



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:46 PM EDT

PDB ID : 5LHY / pdb_00005lhy
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

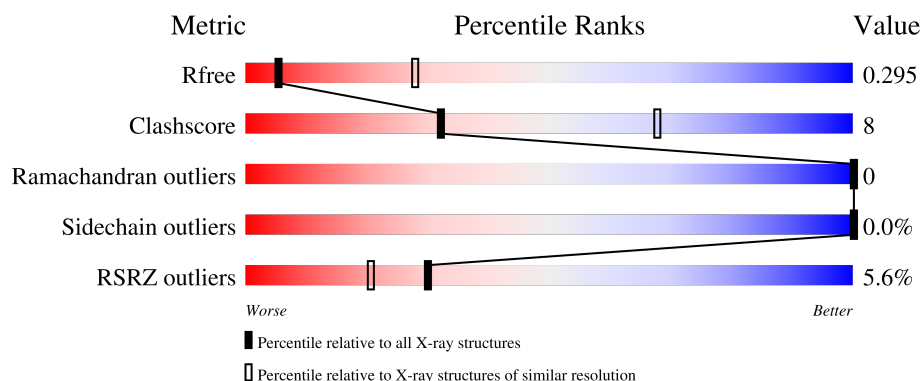
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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.



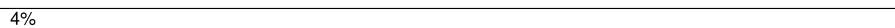
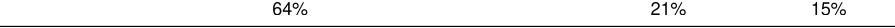
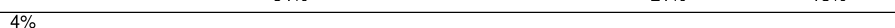
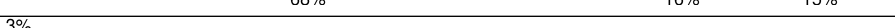
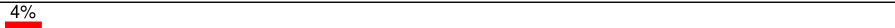
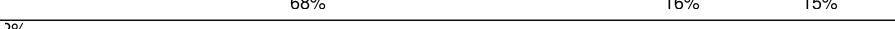
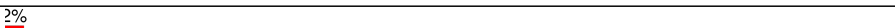
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	91	4% 67% 18% 15%
1	2	91	8% 60% 24% 15%
1	3	91	4% 66% 19% 15%
1	4	91	2% 70% 14% 15%
1	5	91	% 63% 22% 15%

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Mol	Chain	Length	Quality of chain
1	6	91	
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	

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Mol	Chain	Length	Quality of chain
1	V	91	
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	

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Mol	Chain	Length	Quality of chain
1	u	91	2% 70% 14% 15%
1	v	91	3% 69% 15% 15%
1	w	91	5% 65% 20% 15%
1	x	91	4% 73% 12% 15%
1	y	91	4% 69% 15% 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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Continued from previous page...

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
y	881	PRO	-	expression tag	UNP O00444
y	882	MET	-	expression tag	UNP O00444
y	883	GLY	-	expression tag	UNP O00444

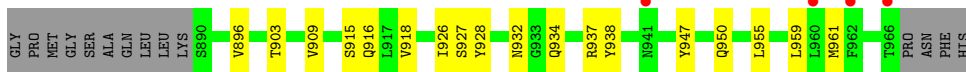
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

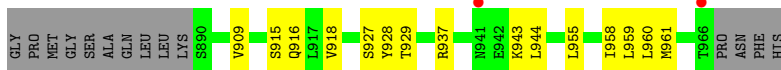
- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



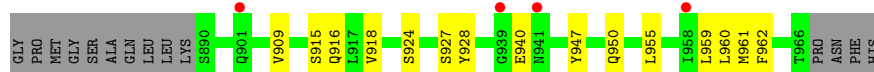
- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



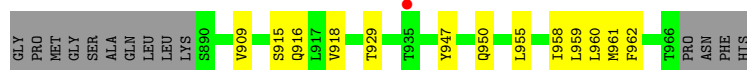
- Molecule 1: Serine/threonine-protein kinase PLK4



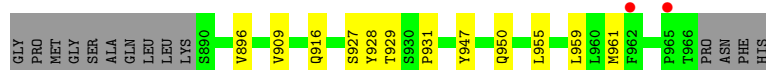
- Molecule 1: Serine/threonine-protein kinase PLK4



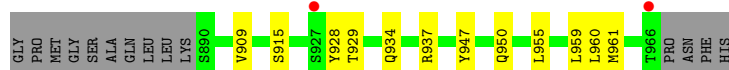
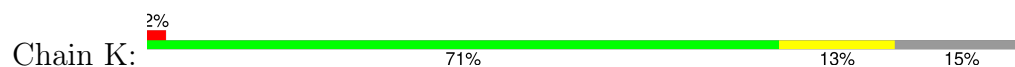
- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



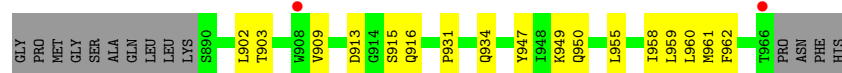
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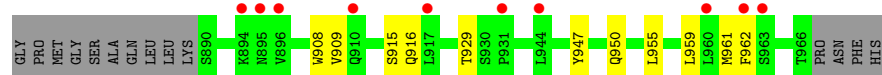
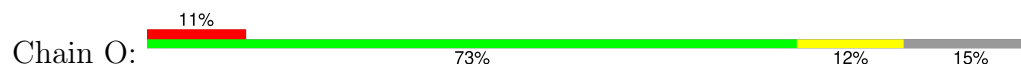
- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



- 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

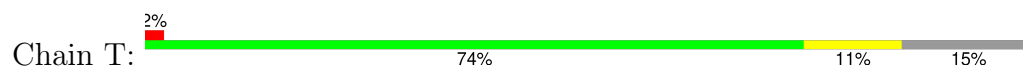


- Molecule 1: Serine/threonine-protein kinase PLK4





- Molecule 1: Serine/threonine-protein kinase PLK4



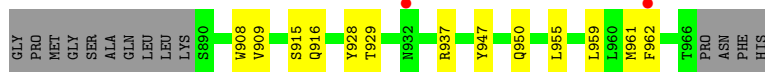
- Molecule 1: Serine/threonine-protein kinase PLK4



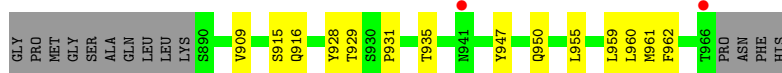
- Molecule 1: Serine/threonine-protein kinase PLK4



- 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



- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



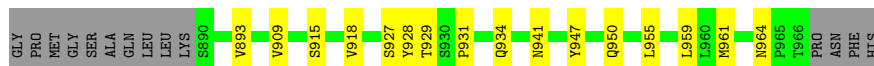
- Molecule 1: Serine/threonine-protein kinase PLK4



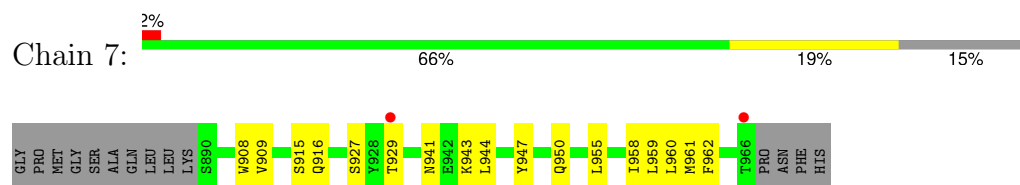
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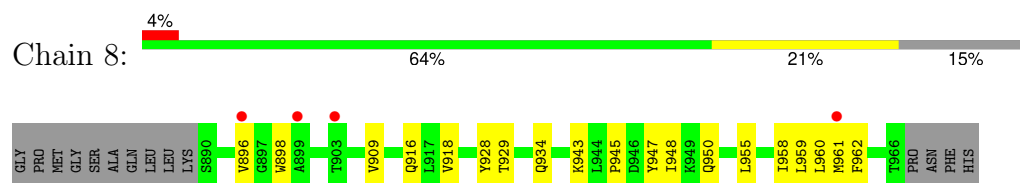
- Molecule 1: Serine/threonine-protein kinase PLK4



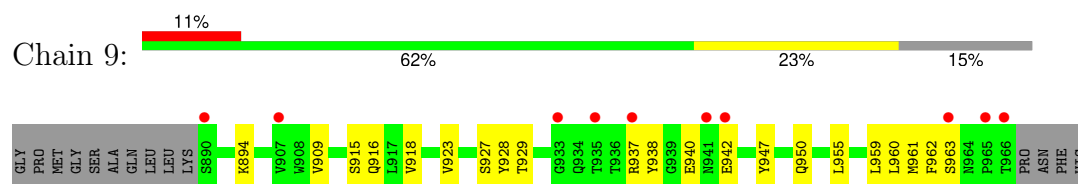
● Molecule 1: Serine/threonine-protein kinase PLK4



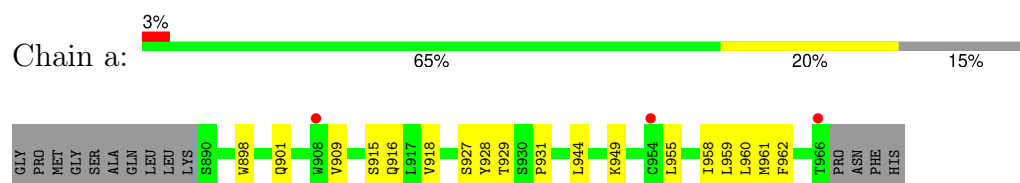
● Molecule 1: Serine/threonine-protein kinase PLK4



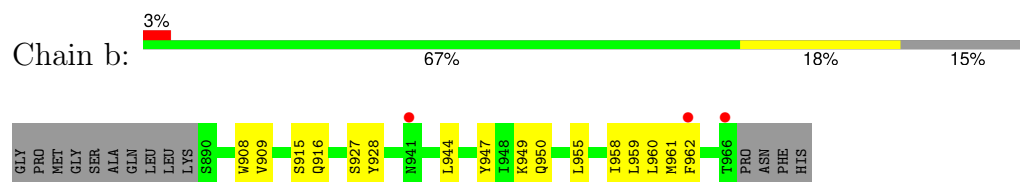
● Molecule 1: Serine/threonine-protein kinase PLK4



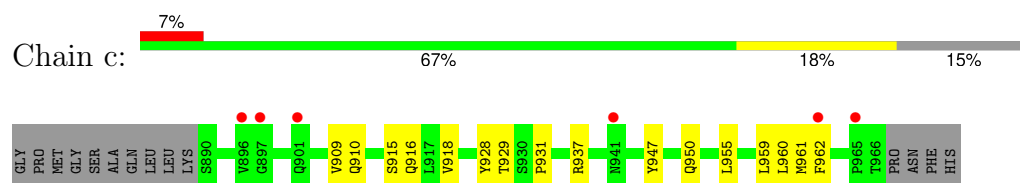
● Molecule 1: Serine/threonine-protein kinase PLK4



● Molecule 1: Serine/threonine-protein kinase PLK4

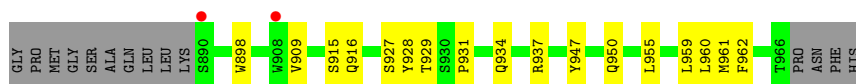


● Molecule 1: Serine/threonine-protein kinase PLK4



● Molecule 1: Serine/threonine-protein kinase PLK4





- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



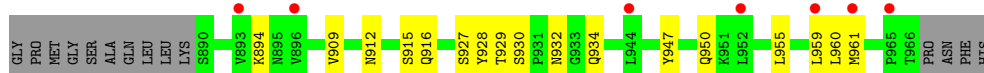
- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



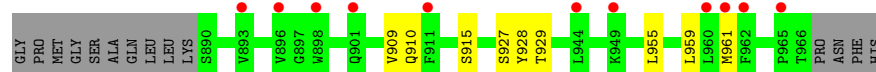
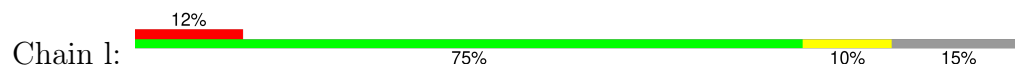
- Molecule 1: Serine/threonine-protein kinase PLK4



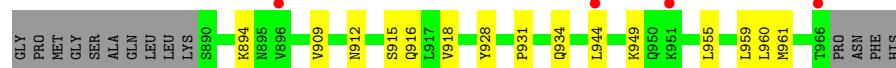
- Molecule 1: Serine/threonine-protein kinase PLK4



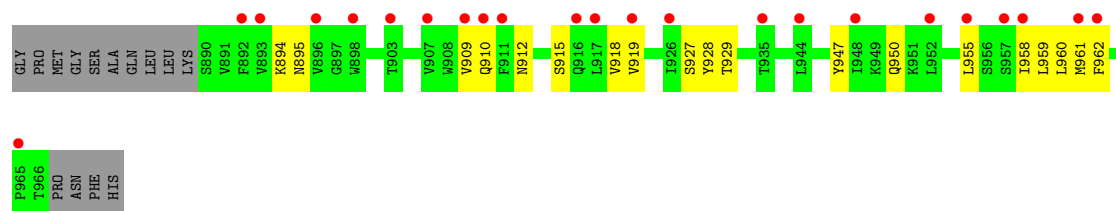
- Molecule 1: Serine/threonine-protein kinase PLK4



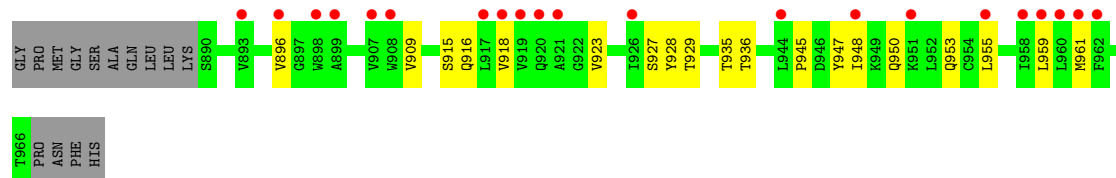
- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



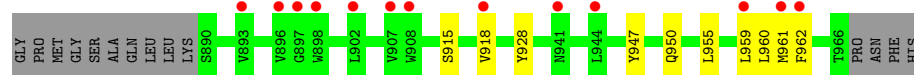
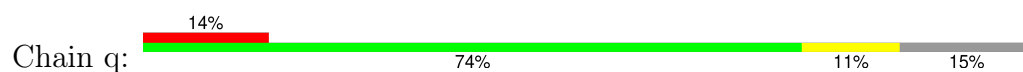
- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



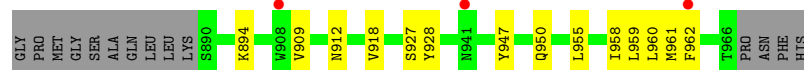
- Molecule 1: Serine/threonine-protein kinase PLK4



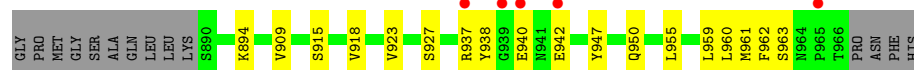
- Molecule 1: Serine/threonine-protein kinase PLK4



- Molecule 1: Serine/threonine-protein kinase PLK4



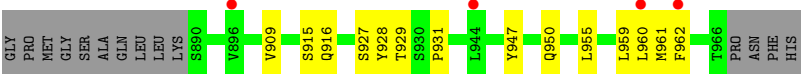
- Molecule 1: Serine/threonine-protein kinase PLK4



● Molecule 1: Serine/threonine-protein kinase PLK4



● 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 – 3.31 104.37 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (104.37-3.31) 99.9 (104.37-3.31)	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 0.272 , 0.295	Depositor DCC
R_{free} test set	5938 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	103.9	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.0	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	0.90	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

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	1	0.11	0/605	0.29	0/823
1	2	0.15	0/605	0.34	0/823
1	3	0.25	0/605	0.34	0/823
1	4	0.10	0/605	0.28	0/823
1	5	0.11	0/605	0.26	0/823
1	6	0.12	0/605	0.33	0/823
1	7	0.11	0/605	0.30	0/823
1	8	0.10	0/605	0.29	0/823
1	9	0.11	0/605	0.29	0/823
1	A	0.11	0/605	0.32	0/823
1	B	0.11	0/605	0.33	0/823
1	C	0.10	0/605	0.27	0/823
1	D	0.10	0/605	0.27	0/823
1	E	0.12	0/605	0.31	0/823
1	F	0.14	0/605	0.34	0/823
1	G	0.11	0/605	0.34	0/823
1	H	0.10	0/605	0.26	0/823
1	I	0.10	0/605	0.28	0/823
1	J	0.09	0/605	0.27	0/823
1	K	0.11	0/605	0.30	0/823
1	L	0.10	0/605	0.25	0/823
1	M	0.12	0/605	0.29	0/823
1	N	0.11	0/605	0.29	0/823
1	O	0.11	0/605	0.30	0/823
1	P	0.10	0/605	0.29	0/823
1	Q	0.10	0/605	0.27	0/823
1	R	0.10	0/605	0.27	0/823
1	S	0.11	0/605	0.30	0/823
1	T	0.11	0/605	0.30	0/823
1	U	0.10	0/605	0.27	0/823
1	V	0.13	0/605	0.36	0/823
1	W	0.10	0/605	0.26	0/823
1	X	0.11	0/605	0.31	0/823
1	Y	0.13	0/605	0.34	0/823

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Z	0.11	0/605	0.30	0/823
1	a	0.10	0/605	0.31	0/823
1	b	0.10	0/605	0.27	0/823
1	c	0.10	0/605	0.26	0/823
1	d	0.10	0/605	0.26	0/823
1	e	0.10	0/605	0.29	0/823
1	f	0.10	0/605	0.28	0/823
1	g	0.11	0/605	0.29	0/823
1	h	0.11	0/605	0.30	0/823
1	i	0.12	0/605	0.32	0/823
1	j	0.10	0/605	0.29	0/823
1	k	0.10	0/605	0.29	0/823
1	l	0.10	0/605	0.28	0/823
1	m	0.09	0/605	0.28	0/823
1	n	0.10	0/605	0.29	0/823
1	o	0.09	0/605	0.29	0/823
1	p	0.10	0/605	0.29	0/823
1	q	0.09	0/605	0.26	0/823
1	r	0.10	0/605	0.29	0/823
1	s	0.13	0/605	0.33	0/823
1	t	0.10	0/605	0.28	0/823
1	u	0.10	0/605	0.30	0/823
1	v	0.09	0/605	0.27	0/823
1	w	0.11	0/605	0.26	0/823
1	x	0.10	0/605	0.26	0/823
1	y	0.10	0/605	0.26	0/823
All	All	0.11	0/36300	0.29	0/49380

There are no bond length outliers.

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	16	0
1	2	593	0	586	26	0
1	3	593	0	586	12	0
1	4	593	0	586	11	0
1	5	593	0	586	23	0
1	6	593	0	586	16	0
1	7	593	0	586	16	0
1	8	593	0	586	19	0
1	9	593	0	586	18	0
1	A	593	0	586	18	0
1	B	593	0	586	17	0
1	C	593	0	586	15	0
1	D	593	0	586	18	0
1	E	593	0	586	9	0
1	F	593	0	586	13	0
1	G	593	0	586	12	0
1	H	593	0	586	13	0
1	I	593	0	586	13	0
1	J	593	0	586	11	0
1	K	593	0	586	11	0
1	L	593	0	586	14	0
1	M	593	0	586	12	0
1	N	593	0	586	16	0
1	O	593	0	586	10	0
1	P	593	0	586	12	0
1	Q	593	0	586	14	0
1	R	593	0	586	21	0
1	S	593	0	586	15	0
1	T	593	0	586	9	0
1	U	593	0	586	18	0
1	V	593	0	586	16	0
1	W	593	0	586	15	0
1	X	593	0	586	13	0
1	Y	593	0	586	18	0
1	Z	593	0	586	13	0
1	a	593	0	586	16	0
1	b	593	0	586	16	0
1	c	593	0	586	14	0
1	d	593	0	586	19	0
1	e	593	0	586	20	0
1	f	593	0	586	18	0
1	g	593	0	586	16	0
1	h	593	0	586	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	i	593	0	586	16	0
1	j	593	0	586	14	0
1	k	593	0	586	15	0
1	l	593	0	586	10	0
1	m	593	0	586	13	0
1	n	593	0	586	17	0
1	o	593	0	586	16	0
1	p	593	0	586	12	0
1	q	593	0	586	10	0
1	r	593	0	586	14	0
1	s	593	0	586	12	0
1	t	593	0	586	18	0
1	u	593	0	586	12	0
1	v	593	0	586	12	0
1	w	593	0	586	14	0
1	x	593	0	586	12	0
1	y	593	0	586	16	0
All	All	35580	0	35160	569	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 8.

All (569) 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	1.18	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	2.02	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	1.68	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
1:F:940:GLU:HB3	1:6:934:GLN:HE21	1.54	0.71
1:9:918:VAL:HB	1:a:927:SER:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:909:VAL:HG21	1:i:955:LEU:HD21	1.71	0.70
1:I:955:LEU:HD11	1:J:909:VAL:HG21	1.73	0.70
1:b:955:LEU:HD11	1:c: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	1.73	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	1.73	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	1.75	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	1.74	0.68
1:V:901:GLN:NE2	1:y:916:GLN:OE1	2.25	0.68
1:m:944:LEU:HD13	1:m:949:LYS:HB2	1.75	0.68
1:A:944:LEU:HD13	1:A:949:LYS:HB2	1.76	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	1.76	0.67
1:A:927:SER:HB3	1:B:918:VAL:HB	1.76	0.67
1:F:939:GLY:H	1:F:942:GLU:CD	2.03	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	1.93	0.66
1:t:960:LEU:HD13	1:t:962:PHE:HE1	1.61	0.66
1:d:955:LEU:HD11	1:e:909:VAL:HG21	1.76	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	1.77	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	2.14	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	1.80	0.63
1:v:955:LEU:HD11	1:w:909:VAL:HG21	1.80	0.62
1:O:909:VAL:HG21	1:P:955:LEU:HD11	1.79	0.62
1:M:939:GLY:H	1:M:942:GLU:CD	2.07	0.62
1:N:960:LEU:HD13	1:N:962:PHE:HE1	1.63	0.61
1:8:943:LYS:HB2	1:d:934:GLN:HG3	1.82	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	1.83	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	1.80	0.61
1:l:927:SER:HB3	1:m:918:VAL:HB	1.82	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
1:8:958:ILE:HD12	1:n:962:PHE:HZ	1.66	0.60
1:x:909:VAL:HG21	1:y:955:LEU:HD11	1.84	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	1.66	0.59
1:t:909:VAL:HG21	1:u:955:LEU:HD11	1.85	0.59
1:G:955:LEU:HD11	1:H:909:VAL:HG21	1.84	0.59
1:9:955:LEU:HD11	1:a:909:VAL:HG21	1.84	0.59
1:O:908:TRP:HE1	1:O:916:GLN:NE2	2.01	0.59
1:1:909:VAL:HG21	1:2:955:LEU:HD21	1.85	0.59
1:n:894:LYS:HE3	1:n:912:ASN:HA	1.84	0.59
1:C:927:SER:HB3	1:D:918:VAL:HB	1.85	0.59
1:S:909:VAL:HG21	1:T:955:LEU:HD11	1.84	0.59
1:h:955:LEU:HD21	1:i:909:VAL:HG21	1.85	0.59
1:E:955:LEU:HD21	1:F:909:VAL:HG21	1.83	0.58
1:L:960:LEU:HD13	1:L:962:PHE:HE1	1.68	0.58
1:b:915:SER:HB3	1:c:931:PRO:HD3	1.85	0.58
1:v:961:MET:HE3	1:y:959:LEU:HD12	1.85	0.58
1:X:947:TYR:HA	1:X:950:GLN:HG2	1.85	0.58
1:G:909:VAL:HG21	1:H:955:LEU:HD21	1.85	0.58
1:9:909:VAL:HG21	1:a:955:LEU:HD11	1.86	0.58
1:n:955:LEU:HD11	1:o:909:VAL:HG21	1.86	0.58
1:c:960:LEU:HD12	1:r:960:LEU:HG	1.85	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	1.53	0.57
1:O:962:PHE:HE2	1:s:958:ILE:HD12	1.68	0.57
1:I:961:MET:HE3	1:L:959:LEU:HD12	1.87	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
1:8:943:LYS:HD3	1:d:934:GLN:HG3	1.87	0.57
1:L:962:PHE:HE2	1:a:958:ILE:HD12	1.69	0.56
1:5:908:TRP:HE1	1:5:916:GLN:NE2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:959:LEU:HD12	1:S:961:MET:HE3	1.87	0.56
1:W:955:LEU:HD11	1:X:909:VAL:HG21	1.87	0.56
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:V:961:MET:HE3	1:W:959:LEU:HD12	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:j:959:LEU:HD12	1:m:961:MET:HE3	1.88	0.55
1:J:961:MET:HE3	1:K:959:LEU:HD12	1.88	0.55
1:A:958:ILE:HD12	1:b:962:PHE:HE2	1.70	0.55
1:I:959:LEU:HD12	1:L:961:MET:HE3	1.87	0.55
1:h:944:LEU:HD13	1:h:949:LYS:HB2	1.89	0.55
1:j:961:MET:HE3	1:m:959:LEU:HD12	1.89	0.55
1:n:895:ASN:HB2	1:n:910:GLN:HB3	1.87	0.55
1:E:959:LEU:HD12	1:H:961:MET:HE3	1.89	0.55
1:S:960:LEU:HD12	1:S:962:PHE:CE1	2.42	0.55
1:g:961:MET:HE3	1:h:959:LEU:HD12	1.89	0.55
1:v:959:LEU:HD12	1:y:961:MET:HE3	1.89	0.55
1:C:918:VAL:HB	1:D:927:SER:HB3	1.89	0.55
1:Z:959:LEU:HD12	1:l:961:MET:HE3	1.89	0.55
1:f:909:VAL:HG21	1:g:955:LEU:HD11	1.89	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	1.90	0.54
1:7:959:LEU:HD12	1:a:961:MET:HE3	1.89	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	1.89	0.54
1:F:961:MET:HE3	1:G:959:LEU:HD12	1.90	0.53
1:N:903:THR:OG1	1:u:932:ASN:O	2.26	0.53
1:Z:961:MET:HE3	1:l:959:LEU:HD12	1.90	0.53
1:n:927:SER:HB3	1:o:918:VAL:HB	1.90	0.53
1:x:918:VAL:HB	1:y:927:SER:HB3	1.89	0.53
1:o:959:LEU:HD12	1:p:961:MET:HE3	1.89	0.53
1:A:961:MET:HE3	1:D:959:LEU:HD12	1.91	0.53
1:n:928:TYR:HE1	1:o:915:SER:HB2	1.74	0.53
1:N:959:LEU:HD12	1:O:961:MET:HE3	1.91	0.53
1:R:961:MET:HE3	1:S:959:LEU:HD12	1.90	0.53
1:U:909:VAL:HG21	1:V:955:LEU:HD11	1.90	0.53
1:k:894:LYS:HE3	1:k:912:ASN:HA	1.89	0.53
1:o:961:MET:HE3	1:p:959:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:908:TRP:HE1	1:t:916:GLN:NE2	2.06	0.53
1:d:909:VAL:HG21	1:e:955:LEU:HD21	1.91	0.53
1:b:909:VAL:HG21	1:c:955:LEU:HD21	1.91	0.53
1:G:915:SER:HB2	1:H:928:TYR:HE1	1.74	0.53
1:4:959:LEU:HD12	1:5:961:MET:HE3	1.90	0.53
1:h:960:LEU:HD11	1:h:962:PHE:CE1	2.44	0.53
1:f:918:VAL:HB	1:g:927:SER:HB3	1.91	0.53
1:y:960:LEU:HD13	1:y:962:PHE:CE1	2.44	0.53
1:7:915:SER:HB2	1:8:928:TYR:HE1	1.74	0.52
1:Q:961:MET:HE3	1:T:959:LEU:HD12	1.91	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:c:959:LEU:HD12	1:d:961:MET:HE3	1.91	0.52
1:2:941:ASN:HD22	1:i:932:ASN:HD21	1.57	0.52
1:N:961:MET:HE3	1:O:959:LEU:HD12	1.91	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:E:961:MET:HE3	1:H:959:LEU:HD12	1.90	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	1.91	0.52
1:w:959:LEU:HD12	1:x:961:MET:HE3	1.90	0.52
1:7:961:MET:HE3	1:a:959:LEU:HD12	1.92	0.52
1:9:915:SER:HB3	1:a:931:PRO:HD3	1.92	0.52
1:F:960:LEU:HD11	1:F:962:PHE:CZ	2.45	0.52
1:M:959:LEU:HD12	1:P:961:MET:HE3	1.92	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
1:4:953:GLN:OE1	1:5:966:THR:N	2.43	0.51
1:d:962:PHE:HZ	1:u:958:ILE:HD12	1.75	0.51
1:f:959:LEU:HD12	1:i:961:MET:HE3	1.92	0.51
1:j:928:TYR:HE1	1:k:915:SER:HB2	1.76	0.51
1:u:934:GLN:OE1	1:u:934:GLN:N	2.40	0.51
1:B:961:MET:HE3	1:C:959:LEU:HD12	1.92	0.51
1:J:959:LEU:HD12	1:K:961:MET:HE3	1.91	0.51
1:O:955:LEU:HD21	1:P:909:VAL:HG21	1.91	0.51
1:9:960:LEU:HD11	1:9:962:PHE:CE1	2.44	0.51
1:a:960:LEU:HD13	1:a:962:PHE:HE1	1.75	0.51
1:b:961:MET:HE3	1:e:959:LEU:HD12	1.92	0.51
1:l:915:SER:HB3	1:m:931:PRO:HD3	1.93	0.51
1:b:960:LEU:HD13	1:b:962:PHE:CE1	2.46	0.51
1:t:955:LEU:HD21	1:u:909:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:916:GLN:HB2	1:u:929:THR:OG1	2.11	0.51
1:w:961:MET:HE3	1:x:959:LEU:HD12	1.92	0.51
1:Q:959:LEU:HD12	1:T:961:MET:HE3	1.92	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	1.75	0.51
1:q:960:LEU:HD13	1:q:962:PHE:HE1	1.76	0.51
1:Y:959:LEU:HD12	1:2:961:MET:HE3	1.93	0.51
1:Y:961:MET:HE3	1:2:959:LEU:HD12	1.93	0.51
1:b:959:LEU:HD12	1:e:961:MET:HE3	1.92	0.51
1:7:908:TRP:HE1	1:7:916:GLN:NE2	2.09	0.50
1:f:961:MET:HE3	1:i:959:LEU:HD12	1.93	0.50
1:j:927:SER:HB3	1:k:918:VAL:HB	1.93	0.50
1:e:960:LEU:HD13	1:e:962:PHE:HE1	1.75	0.50
1:r:959:LEU:HD12	1:u:961:MET:HE3	1.92	0.50
1:I:915:SER:HB3	1:J:931:PRO:HD3	1.94	0.50
1:3:928:TYR:OH	1:3:951:LYS:NZ	2.36	0.50
1:9:915:SER:HB2	1:a:928:TYR:HE1	1.77	0.50
1:j:909:VAL:HG21	1:k:955:LEU:HD11	1.94	0.50
1:t:960:LEU:HD13	1:t:962:PHE:CE1	2.45	0.50
1:w:960:LEU:HD13	1:w:962:PHE:HE1	1.77	0.50
1:B:959:LEU:HD12	1:C:961:MET:HE3	1.93	0.50
1:V:959:LEU:HD12	1:W:961:MET:HE3	1.93	0.50
1:e:960:LEU:HD13	1:e:962:PHE:CE1	2.46	0.50
1:N:958:ILE:HD12	1:t:962:PHE:HE2	1.76	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:k:961:MET:HE3	1:l:959:LEU:HD12	1.93	0.50
1:p:960:LEU:HD13	1:p:962:PHE:HE1	1.75	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	1.94	0.49
1:Y:931:PRO:HD3	1:Z:915:SER:HB3	1.94	0.49
1:3:959:LEU:HD12	1:6:961:MET:HE3	1.93	0.49
1:3:961:MET:HE3	1:6:959:LEU:HD12	1.92	0.49
1:t:928:TYR:HE1	1:u:915:SER:HB2	1.78	0.49
1:3:960:LEU:HD13	1:3:962:PHE:HE1	1.77	0.49
1:r:961:MET:HE3	1:u:959:LEU:HD12	1.94	0.49
1:s:961:MET:HE3	1:t:959:LEU:HD12	1.95	0.49
1:d:927:SER:HB3	1:e:918:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:961:MET:HE3	1:q:959:LEU:HD12	1.94	0.49
1:l:909:VAL:HG21	1:m:955:LEU:HD11	1.95	0.49
1:B:916:GLN:HE22	1:Q:901:GLN:HE21	1.59	0.49
1:K:928:TYR:HE1	1:L:915:SER:HB2	1.78	0.49
1:e:928:TYR:OH	1:e:951:LYS:NZ	2.46	0.49
1:f:915:SER:HB3	1:g:931:PRO:HD3	1.93	0.49
1:F:959:LEU:HD12	1:G:961:MET:HE3	1.93	0.49
1:G:928:TYR:HE1	1:H:915:SER:HB2	1.78	0.49
1:D:960:LEU:HD12	1:e:960:LEU:HD12	1.95	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
1:1:955:LEU:HD21	1:2:909:VAL:HG21	1.94	0.49
1:A:962:PHE:HE2	1:b:958:ILE:HD12	1.77	0.49
1:U:901:GLN:NE2	1:f:916:GLN:OE1	2.43	0.49
1:4:961:MET:HE3	1:5:959:LEU:HD12	1.95	0.49
1:j:915:SER:HB3	1:k:928:TYR:HE1	1.78	0.49
1:n:959:LEU:HD12	1:q:961:MET:HE3	1.95	0.49
1:U:918:VAL:HB	1:V:927:SER:HB3	1.94	0.48
1:U:961:MET:HE3	1:X:959:LEU:HD12	1.94	0.48
1:5:928:TYR:HE1	1:6:915:SER:HB2	1.77	0.48
1:g:959:LEU:HD12	1:h:961:MET:HE3	1.95	0.48
1:h:915:SER:HB2	1:i:928:TYR:HE1	1.78	0.48
1:p:931:PRO:HD3	1:q:915:SER:HB3	1.95	0.48
1:y:947:TYR:HA	1:y:950:GLN:HG2	1.96	0.48
1:X:960:LEU:HD13	1:X:962:PHE:HE1	1.79	0.48
1:8:962:PHE:HZ	1:n:958:ILE:HD12	1.78	0.48
1:b:960:LEU:HD13	1:b:962:PHE:HE1	1.77	0.48
1:c:960:LEU:HD13	1:c:962:PHE:HE1	1.78	0.48
1:p:915:SER:HB2	1:q:928:TYR:HE1	1.78	0.48
1:r:915:SER:HB2	1:s:928:TYR:HE1	1.77	0.48
1:A:959:LEU:HD12	1:D:961:MET:HE3	1.94	0.48
1:U:947:TYR:HA	1:U:950:GLN:HG2	1.96	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	1.78	0.48
1:W:916:GLN:HB2	1:X:929:THR:OG1	2.14	0.48
1:M:961:MET:HE3	1:P:959:LEU:HD12	1.95	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:L:947:TYR:HA	1:L:950:GLN:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:959:LEU:HD12	1:X:961:MET:HE3	1.95	0.48
1:d:928:TYR:HE1	1:e:915:SER:HB2	1.79	0.48
1:1:931:PRO:HD3	1:2:915:SER:HB3	1.96	0.47
1:9:960:LEU:HG	1:q:960:LEU:HD12	1.95	0.47
1:Q:908:TRP:NE1	1:Q:916:GLN:HE21	1.99	0.47
1:3:938:TYR:HA	1:3:942:GLU:OE2	2.14	0.47
1:c:961:MET:HE3	1:d:959:LEU:HD12	1.95	0.47
1:f:915:SER:HB2	1:g:928:TYR:HE1	1.80	0.47
1:k:896:VAL:HG12	1:k:909:VAL:HG22	1.96	0.47
1:L:897:GLY:HA3	1:L:960:LEU:HD23	1.96	0.47
1:2:941:ASN:ND2	1:i:932:ASN:HD21	2.13	0.47
1:5:941:ASN:HD22	1:5:941:ASN:C	2.21	0.47
1:v:928:TYR:HE1	1:w:915:SER:HB2	1.80	0.47
1:v:947:TYR:HA	1:v:950:GLN:HG2	1.97	0.47
1:H:958:ILE:HD12	1:g:962:PHE:CE2	2.50	0.47
1:R:962:PHE:HZ	1:2:958:ILE:HG21	1.79	0.47
1:W:928:TYR:HE1	1:X:915:SER:HB2	1.79	0.47
1:8:961:MET:HE3	1:9:959:LEU:HD12	1.97	0.47
1:s:960:LEU:HD11	1:s:962:PHE:CZ	2.50	0.47
1:K:960:LEU:HD23	1:K:960:LEU:HA	1.77	0.47
1:Y:953:GLN:OE1	1:2:966:THR:N	2.30	0.47
1:5:916:GLN:HB2	1:6:929:THR:OG1	2.15	0.47
1:d:947:TYR:HA	1:d:950:GLN:HG2	1.97	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	2.15	0.47
1:u:960:LEU:HD23	1:u:960:LEU:HA	1.83	0.47
1:x:928:TYR:HE1	1:y:915:SER:HB3	1.80	0.47
1:S:962:PHE:HE2	1:Y:958:ILE:HD12	1.79	0.47
1:b:908:TRP:HE1	1:b:916:GLN:NE2	2.13	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	1.79	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	2.49	0.46
1:k:947:TYR:HA	1:k:950:GLN:HG2	1.98	0.46
1:t:960:LEU:HD23	1:t:960:LEU:HA	1.77	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:c:910:GLN:HG3	1:c:916: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	1.98	0.46
1:R:947:TYR:HA	1:R:950:GLN:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:929:THR:OG1	1:k:916:GLN:HB2	2.16	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	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
1:4:947:TYR:HA	1:4:950:GLN:HG2	1.97	0.46
1:A:918:VAL:HB	1:B:927:SER:HB3	1.96	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:Z:947:TYR:HA	1:Z:950:GLN:HG2	1.97	0.46
1:d:929:THR:OG1	1:e:916:GLN:HB2	2.15	0.46
1:v:909:VAL:HG21	1:w:955:LEU:HD21	1.98	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
1:9:938:TYR:HA	1:9:942:GLU:OE2	2.15	0.46
1:C:915:SER:HB2	1:D:928:TYR:HE1	1.81	0.46
1:k:959:LEU:HD12	1:l:961:MET:HE3	1.97	0.46
1:r:928:TYR:HE1	1:s:915:SER:HB2	1.80	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	2.50	0.45
1:w:947:TYR:HA	1:w:950:GLN:HG2	1.98	0.45
1:P:960:LEU:HD23	1:P:960:LEU:HA	1.81	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	1.99	0.45
1:N:960:LEU:HD12	1:t:960:LEU:HD12	1.99	0.45
1:h:915:SER:HB2	1:i:928:TYR:CE1	2.51	0.45
1:p:894:LYS:HG2	1:p:963:SER:HB2	1.98	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:E:960:LEU:HD23	1:E:960:LEU:HA	1.84	0.45
1:5:898:TRP:CH2	1:5:959:LEU:HD13	2.52	0.45
1:j:959:LEU:O	1:j:960:LEU:HD22	2.16	0.45
1:w:894:LYS:HG2	1:w:963:SER:HB2	1.98	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	1.81	0.45
1:g:925:SER:HB2	1:g:937:ARG:HE	1.82	0.45
1:m:960:LEU:HD23	1:m:960:LEU:HA	1.81	0.45
1:r:960:LEU:HD11	1:r:962:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:VAL:HG12	1:B:909:VAL:HG22	1.99	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:b:928:TYR:HE1	1:c:915:SER:HB2	1.82	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	1.82	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	1.99	0.44
1:M:894:LYS:HG2	1:M:963:SER:HB2	1.99	0.44
1:1:929:THR:OG1	1:2:916:GLN:HB2	2.18	0.44
1:p:947:TYR:HA	1:p:950:GLN:HG2	1.98	0.44
1:W:962:PHE:HE2	1:v:958:ILE:HD12	1.82	0.44
1:Y:928:TYR:HE2	1:Y:947:TYR:HH	1.66	0.44
1:k:934:GLN:OE1	1:k:934:GLN:N	2.46	0.44
1:p:960:LEU:HD23	1:p:960:LEU:HA	1.76	0.44
1:v:894:LYS:HE3	1:v:912:ASN:HA	1.99	0.44
1:C:929:THR:OG1	1:D:916:GLN:HB2	2.18	0.44
1:L:916:GLN:HE22	1:a:901:GLN:HE21	1.66	0.44
1:b:915:SER:HB2	1:c:928:TYR:HE1	1.82	0.44
1:n:915:SER:HB2	1:o:928:TYR:HE1	1.82	0.44
1:M:896:VAL:HG12	1:M:909:VAL:HG22	1.99	0.44
1:6:964:ASN:OD1	1:l:910:GLN:NE2	2.51	0.44
1:B:926:ILE:HB	1:B:938:TYR:HB2	2.00	0.44
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	1.82	0.44
1:6:941:ASN:HD22	1:6:941:ASN:C	2.21	0.44
1:7:943:LYS:HG3	1:7:944:LEU:N	2.32	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:U:958:ILE:HB	1:f:962:PHE:HZ	1.83	0.44
1:d:931:PRO:HD3	1:e:915:SER:HB3	2.00	0.44
1:I:929:THR:OG1	1:J:916:GLN:HB2	2.18	0.44
1:8:898:TRP:CH2	1:8:959:LEU:HD13	2.52	0.44
1:8:947:TYR:HA	1:8:950:GLN:HG2	1.98	0.44
1:b:927:SER:HB3	1:c: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:927:SER:HB3	1:2:918:VAL:HB	2.00	0.44
1:v:927:SER:HB3	1:w:918:VAL:HB	1.99	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	2.47	0.43
1:w:960:LEU:HD23	1:w:960:LEU:HA	1.81	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
1:6:934:GLN:OE1	1:6:934:GLN:N	2.44	0.43
1:e:945:PRO:HD2	1:e:948:ILE:HG13	2.01	0.43
1:E:928:TYR:OH	1:E:951:LYS:NZ	2.52	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
1:9:916:GLN:HB2	1:a:929:THR:OG1	2.18	0.43
1:h:947:TYR:HA	1:h:950:GLN:HG2	2.01	0.43
1:s:896:VAL:HG12	1:s:909:VAL:HG22	2.01	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
1:9:928:TYR:HE1	1:a:915:SER:HB2	1.83	0.43
1:h:918:VAL:HB	1:i:927:SER:HB3	2.00	0.43
1:n:929:THR:OG1	1:o:916:GLN:HB2	2.18	0.43
1:S:959:LEU:O	1:S:960:LEU:HD22	2.18	0.43
1:1:916:GLN:HB2	1:2:929:THR:OG1	2.18	0.43
1:t:897:GLY:HA3	1:t:960:LEU:HD23	2.01	0.43
1:J:896:VAL:HG12	1:J:909:VAL:HG22	2.01	0.43
1:W:908:TRP:NE1	1:W:916:GLN:HE21	2.06	0.43
1:7:929:THR:OG1	1:8:916:GLN:HB2	2.19	0.43
1:8:896:VAL:HG12	1:8:909:VAL:HG22	2.00	0.43
1:8:943:LYS:HB2	1:d:934:GLN:CG	2.48	0.43
1:d:960:LEU:HD23	1:d:960:LEU:HA	1.84	0.43
1:e:960:LEU:HD23	1:e:960:LEU:HA	1.82	0.43
1:j:947:TYR:HA	1:j:950:GLN:HG2	2.01	0.43
1:r:896:VAL:HG12	1:r:909:VAL:HG22	2.00	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
1:6:893:VAL:HG13	1:6:909:VAL:HG13	2.01	0.43
1:f:916:GLN:HB2	1:g:929:THR:OG1	2.18	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:U:916:GLN:HE22	1:f:901:GLN:HE21	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:960:LEU:HD13	1:5:962:PHE:CE1	2.54	0.42
1:8:959:LEU:HD12	1:9:961:MET:HE3	2.01	0.42
1:f:947:TYR:HA	1:f:950:GLN:HG2	2.01	0.42
1:v:960:LEU:O	1:y:960:LEU:N	2.51	0.42
1:F:934:GLN:OE1	1:F:934:GLN:N	2.45	0.42
1:H:960:LEU:HD23	1:H:960:LEU:HA	1.83	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:928:TYR:HE1	1:g:915:SER:HB2	1.83	0.42
1:q:947:TYR:HA	1:q:950:GLN:HG2	2.01	0.42
1:U:960:LEU:HD11	1:U:962:PHE:CE1	2.55	0.42
1:X:935:THR:HG21	1:w:937:ARG:HH22	1.85	0.42
1:A:896:VAL:HG12	1:A:909:VAL:HG22	2.02	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
1:5:918:VAL:HB	1:6:927:SER:HB3	2.02	0.42
1:5:947:TYR:HA	1:5:950:GLN:HG2	2.02	0.42
1:j:934:GLN:OE1	1:j:934:GLN:N	2.49	0.42
1:n:960:LEU:HD11	1:n:962:PHE:HE1	1.84	0.42
1:x:929:THR:OG1	1:y:916:GLN:HB2	2.20	0.42
1:B:934:GLN:OE1	1:B:934:GLN:N	2.46	0.42
1:F:926:ILE:HD12	1:F:944:LEU:HD21	2.01	0.42
1:J:947:TYR:HA	1:J:950:GLN:HG2	2.00	0.42
1:L:928:TYR:OH	1:L:951:LYS:NZ	2.52	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:f:896:VAL:HG12	1:f:909:VAL:HG22	1.99	0.42
1:A:934:GLN:OE1	1:A:934:GLN:N	2.47	0.42
1:r:931:PRO:HD3	1:s:915:SER:HB3	2.02	0.42
1:r:947:TYR:HA	1:r:950:GLN:HG2	2.01	0.42
1:u:898:TRP:CH2	1:u:959:LEU:HD13	2.54	0.42
1:C:937:ARG:HH11	1:d:937:ARG:HD2	1.85	0.42
1:G:960:LEU:HD11	1:G:962:PHE:CE1	2.55	0.42
1:I:960:LEU:HD11	1:I:962:PHE:CZ	2.55	0.42
1:3:947:TYR:HA	1:3:950:GLN:HG2	2.02	0.42
1:o:896:VAL:HG12	1:o:909:VAL:HG22	2.01	0.42
1:M:960:LEU:HD23	1:M:960:LEU:HA	1.84	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	2.02	0.42
1:v:960:LEU:HD11	1:v:962:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:915:SER:HB2	1:6:928:TYR:HE1	1.85	0.42
1:e:947:TYR:HA	1:e:950:GLN:HG2	2.01	0.42
1:g:934:GLN:OE1	1:g:934:GLN:N	2.46	0.42
1:i:960:LEU:HD23	1:i:960:LEU:HA	1.83	0.42
1:l:915:SER:HB2	1:m:928:TYR:HE1	1.83	0.42
1:y:960:LEU:HD23	1:y:960:LEU:HA	1.76	0.42
1:I:915:SER:HB2	1:J:928:TYR:HE1	1.84	0.41
1:R:958:ILE:HB	1:2:962:PHE:HZ	1.86	0.41
1:S:962:PHE:CE2	1:Y:958:ILE:HD12	2.55	0.41
1:U:958:ILE:HD12	1:f:962:PHE:HE2	1.85	0.41
1:V:934:GLN:OE1	1:V:934:GLN:N	2.48	0.41
1:d:934:GLN:OE1	1:d:934:GLN:N	2.42	0.41
1:s:959:LEU:HD12	1:t:961:MET:HE3	2.01	0.41
1:C:916:GLN:HB2	1:D:929:THR:OG1	2.20	0.41
1:Q:918:VAL:HB	1:R:927:SER:HB3	2.02	0.41
1:o:929:THR:HA	1:o:935:THR:HA	2.01	0.41
1:N:947:TYR:HA	1:N:950:GLN:HG2	2.01	0.41
1:V:939:GLY:H	1:V:942:GLU:HG3	1.85	0.41
1:Z:908:TRP:HE1	1:Z:916:GLN:NE2	2.17	0.41
1:h:908:TRP:HD1	1:h:918:VAL:HG22	1.85	0.41
1:p:927:SER:HB3	1:q:918:VAL:HB	2.02	0.41
1:x:960:LEU:HD23	1:x:960:LEU:HA	1.85	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:W:937:ARG:HH11	1:h:937:ARG:HH11	1.69	0.41
1:2:934:GLN:OE1	1:2:934:GLN:N	2.44	0.41
1:3:896:VAL:HG12	1:3:909:VAL:HG22	2.01	0.41
1:w:938:TYR:HA	1:w:942:GLU:OE2	2.21	0.41
1:O:947:TYR:HA	1:O:950:GLN:HG2	2.01	0.41
1:R:934:GLN:OE1	1:R:934:GLN:N	2.45	0.41
1:Y:934:GLN:OE1	1:Y:934:GLN:N	2.45	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	1.83	0.41
1:j:916:GLN:HB2	1:k:929:THR:OG1	2.20	0.41
1:m:934:GLN:OE1	1:m:934:GLN:N	2.45	0.41
1:U:916:GLN:HB2	1:V:929:THR:OG1	2.20	0.41
1:a:898:TRP:CH2	1:a:959:LEU:HD13	2.56	0.41
1:g:947:TYR:HA	1:g:950:GLN:HG2	2.02	0.41
1:p:928:TYR:HE1	1:q:915:SER:HB2	1.86	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

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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	0.41
1:2:937:ARG:O	1:i:938:TYR:OH	2.27	0.41
1:9:927:SER:HB3	1:a:918:VAL:HB	2.02	0.41
1:9:929:THR:OG1	1:a:916:GLN:HB2	2.21	0.41
1:b:916:GLN:HB2	1:c:929:THR:OG1	2.20	0.41
1:y:960:LEU:HD13	1:y:962:PHE:HE1	1.84	0.41
1:S:947:TYR:HA	1:S:950:GLN:HG2	2.03	0.41
1:n:947:TYR:HA	1:n:950:GLN:HG2	2.02	0.41
1:D:944:LEU:O	1:D:944:LEU:HD12	2.21	0.41
1:F:896:VAL:HG12	1:F:909:VAL:HG22	2.02	0.41
1:P:960:LEU:HD13	1:P:962:PHE:HE1	1.85	0.41
1:U:915:SER:HB2	1:V:928:TYR:HE1	1.86	0.41
1:U:929:THR:OG1	1:V:916:GLN:HB2	2.21	0.41
1:V:894:LYS:HG2	1:V:963:SER:HB2	2.02	0.41
1:V:924:SER:HA	1:V:940:GLU:HG3	2.03	0.41
1:Z:934:GLN:OE1	1:Z:934:GLN:N	2.46	0.41
1:3:915:SER:HB2	1:4:928:TYR:HE1	1.86	0.41
1:d:916:GLN:HB2	1:e:929:THR:OG1	2.20	0.41
1:k:910:GLN:HG3	1:k:916:GLN:HG2	2.02	0.41
1:o:945:PRO:HD2	1:o:948:ILE:HG13	2.02	0.41
1:r:916:GLN:HB2	1:s:929:THR:OG1	2.21	0.41
1:x:916:GLN:HB2	1:y:929:THR:OG1	2.20	0.41
1:B:932:ASN:OD1	1:B:932:ASN:N	2.54	0.41
1:K:934:GLN:OE1	1:K:934:GLN:N	2.45	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
1:5:902:LEU:HD13	1:5:953:GLN:NE2	2.36	0.41
1:8:934:GLN:OE1	1:8:934:GLN:N	2.49	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	2.46	0.40
1:l:929:THR:OG1	1:m:916:GLN:HB2	2.21	0.40
1:o:947:TYR:HA	1:o:950:GLN:HG2	2.02	0.40
1:o:953:GLN:OE1	1:p:966:THR:N	2.54	0.40
1:t:947:TYR:HA	1:t:950:GLN:HG2	2.02	0.40
1:H:947:TYR:HA	1:H:950:GLN:HG2	2.04	0.40
1:I:918:VAL:HB	1:J:927:SER:HB3	2.03	0.40
1:1:896:VAL:HG12	1:1:909:VAL:HG22	2.03	0.40
1:1:958:ILE:HD12	1:5:962:PHE:HE2	1.86	0.40
1:2:902:LEU:HD21	1:2:949:LYS:HG3	2.03	0.40
1:7:947:TYR:HA	1:7:950:GLN:HG2	2.03	0.40
1:w:923:VAL:O	1:w:940:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:915:SER:HB2	1:y:928:TYR:HE1	1.87	0.40
1:A:960:LEU:HD23	1:A:960:LEU:HA	1.85	0.40
1:R:960:LEU:HD11	1:R:962:PHE:CE1	2.56	0.40
1:X:960:LEU:HD23	1:X:960:LEU:HA	1.81	0.40
1:e:934:GLN:OE1	1:e:934:GLN:N	2.44	0.40
1:x:915:SER:HB3	1:y:931:PRO:HD3	2.02	0.40
1:F:939:GLY:H	1:F:942:GLU:HG3	1.86	0.40
1:N:913:ASP:OD1	1:N:915:SER:OG	2.39	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
1:9:947:TYR:HA	1:9:950:GLN:HG2	2.03	0.40
1:b:947:TYR:HA	1:b:950:GLN:HG2	2.02	0.40
1:d:898:TRP:CH2	1:d:959:LEU:HD13	2.57	0.40
1:i:947:TYR:HA	1:i:950:GLN:HG2	2.04	0.40
1:n:960:LEU:HD11	1:n:962:PHE:CE1	2.56	0.40
1:H:958:ILE:HD12	1:g:962:PHE:HE2	1.85	0.40
1:U:958:ILE:HD12	1:f:962:PHE:CE2	2.56	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
1:n:919:VAL:HG13	1:o:923:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	68 (100%)	0	100	100
1	2	68/79 (86%)	68 (100%)	0	100	100
1	3	68/79 (86%)	68 (100%)	0	100	100
1	4	68/79 (86%)	67 (98%)	1 (2%)	57	71
1	5	68/79 (86%)	68 (100%)	0	100	100
1	6	68/79 (86%)	68 (100%)	0	100	100
1	7	68/79 (86%)	68 (100%)	0	100	100
1	8	68/79 (86%)	68 (100%)	0	100	100
1	9	68/79 (86%)	68 (100%)	0	100	100
1	A	68/79 (86%)	68 (100%)	0	100	100
1	B	68/79 (86%)	68 (100%)	0	100	100
1	C	68/79 (86%)	68 (100%)	0	100	100
1	D	68/79 (86%)	68 (100%)	0	100	100
1	E	68/79 (86%)	68 (100%)	0	100	100
1	F	68/79 (86%)	68 (100%)	0	100	100
1	G	68/79 (86%)	68 (100%)	0	100	100
1	H	68/79 (86%)	68 (100%)	0	100	100
1	I	68/79 (86%)	68 (100%)	0	100	100
1	J	68/79 (86%)	68 (100%)	0	100	100
1	K	68/79 (86%)	68 (100%)	0	100	100
1	L	68/79 (86%)	68 (100%)	0	100	100
1	M	68/79 (86%)	68 (100%)	0	100	100
1	N	68/79 (86%)	68 (100%)	0	100	100
1	O	68/79 (86%)	68 (100%)	0	100	100
1	P	68/79 (86%)	68 (100%)	0	100	100
1	Q	68/79 (86%)	68 (100%)	0	100	100
1	R	68/79 (86%)	68 (100%)	0	100	100
1	S	68/79 (86%)	68 (100%)	0	100	100
1	T	68/79 (86%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	68/79 (86%)	68 (100%)	0	100	100
1	V	68/79 (86%)	68 (100%)	0	100	100
1	W	68/79 (86%)	68 (100%)	0	100	100
1	X	68/79 (86%)	68 (100%)	0	100	100
1	Y	68/79 (86%)	68 (100%)	0	100	100
1	Z	68/79 (86%)	68 (100%)	0	100	100
1	a	68/79 (86%)	68 (100%)	0	100	100
1	b	68/79 (86%)	68 (100%)	0	100	100
1	c	68/79 (86%)	68 (100%)	0	100	100
1	d	68/79 (86%)	68 (100%)	0	100	100
1	e	68/79 (86%)	68 (100%)	0	100	100
1	f	68/79 (86%)	68 (100%)	0	100	100
1	g	68/79 (86%)	68 (100%)	0	100	100
1	h	68/79 (86%)	68 (100%)	0	100	100
1	i	68/79 (86%)	68 (100%)	0	100	100
1	j	68/79 (86%)	68 (100%)	0	100	100
1	k	68/79 (86%)	68 (100%)	0	100	100
1	l	68/79 (86%)	68 (100%)	0	100	100
1	m	68/79 (86%)	68 (100%)	0	100	100
1	n	68/79 (86%)	68 (100%)	0	100	100
1	o	68/79 (86%)	68 (100%)	0	100	100
1	p	68/79 (86%)	68 (100%)	0	100	100
1	q	68/79 (86%)	68 (100%)	0	100	100
1	r	68/79 (86%)	68 (100%)	0	100	100
1	s	68/79 (86%)	68 (100%)	0	100	100
1	t	68/79 (86%)	68 (100%)	0	100	100
1	u	68/79 (86%)	68 (100%)	0	100	100
1	v	68/79 (86%)	68 (100%)	0	100	100
1	w	68/79 (86%)	68 (100%)	0	100	100
1	x	68/79 (86%)	68 (100%)	0	100	100
1	y	68/79 (86%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4080/4740 (86%)	4079 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	4	954	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	941	ASN
1	F	895	ASN
1	F	910	GLN
1	F	950	GLN
1	G	910	GLN
1	H	895	ASN
1	H	910	GLN
1	J	916	GLN
1	J	950	GLN
1	K	953	GLN
1	L	950	GLN
1	L	964	ASN
1	N	910	GLN
1	N	916	GLN
1	O	895	ASN
1	O	910	GLN
1	O	950	GLN
1	O	964	ASN
1	R	895	ASN
1	R	910	GLN
1	R	941	ASN
1	S	950	GLN
1	T	941	ASN
1	T	950	GLN
1	U	950	GLN
1	V	950	GLN
1	W	941	ASN
1	W	964	ASN
1	X	950	GLN
1	Y	950	GLN
1	Y	964	ASN

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Mol	Chain	Res	Type
1	Z	941	ASN
1	2	895	ASN
1	2	941	ASN
1	3	895	ASN
1	3	950	GLN
1	4	895	ASN
1	4	910	GLN
1	5	953	GLN
1	6	953	GLN
1	7	895	ASN
1	7	910	GLN
1	7	964	ASN
1	b	950	GLN
1	c	964	ASN
1	d	941	ASN
1	e	895	ASN
1	g	895	ASN
1	h	964	ASN
1	k	953	GLN
1	l	941	ASN
1	l	950	GLN
1	l	953	GLN
1	n	950	GLN
1	o	941	ASN
1	o	950	GLN
1	p	953	GLN
1	q	895	ASN
1	s	895	ASN
1	s	916	GLN
1	t	895	ASN
1	t	910	GLN
1	u	895	ASN
1	u	910	GLN
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 oligosaccharides 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%)	0.59	4 (5%) 33 22	58, 88, 156, 303	0
1	2	77/91 (84%)	0.75	7 (9%) 15 12	60, 84, 174, 300	0
1	3	77/91 (84%)	0.52	4 (5%) 33 22	76, 95, 159, 253	0
1	4	77/91 (84%)	0.50	2 (2%) 57 38	68, 96, 156, 183	0
1	5	77/91 (84%)	0.17	1 (1%) 75 57	59, 86, 170, 203	0
1	6	77/91 (84%)	0.31	0 100 100	69, 90, 138, 181	0
1	7	77/91 (84%)	0.50	2 (2%) 57 38	82, 124, 171, 224	0
1	8	77/91 (84%)	0.65	4 (5%) 33 22	103, 135, 197, 223	0
1	9	77/91 (84%)	0.67	10 (12%) 7 6	90, 109, 186, 248	0
1	A	77/91 (84%)	0.38	1 (1%) 75 57	72, 109, 172, 257	0
1	B	77/91 (84%)	0.62	4 (5%) 33 22	79, 106, 160, 197	0
1	C	77/91 (84%)	0.47	2 (2%) 57 38	79, 113, 162, 207	0
1	D	77/91 (84%)	0.48	3 (3%) 43 29	79, 115, 188, 229	0
1	E	77/91 (84%)	0.31	3 (3%) 43 29	61, 81, 119, 163	0
1	F	77/91 (84%)	0.47	4 (5%) 33 22	64, 77, 142, 246	0
1	G	77/91 (84%)	0.50	4 (5%) 33 22	74, 100, 158, 172	0
1	H	77/91 (84%)	0.45	2 (2%) 57 38	72, 108, 157, 208	0
1	I	77/91 (84%)	0.47	1 (1%) 75 57	86, 119, 200, 242	0
1	J	77/91 (84%)	0.49	2 (2%) 57 38	84, 120, 181, 199	0
1	K	77/91 (84%)	0.39	2 (2%) 57 38	81, 102, 145, 275	0
1	L	77/91 (84%)	0.35	0 100 100	77, 109, 171, 223	0
1	M	77/91 (84%)	0.62	7 (9%) 15 12	65, 83, 147, 262	0
1	N	77/91 (84%)	0.47	2 (2%) 57 38	72, 95, 141, 166	0
1	O	77/91 (84%)	0.98	10 (12%) 7 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%)	0.81	7 (9%)	15 12	74, 122, 195, 209	0
1	Q	77/91 (84%)	0.51	2 (2%)	57 38	80, 110, 176, 215	0
1	R	77/91 (84%)	0.55	4 (5%)	33 22	73, 100, 154, 250	0
1	S	77/91 (84%)	0.26	1 (1%)	75 57	75, 107, 157, 188	0
1	T	77/91 (84%)	0.58	2 (2%)	57 38	78, 117, 172, 231	0
1	U	77/91 (84%)	0.36	2 (2%)	57 38	74, 95, 166, 193	0
1	V	77/91 (84%)	0.53	6 (7%)	19 14	73, 100, 152, 235	0
1	W	77/91 (84%)	0.36	2 (2%)	57 38	67, 94, 164, 213	0
1	X	77/91 (84%)	0.47	2 (2%)	57 38	73, 98, 135, 180	0
1	Y	77/91 (84%)	0.44	3 (3%)	43 29	68, 90, 131, 183	0
1	Z	77/91 (84%)	0.38	3 (3%)	43 29	57, 89, 161, 180	0
1	a	77/91 (84%)	0.50	3 (3%)	43 29	83, 112, 164, 214	0
1	b	77/91 (84%)	0.47	3 (3%)	43 29	82, 125, 191, 234	0
1	c	77/91 (84%)	0.60	6 (7%)	19 14	95, 132, 196, 231	0
1	d	77/91 (84%)	0.54	2 (2%)	57 38	93, 152, 221, 290	0
1	e	77/91 (84%)	0.59	2 (2%)	57 38	89, 132, 196, 217	0
1	f	77/91 (84%)	0.76	2 (2%)	57 38	81, 128, 213, 268	0
1	g	77/91 (84%)	0.71	3 (3%)	43 29	86, 145, 197, 298	0
1	h	77/91 (84%)	0.44	2 (2%)	57 38	65, 102, 185, 227	0
1	i	77/91 (84%)	0.63	4 (5%)	33 22	68, 104, 158, 183	0
1	j	77/91 (84%)	0.79	7 (9%)	15 12	122, 175, 245, 293	0
1	k	77/91 (84%)	0.77	5 (6%)	25 17	112, 181, 249, 325	0
1	l	77/91 (84%)	1.06	11 (14%)	6 5	121, 169, 228, 272	0
1	m	77/91 (84%)	0.81	4 (5%)	33 22	126, 170, 236, 303	0
1	n	77/91 (84%)	1.58	23 (29%)	1 1	137, 225, 338, 372	0
1	o	77/91 (84%)	1.59	21 (27%)	1 1	149, 237, 315, 383	0
1	p	77/91 (84%)	0.90	9 (11%)	9 8	123, 180, 281, 372	0
1	q	77/91 (84%)	1.23	13 (16%)	4 4	130, 174, 242, 343	0
1	r	77/91 (84%)	0.45	1 (1%)	75 57	79, 103, 169, 191	0
1	s	77/91 (84%)	0.53	1 (1%)	75 57	79, 112, 151, 174	0
1	t	77/91 (84%)	0.47	3 (3%)	43 29	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%)	0.52	2 (2%)	57 38	80, 107, 158, 182	0
1	v	77/91 (84%)	0.35	3 (3%)	43 29	79, 104, 157, 222	0
1	w	77/91 (84%)	0.55	5 (6%)	25 17	92, 110, 189, 313	0
1	x	77/91 (84%)	0.54	4 (5%)	33 22	101, 124, 156, 203	0
1	y	77/91 (84%)	0.34	4 (5%)	33 22	84, 116, 172, 201	0
All	All	4620/5460 (84%)	0.58	258 (5%)	30 20	57, 115, 217, 383	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	o	919	VAL	6.7
1	2	942	GLU	5.5
1	o	907	VAL	5.2
1	n	893	VAL	4.7
1	4	914	GLY	4.5
1	p	964	ASN	4.5
1	p	965	PRO	4.2
1	O	963	SER	4.1
1	l	962	PHE	4.1
1	e	918	VAL	4.1
1	o	898	TRP	4.1
1	U	962	PHE	4.0
1	n	944	LEU	4.0
1	S	962	PHE	4.0
1	O	894	LYS	4.0
1	j	944	LEU	3.9
1	o	899	ALA	3.8
1	l	961	MET	3.8
1	n	926	ILE	3.8
1	q	898	TRP	3.7
1	1	941	ASN	3.6
1	B	960	LEU	3.6
1	3	942	GLU	3.6
1	h	955	LEU	3.5
1	o	961	MET	3.5
1	q	962	PHE	3.5
1	P	932	ASN	3.5
1	b	941	ASN	3.5
1	c	941	ASN	3.4
1	g	896	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	N	966	THR	3.4
1	m	944	LEU	3.4
1	9	890	SER	3.4
1	o	920	GLN	3.4
1	q	893	VAL	3.3
1	w	942	GLU	3.3
1	q	944	LEU	3.3
1	X	966	THR	3.3
1	q	896	VAL	3.3
1	l	893	VAL	3.2
1	G	901	GLN	3.2
1	o	926	ILE	3.2
1	o	948	ILE	3.2
1	s	939	GLY	3.2
1	n	952	LEU	3.2
1	V	941	ASN	3.2
1	j	961	MET	3.2
1	O	962	PHE	3.1
1	k	948	ILE	3.1
1	o	917	LEU	3.1
1	o	896	VAL	3.1
1	o	908	TRP	3.1
1	n	948	ILE	3.1
1	p	955	LEU	3.0
1	n	896	VAL	3.0
1	O	917	LEU	3.0
1	e	944	LEU	3.0
1	y	960	LEU	3.0
1	t	963	SER	2.9
1	n	907	VAL	2.9
1	p	961	MET	2.9
1	J	965	PRO	2.9
1	x	896	VAL	2.9
1	n	892	PHE	2.9
1	n	919	VAL	2.9
1	k	944	LEU	2.9
1	F	966	THR	2.9
1	2	937	ARG	2.9
1	n	903	THR	2.9
1	y	962	PHE	2.9
1	o	960	LEU	2.9
1	I	935	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	941	ASN	2.8
1	n	917	LEU	2.8
1	r	962	PHE	2.8
1	9	966	THR	2.8
1	i	966	THR	2.8
1	9	942	GLU	2.8
1	l	949	LYS	2.8
1	9	941	ASN	2.8
1	c	965	PRO	2.8
1	O	931	PRO	2.8
1	P	946	ASP	2.7
1	q	907	VAL	2.7
1	M	942	GLU	2.7
1	Z	962	PHE	2.7
1	9	963	SER	2.7
1	2	944	LEU	2.7
1	m	966	THR	2.7
1	n	957	SER	2.7
1	k	898	TRP	2.7
1	o	955	LEU	2.7
1	G	958	ILE	2.7
1	l	901	GLN	2.7
1	Y	962	PHE	2.6
1	R	966	THR	2.6
1	n	911	PHE	2.6
1	o	962	PHE	2.6
1	8	899	ALA	2.6
1	k	955	LEU	2.6
1	R	962	PHE	2.6
1	1	965	PRO	2.6
1	2	941	ASN	2.6
1	n	916	GLN	2.6
1	A	944	LEU	2.6
1	D	944	LEU	2.6
1	y	896	VAL	2.6
1	B	962	PHE	2.6
1	F	935	THR	2.6
1	p	963	SER	2.6
1	3	941	ASN	2.6
1	l	944	LEU	2.6
1	o	959	LEU	2.5
1	t	955	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	895	ASN	2.5
1	o	951	LYS	2.5
1	a	966	THR	2.5
1	b	966	THR	2.5
1	4	965	PRO	2.5
1	n	935	THR	2.5
1	P	939	GLY	2.5
1	C	941	ASN	2.5
1	D	966	THR	2.5
1	Z	966	THR	2.5
1	O	944	LEU	2.5
1	P	951	LYS	2.5
1	m	951	LYS	2.5
1	c	901	GLN	2.5
1	2	962	PHE	2.5
1	x	898	TRP	2.5
1	Q	955	LEU	2.5
1	n	965	PRO	2.5
1	B	966	THR	2.4
1	a	908	TRP	2.4
1	w	939	GLY	2.4
1	o	958	ILE	2.4
1	Y	960	LEU	2.4
1	l	965	PRO	2.4
1	o	918	VAL	2.4
1	Q	901	GLN	2.4
1	H	903	THR	2.4
1	V	966	THR	2.4
1	8	903	THR	2.4
1	l	896	VAL	2.4
1	c	897	GLY	2.4
1	q	961	MET	2.4
1	Y	966	THR	2.4
1	3	965	PRO	2.4
1	5	966	THR	2.4
1	X	941	ASN	2.4
1	K	927	SER	2.4
1	M	963	SER	2.4
1	p	919	VAL	2.4
1	9	933	GLY	2.3
1	h	966	THR	2.3
1	G	941	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	d	908	TRP	2.3
1	O	910	GLN	2.3
1	j	896	VAL	2.3
1	9	937	ARG	2.3
1	y	944	LEU	2.3
1	T	962	PHE	2.3
1	9	907	VAL	2.3
1	o	921	ALA	2.3
1	Z	929	THR	2.3
1	p	951	LYS	2.3
1	p	966	THR	2.3
1	t	966	THR	2.3
1	M	894	LYS	2.3
1	D	896	VAL	2.3
1	V	965	PRO	2.2
1	i	965	PRO	2.2
1	q	902	LEU	2.2
1	n	898	TRP	2.2
1	E	941	ASN	2.2
1	U	965	PRO	2.2
1	n	955	LEU	2.2
1	i	963	SER	2.2
1	f	941	ASN	2.2
1	M	965	PRO	2.2
1	j	952	LEU	2.2
1	w	937	ARG	2.2
1	E	966	THR	2.2
1	7	966	THR	2.2
1	n	909	VAL	2.2
1	2	934	GLN	2.2
1	B	941	ASN	2.2
1	W	932	ASN	2.2
1	V	933	GLY	2.2
1	a	954	CYS	2.2
1	J	962	PHE	2.2
1	N	908	TRP	2.2
1	F	963	SER	2.2
1	8	961	MET	2.2
1	u	961	MET	2.2
1	M	964	ASN	2.2
1	c	896	VAL	2.1
1	q	918	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	942	GLU	2.1
1	3	939	GLY	2.1
1	8	896	VAL	2.1
1	j	893	VAL	2.1
1	i	890	SER	2.1
1	j	965	PRO	2.1
1	l	962	PHE	2.1
1	b	962	PHE	2.1
1	g	941	ASN	2.1
1	E	908	TRP	2.1
1	H	913	ASP	2.1
1	m	896	VAL	2.1
1	x	908	TRP	2.1
1	7	929	THR	2.1
1	u	966	THR	2.1
1	n	961	MET	2.1
1	x	961	MET	2.1
1	w	965	PRO	2.1
1	d	890	SER	2.1
1	g	962	PHE	2.1
1	V	932	ASN	2.1
1	q	941	ASN	2.1
1	l	960	LEU	2.1
1	n	958	ILE	2.1
1	M	935	THR	2.1
1	9	965	PRO	2.1
1	c	962	PHE	2.1
1	v	962	PHE	2.1
1	P	924	SER	2.1
1	O	896	VAL	2.1
1	p	891	VAL	2.1
1	R	958	ILE	2.1
1	V	908	TRP	2.1
1	l	898	TRP	2.1
1	q	908	TRP	2.1
1	K	966	THR	2.1
1	2	935	THR	2.1
1	W	962	PHE	2.1
1	n	962	PHE	2.1
1	M	941	ASN	2.0
1	O	960	LEU	2.0
1	v	908	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	966	THR	2.0
1	9	935	THR	2.0
1	G	939	GLY	2.0
1	P	965	PRO	2.0
1	R	965	PRO	2.0
1	l	911	PHE	2.0
1	f	944	LEU	2.0
1	o	944	LEU	2.0
1	q	959	LEU	2.0
1	v	941	ASN	2.0
1	T	966	THR	2.0
1	l	936	THR	2.0
1	k	966	THR	2.0
1	q	897	GLY	2.0
1	n	910	GLN	2.0
1	o	893	VAL	2.0
1	w	940	GLU	2.0
1	j	959	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.