



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2017 – 10:54 PM EST

PDB ID : 5LHY
Title : PB3 Domain of Human PLK4 (apo)
Authors : Cottee, M.A.; Johnson, S.; Lea, S.M.
Deposited on : 2016-07-13
Resolution : 3.31 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

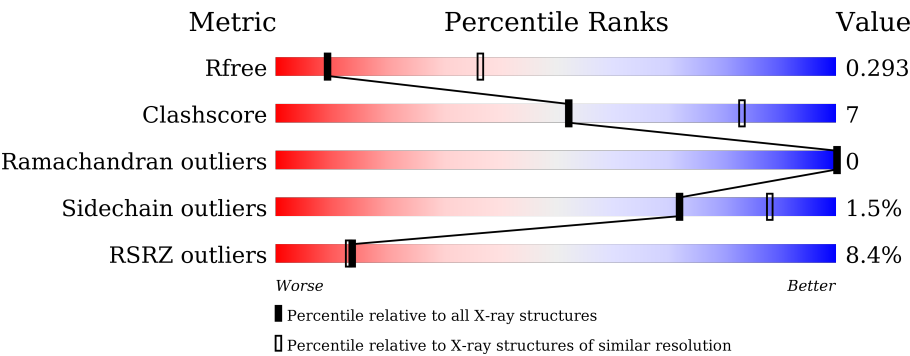
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1198 (3.40-3.24)
Clashscore	102246	1280 (3.40-3.24)
Ramachandran outliers	100387	1260 (3.40-3.24)
Sidechain outliers	100360	1259 (3.40-3.24)
RSRZ outliers	91569	1203 (3.40-3.24)

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 $\leq 5\%$. 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	1	91	<div><div>3%</div><div><div></div><div>69%</div><div>14%</div><div>•</div><div>15%</div></div></div>
1	2	91	<div><div>7%</div><div><div></div><div>63%</div><div>21%</div><div>•</div><div>15%</div></div></div>
1	3	91	<div><div>2%</div><div><div></div><div>69%</div><div>13%</div><div>•</div><div>15%</div></div></div>
1	4	91	<div><div>2%</div><div><div></div><div>73%</div><div>11%</div><div>•</div><div>15%</div></div></div>
1	5	91	<div><div></div><div><div></div><div>64%</div><div>20%</div><div>•</div><div>15%</div></div></div>
1	6	91	<div><div></div><div><div></div><div>69%</div><div>15%</div><div></div><div>15%</div></div></div>


























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Mol	Chain	Length	Quality of chain
1	7	91	
1	8	91	
1	9	91	
1	A	91	
1	B	91	
1	C	91	
1	D	91	
1	E	91	
1	F	91	
1	G	91	
1	H	91	
1	I	91	
1	J	91	
1	K	91	
1	L	91	
1	M	91	
1	N	91	
1	O	91	
1	P	91	
1	Q	91	
1	R	91	
1	S	91	
1	T	91	
1	U	91	
1	V	91	





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Mol	Chain	Length	Quality of chain
1	W	91	
1	X	91	
1	Y	91	
1	Z	91	
1	a	91	
1	b	91	
1	c	91	
1	d	91	
1	e	91	
1	f	91	
1	g	91	
1	h	91	
1	i	91	
1	j	91	
1	k	91	
1	l	91	
1	m	91	
1	n	91	
1	o	91	
1	p	91	
1	q	91	
1	r	91	
1	s	91	
1	t	91	
1	u	91	

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Mol	Chain	Length	Quality of chain
1	v	91	 4%85%15%
1	w	91	 8%84%15%
1	x	91	 4%84%15%
1	y	91	 3%84%15%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 35580 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 Serine/threonine-protein kinase PLK4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	B	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	C	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	D	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	E	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	F	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	G	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	H	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	I	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	J	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	K	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	L	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	M	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	N	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	O	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	P	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	R	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	S	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	T	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	U	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	V	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	W	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	X	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	Y	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	Z	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	1	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	2	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	3	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	4	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	5	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	6	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	7	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	8	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	9	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	a	77	Total 593	C 377	N 98	O 116	S 2	0	0	0
1	b	77	Total 593	C 377	N 98	O 116	S 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	c	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	d	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	e	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	f	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	g	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	h	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	i	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	j	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	k	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	l	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	m	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	n	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	o	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	p	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	q	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	r	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	s	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	t	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	u	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	v	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	w	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	x	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			
1	y	77	Total	C	N	O	S	0	0	0
			593	377	98	116	2			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	880	GLY	-	expression tag	UNP O00444
A	881	PRO	-	expression tag	UNP O00444
A	882	MET	-	expression tag	UNP O00444
A	883	GLY	-	expression tag	UNP O00444
B	880	GLY	-	expression tag	UNP O00444
B	881	PRO	-	expression tag	UNP O00444
B	882	MET	-	expression tag	UNP O00444
B	883	GLY	-	expression tag	UNP O00444
C	880	GLY	-	expression tag	UNP O00444
C	881	PRO	-	expression tag	UNP O00444
C	882	MET	-	expression tag	UNP O00444
C	883	GLY	-	expression tag	UNP O00444
D	880	GLY	-	expression tag	UNP O00444
D	881	PRO	-	expression tag	UNP O00444
D	882	MET	-	expression tag	UNP O00444
D	883	GLY	-	expression tag	UNP O00444
E	880	GLY	-	expression tag	UNP O00444
E	881	PRO	-	expression tag	UNP O00444
E	882	MET	-	expression tag	UNP O00444
E	883	GLY	-	expression tag	UNP O00444
F	880	GLY	-	expression tag	UNP O00444
F	881	PRO	-	expression tag	UNP O00444
F	882	MET	-	expression tag	UNP O00444
F	883	GLY	-	expression tag	UNP O00444
G	880	GLY	-	expression tag	UNP O00444
G	881	PRO	-	expression tag	UNP O00444
G	882	MET	-	expression tag	UNP O00444
G	883	GLY	-	expression tag	UNP O00444
H	880	GLY	-	expression tag	UNP O00444
H	881	PRO	-	expression tag	UNP O00444
H	882	MET	-	expression tag	UNP O00444
H	883	GLY	-	expression tag	UNP O00444
I	880	GLY	-	expression tag	UNP O00444
I	881	PRO	-	expression tag	UNP O00444

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Chain	Residue	Modelled	Actual	Comment	Reference
I	882	MET	-	expression tag	UNP O00444
I	883	GLY	-	expression tag	UNP O00444
J	880	GLY	-	expression tag	UNP O00444
J	881	PRO	-	expression tag	UNP O00444
J	882	MET	-	expression tag	UNP O00444
J	883	GLY	-	expression tag	UNP O00444
K	880	GLY	-	expression tag	UNP O00444
K	881	PRO	-	expression tag	UNP O00444
K	882	MET	-	expression tag	UNP O00444
K	883	GLY	-	expression tag	UNP O00444
L	880	GLY	-	expression tag	UNP O00444
L	881	PRO	-	expression tag	UNP O00444
L	882	MET	-	expression tag	UNP O00444
L	883	GLY	-	expression tag	UNP O00444
M	880	GLY	-	expression tag	UNP O00444
M	881	PRO	-	expression tag	UNP O00444
M	882	MET	-	expression tag	UNP O00444
M	883	GLY	-	expression tag	UNP O00444
N	880	GLY	-	expression tag	UNP O00444
N	881	PRO	-	expression tag	UNP O00444
N	882	MET	-	expression tag	UNP O00444
N	883	GLY	-	expression tag	UNP O00444
O	880	GLY	-	expression tag	UNP O00444
O	881	PRO	-	expression tag	UNP O00444
O	882	MET	-	expression tag	UNP O00444
O	883	GLY	-	expression tag	UNP O00444
P	880	GLY	-	expression tag	UNP O00444
P	881	PRO	-	expression tag	UNP O00444
P	882	MET	-	expression tag	UNP O00444
P	883	GLY	-	expression tag	UNP O00444
Q	880	GLY	-	expression tag	UNP O00444
Q	881	PRO	-	expression tag	UNP O00444
Q	882	MET	-	expression tag	UNP O00444
Q	883	GLY	-	expression tag	UNP O00444
R	880	GLY	-	expression tag	UNP O00444
R	881	PRO	-	expression tag	UNP O00444
R	882	MET	-	expression tag	UNP O00444
R	883	GLY	-	expression tag	UNP O00444
S	880	GLY	-	expression tag	UNP O00444
S	881	PRO	-	expression tag	UNP O00444
S	882	MET	-	expression tag	UNP O00444
S	883	GLY	-	expression tag	UNP O00444

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Chain	Residue	Modelled	Actual	Comment	Reference
T	880	GLY	-	expression tag	UNP O00444
T	881	PRO	-	expression tag	UNP O00444
T	882	MET	-	expression tag	UNP O00444
T	883	GLY	-	expression tag	UNP O00444
U	880	GLY	-	expression tag	UNP O00444
U	881	PRO	-	expression tag	UNP O00444
U	882	MET	-	expression tag	UNP O00444
U	883	GLY	-	expression tag	UNP O00444
V	880	GLY	-	expression tag	UNP O00444
V	881	PRO	-	expression tag	UNP O00444
V	882	MET	-	expression tag	UNP O00444
V	883	GLY	-	expression tag	UNP O00444
W	880	GLY	-	expression tag	UNP O00444
W	881	PRO	-	expression tag	UNP O00444
W	882	MET	-	expression tag	UNP O00444
W	883	GLY	-	expression tag	UNP O00444
X	880	GLY	-	expression tag	UNP O00444
X	881	PRO	-	expression tag	UNP O00444
X	882	MET	-	expression tag	UNP O00444
X	883	GLY	-	expression tag	UNP O00444
Y	880	GLY	-	expression tag	UNP O00444
Y	881	PRO	-	expression tag	UNP O00444
Y	882	MET	-	expression tag	UNP O00444
Y	883	GLY	-	expression tag	UNP O00444
Z	880	GLY	-	expression tag	UNP O00444
Z	881	PRO	-	expression tag	UNP O00444
Z	882	MET	-	expression tag	UNP O00444
Z	883	GLY	-	expression tag	UNP O00444
1	880	GLY	-	expression tag	UNP O00444
1	881	PRO	-	expression tag	UNP O00444
1	882	MET	-	expression tag	UNP O00444
1	883	GLY	-	expression tag	UNP O00444
2	880	GLY	-	expression tag	UNP O00444
2	881	PRO	-	expression tag	UNP O00444
2	882	MET	-	expression tag	UNP O00444
2	883	GLY	-	expression tag	UNP O00444
3	880	GLY	-	expression tag	UNP O00444
3	881	PRO	-	expression tag	UNP O00444
3	882	MET	-	expression tag	UNP O00444
3	883	GLY	-	expression tag	UNP O00444
4	880	GLY	-	expression tag	UNP O00444
4	881	PRO	-	expression tag	UNP O00444

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Chain	Residue	Modelled	Actual	Comment	Reference
4	882	MET	-	expression tag	UNP O00444
4	883	GLY	-	expression tag	UNP O00444
5	880	GLY	-	expression tag	UNP O00444
5	881	PRO	-	expression tag	UNP O00444
5	882	MET	-	expression tag	UNP O00444
5	883	GLY	-	expression tag	UNP O00444
6	880	GLY	-	expression tag	UNP O00444
6	881	PRO	-	expression tag	UNP O00444
6	882	MET	-	expression tag	UNP O00444
6	883	GLY	-	expression tag	UNP O00444
7	880	GLY	-	expression tag	UNP O00444
7	881	PRO	-	expression tag	UNP O00444
7	882	MET	-	expression tag	UNP O00444
7	883	GLY	-	expression tag	UNP O00444
8	880	GLY	-	expression tag	UNP O00444
8	881	PRO	-	expression tag	UNP O00444
8	882	MET	-	expression tag	UNP O00444
8	883	GLY	-	expression tag	UNP O00444
9	880	GLY	-	expression tag	UNP O00444
9	881	PRO	-	expression tag	UNP O00444
9	882	MET	-	expression tag	UNP O00444
9	883	GLY	-	expression tag	UNP O00444
a	880	GLY	-	expression tag	UNP O00444
a	881	PRO	-	expression tag	UNP O00444
a	882	MET	-	expression tag	UNP O00444
a	883	GLY	-	expression tag	UNP O00444
b	880	GLY	-	expression tag	UNP O00444
b	881	PRO	-	expression tag	UNP O00444
b	882	MET	-	expression tag	UNP O00444
b	883	GLY	-	expression tag	UNP O00444
c	880	GLY	-	expression tag	UNP O00444
c	881	PRO	-	expression tag	UNP O00444
c	882	MET	-	expression tag	UNP O00444
c	883	GLY	-	expression tag	UNP O00444
d	880	GLY	-	expression tag	UNP O00444
d	881	PRO	-	expression tag	UNP O00444
d	882	MET	-	expression tag	UNP O00444
d	883	GLY	-	expression tag	UNP O00444
e	880	GLY	-	expression tag	UNP O00444
e	881	PRO	-	expression tag	UNP O00444
e	882	MET	-	expression tag	UNP O00444
e	883	GLY	-	expression tag	UNP O00444

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Chain	Residue	Modelled	Actual	Comment	Reference
f	880	GLY	-	expression tag	UNP O00444
f	881	PRO	-	expression tag	UNP O00444
f	882	MET	-	expression tag	UNP O00444
f	883	GLY	-	expression tag	UNP O00444
g	880	GLY	-	expression tag	UNP O00444
g	881	PRO	-	expression tag	UNP O00444
g	882	MET	-	expression tag	UNP O00444
g	883	GLY	-	expression tag	UNP O00444
h	880	GLY	-	expression tag	UNP O00444
h	881	PRO	-	expression tag	UNP O00444
h	882	MET	-	expression tag	UNP O00444
h	883	GLY	-	expression tag	UNP O00444
i	880	GLY	-	expression tag	UNP O00444
i	881	PRO	-	expression tag	UNP O00444
i	882	MET	-	expression tag	UNP O00444
i	883	GLY	-	expression tag	UNP O00444
j	880	GLY	-	expression tag	UNP O00444
j	881	PRO	-	expression tag	UNP O00444
j	882	MET	-	expression tag	UNP O00444
j	883	GLY	-	expression tag	UNP O00444
k	880	GLY	-	expression tag	UNP O00444
k	881	PRO	-	expression tag	UNP O00444
k	882	MET	-	expression tag	UNP O00444
k	883	GLY	-	expression tag	UNP O00444
l	880	GLY	-	expression tag	UNP O00444
l	881	PRO	-	expression tag	UNP O00444
l	882	MET	-	expression tag	UNP O00444
l	883	GLY	-	expression tag	UNP O00444
m	880	GLY	-	expression tag	UNP O00444
m	881	PRO	-	expression tag	UNP O00444
m	882	MET	-	expression tag	UNP O00444
m	883	GLY	-	expression tag	UNP O00444
n	880	GLY	-	expression tag	UNP O00444
n	881	PRO	-	expression tag	UNP O00444
n	882	MET	-	expression tag	UNP O00444
n	883	GLY	-	expression tag	UNP O00444
o	880	GLY	-	expression tag	UNP O00444
o	881	PRO	-	expression tag	UNP O00444
o	882	MET	-	expression tag	UNP O00444
o	883	GLY	-	expression tag	UNP O00444
p	880	GLY	-	expression tag	UNP O00444
p	881	PRO	-	expression tag	UNP O00444

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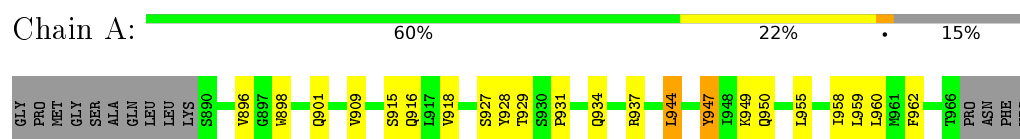
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Chain	Residue	Modelled	Actual	Comment	Reference
p	882	MET	-	expression tag	UNP O00444
p	883	GLY	-	expression tag	UNP O00444
q	880	GLY	-	expression tag	UNP O00444
q	881	PRO	-	expression tag	UNP O00444
q	882	MET	-	expression tag	UNP O00444
q	883	GLY	-	expression tag	UNP O00444
r	880	GLY	-	expression tag	UNP O00444
r	881	PRO	-	expression tag	UNP O00444
r	882	MET	-	expression tag	UNP O00444
r	883	GLY	-	expression tag	UNP O00444
s	880	GLY	-	expression tag	UNP O00444
s	881	PRO	-	expression tag	UNP O00444
s	882	MET	-	expression tag	UNP O00444
s	883	GLY	-	expression tag	UNP O00444
t	880	GLY	-	expression tag	UNP O00444
t	881	PRO	-	expression tag	UNP O00444
t	882	MET	-	expression tag	UNP O00444
t	883	GLY	-	expression tag	UNP O00444
u	880	GLY	-	expression tag	UNP O00444
u	881	PRO	-	expression tag	UNP O00444
u	882	MET	-	expression tag	UNP O00444
u	883	GLY	-	expression tag	UNP O00444
v	880	GLY	-	expression tag	UNP O00444
v	881	PRO	-	expression tag	UNP O00444
v	882	MET	-	expression tag	UNP O00444
v	883	GLY	-	expression tag	UNP O00444
w	880	GLY	-	expression tag	UNP O00444
w	881	PRO	-	expression tag	UNP O00444
w	882	MET	-	expression tag	UNP O00444
w	883	GLY	-	expression tag	UNP O00444
x	880	GLY	-	expression tag	UNP O00444
x	881	PRO	-	expression tag	UNP O00444
x	882	MET	-	expression tag	UNP O00444
x	883	GLY	-	expression tag	UNP O00444
y	880	GLY	-	expression tag	UNP O00444
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y	883	GLY	-	expression tag	UNP O00444

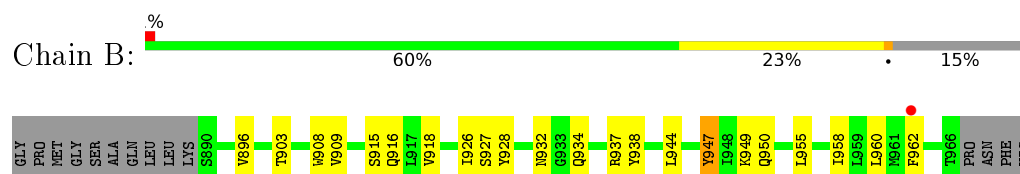
3 Residue-property plots [i](#)

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.

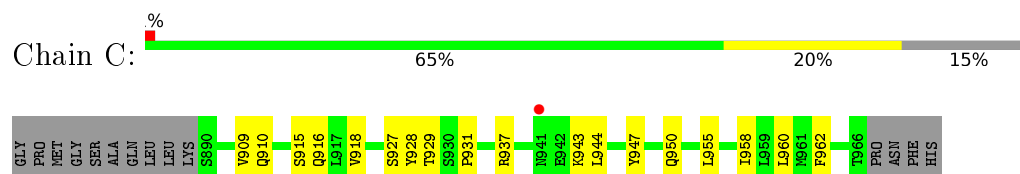
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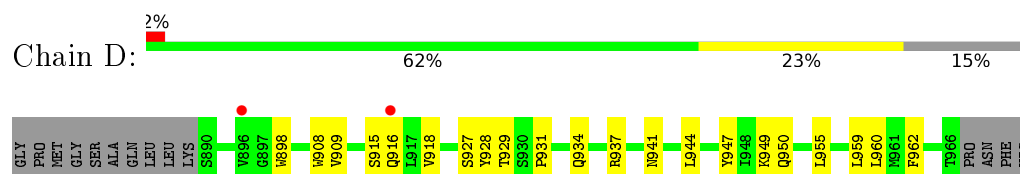
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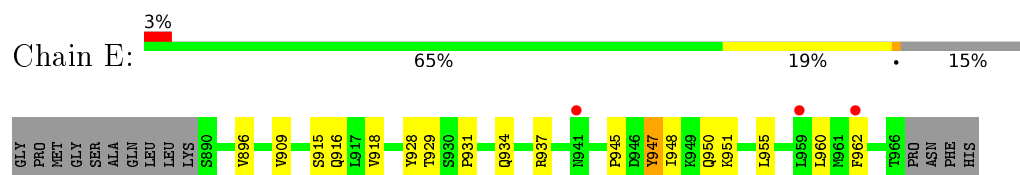
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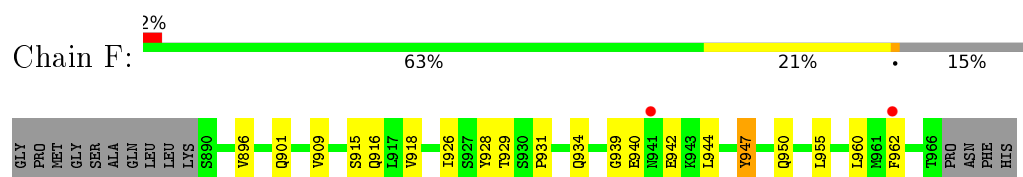
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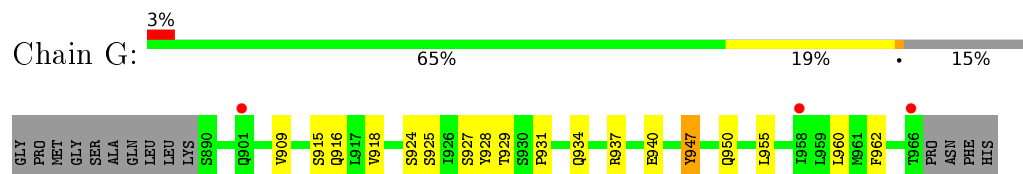
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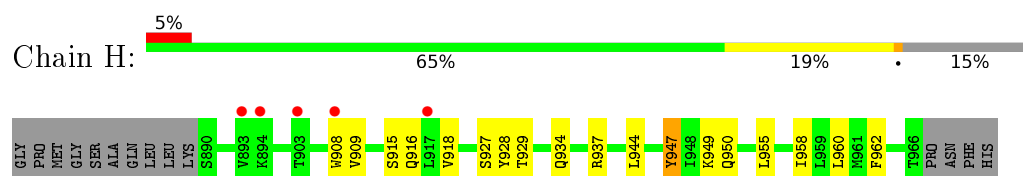
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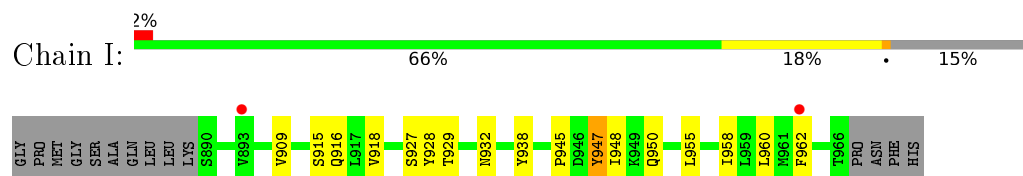
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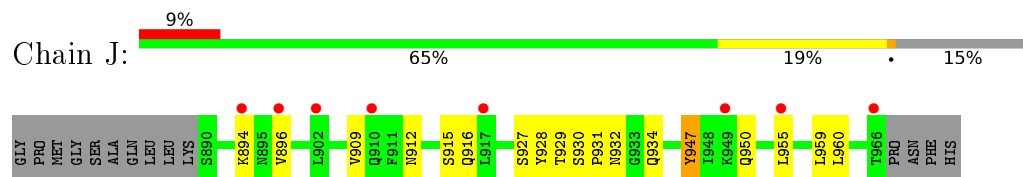
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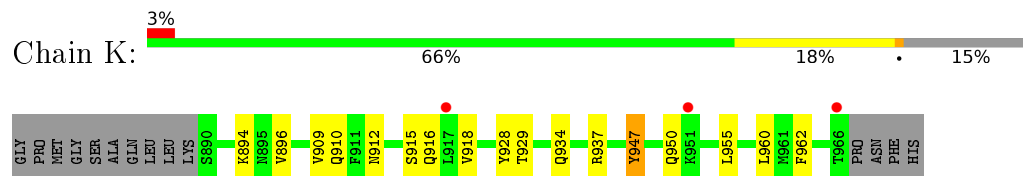
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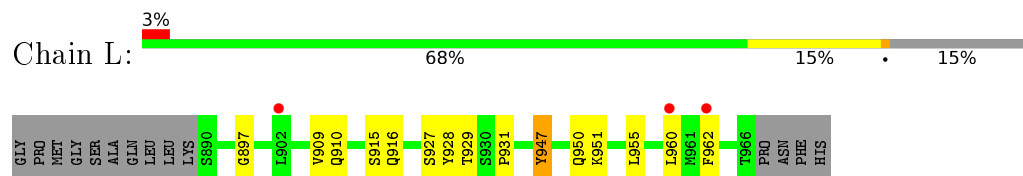
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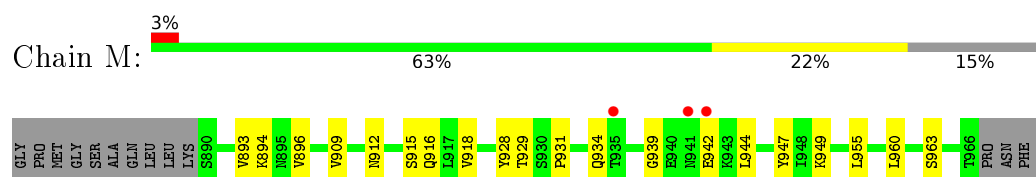
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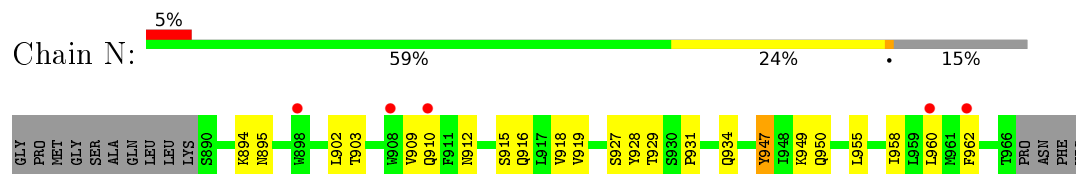
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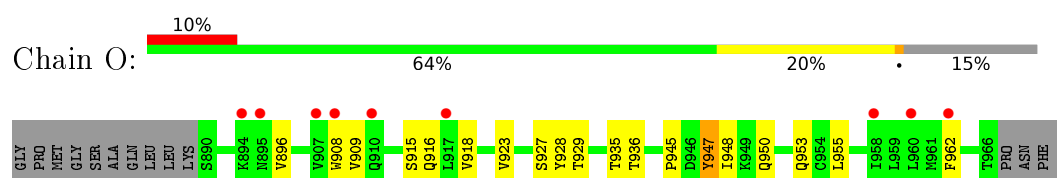
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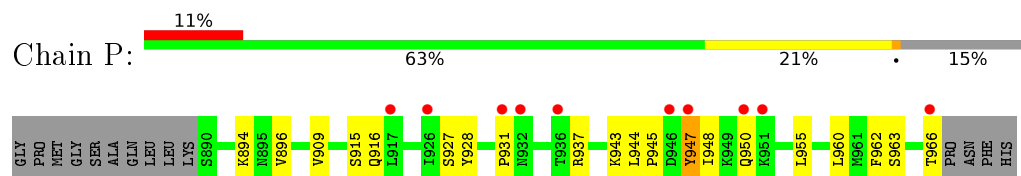
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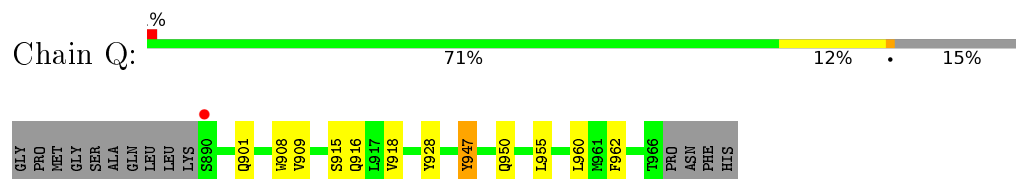
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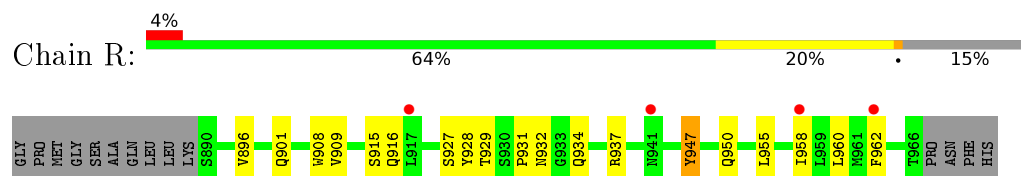
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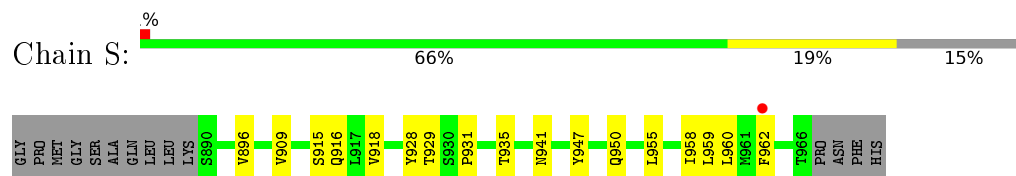
- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4

Chain T: 



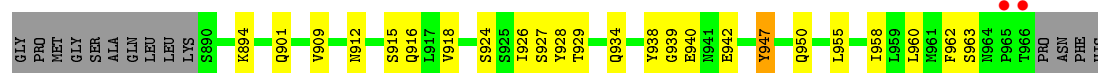
- Molecule 1: Serine/threonine-protein kinase PLK4

Chain U: 



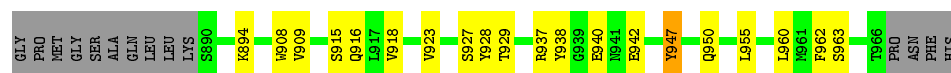
- Molecule 1: Serine/threonine-protein kinase PLK4

Chain V: 



- Molecule 1: Serine/threonine-protein kinase PLK4

Chain W: 



- Molecule 1: Serine/threonine-protein kinase PLK4

Chain X: 




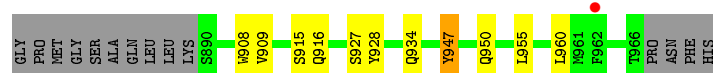
- Molecule 1: Serine/threonine-protein kinase PLK4

Chain Y: 

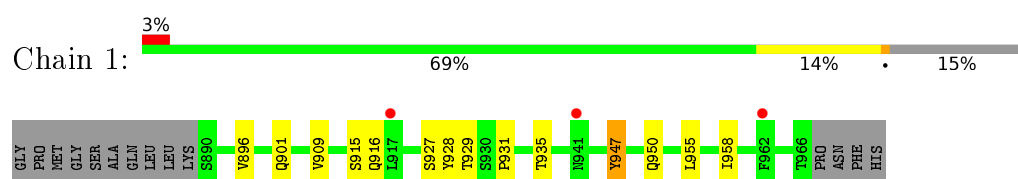


- Molecule 1: Serine/threonine-protein kinase PLK4

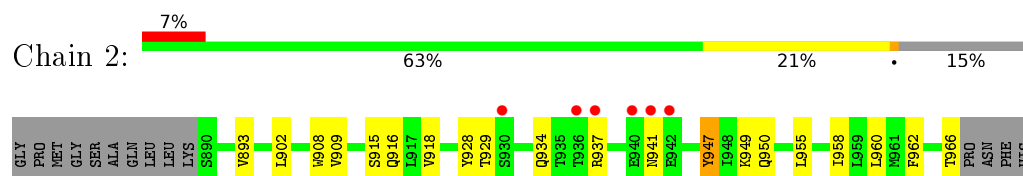
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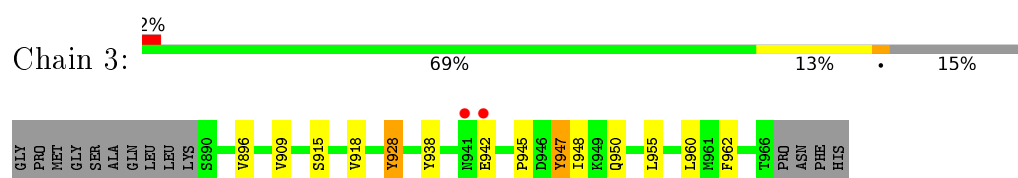
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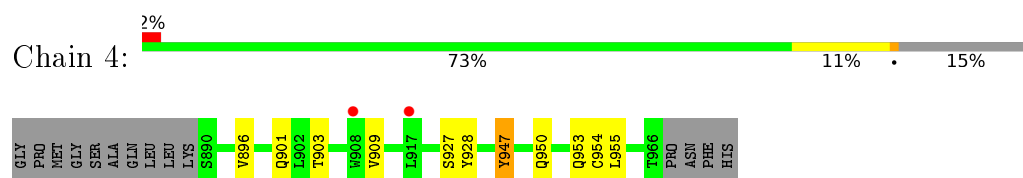
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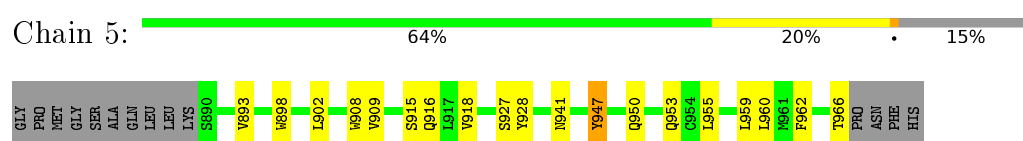
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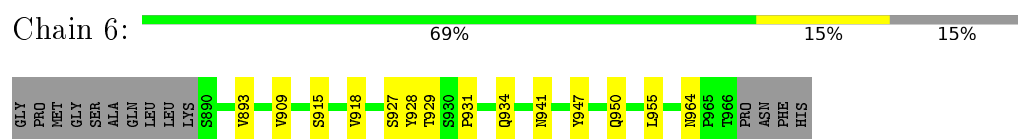
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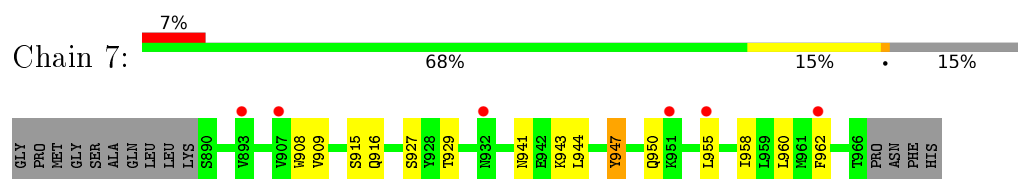
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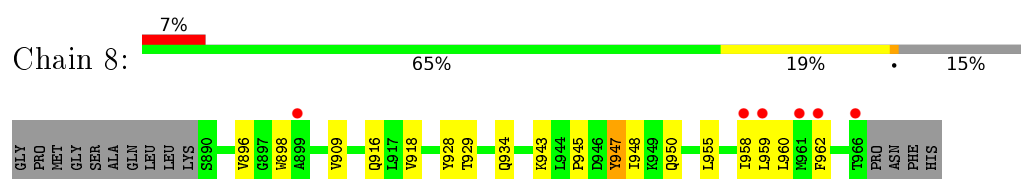
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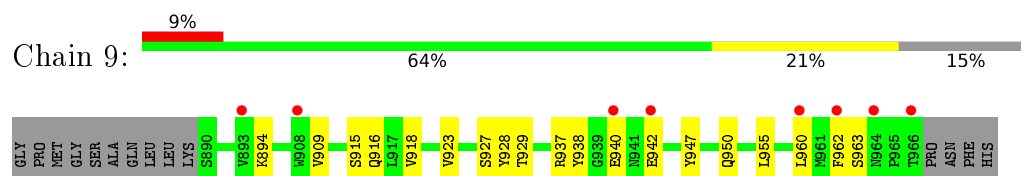
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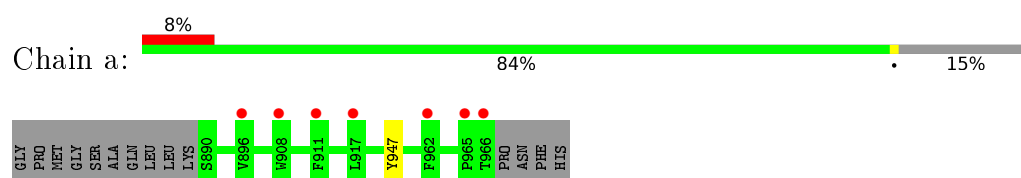
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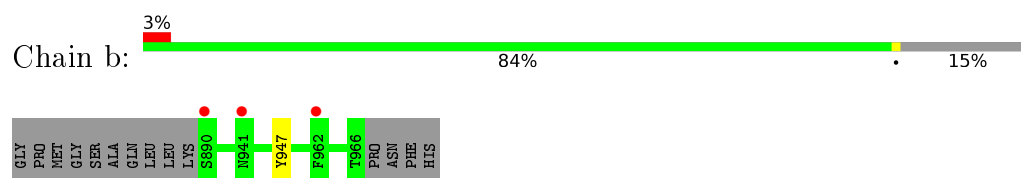
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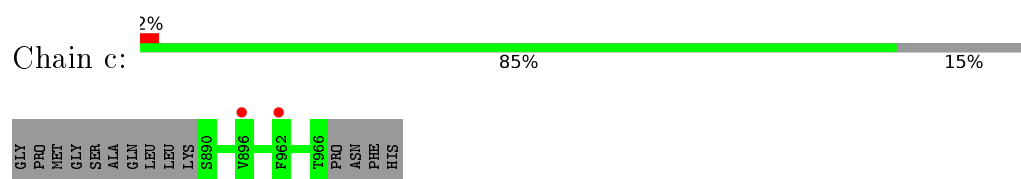
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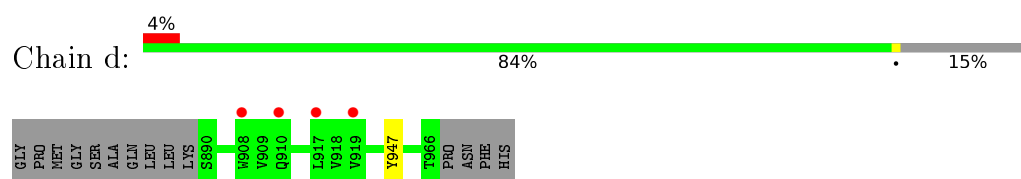
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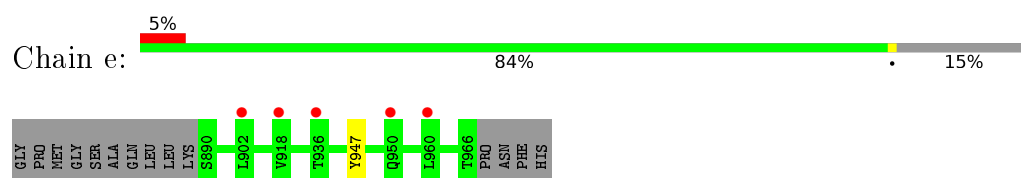
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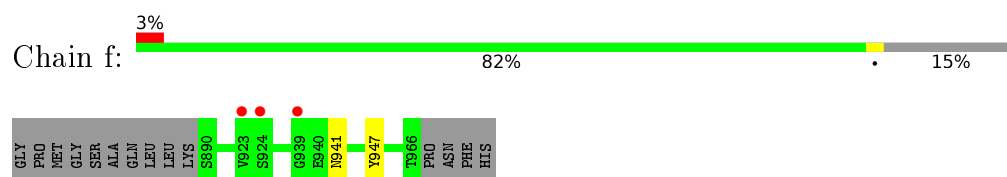
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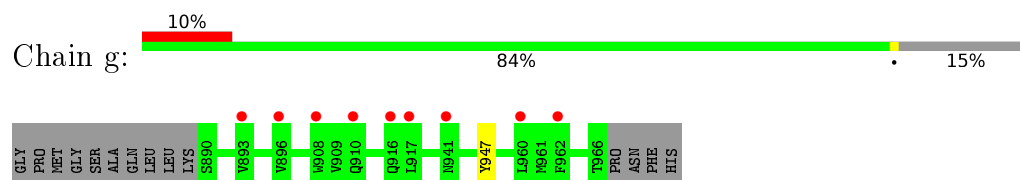
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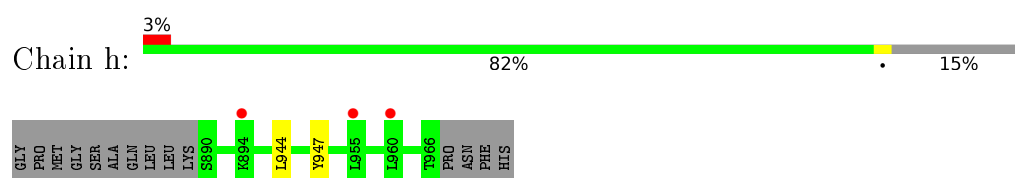
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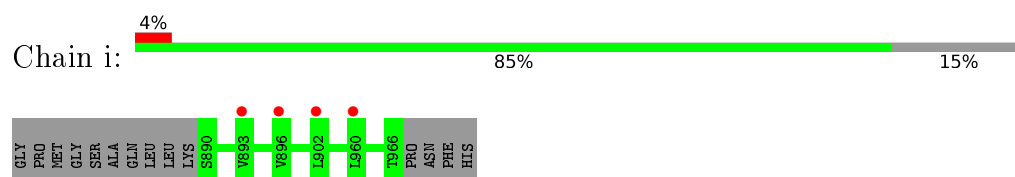
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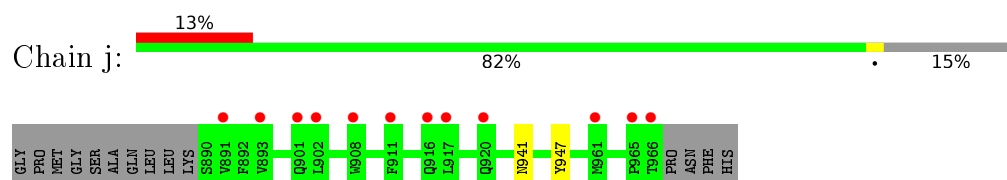
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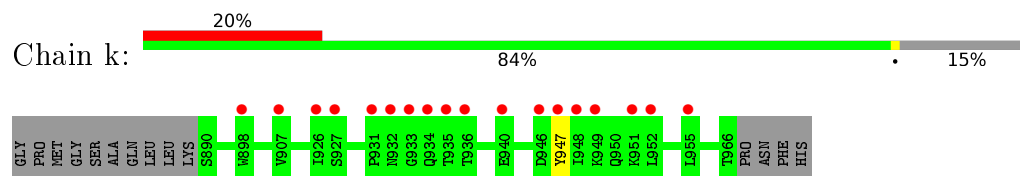
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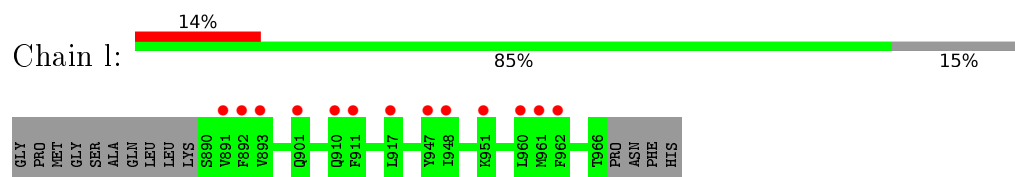
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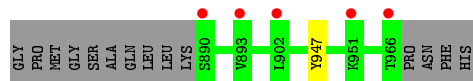
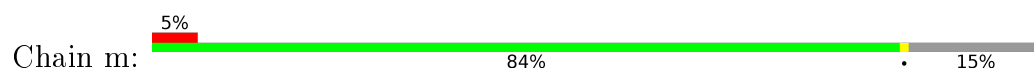
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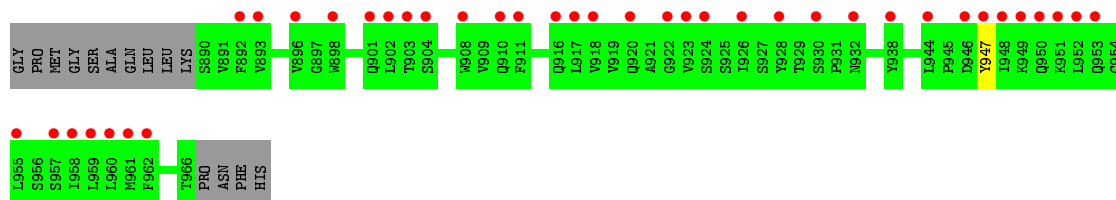
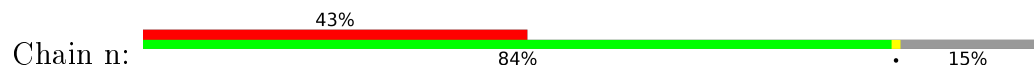
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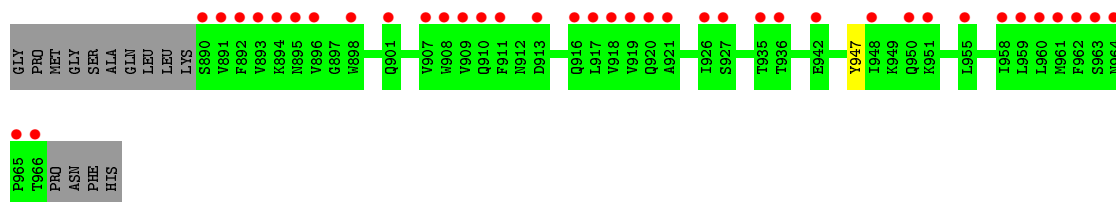
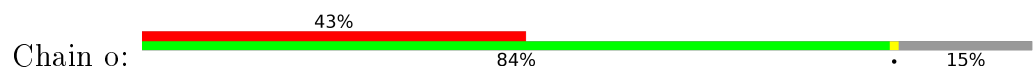
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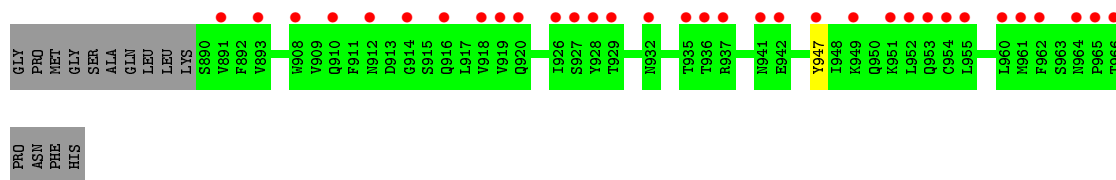
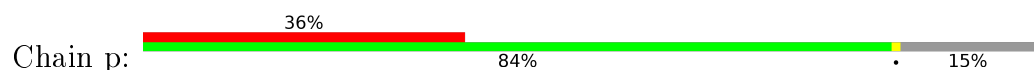
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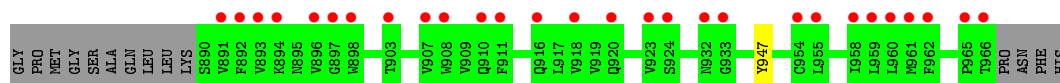
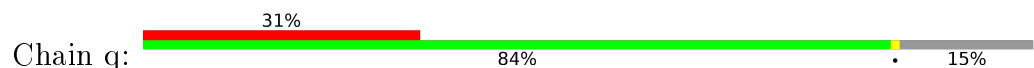
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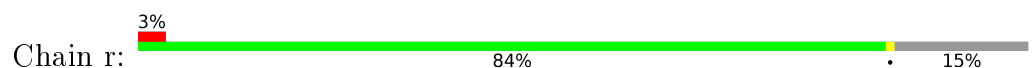
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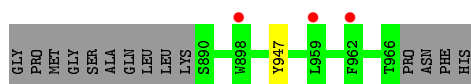


- Molecule 1: Serine/threonine-protein kinase PLK4

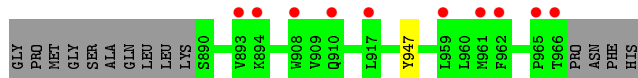
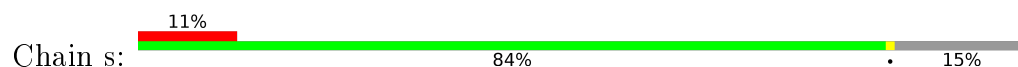


- Molecule 1: Serine/threonine-protein kinase PLK4

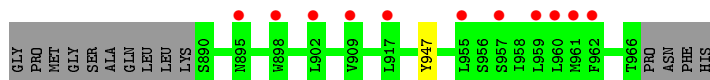
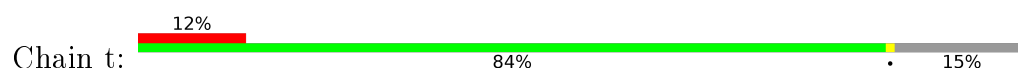




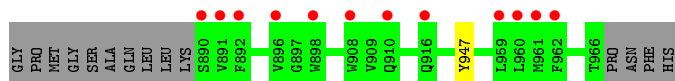
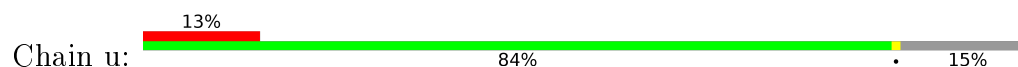
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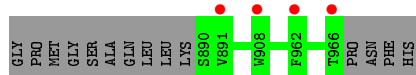
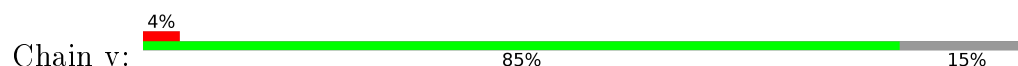
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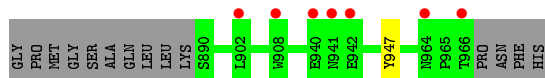
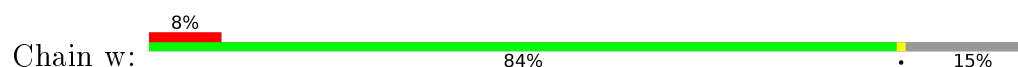
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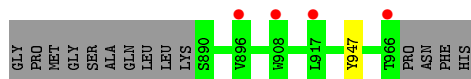
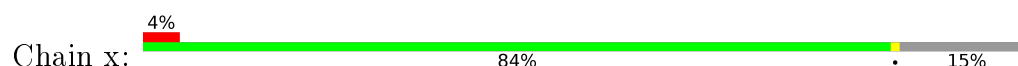
- Molecule 1: Serine/threonine-protein kinase PLK4



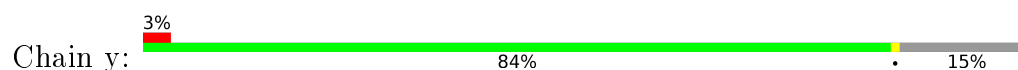
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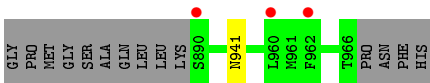


- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	220.35Å 220.35Å 325.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	104.37 – 3.31 110.17 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (104.37-3.31) 100.0 (110.17-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.269 , 0.295 0.267 , 0.293	Depositor DCC
R_{free} test set	5941 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	103.9	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	35580	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1	0.26	0/605	0.47	0/823
1	2	0.28	0/605	0.50	0/823
1	3	0.47	1/605 (0.2%)	0.51	0/823
1	4	0.26	0/605	0.47	0/823
1	5	0.27	0/605	0.46	0/823
1	6	0.27	0/605	0.50	0/823
1	7	0.26	0/605	0.47	0/823
1	8	0.25	0/605	0.47	0/823
1	9	0.26	0/605	0.47	0/823
1	A	0.26	0/605	0.48	0/823
1	B	0.26	0/605	0.49	0/823
1	C	0.25	0/605	0.45	0/823
1	D	0.26	0/605	0.46	0/823
1	E	0.26	0/605	0.48	0/823
1	F	0.27	0/605	0.49	0/823
1	G	0.26	0/605	0.49	0/823
1	H	0.25	0/605	0.44	0/823
1	I	0.26	0/605	0.46	0/823
1	J	0.26	0/605	0.46	0/823
1	K	0.27	0/605	0.47	0/823
1	L	0.25	0/605	0.45	0/823
1	M	0.27	0/605	0.47	0/823
1	N	0.26	0/605	0.45	0/823
1	O	0.26	0/605	0.48	0/823
1	P	0.25	0/605	0.46	0/823
1	Q	0.26	0/605	0.45	0/823
1	R	0.26	0/605	0.45	0/823
1	S	0.26	0/605	0.48	0/823
1	T	0.25	0/605	0.49	0/823
1	U	0.26	0/605	0.45	0/823
1	V	0.26	0/605	0.52	0/823
1	W	0.26	0/605	0.46	0/823
1	X	0.27	0/605	0.50	0/823
1	Y	0.27	0/605	0.50	0/823

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Z	0.26	0/605	0.47	0/823
1	a	0.26	0/605	0.48	0/823
1	b	0.26	0/605	0.47	0/823
1	c	0.26	0/605	0.44	0/823
1	d	0.25	0/605	0.45	0/823
1	e	0.25	0/605	0.45	0/823
1	f	0.26	0/605	0.47	0/823
1	g	0.26	0/605	0.46	0/823
1	h	0.25	0/605	0.48	0/823
1	i	0.26	0/605	0.48	0/823
1	j	0.26	0/605	0.48	0/823
1	k	0.26	0/605	0.49	0/823
1	l	0.25	0/605	0.45	0/823
1	m	0.26	0/605	0.47	0/823
1	n	0.25	0/605	0.47	0/823
1	o	0.25	0/605	0.46	0/823
1	p	0.25	0/605	0.46	0/823
1	q	0.25	0/605	0.45	0/823
1	r	0.26	0/605	0.47	0/823
1	s	0.27	0/605	0.48	0/823
1	t	0.26	0/605	0.45	0/823
1	u	0.27	0/605	0.48	0/823
1	v	0.25	0/605	0.46	0/823
1	w	0.26	0/605	0.45	0/823
1	x	0.25	0/605	0.44	0/823
1	y	0.26	0/605	0.45	0/823
All	All	0.26	1/36300 (0.0%)	0.47	0/49380

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	928	TYR	CE1-CZ	-5.05	1.31	1.38

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	593	0	586	14	0
1	2	593	0	586	24	0
1	3	593	0	586	9	0
1	4	593	0	586	9	0
1	5	593	0	586	20	0
1	6	593	0	586	14	0
1	7	593	0	586	14	0
1	8	593	0	586	17	0
1	9	593	0	586	16	0
1	A	593	0	586	28	0
1	B	593	0	586	28	0
1	C	593	0	586	25	0
1	D	593	0	586	32	0
1	E	593	0	586	22	0
1	F	593	0	586	26	0
1	G	593	0	586	23	0
1	H	593	0	586	23	0
1	I	593	0	586	24	0
1	J	593	0	586	20	0
1	K	593	0	586	20	0
1	L	593	0	586	20	0
1	M	593	0	586	20	0
1	N	593	0	586	27	0
1	O	593	0	586	21	0
1	P	593	0	586	18	0
1	Q	593	0	586	18	0
1	R	593	0	586	29	0
1	S	593	0	586	23	0
1	T	593	0	586	22	0
1	U	593	0	586	25	0
1	V	593	0	586	24	0
1	W	593	0	586	23	0
1	X	593	0	586	20	0
1	Y	593	0	586	29	0
1	Z	593	0	586	11	0
1	a	593	0	586	0	0
1	b	593	0	586	0	0
1	c	593	0	586	0	0
1	d	593	0	586	0	0
1	e	593	0	586	0	0
1	f	593	0	586	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	g	593	0	586	0	0
1	h	593	0	586	0	0
1	i	593	0	586	0	0
1	j	593	0	586	0	0
1	k	593	0	586	0	0
1	l	593	0	586	0	0
1	m	593	0	586	0	0
1	n	593	0	586	0	0
1	o	593	0	586	0	0
1	p	593	0	586	0	0
1	q	593	0	586	0	0
1	r	593	0	586	0	0
1	s	593	0	586	0	0
1	t	593	0	586	0	0
1	u	593	0	586	0	0
1	v	593	0	586	0	0
1	w	593	0	586	0	0
1	x	593	0	586	0	0
1	y	593	0	586	0	0
All	All	35580	0	35160	477	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (477) 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:Q:908:TRP:HE1	1:Q:916:GLN:HE21	1.19	0.90
1:E:937:ARG:HH12	1:T:937:ARG:HH12	61.45	0.89
1:5:908:TRP:HE1	1:5:916:GLN:HE21	1.20	0.87
1:D:908:TRP:HE1	1:D:916:GLN:HE21	1.25	0.83
1:W:908:TRP:HE1	1:W:916:GLN:HE21	1.27	0.83
1:2:908:TRP:HE1	1:2:916:GLN:HE21	1.32	0.78
1:J:930:SER:OG	1:J:932:ASN:OD1	4.78	0.77
1:3:909:VAL:HG21	1:4:955:LEU:HD11	1.68	0.76
1:K:947:TYR:HA	1:K:950:GLN:HG2	1.65	0.75
1:B:944:LEU:HD13	1:B:949:LYS:HB2	4.59	0.74
1:D:944:LEU:HD13	1:D:949:LYS:HB2	1.70	0.74
1:Y:947:TYR:HA	1:Y:950:GLN:HG2	1.69	0.73
1:A:909:VAL:HG21	1:B:955:LEU:HD11	1.71	0.73
1:Q:909:VAL:HG21	1:R:955:LEU:HD21	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:940:GLU:HB3	1:6:934:GLN:HE21	1.54	0.71
1:A:927:SER:HB3	1:9:918:VAL:HB	90.05	0.71
1:H:909:VAL:HG21	1:I:955:LEU:HD21	103.56	0.70
1:B:955:LEU:HD11	1:C:909:VAL:HG21	18.40	0.70
1:I:955:LEU:HD11	1:J:909:VAL:HG21	1.73	0.70
1:R:908:TRP:HE1	1:R:916:GLN:HE21	1.39	0.69
1:K:955:LEU:HD21	1:L:909:VAL:HG21	1.74	0.69
1:N:909:VAL:HG21	1:O:955:LEU:HD11	19.89	0.69
1:5:909:VAL:HG21	1:6:955:LEU:HD11	1.75	0.69
1:A:944:LEU:HD13	1:A:949:LYS:HB2	1.76	0.69
1:A:955:LEU:HD11	1:B:909:VAL:HG21	1.75	0.69
1:X:955:LEU:HD21	1:Y:909:VAL:HG21	84.42	0.69
1:C:958:ILE:HD12	1:T:962:PHE:HZ	1.56	0.68
1:P:909:VAL:HG21	1:Q:955:LEU:HD11	117.64	0.68
1:V:901:GLN:NE2	1:Y:916:GLN:OE1	85.85	0.68
1:M:944:LEU:HD13	1:M:949:LYS:HB2	4.78	0.68
1:R:901:GLN:NE2	1:2:916:GLN:OE1	2.27	0.67
1:R:909:VAL:HG21	1:S:955:LEU:HD11	18.61	0.67
1:A:927:SER:HB3	1:B:918:VAL:HB	1.76	0.67
1:3:955:LEU:HD11	1:4:909:VAL:HG21	1.76	0.67
1:Y:955:LEU:HD21	1:Z:909:VAL:HG21	1.77	0.67
1:E:937:ARG:HH12	1:T:937:ARG:NH1	61.71	0.66
1:T:960:LEU:HD13	1:T:962:PHE:HE1	2.66	0.66
1:D:955:LEU:HD11	1:E:909:VAL:HG21	88.29	0.66
1:5:927:SER:HB3	1:6:918:VAL:HB	1.77	0.66
1:J:955:LEU:HD11	1:K:909:VAL:HG21	18.26	0.65
1:1:901:GLN:NE2	1:5:916:GLN:OE1	2.30	0.65
1:7:909:VAL:HG21	1:8:955:LEU:HD11	1.79	0.63
1:W:909:VAL:HG21	1:X:955:LEU:HD11	1.79	0.63
1:P:937:ARG:HD3	1:R:937:ARG:NH1	91.00	0.63
1:Q:908:TRP:HE1	1:Q:916:GLN:NE2	1.91	0.63
1:R:955:LEU:HD11	1:S:909:VAL:HG21	19.81	0.63
1:V:955:LEU:HD11	1:W:909:VAL:HG21	18.59	0.62
1:O:909:VAL:HG21	1:P:955:LEU:HD11	1.79	0.62
1:F:939:GLY:H	1:F:942:GLU:CD	2.03	0.62
1:N:960:LEU:HD13	1:N:962:PHE:HE1	1.63	0.61
1:D:934:GLN:HG3	1:8:943:LYS:HB2	33.92	0.61
1:A:960:LEU:HD13	1:A:962:PHE:HE1	1.65	0.61
1:L:955:LEU:HD21	1:M:909:VAL:HG21	120.19	0.61
1:6:947:TYR:HA	1:6:950:GLN:HG2	1.82	0.61
1:U:955:LEU:HD11	1:V:909:VAL:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:955:LEU:HD11	1:G:909:VAL:HG21	19.52	0.61
1:L:927:SER:HB3	1:M:918:VAL:HB	135.06	0.60
1:7:908:TRP:HE1	1:7:916:GLN:HE21	1.48	0.60
1:Z:916:GLN:OE1	1:4:901:GLN:NE2	2.27	0.60
1:N:962:PHE:HZ	1:8:958:ILE:HD12	81.59	0.60
1:X:909:VAL:HG21	1:Y:955:LEU:HD11	74.05	0.60
1:Q:955:LEU:HD21	1:R:909:VAL:HG21	1.84	0.59
1:U:937:ARG:HH11	1:X:937:ARG:HD2	46.87	0.59
1:T:909:VAL:HG21	1:U:955:LEU:HD11	74.58	0.59
1:A:909:VAL:HG21	1:9:955:LEU:HD11	74.47	0.59
1:G:955:LEU:HD11	1:H:909:VAL:HG21	1.84	0.59
1:1:909:VAL:HG21	1:2:955:LEU:HD21	1.85	0.59
1:O:908:TRP:HE1	1:O:916:GLN:NE2	2.01	0.59
1:N:894:LYS:HE3	1:N:912:ASN:HA	2.50	0.59
1:C:927:SER:HB3	1:D:918:VAL:HB	1.85	0.59
1:H:955:LEU:HD21	1:I:909:VAL:HG21	103.32	0.59
1:S:909:VAL:HG21	1:T:955:LEU:HD11	1.84	0.59
1:E:955:LEU:HD21	1:F:909:VAL:HG21	1.83	0.58
1:B:915:SER:HB3	1:C:931:PRO:HD3	28.65	0.58
1:L:960:LEU:HD13	1:L:962:PHE:HE1	1.68	0.58
1:M:939:GLY:H	1:M:942:GLU:CD	2.07	0.58
1:X:947:TYR:HA	1:X:950:GLN:HG2	1.85	0.58
1:A:955:LEU:HD11	1:9:909:VAL:HG21	73.77	0.58
1:G:909:VAL:HG21	1:H:955:LEU:HD21	1.85	0.58
1:N:955:LEU:HD11	1:O:909:VAL:HG21	20.03	0.58
1:C:960:LEU:HD12	1:R:960:LEU:HG	26.80	0.58
1:7:955:LEU:HD11	1:8:909:VAL:HG21	1.86	0.57
1:C:909:VAL:HG21	1:D:955:LEU:HD11	1.86	0.57
1:5:955:LEU:HD21	1:6:909:VAL:HG21	1.85	0.57
1:T:908:TRP:HE1	1:T:916:GLN:HE21	4.81	0.57
1:O:962:PHE:HE2	1:S:958:ILE:HD12	107.87	0.57
1:3:945:PRO:HD2	1:3:948:ILE:HG13	1.86	0.57
1:D:908:TRP:HE1	1:D:916:GLN:NE2	1.99	0.57
1:D:934:GLN:HG3	1:8:943:LYS:HD3	33.98	0.57
1:5:908:TRP:HE1	1:5:916:GLN:NE2	1.98	0.56
1:A:958:ILE:HD12	1:L:962:PHE:HE2	67.93	0.56
1:C:955:LEU:HD21	1:D:909:VAL:HG21	1.86	0.56
1:K:909:VAL:HG21	1:L:955:LEU:HD21	1.87	0.56
1:M:955:LEU:HD11	1:N:909:VAL:HG21	1.87	0.56
1:Q:915:SER:HB3	1:R:931:PRO:HD3	1.86	0.56
1:W:955:LEU:HD11	1:X:909:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:908:TRP:HE1	1:2:916:GLN:NE2	2.00	0.56
1:S:955:LEU:HD11	1:T:909:VAL:HG21	1.88	0.56
1:B:903:THR:OG1	1:R:932:ASN:O	2.24	0.56
1:Y:909:VAL:HG21	1:Z:955:LEU:HD21	1.88	0.55
1:A:958:ILE:HD12	1:B:962:PHE:HE2	26.54	0.55
1:H:944:LEU:HD13	1:H:949:LYS:HB2	4.66	0.55
1:N:895:ASN:HB2	1:N:910:GLN:HB3	2.48	0.55
1:S:960:LEU:HD12	1:S:962:PHE:CE1	2.42	0.55
1:C:918:VAL:HB	1:D:927:SER:HB3	1.89	0.55
1:F:909:VAL:HG21	1:G:955:LEU:HD11	18.75	0.55
1:W:908:TRP:HE1	1:W:916:GLN:NE2	2.01	0.54
1:E:960:LEU:HD13	1:E:962:PHE:HE1	1.72	0.54
1:R:915:SER:HB3	1:S:931:PRO:HD3	29.07	0.54
1:7:927:SER:HB3	1:8:918:VAL:HB	1.89	0.54
1:K:915:SER:HB3	1:L:931:PRO:HD3	1.89	0.54
1:N:918:VAL:HB	1:O:927:SER:HB3	37.97	0.54
1:N:927:SER:HB3	1:O:918:VAL:HB	37.91	0.53
1:N:903:THR:OG1	1:U:932:ASN:O	162.56	0.53
1:X:918:VAL:HB	1:Y:927:SER:HB3	73.02	0.53
1:N:928:TYR:HE1	1:O:915:SER:HB2	27.67	0.53
1:K:894:LYS:HE3	1:K:912:ASN:HA	2.37	0.53
1:U:909:VAL:HG21	1:V:955:LEU:HD11	1.90	0.53
1:T:908:TRP:HE1	1:T:916:GLN:NE2	4.07	0.53
1:D:909:VAL:HG21	1:E:955:LEU:HD21	69.56	0.53
1:B:909:VAL:HG21	1:C:955:LEU:HD21	17.20	0.53
1:G:915:SER:HB2	1:H:928:TYR:HE1	1.74	0.53
1:H:960:LEU:HD11	1:H:962:PHE:CE1	3.98	0.53
1:F:918:VAL:HB	1:G:927:SER:HB3	37.90	0.53
1:Y:960:LEU:HD13	1:Y:962:PHE:CE1	2.71	0.53
1:7:915:SER:HB2	1:8:928:TYR:HE1	1.74	0.52
1:M:909:VAL:HG21	1:N:955:LEU:HD21	1.91	0.52
1:S:916:GLN:HE22	1:Y:901:GLN:HE21	1.57	0.52
1:I:932:ASN:HD21	1:2:941:ASN:HD22	102.19	0.52
1:O:915:SER:HB3	1:P:931:PRO:HD3	1.92	0.52
1:U:927:SER:HB3	1:V:918:VAL:HB	1.91	0.52
1:R:908:TRP:HE1	1:R:916:GLN:NE2	2.04	0.52
1:U:947:TYR:HA	1:U:950:GLN:HG2	1.96	0.52
1:A:931:PRO:HD3	1:9:915:SER:HB3	85.02	0.52
1:F:960:LEU:HD11	1:F:962:PHE:CZ	2.45	0.52
1:D:960:LEU:HD13	1:D:962:PHE:CE1	2.44	0.52
1:S:958:ILE:HD12	1:Y:962:PHE:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:953:GLN:OE1	1:5:966:THR:N	2.43	0.51
1:D:962:PHE:HZ	1:U:958:ILE:HD12	97.79	0.51
1:J:928:TYR:HE1	1:K:915:SER:HB2	28.08	0.51
1:U:934:GLN:N	1:U:934:GLN:OE1	2.45	0.51
1:9:960:LEU:HD11	1:9:962:PHE:CE1	2.44	0.51
1:O:955:LEU:HD21	1:P:909:VAL:HG21	1.91	0.51
1:L:915:SER:HB3	1:M:931:PRO:HD3	86.95	0.51
1:B:960:LEU:HD13	1:B:962:PHE:CE1	3.69	0.51
1:T:955:LEU:HD21	1:U:909:VAL:HG21	97.86	0.51
1:T:916:GLN:HB2	1:U:929:THR:OG1	77.46	0.51
1:8:960:LEU:HD11	1:8:962:PHE:CE1	2.45	0.51
1:L:928:TYR:HE1	1:M:915:SER:HB2	135.74	0.51
1:Q:960:LEU:HD13	1:Q:962:PHE:HE1	3.94	0.51
1:7:908:TRP:HE1	1:7:916:GLN:NE2	2.09	0.50
1:J:927:SER:HB3	1:K:918:VAL:HB	37.70	0.50
1:I:915:SER:HB3	1:J:931:PRO:HD3	1.94	0.50
1:6:928:TYR:HE2	1:6:947:TYR:HH	1.60	0.50
1:A:928:TYR:HE1	1:9:915:SER:HB2	84.93	0.50
1:J:909:VAL:HG21	1:K:955:LEU:HD11	19.62	0.50
1:T:960:LEU:HD13	1:T:962:PHE:CE1	3.14	0.50
1:W:960:LEU:HD13	1:W:962:PHE:HE1	1.91	0.50
1:E:960:LEU:HD13	1:E:962:PHE:CE1	2.58	0.50
1:N:958:ILE:HD12	1:T:962:PHE:HE2	82.77	0.50
1:S:915:SER:HB2	1:T:928:TYR:HE1	1.76	0.50
1:U:931:PRO:HD3	1:V:915:SER:HB3	1.93	0.50
1:P:960:LEU:HD13	1:P:962:PHE:HE1	1.85	0.50
1:A:928:TYR:HE1	1:B:915:SER:HB2	1.76	0.50
1:Q:928:TYR:HE1	1:R:915:SER:HB2	1.77	0.50
1:2:960:LEU:HD11	1:2:962:PHE:CE1	2.47	0.49
1:3:918:VAL:HB	1:4:927:SER:HB3	1.94	0.49
1:C:947:TYR:HA	1:C:950:GLN:HG2	2.04	0.49
1:T:928:TYR:HE1	1:U:915:SER:HB2	108.25	0.49
1:Y:931:PRO:HD3	1:Z:915:SER:HB3	1.94	0.49
1:3:960:LEU:HD13	1:3:962:PHE:HE1	1.77	0.49
1:D:927:SER:HB3	1:E:918:VAL:HB	81.24	0.49
1:L:909:VAL:HG21	1:M:955:LEU:HD11	100.35	0.49
1:E:928:TYR:OH	1:E:951:LYS:NZ	2.52	0.49
1:F:915:SER:HB3	1:G:931:PRO:HD3	28.84	0.49
1:K:928:TYR:HE1	1:L:915:SER:HB2	1.78	0.49
1:B:916:GLN:HE22	1:Q:901:GLN:HE21	1.59	0.49
1:G:928:TYR:HE1	1:H:915:SER:HB2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:955:LEU:HD21	1:2:909:VAL:HG21	1.94	0.49
1:D:960:LEU:HD12	1:E:960:LEU:HD12	94.46	0.49
1:I:909:VAL:HG21	1:J:955:LEU:HD11	1.93	0.49
1:S:935:THR:HG23	1:7:941:ASN:OD1	2.13	0.49
1:Y:915:SER:HB3	1:Z:928:TYR:HE1	1.77	0.49
1:A:962:PHE:HE2	1:B:958:ILE:HD12	27.02	0.49
1:F:916:GLN:OE1	1:U:901:GLN:NE2	58.56	0.49
1:J:915:SER:HB3	1:K:928:TYR:HE1	27.78	0.49
1:5:928:TYR:HE1	1:6:915:SER:HB2	1.77	0.48
1:U:918:VAL:HB	1:V:927:SER:HB3	1.94	0.48
1:H:915:SER:HB2	1:I:928:TYR:HE1	100.95	0.48
1:P:931:PRO:HD3	1:Q:915:SER:HB3	85.55	0.48
1:Y:928:TYR:HE2	1:Y:947:TYR:HH	1.62	0.48
1:B:960:LEU:HD13	1:B:962:PHE:HE1	3.93	0.48
1:C:960:LEU:HD13	1:C:962:PHE:HE1	2.23	0.48
1:N:958:ILE:HD12	1:8:962:PHE:HZ	102.29	0.48
1:P:915:SER:HB2	1:Q:928:TYR:HE1	130.81	0.48
1:R:915:SER:HB2	1:S:928:TYR:HE1	28.34	0.48
1:X:960:LEU:HD13	1:X:962:PHE:HE1	1.79	0.48
1:W:915:SER:HB3	1:X:931:PRO:HD3	1.95	0.48
1:B:937:ARG:HD2	1:C:937:ARG:HH11	47.43	0.48
1:W:916:GLN:HB2	1:X:929:THR:OG1	2.14	0.48
1:I:962:PHE:HZ	1:7:958:ILE:HG21	1.79	0.48
1:Y:932:ASN:O	1:4:903:THR:OG1	2.31	0.48
1:C:928:TYR:HE1	1:D:915:SER:HB2	1.77	0.48
1:D:928:TYR:HE1	1:E:915:SER:HB2	95.79	0.48
1:L:947:TYR:HA	1:L:950:GLN:HG2	1.96	0.48
1:1:931:PRO:HD3	1:2:915:SER:HB3	1.96	0.47
1:Q:960:LEU:HD12	1:9:960:LEU:HG	61.34	0.47
1:3:938:TYR:HA	1:3:942:GLU:OE2	2.14	0.47
1:F:915:SER:HB2	1:G:928:TYR:HE1	28.35	0.47
1:K:896:VAL:HG12	1:K:909:VAL:HG22	2.07	0.47
1:L:897:GLY:HA3	1:L:960:LEU:HD23	1.96	0.47
1:I:932:ASN:HD21	1:2:941:ASN:ND2	101.61	0.47
1:V:947:TYR:HA	1:V:950:GLN:HG2	2.02	0.47
1:V:928:TYR:HE1	1:W:915:SER:HB2	28.17	0.47
1:R:962:PHE:HZ	1:2:958:ILE:HG21	1.79	0.47
1:G:962:PHE:CE2	1:H:958:ILE:HD12	25.40	0.47
1:W:928:TYR:HE1	1:X:915:SER:HB2	1.79	0.47
1:S:960:LEU:HD11	1:S:962:PHE:CZ	3.92	0.47
1:5:916:GLN:HB2	1:6:929:THR:OG1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:947:TYR:HA	1:D:950:GLN:HG2	2.03	0.47
1:K:960:LEU:HA	1:K:960:LEU:HD23	1.77	0.47
1:Y:953:GLN:OE1	1:2:966:THR:N	2.30	0.47
1:C:943:LYS:HG3	1:C:944:LEU:N	2.30	0.47
1:H:916:GLN:HB2	1:I:929:THR:OG1	100.24	0.47
1:U:960:LEU:HD23	1:U:960:LEU:HA	2.69	0.47
1:X:928:TYR:HE1	1:Y:915:SER:HB3	92.93	0.47
1:B:908:TRP:HE1	1:B:916:GLN:NE2	4.00	0.47
1:S:962:PHE:HE2	1:Y:958:ILE:HD12	1.79	0.47
1:9:923:VAL:O	1:9:940:GLU:HG3	2.15	0.46
1:H:928:TYR:HE1	1:I:915:SER:HB2	106.38	0.46
1:5:960:LEU:HD13	1:5:962:PHE:HE1	1.80	0.46
1:F:960:LEU:HD11	1:F:962:PHE:CE1	2.60	0.46
1:T:960:LEU:HD23	1:T:960:LEU:HA	2.76	0.46
1:C:910:GLN:HG3	1:C:916:GLN:HG2	2.16	0.46
1:N:934:GLN:OE1	1:N:934:GLN:N	2.42	0.46
1:Q:947:TYR:HA	1:Q:950:GLN:HG2	1.97	0.46
1:A:947:TYR:HA	1:A:950:GLN:HG2	1.98	0.46
1:J:894:LYS:HE3	1:J:912:ASN:HA	2.50	0.46
1:J:929:THR:OG1	1:K:916:GLN:HB2	34.28	0.46
1:R:947:TYR:HA	1:R:950:GLN:HG2	1.98	0.46
1:L:960:LEU:HD13	1:L:962:PHE:CE1	2.48	0.46
1:V:918:VAL:HB	1:W:927:SER:HB3	38.10	0.46
1:4:947:TYR:HA	1:4:950:GLN:HG2	1.97	0.46
1:I:947:TYR:HA	1:I:950:GLN:HG2	1.97	0.46
1:O:908:TRP:HE1	1:O:916:GLN:HE21	1.62	0.46
1:A:918:VAL:HB	1:B:927:SER:HB3	1.96	0.46
1:D:929:THR:OG1	1:E:916:GLN:HB2	87.09	0.46
1:G:947:TYR:HA	1:G:950:GLN:HG2	1.98	0.46
1:R:960:LEU:HD11	1:R:962:PHE:CZ	2.51	0.46
1:V:909:VAL:HG21	1:W:955:LEU:HD21	19.10	0.46
1:Z:947:TYR:HA	1:Z:950:GLN:HG2	1.97	0.46
1:9:938:TYR:HA	1:9:942:GLU:OE2	2.15	0.46
1:A:915:SER:HB2	1:B:928:TYR:HE1	1.81	0.46
1:T:947:TYR:HA	1:T:950:GLN:HG2	1.98	0.46
1:C:915:SER:HB2	1:D:928:TYR:HE1	1.81	0.46
1:R:928:TYR:HE1	1:S:915:SER:HB2	28.04	0.46
1:G:918:VAL:HB	1:H:927:SER:HB3	1.98	0.45
1:W:915:SER:HB2	1:X:928:TYR:HE1	1.80	0.45
1:I:916:GLN:HB2	1:J:929:THR:OG1	2.17	0.45
1:K:960:LEU:HD12	1:K:962:PHE:CE1	4.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:947:TYR:HA	1:W:950:GLN:HG2	2.01	0.45
1:5:915:SER:HB3	1:6:931:PRO:HD3	1.98	0.45
1:F:931:PRO:HD3	1:G:915:SER:HB3	27.98	0.45
1:P:960:LEU:HA	1:P:960:LEU:HD23	1.81	0.45
1:H:915:SER:HB2	1:I:928:TYR:CE1	100.93	0.45
1:P:894:LYS:HG2	1:P:963:SER:HB2	2.04	0.45
1:N:960:LEU:HD12	1:T:960:LEU:HD12	82.83	0.45
1:7:960:LEU:HD11	1:7:962:PHE:CE1	2.51	0.45
1:8:945:PRO:HD2	1:8:948:ILE:HG13	1.98	0.45
1:5:898:TRP:CH2	1:5:959:LEU:HD13	2.52	0.45
1:E:960:LEU:HD23	1:E:960:LEU:HA	1.84	0.45
1:J:959:LEU:O	1:J:960:LEU:HD22	4.33	0.45
1:W:894:LYS:HG2	1:W:963:SER:HB2	2.04	0.45
1:1:928:TYR:HE1	1:2:915:SER:HB2	1.82	0.45
1:5:960:LEU:HD23	1:5:960:LEU:HA	1.80	0.45
1:D:915:SER:HB2	1:E:928:TYR:HE1	61.23	0.45
1:G:925:SER:HB2	1:G:937:ARG:HE	2.31	0.45
1:M:960:LEU:HD23	1:M:960:LEU:HA	1.84	0.45
1:B:896:VAL:HG12	1:B:909:VAL:HG22	1.99	0.45
1:B:928:TYR:HE1	1:C:915:SER:HB2	28.05	0.45
1:G:916:GLN:HB2	1:H:929:THR:OG1	2.17	0.45
1:M:929:THR:OG1	1:N:916:GLN:HB2	2.17	0.45
1:P:896:VAL:HG12	1:P:909:VAL:HG22	1.99	0.45
1:E:896:VAL:HG12	1:E:909:VAL:HG22	1.97	0.45
1:I:960:LEU:HD13	1:I:962:PHE:HE1	4.18	0.45
1:G:924:SER:HA	1:G:940:GLU:HG3	1.98	0.44
1:M:894:LYS:HE3	1:M:912:ASN:HA	2.83	0.44
1:1:929:THR:OG1	1:2:916:GLN:HB2	2.18	0.44
1:M:894:LYS:HG2	1:M:963:SER:HB2	1.99	0.44
1:P:947:TYR:HA	1:P:950:GLN:HG2	2.08	0.44
1:K:934:GLN:N	1:K:934:GLN:OE1	2.45	0.44
1:V:894:LYS:HE3	1:V:912:ASN:HA	2.08	0.44
1:V:958:ILE:HD12	1:W:962:PHE:HE2	8.35	0.44
1:B:915:SER:HB2	1:C:928:TYR:HE1	28.06	0.44
1:C:929:THR:OG1	1:D:916:GLN:HB2	2.18	0.44
1:A:901:GLN:HE21	1:L:916:GLN:HE22	84.00	0.44
1:N:915:SER:HB2	1:O:928:TYR:HE1	28.05	0.44
1:L:910:GLN:NE2	1:6:964:ASN:OD1	126.54	0.44
1:M:896:VAL:HG12	1:M:909:VAL:HG22	1.99	0.44
1:7:943:LYS:HG3	1:7:944:LEU:N	2.32	0.44
1:B:926:ILE:HB	1:B:938:TYR:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:947:TYR:HA	1:B:950:GLN:HG2	2.00	0.44
1:C:960:LEU:HD23	1:C:960:LEU:HA	1.83	0.44
1:D:960:LEU:HD23	1:D:960:LEU:HA	1.77	0.44
1:I:958:ILE:HD12	1:7:962:PHE:CE2	2.52	0.44
1:N:962:PHE:HE2	1:T:958:ILE:HD12	83.66	0.44
1:D:931:PRO:HD3	1:E:915:SER:HB3	96.41	0.44
1:Q:916:GLN:HB2	1:R:929:THR:OG1	2.18	0.44
1:R:958:ILE:HD12	1:2:962:PHE:CE2	2.53	0.44
1:F:962:PHE:HZ	1:U:958:ILE:HB	57.29	0.44
1:8:947:TYR:HA	1:8:950:GLN:HG2	1.98	0.44
1:8:898:TRP:CH2	1:8:959:LEU:HD13	2.52	0.44
1:B:927:SER:HB3	1:C:918:VAL:HB	37.70	0.44
1:I:929:THR:OG1	1:J:916:GLN:HB2	2.18	0.44
1:I:927:SER:HB3	1:2:918:VAL:HB	2.00	0.44
1:F:939:GLY:H	1:F:942:GLU:CG	2.31	0.44
1:P:945:PRO:HD2	1:P:948:ILE:HG13	2.00	0.44
1:V:927:SER:HB3	1:W:918:VAL:HB	37.67	0.44
1:E:931:PRO:HD3	1:F:915:SER:HB3	2.00	0.43
1:K:929:THR:OG1	1:L:916:GLN:HB2	2.18	0.43
1:O:928:TYR:O	1:O:936:THR:N	2.91	0.43
1:W:960:LEU:HD23	1:W:960:LEU:HA	1.81	0.43
1:6:934:GLN:N	1:6:934:GLN:OE1	2.44	0.43
1:M:893:VAL:HG13	1:M:909:VAL:HG13	1.99	0.43
1:M:928:TYR:HE1	1:N:915:SER:HB2	1.83	0.43
1:S:931:PRO:HD3	1:T:915:SER:HB3	2.00	0.43
1:E:945:PRO:HD2	1:E:948:ILE:HG13	2.20	0.43
1:2:947:TYR:HA	1:2:950:GLN:HG2	1.99	0.43
1:5:893:VAL:HG13	1:5:909:VAL:HG13	2.00	0.43
1:A:929:THR:OG1	1:9:916:GLN:HB2	85.53	0.43
1:H:947:TYR:HA	1:H:950:GLN:HG2	2.04	0.43
1:S:896:VAL:HG12	1:S:909:VAL:HG22	2.28	0.43
1:A:915:SER:HB2	1:9:928:TYR:HE1	86.64	0.43
1:H:918:VAL:HB	1:I:927:SER:HB3	102.16	0.43
1:N:929:THR:OG1	1:O:916:GLN:HB2	34.05	0.43
1:P:943:LYS:HG3	1:P:944:LEU:N	2.32	0.43
1:S:918:VAL:HB	1:T:927:SER:HB3	2.01	0.43
1:I:916:GLN:HB2	1:2:929:THR:OG1	2.18	0.43
1:S:959:LEU:O	1:S:960:LEU:HD22	2.18	0.43
1:T:897:GLY:HA3	1:T:960:LEU:HD23	3.42	0.43
1:8:896:VAL:HG12	1:8:909:VAL:HG22	2.00	0.43
1:7:929:THR:OG1	1:8:916:GLN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:934:GLN:CG	1:8:943:LYS:HB2	34.17	0.43
1:J:896:VAL:HG12	1:J:909:VAL:HG22	2.01	0.43
1:J:947:TYR:HA	1:J:950:GLN:HG2	2.00	0.43
1:R:896:VAL:HG12	1:R:909:VAL:HG22	2.16	0.43
1:6:893:VAL:HG13	1:6:909:VAL:HG13	2.01	0.43
1:F:916:GLN:HB2	1:G:929:THR:OG1	34.49	0.43
1:M:915:SER:HB3	1:N:931:PRO:HD3	2.01	0.43
1:V:926:ILE:HB	1:V:938:TYR:HB2	1.99	0.43
1:A:929:THR:OG1	1:B:916:GLN:HB2	2.19	0.43
1:C:955:LEU:HD11	1:D:909:VAL:HG21	2.01	0.43
1:F:901:GLN:HE21	1:U:916:GLN:HE22	57.38	0.43
1:5:960:LEU:HD13	1:5:962:PHE:CE1	2.54	0.42
1:F:947:TYR:HA	1:F:950:GLN:HG2	2.24	0.42
1:V:960:LEU:O	1:Y:960:LEU:N	80.37	0.42
1:1:915:SER:HB2	1:2:928:TYR:HE1	1.84	0.42
1:1:955:LEU:HD11	1:2:909:VAL:HG21	2.00	0.42
1:F:934:GLN:N	1:F:934:GLN:OE1	2.45	0.42
1:F:928:TYR:HE1	1:G:915:SER:HB2	27.52	0.42
1:H:960:LEU:HA	1:H:960:LEU:HD23	1.83	0.42
1:U:960:LEU:HD11	1:U:962:PHE:CE1	2.55	0.42
1:W:937:ARG:HH22	1:X:935:THR:HG21	32.87	0.42
1:5:947:TYR:HA	1:5:950:GLN:HG2	2.02	0.42
1:5:918:VAL:HB	1:6:927:SER:HB3	2.02	0.42
1:A:896:VAL:HG12	1:A:909:VAL:HG22	2.02	0.42
1:J:934:GLN:OE1	1:J:934:GLN:N	2.44	0.42
1:N:960:LEU:HD11	1:N:962:PHE:HE1	2.87	0.42
1:A:937:ARG:HH11	1:R:937:ARG:HD2	1.84	0.42
1:Y:902:LEU:HD13	1:Y:953:GLN:HE21	1.83	0.42
1:X:929:THR:OG1	1:Y:916:GLN:HB2	96.50	0.42
1:2:893:VAL:HG13	1:2:909:VAL:HG13	2.01	0.42
1:4:896:VAL:HG12	1:4:909:VAL:HG22	2.01	0.42
1:B:934:GLN:N	1:B:934:GLN:OE1	2.46	0.42
1:F:896:VAL:HG12	1:F:909:VAL:HG22	2.02	0.42
1:F:926:ILE:HD12	1:F:944:LEU:HD21	2.01	0.42
1:L:928:TYR:OH	1:L:951:LYS:NZ	2.52	0.42
1:A:934:GLN:N	1:A:934:GLN:OE1	2.47	0.42
1:R:931:PRO:HD3	1:S:915:SER:HB3	28.41	0.42
1:U:898:TRP:CH2	1:U:959:LEU:HD13	2.60	0.42
1:3:947:TYR:HA	1:3:950:GLN:HG2	2.02	0.42
1:C:937:ARG:HH11	1:D:937:ARG:HD2	29.84	0.42
1:G:960:LEU:HD11	1:G:962:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:960:LEU:HD11	1:I:962:PHE:CZ	2.55	0.42
1:O:896:VAL:HG12	1:O:909:VAL:HG22	2.28	0.42
1:1:929:THR:HA	1:1:935:THR:HA	2.01	0.42
1:9:894:LYS:HG2	1:9:963:SER:HB2	2.01	0.42
1:I:945:PRO:HD2	1:I:948:ILE:HG13	2.19	0.42
1:V:960:LEU:HD11	1:V:962:PHE:CE1	3.87	0.42
1:5:915:SER:HB2	1:6:928:TYR:HE1	1.85	0.42
1:E:947:TYR:HA	1:E:950:GLN:HG2	2.04	0.42
1:G:934:GLN:N	1:G:934:GLN:OE1	2.48	0.42
1:I:960:LEU:HA	1:I:960:LEU:HD23	2.70	0.42
1:L:915:SER:HB2	1:M:928:TYR:HE1	91.87	0.42
1:Y:960:LEU:HA	1:Y:960:LEU:HD23	1.86	0.42
1:R:958:ILE:HB	1:2:962:PHE:HZ	1.86	0.41
1:D:934:GLN:OE1	1:D:934:GLN:N	2.45	0.41
1:I:915:SER:HB2	1:J:928:TYR:HE1	1.84	0.41
1:S:962:PHE:CE2	1:Y:958:ILE:HD12	2.55	0.41
1:F:962:PHE:HE2	1:U:958:ILE:HD12	53.44	0.41
1:V:934:GLN:N	1:V:934:GLN:OE1	2.48	0.41
1:C:916:GLN:HB2	1:D:929:THR:OG1	2.20	0.41
1:O:929:THR:HA	1:O:935:THR:HA	2.45	0.41
1:Q:918:VAL:HB	1:R:927:SER:HB3	2.02	0.41
1:H:908:TRP:HD1	1:H:918:VAL:HG22	2.10	0.41
1:N:947:TYR:HA	1:N:950:GLN:HG2	2.01	0.41
1:P:927:SER:HB3	1:Q:918:VAL:HB	89.37	0.41
1:V:939:GLY:H	1:V:942:GLU:HG3	1.85	0.41
1:X:960:LEU:HA	1:X:960:LEU:HD23	1.81	0.41
1:Z:908:TRP:HE1	1:Z:916:GLN:NE2	2.17	0.41
1:2:934:GLN:N	1:2:934:GLN:OE1	2.44	0.41
1:3:896:VAL:HG12	1:3:909:VAL:HG22	2.01	0.41
1:G:927:SER:HB3	1:H:918:VAL:HB	2.01	0.41
1:N:902:LEU:HD21	1:N:949:LYS:HG3	2.03	0.41
1:H:937:ARG:HH11	1:W:937:ARG:HH11	67.46	0.41
1:W:938:TYR:HA	1:W:942:GLU:OE2	2.29	0.41
1:7:916:GLN:HB2	1:8:929:THR:OG1	2.21	0.41
1:G:960:LEU:HD23	1:G:960:LEU:HA	2.74	0.41
1:J:916:GLN:HB2	1:K:929:THR:OG1	33.70	0.41
1:M:934:GLN:N	1:M:934:GLN:OE1	2.44	0.41
1:O:947:TYR:HA	1:O:950:GLN:HG2	2.01	0.41
1:R:934:GLN:N	1:R:934:GLN:OE1	2.45	0.41
1:Y:934:GLN:N	1:Y:934:GLN:OE1	2.45	0.41
1:A:898:TRP:CH2	1:A:959:LEU:HD13	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:928:TYR:HE1	1:Q:915:SER:HB2	89.35	0.41
1:U:916:GLN:HB2	1:V:929:THR:OG1	2.20	0.41
1:I:938:TYR:OH	1:2:937:ARG:O	102.29	0.41
1:A:918:VAL:HB	1:9:927:SER:HB3	91.50	0.41
1:A:916:GLN:HB2	1:9:929:THR:OG1	87.41	0.41
1:B:916:GLN:HB2	1:C:929:THR:OG1	34.06	0.41
1:E:916:GLN:HB2	1:F:929:THR:OG1	2.21	0.41
1:K:937:ARG:HD2	1:9:937:ARG:HH11	1.85	0.41
1:Y:960:LEU:HD13	1:Y:962:PHE:HE1	1.91	0.41
1:S:947:TYR:HA	1:S:950:GLN:HG2	2.03	0.41
1:D:916:GLN:HB2	1:E:929:THR:OG1	67.75	0.41
1:K:910:GLN:HG3	1:K:916:GLN:HG2	2.13	0.41
1:O:945:PRO:HD2	1:O:948:ILE:HG13	2.21	0.41
1:U:915:SER:HB2	1:V:928:TYR:HE1	1.86	0.41
1:Z:934:GLN:N	1:Z:934:GLN:OE1	2.46	0.41
1:3:915:SER:HB2	1:4:928:TYR:HE1	1.86	0.41
1:D:944:LEU:HD12	1:D:944:LEU:O	2.21	0.41
1:R:916:GLN:HB2	1:S:929:THR:OG1	34.45	0.41
1:U:929:THR:OG1	1:V:916:GLN:HB2	2.21	0.41
1:V:924:SER:HA	1:V:940:GLU:HG3	2.03	0.41
1:V:894:LYS:HG2	1:V:963:SER:HB2	2.02	0.41
1:X:916:GLN:HB2	1:Y:929:THR:OG1	68.29	0.41
1:5:902:LEU:HD13	1:5:953:GLN:NE2	2.36	0.41
1:8:934:GLN:N	1:8:934:GLN:OE1	2.49	0.41
1:B:932:ASN:OD1	1:B:932:ASN:N	2.54	0.41
1:O:929:THR:OG1	1:P:916:GLN:HB2	2.21	0.41
1:Y:918:VAL:HB	1:Z:927:SER:HB3	2.03	0.41
1:1:947:TYR:HA	1:1:950:GLN:HG2	2.03	0.40
1:H:934:GLN:OE1	1:H:934:GLN:N	2.43	0.40
1:L:929:THR:OG1	1:M:916:GLN:HB2	135.92	0.40
1:O:953:GLN:OE1	1:P:966:THR:N	28.32	0.40
1:1:896:VAL:HG12	1:1:909:VAL:HG22	2.03	0.40
1:2:902:LEU:HD21	1:2:949:LYS:HG3	2.03	0.40
1:1:958:ILE:HD12	1:5:962:PHE:HE2	1.86	0.40
1:7:947:TYR:HA	1:7:950:GLN:HG2	2.03	0.40
1:I:918:VAL:HB	1:J:927:SER:HB3	2.03	0.40
1:W:923:VAL:O	1:W:940:GLU:HG3	2.64	0.40
1:X:915:SER:HB2	1:Y:928:TYR:HE1	70.36	0.40
1:A:960:LEU:HA	1:A:960:LEU:HD23	1.85	0.40
1:E:934:GLN:N	1:E:934:GLN:OE1	2.47	0.40
1:R:960:LEU:HD11	1:R:962:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:915:SER:HB3	1:Y:931:PRO:HD3	70.29	0.40
1:9:947:TYR:HA	1:9:950:GLN:HG2	2.03	0.40
1:D:898:TRP:CH2	1:D:959:LEU:HD13	2.66	0.40
1:F:939:GLY:H	1:F:942:GLU:HG3	1.86	0.40
1:N:960:LEU:HD11	1:N:962:PHE:CE1	3.70	0.40
1:Q:915:SER:HB2	1:R:928:TYR:HE1	1.86	0.40
1:Y:929:THR:OG1	1:Z:916:GLN:HB2	2.21	0.40
1:F:962:PHE:CE2	1:U:958:ILE:HD12	53.62	0.40
1:G:962:PHE:HE2	1:H:958:ILE:HD12	25.01	0.40
1:N:919:VAL:HG13	1:O:923:VAL:HG13	35.82	0.40
1:W:929:THR:OG1	1:X:916:GLN:HB2	2.22	0.40
1:Z:960:LEU:HD23	1:Z:960:LEU:HA	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	2	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	3	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	4	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	5	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	6	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	7	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	8	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	9	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	A	75/91 (82%)	74 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	C	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	D	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	E	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	F	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	G	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	H	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	I	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	J	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	K	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	L	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	M	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	N	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	O	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	P	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	Q	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	R	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	S	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	T	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	U	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	V	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	W	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	X	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	Y	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	Z	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	a	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	b	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	c	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	d	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	e	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	f	75/91 (82%)	74 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	g	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	h	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	i	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	j	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	k	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	l	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	m	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	n	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	o	75/91 (82%)	73 (97%)	2 (3%)	0	100	100
1	p	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	q	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	r	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	s	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	t	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	u	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	v	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	w	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	x	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
1	y	75/91 (82%)	74 (99%)	1 (1%)	0	100	100
All	All	4500/5460 (82%)	4439 (99%)	61 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	1	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	2	68/79 (86%)	67 (98%)	1 (2%)	72	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	68/79 (86%)	66 (97%)	2 (3%)	50	80
1	4	68/79 (86%)	66 (97%)	2 (3%)	50	80
1	5	68/79 (86%)	66 (97%)	2 (3%)	50	80
1	6	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	7	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	8	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	9	68/79 (86%)	68 (100%)	0	100	100
1	A	68/79 (86%)	66 (97%)	2 (3%)	50	80
1	B	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	C	68/79 (86%)	68 (100%)	0	100	100
1	D	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	E	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	F	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	G	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	H	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	I	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	J	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	K	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	L	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	M	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	N	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	O	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	P	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	Q	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	R	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	S	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	T	68/79 (86%)	68 (100%)	0	100	100
1	U	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	V	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	W	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	X	68/79 (86%)	67 (98%)	1 (2%)	72	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	Z	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	a	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	b	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	c	68/79 (86%)	68 (100%)	0	100	100
1	d	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	e	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	f	68/79 (86%)	66 (97%)	2 (3%)	50	80
1	g	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	h	68/79 (86%)	66 (97%)	2 (3%)	50	80
1	i	68/79 (86%)	68 (100%)	0	100	100
1	j	68/79 (86%)	66 (97%)	2 (3%)	50	80
1	k	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	l	68/79 (86%)	68 (100%)	0	100	100
1	m	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	n	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	o	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	p	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	q	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	r	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	s	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	t	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	u	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	v	68/79 (86%)	68 (100%)	0	100	100
1	w	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	x	68/79 (86%)	67 (98%)	1 (2%)	72	88
1	y	68/79 (86%)	67 (98%)	1 (2%)	72	88
All	All	4080/4740 (86%)	4020 (98%)	60 (2%)	72	88

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	944	LEU

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Mol	Chain	Res	Type
1	A	947	TYR
1	B	947	TYR
1	D	941	ASN
1	E	947	TYR
1	F	947	TYR
1	G	947	TYR
1	H	947	TYR
1	I	947	TYR
1	J	947	TYR
1	K	947	TYR
1	L	947	TYR
1	M	947	TYR
1	N	947	TYR
1	O	947	TYR
1	P	947	TYR
1	Q	947	TYR
1	R	947	TYR
1	S	941	ASN
1	U	947	TYR
1	V	947	TYR
1	W	947	TYR
1	X	947	TYR
1	Y	947	TYR
1	Z	947	TYR
1	1	947	TYR
1	2	947	TYR
1	3	928	TYR
1	3	947	TYR
1	4	947	TYR
1	4	954	CYS
1	5	941	ASN
1	5	947	TYR
1	6	941	ASN
1	7	947	TYR
1	8	947	TYR
1	a	947	TYR
1	b	947	TYR
1	d	947	TYR
1	e	947	TYR
1	f	941	ASN
1	f	947	TYR
1	g	947	TYR

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Mol	Chain	Res	Type
1	h	944	LEU
1	h	947	TYR
1	j	941	ASN
1	j	947	TYR
1	k	947	TYR
1	m	947	TYR
1	n	947	TYR
1	o	947	TYR
1	p	947	TYR
1	q	947	TYR
1	r	947	TYR
1	s	947	TYR
1	t	947	TYR
1	u	947	TYR
1	w	947	TYR
1	x	947	TYR
1	y	941	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	910	GLN
1	N	916	GLN
1	W	964	ASN
1	2	941	ASN
1	l	941	ASN
1	o	941	ASN
1	s	964	ASN
1	y	910	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	1	77/91 (84%)	0.69	3 (3%)	43 41	58, 88, 156, 303	0
1	2	77/91 (84%)	0.91	6 (7%)	16 16	60, 84, 174, 300	0
1	3	77/91 (84%)	0.54	2 (2%)	59 58	76, 95, 159, 253	0
1	4	77/91 (84%)	0.53	2 (2%)	59 58	68, 96, 156, 183	0
1	5	77/91 (84%)	0.33	0	100 100	59, 86, 170, 203	0
1	6	77/91 (84%)	0.40	0	100 100	69, 90, 138, 181	0
1	7	77/91 (84%)	0.69	6 (7%)	16 16	82, 124, 171, 224	0
1	8	77/91 (84%)	0.64	6 (7%)	16 16	103, 135, 197, 223	0
1	9	77/91 (84%)	0.95	8 (10%)	8 8	90, 109, 186, 248	0
1	A	77/91 (84%)	0.18	0	100 100	72, 109, 172, 257	0
1	B	77/91 (84%)	0.53	1 (1%)	79 79	79, 106, 160, 197	0
1	C	77/91 (84%)	0.36	1 (1%)	79 79	79, 113, 162, 207	0
1	D	77/91 (84%)	0.40	2 (2%)	59 58	79, 115, 188, 229	0
1	E	77/91 (84%)	0.51	3 (3%)	43 41	61, 81, 119, 163	0
1	F	77/91 (84%)	0.56	2 (2%)	59 58	64, 77, 142, 246	0
1	G	77/91 (84%)	0.69	3 (3%)	43 41	74, 100, 158, 172	0
1	H	77/91 (84%)	0.62	5 (6%)	22 22	72, 108, 157, 208	0
1	I	77/91 (84%)	0.55	2 (2%)	59 58	86, 119, 200, 242	0
1	J	77/91 (84%)	0.85	8 (10%)	8 8	84, 120, 181, 199	0
1	K	77/91 (84%)	0.86	3 (3%)	43 41	81, 102, 145, 275	0
1	L	77/91 (84%)	0.47	3 (3%)	43 41	77, 109, 171, 223	0
1	M	77/91 (84%)	0.68	3 (3%)	43 41	65, 83, 147, 262	0
1	N	77/91 (84%)	0.78	5 (6%)	22 22	72, 95, 141, 166	0
1	O	77/91 (84%)	0.76	9 (11%)	6 6	80, 120, 163, 250	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	P	77/91 (84%)	0.90	10 (12%) 5 4	74, 122, 195, 209	0
1	Q	77/91 (84%)	0.51	1 (1%) 79 79	80, 110, 176, 215	0
1	R	77/91 (84%)	0.59	4 (5%) 31 29	73, 100, 154, 250	0
1	S	77/91 (84%)	0.19	1 (1%) 79 79	75, 107, 157, 188	0
1	T	77/91 (84%)	0.38	0 100 100	78, 117, 172, 231	0
1	U	77/91 (84%)	0.26	1 (1%) 79 79	74, 95, 166, 193	0
1	V	77/91 (84%)	0.49	2 (2%) 59 58	73, 100, 152, 235	0
1	W	77/91 (84%)	0.25	0 100 100	67, 94, 164, 213	0
1	X	77/91 (84%)	0.45	1 (1%) 79 79	73, 98, 135, 180	0
1	Y	77/91 (84%)	0.67	2 (2%) 59 58	68, 90, 131, 183	0
1	Z	77/91 (84%)	0.45	1 (1%) 79 79	57, 89, 161, 180	0
1	a	77/91 (84%)	0.80	7 (9%) 11 11	83, 112, 164, 214	0
1	b	77/91 (84%)	0.47	3 (3%) 43 41	82, 125, 191, 234	0
1	c	77/91 (84%)	0.48	2 (2%) 59 58	95, 132, 196, 231	0
1	d	77/91 (84%)	0.64	4 (5%) 31 29	93, 152, 221, 290	0
1	e	77/91 (84%)	0.53	5 (6%) 22 22	89, 132, 196, 217	0
1	f	77/91 (84%)	0.61	3 (3%) 43 41	81, 128, 213, 268	0
1	g	77/91 (84%)	0.71	9 (11%) 6 6	86, 145, 197, 298	0
1	h	77/91 (84%)	0.45	3 (3%) 43 41	65, 102, 185, 227	0
1	i	77/91 (84%)	0.68	4 (5%) 31 29	68, 104, 158, 183	0
1	j	77/91 (84%)	0.78	12 (15%) 3 3	122, 175, 245, 293	0
1	k	77/91 (84%)	1.12	18 (23%) 1 1	112, 181, 249, 325	0
1	l	77/91 (84%)	1.01	13 (16%) 2 2	121, 169, 228, 272	0
1	m	77/91 (84%)	0.66	5 (6%) 22 22	126, 170, 236, 303	0
1	n	77/91 (84%)	2.17	39 (50%) 0 0	137, 225, 338, 372	0
1	o	77/91 (84%)	2.10	39 (50%) 0 0	149, 237, 315, 383	0
1	p	77/91 (84%)	1.91	33 (42%) 0 1	123, 180, 281, 372	0
1	q	77/91 (84%)	1.60	28 (36%) 0 1	130, 174, 242, 343	0
1	r	77/91 (84%)	0.50	3 (3%) 43 41	79, 103, 169, 191	0
1	s	77/91 (84%)	0.86	10 (12%) 5 4	79, 112, 151, 174	0
1	t	77/91 (84%)	0.78	11 (14%) 4 3	76, 108, 183, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	u	77/91 (84%)	1.03	12 (15%)	3 3	80, 107, 158, 182	0
1	v	77/91 (84%)	0.53	4 (5%)	31 29	79, 104, 157, 222	0
1	w	77/91 (84%)	0.92	7 (9%)	11 11	92, 110, 189, 313	0
1	x	77/91 (84%)	0.59	4 (5%)	31 29	101, 124, 156, 203	0
1	y	77/91 (84%)	0.30	3 (3%)	43 41	84, 116, 172, 201	0
All	All	4620/5460 (84%)	0.70	387 (8%)	14 13	57, 115, 217, 383	0

All (387) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	966	THR	13.1
1	n	893	VAL	9.4
1	w	941	ASN	7.9
1	p	966	THR	7.9
1	p	951	LYS	7.8
1	j	966	THR	7.4
1	n	903	THR	7.3
1	q	891	VAL	7.3
1	n	949	LYS	7.1
1	o	919	VAL	7.1
1	o	891	VAL	6.9
1	2	941	ASN	6.5
1	p	936	THR	6.4
1	o	890	SER	6.1
1	o	951	LYS	6.0
1	n	924	SER	5.9
1	m	966	THR	5.8
1	u	891	VAL	5.8
1	o	893	VAL	5.7
1	q	893	VAL	5.7
1	w	966	THR	5.4
1	q	908	TRP	5.3
1	w	942	GLU	5.2
1	p	964	ASN	5.1
1	k	948	ILE	5.0
1	o	965	PRO	5.0
1	n	953	GLN	4.9
1	o	898	TRP	4.8
1	n	902	LEU	4.6
1	n	926	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	q	955	LEU	4.6
1	q	898	TRP	4.6
1	q	916	GLN	4.6
1	s	962	PHE	4.5
1	o	892	PHE	4.5
1	V	966	THR	4.4
1	o	894	LYS	4.4
1	d	908	TRP	4.4
1	J	966	THR	4.3
1	p	953	GLN	4.3
1	9	964	ASN	4.3
1	P	947	TYR	4.3
1	o	908	TRP	4.3
1	3	942	GLU	4.3
1	l	892	PHE	4.2
1	p	941	ASN	4.1
1	n	901	GLN	4.0
1	n	911	PHE	4.0
1	p	928	TYR	4.0
1	n	892	PHE	4.0
1	p	927	SER	4.0
1	2	942	GLU	4.0
1	o	917	LEU	4.0
1	j	901	GLN	3.9
1	n	923	VAL	3.9
1	q	962	PHE	3.9
1	m	951	LYS	3.9
1	F	941	ASN	3.8
1	n	928	TYR	3.8
1	l	941	ASN	3.8
1	q	910	GLN	3.8
1	k	927	SER	3.8
1	o	910	GLN	3.7
1	m	893	VAL	3.7
1	j	893	VAL	3.7
1	k	951	LYS	3.7
1	o	964	ASN	3.7
1	o	966	THR	3.6
1	u	916	GLN	3.6
1	2	940	GLU	3.6
1	q	918	VAL	3.6
1	u	890	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	l	962	PHE	3.6
1	l	893	VAL	3.6
1	P	966	THR	3.6
1	O	894	LYS	3.5
1	o	962	PHE	3.5
1	n	917	LEU	3.5
1	P	951	LYS	3.5
1	w	964	ASN	3.4
1	o	896	VAL	3.4
1	m	890	SER	3.4
1	3	941	ASN	3.4
1	k	955	LEU	3.4
1	j	965	PRO	3.4
1	o	935	THR	3.4
1	P	932	ASN	3.3
1	g	896	VAL	3.3
1	q	892	PHE	3.3
1	k	947	TYR	3.3
1	P	946	ASP	3.3
1	n	930	SER	3.3
1	j	908	TRP	3.3
1	O	962	PHE	3.3
1	l	961	MET	3.3
1	p	955	LEU	3.3
1	n	950	GLN	3.2
1	a	965	PRO	3.2
1	k	926	ILE	3.2
1	s	893	VAL	3.2
1	o	913	ASP	3.2
1	E	941	ASN	3.2
1	O	917	LEU	3.2
1	l	901	GLN	3.2
1	a	966	THR	3.2
1	x	966	THR	3.2
1	q	924	SER	3.1
1	n	904	SER	3.1
1	8	962	PHE	3.1
1	o	961	MET	3.1
1	n	959	LEU	3.1
1	q	932	ASN	3.1
1	n	962	PHE	3.0
1	n	898	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	9	962	PHE	3.0
1	m	902	LEU	3.0
1	v	966	THR	3.0
1	s	908	TRP	3.0
1	n	896	VAL	3.0
1	n	946	ASP	3.0
1	s	917	LEU	3.0
1	8	966	THR	3.0
1	j	961	MET	3.0
1	u	910	GLN	3.0
1	N	908	TRP	3.0
1	g	910	GLN	3.0
1	o	920	GLN	2.9
1	o	942	GLU	2.9
1	J	955	LEU	2.9
1	o	911	PHE	2.9
1	l	948	ILE	2.9
1	r	959	LEU	2.9
1	e	918	VAL	2.9
1	g	962	PHE	2.9
1	p	929	THR	2.9
1	l	951	LYS	2.9
1	O	910	GLN	2.9
1	q	896	VAL	2.9
1	4	917	LEU	2.9
1	U	962	PHE	2.9
1	o	907	VAL	2.9
1	q	923	VAL	2.9
1	p	932	ASN	2.9
1	N	962	PHE	2.8
1	P	950	GLN	2.8
1	g	916	GLN	2.8
1	p	935	THR	2.8
1	t	902	LEU	2.8
1	g	893	VAL	2.8
1	o	895	ASN	2.8
1	2	936	THR	2.8
1	p	908	TRP	2.8
1	p	914	GLY	2.8
1	y	962	PHE	2.8
1	s	961	MET	2.8
1	n	916	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	p	919	VAL	2.8
1	9	966	THR	2.8
1	k	935	THR	2.8
1	p	949	LYS	2.8
1	N	910	GLN	2.7
1	O	895	ASN	2.7
1	g	917	LEU	2.7
1	p	942	GLU	2.7
1	q	960	LEU	2.7
1	9	908	TRP	2.7
1	u	908	TRP	2.7
1	n	951	LYS	2.7
1	q	933	GLY	2.7
1	q	897	GLY	2.7
1	H	917	LEU	2.6
1	f	924	SER	2.6
1	p	952	LEU	2.6
1	l	891	VAL	2.6
1	n	922	GLY	2.6
1	P	931	PRO	2.6
1	o	963	SER	2.6
1	p	961	MET	2.6
1	8	959	LEU	2.6
1	n	948	ILE	2.6
1	n	960	LEU	2.6
1	x	908	TRP	2.6
1	p	937	ARG	2.6
1	d	919	VAL	2.6
1	o	909	VAL	2.6
1	k	932	ASN	2.6
1	i	893	VAL	2.6
1	u	898	TRP	2.6
1	w	902	LEU	2.6
1	u	961	MET	2.6
1	p	920	GLN	2.6
1	G	966	THR	2.6
1	n	952	LEU	2.6
1	L	902	LEU	2.6
1	t	898	TRP	2.5
1	9	893	VAL	2.5
1	o	927	SER	2.5
1	8	961	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	k	936	THR	2.5
1	2	937	ARG	2.5
1	H	894	LYS	2.5
1	n	938	TYR	2.5
1	k	907	VAL	2.5
1	n	908	TRP	2.5
1	o	936	THR	2.5
1	l	911	PHE	2.5
1	M	935	THR	2.5
1	p	954	CYS	2.5
1	o	921	ALA	2.5
1	s	910	GLN	2.5
1	n	932	ASN	2.5
1	q	894	LYS	2.5
1	j	911	PHE	2.5
1	Z	962	PHE	2.5
1	o	926	ILE	2.5
1	q	961	MET	2.5
1	g	960	LEU	2.5
1	d	910	GLN	2.5
1	p	916	GLN	2.5
1	q	911	PHE	2.5
1	l	947	TYR	2.5
1	S	962	PHE	2.5
1	p	965	PRO	2.5
1	k	898	TRP	2.4
1	p	893	VAL	2.4
1	k	934	GLN	2.4
1	Y	960	LEU	2.4
1	j	891	VAL	2.4
1	Y	962	PHE	2.4
1	J	896	VAL	2.4
1	p	918	VAL	2.4
1	s	965	PRO	2.4
1	e	902	LEU	2.4
1	7	932	ASN	2.4
1	k	946	ASP	2.4
1	o	958	ILE	2.4
1	o	959	LEU	2.4
1	y	960	LEU	2.4
1	o	916	GLN	2.4
1	7	907	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	n	910	GLN	2.4
1	q	965	PRO	2.4
1	l	960	LEU	2.4
1	V	965	PRO	2.3
1	c	962	PHE	2.3
1	Q	890	SER	2.3
1	E	959	LEU	2.3
1	n	958	ILE	2.3
1	q	958	ILE	2.3
1	u	960	LEU	2.3
1	7	893	VAL	2.3
1	n	918	VAL	2.3
1	J	894	LYS	2.3
1	k	931	PRO	2.3
1	s	959	LEU	2.3
1	L	962	PHE	2.3
1	R	962	PHE	2.3
1	7	962	PHE	2.3
1	u	962	PHE	2.3
1	4	908	TRP	2.3
1	l	917	LEU	2.3
1	f	923	VAL	2.3
1	t	909	VAL	2.3
1	p	960	LEU	2.3
1	t	955	LEU	2.3
1	w	908	TRP	2.3
1	s	966	THR	2.3
1	t	957	SER	2.3
1	J	910	GLN	2.3
1	N	960	LEU	2.3
1	H	903	THR	2.3
1	r	962	PHE	2.3
1	s	894	LYS	2.3
1	q	903	THR	2.3
1	K	951	LYS	2.3
1	k	940	GLU	2.3
1	P	917	LEU	2.3
1	7	955	LEU	2.3
1	i	960	LEU	2.3
1	g	908	TRP	2.3
1	t	959	LEU	2.3
1	P	926	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	908	TRP	2.2
1	q	959	LEU	2.2
1	O	958	ILE	2.2
1	o	948	ILE	2.2
1	p	962	PHE	2.2
1	e	936	THR	2.2
1	x	896	VAL	2.2
1	n	957	SER	2.2
1	R	958	ILE	2.2
1	l	910	GLN	2.2
1	n	947	TYR	2.2
1	p	947	TYR	2.2
1	C	941	ASN	2.2
1	l	917	LEU	2.2
1	q	954	CYS	2.2
1	F	962	PHE	2.2
1	a	908	TRP	2.2
1	I	893	VAL	2.2
1	i	896	VAL	2.2
1	u	896	VAL	2.2
1	h	955	LEU	2.2
1	j	917	LEU	2.2
1	o	955	LEU	2.2
1	x	917	LEU	2.2
1	q	907	VAL	2.2
1	G	901	GLN	2.2
1	q	920	GLN	2.2
1	u	892	PHE	2.2
1	r	898	TRP	2.2
1	b	890	SER	2.2
1	a	962	PHE	2.2
1	M	941	ASN	2.2
1	q	966	THR	2.2
1	t	961	MET	2.2
1	a	896	VAL	2.2
1	O	960	LEU	2.1
1	E	962	PHE	2.1
1	j	920	GLN	2.1
1	p	910	GLN	2.1
1	g	941	ASN	2.1
1	o	960	LEU	2.1
1	G	958	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	8	958	ILE	2.1
1	h	894	LYS	2.1
1	o	918	VAL	2.1
1	R	917	LEU	2.1
1	a	917	LEU	2.1
1	h	960	LEU	2.1
1	j	902	LEU	2.1
1	u	959	LEU	2.1
1	I	962	PHE	2.1
1	D	896	VAL	2.1
1	2	930	SER	2.1
1	K	917	LEU	2.1
1	O	908	TRP	2.1
1	J	902	LEU	2.1
1	y	890	SER	2.1
1	9	942	GLU	2.1
1	k	952	LEU	2.1
1	n	955	LEU	2.1
1	J	949	LYS	2.1
1	L	960	LEU	2.1
1	f	939	GLY	2.1
1	M	942	GLU	2.1
1	9	940	GLU	2.1
1	N	898	TRP	2.1
1	p	926	ILE	2.1
1	i	902	LEU	2.1
1	o	950	GLN	2.1
1	a	911	PHE	2.1
1	p	912	ASN	2.1
1	B	962	PHE	2.1
1	t	895	ASN	2.1
1	k	949	LYS	2.0
1	k	933	GLY	2.0
1	t	960	LEU	2.0
1	t	962	PHE	2.0
1	H	893	VAL	2.0
1	J	917	LEU	2.0
1	b	941	ASN	2.0
1	d	917	LEU	2.0
1	n	920	GLN	2.0
1	n	961	MET	2.0
1	v	908	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	w	940	GLU	2.0
1	O	907	VAL	2.0
1	v	891	VAL	2.0
1	X	960	LEU	2.0
1	n	944	LEU	2.0
1	l	962	PHE	2.0
1	D	916	GLN	2.0
1	e	950	GLN	2.0
1	j	916	GLN	2.0
1	p	891	VAL	2.0
1	8	899	ALA	2.0
1	b	962	PHE	2.0
1	v	962	PHE	2.0
1	P	936	THR	2.0
1	R	941	ASN	2.0
1	7	951	LYS	2.0
1	o	901	GLN	2.0
1	9	960	LEU	2.0
1	c	896	VAL	2.0
1	e	960	LEU	2.0
1	t	917	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.