	0.47
1:1:68:VAL:HA	1:1:105:PRO:HB3	1.97	0.46
1:C:153:SER:OG	1:C:177:LEU:HA	2.67	0.46
1:O:96:GLN:HG2	1:O:101:LEU:HD12	1.97	0.46
1:Q:120:LYS:HE2	1:Q:129:VAL:HG13	1.98	0.46
1:M:187:LEU:HD23	1:M:191:PHE:HE2	3.58	0.46
1:4:69:GLY:HA3	1:4:101:LEU:HD22	1.96	0.46
1:E:148:LEU:O	1:G:128:ASP:HA	41.14	0.46
1:E:153:SER:OG	1:E:177:LEU:HA	2.87	0.46
1:4:145:ASP:HA	1:4:153:SER:HA	1.96	0.46
1:M:84:GLY:HA3	1:M:87:ASP:HB2	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:146:ASP:OD1	1:I:146:ASP:N	2.41	0.46
1:G:109:GLU:H	1:G:109:GLU:CD	2.18	0.46
1:G:85:PRO:HG2	1:G:86:LEU:HD12	1.97	0.46
1:3:65:ILE:HG12	1:3:112:MSE:HB2	1.98	0.46
1:1:119:ILE:HD11	1:1:187:LEU:HD13	1.98	0.46
1:M:107:GLU:OE2	1:M:108:GLU:HB3	9.61	0.46
1:W:146:ASP:HB2	1:W:148:LEU:HD12	1.98	0.46
1:I:185:LYS:HG3	1:M:178:GLU:HB3	1.97	0.46
1:I:172:TYR:N	1:I:172:TYR:CD1	3.22	0.46
2:H:789:THR:O	2:F:784:LYS:HB3	2.16	0.46
1:U:153:SER:OG	1:U:177:LEU:HA	2.83	0.46
1:K:142:VAL:HB	1:K:156:ALA:HB3	1.97	0.46
1:U:155:LEU:HB3	1:U:172:TYR:HB2	1.98	0.46
1:I:139:ILE:HD12	1:I:158:LYS:HG2	1.97	0.46
1:Y:155:LEU:HB3	1:Y:172:TYR:HB2	1.98	0.45
1:K:149:GLY:HA3	1:Q:148:LEU:HB3	1.98	0.45
1:A:141:MSE:HE3	1:A:155:LEU:HD11	1.98	0.45
1:1:138:ILE:HG12	1:1:157:LEU:HD21	1.98	0.45
1:O:175:ASN:O	1:O:176:SER:HB3	2.16	0.45
1:M:155:LEU:HB3	1:M:172:TYR:HB2	1.97	0.45
1:K:142:VAL:O	1:K:155:LEU:HA	2.66	0.45
1:0:135:LEU:HA	1:0:138:ILE:HD12	1.98	0.45
1:Y:85:PRO:HB3	2:Z:789:THR:HG21	1.99	0.45
1:O:181:GLN:O	1:O:185:LYS:HG2	2.17	0.45
1:K:146:ASP:HB3	1:K:154:LEU:HG	1.99	0.45
1:S:155:LEU:HB3	1:S:172:TYR:HB2	1.98	0.45
1:5:187:LEU:HD23	2:6:790:VAL:HG11	1.99	0.45
1:G:155:LEU:HB3	1:G:172:TYR:HB2	3.50	0.45
1:A:189:THR:HG21	1:C:176:SER:HB2	25.73	0.45
1:5:139:ILE:HG22	1:5:140:ARG:HG3	1.98	0.45
1:E:153:SER:HB3	1:E:174:CYS:HB2	1.99	0.44
1:E:85:PRO:HG2	1:E:86:LEU:HD12	5.31	0.44
1:I:119:ILE:HD12	1:I:157:LEU:HD21	1.99	0.44
1:W:155:LEU:HB3	1:W:172:TYR:HB2	1.99	0.44
1:5:146:ASP:OD1	1:5:146:ASP:N	2.50	0.44
1:3:181:GLN:HG2	2:8:788:THR:HG21	2.00	0.44
1:G:143:CYS:HA	1:G:154:LEU:O	2.17	0.44
1:I:176:SER:OG	1:I:179:GLN:HB2	3.83	0.44
1:A:141:MSE:HE2	1:A:155:LEU:HD23	4.92	0.44
1:4:85:PRO:O	1:4:89:ILE:HD12	2.16	0.44
1:E:139:ILE:HG23	2:F:794:LYS:HD2	6.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:68:VAL:HA	1:Y:105:PRO:HB3	1.99	0.44
1:G:68:VAL:HA	1:G:105:PRO:HB3	2.64	0.44
1:K:142:VAL:HG22	2:L:789:THR:HG22	2.00	0.44
1:0:181:GLN:HG2	2:9:788:THR:HG21	2.00	0.44
1:4:72:GLU:C	1:4:74:LEU:HD23	2.38	0.44
1:G:104:VAL:HG21	1:W:148:LEU:HB3	96.66	0.44
1:E:68:VAL:HG22	1:E:105:PRO:HB3	2.95	0.44
1:A:135:LEU:HD21	1:A:191:PHE:HA	3.57	0.44
1:Y:83:GLU:N	1:Y:158:LYS:HZ3	2.16	0.43
1:O:157:LEU:HB2	1:O:170:TRP:HB2	2.47	0.43
1:2:179:GLN:HG2	1:3:186:VAL:HG22	1.98	0.43
1:Q:150:ALA:O	1:Q:152:LYS:N	2.50	0.43
1:I:68:VAL:HA	1:I:105:PRO:HB3	1.98	0.43
1:Q:181:GLN:HG2	2:R:788:THR:CG2	2.47	0.43
1:0:68:VAL:HB	1:0:171:VAL:HB	2.00	0.43
1:C:135:LEU:HA	1:C:138:ILE:HD12	2.01	0.43
1:0:144:TYR:HB3	2:9:787:VAL:HG13	1.99	0.43
1:U:68:VAL:HA	1:U:105:PRO:HB3	2.00	0.43
1:G:107:GLU:OE1	1:W:106:PRO:C	96.56	0.43
2:N:785:SER:HA	2:P:788:THR:HA	1.99	0.43
1:3:155:LEU:HB2	1:3:172:TYR:HB2	1.99	0.43
1:O:153:SER:HG	1:O:177:LEU:N	5.68	0.43
1:U:119:ILE:HB	1:U:133:HIS:CD2	3.70	0.43
1:1:153:SER:HB3	1:1:174:CYS:HB2	2.00	0.43
2:H:785:SER:HA	2:F:788:THR:HG22	2.00	0.43
1:C:68:VAL:HG22	1:C:105:PRO:HB3	2.54	0.43
1:U:135:LEU:HA	1:U:138:ILE:HD12	2.13	0.43
1:K:106:PRO:C	1:K:108:GLU:H	2.23	0.43
1:O:146:ASP:H	1:O:154:LEU:HD23	1.83	0.42
2:J:792:ASN:HA	2:J:793:PRO:HD3	1.85	0.42
1:O:86:LEU:HA	1:O:89:ILE:HD12	2.36	0.42
1:1:120:LYS:HE3	1:1:122:SER:HB3	2.01	0.42
1:S:138:ILE:O	2:T:792:ASN:HB3	3.58	0.42
1:S:68:VAL:HA	1:S:105:PRO:HB3	2.00	0.42
2:7:785:SER:HA	2:X:788:THR:HB	87.49	0.42
1:Q:191:PHE:O	1:Q:194:VAL:HG22	2.19	0.42
1:G:139:ILE:HD12	1:G:158:LYS:HG2	2.02	0.42
1:Q:119:ILE:HD12	1:Q:119:ILE:N	2.34	0.42
1:C:71:ILE:HD11	1:C:95:ALA:HB1	2.00	0.42
1:W:68:VAL:HA	1:W:105:PRO:HB3	2.01	0.42
1:G:142:VAL:HB	1:G:156:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:LEU:HD23	1:C:89:ILE:HD12	2.01	0.42
1:Y:68:VAL:HG22	1:Y:105:PRO:HB3	2.76	0.42
1:1:112:MSE:HG3	1:1:121:VAL:HG22	2.02	0.42
1:I:135:LEU:HA	1:I:138:ILE:HD12	2.01	0.42
1:M:68:VAL:HA	1:M:105:PRO:HB3	2.01	0.42
1:S:155:LEU:HD11	1:S:183:ILE:HD12	4.51	0.42
1:E:135:LEU:HA	1:E:138:ILE:HD12	2.33	0.42
1:A:65:ILE:HG12	1:A:112:MSE:HB2	2.00	0.42
1:3:143:CYS:HB3	1:3:155:LEU:HD23	2.02	0.42
1:W:65:ILE:HG12	1:W:112:MSE:HG2	4.69	0.42
1:4:143:CYS:SG	1:4:181:GLN:HG3	2.60	0.42
1:U:68:VAL:HG22	1:U:105:PRO:HB3	2.75	0.42
1:Y:101:LEU:HA	1:Y:102:PRO:HD3	2.00	0.42
1:M:125:ASP:HB2	1:M:127:TYR:HB2	2.02	0.42
1:Y:135:LEU:HA	1:Y:138:ILE:HD12	2.14	0.42
1:M:135:LEU:HA	1:M:138:ILE:HD12	2.13	0.41
1:M:104:VAL:HG11	1:M:105:PRO:O	4.78	0.41
1:G:85:PRO:CB	2:H:789:THR:HG21	2.45	0.41
1:Q:135:LEU:HD11	1:Q:191:PHE:HA	2.01	0.41
1:1:153:SER:O	1:1:173:GLN:HG3	2.19	0.41
2:H:786:ALA:HB2	2:F:789:THR:HG22	2.02	0.41
1:S:88:LEU:HD12	1:S:88:LEU:HA	3.83	0.41
1:M:68:VAL:HG22	1:M:105:PRO:HB3	2.77	0.41
1:O:68:VAL:HG22	1:O:173:GLN:HB2	2.02	0.41
1:C:96:GLN:HB3	1:C:103:PHE:CZ	2.71	0.41
1:5:135:LEU:HA	1:5:138:ILE:HD12	2.02	0.41
2:B:788:THR:HG22	2:Z:785:SER:HA	100.02	0.41
1:I:129:VAL:HB	1:I:132:ARG:NH1	2.36	0.41
1:C:141:MSE:O	2:D:789:THR:HA	2.51	0.41
1:K:130:LEU:HB3	1:K:131:HIS:H	1.55	0.41
1:K:143:CYS:SG	1:K:180:ALA:CB	3.09	0.41
1:K:60:CYS:N	1:K:116:LYS:HZ2	8.87	0.41
1:C:178:GLU:O	1:G:185:LYS:HB3	2.21	0.41
1:Q:92:ILE:O	1:Q:96:GLN:HB2	2.21	0.41
1:E:141:MSE:SE	1:E:184:CYS:SG	3.29	0.41
1:5:143:CYS:HB3	1:5:155:LEU:HD12	2.03	0.41
1:Q:88:LEU:HD12	1:Q:88:LEU:HA	1.98	0.41
1:4:157:LEU:HD12	1:4:172:TYR:HE1	1.86	0.41
1:I:141:MSE:SE	1:I:155:LEU:HD21	2.70	0.41
1:C:159:THR:OG1	1:C:170:TRP:NE1	2.54	0.41
1:4:101:LEU:HA	1:4:102:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LEU:HA	1:A:88:LEU:HD12	3.03	0.41
1:G:108:GLU:HG2	1:W:107:GLU:OE2	89.84	0.41
1:I:121:VAL:HB	1:I:131:HIS:HB2	2.19	0.41
1:M:104:VAL:HA	1:M:105:PRO:HD2	1.89	0.40
2:V:792:ASN:HA	2:V:793:PRO:HD3	2.37	0.40
1:5:148:LEU:HD13	1:5:148:LEU:HA	1.91	0.40
1:C:72:GLU:H	1:C:72:GLU:HG2	1.72	0.40
1:3:145:ASP:HB2	1:3:177:LEU:HD22	2.03	0.40
1:5:152:LYS:HD3	1:5:175:ASN:O	2.21	0.40
1:I:157:LEU:HB3	1:I:170:TRP:HD1	2.98	0.40
1:E:85:PRO:HA	1:E:88:LEU:HD13	2.02	0.40
1:U:104:VAL:HA	1:U:105:PRO:HD2	1.89	0.40
1:K:152:LYS:HE2	1:K:175:ASN:HA	2.04	0.40
1:I:105:PRO:CG	1:I:173:GLN:HE21	3.96	0.40
1:1:65:ILE:HD13	1:1:172:TYR:CD2	2.56	0.40
1:O:145:ASP:HB2	1:O:177:LEU:HD22	3.46	0.40
1:I:130:LEU:HD13	1:I:130:LEU:H	1.87	0.40
1:Q:150:ALA:O	1:Q:152:LYS:HE3	2.22	0.40
1:1:151:GLY:HA3	1:O:104:VAL:HG13	87.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:148:LEU:O	1:Y:97:GLN:OE1[1_655]	2.04	0.16

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	100/157 (64%)	92 (92%)	7 (7%)	1 (1%)	19 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	24	66
1	A	96/157 (61%)	88 (92%)	7 (7%)	1 (1%)	19	61
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%)	21	64
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%)	11	45
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%)	24	66
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%)	24	66
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	46	84

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 (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%)	61	89
1	1	100/132 (76%)	98 (98%)	2 (2%)	63	89
1	2	79/132 (60%)	75 (95%)	4 (5%)	29	69
1	3	88/132 (67%)	85 (97%)	3 (3%)	44	81
1	4	110/132 (83%)	106 (96%)	4 (4%)	42	79
1	5	110/132 (83%)	103 (94%)	7 (6%)	22	59
1	A	92/132 (70%)	88 (96%)	4 (4%)	35	75
1	C	109/132 (83%)	101 (93%)	8 (7%)	17	52
1	E	96/132 (73%)	92 (96%)	4 (4%)	36	76
1	G	109/132 (83%)	106 (97%)	3 (3%)	51	84
1	I	107/132 (81%)	102 (95%)	5 (5%)	32	72
1	K	98/132 (74%)	92 (94%)	6 (6%)	23	61
1	M	107/132 (81%)	101 (94%)	6 (6%)	26	65
1	O	89/132 (67%)	86 (97%)	3 (3%)	44	81
1	Q	104/132 (79%)	98 (94%)	6 (6%)	25	63
1	S	108/132 (82%)	105 (97%)	3 (3%)	51	84
1	U	89/132 (67%)	86 (97%)	3 (3%)	44	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	W	111/132 (84%)	107 (96%)	4 (4%)	42 79
1	Y	111/132 (84%)	105 (95%)	6 (5%)	27 66
1	a	84/132 (64%)	77 (92%)	7 (8%)	14 46
1	c	102/132 (77%)	96 (94%)	6 (6%)	24 63
1	e	108/132 (82%)	100 (93%)	8 (7%)	17 52
1	g	109/132 (83%)	104 (95%)	5 (5%)	33 73
1	i	85/132 (64%)	75 (88%)	10 (12%)	6 26
1	k	91/132 (69%)	85 (93%)	6 (7%)	21 57
1	m	109/132 (83%)	102 (94%)	7 (6%)	22 59
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%)	44 81
1	u	89/132 (67%)	83 (93%)	6 (7%)	20 57
1	w	43/132 (33%)	42 (98%)	1 (2%)	58 87
1	y	83/132 (63%)	77 (93%)	6 (7%)	18 53
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%)	4 19
2	9	7/13 (54%)	7 (100%)	0	100 100
2	B	9/13 (69%)	8 (89%)	1 (11%)	8 29
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 8
2	P	10/13 (77%)	8 (80%)	2 (20%)	1 8
2	R	10/13 (77%)	9 (90%)	1 (10%)	9 34
2	T	10/13 (77%)	10 (100%)	0	100 100
2	V	9/13 (69%)	8 (89%)	1 (11%)	8 29
2	X	11/13 (85%)	10 (91%)	1 (9%)	12 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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%)	9 34
2	h	9/13 (69%)	8 (89%)	1 (11%)	8 29
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%)	4 19
2	v	7/13 (54%)	6 (86%)	1 (14%)	4 19
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%)	30 70

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Some 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 carbohydrates 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%)	0.27	5 (4%) 36 14	65, 77, 88, 97	0
1	1	116/157 (73%)	0.21	0 100 100	66, 72, 83, 91	0
1	2	89/157 (56%)	0.71	8 (8%) 12 4	76, 85, 94, 97	0
1	3	102/157 (64%)	0.60	12 (11%) 6 2	75, 91, 105, 110	0
1	4	127/157 (80%)	0.52	7 (5%) 29 11	58, 76, 87, 90	0
1	5	126/157 (80%)	0.30	0 100 100	55, 72, 82, 86	0
1	A	104/157 (66%)	0.28	4 (3%) 44 18	64, 77, 85, 90	0
1	C	125/157 (79%)	-0.06	0 100 100	46, 50, 56, 67	0
1	E	111/157 (70%)	0.19	2 (1%) 71 43	60, 73, 86, 95	0
1	G	125/157 (79%)	0.12	0 100 100	58, 67, 79, 91	0
1	I	123/157 (78%)	0.06	2 (1%) 74 47	49, 57, 66, 77	0
1	K	114/157 (72%)	0.12	1 (0%) 85 64	55, 70, 82, 85	0
1	M	122/157 (77%)	0.46	2 (1%) 74 47	64, 78, 92, 105	0
1	O	100/157 (63%)	0.68	10 (10%) 9 4	73, 97, 116, 124	0
1	Q	120/157 (76%)	0.58	12 (10%) 9 4	72, 94, 106, 113	0
1	S	124/157 (78%)	0.47	5 (4%) 42 17	71, 87, 101, 110	0
1	U	99/157 (63%)	1.24	21 (21%) 1 1	82, 116, 134, 149	0
1	W	126/157 (80%)	0.78	9 (7%) 19 7	67, 89, 106, 115	0
1	Y	127/157 (80%)	0.65	7 (5%) 29 11	67, 85, 107, 123	0
1	a	97/157 (61%)	1.39	27 (27%) 1 0	101, 119, 153, 158	0
1	c	118/157 (75%)	1.58	27 (22%) 1 1	91, 116, 149, 159	0
1	e	124/157 (78%)	0.74	13 (10%) 8 3	68, 92, 108, 116	0
1	g	125/157 (79%)	1.16	28 (22%) 1 1	87, 106, 120, 134	0
1	i	99/157 (63%)	0.75	17 (17%) 2 1	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%)	1.10	22 (21%) 1 1	90, 110, 125, 131	0
1	m	125/157 (79%)	0.83	17 (13%) 4 1	75, 98, 110, 120	0
1	o	61/157 (38%)	1.61	20 (32%) 0 0	64, 112, 132, 147	0
1	q	45/157 (28%)	0.86	5 (11%) 7 3	73, 107, 121, 127	0
1	s	100/157 (63%)	1.28	22 (22%) 1 1	89, 112, 129, 134	0
1	u	104/157 (66%)	1.35	30 (28%) 1 0	88, 116, 139, 147	0
1	w	47/157 (29%)	0.93	8 (17%) 2 1	77, 107, 133, 139	0
1	y	91/157 (57%)	2.18	42 (46%) 0 0	106, 134, 155, 168	0
2	6	11/15 (73%)	0.04	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%)	0.33	1 (12%) 5 2	68, 73, 79, 80	0
2	9	8/15 (53%)	0.05	0 100 100	64, 70, 78, 79	0
2	B	10/15 (66%)	0.66	1 (10%) 9 4	54, 69, 74, 75	0
2	D	11/15 (73%)	0.03	0 100 100	36, 38, 64, 71	0
2	F	11/15 (73%)	0.29	0 100 100	44, 65, 79, 80	0
2	H	11/15 (73%)	0.03	0 100 100	46, 54, 63, 63	0
2	J	11/15 (73%)	0.71	1 (9%) 11 4	78, 83, 104, 112	0
2	L	11/15 (73%)	-0.03	0 100 100	59, 64, 70, 72	0
2	N	11/15 (73%)	0.41	0 100 100	61, 66, 75, 80	0
2	P	11/15 (73%)	0.23	0 100 100	45, 70, 90, 92	0
2	R	11/15 (73%)	0.73	1 (9%) 11 4	75, 85, 102, 104	0
2	T	11/15 (73%)	0.14	0 100 100	80, 84, 87, 87	0
2	V	10/15 (66%)	0.49	0 100 100	67, 71, 92, 93	0
2	X	12/15 (80%)	0.34	0 100 100	64, 73, 80, 81	0
2	Z	11/15 (73%)	0.81	1 (9%) 11 4	87, 90, 92, 93	0
2	b	10/15 (66%)	0.59	0 100 100	88, 100, 116, 117	0
2	d	11/15 (73%)	0.48	0 100 100	65, 90, 99, 101	0
2	f	11/15 (73%)	0.46	1 (9%) 11 4	73, 78, 81, 83	0
2	h	10/15 (66%)	0.82	1 (10%) 9 4	78, 88, 93, 94	0
2	j	4/15 (26%)	-0.00	0 100 100	90, 92, 92, 95	0
2	l	7/15 (46%)	0.04	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%)	0.67	2 (18%) 2 1	89, 92, 94, 95	0
2	p	5/15 (33%)	1.13	2 (40%) 0 0	111, 117, 118, 121	0
2	r	2/15 (13%)	-0.07	0 100 100	76, 76, 76, 82	0
2	t	8/15 (53%)	0.05	1 (12%) 5 2	53, 57, 92, 94	0
2	v	8/15 (53%)	0.47	0 100 100	80, 88, 104, 104	0
2	x	4/15 (26%)	0.47	0 100 100	74, 78, 80, 83	0
2	z	5/15 (33%)	0.60	0 100 100	99, 102, 108, 109	0
All	All	3703/5474 (67%)	0.68	397 (10%) 8 3	36, 87, 129, 168	0

All (397) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	c	60	CYS	23.6
1	a	70	ALA	12.5
1	y	70	ALA	11.6
1	y	169	LEU	11.5
1	c	109	GLU	9.7
1	c	110	PHE	9.0
1	U	194	VAL	8.6
1	o	142	VAL	8.6
1	u	70	ALA	8.5
1	c	132	ARG	8.0
1	y	92	ILE	8.0
1	k	178	GLU	7.4
1	M	195	LEU	7.2
1	4	142	VAL	7.2
1	o	121	VAL	7.1
1	u	100	LYS	6.9
1	k	91	TYR	6.9
1	W	167	TYR	6.5
1	m	142	VAL	6.5
1	U	70	ALA	6.4
1	c	117	TYR	6.2
1	y	62	GLU	6.1
1	g	139	ILE	6.0
1	y	142	VAL	5.9
1	s	187	LEU	5.8
1	i	69	GLY	5.8
1	u	170	TRP	5.8
1	Y	195	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	s	188	SER	5.8
1	y	105	PRO	5.7
1	W	136	TYR	5.7
1	a	86	LEU	5.7
1	s	70	ALA	5.6
1	m	167	TYR	5.5
1	y	88	LEU	5.5
1	g	138	ILE	5.5
1	U	120	LYS	5.4
1	q	68	VAL	5.3
1	W	91	TYR	5.3
1	w	187	LEU	5.3
1	o	144	TYR	5.2
1	c	111	ILE	5.2
1	u	103	PHE	5.2
1	w	104	VAL	5.1
1	a	175	ASN	5.0
1	o	114	VAL	5.0
1	c	61	ALA	5.0
1	a	111	ILE	4.9
1	i	120	LYS	4.9
1	y	136	TYR	4.8
1	s	133	HIS	4.8
1	a	65	ILE	4.8
1	0	111	ILE	4.7
1	3	100	LYS	4.7
1	g	144	TYR	4.7
1	W	174	CYS	4.7
1	u	157	LEU	4.7
1	o	184	CYS	4.7
1	k	179	GLN	4.7
1	o	140	ARG	4.6
1	3	99	GLY	4.6
1	s	142	VAL	4.6
1	2	69	GLY	4.6
1	2	142	VAL	4.6
1	g	134	ALA	4.5
1	k	64	ARG	4.5
1	2	191	PHE	4.5
1	s	195	LEU	4.5
1	a	92	ILE	4.5
1	W	124	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	y	71	ILE	4.4
1	i	177	LEU	4.4
1	c	64	ARG	4.4
1	w	109	GLU	4.4
1	o	143	CYS	4.4
1	o	92	ILE	4.3
1	y	106	PRO	4.3
1	g	167	TYR	4.3
1	a	167	TYR	4.2
2	R	789	THR	4.2
1	g	135	LEU	4.2
1	u	177	LEU	4.2
1	u	69	GLY	4.2
1	u	153	SER	4.1
1	u	158	LYS	4.1
1	o	183	ILE	4.1
1	g	59	THR	4.1
1	U	193	SER	4.1
1	2	187	LEU	4.1
1	i	149	GLY	4.0
1	Q	135	LEU	4.0
1	y	64	ARG	4.0
1	a	72	GLU	4.0
1	a	71	ILE	4.0
1	g	89	ILE	4.0
1	u	97	GLN	4.0
1	g	158	LYS	4.0
1	m	137	LEU	4.0
1	y	108	GLU	3.9
1	g	133	HIS	3.9
1	y	154	LEU	3.9
1	i	133	HIS	3.9
1	k	167	TYR	3.9
1	O	159	THR	3.9
1	a	91	TYR	3.9
1	a	120	LYS	3.9
2	B	789	THR	3.9
1	O	172	TYR	3.9
1	k	134	ALA	3.8
1	y	187	LEU	3.8
1	o	169	LEU	3.8
1	g	170	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
1	Q	89	ILE	3.8
1	e	136	TYR	3.8
1	y	139	ILE	3.7
1	m	116	LYS	3.7
1	k	63	PHE	3.7
1	c	191	PHE	3.7
1	u	62	GLU	3.7
1	y	116	LYS	3.7
1	U	65	ILE	3.7
1	u	171	VAL	3.7
1	s	67	TYR	3.7
1	c	136	TYR	3.7
1	a	173	GLN	3.7
1	2	155	LEU	3.6
1	u	151	GLY	3.6
1	k	113	GLY	3.6
1	s	71	ILE	3.6
1	w	108	GLU	3.6
1	O	138	ILE	3.6
1	3	156	ALA	3.5
1	o	172	TYR	3.5
1	O	92	ILE	3.5
1	e	111	ILE	3.5
1	y	63	PHE	3.5
1	W	175	ASN	3.5
1	g	142	VAL	3.5
1	k	65	ILE	3.5
1	U	135	LEU	3.5
1	c	63	PHE	3.5
1	u	67	TYR	3.5
1	a	133	HIS	3.4
1	i	70	ALA	3.4
1	i	121	VAL	3.4
1	m	136	TYR	3.4
1	y	174	CYS	3.4
1	g	196	THR	3.4
1	Q	162	ALA	3.4
1	U	136	TYR	3.4
1	y	189	THR	3.4
1	s	132	ARG	3.4
1	y	153	SER	3.4
1	c	129	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	y	172	TYR	3.4
1	a	68	VAL	3.4
1	Q	195	LEU	3.4
1	u	104	VAL	3.4
1	U	67	TYR	3.3
1	y	134	ALA	3.3
1	y	65	ILE	3.3
1	a	95	ALA	3.3
1	u	174	CYS	3.3
1	s	144	TYR	3.3
1	g	136	TYR	3.3
1	y	140	ARG	3.3
1	2	182	ALA	3.2
1	e	63	PHE	3.2
1	k	160	THR	3.2
1	s	64	ARG	3.2
1	y	143	CYS	3.2
1	4	94	VAL	3.2
1	i	155	LEU	3.2
1	c	167	TYR	3.2
1	c	120	LYS	3.2
1	m	111	ILE	3.1
1	y	121	VAL	3.1
1	g	183	ILE	3.1
1	O	71	ILE	3.1
1	a	170	TRP	3.1
1	m	63	PHE	3.1
1	g	63	PHE	3.1
1	4	177	LEU	3.1
1	m	114	VAL	3.1
1	i	119	ILE	3.1
1	3	92	ILE	3.1
1	y	86	LEU	3.1
1	Q	172	TYR	3.1
1	c	162	ALA	3.1
1	U	71	ILE	3.1
1	g	137	LEU	3.1
1	m	59	THR	3.0
1	a	101	LEU	3.0
1	3	129	VAL	3.0
1	g	114	VAL	3.0
1	w	65	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	k	88	LEU	3.0
1	o	86	LEU	3.0
1	c	123	THR	3.0
1	e	187	LEU	3.0
1	o	115	SER	3.0
1	q	106	PRO	2.9
1	U	119	ILE	2.9
1	a	177	LEU	2.9
1	a	114	VAL	2.9
1	Y	85	PRO	2.9
1	o	88	LEU	2.9
1	e	114	VAL	2.9
1	4	92	ILE	2.9
1	O	86	LEU	2.9
1	O	173	GLN	2.9
1	m	179	GLN	2.9
1	w	171	VAL	2.9
1	3	94	VAL	2.9
1	u	137	LEU	2.9
1	s	120	LYS	2.9
1	U	131	HIS	2.9
1	a	172	TYR	2.8
1	s	186	VAL	2.8
1	S	91	TYR	2.8
1	g	90	ASN	2.8
1	m	184	CYS	2.8
1	e	191	PHE	2.8
1	U	191	PHE	2.8
1	q	69	GLY	2.8
2	p	791	VAL	2.8
1	3	97	GLN	2.7
1	S	107	GLU	2.7
1	o	153	SER	2.7
1	s	157	LEU	2.7
1	Q	120	LYS	2.7
1	O	70	ALA	2.7
1	g	156	ALA	2.7
1	U	62	GLU	2.7
1	c	192	ASP	2.7
1	g	98	ASP	2.7
1	c	62	GLU	2.7
1	g	132	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	e	86	LEU	2.7
1	e	126	GLN	2.7
1	u	156	ALA	2.7
1	c	114	VAL	2.7
1	i	167	TYR	2.7
1	E	122	SER	2.7
1	e	142	VAL	2.6
1	Q	110	PHE	2.6
1	2	144	TYR	2.6
1	u	159	THR	2.6
1	S	89	ILE	2.6
1	a	116	LYS	2.6
1	A	157	LEU	2.6
1	u	169	LEU	2.6
1	c	187	LEU	2.6
1	S	88	LEU	2.6
1	a	179	GLN	2.6
2	n	790	VAL	2.6
2	p	790	VAL	2.6
1	m	169	LEU	2.6
1	U	137	LEU	2.6
1	U	90	ASN	2.6
1	c	153	SER	2.6
1	u	98	ASP	2.6
1	A	120	LYS	2.6
1	k	185	LYS	2.6
1	c	160	THR	2.6
1	k	86	LEU	2.6
1	k	146	ASP	2.6
1	y	87	ASP	2.6
1	u	94	VAL	2.6
1	g	86	LEU	2.5
1	m	158	LYS	2.5
1	S	65	ILE	2.5
1	q	187	LEU	2.5
1	a	69	GLY	2.5
1	y	60	CYS	2.5
1	c	100	LYS	2.5
1	y	185	LYS	2.5
2	J	791	VAL	2.5
1	i	118	GLY	2.5
1	c	89	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	191	PHE	2.5
1	u	71	ILE	2.5
1	o	113	GLY	2.5
1	Q	64	ARG	2.5
1	s	175	ASN	2.5
1	k	97	GLN	2.5
1	y	182	ALA	2.5
1	a	64	ARG	2.5
1	I	191	PHE	2.5
1	o	182	ALA	2.5
1	U	111	ILE	2.5
1	A	194	VAL	2.5
1	E	186	VAL	2.5
1	3	103	PHE	2.5
1	s	169	LEU	2.4
1	U	86	LEU	2.4
1	i	62	GLU	2.4
1	y	181	GLN	2.4
1	I	142	VAL	2.4
1	s	166	GLU	2.4
1	m	187	LEU	2.4
1	W	190	ALA	2.4
2	n	789	THR	2.4
1	U	169	LEU	2.4
1	Y	154	LEU	2.4
1	k	98	ASP	2.4
1	i	187	LEU	2.4
1	U	110	PHE	2.4
1	0	120	LYS	2.4
1	o	156	ALA	2.4
1	q	103	PHE	2.4
1	O	157	LEU	2.3
1	Q	177	LEU	2.3
1	Y	175	ASN	2.3
1	y	144	TYR	2.3
1	c	186	VAL	2.3
1	s	172	TYR	2.3
2	h	790	VAL	2.3
1	y	138	ILE	2.3
1	Q	144	TYR	2.3
1	k	183	ILE	2.3
1	3	158	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	k	145	ASP	2.3
1	3	86	LEU	2.3
1	c	169	LEU	2.3
1	g	88	LEU	2.3
1	m	170	TRP	2.3
1	u	183	ILE	2.3
2	f	789	THR	2.3
1	k	171	VAL	2.3
1	Q	186	VAL	2.3
1	a	87	ASP	2.3
1	a	181	GLN	2.3
1	y	179	GLN	2.3
1	u	150	ALA	2.3
1	0	98	ASP	2.3
1	y	183	ILE	2.3
1	4	122	SER	2.2
1	y	175	ASN	2.2
1	k	90	ASN	2.2
1	0	102	PRO	2.2
1	K	110	PHE	2.2
1	i	92	ILE	2.2
1	y	117	TYR	2.2
1	4	186	VAL	2.2
2	8	787	VAL	2.2
1	U	64	ARG	2.2
1	i	68	VAL	2.2
1	m	191	PHE	2.2
1	3	157	LEU	2.2
1	O	91	TYR	2.2
1	e	169	LEU	2.2
1	g	145	ASP	2.1
1	g	177	LEU	2.1
1	y	195	LEU	2.1
1	0	88	LEU	2.1
1	U	157	LEU	2.1
1	y	184	CYS	2.1
1	u	167	TYR	2.1
1	2	154	LEU	2.1
1	c	142	VAL	2.1
1	W	189	THR	2.1
1	A	191	PHE	2.1
1	s	105	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	u	107	GLU	2.1
1	s	189	THR	2.1
1	k	102	PRO	2.1
1	a	135	LEU	2.1
1	g	72	GLU	2.1
2	t	787	VAL	2.1
1	u	190	ALA	2.1
1	4	144	TYR	2.1
1	i	90	ASN	2.1
1	Y	135	LEU	2.1
1	o	93	ASP	2.1
1	u	99	GLY	2.1
1	w	172	TYR	2.1
1	y	109	GLU	2.1
1	k	177	LEU	2.1
1	o	103	PHE	2.1
1	Y	159	THR	2.1
1	W	116	LYS	2.1
1	3	171	VAL	2.1
1	s	102	PRO	2.1
1	s	140	ARG	2.1
1	e	64	ARG	2.1
1	Q	167	TYR	2.0
1	e	135	LEU	2.0
1	g	60	CYS	2.0
1	y	114	VAL	2.0
1	e	100	LYS	2.0
1	u	65	ILE	2.0
1	Y	91	TYR	2.0
1	m	90	ASN	2.0
1	w	68	VAL	2.0
1	i	158	LYS	2.0
2	Z	791	VAL	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.