



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:34 PM UTC

PDB ID : 5ZJU / pdb_00005zju
Title : Crystal structure of in vitro expressed and assembled PCV2 Virus-like Particle
Authors : Yuan, Y.A.; Mo, X.
Deposited on : 2018-03-22
Resolution : 2.80 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

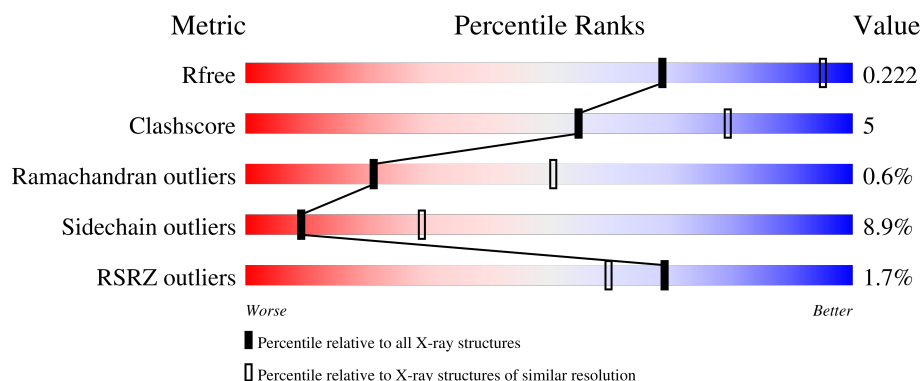
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



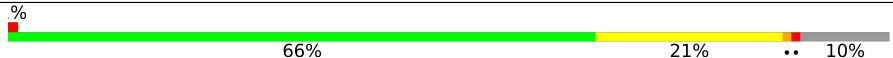
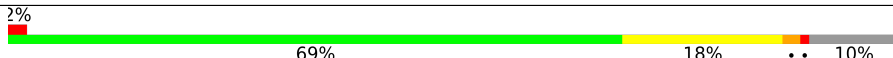
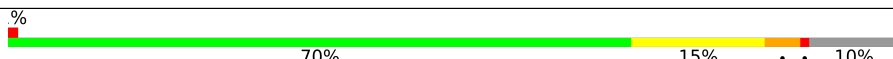
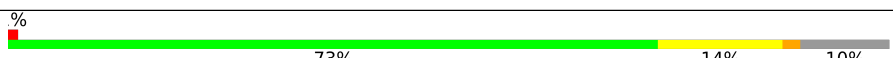
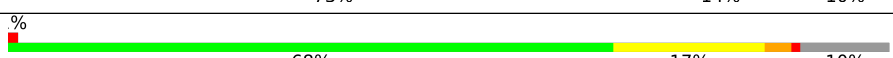
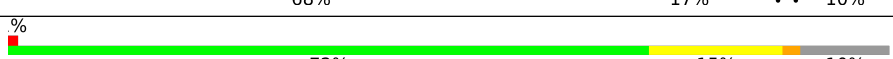
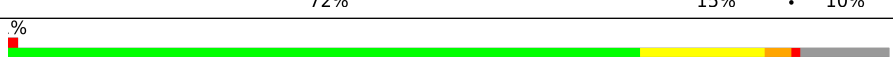
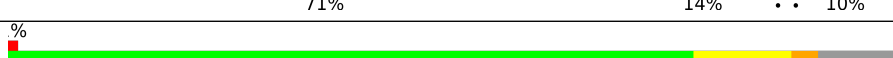
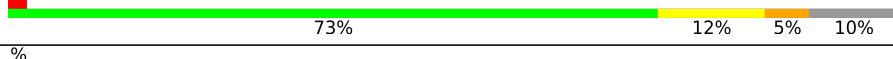
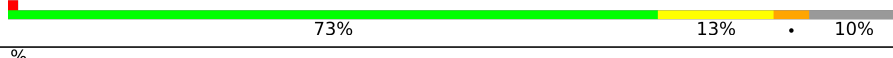
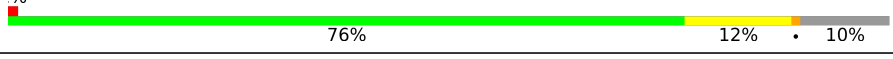
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	209	% 73% 14% • 10%
1	2	209	3% 72% 15% • 10%
1	3	209	% 70% 17% •• 10%
1	4	209	% 75% 13% • 10%
1	5	209	% 74% 12% • 10%

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Mol	Chain	Length	Quality of chain
1	6	209	
1	7	209	
1	8	209	
1	9	209	
1	A	209	
1	B	209	
1	C	209	
1	D	209	
1	E	209	
1	F	209	
1	G	209	
1	H	209	
1	I	209	
1	J	209	
1	K	209	
1	L	209	
1	M	209	
1	N	209	
1	O	209	
1	P	209	
1	Q	209	
1	R	209	
1	S	209	
1	T	209	
1	U	209	

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Mol	Chain	Length	Quality of chain
1	V	209	
1	W	209	
1	X	209	
1	Y	209	
1	Z	209	
1	a	209	
1	b	209	
1	c	209	
1	d	209	
1	e	209	
1	f	209	
1	g	209	
1	h	209	
1	i	209	
1	j	209	
1	k	209	
1	l	209	
1	m	209	
1	n	209	
1	o	209	
1	p	209	
1	q	209	
1	r	209	
1	s	209	
1	t	209	

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Mol	Chain	Length	Quality of chain
1	u	209	2% 73% 14% •• 10%
1	v	209	2% 71% 14% • 10%
1	w	209	73% 12% • 10%
1	x	209	2% 72% 14% •• 10%
1	y	209	2% 69% 17% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 97686 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	B	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	C	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	D	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	E	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	F	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	G	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	H	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	I	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	J	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	K	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	L	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			
1	M	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	N	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	O	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	P	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	R	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	S	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	T	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	U	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	V	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	W	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	X	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	Y	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	Z	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	1	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	2	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			
1	3	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	4	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	5	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	6	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	7	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	8	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	9	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			
1	a	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			
1	b	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	c	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	d	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	e	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			
1	f	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	g	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	h	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	i	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	j	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	k	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			
1	l	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	m	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	n	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	o	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	p	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			
1	q	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	r	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			
1	s	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	t	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	u	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	v	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	w	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	x	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			
1	y	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			

There are 1200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	expression tag	UNP G0Y2B2
A	26	GLY	-	expression tag	UNP G0Y2B2
A	27	SER	-	expression tag	UNP G0Y2B2
A	28	SER	-	expression tag	UNP G0Y2B2
A	29	HIS	-	expression tag	UNP G0Y2B2
A	30	HIS	-	expression tag	UNP G0Y2B2
A	31	HIS	-	expression tag	UNP G0Y2B2
A	32	HIS	-	expression tag	UNP G0Y2B2
A	33	HIS	-	expression tag	UNP G0Y2B2
A	34	HIS	-	expression tag	UNP G0Y2B2
A	35	SER	-	expression tag	UNP G0Y2B2
A	36	SER	-	expression tag	UNP G0Y2B2
A	37	GLY	-	expression tag	UNP G0Y2B2
A	38	LEU	-	expression tag	UNP G0Y2B2
A	39	VAL	-	expression tag	UNP G0Y2B2
A	40	PRO	-	expression tag	UNP G0Y2B2
A	41	ARG	-	expression tag	UNP G0Y2B2
A	42	GLY	-	expression tag	UNP G0Y2B2
A	43	SER	-	expression tag	UNP G0Y2B2
A	44	HIS	-	expression tag	UNP G0Y2B2
B	25	MET	-	expression tag	UNP G0Y2B2
B	26	GLY	-	expression tag	UNP G0Y2B2
B	27	SER	-	expression tag	UNP G0Y2B2
B	28	SER	-	expression tag	UNP G0Y2B2
B	29	HIS	-	expression tag	UNP G0Y2B2
B	30	HIS	-	expression tag	UNP G0Y2B2
B	31	HIS	-	expression tag	UNP G0Y2B2
B	32	HIS	-	expression tag	UNP G0Y2B2
B	33	HIS	-	expression tag	UNP G0Y2B2
B	34	HIS	-	expression tag	UNP G0Y2B2
B	35	SER	-	expression tag	UNP G0Y2B2
B	36	SER	-	expression tag	UNP G0Y2B2
B	37	GLY	-	expression tag	UNP G0Y2B2
B	38	LEU	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	39	VAL	-	expression tag	UNP G0Y2B2
B	40	PRO	-	expression tag	UNP G0Y2B2
B	41	ARG	-	expression tag	UNP G0Y2B2
B	42	GLY	-	expression tag	UNP G0Y2B2
B	43	SER	-	expression tag	UNP G0Y2B2
B	44	HIS	-	expression tag	UNP G0Y2B2
C	25	MET	-	expression tag	UNP G0Y2B2
C	26	GLY	-	expression tag	UNP G0Y2B2
C	27	SER	-	expression tag	UNP G0Y2B2
C	28	SER	-	expression tag	UNP G0Y2B2
C	29	HIS	-	expression tag	UNP G0Y2B2
C	30	HIS	-	expression tag	UNP G0Y2B2
C	31	HIS	-	expression tag	UNP G0Y2B2
C	32	HIS	-	expression tag	UNP G0Y2B2
C	33	HIS	-	expression tag	UNP G0Y2B2
C	34	HIS	-	expression tag	UNP G0Y2B2
C	35	SER	-	expression tag	UNP G0Y2B2
C	36	SER	-	expression tag	UNP G0Y2B2
C	37	GLY	-	expression tag	UNP G0Y2B2
C	38	LEU	-	expression tag	UNP G0Y2B2
C	39	VAL	-	expression tag	UNP G0Y2B2
C	40	PRO	-	expression tag	UNP G0Y2B2
C	41	ARG	-	expression tag	UNP G0Y2B2
C	42	GLY	-	expression tag	UNP G0Y2B2
C	43	SER	-	expression tag	UNP G0Y2B2
C	44	HIS	-	expression tag	UNP G0Y2B2
D	25	MET	-	expression tag	UNP G0Y2B2
D	26	GLY	-	expression tag	UNP G0Y2B2
D	27	SER	-	expression tag	UNP G0Y2B2
D	28	SER	-	expression tag	UNP G0Y2B2
D	29	HIS	-	expression tag	UNP G0Y2B2
D	30	HIS	-	expression tag	UNP G0Y2B2
D	31	HIS	-	expression tag	UNP G0Y2B2
D	32	HIS	-	expression tag	UNP G0Y2B2
D	33	HIS	-	expression tag	UNP G0Y2B2
D	34	HIS	-	expression tag	UNP G0Y2B2
D	35	SER	-	expression tag	UNP G0Y2B2
D	36	SER	-	expression tag	UNP G0Y2B2
D	37	GLY	-	expression tag	UNP G0Y2B2
D	38	LEU	-	expression tag	UNP G0Y2B2
D	39	VAL	-	expression tag	UNP G0Y2B2
D	40	PRO	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	41	ARG	-	expression tag	UNP G0Y2B2
D	42	GLY	-	expression tag	UNP G0Y2B2
D	43	SER	-	expression tag	UNP G0Y2B2
D	44	HIS	-	expression tag	UNP G0Y2B2
E	25	MET	-	expression tag	UNP G0Y2B2
E	26	GLY	-	expression tag	UNP G0Y2B2
E	27	SER	-	expression tag	UNP G0Y2B2
E	28	SER	-	expression tag	UNP G0Y2B2
E	29	HIS	-	expression tag	UNP G0Y2B2
E	30	HIS	-	expression tag	UNP G0Y2B2
E	31	HIS	-	expression tag	UNP G0Y2B2
E	32	HIS	-	expression tag	UNP G0Y2B2
E	33	HIS	-	expression tag	UNP G0Y2B2
E	34	HIS	-	expression tag	UNP G0Y2B2
E	35	SER	-	expression tag	UNP G0Y2B2
E	36	SER	-	expression tag	UNP G0Y2B2
E	37	GLY	-	expression tag	UNP G0Y2B2
E	38	LEU	-	expression tag	UNP G0Y2B2
E	39	VAL	-	expression tag	UNP G0Y2B2
E	40	PRO	-	expression tag	UNP G0Y2B2
E	41	ARG	-	expression tag	UNP G0Y2B2
E	42	GLY	-	expression tag	UNP G0Y2B2
E	43	SER	-	expression tag	UNP G0Y2B2
E	44	HIS	-	expression tag	UNP G0Y2B2
F	25	MET	-	expression tag	UNP G0Y2B2
F	26	GLY	-	expression tag	UNP G0Y2B2
F	27	SER	-	expression tag	UNP G0Y2B2
F	28	SER	-	expression tag	UNP G0Y2B2
F	29	HIS	-	expression tag	UNP G0Y2B2
F	30	HIS	-	expression tag	UNP G0Y2B2
F	31	HIS	-	expression tag	UNP G0Y2B2
F	32	HIS	-	expression tag	UNP G0Y2B2
F	33	HIS	-	expression tag	UNP G0Y2B2
F	34	HIS	-	expression tag	UNP G0Y2B2
F	35	SER	-	expression tag	UNP G0Y2B2
F	36	SER	-	expression tag	UNP G0Y2B2
F	37	GLY	-	expression tag	UNP G0Y2B2
F	38	LEU	-	expression tag	UNP G0Y2B2
F	39	VAL	-	expression tag	UNP G0Y2B2
F	40	PRO	-	expression tag	UNP G0Y2B2
F	41	ARG	-	expression tag	UNP G0Y2B2
F	42	GLY	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	43	SER	-	expression tag	UNP G0Y2B2
F	44	HIS	-	expression tag	UNP G0Y2B2
G	25	MET	-	expression tag	UNP G0Y2B2
G	26	GLY	-	expression tag	UNP G0Y2B2
G	27	SER	-	expression tag	UNP G0Y2B2
G	28	SER	-	expression tag	UNP G0Y2B2
G	29	HIS	-	expression tag	UNP G0Y2B2
G	30	HIS	-	expression tag	UNP G0Y2B2
G	31	HIS	-	expression tag	UNP G0Y2B2
G	32	HIS	-	expression tag	UNP G0Y2B2
G	33	HIS	-	expression tag	UNP G0Y2B2
G	34	HIS	-	expression tag	UNP G0Y2B2
G	35	SER	-	expression tag	UNP G0Y2B2
G	36	SER	-	expression tag	UNP G0Y2B2
G	37	GLY	-	expression tag	UNP G0Y2B2
G	38	LEU	-	expression tag	UNP G0Y2B2
G	39	VAL	-	expression tag	UNP G0Y2B2
G	40	PRO	-	expression tag	UNP G0Y2B2
G	41	ARG	-	expression tag	UNP G0Y2B2
G	42	GLY	-	expression tag	UNP G0Y2B2
G	43	SER	-	expression tag	UNP G0Y2B2
G	44	HIS	-	expression tag	UNP G0Y2B2
H	25	MET	-	expression tag	UNP G0Y2B2
H	26	GLY	-	expression tag	UNP G0Y2B2
H	27	SER	-	expression tag	UNP G0Y2B2
H	28	SER	-	expression tag	UNP G0Y2B2
H	29	HIS	-	expression tag	UNP G0Y2B2
H	30	HIS	-	expression tag	UNP G0Y2B2
H	31	HIS	-	expression tag	UNP G0Y2B2
H	32	HIS	-	expression tag	UNP G0Y2B2
H	33	HIS	-	expression tag	UNP G0Y2B2
H	34	HIS	-	expression tag	UNP G0Y2B2
H	35	SER	-	expression tag	UNP G0Y2B2
H	36	SER	-	expression tag	UNP G0Y2B2
H	37	GLY	-	expression tag	UNP G0Y2B2
H	38	LEU	-	expression tag	UNP G0Y2B2
H	39	VAL	-	expression tag	UNP G0Y2B2
H	40	PRO	-	expression tag	UNP G0Y2B2
H	41	ARG	-	expression tag	UNP G0Y2B2
H	42	GLY	-	expression tag	UNP G0Y2B2
H	43	SER	-	expression tag	UNP G0Y2B2
H	44	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	25	MET	-	expression tag	UNP G0Y2B2
I	26	GLY	-	expression tag	UNP G0Y2B2
I	27	SER	-	expression tag	UNP G0Y2B2
I	28	SER	-	expression tag	UNP G0Y2B2
I	29	HIS	-	expression tag	UNP G0Y2B2
I	30	HIS	-	expression tag	UNP G0Y2B2
I	31	HIS	-	expression tag	UNP G0Y2B2
I	32	HIS	-	expression tag	UNP G0Y2B2
I	33	HIS	-	expression tag	UNP G0Y2B2
I	34	HIS	-	expression tag	UNP G0Y2B2
I	35	SER	-	expression tag	UNP G0Y2B2
I	36	SER	-	expression tag	UNP G0Y2B2
I	37	GLY	-	expression tag	UNP G0Y2B2
I	38	LEU	-	expression tag	UNP G0Y2B2
I	39	VAL	-	expression tag	UNP G0Y2B2
I	40	PRO	-	expression tag	UNP G0Y2B2
I	41	ARG	-	expression tag	UNP G0Y2B2
I	42	GLY	-	expression tag	UNP G0Y2B2
I	43	SER	-	expression tag	UNP G0Y2B2
I	44	HIS	-	expression tag	UNP G0Y2B2
J	25	MET	-	expression tag	UNP G0Y2B2
J	26	GLY	-	expression tag	UNP G0Y2B2
J	27	SER	-	expression tag	UNP G0Y2B2
J	28	SER	-	expression tag	UNP G0Y2B2
J	29	HIS	-	expression tag	UNP G0Y2B2
J	30	HIS	-	expression tag	UNP G0Y2B2
J	31	HIS	-	expression tag	UNP G0Y2B2
J	32	HIS	-	expression tag	UNP G0Y2B2
J	33	HIS	-	expression tag	UNP G0Y2B2
J	34	HIS	-	expression tag	UNP G0Y2B2
J	35	SER	-	expression tag	UNP G0Y2B2
J	36	SER	-	expression tag	UNP G0Y2B2
J	37	GLY	-	expression tag	UNP G0Y2B2
J	38	LEU	-	expression tag	UNP G0Y2B2
J	39	VAL	-	expression tag	UNP G0Y2B2
J	40	PRO	-	expression tag	UNP G0Y2B2
J	41	ARG	-	expression tag	UNP G0Y2B2
J	42	GLY	-	expression tag	UNP G0Y2B2
J	43	SER	-	expression tag	UNP G0Y2B2
J	44	HIS	-	expression tag	UNP G0Y2B2
K	25	MET	-	expression tag	UNP G0Y2B2
K	26	GLY	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	27	SER	-	expression tag	UNP G0Y2B2
K	28	SER	-	expression tag	UNP G0Y2B2
K	29	HIS	-	expression tag	UNP G0Y2B2
K	30	HIS	-	expression tag	UNP G0Y2B2
K	31	HIS	-	expression tag	UNP G0Y2B2
K	32	HIS	-	expression tag	UNP G0Y2B2
K	33	HIS	-	expression tag	UNP G0Y2B2
K	34	HIS	-	expression tag	UNP G0Y2B2
K	35	SER	-	expression tag	UNP G0Y2B2
K	36	SER	-	expression tag	UNP G0Y2B2
K	37	GLY	-	expression tag	UNP G0Y2B2
K	38	LEU	-	expression tag	UNP G0Y2B2
K	39	VAL	-	expression tag	UNP G0Y2B2
K	40	PRO	-	expression tag	UNP G0Y2B2
K	41	ARG	-	expression tag	UNP G0Y2B2
K	42	GLY	-	expression tag	UNP G0Y2B2
K	43	SER	-	expression tag	UNP G0Y2B2
K	44	HIS	-	expression tag	UNP G0Y2B2
L	25	MET	-	expression tag	UNP G0Y2B2
L	26	GLY	-	expression tag	UNP G0Y2B2
L	27	SER	-	expression tag	UNP G0Y2B2
L	28	SER	-	expression tag	UNP G0Y2B2
L	29	HIS	-	expression tag	UNP G0Y2B2
L	30	HIS	-	expression tag	UNP G0Y2B2
L	31	HIS	-	expression tag	UNP G0Y2B2
L	32	HIS	-	expression tag	UNP G0Y2B2
L	33	HIS	-	expression tag	UNP G0Y2B2
L	34	HIS	-	expression tag	UNP G0Y2B2
L	35	SER	-	expression tag	UNP G0Y2B2
L	36	SER	-	expression tag	UNP G0Y2B2
L	37	GLY	-	expression tag	UNP G0Y2B2
L	38	LEU	-	expression tag	UNP G0Y2B2
L	39	VAL	-	expression tag	UNP G0Y2B2
L	40	PRO	-	expression tag	UNP G0Y2B2
L	41	ARG	-	expression tag	UNP G0Y2B2
L	42	GLY	-	expression tag	UNP G0Y2B2
L	43	SER	-	expression tag	UNP G0Y2B2
L	44	HIS	-	expression tag	UNP G0Y2B2
M	25	MET	-	expression tag	UNP G0Y2B2
M	26	GLY	-	expression tag	UNP G0Y2B2
M	27	SER	-	expression tag	UNP G0Y2B2
M	28	SER	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
M	29	HIS	-	expression tag	UNP G0Y2B2
M	30	HIS	-	expression tag	UNP G0Y2B2
M	31	HIS	-	expression tag	UNP G0Y2B2
M	32	HIS	-	expression tag	UNP G0Y2B2
M	33	HIS	-	expression tag	UNP G0Y2B2
M	34	HIS	-	expression tag	UNP G0Y2B2
M	35	SER	-	expression tag	UNP G0Y2B2
M	36	SER	-	expression tag	UNP G0Y2B2
M	37	GLY	-	expression tag	UNP G0Y2B2
M	38	LEU	-	expression tag	UNP G0Y2B2
M	39	VAL	-	expression tag	UNP G0Y2B2
M	40	PRO	-	expression tag	UNP G0Y2B2
M	41	ARG	-	expression tag	UNP G0Y2B2
M	42	GLY	-	expression tag	UNP G0Y2B2
M	43	SER	-	expression tag	UNP G0Y2B2
M	44	HIS	-	expression tag	UNP G0Y2B2
N	25	MET	-	expression tag	UNP G0Y2B2
N	26	GLY	-	expression tag	UNP G0Y2B2
N	27	SER	-	expression tag	UNP G0Y2B2
N	28	SER	-	expression tag	UNP G0Y2B2
N	29	HIS	-	expression tag	UNP G0Y2B2
N	30	HIS	-	expression tag	UNP G0Y2B2
N	31	HIS	-	expression tag	UNP G0Y2B2
N	32	HIS	-	expression tag	UNP G0Y2B2
N	33	HIS	-	expression tag	UNP G0Y2B2
N	34	HIS	-	expression tag	UNP G0Y2B2
N	35	SER	-	expression tag	UNP G0Y2B2
N	36	SER	-	expression tag	UNP G0Y2B2
N	37	GLY	-	expression tag	UNP G0Y2B2
N	38	LEU	-	expression tag	UNP G0Y2B2
N	39	VAL	-	expression tag	UNP G0Y2B2
N	40	PRO	-	expression tag	UNP G0Y2B2
N	41	ARG	-	expression tag	UNP G0Y2B2
N	42	GLY	-	expression tag	UNP G0Y2B2
N	43	SER	-	expression tag	UNP G0Y2B2
N	44	HIS	-	expression tag	UNP G0Y2B2
O	25	MET	-	expression tag	UNP G0Y2B2
O	26	GLY	-	expression tag	UNP G0Y2B2
O	27	SER	-	expression tag	UNP G0Y2B2
O	28	SER	-	expression tag	UNP G0Y2B2
O	29	HIS	-	expression tag	UNP G0Y2B2
O	30	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
O	31	HIS	-	expression tag	UNP G0Y2B2
O	32	HIS	-	expression tag	UNP G0Y2B2
O	33	HIS	-	expression tag	UNP G0Y2B2
O	34	HIS	-	expression tag	UNP G0Y2B2
O	35	SER	-	expression tag	UNP G0Y2B2
O	36	SER	-	expression tag	UNP G0Y2B2
O	37	GLY	-	expression tag	UNP G0Y2B2
O	38	LEU	-	expression tag	UNP G0Y2B2
O	39	VAL	-	expression tag	UNP G0Y2B2
O	40	PRO	-	expression tag	UNP G0Y2B2
O	41	ARG	-	expression tag	UNP G0Y2B2
O	42	GLY	-	expression tag	UNP G0Y2B2
O	43	SER	-	expression tag	UNP G0Y2B2
O	44	HIS	-	expression tag	UNP G0Y2B2
P	25	MET	-	expression tag	UNP G0Y2B2
P	26	GLY	-	expression tag	UNP G0Y2B2
P	27	SER	-	expression tag	UNP G0Y2B2
P	28	SER	-	expression tag	UNP G0Y2B2
P	29	HIS	-	expression tag	UNP G0Y2B2
P	30	HIS	-	expression tag	UNP G0Y2B2
P	31	HIS	-	expression tag	UNP G0Y2B2
P	32	HIS	-	expression tag	UNP G0Y2B2
P	33	HIS	-	expression tag	UNP G0Y2B2
P	34	HIS	-	expression tag	UNP G0Y2B2
P	35	SER	-	expression tag	UNP G0Y2B2
P	36	SER	-	expression tag	UNP G0Y2B2
P	37	GLY	-	expression tag	UNP G0Y2B2
P	38	LEU	-	expression tag	UNP G0Y2B2
P	39	VAL	-	expression tag	UNP G0Y2B2
P	40	PRO	-	expression tag	UNP G0Y2B2
P	41	ARG	-	expression tag	UNP G0Y2B2
P	42	GLY	-	expression tag	UNP G0Y2B2
P	43	SER	-	expression tag	UNP G0Y2B2
P	44	HIS	-	expression tag	UNP G0Y2B2
Q	25	MET	-	expression tag	UNP G0Y2B2
Q	26	GLY	-	expression tag	UNP G0Y2B2
Q	27	SER	-	expression tag	UNP G0Y2B2
Q	28	SER	-	expression tag	UNP G0Y2B2
Q	29	HIS	-	expression tag	UNP G0Y2B2
Q	30	HIS	-	expression tag	UNP G0Y2B2
Q	31	HIS	-	expression tag	UNP G0Y2B2
Q	32	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	33	HIS	-	expression tag	UNP G0Y2B2
Q	34	HIS	-	expression tag	UNP G0Y2B2
Q	35	SER	-	expression tag	UNP G0Y2B2
Q	36	SER	-	expression tag	UNP G0Y2B2
Q	37	GLY	-	expression tag	UNP G0Y2B2
Q	38	LEU	-	expression tag	UNP G0Y2B2
Q	39	VAL	-	expression tag	UNP G0Y2B2
Q	40	PRO	-	expression tag	UNP G0Y2B2
Q	41	ARG	-	expression tag	UNP G0Y2B2
Q	42	GLY	-	expression tag	UNP G0Y2B2
Q	43	SER	-	expression tag	UNP G0Y2B2
Q	44	HIS	-	expression tag	UNP G0Y2B2
R	25	MET	-	expression tag	UNP G0Y2B2
R	26	GLY	-	expression tag	UNP G0Y2B2
R	27	SER	-	expression tag	UNP G0Y2B2
R	28	SER	-	expression tag	UNP G0Y2B2
R	29	HIS	-	expression tag	UNP G0Y2B2
R	30	HIS	-	expression tag	UNP G0Y2B2
R	31	HIS	-	expression tag	UNP G0Y2B2
R	32	HIS	-	expression tag	UNP G0Y2B2
R	33	HIS	-	expression tag	UNP G0Y2B2
R	34	HIS	-	expression tag	UNP G0Y2B2
R	35	SER	-	expression tag	UNP G0Y2B2
R	36	SER	-	expression tag	UNP G0Y2B2
R	37	GLY	-	expression tag	UNP G0Y2B2
R	38	LEU	-	expression tag	UNP G0Y2B2
R	39	VAL	-	expression tag	UNP G0Y2B2
R	40	PRO	-	expression tag	UNP G0Y2B2
R	41	ARG	-	expression tag	UNP G0Y2B2
R	42	GLY	-	expression tag	UNP G0Y2B2
R	43	SER	-	expression tag	UNP G0Y2B2
R	44	HIS	-	expression tag	UNP G0Y2B2
S	25	MET	-	expression tag	UNP G0Y2B2
S	26	GLY	-	expression tag	UNP G0Y2B2
S	27	SER	-	expression tag	UNP G0Y2B2
S	28	SER	-	expression tag	UNP G0Y2B2
S	29	HIS	-	expression tag	UNP G0Y2B2
S	30	HIS	-	expression tag	UNP G0Y2B2
S	31	HIS	-	expression tag	UNP G0Y2B2
S	32	HIS	-	expression tag	UNP G0Y2B2
S	33	HIS	-	expression tag	UNP G0Y2B2
S	34	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
S	35	SER	-	expression tag	UNP G0Y2B2
S	36	SER	-	expression tag	UNP G0Y2B2
S	37	GLY	-	expression tag	UNP G0Y2B2
S	38	LEU	-	expression tag	UNP G0Y2B2
S	39	VAL	-	expression tag	UNP G0Y2B2
S	40	PRO	-	expression tag	UNP G0Y2B2
S	41	ARG	-	expression tag	UNP G0Y2B2
S	42	GLY	-	expression tag	UNP G0Y2B2
S	43	SER	-	expression tag	UNP G0Y2B2
S	44	HIS	-	expression tag	UNP G0Y2B2
T	25	MET	-	expression tag	UNP G0Y2B2
T	26	GLY	-	expression tag	UNP G0Y2B2
T	27	SER	-	expression tag	UNP G0Y2B2
T	28	SER	-	expression tag	UNP G0Y2B2
T	29	HIS	-	expression tag	UNP G0Y2B2
T	30	HIS	-	expression tag	UNP G0Y2B2
T	31	HIS	-	expression tag	UNP G0Y2B2
T	32	HIS	-	expression tag	UNP G0Y2B2
T	33	HIS	-	expression tag	UNP G0Y2B2
T	34	HIS	-	expression tag	UNP G0Y2B2
T	35	SER	-	expression tag	UNP G0Y2B2
T	36	SER	-	expression tag	UNP G0Y2B2
T	37	GLY	-	expression tag	UNP G0Y2B2
T	38	LEU	-	expression tag	UNP G0Y2B2
T	39	VAL	-	expression tag	UNP G0Y2B2
T	40	PRO	-	expression tag	UNP G0Y2B2
T	41	ARG	-	expression tag	UNP G0Y2B2
T	42	GLY	-	expression tag	UNP G0Y2B2
T	43	SER	-	expression tag	UNP G0Y2B2
T	44	HIS	-	expression tag	UNP G0Y2B2
U	25	MET	-	expression tag	UNP G0Y2B2
U	26	GLY	-	expression tag	UNP G0Y2B2
U	27	SER	-	expression tag	UNP G0Y2B2
U	28	SER	-	expression tag	UNP G0Y2B2
U	29	HIS	-	expression tag	UNP G0Y2B2
U	30	HIS	-	expression tag	UNP G0Y2B2
U	31	HIS	-	expression tag	UNP G0Y2B2
U	32	HIS	-	expression tag	UNP G0Y2B2
U	33	HIS	-	expression tag	UNP G0Y2B2
U	34	HIS	-	expression tag	UNP G0Y2B2
U	35	SER	-	expression tag	UNP G0Y2B2
U	36	SER	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
U	37	GLY	-	expression tag	UNP G0Y2B2
U	38	LEU	-	expression tag	UNP G0Y2B2
U	39	VAL	-	expression tag	UNP G0Y2B2
U	40	PRO	-	expression tag	UNP G0Y2B2
U	41	ARG	-	expression tag	UNP G0Y2B2
U	42	GLY	-	expression tag	UNP G0Y2B2
U	43	SER	-	expression tag	UNP G0Y2B2
U	44	HIS	-	expression tag	UNP G0Y2B2
V	25	MET	-	expression tag	UNP G0Y2B2
V	26	GLY	-	expression tag	UNP G0Y2B2
V	27	SER	-	expression tag	UNP G0Y2B2
V	28	SER	-	expression tag	UNP G0Y2B2
V	29	HIS	-	expression tag	UNP G0Y2B2
V	30	HIS	-	expression tag	UNP G0Y2B2
V	31	HIS	-	expression tag	UNP G0Y2B2
V	32	HIS	-	expression tag	UNP G0Y2B2
V	33	HIS	-	expression tag	UNP G0Y2B2
V	34	HIS	-	expression tag	UNP G0Y2B2
V	35	SER	-	expression tag	UNP G0Y2B2
V	36	SER	-	expression tag	UNP G0Y2B2
V	37	GLY	-	expression tag	UNP G0Y2B2
V	38	LEU	-	expression tag	UNP G0Y2B2
V	39	VAL	-	expression tag	UNP G0Y2B2
V	40	PRO	-	expression tag	UNP G0Y2B2
V	41	ARG	-	expression tag	UNP G0Y2B2
V	42	GLY	-	expression tag	UNP G0Y2B2
V	43	SER	-	expression tag	UNP G0Y2B2
V	44	HIS	-	expression tag	UNP G0Y2B2
W	25	MET	-	expression tag	UNP G0Y2B2
W	26	GLY	-	expression tag	UNP G0Y2B2
W	27	SER	-	expression tag	UNP G0Y2B2
W	28	SER	-	expression tag	UNP G0Y2B2
W	29	HIS	-	expression tag	UNP G0Y2B2
W	30	HIS	-	expression tag	UNP G0Y2B2
W	31	HIS	-	expression tag	UNP G0Y2B2
W	32	HIS	-	expression tag	UNP G0Y2B2
W	33	HIS	-	expression tag	UNP G0Y2B2
W	34	HIS	-	expression tag	UNP G0Y2B2
W	35	SER	-	expression tag	UNP G0Y2B2
W	36	SER	-	expression tag	UNP G0Y2B2
W	37	GLY	-	expression tag	UNP G0Y2B2
W	38	LEU	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
W	39	VAL	-	expression tag	UNP G0Y2B2
W	40	PRO	-	expression tag	UNP G0Y2B2
W	41	ARG	-	expression tag	UNP G0Y2B2
W	42	GLY	-	expression tag	UNP G0Y2B2
W	43	SER	-	expression tag	UNP G0Y2B2
W	44	HIS	-	expression tag	UNP G0Y2B2
X	25	MET	-	expression tag	UNP G0Y2B2
X	26	GLY	-	expression tag	UNP G0Y2B2
X	27	SER	-	expression tag	UNP G0Y2B2
X	28	SER	-	expression tag	UNP G0Y2B2
X	29	HIS	-	expression tag	UNP G0Y2B2
X	30	HIS	-	expression tag	UNP G0Y2B2
X	31	HIS	-	expression tag	UNP G0Y2B2
X	32	HIS	-	expression tag	UNP G0Y2B2
X	33	HIS	-	expression tag	UNP G0Y2B2
X	34	HIS	-	expression tag	UNP G0Y2B2
X	35	SER	-	expression tag	UNP G0Y2B2
X	36	SER	-	expression tag	UNP G0Y2B2
X	37	GLY	-	expression tag	UNP G0Y2B2
X	38	LEU	-	expression tag	UNP G0Y2B2
X	39	VAL	-	expression tag	UNP G0Y2B2
X	40	PRO	-	expression tag	UNP G0Y2B2
X	41	ARG	-	expression tag	UNP G0Y2B2
X	42	GLY	-	expression tag	UNP G0Y2B2
X	43	SER	-	expression tag	UNP G0Y2B2
X	44	HIS	-	expression tag	UNP G0Y2B2
Y	25	MET	-	expression tag	UNP G0Y2B2
Y	26	GLY	-	expression tag	UNP G0Y2B2
Y	27	SER	-	expression tag	UNP G0Y2B2
Y	28	SER	-	expression tag	UNP G0Y2B2
Y	29	HIS	-	expression tag	UNP G0Y2B2
Y	30	HIS	-	expression tag	UNP G0Y2B2
Y	31	HIS	-	expression tag	UNP G0Y2B2
Y	32	HIS	-	expression tag	UNP G0Y2B2
Y	33	HIS	-	expression tag	UNP G0Y2B2
Y	34	HIS	-	expression tag	UNP G0Y2B2
Y	35	SER	-	expression tag	UNP G0Y2B2
Y	36	SER	-	expression tag	UNP G0Y2B2
Y	37	GLY	-	expression tag	UNP G0Y2B2
Y	38	LEU	-	expression tag	UNP G0Y2B2
Y	39	VAL	-	expression tag	UNP G0Y2B2
Y	40	PRO	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	41	ARG	-	expression tag	UNP G0Y2B2
Y	42	GLY	-	expression tag	UNP G0Y2B2
Y	43	SER	-	expression tag	UNP G0Y2B2
Y	44	HIS	-	expression tag	UNP G0Y2B2
Z	25	MET	-	expression tag	UNP G0Y2B2
Z	26	GLY	-	expression tag	UNP G0Y2B2
Z	27	SER	-	expression tag	UNP G0Y2B2
Z	28	SER	-	expression tag	UNP G0Y2B2
Z	29	HIS	-	expression tag	UNP G0Y2B2
Z	30	HIS	-	expression tag	UNP G0Y2B2
Z	31	HIS	-	expression tag	UNP G0Y2B2
Z	32	HIS	-	expression tag	UNP G0Y2B2
Z	33	HIS	-	expression tag	UNP G0Y2B2
Z	34	HIS	-	expression tag	UNP G0Y2B2
Z	35	SER	-	expression tag	UNP G0Y2B2
Z	36	SER	-	expression tag	UNP G0Y2B2
Z	37	GLY	-	expression tag	UNP G0Y2B2
Z	38	LEU	-	expression tag	UNP G0Y2B2
Z	39	VAL	-	expression tag	UNP G0Y2B2
Z	40	PRO	-	expression tag	UNP G0Y2B2
Z	41	ARG	-	expression tag	UNP G0Y2B2
Z	42	GLY	-	expression tag	UNP G0Y2B2
Z	43	SER	-	expression tag	UNP G0Y2B2
Z	44	HIS	-	expression tag	UNP G0Y2B2
1	25	MET	-	expression tag	UNP G0Y2B2
1	26	GLY	-	expression tag	UNP G0Y2B2
1	27	SER	-	expression tag	UNP G0Y2B2
1	28	SER	-	expression tag	UNP G0Y2B2
1	29	HIS	-	expression tag	UNP G0Y2B2
1	30	HIS	-	expression tag	UNP G0Y2B2
1	31	HIS	-	expression tag	UNP G0Y2B2
1	32	HIS	-	expression tag	UNP G0Y2B2
1	33	HIS	-	expression tag	UNP G0Y2B2
1	34	HIS	-	expression tag	UNP G0Y2B2
1	35	SER	-	expression tag	UNP G0Y2B2
1	36	SER	-	expression tag	UNP G0Y2B2
1	37	GLY	-	expression tag	UNP G0Y2B2
1	38	LEU	-	expression tag	UNP G0Y2B2
1	39	VAL	-	expression tag	UNP G0Y2B2
1	40	PRO	-	expression tag	UNP G0Y2B2
1	41	ARG	-	expression tag	UNP G0Y2B2
1	42	GLY	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
1	43	SER	-	expression tag	UNP G0Y2B2
1	44	HIS	-	expression tag	UNP G0Y2B2
2	25	MET	-	expression tag	UNP G0Y2B2
2	26	GLY	-	expression tag	UNP G0Y2B2
2	27	SER	-	expression tag	UNP G0Y2B2
2	28	SER	-	expression tag	UNP G0Y2B2
2	29	HIS	-	expression tag	UNP G0Y2B2
2	30	HIS	-	expression tag	UNP G0Y2B2
2	31	HIS	-	expression tag	UNP G0Y2B2
2	32	HIS	-	expression tag	UNP G0Y2B2
2	33	HIS	-	expression tag	UNP G0Y2B2
2	34	HIS	-	expression tag	UNP G0Y2B2
2	35	SER	-	expression tag	UNP G0Y2B2
2	36	SER	-	expression tag	UNP G0Y2B2
2	37	GLY	-	expression tag	UNP G0Y2B2
2	38	LEU	-	expression tag	UNP G0Y2B2
2	39	VAL	-	expression tag	UNP G0Y2B2
2	40	PRO	-	expression tag	UNP G0Y2B2
2	41	ARG	-	expression tag	UNP G0Y2B2
2	42	GLY	-	expression tag	UNP G0Y2B2
2	43	SER	-	expression tag	UNP G0Y2B2
2	44	HIS	-	expression tag	UNP G0Y2B2
3	25	MET	-	expression tag	UNP G0Y2B2
3	26	GLY	-	expression tag	UNP G0Y2B2
3	27	SER	-	expression tag	UNP G0Y2B2
3	28	SER	-	expression tag	UNP G0Y2B2
3	29	HIS	-	expression tag	UNP G0Y2B2
3	30	HIS	-	expression tag	UNP G0Y2B2
3	31	HIS	-	expression tag	UNP G0Y2B2
3	32	HIS	-	expression tag	UNP G0Y2B2
3	33	HIS	-	expression tag	UNP G0Y2B2
3	34	HIS	-	expression tag	UNP G0Y2B2
3	35	SER	-	expression tag	UNP G0Y2B2
3	36	SER	-	expression tag	UNP G0Y2B2
3	37	GLY	-	expression tag	UNP G0Y2B2
3	38	LEU	-	expression tag	UNP G0Y2B2
3	39	VAL	-	expression tag	UNP G0Y2B2
3	40	PRO	-	expression tag	UNP G0Y2B2
3	41	ARG	-	expression tag	UNP G0Y2B2
3	42	GLY	-	expression tag	UNP G0Y2B2
3	43	SER	-	expression tag	UNP G0Y2B2
3	44	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
4	25	MET	-	expression tag	UNP G0Y2B2
4	26	GLY	-	expression tag	UNP G0Y2B2
4	27	SER	-	expression tag	UNP G0Y2B2
4	28	SER	-	expression tag	UNP G0Y2B2
4	29	HIS	-	expression tag	UNP G0Y2B2
4	30	HIS	-	expression tag	UNP G0Y2B2
4	31	HIS	-	expression tag	UNP G0Y2B2
4	32	HIS	-	expression tag	UNP G0Y2B2
4	33	HIS	-	expression tag	UNP G0Y2B2
4	34	HIS	-	expression tag	UNP G0Y2B2
4	35	SER	-	expression tag	UNP G0Y2B2
4	36	SER	-	expression tag	UNP G0Y2B2
4	37	GLY	-	expression tag	UNP G0Y2B2
4	38	LEU	-	expression tag	UNP G0Y2B2
4	39	VAL	-	expression tag	UNP G0Y2B2
4	40	PRO	-	expression tag	UNP G0Y2B2
4	41	ARG	-	expression tag	UNP G0Y2B2
4	42	GLY	-	expression tag	UNP G0Y2B2
4	43	SER	-	expression tag	UNP G0Y2B2
4	44	HIS	-	expression tag	UNP G0Y2B2
5	25	MET	-	expression tag	UNP G0Y2B2
5	26	GLY	-	expression tag	UNP G0Y2B2
5	27	SER	-	expression tag	UNP G0Y2B2
5	28	SER	-	expression tag	UNP G0Y2B2
5	29	HIS	-	expression tag	UNP G0Y2B2
5	30	HIS	-	expression tag	UNP G0Y2B2
5	31	HIS	-	expression tag	UNP G0Y2B2
5	32	HIS	-	expression tag	UNP G0Y2B2
5	33	HIS	-	expression tag	UNP G0Y2B2
5	34	HIS	-	expression tag	UNP G0Y2B2
5	35	SER	-	expression tag	UNP G0Y2B2
5	36	SER	-	expression tag	UNP G0Y2B2
5	37	GLY	-	expression tag	UNP G0Y2B2
5	38	LEU	-	expression tag	UNP G0Y2B2
5	39	VAL	-	expression tag	UNP G0Y2B2
5	40	PRO	-	expression tag	UNP G0Y2B2
5	41	ARG	-	expression tag	UNP G0Y2B2
5	42	GLY	-	expression tag	UNP G0Y2B2
5	43	SER	-	expression tag	UNP G0Y2B2
5	44	HIS	-	expression tag	UNP G0Y2B2
6	25	MET	-	expression tag	UNP G0Y2B2
6	26	GLY	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
6	27	SER	-	expression tag	UNP G0Y2B2
6	28	SER	-	expression tag	UNP G0Y2B2
6	29	HIS	-	expression tag	UNP G0Y2B2
6	30	HIS	-	expression tag	UNP G0Y2B2
6	31	HIS	-	expression tag	UNP G0Y2B2
6	32	HIS	-	expression tag	UNP G0Y2B2
6	33	HIS	-	expression tag	UNP G0Y2B2
6	34	HIS	-	expression tag	UNP G0Y2B2
6	35	SER	-	expression tag	UNP G0Y2B2
6	36	SER	-	expression tag	UNP G0Y2B2
6	37	GLY	-	expression tag	UNP G0Y2B2
6	38	LEU	-	expression tag	UNP G0Y2B2
6	39	VAL	-	expression tag	UNP G0Y2B2
6	40	PRO	-	expression tag	UNP G0Y2B2
6	41	ARG	-	expression tag	UNP G0Y2B2
6	42	GLY	-	expression tag	UNP G0Y2B2
6	43	SER	-	expression tag	UNP G0Y2B2
6	44	HIS	-	expression tag	UNP G0Y2B2
7	25	MET	-	expression tag	UNP G0Y2B2
7	26	GLY	-	expression tag	UNP G0Y2B2
7	27	SER	-	expression tag	UNP G0Y2B2
7	28	SER	-	expression tag	UNP G0Y2B2
7	29	HIS	-	expression tag	UNP G0Y2B2
7	30	HIS	-	expression tag	UNP G0Y2B2
7	31	HIS	-	expression tag	UNP G0Y2B2
7	32	HIS	-	expression tag	UNP G0Y2B2
7	33	HIS	-	expression tag	UNP G0Y2B2
7	34	HIS	-	expression tag	UNP G0Y2B2
7	35	SER	-	expression tag	UNP G0Y2B2
7	36	SER	-	expression tag	UNP G0Y2B2
7	37	GLY	-	expression tag	UNP G0Y2B2
7	38	LEU	-	expression tag	UNP G0Y2B2
7	39	VAL	-	expression tag	UNP G0Y2B2
7	40	PRO	-	expression tag	UNP G0Y2B2
7	41	ARG	-	expression tag	UNP G0Y2B2
7	42	GLY	-	expression tag	UNP G0Y2B2
7	43	SER	-	expression tag	UNP G0Y2B2
7	44	HIS	-	expression tag	UNP G0Y2B2
8	25	MET	-	expression tag	UNP G0Y2B2
8	26	GLY	-	expression tag	UNP G0Y2B2
8	27	SER	-	expression tag	UNP G0Y2B2
8	28	SER	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
8	29	HIS	-	expression tag	UNP G0Y2B2
8	30	HIS	-	expression tag	UNP G0Y2B2
8	31	HIS	-	expression tag	UNP G0Y2B2
8	32	HIS	-	expression tag	UNP G0Y2B2
8	33	HIS	-	expression tag	UNP G0Y2B2
8	34	HIS	-	expression tag	UNP G0Y2B2
8	35	SER	-	expression tag	UNP G0Y2B2
8	36	SER	-	expression tag	UNP G0Y2B2
8	37	GLY	-	expression tag	UNP G0Y2B2
8	38	LEU	-	expression tag	UNP G0Y2B2
8	39	VAL	-	expression tag	UNP G0Y2B2
8	40	PRO	-	expression tag	UNP G0Y2B2
8	41	ARG	-	expression tag	UNP G0Y2B2
8	42	GLY	-	expression tag	UNP G0Y2B2
8	43	SER	-	expression tag	UNP G0Y2B2
8	44	HIS	-	expression tag	UNP G0Y2B2
9	25	MET	-	expression tag	UNP G0Y2B2
9	26	GLY	-	expression tag	UNP G0Y2B2
9	27	SER	-	expression tag	UNP G0Y2B2
9	28	SER	-	expression tag	UNP G0Y2B2
9	29	HIS	-	expression tag	UNP G0Y2B2
9	30	HIS	-	expression tag	UNP G0Y2B2
9	31	HIS	-	expression tag	UNP G0Y2B2
9	32	HIS	-	expression tag	UNP G0Y2B2
9	33	HIS	-	expression tag	UNP G0Y2B2
9	34	HIS	-	expression tag	UNP G0Y2B2
9	35	SER	-	expression tag	UNP G0Y2B2
9	36	SER	-	expression tag	UNP G0Y2B2
9	37	GLY	-	expression tag	UNP G0Y2B2
9	38	LEU	-	expression tag	UNP G0Y2B2
9	39	VAL	-	expression tag	UNP G0Y2B2
9	40	PRO	-	expression tag	UNP G0Y2B2
9	41	ARG	-	expression tag	UNP G0Y2B2
9	42	GLY	-	expression tag	UNP G0Y2B2
9	43	SER	-	expression tag	UNP G0Y2B2
9	44	HIS	-	expression tag	UNP G0Y2B2
a	25	MET	-	expression tag	UNP G0Y2B2
a	26	GLY	-	expression tag	UNP G0Y2B2
a	27	SER	-	expression tag	UNP G0Y2B2
a	28	SER	-	expression tag	UNP G0Y2B2
a	29	HIS	-	expression tag	UNP G0Y2B2
a	30	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
a	31	HIS	-	expression tag	UNP G0Y2B2
a	32	HIS	-	expression tag	UNP G0Y2B2
a	33	HIS	-	expression tag	UNP G0Y2B2
a	34	HIS	-	expression tag	UNP G0Y2B2
a	35	SER	-	expression tag	UNP G0Y2B2
a	36	SER	-	expression tag	UNP G0Y2B2
a	37	GLY	-	expression tag	UNP G0Y2B2
a	38	LEU	-	expression tag	UNP G0Y2B2
a	39	VAL	-	expression tag	UNP G0Y2B2
a	40	PRO	-	expression tag	UNP G0Y2B2
a	41	ARG	-	expression tag	UNP G0Y2B2
a	42	GLY	-	expression tag	UNP G0Y2B2
a	43	SER	-	expression tag	UNP G0Y2B2
a	44	HIS	-	expression tag	UNP G0Y2B2
b	25	MET	-	expression tag	UNP G0Y2B2
b	26	GLY	-	expression tag	UNP G0Y2B2
b	27	SER	-	expression tag	UNP G0Y2B2
b	28	SER	-	expression tag	UNP G0Y2B2
b	29	HIS	-	expression tag	UNP G0Y2B2
b	30	HIS	-	expression tag	UNP G0Y2B2
b	31	HIS	-	expression tag	UNP G0Y2B2
b	32	HIS	-	expression tag	UNP G0Y2B2
b	33	HIS	-	expression tag	UNP G0Y2B2
b	34	HIS	-	expression tag	UNP G0Y2B2
b	35	SER	-	expression tag	UNP G0Y2B2
b	36	SER	-	expression tag	UNP G0Y2B2
b	37	GLY	-	expression tag	UNP G0Y2B2
b	38	LEU	-	expression tag	UNP G0Y2B2
b	39	VAL	-	expression tag	UNP G0Y2B2
b	40	PRO	-	expression tag	UNP G0Y2B2
b	41	ARG	-	expression tag	UNP G0Y2B2
b	42	GLY	-	expression tag	UNP G0Y2B2
b	43	SER	-	expression tag	UNP G0Y2B2
b	44	HIS	-	expression tag	UNP G0Y2B2
c	25	MET	-	expression tag	UNP G0Y2B2
c	26	GLY	-	expression tag	UNP G0Y2B2
c	27	SER	-	expression tag	UNP G0Y2B2
c	28	SER	-	expression tag	UNP G0Y2B2
c	29	HIS	-	expression tag	UNP G0Y2B2
c	30	HIS	-	expression tag	UNP G0Y2B2
c	31	HIS	-	expression tag	UNP G0Y2B2
c	32	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
c	33	HIS	-	expression tag	UNP G0Y2B2
c	34	HIS	-	expression tag	UNP G0Y2B2
c	35	SER	-	expression tag	UNP G0Y2B2
c	36	SER	-	expression tag	UNP G0Y2B2
c	37	GLY	-	expression tag	UNP G0Y2B2
c	38	LEU	-	expression tag	UNP G0Y2B2
c	39	VAL	-	expression tag	UNP G0Y2B2
c	40	PRO	-	expression tag	UNP G0Y2B2
c	41	ARG	-	expression tag	UNP G0Y2B2
c	42	GLY	-	expression tag	UNP G0Y2B2
c	43	SER	-	expression tag	UNP G0Y2B2
c	44	HIS	-	expression tag	UNP G0Y2B2
d	25	MET	-	expression tag	UNP G0Y2B2
d	26	GLY	-	expression tag	UNP G0Y2B2
d	27	SER	-	expression tag	UNP G0Y2B2
d	28	SER	-	expression tag	UNP G0Y2B2
d	29	HIS	-	expression tag	UNP G0Y2B2
d	30	HIS	-	expression tag	UNP G0Y2B2
d	31	HIS	-	expression tag	UNP G0Y2B2
d	32	HIS	-	expression tag	UNP G0Y2B2
d	33	HIS	-	expression tag	UNP G0Y2B2
d	34	HIS	-	expression tag	UNP G0Y2B2
d	35	SER	-	expression tag	UNP G0Y2B2
d	36	SER	-	expression tag	UNP G0Y2B2
d	37	GLY	-	expression tag	UNP G0Y2B2
d	38	LEU	-	expression tag	UNP G0Y2B2
d	39	VAL	-	expression tag	UNP G0Y2B2
d	40	PRO	-	expression tag	UNP G0Y2B2
d	41	ARG	-	expression tag	UNP G0Y2B2
d	42	GLY	-	expression tag	UNP G0Y2B2
d	43	SER	-	expression tag	UNP G0Y2B2
d	44	HIS	-	expression tag	UNP G0Y2B2
e	25	MET	-	expression tag	UNP G0Y2B2
e	26	GLY	-	expression tag	UNP G0Y2B2
e	27	SER	-	expression tag	UNP G0Y2B2
e	28	SER	-	expression tag	UNP G0Y2B2
e	29	HIS	-	expression tag	UNP G0Y2B2
e	30	HIS	-	expression tag	UNP G0Y2B2
e	31	HIS	-	expression tag	UNP G0Y2B2
e	32	HIS	-	expression tag	UNP G0Y2B2
e	33	HIS	-	expression tag	UNP G0Y2B2
e	34	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
e	35	SER	-	expression tag	UNP G0Y2B2
e	36	SER	-	expression tag	UNP G0Y2B2
e	37	GLY	-	expression tag	UNP G0Y2B2
e	38	LEU	-	expression tag	UNP G0Y2B2
e	39	VAL	-	expression tag	UNP G0Y2B2
e	40	PRO	-	expression tag	UNP G0Y2B2
e	41	ARG	-	expression tag	UNP G0Y2B2
e	42	GLY	-	expression tag	UNP G0Y2B2
e	43	SER	-	expression tag	UNP G0Y2B2
e	44	HIS	-	expression tag	UNP G0Y2B2
f	25	MET	-	expression tag	UNP G0Y2B2
f	26	GLY	-	expression tag	UNP G0Y2B2
f	27	SER	-	expression tag	UNP G0Y2B2
f	28	SER	-	expression tag	UNP G0Y2B2
f	29	HIS	-	expression tag	UNP G0Y2B2
f	30	HIS	-	expression tag	UNP G0Y2B2
f	31	HIS	-	expression tag	UNP G0Y2B2
f	32	HIS	-	expression tag	UNP G0Y2B2
f	33	HIS	-	expression tag	UNP G0Y2B2
f	34	HIS	-	expression tag	UNP G0Y2B2
f	35	SER	-	expression tag	UNP G0Y2B2
f	36	SER	-	expression tag	UNP G0Y2B2
f	37	GLY	-	expression tag	UNP G0Y2B2
f	38	LEU	-	expression tag	UNP G0Y2B2
f	39	VAL	-	expression tag	UNP G0Y2B2
f	40	PRO	-	expression tag	UNP G0Y2B2
f	41	ARG	-	expression tag	UNP G0Y2B2
f	42	GLY	-	expression tag	UNP G0Y2B2
f	43	SER	-	expression tag	UNP G0Y2B2
f	44	HIS	-	expression tag	UNP G0Y2B2
g	25	MET	-	expression tag	UNP G0Y2B2
g	26	GLY	-	expression tag	UNP G0Y2B2
g	27	SER	-	expression tag	UNP G0Y2B2
g	28	SER	-	expression tag	UNP G0Y2B2
g	29	HIS	-	expression tag	UNP G0Y2B2
g	30	HIS	-	expression tag	UNP G0Y2B2
g	31	HIS	-	expression tag	UNP G0Y2B2
g	32	HIS	-	expression tag	UNP G0Y2B2
g	33	HIS	-	expression tag	UNP G0Y2B2
g	34	HIS	-	expression tag	UNP G0Y2B2
g	35	SER	-	expression tag	UNP G0Y2B2
g	36	SER	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
g	37	GLY	-	expression tag	UNP G0Y2B2
g	38	LEU	-	expression tag	UNP G0Y2B2
g	39	VAL	-	expression tag	UNP G0Y2B2
g	40	PRO	-	expression tag	UNP G0Y2B2
g	41	ARG	-	expression tag	UNP G0Y2B2
g	42	GLY	-	expression tag	UNP G0Y2B2
g	43	SER	-	expression tag	UNP G0Y2B2
g	44	HIS	-	expression tag	UNP G0Y2B2
h	25	MET	-	expression tag	UNP G0Y2B2
h	26	GLY	-	expression tag	UNP G0Y2B2
h	27	SER	-	expression tag	UNP G0Y2B2
h	28	SER	-	expression tag	UNP G0Y2B2
h	29	HIS	-	expression tag	UNP G0Y2B2
h	30	HIS	-	expression tag	UNP G0Y2B2
h	31	HIS	-	expression tag	UNP G0Y2B2
h	32	HIS	-	expression tag	UNP G0Y2B2
h	33	HIS	-	expression tag	UNP G0Y2B2
h	34	HIS	-	expression tag	UNP G0Y2B2
h	35	SER	-	expression tag	UNP G0Y2B2
h	36	SER	-	expression tag	UNP G0Y2B2
h	37	GLY	-	expression tag	UNP G0Y2B2
h	38	LEU	-	expression tag	UNP G0Y2B2
h	39	VAL	-	expression tag	UNP G0Y2B2
h	40	PRO	-	expression tag	UNP G0Y2B2
h	41	ARG	-	expression tag	UNP G0Y2B2
h	42	GLY	-	expression tag	UNP G0Y2B2
h	43	SER	-	expression tag	UNP G0Y2B2
h	44	HIS	-	expression tag	UNP G0Y2B2
i	25	MET	-	expression tag	UNP G0Y2B2
i	26	GLY	-	expression tag	UNP G0Y2B2
i	27	SER	-	expression tag	UNP G0Y2B2
i	28	SER	-	expression tag	UNP G0Y2B2
i	29	HIS	-	expression tag	UNP G0Y2B2
i	30	HIS	-	expression tag	UNP G0Y2B2
i	31	HIS	-	expression tag	UNP G0Y2B2
i	32	HIS	-	expression tag	UNP G0Y2B2
i	33	HIS	-	expression tag	UNP G0Y2B2
i	34	HIS	-	expression tag	UNP G0Y2B2
i	35	SER	-	expression tag	UNP G0Y2B2
i	36	SER	-	expression tag	UNP G0Y2B2
i	37	GLY	-	expression tag	UNP G0Y2B2
i	38	LEU	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
i	39	VAL	-	expression tag	UNP G0Y2B2
i	40	PRO	-	expression tag	UNP G0Y2B2
i	41	ARG	-	expression tag	UNP G0Y2B2
i	42	GLY	-	expression tag	UNP G0Y2B2
i	43	SER	-	expression tag	UNP G0Y2B2
i	44	HIS	-	expression tag	UNP G0Y2B2
j	25	MET	-	expression tag	UNP G0Y2B2
j	26	GLY	-	expression tag	UNP G0Y2B2
j	27	SER	-	expression tag	UNP G0Y2B2
j	28	SER	-	expression tag	UNP G0Y2B2
j	29	HIS	-	expression tag	UNP G0Y2B2
j	30	HIS	-	expression tag	UNP G0Y2B2
j	31	HIS	-	expression tag	UNP G0Y2B2
j	32	HIS	-	expression tag	UNP G0Y2B2
j	33	HIS	-	expression tag	UNP G0Y2B2
j	34	HIS	-	expression tag	UNP G0Y2B2
j	35	SER	-	expression tag	UNP G0Y2B2
j	36	SER	-	expression tag	UNP G0Y2B2
j	37	GLY	-	expression tag	UNP G0Y2B2
j	38	LEU	-	expression tag	UNP G0Y2B2
j	39	VAL	-	expression tag	UNP G0Y2B2
j	40	PRO	-	expression tag	UNP G0Y2B2
j	41	ARG	-	expression tag	UNP G0Y2B2
j	42	GLY	-	expression tag	UNP G0Y2B2
j	43	SER	-	expression tag	UNP G0Y2B2
j	44	HIS	-	expression tag	UNP G0Y2B2
k	25	MET	-	expression tag	UNP G0Y2B2
k	26	GLY	-	expression tag	UNP G0Y2B2
k	27	SER	-	expression tag	UNP G0Y2B2
k	28	SER	-	expression tag	UNP G0Y2B2
k	29	HIS	-	expression tag	UNP G0Y2B2
k	30	HIS	-	expression tag	UNP G0Y2B2
k	31	HIS	-	expression tag	UNP G0Y2B2
k	32	HIS	-	expression tag	UNP G0Y2B2
k	33	HIS	-	expression tag	UNP G0Y2B2
k	34	HIS	-	expression tag	UNP G0Y2B2
k	35	SER	-	expression tag	UNP G0Y2B2
k	36	SER	-	expression tag	UNP G0Y2B2
k	37	GLY	-	expression tag	UNP G0Y2B2
k	38	LEU	-	expression tag	UNP G0Y2B2
k	39	VAL	-	expression tag	UNP G0Y2B2
k	40	PRO	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
k	41	ARG	-	expression tag	UNP G0Y2B2
k	42	GLY	-	expression tag	UNP G0Y2B2
k	43	SER	-	expression tag	UNP G0Y2B2
k	44	HIS	-	expression tag	UNP G0Y2B2
l	25	MET	-	expression tag	UNP G0Y2B2
l	26	GLY	-	expression tag	UNP G0Y2B2
l	27	SER	-	expression tag	UNP G0Y2B2
l	28	SER	-	expression tag	UNP G0Y2B2
l	29	HIS	-	expression tag	UNP G0Y2B2
l	30	HIS	-	expression tag	UNP G0Y2B2
l	31	HIS	-	expression tag	UNP G0Y2B2
l	32	HIS	-	expression tag	UNP G0Y2B2
l	33	HIS	-	expression tag	UNP G0Y2B2
l	34	HIS	-	expression tag	UNP G0Y2B2
l	35	SER	-	expression tag	UNP G0Y2B2
l	36	SER	-	expression tag	UNP G0Y2B2
l	37	GLY	-	expression tag	UNP G0Y2B2
l	38	LEU	-	expression tag	UNP G0Y2B2
l	39	VAL	-	expression tag	UNP G0Y2B2
l	40	PRO	-	expression tag	UNP G0Y2B2
l	41	ARG	-	expression tag	UNP G0Y2B2
l	42	GLY	-	expression tag	UNP G0Y2B2
l	43	SER	-	expression tag	UNP G0Y2B2
l	44	HIS	-	expression tag	UNP G0Y2B2
m	25	MET	-	expression tag	UNP G0Y2B2
m	26	GLY	-	expression tag	UNP G0Y2B2
m	27	SER	-	expression tag	UNP G0Y2B2
m	28	SER	-	expression tag	UNP G0Y2B2
m	29	HIS	-	expression tag	UNP G0Y2B2
m	30	HIS	-	expression tag	UNP G0Y2B2
m	31	HIS	-	expression tag	UNP G0Y2B2
m	32	HIS	-	expression tag	UNP G0Y2B2
m	33	HIS	-	expression tag	UNP G0Y2B2
m	34	HIS	-	expression tag	UNP G0Y2B2
m	35	SER	-	expression tag	UNP G0Y2B2
m	36	SER	-	expression tag	UNP G0Y2B2
m	37	GLY	-	expression tag	UNP G0Y2B2
m	38	LEU	-	expression tag	UNP G0Y2B2
m	39	VAL	-	expression tag	UNP G0Y2B2
m	40	PRO	-	expression tag	UNP G0Y2B2
m	41	ARG	-	expression tag	UNP G0Y2B2
m	42	GLY	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
m	43	SER	-	expression tag	UNP G0Y2B2
m	44	HIS	-	expression tag	UNP G0Y2B2
n	25	MET	-	expression tag	UNP G0Y2B2
n	26	GLY	-	expression tag	UNP G0Y2B2
n	27	SER	-	expression tag	UNP G0Y2B2
n	28	SER	-	expression tag	UNP G0Y2B2
n	29	HIS	-	expression tag	UNP G0Y2B2
n	30	HIS	-	expression tag	UNP G0Y2B2
n	31	HIS	-	expression tag	UNP G0Y2B2
n	32	HIS	-	expression tag	UNP G0Y2B2
n	33	HIS	-	expression tag	UNP G0Y2B2
n	34	HIS	-	expression tag	UNP G0Y2B2
n	35	SER	-	expression tag	UNP G0Y2B2
n	36	SER	-	expression tag	UNP G0Y2B2
n	37	GLY	-	expression tag	UNP G0Y2B2
n	38	LEU	-	expression tag	UNP G0Y2B2
n	39	VAL	-	expression tag	UNP G0Y2B2
n	40	PRO	-	expression tag	UNP G0Y2B2
n	41	ARG	-	expression tag	UNP G0Y2B2
n	42	GLY	-	expression tag	UNP G0Y2B2
n	43	SER	-	expression tag	UNP G0Y2B2
n	44	HIS	-	expression tag	UNP G0Y2B2
o	25	MET	-	expression tag	UNP G0Y2B2
o	26	GLY	-	expression tag	UNP G0Y2B2
o	27	SER	-	expression tag	UNP G0Y2B2
o	28	SER	-	expression tag	UNP G0Y2B2
o	29	HIS	-	expression tag	UNP G0Y2B2
o	30	HIS	-	expression tag	UNP G0Y2B2
o	31	HIS	-	expression tag	UNP G0Y2B2
o	32	HIS	-	expression tag	UNP G0Y2B2
o	33	HIS	-	expression tag	UNP G0Y2B2
o	34	HIS	-	expression tag	UNP G0Y2B2
o	35	SER	-	expression tag	UNP G0Y2B2
o	36	SER	-	expression tag	UNP G0Y2B2
o	37	GLY	-	expression tag	UNP G0Y2B2
o	38	LEU	-	expression tag	UNP G0Y2B2
o	39	VAL	-	expression tag	UNP G0Y2B2
o	40	PRO	-	expression tag	UNP G0Y2B2
o	41	ARG	-	expression tag	UNP G0Y2B2
o	42	GLY	-	expression tag	UNP G0Y2B2
o	43	SER	-	expression tag	UNP G0Y2B2
o	44	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
p	25	MET	-	expression tag	UNP G0Y2B2
p	26	GLY	-	expression tag	UNP G0Y2B2
p	27	SER	-	expression tag	UNP G0Y2B2
p	28	SER	-	expression tag	UNP G0Y2B2
p	29	HIS	-	expression tag	UNP G0Y2B2
p	30	HIS	-	expression tag	UNP G0Y2B2
p	31	HIS	-	expression tag	UNP G0Y2B2
p	32	HIS	-	expression tag	UNP G0Y2B2
p	33	HIS	-	expression tag	UNP G0Y2B2
p	34	HIS	-	expression tag	UNP G0Y2B2
p	35	SER	-	expression tag	UNP G0Y2B2
p	36	SER	-	expression tag	UNP G0Y2B2
p	37	GLY	-	expression tag	UNP G0Y2B2
p	38	LEU	-	expression tag	UNP G0Y2B2
p	39	VAL	-	expression tag	UNP G0Y2B2
p	40	PRO	-	expression tag	UNP G0Y2B2
p	41	ARG	-	expression tag	UNP G0Y2B2
p	42	GLY	-	expression tag	UNP G0Y2B2
p	43	SER	-	expression tag	UNP G0Y2B2
p	44	HIS	-	expression tag	UNP G0Y2B2
q	25	MET	-	expression tag	UNP G0Y2B2
q	26	GLY	-	expression tag	UNP G0Y2B2
q	27	SER	-	expression tag	UNP G0Y2B2
q	28	SER	-	expression tag	UNP G0Y2B2
q	29	HIS	-	expression tag	UNP G0Y2B2
q	30	HIS	-	expression tag	UNP G0Y2B2
q	31	HIS	-	expression tag	UNP G0Y2B2
q	32	HIS	-	expression tag	UNP G0Y2B2
q	33	HIS	-	expression tag	UNP G0Y2B2
q	34	HIS	-	expression tag	UNP G0Y2B2
q	35	SER	-	expression tag	UNP G0Y2B2
q	36	SER	-	expression tag	UNP G0Y2B2
q	37	GLY	-	expression tag	UNP G0Y2B2
q	38	LEU	-	expression tag	UNP G0Y2B2
q	39	VAL	-	expression tag	UNP G0Y2B2
q	40	PRO	-	expression tag	UNP G0Y2B2
q	41	ARG	-	expression tag	UNP G0Y2B2
q	42	GLY	-	expression tag	UNP G0Y2B2
q	43	SER	-	expression tag	UNP G0Y2B2
q	44	HIS	-	expression tag	UNP G0Y2B2
r	25	MET	-	expression tag	UNP G0Y2B2
r	26	GLY	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
r	27	SER	-	expression tag	UNP G0Y2B2
r	28	SER	-	expression tag	UNP G0Y2B2
r	29	HIS	-	expression tag	UNP G0Y2B2
r	30	HIS	-	expression tag	UNP G0Y2B2
r	31	HIS	-	expression tag	UNP G0Y2B2
r	32	HIS	-	expression tag	UNP G0Y2B2
r	33	HIS	-	expression tag	UNP G0Y2B2
r	34	HIS	-	expression tag	UNP G0Y2B2
r	35	SER	-	expression tag	UNP G0Y2B2
r	36	SER	-	expression tag	UNP G0Y2B2
r	37	GLY	-	expression tag	UNP G0Y2B2
r	38	LEU	-	expression tag	UNP G0Y2B2
r	39	VAL	-	expression tag	UNP G0Y2B2
r	40	PRO	-	expression tag	UNP G0Y2B2
r	41	ARG	-	expression tag	UNP G0Y2B2
r	42	GLY	-	expression tag	UNP G0Y2B2
r	43	SER	-	expression tag	UNP G0Y2B2
r	44	HIS	-	expression tag	UNP G0Y2B2
s	25	MET	-	expression tag	UNP G0Y2B2
s	26	GLY	-	expression tag	UNP G0Y2B2
s	27	SER	-	expression tag	UNP G0Y2B2
s	28	SER	-	expression tag	UNP G0Y2B2
s	29	HIS	-	expression tag	UNP G0Y2B2
s	30	HIS	-	expression tag	UNP G0Y2B2
s	31	HIS	-	expression tag	UNP G0Y2B2
s	32	HIS	-	expression tag	UNP G0Y2B2
s	33	HIS	-	expression tag	UNP G0Y2B2
s	34	HIS	-	expression tag	UNP G0Y2B2
s	35	SER	-	expression tag	UNP G0Y2B2
s	36	SER	-	expression tag	UNP G0Y2B2
s	37	GLY	-	expression tag	UNP G0Y2B2
s	38	LEU	-	expression tag	UNP G0Y2B2
s	39	VAL	-	expression tag	UNP G0Y2B2
s	40	PRO	-	expression tag	UNP G0Y2B2
s	41	ARG	-	expression tag	UNP G0Y2B2
s	42	GLY	-	expression tag	UNP G0Y2B2
s	43	SER	-	expression tag	UNP G0Y2B2
s	44	HIS	-	expression tag	UNP G0Y2B2
t	25	MET	-	expression tag	UNP G0Y2B2
t	26	GLY	-	expression tag	UNP G0Y2B2
t	27	SER	-	expression tag	UNP G0Y2B2
t	28	SER	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
t	29	HIS	-	expression tag	UNP G0Y2B2
t	30	HIS	-	expression tag	UNP G0Y2B2
t	31	HIS	-	expression tag	UNP G0Y2B2
t	32	HIS	-	expression tag	UNP G0Y2B2
t	33	HIS	-	expression tag	UNP G0Y2B2
t	34	HIS	-	expression tag	UNP G0Y2B2
t	35	SER	-	expression tag	UNP G0Y2B2
t	36	SER	-	expression tag	UNP G0Y2B2
t	37	GLY	-	expression tag	UNP G0Y2B2
t	38	LEU	-	expression tag	UNP G0Y2B2
t	39	VAL	-	expression tag	UNP G0Y2B2
t	40	PRO	-	expression tag	UNP G0Y2B2
t	41	ARG	-	expression tag	UNP G0Y2B2
t	42	GLY	-	expression tag	UNP G0Y2B2
t	43	SER	-	expression tag	UNP G0Y2B2
t	44	HIS	-	expression tag	UNP G0Y2B2
u	25	MET	-	expression tag	UNP G0Y2B2
u	26	GLY	-	expression tag	UNP G0Y2B2
u	27	SER	-	expression tag	UNP G0Y2B2
u	28	SER	-	expression tag	UNP G0Y2B2
u	29	HIS	-	expression tag	UNP G0Y2B2
u	30	HIS	-	expression tag	UNP G0Y2B2
u	31	HIS	-	expression tag	UNP G0Y2B2
u	32	HIS	-	expression tag	UNP G0Y2B2
u	33	HIS	-	expression tag	UNP G0Y2B2
u	34	HIS	-	expression tag	UNP G0Y2B2
u	35	SER	-	expression tag	UNP G0Y2B2
u	36	SER	-	expression tag	UNP G0Y2B2
u	37	GLY	-	expression tag	UNP G0Y2B2
u	38	LEU	-	expression tag	UNP G0Y2B2
u	39	VAL	-	expression tag	UNP G0Y2B2
u	40	PRO	-	expression tag	UNP G0Y2B2
u	41	ARG	-	expression tag	UNP G0Y2B2
u	42	GLY	-	expression tag	UNP G0Y2B2
u	43	SER	-	expression tag	UNP G0Y2B2
u	44	HIS	-	expression tag	UNP G0Y2B2
v	25	MET	-	expression tag	UNP G0Y2B2
v	26	GLY	-	expression tag	UNP G0Y2B2
v	27	SER	-	expression tag	UNP G0Y2B2
v	28	SER	-	expression tag	UNP G0Y2B2
v	29	HIS	-	expression tag	UNP G0Y2B2
v	30	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
v	31	HIS	-	expression tag	UNP G0Y2B2
v	32	HIS	-	expression tag	UNP G0Y2B2
v	33	HIS	-	expression tag	UNP G0Y2B2
v	34	HIS	-	expression tag	UNP G0Y2B2
v	35	SER	-	expression tag	UNP G0Y2B2
v	36	SER	-	expression tag	UNP G0Y2B2
v	37	GLY	-	expression tag	UNP G0Y2B2
v	38	LEU	-	expression tag	UNP G0Y2B2
v	39	VAL	-	expression tag	UNP G0Y2B2
v	40	PRO	-	expression tag	UNP G0Y2B2
v	41	ARG	-	expression tag	UNP G0Y2B2
v	42	GLY	-	expression tag	UNP G0Y2B2
v	43	SER	-	expression tag	UNP G0Y2B2
v	44	HIS	-	expression tag	UNP G0Y2B2
w	25	MET	-	expression tag	UNP G0Y2B2
w	26	GLY	-	expression tag	UNP G0Y2B2
w	27	SER	-	expression tag	UNP G0Y2B2
w	28	SER	-	expression tag	UNP G0Y2B2
w	29	HIS	-	expression tag	UNP G0Y2B2
w	30	HIS	-	expression tag	UNP G0Y2B2
w	31	HIS	-	expression tag	UNP G0Y2B2
w	32	HIS	-	expression tag	UNP G0Y2B2
w	33	HIS	-	expression tag	UNP G0Y2B2
w	34	HIS	-	expression tag	UNP G0Y2B2
w	35	SER	-	expression tag	UNP G0Y2B2
w	36	SER	-	expression tag	UNP G0Y2B2
w	37	GLY	-	expression tag	UNP G0Y2B2
w	38	LEU	-	expression tag	UNP G0Y2B2
w	39	VAL	-	expression tag	UNP G0Y2B2
w	40	PRO	-	expression tag	UNP G0Y2B2
w	41	ARG	-	expression tag	UNP G0Y2B2
w	42	GLY	-	expression tag	UNP G0Y2B2
w	43	SER	-	expression tag	UNP G0Y2B2
w	44	HIS	-	expression tag	UNP G0Y2B2
x	25	MET	-	expression tag	UNP G0Y2B2
x	26	GLY	-	expression tag	UNP G0Y2B2
x	27	SER	-	expression tag	UNP G0Y2B2
x	28	SER	-	expression tag	UNP G0Y2B2
x	29	HIS	-	expression tag	UNP G0Y2B2
x	30	HIS	-	expression tag	UNP G0Y2B2
x	31	HIS	-	expression tag	UNP G0Y2B2
x	32	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
x	33	HIS	-	expression tag	UNP G0Y2B2
x	34	HIS	-	expression tag	UNP G0Y2B2
x	35	SER	-	expression tag	UNP G0Y2B2
x	36	SER	-	expression tag	UNP G0Y2B2
x	37	GLY	-	expression tag	UNP G0Y2B2
x	38	LEU	-	expression tag	UNP G0Y2B2
x	39	VAL	-	expression tag	UNP G0Y2B2
x	40	PRO	-	expression tag	UNP G0Y2B2
x	41	ARG	-	expression tag	UNP G0Y2B2
x	42	GLY	-	expression tag	UNP G0Y2B2
x	43	SER	-	expression tag	UNP G0Y2B2
x	44	HIS	-	expression tag	UNP G0Y2B2
y	25	MET	-	expression tag	UNP G0Y2B2
y	26	GLY	-	expression tag	UNP G0Y2B2
y	27	SER	-	expression tag	UNP G0Y2B2
y	28	SER	-	expression tag	UNP G0Y2B2
y	29	HIS	-	expression tag	UNP G0Y2B2
y	30	HIS	-	expression tag	UNP G0Y2B2
y	31	HIS	-	expression tag	UNP G0Y2B2
y	32	HIS	-	expression tag	UNP G0Y2B2
y	33	HIS	-	expression tag	UNP G0Y2B2
y	34	HIS	-	expression tag	UNP G0Y2B2
y	35	SER	-	expression tag	UNP G0Y2B2
y	36	SER	-	expression tag	UNP G0Y2B2
y	37	GLY	-	expression tag	UNP G0Y2B2
y	38	LEU	-	expression tag	UNP G0Y2B2
y	39	VAL	-	expression tag	UNP G0Y2B2
y	40	PRO	-	expression tag	UNP G0Y2B2
y	41	ARG	-	expression tag	UNP G0Y2B2
y	42	GLY	-	expression tag	UNP G0Y2B2
y	43	SER	-	expression tag	UNP G0Y2B2
y	44	HIS	-	expression tag	UNP G0Y2B2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	94	Total O 94 94	0	0
2	B	78	Total O 78 78	0	0
2	C	98	Total O 98 98	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	91	Total 91	O 91	0	0
2	E	107	Total 107	O 107	0	0
2	F	95	Total 95	O 95	0	0
2	G	90	Total 90	O 90	0	0
2	H	52	Total 52	O 52	0	0
2	I	63	Total 63	O 63	0	0
2	J	65	Total 65	O 65	0	0
2	K	75	Total 75	O 75	0	0
2	L	81	Total 81	O 81	0	0
2	M	96	Total 96	O 96	0	0
2	N	83	Total 83	O 83	0	0
2	O	74	Total 74	O 74	0	0
2	P	94	Total 94	O 94	0	0
2	Q	83	Total 83	O 83	0	0
2	R	86	Total 86	O 86	0	0
2	S	87	Total 87	O 87	0	0
2	T	74	Total 74	O 74	0	0
2	U	68	Total 68	O 68	0	0
2	V	53	Total 53	O 53	0	0
2	W	55	Total 55	O 55	0	0
2	X	72	Total 72	O 72	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Y	57	Total O 57 57	0	0
2	Z	63	Total O 63 63	0	0
2	1	66	Total O 66 66	0	0
2	2	79	Total O 79 79	0	0
2	3	98	Total O 98 98	0	0
2	4	96	Total O 96 96	0	0
2	5	92	Total O 92 92	0	0
2	6	104	Total O 104 104	0	0
2	7	88	Total O 88 88	0	0
2	8	91	Total O 91 91	0	0
2	9	91	Total O 91 91	0	0
2	a	90	Total O 90 90	0	0
2	b	63	Total O 63 63	0	0
2	c	50	Total O 50 50	0	0
2	d	69	Total O 69 69	0	0
2	e	76	Total O 76 76	0	0
2	f	78	Total O 78 78	0	0
2	g	70	Total O 70 70	0	0
2	h	80	Total O 80 80	0	0
2	i	81	Total O 81 81	0	0
2	j	69	Total O 69 69	0	0

Continued on next page...

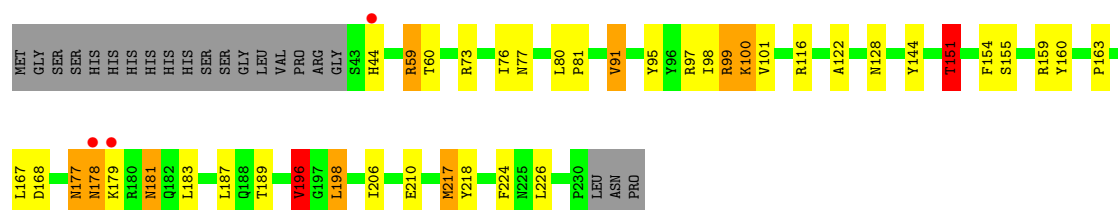
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	k	78	Total 78	O 78	0	0
2	l	81	Total 81	O 81	0	0
2	m	78	Total 78	O 78	0	0
2	n	94	Total 94	O 94	0	0
2	o	79	Total 79	O 79	0	0
2	p	78	Total 78	O 78	0	0
2	q	102	Total 102	O 102	0	0
2	r	74	Total 74	O 74	0	0
2	s	113	Total 113	O 113	0	0
2	t	76	Total 76	O 76	0	0
2	u	93	Total 93	O 93	0	0
2	v	82	Total 82	O 82	0	0
2	w	94	Total 94	O 94	0	0
2	x	81	Total 81	O 81	0	0
2	y	78	Total 78	O 78	0	0

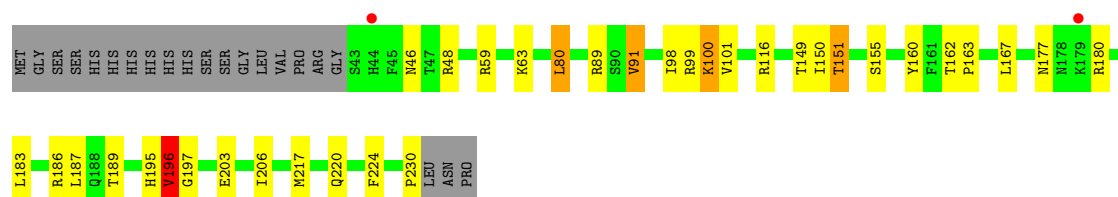
3 Residue-property plots [i](#)

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.

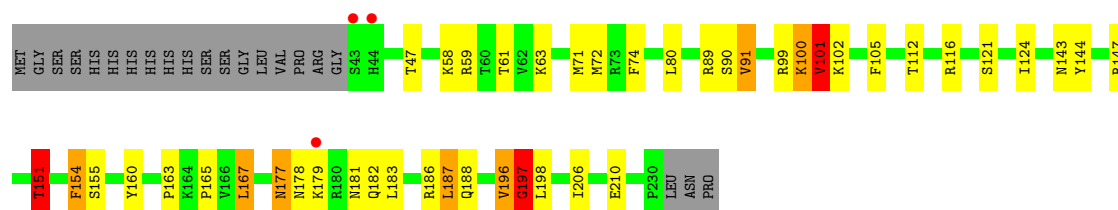
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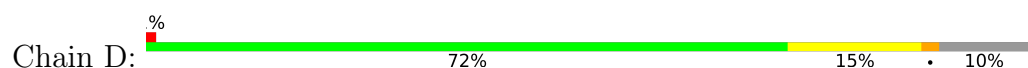
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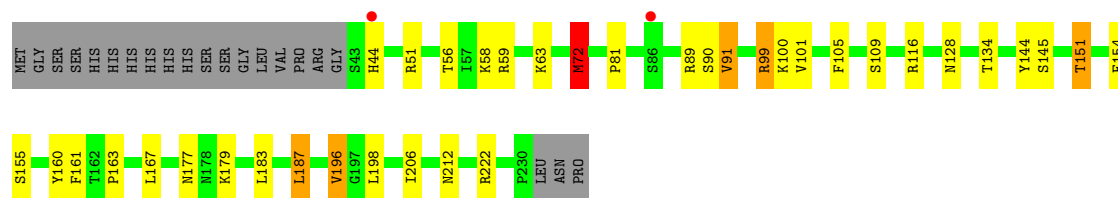


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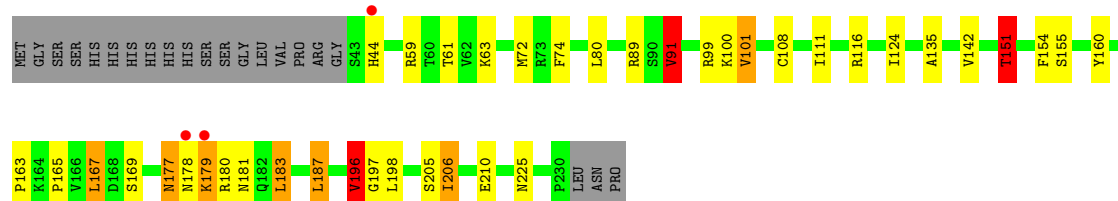


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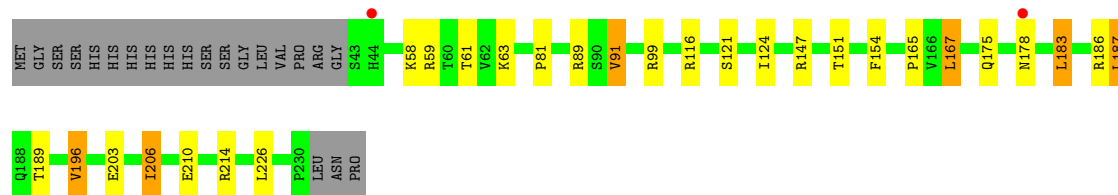
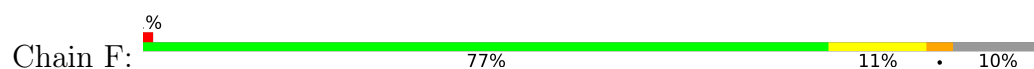




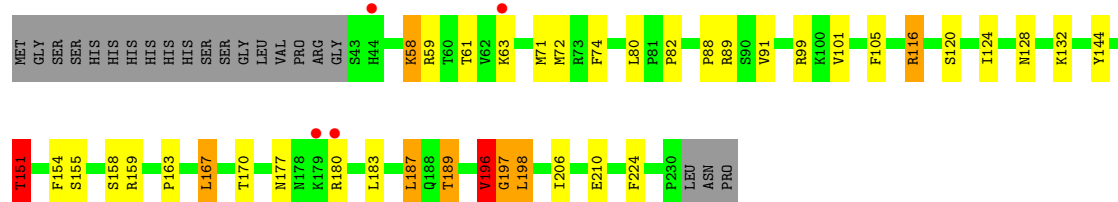
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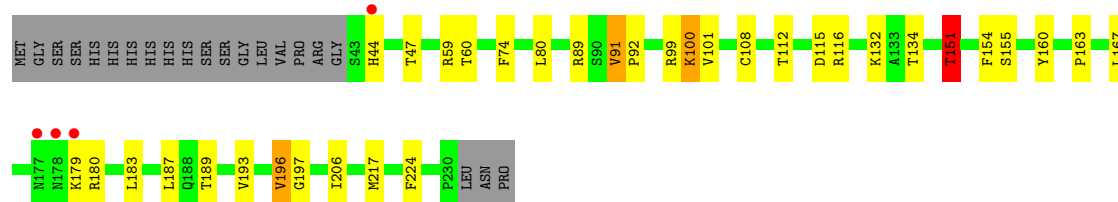
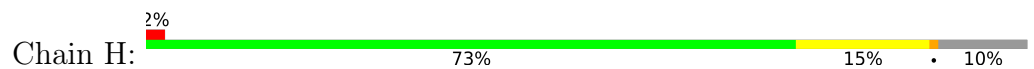
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• Molecule 1: Capsid protein

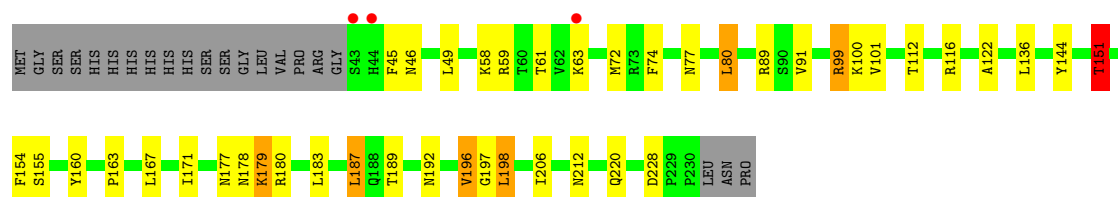


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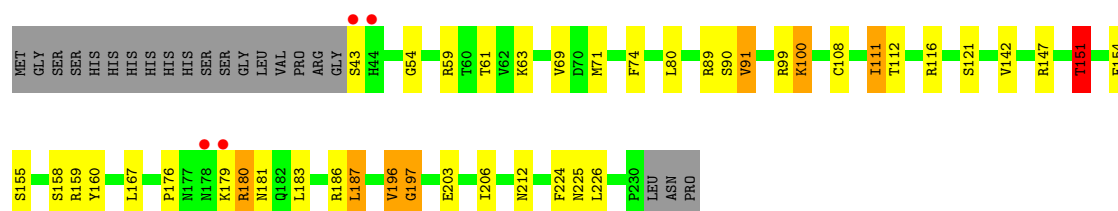
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Chain I: 



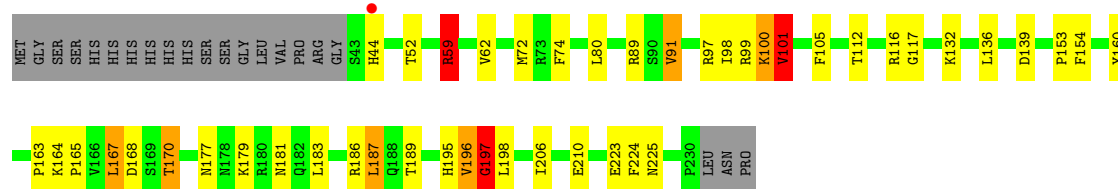
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Chain J: 



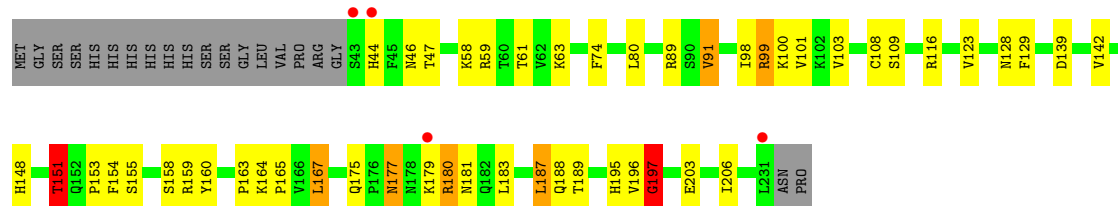
- Molecule 1: Capsid protein

Chain K: 



- Molecule 1: Capsid protein

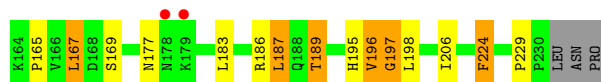
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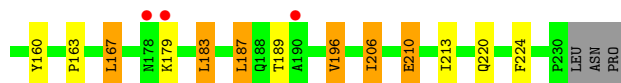
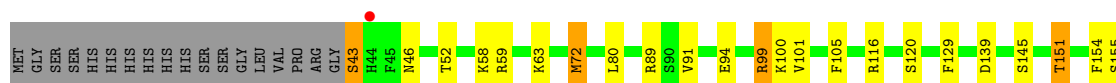
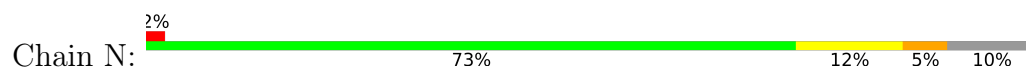
- Molecule 1: Capsid protein

Chain M: 

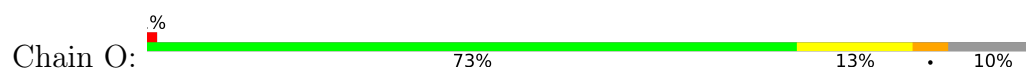




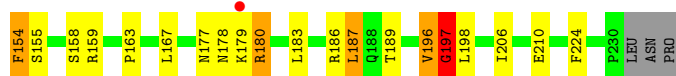
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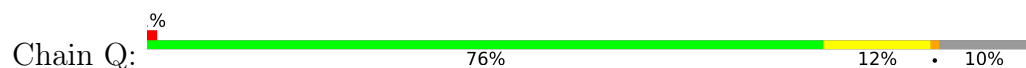
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein

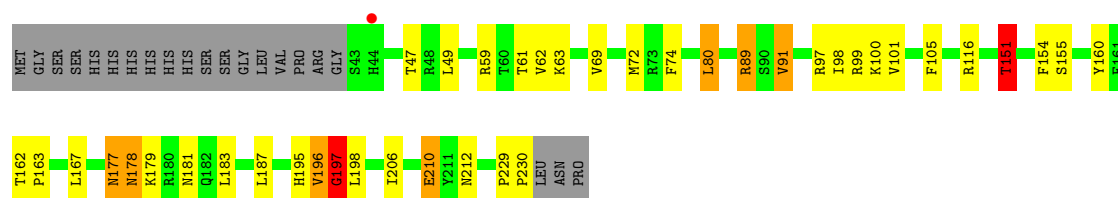


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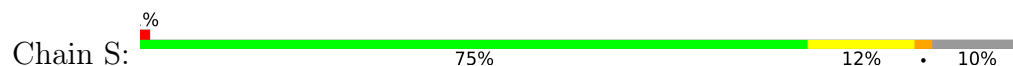


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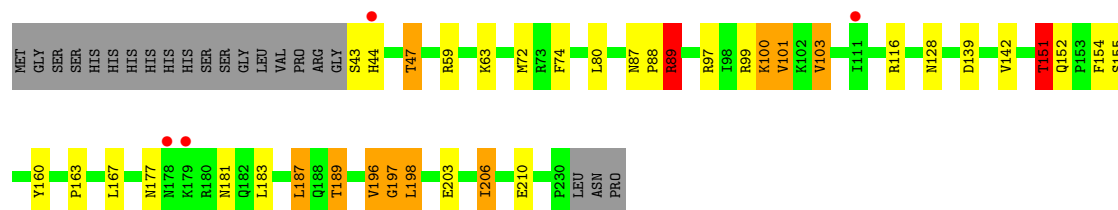




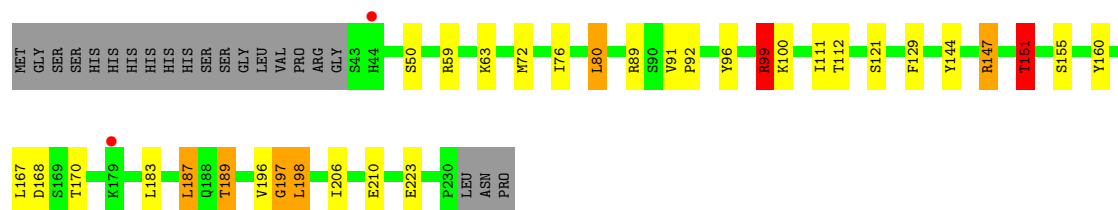
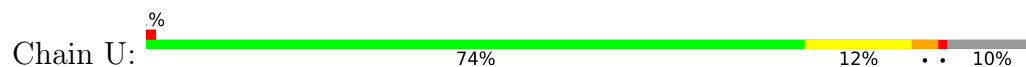
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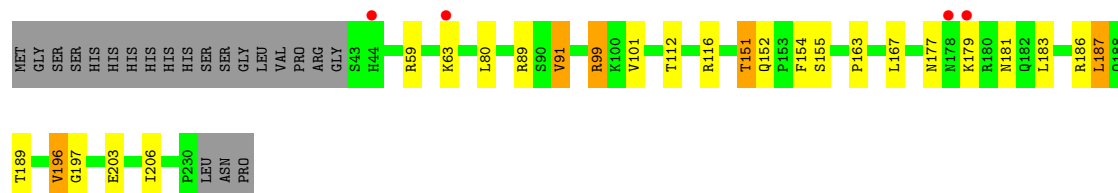
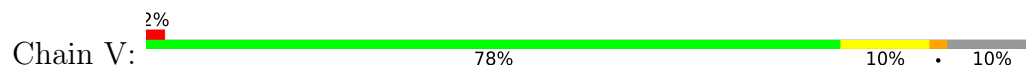
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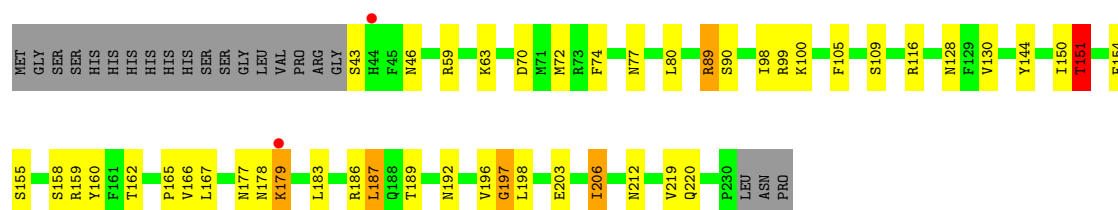
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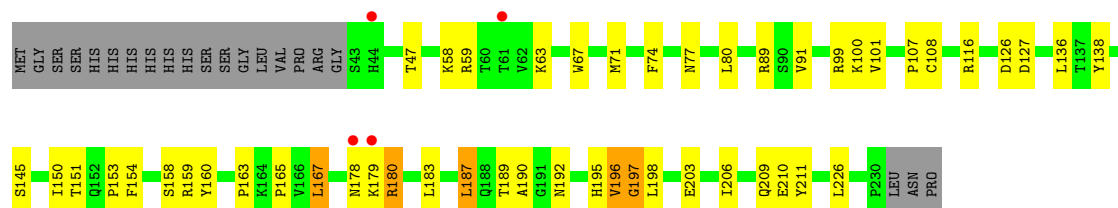
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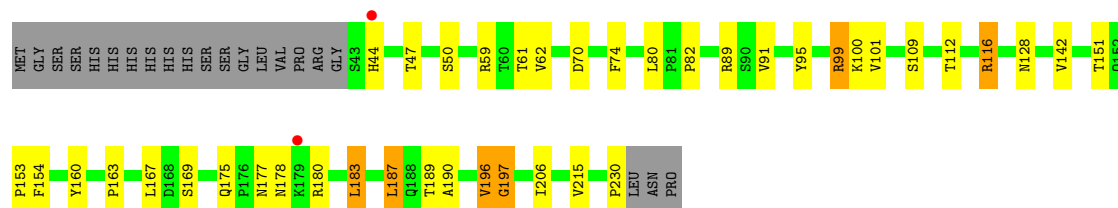
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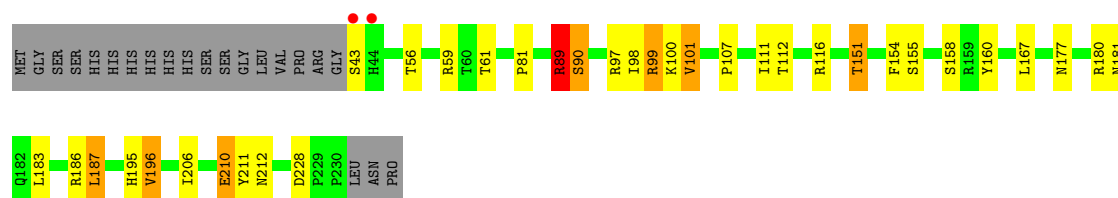
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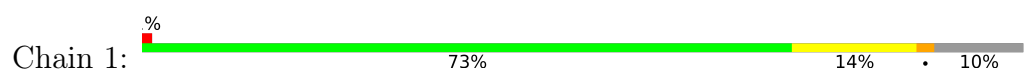
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- Molecule 1: Capsid protein

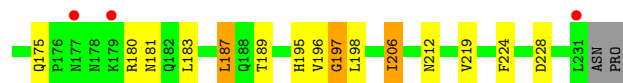
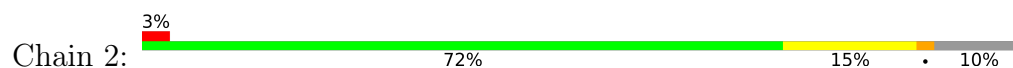


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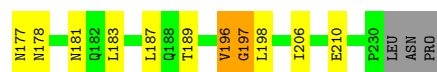
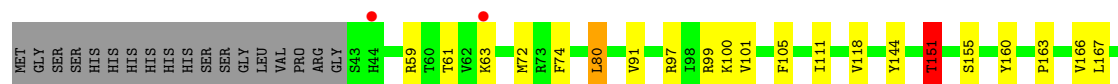
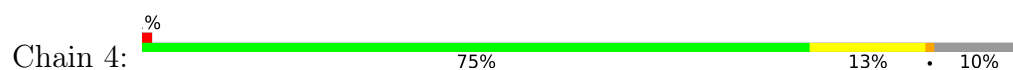
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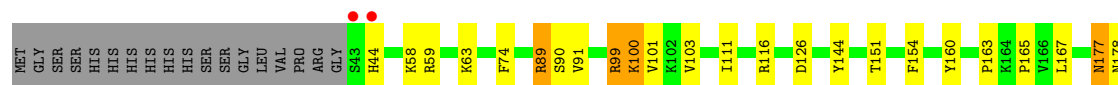
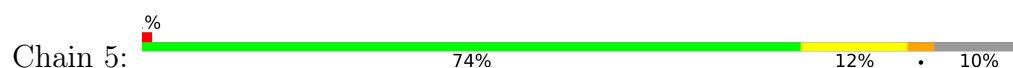
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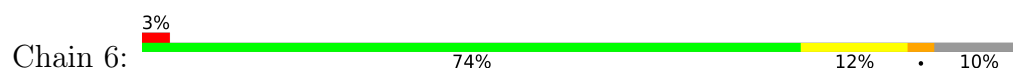
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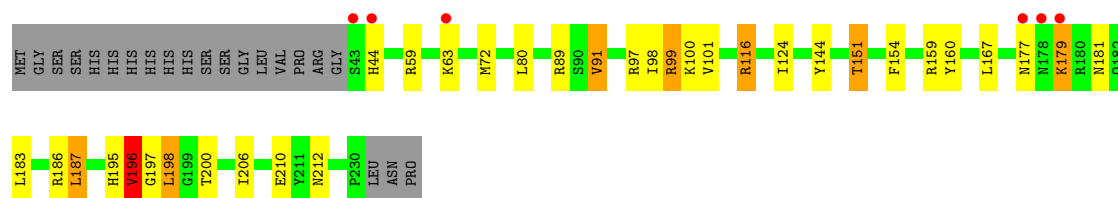


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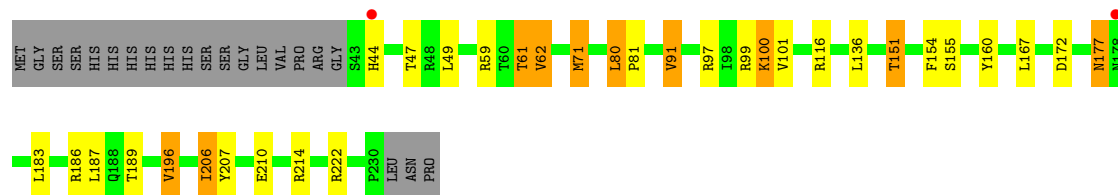
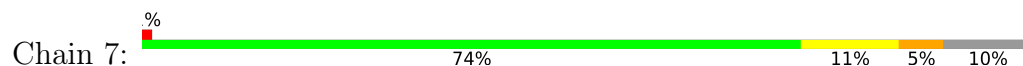


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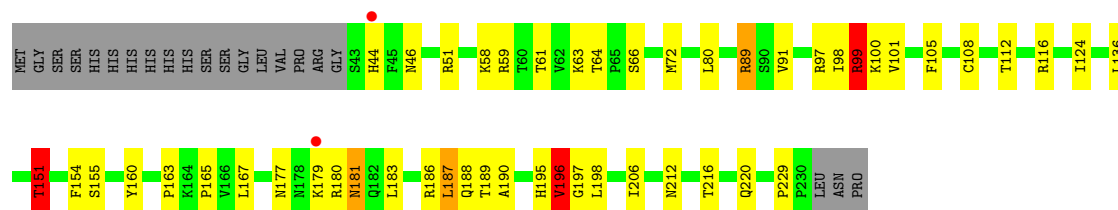




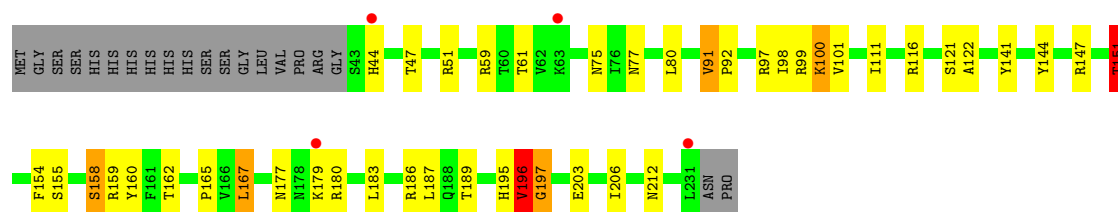
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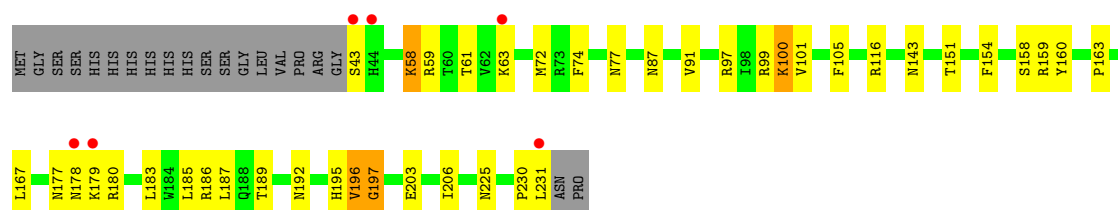
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein

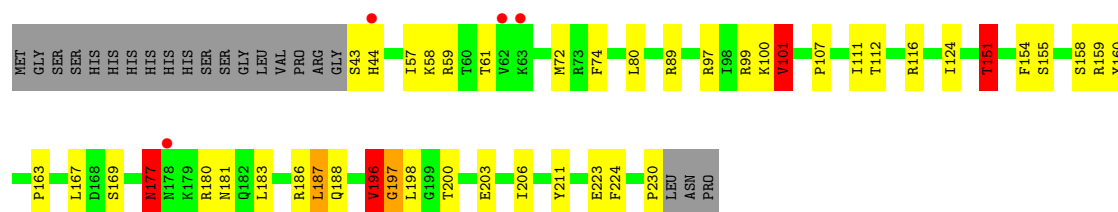


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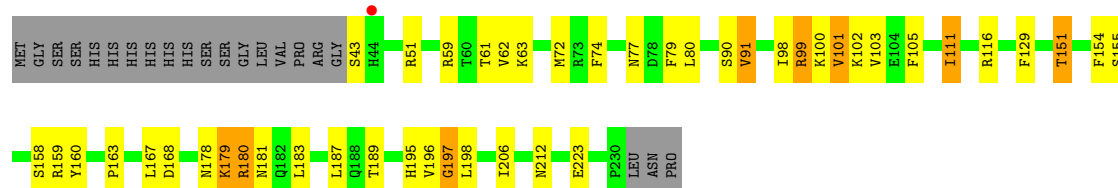
- Molecule 1: Capsid protein

Chain b: 



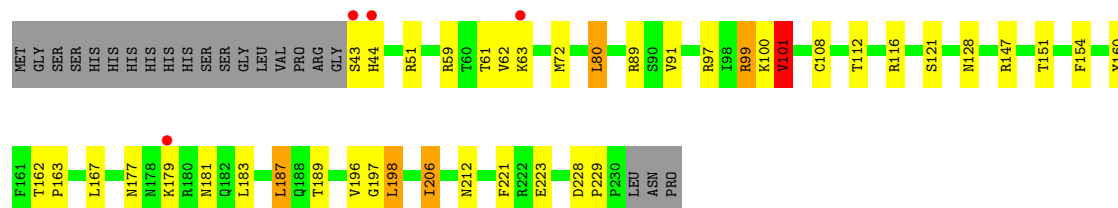
- Molecule 1: Capsid protein

Chain c: 



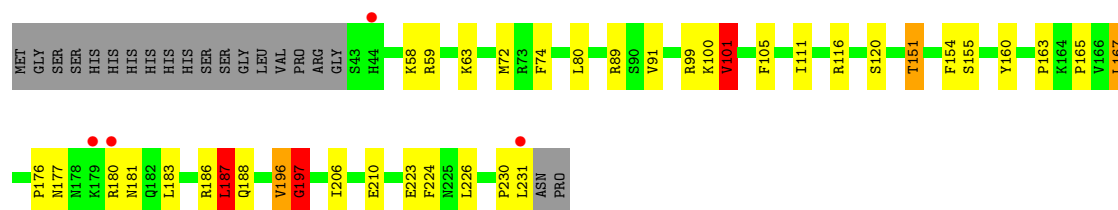
- Molecule 1: Capsid protein

Chain d: 



- Molecule 1: Capsid protein

Chain e: 



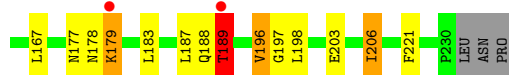
- Molecule 1: Capsid protein

Chain f: 

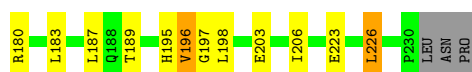
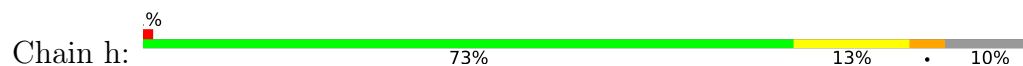




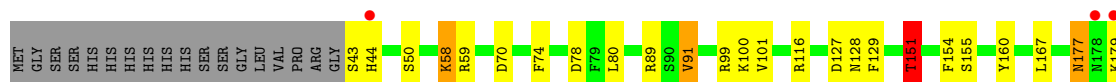
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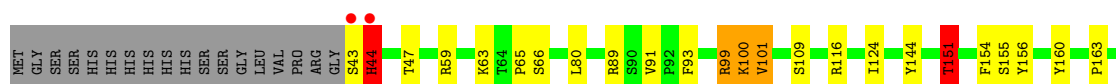
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein

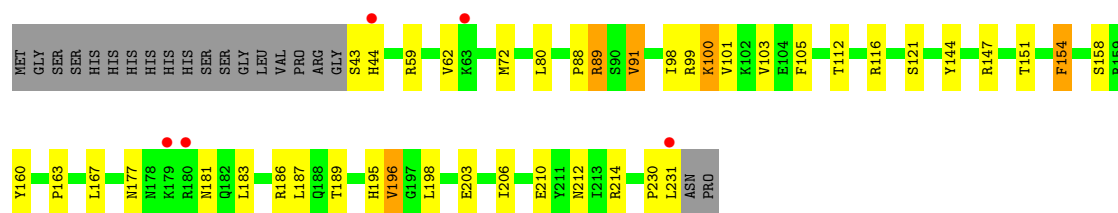


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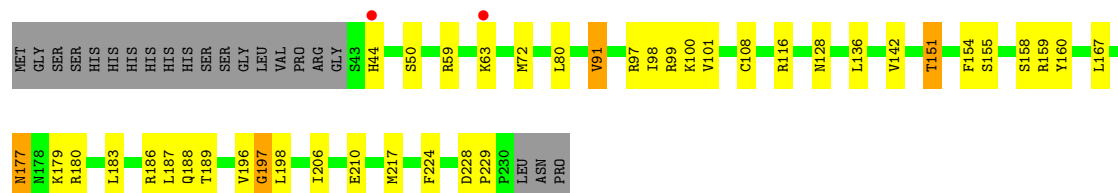


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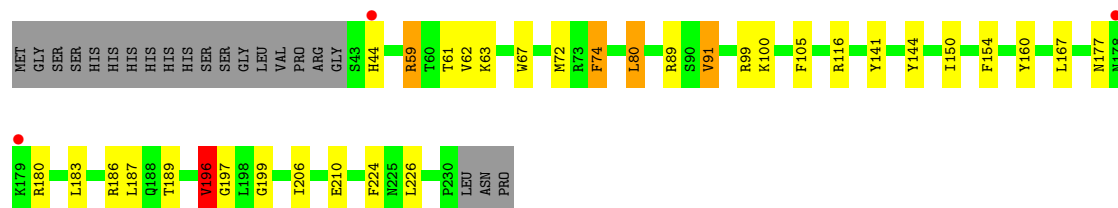
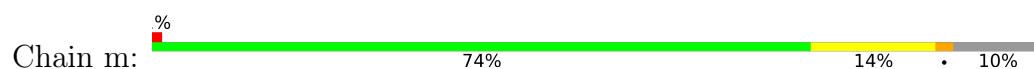




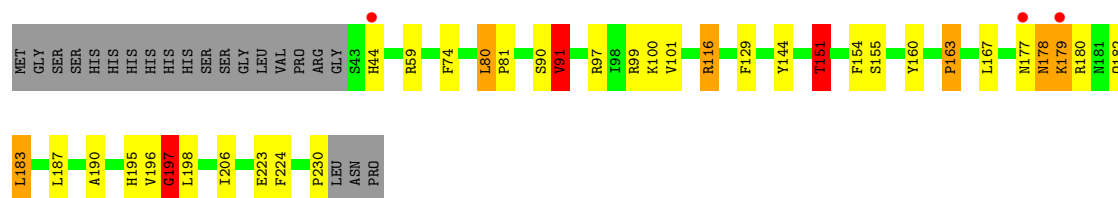
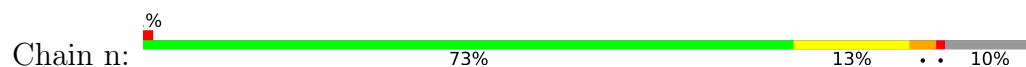
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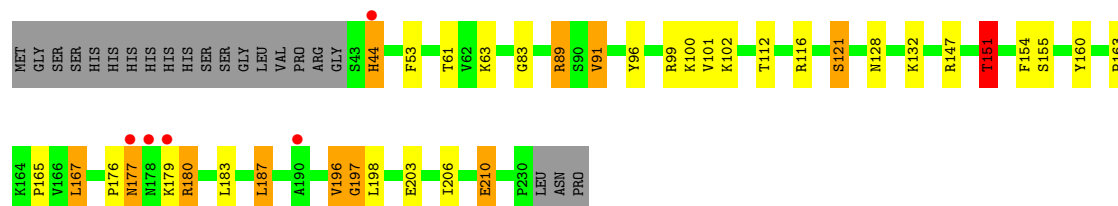
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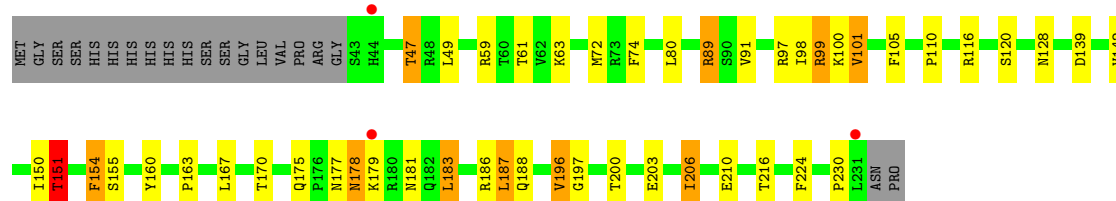
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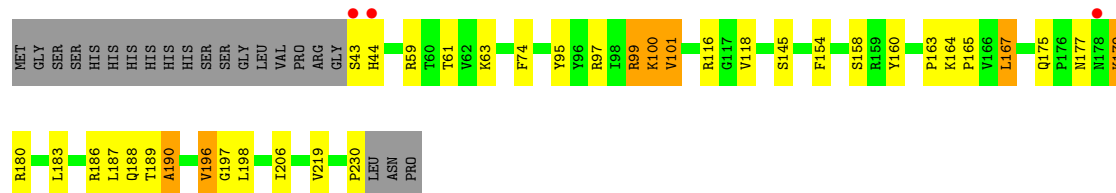
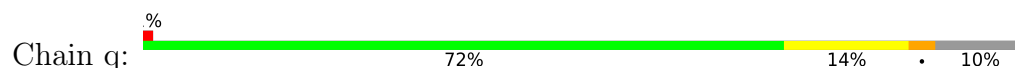
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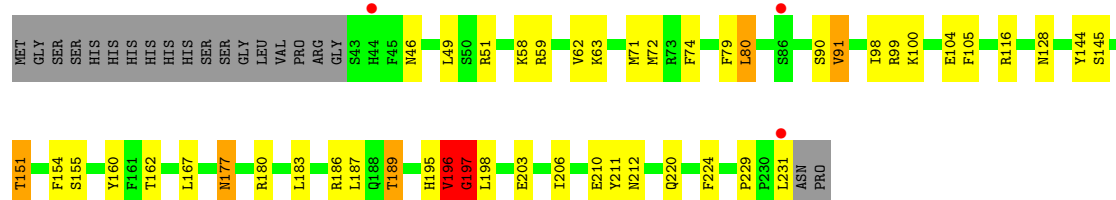
- Molecule 1: Capsid protein



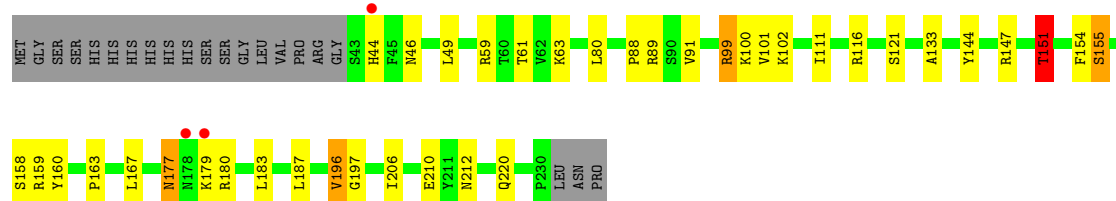
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

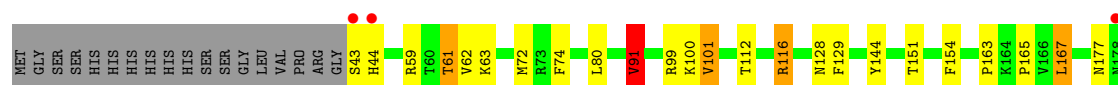
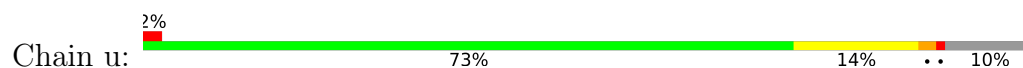


- Molecule 1: Capsid protein

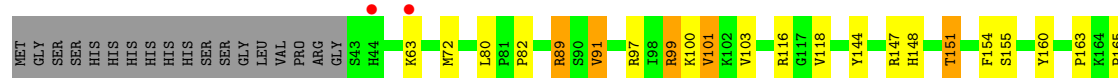




• Molecule 1: Capsid protein



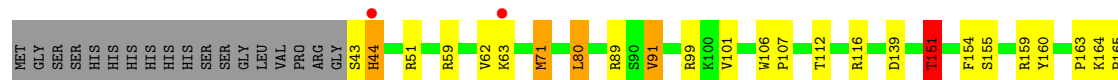
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein

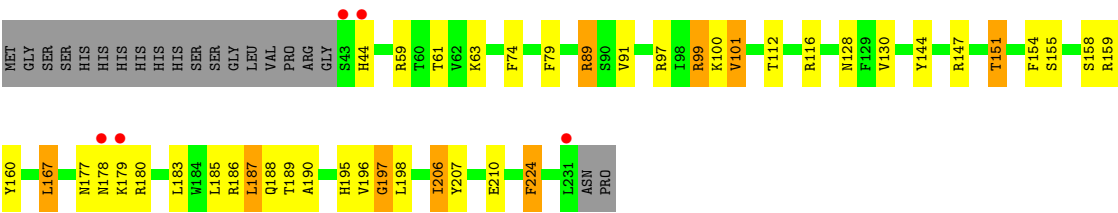


• Molecule 1: Capsid protein



• Molecule 1: Capsid protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	194.12Å 201.88Å 231.28Å 90.00° 90.72° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.80) 99.0 (50.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.163 , 0.224 0.167 , 0.222	Depositor DCC
R_{free} test set	21255 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l 0.000 for k,h,-l 0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	97686	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.36% 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	1.21	4/1594 (0.3%)	1.23	4/2171 (0.2%)
1	2	1.21	2/1602 (0.1%)	1.25	11/2182 (0.5%)
1	3	1.30	4/1594 (0.3%)	1.21	7/2171 (0.3%)
1	4	1.26	3/1594 (0.2%)	1.29	9/2171 (0.4%)
1	5	1.26	6/1594 (0.4%)	1.24	3/2171 (0.1%)
1	6	1.35	6/1594 (0.4%)	1.31	10/2171 (0.5%)
1	7	1.32	4/1594 (0.3%)	1.26	8/2171 (0.4%)
1	8	1.31	8/1594 (0.5%)	1.29	13/2171 (0.6%)
1	9	1.30	3/1602 (0.2%)	1.25	7/2182 (0.3%)
1	A	1.36	8/1594 (0.5%)	1.33	10/2171 (0.5%)
1	B	1.30	6/1594 (0.4%)	1.25	5/2171 (0.2%)
1	C	1.31	4/1594 (0.3%)	1.25	8/2171 (0.4%)
1	D	1.34	3/1594 (0.2%)	1.27	8/2171 (0.4%)
1	E	1.32	7/1594 (0.4%)	1.27	11/2171 (0.5%)
1	F	1.33	1/1594 (0.1%)	1.24	6/2171 (0.3%)
1	G	1.26	4/1594 (0.3%)	1.27	5/2171 (0.2%)
1	H	1.22	2/1594 (0.1%)	1.17	2/2171 (0.1%)
1	I	1.20	1/1594 (0.1%)	1.22	8/2171 (0.4%)
1	J	1.23	2/1594 (0.1%)	1.25	5/2171 (0.2%)
1	K	1.33	10/1594 (0.6%)	1.30	9/2171 (0.4%)
1	L	1.21	7/1602 (0.4%)	1.25	9/2182 (0.4%)
1	M	1.28	2/1594 (0.1%)	1.25	11/2171 (0.5%)
1	N	1.28	2/1594 (0.1%)	1.22	3/2171 (0.1%)
1	O	1.36	7/1594 (0.4%)	1.26	5/2171 (0.2%)
1	P	1.35	7/1594 (0.4%)	1.32	14/2171 (0.6%)
1	Q	1.27	2/1594 (0.1%)	1.24	3/2171 (0.1%)
1	R	1.34	7/1594 (0.4%)	1.32	9/2171 (0.4%)
1	S	1.32	3/1594 (0.2%)	1.19	3/2171 (0.1%)
1	T	1.26	2/1594 (0.1%)	1.30	11/2171 (0.5%)
1	U	1.22	3/1594 (0.2%)	1.23	7/2171 (0.3%)
1	V	1.19	2/1594 (0.1%)	1.19	1/2171 (0.0%)
1	W	1.25	1/1594 (0.1%)	1.22	9/2171 (0.4%)
1	X	1.17	2/1594 (0.1%)	1.17	4/2171 (0.2%)
1	Y	1.21	1/1594 (0.1%)	1.19	4/2171 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Z	1.21	4/1594 (0.3%)	1.20	5/2171 (0.2%)
1	a	1.23	3/1602 (0.2%)	1.21	6/2182 (0.3%)
1	b	1.23	3/1594 (0.2%)	1.25	12/2171 (0.6%)
1	c	1.24	2/1594 (0.1%)	1.19	3/2171 (0.1%)
1	d	1.21	2/1594 (0.1%)	1.22	14/2171 (0.6%)
1	e	1.29	5/1602 (0.3%)	1.24	3/2182 (0.1%)
1	f	1.17	2/1594 (0.1%)	1.18	4/2171 (0.2%)
1	g	1.29	7/1594 (0.4%)	1.21	7/2171 (0.3%)
1	h	1.27	4/1594 (0.3%)	1.25	5/2171 (0.2%)
1	i	1.29	5/1594 (0.3%)	1.23	6/2171 (0.3%)
1	j	1.23	4/1594 (0.3%)	1.19	6/2171 (0.3%)
1	k	1.28	1/1602 (0.1%)	1.25	4/2182 (0.2%)
1	l	1.30	2/1594 (0.1%)	1.23	13/2171 (0.6%)
1	m	1.30	6/1594 (0.4%)	1.19	3/2171 (0.1%)
1	n	1.30	7/1594 (0.4%)	1.27	16/2171 (0.7%)
1	o	1.30	3/1594 (0.2%)	1.30	8/2171 (0.4%)
1	p	1.31	6/1602 (0.4%)	1.27	10/2182 (0.5%)
1	q	1.31	2/1594 (0.1%)	1.26	7/2171 (0.3%)
1	r	1.26	5/1602 (0.3%)	1.24	9/2182 (0.4%)
1	s	1.30	4/1594 (0.3%)	1.22	2/2171 (0.1%)
1	t	1.29	6/1594 (0.4%)	1.26	4/2171 (0.2%)
1	u	1.28	3/1594 (0.2%)	1.25	8/2171 (0.4%)
1	v	1.28	5/1594 (0.3%)	1.23	8/2171 (0.4%)
1	w	1.32	6/1594 (0.4%)	1.24	5/2171 (0.2%)
1	x	1.30	3/1602 (0.2%)	1.27	11/2182 (0.5%)
1	y	1.28	4/1602 (0.2%)	1.26	6/2182 (0.3%)
All	All	1.28	240/95720 (0.3%)	1.24	427/130370 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
1	4	0	1
1	5	0	1
1	6	0	1
1	7	0	1
1	9	0	1
1	A	0	2
1	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
1	F	0	2
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	M	0	1
1	N	0	2
1	O	0	1
1	P	0	1
1	Q	0	1
1	S	0	1
1	T	0	1
1	U	0	1
1	Y	0	1
1	Z	0	1
1	a	0	1
1	b	0	1
1	e	0	1
1	f	0	1
1	g	0	2
1	h	0	1
1	i	0	1
1	k	0	1
1	m	0	1
1	o	0	2
1	p	0	2
1	q	0	3
1	r	0	2
1	s	0	1
1	t	0	1
1	u	0	1
1	v	0	1
1	w	0	1
1	x	0	1
All	All	0	54

All (240) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	189	THR	CA-C	9.40	1.65	1.52
1	g	189	THR	CA-CB	9.32	1.69	1.53
1	E	177	ASN	CA-CB	8.42	1.63	1.53
1	7	81	PRO	CA-C	7.59	1.59	1.52
1	R	196	VAL	C-O	7.53	1.31	1.24
1	T	103	VAL	C-O	-7.50	1.15	1.24
1	5	103	VAL	C-O	-7.46	1.15	1.24
1	P	197	GLY	N-CA	-7.46	1.34	1.45
1	Q	181	ASN	N-CA	7.31	1.55	1.46
1	R	69	VAL	C-O	-7.11	1.16	1.24
1	K	117	GLY	N-CA	7.11	1.52	1.45
1	P	44	HIS	C-O	-7.09	1.15	1.23
1	w	60	THR	CA-C	-6.91	1.44	1.52
1	H	44	HIS	CA-C	-6.88	1.44	1.52
1	P	154	PHE	C-O	-6.83	1.15	1.24
1	9	44	HIS	CA-C	-6.81	1.44	1.52
1	V	179	LYS	CA-C	6.77	1.57	1.52
1	w	177	ASN	CA-CB	6.73	1.62	1.53
1	8	229	PRO	C-O	-6.72	1.19	1.24
1	G	198	LEU	N-CA	6.71	1.54	1.46
1	n	129	PHE	C-O	-6.62	1.15	1.23
1	3	44	HIS	C-O	-6.58	1.16	1.24
1	R	210	GLU	CA-C	6.57	1.61	1.52
1	b	44	HIS	CA-C	-6.55	1.44	1.52
1	U	96	TYR	C-O	-6.50	1.15	1.23
1	K	179	LYS	CA-C	6.47	1.57	1.52
1	u	198	LEU	N-CA	6.45	1.53	1.46
1	8	229	PRO	CA-C	6.44	1.56	1.52
1	r	197	GLY	N-CA	-6.44	1.36	1.45
1	n	163	PRO	N-CA	-6.42	1.40	1.46
1	t	196	VAL	N-CA	-6.40	1.38	1.46
1	Y	190	ALA	N-CA	-6.40	1.38	1.46
1	K	52	THR	C-O	-6.39	1.16	1.24
1	C	177	ASN	CA-CB	6.38	1.60	1.53
1	B	220	GLN	C-O	-6.35	1.16	1.24
1	U	129	PHE	C-O	-6.32	1.15	1.23
1	g	206	ILE	CA-C	6.32	1.61	1.52
1	s	133	ALA	N-CA	6.30	1.53	1.46
1	E	44	HIS	CA-C	-6.29	1.45	1.52
1	C	143	ASN	C-O	6.27	1.32	1.24
1	N	145	SER	C-O	-6.25	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	150	ILE	C-O	-6.23	1.17	1.24
1	9	196	VAL	N-CA	-6.23	1.39	1.46
1	K	44	HIS	CA-C	-6.22	1.45	1.52
1	2	44	HIS	C-O	-6.22	1.17	1.24
1	e	187	LEU	N-CA	6.20	1.54	1.46
1	W	98	ILE	C-O	-6.19	1.17	1.24
1	u	44	HIS	CA-C	-6.18	1.45	1.52
1	g	154	PHE	C-O	-6.17	1.15	1.24
1	8	196	VAL	N-CA	-6.17	1.39	1.46
1	e	230	PRO	N-CA	6.16	1.52	1.46
1	b	200	THR	CA-C	-6.16	1.45	1.52
1	Z	177	ASN	CA-CB	6.16	1.60	1.53
1	t	149	THR	C-O	-6.14	1.16	1.23
1	w	124	ILE	C-O	-6.14	1.16	1.24
1	R	196	VAL	N-CA	-6.12	1.39	1.46
1	q	145	SER	C-O	-6.10	1.16	1.24
1	A	168	ASP	C-O	-6.09	1.17	1.23
1	n	163	PRO	C-O	6.08	1.31	1.23
1	e	101	VAL	C-O	-6.08	1.17	1.24
1	j	172	ASP	CA-C	-6.06	1.46	1.53
1	B	46	ASN	C-O	-6.05	1.16	1.24
1	i	201	ALA	C-O	-6.04	1.16	1.24
1	r	196	VAL	N-CA	-6.04	1.39	1.46
1	4	177	ASN	CA-CB	6.03	1.62	1.53
1	B	150	ILE	C-O	-6.02	1.16	1.24
1	a	87	ASN	N-CA	6.01	1.52	1.46
1	O	220	GLN	C-O	-5.99	1.16	1.24
1	E	177	ASN	CA-C	5.97	1.60	1.52
1	R	229	PRO	C-O	-5.97	1.20	1.25
1	K	100	LYS	CA-C	5.95	1.60	1.52
1	r	177	ASN	CA-CB	5.92	1.63	1.53
1	L	177	ASN	CA-CB	5.90	1.63	1.53
1	p	110	PRO	N-CA	-5.89	1.40	1.46
1	4	178	ASN	N-CA	5.88	1.53	1.46
1	x	198	LEU	CA-C	5.88	1.59	1.52
1	7	47	THR	CA-C	-5.84	1.45	1.53
1	n	177	ASN	CA-CB	5.84	1.60	1.53
1	m	150	ILE	C-O	-5.83	1.17	1.24
1	E	181	ASN	N-CA	5.82	1.53	1.46
1	m	74	PHE	CA-C	-5.81	1.45	1.52
1	u	129	PHE	C-O	-5.80	1.16	1.23
1	m	196	VAL	N-CA	-5.77	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	d	221	PHE	N-CA	5.77	1.52	1.45
1	c	77	ASN	N-CA	5.74	1.53	1.46
1	v	179	LYS	CA-C	5.74	1.60	1.52
1	m	44	HIS	C-O	-5.73	1.17	1.23
1	B	230	PRO	N-CA	5.72	1.55	1.47
1	1	196	VAL	N-CA	-5.72	1.39	1.46
1	6	200	THR	CA-C	-5.71	1.45	1.52
1	p	150	ILE	CA-CB	-5.71	1.47	1.54
1	w	44	HIS	C-O	-5.70	1.17	1.24
1	E	196	VAL	CA-C	-5.70	1.45	1.52
1	i	129	PHE	C-O	-5.70	1.17	1.23
1	2	149	THR	C-O	-5.70	1.17	1.24
1	4	198	LEU	N-CA	5.67	1.53	1.46
1	A	177	ASN	CA-CB	5.66	1.61	1.53
1	8	177	ASN	CA-CB	5.65	1.62	1.53
1	8	44	HIS	CA-C	-5.65	1.45	1.52
1	t	47	THR	C-O	-5.64	1.17	1.23
1	B	149	THR	C-O	-5.64	1.17	1.23
1	g	123	VAL	C-O	5.63	1.30	1.23
1	j	44	HIS	CA-C	5.63	1.58	1.52
1	8	216	THR	CA-C	5.62	1.59	1.52
1	p	154	PHE	C-O	-5.60	1.16	1.24
1	5	44	HIS	CA-C	-5.59	1.45	1.52
1	x	196	VAL	N-CA	-5.59	1.39	1.46
1	1	188	GLN	C-O	5.59	1.30	1.23
1	m	59	ARG	C-O	-5.58	1.17	1.23
1	v	101	VAL	C-O	-5.58	1.18	1.24
1	k	154	PHE	C-O	-5.58	1.16	1.24
1	o	121	SER	N-CA	5.58	1.52	1.45
1	n	81	PRO	CA-C	5.57	1.57	1.52
1	i	78	ASP	C-O	-5.57	1.16	1.24
1	N	129	PHE	C-O	-5.56	1.16	1.23
1	K	132	LYS	C-O	5.56	1.30	1.23
1	A	59	ARG	C-O	-5.55	1.17	1.23
1	r	79	PHE	N-CA	5.54	1.53	1.45
1	A	218	TYR	C-O	-5.54	1.17	1.24
1	7	222	ARG	CA-C	5.53	1.59	1.52
1	Z	158	SER	C-O	-5.52	1.17	1.23
1	Z	158	SER	CA-C	-5.52	1.46	1.52
1	1	195	HIS	CA-C	-5.49	1.46	1.52
1	L	148	HIS	CA-C	5.48	1.59	1.52
1	P	197	GLY	CA-C	-5.48	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	120	SER	CA-C	-5.48	1.45	1.52
1	d	229	PRO	C-O	-5.48	1.20	1.25
1	x	169	SER	CA-C	5.48	1.60	1.52
1	3	196	VAL	N-CA	-5.47	1.40	1.46
1	t	44	HIS	CA-C	-5.46	1.46	1.52
1	O	92	PRO	CA-C	-5.46	1.48	1.53
1	S	44	HIS	N-CA	5.46	1.52	1.46
1	v	177	ASN	CA-C	5.45	1.59	1.52
1	P	151	THR	N-CA	-5.45	1.39	1.46
1	K	197	GLY	N-CA	-5.45	1.37	1.45
1	5	177	ASN	CA-C	5.45	1.60	1.52
1	6	196	VAL	CA-C	-5.44	1.46	1.52
1	g	164	LYS	CA-C	-5.44	1.47	1.52
1	a	225	ASN	N-CA	5.43	1.51	1.46
1	6	196	VAL	N-CA	-5.43	1.40	1.46
1	n	190	ALA	CA-C	-5.43	1.49	1.52
1	M	134	THR	C-O	5.41	1.31	1.24
1	S	160	TYR	C-O	-5.39	1.17	1.23
1	8	165	PRO	N-CA	-5.38	1.40	1.47
1	E	111	ILE	CA-C	5.37	1.60	1.52
1	8	190	ALA	N-CA	-5.37	1.40	1.46
1	l	229	PRO	C-O	-5.37	1.20	1.24
1	D	56	THR	C-O	-5.36	1.17	1.23
1	m	44	HIS	CA-C	-5.35	1.46	1.52
1	V	177	ASN	CA-CB	5.35	1.59	1.53
1	G	82	PRO	CA-C	5.35	1.59	1.52
1	L	123	VAL	C-O	5.34	1.29	1.24
1	L	142	VAL	C-O	-5.34	1.17	1.24
1	U	147	ARG	C-O	-5.34	1.17	1.23
1	P	177	ASN	CA-CB	5.33	1.61	1.53
1	l	44	HIS	C-O	-5.33	1.17	1.24
1	s	155	SER	CA-C	-5.33	1.46	1.52
1	e	197	GLY	CA-C	-5.33	1.44	1.51
1	L	46	ASN	CA-C	-5.33	1.46	1.52
1	T	103	VAL	CA-C	-5.32	1.46	1.52
1	g	221	PHE	C-O	-5.32	1.17	1.23
1	J	69	VAL	C-O	-5.31	1.18	1.24
1	Q	166	VAL	CA-C	-5.31	1.47	1.53
1	s	44	HIS	CA-C	-5.31	1.46	1.52
1	P	112	THR	CA-CB	5.31	1.62	1.53
1	R	91	VAL	C-O	-5.31	1.18	1.24
1	f	149	THR	C-O	-5.31	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	183	LEU	CA-C	5.30	1.59	1.52
1	t	102	LYS	CA-C	-5.30	1.46	1.52
1	F	124	ILE	C-O	-5.30	1.17	1.24
1	q	61	THR	C-O	-5.29	1.16	1.24
1	L	129	PHE	C-O	-5.28	1.17	1.23
1	Z	228	ASP	CA-C	5.28	1.58	1.52
1	w	229	PRO	CA-C	5.28	1.55	1.52
1	O	179	LYS	CA-C	5.28	1.55	1.52
1	S	44	HIS	CA-C	-5.27	1.46	1.52
1	3	188	GLN	C-O	5.27	1.30	1.23
1	7	214	ARG	CZ-NH2	5.27	1.40	1.33
1	I	45	PHE	N-CA	-5.26	1.40	1.46
1	A	77	ASN	C-O	-5.25	1.18	1.24
1	D	222	ARG	C-O	5.25	1.30	1.23
1	5	165	PRO	CA-C	5.25	1.59	1.52
1	i	214	ARG	CZ-NH2	5.24	1.40	1.33
1	v	196	VAL	N-CA	-5.23	1.40	1.46
1	O	216	THR	C-O	-5.23	1.18	1.24
1	o	91	VAL	C-O	-5.22	1.18	1.24
1	6	212	ASN	CA-C	-5.21	1.46	1.52
1	O	170	THR	C-O	-5.21	1.18	1.24
1	K	177	ASN	CA-CB	5.20	1.60	1.53
1	t	148	HIS	N-CA	5.19	1.52	1.46
1	a	185	LEU	CA-C	5.18	1.58	1.52
1	C	154	PHE	C-O	-5.18	1.17	1.24
1	G	132	LYS	CA-C	5.17	1.59	1.52
1	A	98	ILE	C-O	-5.17	1.17	1.23
1	i	58	LYS	C-O	-5.17	1.17	1.23
1	y	130	VAL	C-O	5.17	1.30	1.24
1	K	62	VAL	CA-C	5.16	1.59	1.52
1	X	190	ALA	CA-C	-5.16	1.47	1.52
1	h	63	LYS	CA-CB	5.16	1.61	1.53
1	J	179	LYS	CA-C	5.15	1.59	1.52
1	l	177	ASN	CA-CB	5.14	1.59	1.53
1	H	92	PRO	CA-C	5.14	1.57	1.52
1	B	230	PRO	CA-C	5.13	1.63	1.52
1	M	229	PRO	C-O	-5.12	1.18	1.24
1	A	44	HIS	CA-C	-5.12	1.46	1.52
1	C	182	GLN	C-O	-5.11	1.17	1.24
1	D	91	VAL	CA-C	5.11	1.57	1.52
1	5	177	ASN	CA-CB	5.11	1.60	1.53
1	p	98	ILE	CA-C	-5.11	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	120	SER	C-O	5.10	1.30	1.23
1	v	225	ASN	N-CA	5.10	1.52	1.46
1	y	44	HIS	CA-C	-5.10	1.46	1.52
1	9	122	ALA	CA-C	5.09	1.58	1.52
1	p	170	THR	C-O	-5.09	1.18	1.24
1	j	156	TYR	C-O	-5.09	1.17	1.23
1	6	124	ILE	C-O	-5.09	1.18	1.24
1	s	102	LYS	CA-C	-5.08	1.46	1.52
1	w	197	GLY	CA-C	-5.08	1.44	1.51
1	A	144	TYR	C-O	-5.08	1.17	1.23
1	3	172	ASP	CA-C	-5.07	1.47	1.53
1	h	96	TYR	CA-C	-5.07	1.46	1.52
1	y	190	ALA	CA-C	-5.07	1.48	1.52
1	6	179	LYS	CA-C	5.06	1.56	1.52
1	L	47	THR	C-O	-5.06	1.19	1.24
1	b	198	LEU	N-CA	5.06	1.52	1.46
1	c	129	PHE	C-O	-5.06	1.17	1.23
1	j	93	PHE	C-O	-5.05	1.17	1.23
1	h	48	ARG	N-CA	-5.05	1.39	1.46
1	y	195	HIS	CA-C	-5.05	1.46	1.52
1	O	195	HIS	CA-C	-5.04	1.46	1.52
1	o	197	GLY	N-CA	-5.04	1.38	1.45
1	h	197	GLY	CA-C	-5.04	1.44	1.51
1	p	200	THR	C-O	-5.04	1.18	1.23
1	K	132	LYS	CA-C	5.04	1.59	1.52
1	R	178	ASN	N-CA	5.03	1.52	1.46
1	f	177	ASN	CA-CB	5.03	1.60	1.53
1	n	178	ASN	N-CA	5.02	1.51	1.46
1	5	196	VAL	N-CA	-5.01	1.40	1.46
1	r	145	SER	C-O	-5.01	1.18	1.24
1	O	47	THR	C-O	-5.00	1.18	1.23

All (427) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ASN	N-CA-C	8.70	123.73	113.20
1	4	80	LEU	CA-C-N	-8.41	111.72	120.38
1	4	80	LEU	C-N-CA	-8.41	111.72	120.38
1	K	101	VAL	CB-CA-C	-8.33	98.20	110.62
1	T	89	ARG	NE-CZ-NH2	8.23	126.61	119.20
1	w	189	THR	N-CA-C	-8.19	102.29	111.14
1	L	181	ASN	N-CA-C	8.17	123.09	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	r	198	LEU	N-CA-C	8.10	121.62	108.34
1	o	177	ASN	CB-CA-C	7.98	122.35	109.90
1	P	83	GLY	N-CA-C	-7.91	103.30	112.79
1	8	177	ASN	N-CA-C	-7.86	98.17	109.96
1	6	80	LEU	CA-C-N	-7.84	112.31	120.38
1	6	80	LEU	C-N-CA	-7.84	112.31	120.38
1	e	101	VAL	CB-CA-C	-7.63	99.06	110.82
1	Z	177	ASN	N-CA-C	-7.56	96.95	108.67
1	J	142	VAL	N-CA-C	7.55	118.32	110.62
1	9	151	THR	CB-CA-C	7.50	122.70	109.72
1	E	177	ASN	CB-CA-C	7.50	122.07	110.67
1	1	181	ASN	N-CA-C	7.42	122.33	113.28
1	P	80	LEU	CA-C-N	-7.33	112.83	120.38
1	P	80	LEU	C-N-CA	-7.33	112.83	120.38
1	I	177	ASN	N-CA-C	-7.27	99.05	109.96
1	n	198	LEU	N-CA-C	7.26	121.03	108.76
1	3	198	LEU	N-CA-C	7.23	120.69	108.90
1	L	103	VAL	N-CA-C	-7.16	98.12	108.36
1	L	151	THR	CB-CA-C	7.15	122.09	109.72
1	l	101	VAL	CB-CA-C	-7.11	100.00	110.81
1	A	179	LYS	N-CA-C	7.08	119.14	107.73
1	c	101	VAL	CB-CA-C	-7.04	100.11	110.81
1	Z	177	ASN	CB-CA-C	7.03	122.52	110.77
1	l	198	LEU	N-CA-C	7.01	119.84	108.41
1	b	198	LEU	N-CA-C	7.00	119.88	108.26
1	A	151	THR	CB-CA-C	7.00	121.82	109.72
1	d	228	ASP	CA-C-N	6.99	124.76	119.66
1	d	228	ASP	C-N-CA	6.99	124.76	119.66
1	g	189	THR	CA-CB-OG1	6.99	120.08	109.60
1	8	198	LEU	N-CA-C	6.97	119.78	108.34
1	p	177	ASN	CB-CA-C	6.96	120.18	110.16
1	u	72	MET	CG-SD-CE	-6.95	85.61	100.90
1	j	198	LEU	N-CA-C	6.91	120.19	109.07
1	J	151	THR	CB-CA-C	6.90	121.65	109.72
1	f	151	THR	CB-CA-C	6.88	121.47	110.19
1	I	177	ASN	CB-CA-C	6.86	120.86	109.89
1	d	101	VAL	CB-CA-C	-6.85	99.96	110.50
1	G	198	LEU	N-CA-C	6.84	119.56	108.34
1	3	97	ARG	NE-CZ-NH2	6.82	125.33	119.20
1	E	181	ASN	N-CA-C	6.81	121.29	112.92
1	s	177	ASN	CB-CA-C	6.80	119.95	110.16
1	O	198	LEU	N-CA-C	6.78	119.52	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	151	THR	CB-CA-C	6.77	121.40	110.16
1	t	80	LEU	CA-C-N	-6.75	113.43	120.38
1	t	80	LEU	C-N-CA	-6.75	113.43	120.38
1	a	177	ASN	CB-CA-C	6.72	119.84	110.16
1	9	97	ARG	NE-CZ-NH2	6.72	125.25	119.20
1	g	101	VAL	CB-CA-C	-6.70	100.63	110.81
1	H	151	THR	CB-CA-C	6.68	121.28	109.72
1	L	197	GLY	CA-C-N	-6.68	113.58	122.99
1	L	197	GLY	C-N-CA	-6.68	113.58	122.99
1	b	181	ASN	N-CA-C	6.67	121.43	113.16
1	h	189	THR	N-CA-C	-6.65	104.11	111.36
1	L	44	HIS	N-CA-C	-6.62	97.57	108.76
1	R	91	VAL	CB-CA-C	6.60	118.44	110.85
1	2	219	VAL	CB-CA-C	-6.60	101.68	110.98
1	i	177	ASN	N-CA-C	-6.59	99.91	109.59
1	P	89	ARG	NE-CZ-NH2	6.58	125.12	119.20
1	R	198	LEU	N-CA-C	6.57	119.11	108.34
1	x	159	ARG	NE-CZ-NH2	6.54	125.08	119.20
1	y	97	ARG	NE-CZ-NH2	6.54	125.08	119.20
1	U	99	ARG	N-CA-C	6.50	118.91	111.11
1	E	151	THR	CB-CA-C	6.48	121.56	109.71
1	c	99	ARG	N-CA-C	6.46	118.32	111.28
1	k	198	LEU	N-CA-C	6.46	118.93	108.34
1	2	44	HIS	N-CA-C	-6.44	97.78	108.34
1	r	62	VAL	N-CA-C	-6.44	101.24	109.80
1	T	97	ARG	NE-CZ-NH2	6.43	124.99	119.20
1	S	230	PRO	N-CA-C	6.43	128.17	112.10
1	a	97	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	d	181	ASN	N-CA-C	6.42	121.11	113.28
1	3	97	ARG	NE-CZ-NH1	-6.41	115.09	121.50
1	P	177	ASN	CB-CA-C	6.41	119.39	110.16
1	2	228	ASP	CA-C-N	6.40	124.27	119.66
1	2	228	ASP	C-N-CA	6.40	124.27	119.66
1	c	198	LEU	N-CA-C	6.39	118.93	108.52
1	o	151	THR	CB-CA-C	6.39	120.77	109.72
1	G	151	THR	CB-CA-C	6.39	121.26	109.70
1	8	80	LEU	CA-C-N	-6.36	113.83	120.38
1	8	80	LEU	C-N-CA	-6.36	113.83	120.38
1	x	177	ASN	N-CA-C	-6.36	100.87	110.28
1	T	151	THR	CB-CA-C	6.34	120.58	110.19
1	q	198	LEU	N-CA-C	6.33	118.73	108.41
1	C	101	VAL	CB-CA-C	-6.32	101.21	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	PRO	CA-C-N	-6.31	113.78	120.03
1	A	81	PRO	C-N-CA	-6.31	113.78	120.03
1	R	177	ASN	N-CA-C	-6.30	100.71	110.10
1	R	151	THR	CB-CA-C	6.30	121.24	109.71
1	I	198	LEU	N-CA-C	6.28	118.69	108.26
1	M	177	ASN	N-CA-C	-6.26	100.38	109.59
1	U	80	LEU	CA-C-N	-6.26	113.93	120.38
1	U	80	LEU	C-N-CA	-6.26	113.93	120.38
1	h	198	LEU	N-CA-C	6.26	119.35	108.76
1	x	198	LEU	N-CA-C	6.26	118.62	108.41
1	g	62	VAL	N-CA-C	-6.26	100.70	109.21
1	d	97	ARG	NE-CZ-NH2	6.24	124.82	119.20
1	T	101	VAL	CB-CA-C	-6.23	101.34	110.62
1	7	97	ARG	NE-CZ-NH2	6.22	124.80	119.20
1	I	151	THR	CB-CA-C	6.21	120.47	110.16
1	V	196	VAL	N-CA-C	6.21	118.98	108.86
1	d	177	ASN	CB-CA-C	6.20	119.55	110.26
1	l	197	GLY	CA-C-N	-6.18	114.28	123.00
1	l	197	GLY	C-N-CA	-6.18	114.28	123.00
1	Z	101	VAL	CB-CA-C	-6.18	101.42	110.81
1	6	91	VAL	N-CA-CB	6.17	118.21	111.61
1	U	197	GLY	CA-C-N	-6.15	114.12	122.86
1	U	197	GLY	C-N-CA	-6.15	114.12	122.86
1	p	151	THR	CB-CA-C	6.14	119.88	109.75
1	l	97	ARG	NE-CZ-NH2	6.14	124.72	119.20
1	C	198	LEU	N-CA-C	6.13	118.41	108.41
1	6	198	LEU	N-CA-C	6.12	119.10	108.76
1	1	180	ARG	N-CA-C	6.07	119.52	111.75
1	r	177	ASN	N-CA-C	-6.07	101.05	110.10
1	2	197	GLY	CA-C-N	-6.07	114.43	122.99
1	2	197	GLY	C-N-CA	-6.07	114.43	122.99
1	3	91	VAL	CA-C-O	6.05	123.12	119.19
1	n	97	ARG	NE-CZ-NH2	6.04	124.64	119.20
1	M	80	LEU	CA-C-N	-6.03	114.17	120.38
1	M	80	LEU	C-N-CA	-6.03	114.17	120.38
1	4	198	LEU	N-CA-C	6.02	118.22	108.34
1	j	151	THR	CB-CA-C	6.02	119.68	109.75
1	A	159	ARG	NE-CZ-NH2	6.01	124.61	119.20
1	P	151	THR	N-CA-CB	-6.00	101.14	110.57
1	4	177	ASN	CB-CA-C	5.99	118.78	110.16
1	x	80	LEU	CA-C-N	-5.97	114.23	120.38
1	x	80	LEU	C-N-CA	-5.97	114.23	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	177	ASN	N-CA-C	-5.96	100.56	109.15
1	P	198	LEU	N-CA-C	5.96	118.12	108.34
1	d	198	LEU	N-CA-C	5.96	118.12	108.34
1	b	101	VAL	CB-CA-C	-5.96	101.76	110.81
1	i	177	ASN	CB-CA-C	5.95	119.19	110.26
1	h	101	VAL	CB-CA-C	-5.95	101.77	110.81
1	d	162	THR	CA-C-N	-5.95	114.62	120.98
1	d	162	THR	C-N-CA	-5.95	114.62	120.98
1	u	101	VAL	CB-CA-C	-5.95	101.76	110.62
1	y	89	ARG	NE-CZ-NH2	5.94	124.55	119.20
1	o	53	PHE	N-CA-C	5.92	117.78	108.96
1	P	151	THR	CB-CA-C	5.91	119.95	109.72
1	8	151	THR	CB-CA-C	5.91	119.95	109.72
1	W	206	ILE	CA-CB-CG2	5.91	120.54	110.50
1	O	229	PRO	O-C-N	5.90	123.92	121.15
1	4	181	ASN	N-CA-C	5.90	120.48	113.16
1	T	47	THR	N-CA-C	5.90	116.88	108.74
1	q	219	VAL	CB-CA-C	-5.89	101.84	110.62
1	r	229	PRO	CA-C-N	-5.89	114.67	120.98
1	r	229	PRO	C-N-CA	-5.89	114.67	120.98
1	E	205	SER	CA-C-N	5.89	129.78	120.47
1	E	205	SER	C-N-CA	5.89	129.78	120.47
1	U	151	THR	CB-CA-C	5.88	119.90	109.72
1	o	198	LEU	N-CA-C	5.88	117.99	108.34
1	u	198	LEU	N-CA-C	5.88	117.98	108.34
1	s	151	THR	CB-CA-C	5.88	120.59	109.37
1	r	80	LEU	CA-C-N	-5.87	114.33	120.38
1	r	80	LEU	C-N-CA	-5.87	114.33	120.38
1	E	101	VAL	CB-CA-C	-5.87	101.46	110.50
1	v	89	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	M	177	ASN	CB-CA-C	5.83	119.01	110.26
1	y	224	PHE	N-CA-C	-5.83	101.01	109.59
1	M	198	LEU	N-CA-C	5.83	117.90	108.34
1	Z	89	ARG	NE-CZ-NH2	5.83	124.44	119.20
1	6	181	ASN	CB-CA-C	-5.82	100.00	110.37
1	n	151	THR	CB-CA-C	5.82	119.86	109.38
1	p	47	THR	N-CA-C	5.82	115.79	108.45
1	x	89	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	E	91	VAL	N-CA-CB	5.81	118.59	111.21
1	7	91	VAL	N-CA-CB	5.81	118.59	111.21
1	q	177	ASN	CB-CA-C	5.81	118.53	110.16
1	C	177	ASN	CB-CA-C	5.81	119.50	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	97	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	i	214	ARG	NE-CZ-NH1	-5.80	115.70	121.50
1	W	219	VAL	CB-CA-C	-5.79	101.99	110.62
1	Q	181	ASN	N-CA-C	5.78	120.33	113.16
1	L	180	ARG	N-CA-C	5.78	117.66	111.36
1	7	177	ASN	CB-CA-C	5.77	118.92	110.26
1	n	177	ASN	CB-CA-C	5.77	119.44	110.67
1	8	97	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	h	151	THR	CB-CA-C	5.76	119.72	110.16
1	v	198	LEU	N-CA-C	5.75	117.77	108.34
1	W	166	VAL	CB-CA-C	-5.75	106.78	113.22
1	R	89	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	t	177	ASN	N-CA-C	-5.74	100.89	109.15
1	E	206	ILE	CA-CB-CG2	5.74	120.25	110.50
1	D	90	SER	CA-C-N	-5.73	117.13	123.43
1	D	90	SER	C-N-CA	-5.73	117.13	123.43
1	K	177	ASN	CB-CA-C	5.72	118.85	110.26
1	n	80	LEU	CA-C-N	-5.72	114.48	120.38
1	n	80	LEU	C-N-CA	-5.72	114.48	120.38
1	8	177	ASN	CB-CA-C	5.72	119.05	109.89
1	8	99	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	d	80	LEU	CA-C-N	-5.71	114.50	120.38
1	d	80	LEU	C-N-CA	-5.71	114.50	120.38
1	l	62	VAL	CB-CA-C	-5.71	101.93	111.29
1	o	210	GLU	N-CA-C	-5.71	100.40	109.76
1	G	170	THR	N-CA-C	5.70	118.70	111.69
1	n	91	VAL	CB-CA-C	5.70	116.46	110.37
1	B	196	VAL	N-CA-C	5.69	118.03	108.81
1	T	181	ASN	N-CA-C	5.69	119.85	113.02
1	w	177	ASN	CB-CA-C	5.69	118.80	110.26
1	I	80	LEU	CA-C-N	-5.68	114.53	120.38
1	I	80	LEU	C-N-CA	-5.68	114.53	120.38
1	4	151	THR	CB-CA-C	5.68	119.54	109.72
1	b	80	LEU	CA-C-N	-5.67	114.54	120.38
1	b	80	LEU	C-N-CA	-5.67	114.54	120.38
1	r	177	ASN	CB-CA-C	5.65	118.71	109.90
1	g	80	LEU	CA-C-N	-5.64	114.57	120.38
1	g	80	LEU	C-N-CA	-5.64	114.57	120.38
1	K	225	ASN	N-CA-C	5.63	119.96	112.30
1	Y	116	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	C	197	GLY	N-CA-C	5.63	126.52	113.18
1	4	177	ASN	N-CA-C	-5.63	101.57	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	198	LEU	N-CA-C	5.62	118.03	108.02
1	u	116	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	m	80	LEU	CA-C-N	-5.62	114.60	120.38
1	m	80	LEU	C-N-CA	-5.62	114.60	120.38
1	6	177	ASN	CB-CA-C	5.61	119.25	109.65
1	3	177	ASN	CB-CA-C	5.61	119.03	109.72
1	x	159	ARG	NE-CZ-NH1	-5.60	115.90	121.50
1	D	198	LEU	N-CA-C	5.60	117.53	108.34
1	9	101	VAL	CB-CA-C	-5.60	102.28	110.62
1	l	228	ASP	CA-C-N	5.60	123.69	119.66
1	l	228	ASP	C-N-CA	5.60	123.69	119.66
1	Q	114	GLY	N-CA-C	-5.59	104.60	112.60
1	O	89	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	q	101	VAL	CB-CA-C	-5.58	102.22	110.82
1	Q	198	LEU	N-CA-C	5.58	117.49	108.34
1	B	230	PRO	N-CA-C	5.58	126.04	112.10
1	7	44	HIS	CB-CA-C	-5.57	99.18	109.37
1	f	177	ASN	CB-CA-C	5.56	118.59	110.26
1	2	51	ARG	NE-CZ-NH2	5.55	124.20	119.20
1	K	198	LEU	N-CA-C	5.55	117.45	108.34
1	n	116	ARG	NE-CZ-NH2	5.55	124.20	119.20
1	X	195	HIS	CA-C-N	-5.55	115.23	122.94
1	X	195	HIS	C-N-CA	-5.55	115.23	122.94
1	C	91	VAL	CB-CA-C	5.53	116.39	110.53
1	K	181	ASN	N-CA-C	5.53	120.14	113.17
1	L	197	GLY	N-CA-C	5.52	126.27	113.18
1	l	177	ASN	N-CA-C	-5.52	101.87	110.10
1	n	197	GLY	CA-C-N	-5.52	114.23	122.74
1	n	197	GLY	C-N-CA	-5.52	114.23	122.74
1	2	198	LEU	N-CA-C	5.52	117.89	108.90
1	q	97	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	l	50	SER	N-CA-C	5.51	118.06	109.52
1	W	198	LEU	N-CA-C	5.50	117.87	108.90
1	b	97	ARG	NE-CZ-NH2	5.50	124.16	119.20
1	p	150	ILE	CB-CA-C	-5.50	103.35	110.84
1	w	80	LEU	CA-C-N	-5.50	114.71	120.38
1	w	80	LEU	C-N-CA	-5.50	114.71	120.38
1	x	151	THR	CB-CA-C	5.49	119.19	110.19
1	6	151	THR	CB-CA-C	5.48	119.20	109.72
1	8	64	THR	CA-C-N	5.48	125.49	119.90
1	8	64	THR	C-N-CA	5.48	125.49	119.90
1	t	198	LEU	N-CA-C	5.48	117.33	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	97	ARG	NE-CZ-NH2	5.47	124.13	119.20
1	5	177	ASN	CB-CA-C	5.47	118.47	110.26
1	k	181	ASN	N-CA-C	5.47	119.95	113.16
1	8	97	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	7	97	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	y	177	ASN	CB-CA-C	5.46	118.63	109.89
1	M	197	GLY	N-CA-C	5.46	126.12	113.18
1	m	67	TRP	N-CA-C	5.46	117.99	108.76
1	A	198	LEU	N-CA-C	5.45	117.30	108.41
1	W	151	THR	CB-CA-C	5.45	118.74	109.75
1	x	177	ASN	CB-CA-C	5.44	118.95	109.65
1	3	151	THR	CB-CA-C	5.44	119.13	109.72
1	r	189	THR	CB-CA-C	-5.43	102.32	110.90
1	R	181	ASN	N-CA-C	5.43	119.89	113.16
1	S	151	THR	CB-CA-C	5.42	119.14	109.38
1	y	101	VAL	CB-CA-C	-5.42	102.58	110.81
1	D	177	ASN	CB-CA-C	5.41	118.34	109.90
1	g	151	THR	CB-CA-C	5.41	119.61	109.71
1	2	80	LEU	CA-C-N	-5.41	114.81	120.38
1	2	80	LEU	C-N-CA	-5.41	114.81	120.38
1	F	91	VAL	N-CA-CB	5.40	117.39	111.61
1	K	164	LYS	CA-C-N	-5.40	114.69	120.03
1	K	164	LYS	C-N-CA	-5.40	114.69	120.03
1	e	177	ASN	N-CA-C	-5.39	101.87	109.96
1	b	230	PRO	N-CA-C	5.39	125.57	112.10
1	y	198	LEU	N-CA-C	5.39	117.19	108.41
1	W	130	VAL	N-CA-C	-5.38	101.89	109.21
1	D	81	PRO	N-CA-C	5.38	117.26	110.70
1	B	89	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	D	51	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	1	99	ARG	N-CA-C	5.34	117.10	111.28
1	G	116	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	X	180	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	9	47	THR	N-CA-C	5.33	116.10	108.74
1	R	62	VAL	N-CA-C	-5.33	101.73	108.93
1	v	186	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	b	151	THR	CB-CA-C	5.32	118.99	110.16
1	d	177	ASN	N-CA-C	-5.32	101.77	109.59
1	E	142	VAL	N-CA-C	5.32	117.69	111.05
1	D	134	THR	N-CA-C	5.31	117.07	111.28
1	f	198	LEU	N-CA-C	5.31	117.05	108.34
1	P	120	SER	N-CA-C	5.31	117.46	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	l	189	THR	N-CA-C	-5.31	104.92	111.40
1	p	101	VAL	CB-CA-C	-5.30	102.33	110.50
1	u	219	VAL	CB-CA-C	-5.29	102.76	110.81
1	F	81	PRO	CA-C-N	5.29	126.45	119.84
1	F	81	PRO	C-N-CA	5.29	126.45	119.84
1	O	89	ARG	NE-CZ-NH1	-5.29	116.21	121.50
1	p	97	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	G	58	LYS	N-CA-CB	5.28	118.31	110.29
1	J	181	ASN	N-CA-C	5.27	119.70	113.16
1	T	87	ASN	CA-C-N	-5.27	114.35	120.04
1	T	87	ASN	C-N-CA	-5.27	114.35	120.04
1	2	64	THR	N-CA-C	5.27	117.42	110.36
1	q	44	HIS	CB-CA-C	-5.27	98.99	109.79
1	7	80	LEU	CA-C-N	-5.26	114.96	120.38
1	7	80	LEU	C-N-CA	-5.26	114.96	120.38
1	q	158	SER	N-CA-C	5.26	117.38	109.23
1	d	97	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	e	181	ASN	N-CA-C	5.25	119.79	113.17
1	K	59	ARG	CA-CB-CG	5.25	124.60	114.10
1	9	197	GLY	N-CA-C	5.24	125.60	113.18
1	W	150	ILE	CB-CA-C	-5.24	103.02	110.83
1	b	177	ASN	N-CA-C	-5.24	102.16	109.96
1	P	90	SER	CA-C-N	-5.23	118.23	123.04
1	P	90	SER	C-N-CA	-5.23	118.23	123.04
1	p	206	ILE	CA-CB-CG2	5.23	119.39	110.50
1	9	51	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	a	177	ASN	N-CA-C	-5.23	102.17	109.96
1	C	151	THR	CB-CA-C	5.22	118.77	109.38
1	k	62	VAL	N-CA-C	-5.22	102.86	109.80
1	O	151	THR	CB-CA-C	5.21	118.74	109.72
1	P	91	VAL	CB-CA-C	5.20	116.04	110.53
1	T	142	VAL	N-CA-C	5.20	115.92	110.62
1	n	90	SER	CA-C-N	-5.20	117.71	123.43
1	n	90	SER	C-N-CA	-5.20	117.71	123.43
1	f	101	VAL	CB-CA-C	-5.20	102.88	110.62
1	M	224	PHE	N-CA-C	-5.19	102.17	109.96
1	o	96	TYR	N-CA-C	5.19	116.96	109.07
1	v	97	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	Y	142	VAL	N-CA-C	5.19	116.54	110.62
1	U	198	LEU	N-CA-C	5.19	117.26	108.02
1	p	142	VAL	N-CA-C	5.19	116.53	110.62
1	N	210	GLU	N-CA-C	-5.18	101.82	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	175	GLN	N-CA-C	5.18	116.36	109.93
1	R	97	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	l	142	VAL	N-CA-C	5.18	118.32	111.17
1	o	83	GLY	N-CA-C	-5.18	103.76	112.77
1	h	226	LEU	N-CA-C	5.18	118.30	110.64
1	5	89	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	F	214	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	I	228	ASP	CA-C-N	5.17	123.38	119.66
1	I	228	ASP	C-N-CA	5.17	123.38	119.66
1	Y	177	ASN	N-CA-C	-5.17	102.40	110.10
1	A	210	GLU	CA-CB-CG	5.16	124.43	114.10
1	C	90	SER	CA-C-N	-5.16	118.29	123.04
1	C	90	SER	C-N-CA	-5.16	118.29	123.04
1	d	206	ILE	N-CA-C	-5.16	105.33	112.50
1	n	195	HIS	CA-C-N	-5.16	115.28	122.71
1	n	195	HIS	C-N-CA	-5.16	115.28	122.71
1	j	181	ASN	N-CA-C	5.16	119.56	113.16
1	E	135	ALA	N-CA-C	5.16	118.55	108.18
1	W	165	PRO	CA-C-N	5.16	126.50	121.65
1	W	165	PRO	C-N-CA	5.16	126.50	121.65
1	A	97	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	L	151	THR	N-CA-C	-5.16	100.77	109.07
1	X	196	VAL	CB-CA-C	5.15	118.44	110.50
1	B	80	LEU	CA-C-N	-5.14	115.08	120.38
1	B	80	LEU	C-N-CA	-5.14	115.08	120.38
1	o	177	ASN	N-CA-C	-5.14	102.44	110.10
1	P	51	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	M	97	ARG	NE-CZ-NH2	5.14	123.82	119.20
1	T	206	ILE	CA-CB-CG2	5.13	119.23	110.50
1	6	116	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	i	189	THR	O-C-N	5.13	128.00	122.15
1	u	91	VAL	N-CA-CB	5.13	117.72	111.21
1	M	195	HIS	CA-C-N	-5.13	115.41	122.69
1	M	195	HIS	C-N-CA	-5.13	115.41	122.69
1	9	158	SER	N-CA-C	5.13	116.98	109.24
1	v	204	ASN	N-CA-C	-5.13	103.62	110.55
1	a	195	HIS	CA-C-N	-5.12	115.00	122.58
1	a	195	HIS	C-N-CA	-5.12	115.00	122.58
1	b	57	ILE	N-CA-CB	5.12	116.84	111.00
1	p	178	ASN	N-CA-C	5.12	116.85	109.07
1	5	180	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	Y	177	ASN	CB-CA-C	5.11	117.87	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	159	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	8	181	ASN	N-CA-C	5.11	119.61	113.17
1	v	91	VAL	N-CA-CB	5.11	117.07	111.61
1	A	210	GLU	N-CA-CB	-5.10	102.47	110.69
1	p	181	ASN	N-CA-C	5.10	119.19	112.92
1	x	197	GLY	CA-C-N	-5.10	115.81	123.00
1	x	197	GLY	C-N-CA	-5.10	115.81	123.00
1	F	178	ASN	N-CA-C	5.09	116.36	107.49
1	H	193	VAL	N-CA-C	5.09	115.66	109.30
1	R	197	GLY	N-CA-C	5.09	125.24	113.18
1	v	80	LEU	CA-C-N	-5.09	115.14	120.38
1	v	80	LEU	C-N-CA	-5.09	115.14	120.38
1	8	51	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	P	180	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	n	91	VAL	N-CA-CB	5.08	117.04	111.61
1	T	198	LEU	N-CA-C	5.08	117.05	108.02
1	l	91	VAL	CB-CA-C	5.08	116.69	110.85
1	J	54	GLY	N-CA-C	5.07	118.68	112.14
1	b	97	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	l	177	ASN	CB-CA-C	5.07	117.81	109.90
1	Z	97	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	N	206	ILE	CA-CB-CG2	5.07	119.11	110.50
1	S	226	LEU	N-CA-C	5.06	117.89	110.30
1	j	80	LEU	CA-C-N	-5.06	115.17	120.38
1	j	80	LEU	C-N-CA	-5.06	115.17	120.38
1	F	206	ILE	CA-CB-CG2	5.05	119.09	110.50
1	i	127	ASP	N-CA-CB	-5.05	104.62	112.30
1	w	180	ARG	N-CA-C	5.05	118.91	112.34
1	K	97	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	b	180	ARG	N-CA-C	5.04	118.21	111.75
1	k	89	ARG	CG-CD-NE	5.04	123.10	112.00
1	n	177	ASN	N-CA-C	-5.03	101.90	109.15
1	J	180	ARG	N-CA-C	5.03	117.50	111.71
1	6	97	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	i	151	THR	CB-CA-C	5.03	118.05	109.75
1	3	50	SER	N-CA-C	5.03	117.31	109.52
1	u	197	GLY	CA-C-N	-5.03	115.68	122.77
1	u	197	GLY	C-N-CA	-5.03	115.68	122.77
1	D	72	MET	CG-SD-CE	-5.02	89.85	100.90
1	N	72	MET	CG-SD-CE	-5.00	89.89	100.90
1	7	214	ARG	NE-CZ-NH1	-5.00	116.50	121.50
1	4	166	VAL	CB-CA-C	-5.00	106.98	112.68

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	196	VAL	Peptide
1	4	196	VAL	Peptide
1	5	196	VAL	Peptide
1	6	196	VAL	Peptide
1	7	196	VAL	Peptide
1	9	196	VAL	Peptide
1	A	177	ASN	Peptide
1	A	196	VAL	Peptide
1	B	196	VAL	Peptide
1	D	196	VAL	Peptide
1	E	196	VAL	Peptide
1	F	189	THR	Peptide
1	F	196	VAL	Peptide
1	G	196	VAL	Peptide
1	H	196	VAL	Peptide
1	I	196	VAL	Peptide
1	J	196	VAL	Peptide
1	K	196	VAL	Peptide
1	M	196	VAL	Peptide
1	N	189	THR	Peptide
1	N	196	VAL	Peptide
1	O	196	VAL	Peptide
1	P	196	VAL	Peptide
1	Q	196	VAL	Peptide
1	S	196	VAL	Peptide
1	T	196	VAL	Peptide
1	U	189	THR	Peptide
1	Y	196	VAL	Peptide
1	Z	196	VAL	Peptide
1	a	196	VAL	Peptide
1	b	196	VAL	Peptide
1	e	196	VAL	Peptide
1	f	196	VAL	Peptide
1	g	188	GLN	Peptide
1	g	196	VAL	Peptide
1	h	196	VAL	Peptide
1	i	196	VAL	Peptide
1	k	196	VAL	Peptide
1	m	196	VAL	Peptide
1	o	196	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	o	61	THR	Peptide
1	p	196	VAL	Peptide
1	p	230	PRO	Peptide
1	q	190	ALA	Peptide
1	q	196	VAL	Peptide
1	q	43	SER	Peptide
1	r	196	VAL	Peptide
1	r	211	TYR	Peptide
1	s	196	VAL	Peptide
1	t	196	VAL	Peptide
1	u	196	VAL	Peptide
1	v	196	VAL	Peptide
1	w	196	VAL	Peptide
1	x	196	VAL	Peptide

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	1546	0	1490	14	0
1	2	1554	0	1501	16	0
1	3	1546	0	1490	14	0
1	4	1546	0	1490	8	0
1	5	1546	0	1490	12	0
1	6	1546	0	1490	16	0
1	7	1546	0	1490	16	0
1	8	1546	0	1490	19	0
1	9	1554	0	1501	18	0
1	A	1546	0	1490	17	0
1	B	1546	0	1490	15	0
1	C	1546	0	1490	20	0
1	D	1546	0	1490	14	0
1	E	1546	0	1490	18	0
1	F	1546	0	1490	10	0
1	G	1546	0	1490	19	0
1	H	1546	0	1490	14	0
1	I	1546	0	1490	20	0
1	J	1546	0	1490	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1546	0	1490	22	0
1	L	1554	0	1501	20	0
1	M	1546	0	1490	20	0
1	N	1546	0	1490	19	0
1	O	1546	0	1490	10	0
1	P	1546	0	1490	19	0
1	Q	1546	0	1490	11	0
1	R	1546	0	1490	15	0
1	S	1546	0	1490	17	0
1	T	1546	0	1490	19	0
1	U	1546	0	1490	12	0
1	V	1546	0	1490	13	0
1	W	1546	0	1490	21	0
1	X	1546	0	1490	19	0
1	Y	1546	0	1490	13	0
1	Z	1546	0	1490	16	0
1	a	1554	0	1501	15	0
1	b	1546	0	1490	18	0
1	c	1546	0	1490	20	0
1	d	1546	0	1490	16	0
1	e	1554	0	1501	14	0
1	f	1546	0	1490	16	0
1	g	1546	0	1490	16	0
1	h	1546	0	1490	14	0
1	i	1546	0	1490	13	0
1	j	1546	0	1490	14	0
1	k	1554	0	1501	17	0
1	l	1546	0	1490	13	0
1	m	1546	0	1490	12	0
1	n	1546	0	1490	14	0
1	o	1546	0	1490	18	0
1	p	1554	0	1501	22	0
1	q	1546	0	1490	12	0
1	r	1554	0	1501	23	0
1	s	1546	0	1490	15	0
1	t	1546	0	1490	18	0
1	u	1546	0	1490	14	0
1	v	1546	0	1490	20	0
1	w	1546	0	1490	20	0
1	x	1554	0	1501	23	0
1	y	1554	0	1501	19	0
2	1	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	79	0	0	3	0
2	3	98	0	0	1	0
2	4	96	0	0	0	0
2	5	92	0	0	1	0
2	6	104	0	0	4	1
2	7	88	0	0	4	0
2	8	91	0	0	2	0
2	9	91	0	0	2	0
2	A	94	0	0	2	0
2	B	78	0	0	1	0
2	C	98	0	0	2	0
2	D	91	0	0	3	0
2	E	107	0	0	2	0
2	F	95	0	0	1	0
2	G	90	0	0	1	0
2	H	52	0	0	0	0
2	I	63	0	0	0	0
2	J	65	0	0	0	0
2	K	75	0	0	4	0
2	L	81	0	0	2	0
2	M	96	0	0	3	0
2	N	83	0	0	2	0
2	O	74	0	0	1	0
2	P	94	0	0	3	0
2	Q	83	0	0	4	0
2	R	86	0	0	1	0
2	S	87	0	0	2	0
2	T	74	0	0	4	0
2	U	68	0	0	2	0
2	V	53	0	0	2	0
2	W	55	0	0	2	0
2	X	72	0	0	2	0
2	Y	57	0	0	1	0
2	Z	63	0	0	0	0
2	a	90	0	0	2	0
2	b	63	0	0	1	0
2	c	50	0	0	1	0
2	d	69	0	0	2	0
2	e	76	0	0	1	0
2	f	78	0	0	1	0
2	g	70	0	0	5	0
2	h	80	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	i	81	0	0	3	0
2	j	69	0	0	4	0
2	k	78	0	0	2	0
2	l	81	0	0	0	0
2	m	78	0	0	1	0
2	n	94	0	0	2	0
2	o	79	0	0	4	0
2	p	78	0	0	0	0
2	q	102	0	0	2	1
2	r	74	0	0	3	0
2	s	113	0	0	1	0
2	t	76	0	0	1	0
2	u	93	0	0	3	0
2	v	82	0	0	2	0
2	w	94	0	0	5	0
2	x	81	0	0	6	0
2	y	78	0	0	2	0
All	All	97686	0	89510	872	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (872) 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:g:44:HIS:HB3	2:g:358:HOH:O	1.46	1.12
1:6:101:VAL:HB	2:6:371:HOH:O	1.47	1.11
1:x:44:HIS:HB2	2:x:371:HOH:O	1.49	1.09
1:i:101:VAL:HB	2:i:343:HOH:O	1.55	1.06
1:M:101:VAL:HB	2:M:367:HOH:O	1.56	1.05
1:g:189:THR:HA	2:g:303:HOH:O	1.57	1.04
1:L:101:VAL:HB	2:L:362:HOH:O	1.59	1.03
1:6:44:HIS:HB3	2:6:303:HOH:O	1.69	0.92
1:g:177:ASN:OD1	2:g:301:HOH:O	1.88	0.92
1:i:177:ASN:HB3	2:i:355:HOH:O	1.69	0.92
1:y:151:THR:HG22	1:y:155:SER:HB2	1.53	0.90
1:D:101:VAL:HB	2:D:370:HOH:O	1.72	0.90
1:w:44:HIS:CB	2:w:355:HOH:O	2.19	0.89
1:1:89:ARG:HD2	1:1:187:LEU:HD13	1.56	0.87
1:f:180:ARG:NH2	2:f:301:HOH:O	2.14	0.81
1:X:145:SER:HG	1:g:43:SER:N	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:177:ASN:OD1	2:G:301:HOH:O	1.99	0.80
1:c:151:THR:HG22	1:c:155:SER:HB2	1.63	0.80
1:E:80:LEU:HD11	1:E:91:VAL:HG13	1.63	0.79
1:r:151:THR:HG22	1:r:155:SER:HB2	1.64	0.79
1:D:145:SER:HG	1:M:43:SER:N	1.80	0.79
1:E:210:GLU:HB2	2:E:325:HOH:O	1.82	0.78
1:B:101:VAL:HB	2:B:351:HOH:O	1.84	0.78
1:w:44:HIS:CA	2:w:355:HOH:O	2.32	0.77
1:o:44:HIS:HB3	2:o:364:HOH:O	1.84	0.77
1:7:177:ASN:HB3	2:7:371:HOH:O	1.83	0.76
1:T:177:ASN:HB3	2:T:334:HOH:O	1.84	0.76
1:k:100:LYS:HG2	1:k:160:TYR:CZ	2.21	0.75
1:3:230:PRO:C	2:3:307:HOH:O	2.30	0.74
1:y:151:THR:HG22	1:y:155:SER:CB	2.17	0.74
1:7:151:THR:HG22	1:7:155:SER:CB	2.19	0.73
1:j:44:HIS:CB	2:j:330:HOH:O	2.35	0.73
1:k:177:ASN:HB3	2:k:323:HOH:O	1.88	0.73
1:Q:89:ARG:HD2	1:Q:187:LEU:HD13	1.71	0.72
1:K:59:ARG:NE	2:K:301:HOH:O	2.21	0.72
1:S:177:ASN:OD1	2:S:301:HOH:O	2.06	0.72
1:O:151:THR:HG22	1:O:155:SER:HB2	1.73	0.71
1:7:151:THR:HG22	1:7:155:SER:OG	1.91	0.71
1:8:151:THR:HG22	1:8:155:SER:HB2	1.72	0.70
1:b:100:LYS:HG2	1:b:160:TYR:CZ	2.26	0.70
1:P:151:THR:HG22	1:P:155:SER:HB2	1.73	0.70
1:L:151:THR:HG22	1:L:155:SER:HB2	1.74	0.70
1:n:230:PRO:C	2:n:333:HOH:O	2.34	0.70
1:K:89:ARG:HD2	1:K:187:LEU:HD13	1.74	0.69
1:v:89:ARG:HD2	1:v:187:LEU:HD13	1.73	0.69
1:3:151:THR:HG22	1:3:155:SER:HB2	1.72	0.69
1:9:151:THR:HG22	1:9:155:SER:HB2	1.74	0.69
1:A:101:VAL:HB	2:A:303:HOH:O	1.93	0.69
1:P:80:LEU:HD11	1:P:91:VAL:HG13	1.74	0.68
1:D:89:ARG:HD2	1:D:187:LEU:HD13	1.74	0.68
1:g:116:ARG:HD3	1:g:154:PHE:CE2	2.28	0.68
1:j:44:HIS:HB2	2:j:330:HOH:O	1.92	0.68
1:Q:210:GLU:HB2	2:Q:378:HOH:O	1.94	0.67
1:5:177:ASN:HB3	2:5:370:HOH:O	1.93	0.67
1:I:151:THR:HG22	1:I:155:SER:CB	2.25	0.67
1:K:59:ARG:CD	2:K:301:HOH:O	2.43	0.67
1:3:151:THR:HG22	1:3:155:SER:CB	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:151:THR:HG22	1:9:155:SER:CB	2.24	0.67
1:u:116:ARG:HD2	2:u:328:HOH:O	1.95	0.67
1:e:186:ARG:NH1	1:e:188:GLN:HG2	2.10	0.66
1:4:151:THR:HG22	1:4:155:SER:CB	2.25	0.66
1:S:100:LYS:HG2	1:S:160:TYR:CZ	2.31	0.66
1:5:116:ARG:HD3	1:5:154:PHE:CE2	2.30	0.66
1:x:44:HIS:CB	2:x:371:HOH:O	2.21	0.66
1:H:151:THR:HG22	1:H:155:SER:CB	2.25	0.66
1:T:100:LYS:HG2	1:T:160:TYR:CZ	2.31	0.66
1:J:151:THR:HG22	1:J:155:SER:HB2	1.78	0.65
1:h:101:VAL:HG23	1:h:163:PRO:HG3	1.76	0.65
1:Y:116:ARG:HD3	1:Y:154:PHE:CE2	2.31	0.65
1:8:151:THR:HG22	1:8:155:SER:CB	2.25	0.65
1:w:210:GLU:HB2	2:w:387:HOH:O	1.96	0.65
1:6:100:LYS:HG2	1:6:160:TYR:CZ	2.31	0.65
1:r:151:THR:HG22	1:r:155:SER:CB	2.26	0.65
1:Y:116:ARG:HD3	1:Y:154:PHE:HE2	1.61	0.65
1:4:151:THR:HG22	1:4:155:SER:HB2	1.78	0.65
1:N:89:ARG:HD2	1:N:187:LEU:HD13	1.78	0.65
1:V:181:ASN:ND2	1:c:181:ASN:HD21	1.95	0.65
1:u:80:LEU:HD11	1:u:91:VAL:HG13	1.79	0.65
1:w:44:HIS:HB2	2:w:355:HOH:O	1.87	0.65
1:I:151:THR:HG22	1:I:155:SER:HB2	1.79	0.64
1:O:116:ARG:HD3	1:O:154:PHE:CE2	2.32	0.64
1:w:80:LEU:HD11	1:w:91:VAL:HG13	1.79	0.64
1:K:59:ARG:HD3	2:K:301:HOH:O	1.97	0.64
1:N:151:THR:HG22	1:N:155:SER:HB2	1.79	0.64
1:q:100:LYS:HG2	1:q:160:TYR:CZ	2.33	0.64
1:o:180:ARG:HB2	2:o:331:HOH:O	1.97	0.64
1:s:101:VAL:HG23	1:s:163:PRO:HG3	1.80	0.64
1:P:151:THR:HG22	1:P:155:SER:CB	2.28	0.63
1:O:100:LYS:HG2	1:O:160:TYR:CZ	2.34	0.63
1:h:80:LEU:HD11	1:h:91:VAL:HG13	1.79	0.63
1:G:151:THR:HG22	1:G:155:SER:CB	2.28	0.63
1:c:151:THR:HG22	1:c:155:SER:CB	2.27	0.63
1:A:151:THR:HG22	1:A:155:SER:CB	2.29	0.63
1:H:151:THR:HG22	1:H:155:SER:HB2	1.81	0.62
1:R:74:PHE:HE2	1:R:197:GLY:HA3	1.64	0.62
1:v:165:PRO:HB2	1:v:167:LEU:HD13	1.80	0.62
1:x:214:ARG:NH2	2:x:301:HOH:O	2.25	0.62
1:X:77:ASN:HD21	1:X:192:ASN:H	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:151:THR:HG22	1:N:155:SER:CB	2.28	0.62
1:1:100:LYS:HG2	1:1:160:TYR:CZ	2.33	0.62
1:N:100:LYS:HG2	1:N:160:TYR:CZ	2.35	0.62
1:a:100:LYS:HG2	1:a:160:TYR:CZ	2.35	0.62
1:w:44:HIS:HA	2:w:355:HOH:O	1.97	0.62
1:o:101:VAL:HG23	1:o:163:PRO:HG3	1.82	0.62
1:O:151:THR:HG22	1:O:155:SER:CB	2.29	0.61
1:A:151:THR:HG22	1:A:155:SER:HB2	1.82	0.61
1:s:177:ASN:HB3	2:s:341:HOH:O	2.00	0.61
1:A:128:ASN:HB2	1:F:186:ARG:HD2	1.82	0.61
1:J:151:THR:HG22	1:J:155:SER:CB	2.31	0.61
1:2:98:ILE:HD12	1:2:195:HIS:CD2	2.36	0.61
1:x:101:VAL:HG23	1:x:163:PRO:HG3	1.83	0.60
1:1:101:VAL:HG23	1:1:163:PRO:HG3	1.82	0.60
1:Z:100:LYS:HG2	1:Z:160:TYR:CZ	2.37	0.60
1:9:116:ARG:HD3	1:9:154:PHE:CE2	2.37	0.60
1:e:116:ARG:HD3	1:e:154:PHE:CE2	2.36	0.60
1:l:100:LYS:HG2	1:l:160:TYR:CZ	2.36	0.60
1:U:151:THR:HG22	1:U:155:SER:HB2	1.83	0.60
1:W:212:ASN:ND2	1:b:203:GLU:OE1	2.35	0.60
1:s:151:THR:HG22	1:s:155:SER:HB2	1.84	0.60
1:x:151:THR:HG22	1:x:155:SER:CB	2.32	0.60
1:H:116:ARG:HD3	1:H:154:PHE:CE2	2.37	0.60
1:T:189:THR:HG23	2:T:316:HOH:O	2.01	0.60
1:d:100:LYS:HG2	1:d:160:TYR:CZ	2.37	0.60
1:Y:74:PHE:HE2	1:Y:197:GLY:HA3	1.65	0.60
1:c:100:LYS:HG2	1:c:160:TYR:CZ	2.36	0.59
1:A:80:LEU:HD11	1:A:91:VAL:HG13	1.84	0.59
1:G:101:VAL:HG23	1:G:163:PRO:HG3	1.84	0.59
1:T:101:VAL:HG23	1:T:163:PRO:HG3	1.83	0.59
1:i:116:ARG:HD3	1:i:154:PHE:CE2	2.37	0.59
1:C:177:ASN:ND2	2:C:301:HOH:O	2.35	0.59
1:J:80:LEU:HD11	1:J:91:VAL:HG13	1.85	0.59
1:L:151:THR:HG22	1:L:155:SER:CB	2.32	0.59
1:R:230:PRO:C	2:R:351:HOH:O	2.44	0.59
1:1:151:THR:HG22	1:1:155:SER:HB2	1.84	0.59
1:J:100:LYS:HG2	1:J:160:TYR:CZ	2.37	0.59
1:c:80:LEU:HD11	1:c:91:VAL:HG13	1.84	0.59
1:E:151:THR:HG22	1:E:155:SER:HB2	1.83	0.59
1:Z:116:ARG:HD3	1:Z:154:PHE:CE2	2.38	0.59
1:k:98:ILE:HD12	1:k:195:HIS:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:116:ARG:NH1	1:V:154:PHE:O	2.36	0.59
1:I:89:ARG:HD2	1:I:187:LEU:HD13	1.84	0.59
1:M:151:THR:HG22	1:M:155:SER:CB	2.33	0.59
1:Y:89:ARG:HD2	1:Y:187:LEU:HD13	1.84	0.59
1:u:177:ASN:ND2	2:u:302:HOH:O	2.33	0.58
1:E:151:THR:HG22	1:E:155:SER:CB	2.33	0.58
1:I:116:ARG:HD3	1:I:154:PHE:CE2	2.38	0.58
1:4:74:PHE:HE2	1:4:197:GLY:HA3	1.68	0.58
1:N:116:ARG:HD3	1:N:154:PHE:CE2	2.38	0.58
1:J:116:ARG:HD3	1:J:154:PHE:CE2	2.38	0.58
1:V:116:ARG:HD3	1:V:154:PHE:CE2	2.38	0.58
1:r:116:ARG:HD3	1:r:154:PHE:CE2	2.38	0.58
1:b:116:ARG:HD3	1:b:154:PHE:CE2	2.38	0.58
1:v:100:LYS:HG2	1:v:160:TYR:CZ	2.39	0.58
1:I:100:LYS:HG2	1:I:160:TYR:CZ	2.39	0.58
1:W:89:ARG:HD2	1:W:187:LEU:HD13	1.85	0.58
1:o:100:LYS:HG2	1:o:160:TYR:CZ	2.38	0.58
1:h:100:LYS:HG2	1:h:160:TYR:CZ	2.39	0.58
1:s:151:THR:HG22	1:s:155:SER:CB	2.33	0.58
1:v:178:ASN:OD1	1:v:179:LYS:N	2.37	0.58
1:K:116:ARG:HD3	1:K:154:PHE:CE2	2.38	0.58
1:V:89:ARG:HD2	1:V:187:LEU:HD13	1.86	0.58
1:H:100:LYS:HG2	1:H:160:TYR:CZ	2.39	0.57
1:M:100:LYS:HG2	1:M:160:TYR:CZ	2.39	0.57
1:o:89:ARG:HD2	1:o:187:LEU:HD13	1.84	0.57
1:p:72:MET:HE1	1:p:105:PHE:CZ	2.39	0.57
1:t:178:ASN:HD21	1:w:180:ARG:HE	1.51	0.57
1:e:231:LEU:HB2	2:e:363:HOH:O	2.03	0.57
1:l:116:ARG:HD3	1:l:154:PHE:CE2	2.39	0.57
1:8:116:ARG:HD3	1:8:154:PHE:CE2	2.38	0.57
1:E:116:ARG:HD3	1:E:154:PHE:CE2	2.40	0.57
1:K:167:LEU:HD22	2:K:314:HOH:O	2.05	0.57
1:7:116:ARG:HD3	1:7:154:PHE:CE2	2.40	0.57
1:p:175:GLN:CD	1:p:183:LEU:HD22	2.30	0.57
1:u:116:ARG:HD3	1:u:154:PHE:CE2	2.40	0.57
1:L:116:ARG:HD2	2:L:339:HOH:O	2.03	0.57
1:Y:74:PHE:CE2	1:Y:197:GLY:HA3	2.38	0.57
1:E:100:LYS:HG2	1:E:160:TYR:CZ	2.40	0.57
1:i:180:ARG:NH2	2:i:301:HOH:O	2.38	0.57
1:r:98:ILE:HD12	1:r:195:HIS:CE1	2.40	0.57
1:g:162:THR:HB	1:g:177:ASN:HD22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ALA:O	1:A:198:LEU:HD12	2.04	0.56
1:x:116:ARG:HD3	1:x:154:PHE:CE2	2.40	0.56
1:6:116:ARG:HD3	1:6:154:PHE:CE2	2.40	0.56
1:q:165:PRO:HB2	1:q:167:LEU:HD13	1.87	0.56
1:N:99:ARG:O	1:N:100:LYS:HD2	2.05	0.56
1:b:151:THR:HG22	1:b:155:SER:CB	2.35	0.56
1:k:116:ARG:HD3	1:k:154:PHE:CE2	2.41	0.56
1:A:116:ARG:HD3	1:A:154:PHE:CE2	2.40	0.56
1:s:100:LYS:HG2	1:s:160:TYR:CZ	2.39	0.56
1:v:101:VAL:HG23	1:v:163:PRO:HG3	1.86	0.56
1:C:89:ARG:HD2	1:C:187:LEU:HD13	1.88	0.56
1:e:89:ARG:HD2	1:e:187:LEU:HD13	1.88	0.56
1:j:101:VAL:HG23	1:j:163:PRO:HD3	1.87	0.56
1:C:178:ASN:OD1	1:C:179:LYS:N	2.39	0.56
1:V:116:ARG:HD2	2:V:326:HOH:O	2.05	0.56
1:x:80:LEU:HD11	1:x:91:VAL:HG13	1.87	0.56
1:f:116:ARG:HD3	1:f:154:PHE:CE2	2.41	0.55
1:k:101:VAL:HG23	1:k:163:PRO:HG3	1.88	0.55
1:m:224:PHE:O	1:y:144:TYR:HA	2.06	0.55
1:n:74:PHE:HE2	1:n:197:GLY:HA3	1.71	0.55
1:6:72:MET:CE	1:6:198:LEU:HD23	2.37	0.55
1:B:162:THR:HB	1:B:177:ASN:HD22	1.72	0.55
1:K:98:ILE:HD12	1:K:195:HIS:CD2	2.41	0.55
1:V:101:VAL:HG23	1:V:163:PRO:HG3	1.87	0.55
1:b:89:ARG:HD2	1:b:187:LEU:HD13	1.89	0.55
1:p:116:ARG:HD3	1:p:154:PHE:CE2	2.42	0.55
1:H:80:LEU:HD11	1:H:91:VAL:HG13	1.88	0.55
1:E:80:LEU:HD12	1:F:226:LEU:HD21	1.89	0.55
1:2:116:ARG:HD2	2:2:350:HOH:O	2.06	0.55
1:w:116:ARG:HD3	1:w:154:PHE:CE2	2.41	0.55
1:t:226:LEU:HD21	1:u:80:LEU:HD12	1.89	0.55
1:Z:89:ARG:HD2	1:Z:187:LEU:HD13	1.89	0.54
1:G:151:THR:HG22	1:G:155:SER:HB2	1.88	0.54
1:x:44:HIS:CE1	2:x:315:HOH:O	2.59	0.54
1:l:151:THR:HG22	1:l:155:SER:HB2	1.89	0.54
1:i:80:LEU:HD11	1:i:91:VAL:HG13	1.88	0.54
1:v:99:ARG:O	1:v:100:LYS:HD2	2.08	0.54
1:G:74:PHE:HE2	1:G:197:GLY:HA3	1.72	0.54
1:J:89:ARG:HD2	1:J:187:LEU:HD13	1.90	0.54
1:d:99:ARG:NH2	2:d:302:HOH:O	2.39	0.54
1:p:72:MET:HE1	1:p:105:PHE:HZ	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:178:ASN:OD1	1:W:179:LYS:N	2.41	0.54
1:I:74:PHE:CE2	1:I:197:GLY:HA3	2.43	0.54
1:U:100:LYS:HG2	1:U:160:TYR:CZ	2.43	0.54
1:3:181:ASN:HD21	1:8:181:ASN:ND2	2.05	0.54
1:b:74:PHE:CE2	1:b:197:GLY:HA3	2.43	0.54
1:r:186:ARG:HD2	1:u:128:ASN:HB2	1.89	0.54
1:M:89:ARG:NH2	1:M:189:THR:OG1	2.40	0.54
1:v:230:PRO:C	2:v:340:HOH:O	2.51	0.54
1:R:151:THR:HG22	1:R:155:SER:CB	2.38	0.53
1:5:99:ARG:O	1:5:100:LYS:HD2	2.08	0.53
1:a:203:GLU:OE1	1:r:212:ASN:ND2	2.39	0.53
1:p:100:LYS:HG2	1:p:160:TYR:CZ	2.43	0.53
1:q:186:ARG:CZ	1:q:188:GLN:HG2	2.38	0.53
1:R:49:LEU:HD13	1:R:80:LEU:HD13	1.89	0.53
1:W:151:THR:HG22	1:W:155:SER:CB	2.38	0.53
1:c:116:ARG:HD3	1:c:154:PHE:CE2	2.43	0.53
1:k:80:LEU:HD11	1:k:91:VAL:HG13	1.89	0.53
1:o:151:THR:HG22	1:o:155:SER:CB	2.38	0.53
1:X:158:SER:O	1:X:159:ARG:HD2	2.09	0.53
1:e:151:THR:HG22	1:e:155:SER:CB	2.39	0.53
1:N:116:ARG:HD2	2:N:334:HOH:O	2.08	0.53
1:X:116:ARG:HD3	1:X:154:PHE:CE2	2.43	0.53
1:f:89:ARG:HD2	1:f:187:LEU:HD13	1.91	0.53
1:h:116:ARG:HD3	1:h:154:PHE:CE2	2.43	0.53
1:L:158:SER:O	1:L:159:ARG:HD2	2.07	0.53
1:y:186:ARG:NH1	1:y:188:GLN:HG2	2.24	0.53
1:a:72:MET:HE1	1:a:105:PHE:CZ	2.44	0.53
1:H:116:ARG:HD3	1:H:154:PHE:HE2	1.73	0.53
1:P:186:ARG:HD2	1:3:128:ASN:HB2	1.91	0.53
1:d:99:ARG:O	1:d:100:LYS:HD2	2.09	0.53
1:g:100:LYS:HG2	1:g:160:TYR:CZ	2.44	0.53
1:h:151:THR:HG22	1:h:155:SER:HB2	1.90	0.53
1:S:74:PHE:CE2	1:S:197:GLY:HA3	2.43	0.53
1:6:72:MET:HE3	1:6:198:LEU:HD23	1.91	0.52
1:Z:151:THR:HG22	1:Z:155:SER:OG	2.08	0.52
1:Z:181:ASN:HD21	1:1:181:ASN:ND2	2.07	0.52
1:E:165:PRO:HB2	1:E:167:LEU:HD13	1.92	0.52
1:L:116:ARG:HD3	1:L:154:PHE:CE2	2.44	0.52
1:R:101:VAL:HG23	1:R:163:PRO:HD3	1.91	0.52
1:4:100:LYS:HG2	1:4:160:TYR:CZ	2.45	0.52
1:C:116:ARG:HD3	1:C:154:PHE:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:44:HIS:HA	2:o:364:HOH:O	2.09	0.52
1:V:80:LEU:HD11	1:V:91:VAL:HG13	1.92	0.52
1:b:116:ARG:HD3	1:b:154:PHE:HE2	1.74	0.52
1:b:151:THR:HG22	1:b:155:SER:HB2	1.91	0.52
1:i:74:PHE:HE2	1:i:197:GLY:HA3	1.74	0.52
1:j:44:HIS:C	2:j:330:HOH:O	2.52	0.52
1:Q:177:ASN:ND2	2:Q:304:HOH:O	2.43	0.52
1:w:112:THR:HG22	1:y:112:THR:HG21	1.91	0.52
1:D:99:ARG:O	1:D:100:LYS:HD2	2.10	0.52
1:T:74:PHE:HE2	1:T:197:GLY:HA3	1.73	0.52
1:m:177:ASN:ND2	2:m:303:HOH:O	2.42	0.52
1:Z:98:ILE:HD12	1:Z:195:HIS:CD2	2.44	0.52
1:2:100:LYS:HG2	1:2:160:TYR:CZ	2.45	0.52
1:6:116:ARG:HD2	2:6:359:HOH:O	2.09	0.52
1:y:100:LYS:HG2	1:y:160:TYR:CZ	2.44	0.52
1:P:61:THR:O	1:P:62:VAL:C	2.52	0.51
1:c:74:PHE:HE2	1:c:197:GLY:HA3	1.75	0.51
1:I:101:VAL:HG23	1:I:163:PRO:HG3	1.93	0.51
1:W:178:ASN:O	2:W:302:HOH:O	2.19	0.51
1:C:151:THR:HG22	1:C:155:SER:HB2	1.91	0.51
1:S:103:VAL:O	1:S:158:SER:HA	2.11	0.51
1:U:151:THR:HG22	1:U:155:SER:CB	2.40	0.51
1:5:89:ARG:HD2	1:5:187:LEU:HD13	1.92	0.51
1:c:101:VAL:HG23	1:c:163:PRO:HD3	1.91	0.51
1:G:116:ARG:HD3	1:G:154:PHE:CE2	2.46	0.51
1:g:178:ASN:OD1	1:g:179:LYS:N	2.43	0.51
1:j:116:ARG:HD3	1:j:154:PHE:CE2	2.46	0.51
1:p:99:ARG:O	1:p:100:LYS:HD2	2.11	0.51
1:H:80:LEU:HD11	1:H:91:VAL:CG1	2.41	0.51
1:L:80:LEU:HD11	1:L:91:VAL:HG13	1.93	0.51
1:R:100:LYS:HG2	1:R:160:TYR:CZ	2.46	0.51
1:d:72:MET:CE	1:d:198:LEU:HD23	2.41	0.51
1:F:116:ARG:HD3	1:F:154:PHE:CE2	2.46	0.51
1:U:168:ASP:OD1	1:U:168:ASP:C	2.53	0.51
1:5:178:ASN:OD1	1:5:179:LYS:N	2.43	0.51
1:a:101:VAL:HG23	1:a:163:PRO:HG3	1.93	0.51
1:p:89:ARG:HD2	1:p:187:LEU:HD13	1.92	0.51
1:I:72:MET:CE	1:I:198:LEU:HD23	2.41	0.50
1:7:100:LYS:HG2	1:7:160:TYR:CZ	2.46	0.50
1:u:61:THR:OG1	2:u:301:HOH:O	2.19	0.50
1:B:98:ILE:HD12	1:B:195:HIS:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:74:PHE:CE2	1:G:197:GLY:HA3	2.46	0.50
2:D:308:HOH:O	1:F:147:ARG:HD3	2.10	0.50
1:3:116:ARG:HD3	1:3:154:PHE:CE2	2.46	0.50
1:f:128:ASN:HB2	1:k:186:ARG:HD2	1.93	0.50
1:K:186:ARG:HD2	1:M:128:ASN:HB2	1.94	0.50
1:L:89:ARG:HD2	1:L:187:LEU:HD13	1.92	0.50
1:A:76:ILE:HG13	1:A:217:MET:HE1	1.94	0.50
1:I:72:MET:HE1	1:I:198:LEU:HD23	1.94	0.50
1:2:206:ILE:HD11	2:2:368:HOH:O	2.11	0.50
1:t:74:PHE:HE2	1:t:197:GLY:HA3	1.76	0.50
1:D:161:PHE:CZ	2:D:370:HOH:O	2.62	0.50
1:O:121:SER:O	1:O:147:ARG:HA	2.12	0.50
1:P:116:ARG:HD3	1:P:154:PHE:CE2	2.47	0.50
1:P:128:ASN:HB2	1:8:186:ARG:HD2	1.94	0.50
1:h:159:ARG:HA	2:h:319:HOH:O	2.11	0.50
1:U:112:THR:HG21	1:d:112:THR:HB	1.93	0.50
1:X:80:LEU:HD23	2:X:344:HOH:O	2.11	0.50
1:p:224:PHE:O	1:s:144:TYR:HA	2.12	0.50
1:G:89:ARG:HD2	1:G:187:LEU:HD13	1.94	0.50
1:P:74:PHE:HE2	1:P:197:GLY:HA3	1.76	0.50
1:T:101:VAL:CG2	1:T:163:PRO:HG3	2.42	0.50
1:V:151:THR:HG22	1:V:155:SER:HB2	1.94	0.50
1:X:101:VAL:HG23	1:X:163:PRO:HD3	1.93	0.50
1:6:144:TYR:HA	1:l:224:PHE:O	2.12	0.50
1:n:151:THR:HG22	1:n:155:SER:HB2	1.94	0.50
1:K:100:LYS:HG2	1:K:160:TYR:CZ	2.47	0.49
1:K:168:ASP:OD1	1:K:168:ASP:C	2.52	0.49
1:V:112:THR:HG22	1:b:112:THR:HG21	1.93	0.49
1:5:100:LYS:HG2	1:5:160:TYR:CZ	2.47	0.49
1:B:101:VAL:HG23	1:B:163:PRO:HG3	1.93	0.49
1:D:212:ASN:ND2	1:F:203:GLU:OE1	2.45	0.49
1:9:158:SER:O	1:9:159:ARG:HD2	2.13	0.49
1:e:151:THR:HG22	1:e:155:SER:HB2	1.93	0.49
1:n:178:ASN:OD1	1:n:179:LYS:N	2.46	0.49
1:r:80:LEU:HD11	1:r:91:VAL:HG13	1.93	0.49
1:t:116:ARG:HD3	1:t:154:PHE:CE2	2.46	0.49
1:C:100:LYS:HG3	1:C:160:TYR:CZ	2.46	0.49
1:X:178:ASN:OD1	1:X:179:LYS:N	2.45	0.49
1:c:178:ASN:OD1	1:c:179:LYS:N	2.45	0.49
1:E:124:ILE:O	1:E:196:VAL:HG13	2.13	0.49
1:L:128:ASN:HB2	1:l:186:ARG:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:100:LYS:HG2	1:k:160:TYR:CE1	2.47	0.49
1:H:74:PHE:CE2	1:H:197:GLY:HA3	2.47	0.49
1:P:101:VAL:CG2	1:P:163:PRO:HG3	2.42	0.49
1:Q:226:LEU:HD21	1:R:80:LEU:HD12	1.95	0.49
1:7:186:ARG:HD2	1:o:128:ASN:HB2	1.93	0.49
1:o:116:ARG:HD3	1:o:154:PHE:CE2	2.48	0.49
1:A:181:ASN:HD21	1:C:181:ASN:ND2	2.11	0.49
1:2:224:PHE:O	1:j:144:TYR:HA	2.13	0.49
1:k:121:SER:O	1:k:147:ARG:HA	2.13	0.49
1:S:151:THR:HG22	1:S:155:SER:HB2	1.95	0.49
1:b:74:PHE:HE2	1:b:197:GLY:HA3	1.77	0.49
1:y:116:ARG:HD3	1:y:154:PHE:CE2	2.48	0.49
1:B:101:VAL:CG2	1:B:163:PRO:HG3	2.43	0.49
1:C:151:THR:HG22	1:C:155:SER:CB	2.43	0.49
1:C:154:PHE:O	1:K:116:ARG:NH1	2.46	0.49
1:u:101:VAL:HG23	1:u:163:PRO:HG3	1.94	0.49
1:M:72:MET:HE1	1:M:105:PHE:HZ	1.77	0.49
1:R:98:ILE:HD12	1:R:195:HIS:CE1	2.48	0.49
1:W:100:LYS:HG2	1:W:160:TYR:CZ	2.48	0.49
1:d:72:MET:HE1	1:d:198:LEU:HD23	1.94	0.49
1:v:72:MET:HE1	1:v:103:VAL:HG11	1.95	0.49
1:G:124:ILE:O	1:G:196:VAL:HG13	2.13	0.48
1:M:72:MET:HE1	1:M:105:PHE:CZ	2.47	0.48
1:G:224:PHE:O	1:I:144:TYR:HA	2.12	0.48
1:Q:162:THR:HB	1:Q:177:ASN:HD22	1.77	0.48
1:2:89:ARG:HD2	1:2:187:LEU:HD13	1.94	0.48
1:3:89:ARG:HD2	1:3:187:LEU:HD13	1.96	0.48
1:d:116:ARG:HD3	1:d:154:PHE:CE2	2.47	0.48
1:m:116:ARG:HD3	1:m:154:PHE:CE2	2.47	0.48
1:6:98:ILE:HD12	1:6:195:HIS:CD2	2.48	0.48
1:B:98:ILE:HD12	1:B:195:HIS:CG	2.48	0.48
1:W:186:ARG:HD2	1:Y:128:ASN:HB2	1.95	0.48
1:1:116:ARG:HD3	1:1:154:PHE:CE2	2.47	0.48
1:F:121:SER:O	1:F:147:ARG:HA	2.13	0.48
1:o:121:SER:O	1:o:147:ARG:HA	2.14	0.48
1:y:147:ARG:HD2	1:y:147:ARG:C	2.39	0.48
1:F:116:ARG:HD2	2:F:343:HOH:O	2.13	0.48
1:V:101:VAL:CG2	1:V:163:PRO:HG3	2.43	0.48
1:W:177:ASN:ND2	2:W:305:HOH:O	2.44	0.48
1:t:188:GLN:O	1:t:192:ASN:ND2	2.41	0.48
1:A:100:LYS:HG2	1:A:160:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:VAL:HG23	1:E:163:PRO:HD3	1.95	0.48
1:K:165:PRO:HB2	1:K:167:LEU:HD13	1.95	0.48
1:n:178:ASN:N	2:n:303:HOH:O	2.46	0.48
1:E:116:ARG:HD2	2:E:358:HOH:O	2.14	0.48
1:T:72:MET:HE3	1:T:198:LEU:HD23	1.95	0.48
1:W:74:PHE:HE2	1:W:197:GLY:HA3	1.78	0.48
1:t:144:TYR:HA	1:w:224:PHE:O	2.14	0.48
1:K:116:ARG:HD3	1:K:154:PHE:HE2	1.76	0.48
1:1:74:PHE:CE2	1:1:197:GLY:HA3	2.48	0.48
1:e:165:PRO:HB2	1:e:167:LEU:HD13	1.95	0.48
1:p:74:PHE:CE2	1:p:197:GLY:HA3	2.49	0.48
1:G:167:LEU:HD12	1:I:171:ILE:HD13	1.96	0.48
1:S:74:PHE:HE2	1:S:197:GLY:HA3	1.78	0.47
1:S:116:ARG:HD3	1:S:154:PHE:CE2	2.49	0.47
1:n:151:THR:HG22	1:n:155:SER:CB	2.44	0.47
1:x:165:PRO:HB2	1:x:167:LEU:HD13	1.96	0.47
1:Q:116:ARG:HD3	1:Q:154:PHE:CE2	2.49	0.47
1:S:151:THR:HG22	1:S:155:SER:CB	2.43	0.47
1:T:88:PRO:HB2	2:T:316:HOH:O	2.13	0.47
1:d:61:THR:O	1:d:62:VAL:C	2.57	0.47
1:g:151:THR:HG22	1:g:155:SER:CB	2.44	0.47
1:q:116:ARG:HD3	1:q:154:PHE:CE2	2.48	0.47
1:H:224:PHE:O	1:S:144:TYR:HA	2.15	0.47
1:Z:186:ARG:HD2	1:1:128:ASN:HB2	1.96	0.47
1:f:151:THR:HG22	1:f:155:SER:CB	2.44	0.47
1:n:100:LYS:HG2	1:n:160:TYR:CZ	2.50	0.47
1:M:89:ARG:HD2	1:M:187:LEU:HD13	1.96	0.47
1:U:72:MET:CE	1:U:198:LEU:HD23	2.44	0.47
1:X:153:PRO:HB3	1:X:209:GLN:OE1	2.15	0.47
1:Y:100:LYS:HG2	1:Y:160:TYR:CZ	2.49	0.47
1:7:100:LYS:HE3	2:7:350:HOH:O	2.14	0.47
1:j:99:ARG:O	1:j:100:LYS:HD2	2.15	0.47
1:q:186:ARG:NH1	1:q:188:GLN:HG2	2.29	0.47
1:s:158:SER:O	1:s:159:ARG:HD2	2.14	0.47
1:t:100:LYS:HG2	1:t:160:TYR:CZ	2.49	0.47
1:H:112:THR:HG21	1:I:112:THR:HG22	1.96	0.47
1:K:224:PHE:O	1:M:144:TYR:HA	2.14	0.47
1:n:116:ARG:HD3	1:n:154:PHE:CE2	2.49	0.47
1:G:72:MET:HE3	1:G:198:LEU:HD23	1.95	0.47
1:N:72:MET:HE1	1:N:105:PHE:HZ	1.80	0.47
1:e:100:LYS:HG2	1:e:160:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:151:THR:HG22	1:h:155:SER:CB	2.44	0.47
1:l:98:ILE:HD13	1:l:217:MET:SD	2.54	0.47
1:B:203:GLU:OE1	1:J:212:ASN:ND2	2.48	0.47
1:H:89:ARG:NH2	1:H:189:THR:OG1	2.47	0.47
1:J:186:ARG:HD2	1:W:128:ASN:HB2	1.97	0.47
1:O:99:ARG:O	1:O:100:LYS:HD2	2.15	0.47
1:P:178:ASN:OD1	1:P:179:LYS:N	2.48	0.47
1:Q:230:PRO:C	2:Q:307:HOH:O	2.57	0.47
1:Y:112:THR:HG21	1:1:112:THR:HB	1.96	0.47
1:9:100:LYS:HG2	1:9:160:TYR:CZ	2.50	0.47
1:a:116:ARG:NH1	1:r:154:PHE:O	2.48	0.47
1:m:80:LEU:HD11	1:m:91:VAL:HG13	1.96	0.47
1:r:71:MET:HE2	2:r:323:HOH:O	2.13	0.47
1:y:178:ASN:OD1	1:y:179:LYS:N	2.48	0.47
1:L:165:PRO:HB2	1:L:167:LEU:HD13	1.96	0.47
1:W:72:MET:HE1	1:W:105:PHE:CZ	2.50	0.47
1:I:122:ALA:O	1:I:198:LEU:HD12	2.15	0.47
1:N:101:VAL:HG23	1:N:163:PRO:HG3	1.96	0.47
1:S:116:ARG:HD2	2:S:328:HOH:O	2.15	0.47
1:X:203:GLU:OE1	1:f:212:ASN:ND2	2.48	0.47
1:s:116:ARG:HD3	1:s:154:PHE:CE2	2.50	0.47
1:f:101:VAL:HG23	1:f:163:PRO:HG3	1.96	0.47
1:r:162:THR:HB	1:r:177:ASN:HD22	1.78	0.47
1:1:151:THR:HG22	1:1:155:SER:CB	2.44	0.46
1:7:61:THR:O	1:7:62:VAL:C	2.57	0.46
1:A:226:LEU:HD21	1:B:80:LEU:HD12	1.98	0.46
1:D:151:THR:HG22	1:D:155:SER:CB	2.45	0.46
1:K:80:LEU:HD21	1:K:91:VAL:HG22	1.97	0.46
1:Q:224:PHE:O	1:9:144:TYR:HA	2.15	0.46
1:W:151:THR:HG22	1:W:155:SER:HB2	1.97	0.46
1:3:100:LYS:HG2	1:3:160:TYR:CZ	2.50	0.46
1:8:212:ASN:ND2	1:o:203:GLU:OE1	2.48	0.46
1:g:43:SER:HA	2:g:361:HOH:O	2.16	0.46
1:k:203:GLU:OE1	1:w:212:ASN:ND2	2.49	0.46
1:l:151:THR:HG22	1:l:155:SER:CB	2.45	0.46
1:w:46:ASN:OD1	1:w:220:GLN:HG3	2.15	0.46
1:I:212:ASN:ND2	1:W:203:GLU:OE1	2.48	0.46
1:T:151:THR:HG22	1:T:155:SER:CB	2.46	0.46
1:T:152:GLN:NE2	1:T:203:GLU:O	2.43	0.46
1:1:108:CYS:HA	1:j:116:ARG:HB2	1.97	0.46
1:2:151:THR:HG22	1:2:155:SER:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:99:ARG:NH2	2:8:304:HOH:O	2.48	0.46
1:m:100:LYS:HG2	1:m:160:TYR:CZ	2.50	0.46
1:p:151:THR:HG22	1:p:155:SER:CB	2.46	0.46
1:1:121:SER:O	1:1:147:ARG:HA	2.16	0.46
1:8:89:ARG:HD2	1:8:187:LEU:HD13	1.97	0.46
1:9:121:SER:O	1:9:147:ARG:HA	2.16	0.46
1:u:212:ASN:ND2	1:x:203:GLU:OE1	2.48	0.46
1:x:151:THR:HG22	1:x:155:SER:HB2	1.96	0.46
1:C:101:VAL:HG23	1:C:163:PRO:HD3	1.98	0.46
1:S:116:ARG:HD3	1:S:154:PHE:HE2	1.81	0.46
1:m:74:PHE:HE2	1:m:197:GLY:HA3	1.81	0.46
1:p:120:SER:OG	1:p:139:ASP:OD2	2.33	0.46
1:v:101:VAL:CG2	1:v:163:PRO:HG3	2.46	0.46
1:x:151:THR:HG22	1:x:155:SER:OG	2.15	0.46
1:D:100:LYS:HG2	1:D:160:TYR:CZ	2.51	0.46
1:M:63:LYS:HB3	2:M:366:HOH:O	2.16	0.46
1:3:101:VAL:HG23	1:3:163:PRO:HG3	1.98	0.46
1:6:99:ARG:NH1	1:6:179:LYS:O	2.49	0.46
1:J:74:PHE:HE2	1:J:197:GLY:HA3	1.80	0.46
1:S:89:ARG:HD2	1:S:187:LEU:HD13	1.97	0.46
1:U:99:ARG:NH2	2:U:302:HOH:O	2.47	0.46
1:W:116:ARG:HD3	1:W:154:PHE:CE2	2.51	0.46
1:3:72:MET:HE1	1:3:105:PHE:CZ	2.51	0.46
1:8:108:CYS:HA	1:o:116:ARG:HB2	1.97	0.46
1:d:89:ARG:HD2	1:d:187:LEU:HD13	1.98	0.46
1:d:101:VAL:CG2	1:d:163:PRO:HG3	2.45	0.46
1:t:101:VAL:HG23	1:t:163:PRO:HD3	1.98	0.46
1:x:101:VAL:CG2	1:x:163:PRO:HG3	2.44	0.46
1:J:203:GLU:OE1	1:Z:212:ASN:ND2	2.49	0.46
1:O:49:LEU:HD13	1:O:80:LEU:HD13	1.96	0.46
1:c:116:ARG:HD3	1:c:154:PHE:HE2	1.80	0.46
1:j:151:THR:HG22	1:j:155:SER:CB	2.45	0.46
1:B:224:PHE:O	1:G:144:TYR:HA	2.14	0.46
1:2:98:ILE:HD12	1:2:195:HIS:CG	2.50	0.46
1:f:116:ARG:HD3	1:f:154:PHE:HE2	1.80	0.46
1:g:101:VAL:HG23	1:g:163:PRO:HG3	1.98	0.46
1:r:74:PHE:HE2	1:r:197:GLY:HA3	1.80	0.46
1:y:206:ILE:HG22	1:y:207:TYR:CE2	2.50	0.46
1:E:74:PHE:CE2	1:E:197:GLY:HA3	2.51	0.46
1:D:144:TYR:HA	1:M:224:PHE:O	2.16	0.45
1:M:101:VAL:HG23	1:M:163:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:100:LYS:HG2	1:X:160:TYR:CZ	2.51	0.45
1:a:101:VAL:CG2	1:a:163:PRO:HG3	2.46	0.45
1:c:212:ASN:ND2	1:g:203:GLU:OE1	2.49	0.45
1:e:72:MET:HE1	1:e:105:PHE:CZ	2.51	0.45
1:m:186:ARG:HD2	1:y:128:ASN:HB2	1.98	0.45
1:C:72:MET:HE1	1:C:105:PHE:CZ	2.51	0.45
1:c:180:ARG:HA	2:c:327:HOH:O	2.15	0.45
1:D:116:ARG:HD3	1:D:154:PHE:CE2	2.52	0.45
1:E:178:ASN:OD1	1:E:179:LYS:N	2.48	0.45
1:R:212:ASN:ND2	1:9:203:GLU:OE1	2.49	0.45
1:7:151:THR:HG22	1:7:155:SER:HB2	1.94	0.45
1:h:99:ARG:NH1	1:h:179:LYS:O	2.49	0.45
1:A:224:PHE:O	1:C:144:TYR:HA	2.16	0.45
1:9:162:THR:HB	1:9:177:ASN:HD22	1.82	0.45
1:C:121:SER:O	1:C:147:ARG:HA	2.17	0.45
1:U:76:ILE:HG22	2:U:322:HOH:O	2.17	0.45
1:4:72:MET:HE1	1:4:105:PHE:CZ	2.52	0.45
1:h:203:GLU:OE1	1:k:212:ASN:ND2	2.49	0.45
1:s:121:SER:O	1:s:147:ARG:HA	2.17	0.45
1:B:80:LEU:HD11	1:B:91:VAL:HG13	1.98	0.45
1:F:89:ARG:HD2	1:F:187:LEU:HD13	1.98	0.45
1:P:158:SER:O	1:P:159:ARG:HD2	2.17	0.45
1:U:72:MET:HE3	1:U:198:LEU:HD23	1.99	0.45
1:Y:101:VAL:HG23	1:Y:163:PRO:HG3	1.98	0.45
1:x:43:SER:HG	1:x:44:HIS:CE1	2.34	0.45
1:H:108:CYS:HA	1:I:116:ARG:HB2	1.99	0.45
1:T:74:PHE:CE2	1:T:197:GLY:HA3	2.52	0.45
1:V:186:ARG:HD2	1:d:128:ASN:HB2	1.99	0.45
1:e:74:PHE:CE2	1:e:197:GLY:HA3	2.52	0.45
1:v:116:ARG:HD3	1:v:154:PHE:CE2	2.52	0.45
1:C:124:ILE:O	1:C:196:VAL:HG13	2.17	0.44
1:H:101:VAL:HG23	1:H:163:PRO:HG3	1.99	0.44
1:S:158:SER:O	1:S:159:ARG:HD2	2.17	0.44
1:T:72:MET:HE1	1:T:103:VAL:HG11	1.99	0.44
1:T:139:ASP:C	1:T:139:ASP:OD1	2.61	0.44
1:c:111:ILE:HD11	1:g:111:ILE:HG13	1.98	0.44
1:h:112:THR:HB	1:k:112:THR:HG21	1.98	0.44
1:k:103:VAL:O	1:k:158:SER:HA	2.17	0.44
1:o:165:PRO:HB2	1:o:167:LEU:HD13	1.99	0.44
1:p:116:ARG:HD3	1:p:154:PHE:HE2	1.80	0.44
1:r:224:PHE:O	1:u:144:TYR:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:THR:HG22	1:B:155:SER:CB	2.47	0.44
1:G:158:SER:O	1:G:159:ARG:HD2	2.17	0.44
1:l:80:LEU:HD12	1:l:80:LEU:HA	1.76	0.44
1:t:127:ASP:HA	1:t:196:VAL:HG21	2.00	0.44
1:L:100:LYS:HG2	1:L:160:TYR:CZ	2.52	0.44
1:V:152:GLN:NE2	1:V:203:GLU:O	2.49	0.44
1:n:101:VAL:HG23	1:n:163:PRO:HG3	2.00	0.44
1:t:74:PHE:CE2	1:t:197:GLY:HA3	2.52	0.44
1:v:72:MET:HE3	1:v:198:LEU:HD23	2.00	0.44
1:D:101:VAL:HG23	1:D:163:PRO:HG3	2.00	0.44
1:I:178:ASN:OD1	1:I:179:LYS:N	2.51	0.44
1:P:224:PHE:O	1:3:144:TYR:HA	2.17	0.44
1:3:165:PRO:HB2	1:3:167:LEU:HD13	1.99	0.44
1:b:107:PRO:HA	1:b:211:TYR:CD2	2.53	0.44
1:w:43:SER:OG	1:w:44:HIS:ND1	2.51	0.44
1:F:165:PRO:HB2	1:F:167:LEU:HD13	1.99	0.44
1:T:189:THR:HA	2:T:316:HOH:O	2.16	0.44
1:f:107:PRO:HA	1:f:211:TYR:CD2	2.52	0.44
1:j:100:LYS:HG2	1:j:160:TYR:CZ	2.53	0.44
1:k:72:MET:HE1	1:k:105:PHE:CZ	2.53	0.44
1:t:99:ARG:O	1:t:100:LYS:HD2	2.18	0.44
1:E:116:ARG:HB2	1:Q:108:CYS:HA	2.00	0.44
1:L:108:CYS:HA	1:M:116:ARG:HB2	2.00	0.44
1:W:89:ARG:NH2	1:W:189:THR:HG23	2.33	0.44
1:W:158:SER:O	1:W:159:ARG:HD2	2.17	0.44
1:Z:107:PRO:HA	1:Z:211:TYR:CD2	2.52	0.44
1:7:49:LEU:HD13	1:7:80:LEU:HD13	1.97	0.44
1:8:112:THR:HG21	1:o:112:THR:HB	2.00	0.44
1:i:151:THR:HG22	1:i:155:SER:CB	2.48	0.44
1:p:101:VAL:HG23	1:p:163:PRO:HG3	1.98	0.44
1:w:72:MET:HE1	1:w:105:PHE:CZ	2.52	0.44
1:K:80:LEU:HD11	1:K:91:VAL:HG13	2.00	0.44
1:P:72:MET:HE1	1:P:105:PHE:CZ	2.53	0.44
1:S:186:ARG:NH1	1:S:188:GLN:HG2	2.33	0.44
1:9:212:ASN:ND2	1:p:203:GLU:OE1	2.51	0.44
1:a:74:PHE:HE2	1:a:197:GLY:HA3	1.83	0.44
1:m:144:TYR:HA	1:n:224:PHE:O	2.18	0.44
1:y:74:PHE:HE2	1:y:197:GLY:HA3	1.83	0.44
1:B:100:LYS:HG2	1:B:160:TYR:CZ	2.53	0.44
1:L:74:PHE:HE1	1:L:197:GLY:HA3	1.83	0.44
1:L:101:VAL:HG23	1:L:163:PRO:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:120:SER:OG	1:N:139:ASP:OD2	2.34	0.44
1:Y:230:PRO:C	2:Y:315:HOH:O	2.60	0.44
1:6:101:VAL:O	1:6:160:TYR:HA	2.17	0.44
1:6:116:ARG:HD3	1:6:154:PHE:HE2	1.79	0.44
1:9:80:LEU:HD11	1:9:91:VAL:HG13	2.00	0.44
1:c:158:SER:O	1:c:159:ARG:HD2	2.18	0.44
1:k:116:ARG:HD2	2:k:313:HOH:O	2.18	0.44
1:p:49:LEU:O	1:p:216:THR:HA	2.18	0.44
1:v:147:ARG:O	1:v:148:HIS:HD2	2.00	0.44
1:N:167:LEU:HD21	1:N:183:LEU:HD23	1.99	0.44
1:R:116:ARG:HD3	1:R:154:PHE:CE2	2.53	0.44
1:S:224:PHE:O	1:U:144:TYR:HA	2.18	0.44
1:4:101:VAL:HG23	1:4:163:PRO:HG3	2.00	0.44
1:r:46:ASN:OD1	1:r:220:GLN:HG3	2.17	0.44
1:x:163:PRO:O	1:x:164:LYS:HD3	2.18	0.44
1:E:89:ARG:HD2	1:E:187:LEU:HD13	1.99	0.43
1:M:151:THR:HG22	1:M:155:SER:HB2	2.00	0.43
1:R:151:THR:HG22	1:R:155:SER:HB2	1.98	0.43
1:S:162:THR:HB	1:S:177:ASN:HD22	1.81	0.43
1:Z:151:THR:HG22	1:Z:155:SER:CB	2.48	0.43
1:y:186:ARG:CZ	1:y:188:GLN:HG2	2.47	0.43
1:D:128:ASN:HB2	1:M:186:ARG:HD2	1.99	0.43
1:L:99:ARG:O	1:L:100:LYS:HD3	2.18	0.43
1:L:164:LYS:NZ	1:L:175:GLN:O	2.50	0.43
1:V:99:ARG:NH2	2:V:303:HOH:O	2.47	0.43
1:X:77:ASN:HD21	1:X:192:ASN:N	2.14	0.43
1:f:203:GLU:OE1	1:j:212:ASN:ND2	2.51	0.43
1:r:104:GLU:HG3	2:r:320:HOH:O	2.18	0.43
1:K:101:VAL:CG2	1:K:163:PRO:HG3	2.49	0.43
1:d:212:ASN:ND2	1:r:203:GLU:OE1	2.51	0.43
1:k:88:PRO:C	1:k:89:ARG:HG3	2.43	0.43
1:B:162:THR:HB	1:B:177:ASN:ND2	2.32	0.43
1:P:159:ARG:HA	2:P:335:HOH:O	2.18	0.43
1:8:116:ARG:HD2	2:8:353:HOH:O	2.18	0.43
1:b:158:SER:O	1:b:159:ARG:HD2	2.19	0.43
1:c:51:ARG:HG2	1:c:79:PHE:CE2	2.54	0.43
1:p:101:VAL:HG23	1:p:163:PRO:HD3	2.01	0.43
1:v:151:THR:HG22	1:v:155:SER:HB2	2.00	0.43
1:E:89:ARG:HH11	1:E:225:ASN:HD21	1.65	0.43
1:8:100:LYS:HG2	1:8:160:TYR:CZ	2.54	0.43
1:a:116:ARG:HD3	1:a:154:PHE:CE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:186:ARG:HD2	1:p:128:ASN:HB2	2.00	0.43
1:r:72:MET:HE1	1:r:105:PHE:CZ	2.52	0.43
1:C:165:PRO:HB2	1:C:167:LEU:HD13	2.00	0.43
1:R:72:MET:HE1	1:R:105:PHE:CZ	2.53	0.43
1:T:151:THR:HG22	1:T:155:SER:HB2	2.01	0.43
1:8:46:ASN:OD1	1:8:220:GLN:HG3	2.18	0.43
1:X:74:PHE:HE2	1:X:197:GLY:HA3	1.82	0.43
1:2:116:ARG:HD3	1:2:154:PHE:CE2	2.54	0.43
1:4:74:PHE:CE2	1:4:197:GLY:HA3	2.51	0.43
1:a:77:ASN:OD1	1:a:192:ASN:HB2	2.19	0.43
1:a:178:ASN:HB3	2:a:369:HOH:O	2.19	0.43
1:w:60:THR:HB	1:w:62:VAL:HG23	2.00	0.43
1:A:101:VAL:HG23	1:A:163:PRO:HG3	2.01	0.43
1:O:89:ARG:HD2	1:O:187:LEU:HD13	1.99	0.43
1:n:182:GLN:O	1:n:183:LEU:C	2.62	0.43
1:q:99:ARG:NH1	1:q:179:LYS:HA	2.34	0.43
1:q:118:VAL:HG13	1:q:118:VAL:O	2.17	0.43
1:A:99:ARG:NH2	2:A:306:HOH:O	2.51	0.43
1:C:186:ARG:CZ	1:C:188:GLN:HG2	2.48	0.43
1:R:80:LEU:HD12	1:R:80:LEU:HA	1.80	0.43
1:8:98:ILE:HD12	1:8:195:HIS:CD2	2.54	0.43
1:d:108:CYS:HA	1:r:116:ARG:HB2	2.00	0.43
1:f:72:MET:HE1	1:f:105:PHE:CZ	2.53	0.43
1:n:101:VAL:CG2	1:n:163:PRO:HG3	2.49	0.43
1:s:49:LEU:HD13	1:s:80:LEU:HD13	2.00	0.43
1:w:80:LEU:HD23	1:w:187:LEU:HD21	2.01	0.43
1:y:89:ARG:HD2	1:y:187:LEU:HD13	2.01	0.43
1:P:43:SER:HB2	2:P:354:HOH:O	2.18	0.42
1:P:74:PHE:CE2	1:P:197:GLY:HA3	2.54	0.42
1:2:151:THR:HG22	1:2:155:SER:OG	2.18	0.42
1:7:100:LYS:CE	2:7:350:HOH:O	2.67	0.42
1:c:98:ILE:HD12	1:c:195:HIS:CG	2.55	0.42
1:e:224:PHE:O	1:r:144:TYR:HA	2.19	0.42
1:w:80:LEU:HD11	1:w:91:VAL:CG1	2.47	0.42
1:N:52:THR:HA	1:N:213:ILE:O	2.19	0.42
1:R:162:THR:HB	1:R:177:ASN:HD22	1.84	0.42
1:T:89:ARG:HD2	1:T:187:LEU:HD13	2.01	0.42
1:Y:175:GLN:CD	1:Y:183:LEU:HD22	2.44	0.42
1:Z:81:PRO:O	1:Z:90:SER:OG	2.34	0.42
1:7:101:VAL:O	1:7:160:TYR:HA	2.18	0.42
1:l:108:CYS:HB2	1:l:210:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:228:ASP:OD2	1:y:79:PHE:HA	2.19	0.42
1:A:151:THR:HG22	1:A:155:SER:OG	2.19	0.42
1:B:116:ARG:HB2	1:J:108:CYS:HA	2.01	0.42
1:D:151:THR:HG22	1:D:155:SER:HB2	2.01	0.42
1:I:77:ASN:HD21	1:I:192:ASN:H	1.66	0.42
1:N:72:MET:HE1	1:N:105:PHE:CZ	2.54	0.42
1:N:80:LEU:HD11	1:N:91:VAL:HG13	2.02	0.42
1:g:189:THR:C	2:g:303:HOH:O	2.62	0.42
1:l:186:ARG:NH1	1:l:188:GLN:HG2	2.35	0.42
1:m:141:TYR:CZ	1:m:199:GLY:HA3	2.54	0.42
1:s:46:ASN:OD1	1:s:220:GLN:HG3	2.20	0.42
1:s:99:ARG:O	1:s:100:LYS:HD2	2.19	0.42
1:O:230:PRO:C	2:O:331:HOH:O	2.63	0.42
1:9:141:TYR:OH	2:9:301:HOH:O	2.21	0.42
1:m:72:MET:HE1	1:m:105:PHE:CZ	2.54	0.42
1:9:98:ILE:HD12	1:9:195:HIS:CG	2.55	0.42
1:e:101:VAL:CG2	1:e:163:PRO:HG3	2.49	0.42
1:n:144:TYR:HA	1:y:224:PHE:O	2.19	0.42
1:p:178:ASN:OD1	1:p:179:LYS:N	2.52	0.42
1:J:158:SER:O	1:J:159:ARG:HD2	2.19	0.42
1:N:46:ASN:OD1	1:N:220:GLN:HG3	2.19	0.42
1:U:121:SER:O	1:U:147:ARG:HA	2.20	0.42
1:2:51:ARG:HG2	1:2:79:PHE:CE2	2.55	0.42
1:7:136:LEU:HD12	1:7:136:LEU:HA	1.90	0.42
1:8:124:ILE:O	1:8:196:VAL:HG13	2.18	0.42
1:a:74:PHE:CE2	1:a:197:GLY:HA3	2.55	0.42
1:d:80:LEU:HD12	1:e:226:LEU:HD21	2.02	0.42
1:g:108:CYS:HA	1:v:116:ARG:HB2	2.01	0.42
1:r:116:ARG:HD3	1:r:154:PHE:HE2	1.82	0.42
1:D:72:MET:HE1	1:D:105:PHE:CZ	2.55	0.42
1:J:112:THR:HG22	1:Z:112:THR:HG21	2.00	0.42
1:X:67:TRP:CE3	1:X:138:TYR:C	2.98	0.42
1:Z:99:ARG:O	1:Z:100:LYS:HD2	2.20	0.42
1:5:101:VAL:HG23	1:5:163:PRO:HG3	2.01	0.42
1:b:72:MET:HE3	1:b:72:MET:HB2	1.94	0.42
1:c:72:MET:HE1	1:c:105:PHE:CZ	2.54	0.42
1:f:100:LYS:HE2	1:f:162:THR:OG1	2.20	0.42
1:t:121:SER:O	1:t:147:ARG:HA	2.19	0.42
1:u:165:PRO:HB2	1:u:167:LEU:HD13	2.01	0.42
1:y:158:SER:O	1:y:159:ARG:HD2	2.20	0.42
1:I:99:ARG:O	1:I:100:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:61:THR:O	1:M:62:VAL:C	2.62	0.42
1:R:101:VAL:CG2	1:R:163:PRO:HG3	2.49	0.42
1:T:101:VAL:HG23	1:T:163:PRO:CG	2.49	0.42
1:1:103:VAL:O	1:1:158:SER:HA	2.19	0.42
1:5:99:ARG:NH1	1:5:179:LYS:HA	2.34	0.42
1:b:224:PHE:O	1:g:144:TYR:HA	2.19	0.42
1:f:151:THR:O	1:f:155:SER:HB2	2.20	0.42
1:j:89:ARG:HD2	1:j:187:LEU:HD13	2.01	0.42
1:o:151:THR:CG2	1:o:155:SER:CB	2.98	0.42
1:q:74:PHE:HE2	1:q:197:GLY:HA3	1.85	0.42
1:C:116:ARG:HD2	2:C:352:HOH:O	2.19	0.42
1:J:225:ASN:HB2	1:W:144:TYR:CZ	2.55	0.42
1:M:167:LEU:HD22	2:M:306:HOH:O	2.18	0.42
1:N:224:PHE:O	1:5:144:TYR:HA	2.20	0.42
1:8:72:MET:HE1	1:8:105:PHE:CZ	2.55	0.42
1:i:186:ARG:HD2	1:l:128:ASN:HB2	2.02	0.42
1:x:106:TRP:HA	1:x:107:PRO:HD2	1.87	0.42
1:X:89:ARG:HD2	1:X:187:LEU:HD13	2.01	0.42
1:X:116:ARG:HD2	2:X:342:HOH:O	2.19	0.42
1:Y:50:SER:HA	1:Y:215:VAL:O	2.20	0.42
1:2:175:GLN:NE2	1:2:181:ASN:O	2.48	0.42
1:t:76:ILE:HD12	1:t:217:MET:HE1	2.01	0.42
1:C:112:THR:HG21	1:K:112:THR:HB	2.02	0.41
1:G:72:MET:HE1	1:G:105:PHE:CZ	2.55	0.41
1:G:80:LEU:HD12	1:G:80:LEU:HA	1.73	0.41
1:M:116:ARG:HD3	1:M:154:PHE:CE2	2.55	0.41
1:U:89:ARG:HD2	1:U:187:LEU:HD13	2.02	0.41
1:6:44:HIS:CG	2:6:303:HOH:O	2.73	0.41
1:b:124:ILE:O	1:b:196:VAL:HG13	2.20	0.41
1:f:124:ILE:O	1:f:196:VAL:HG13	2.19	0.41
1:h:98:ILE:HD12	1:h:195:HIS:CD2	2.55	0.41
1:u:112:THR:HG21	1:x:112:THR:HB	2.01	0.41
1:E:72:MET:CE	1:E:198:LEU:HD23	2.50	0.41
1:I:49:LEU:HD13	1:I:80:LEU:HD13	2.02	0.41
1:L:98:ILE:HD12	1:L:195:HIS:CE1	2.55	0.41
1:W:46:ASN:OD1	1:W:220:GLN:HG3	2.20	0.41
1:Z:56:THR:HG23	1:Z:210:GLU:HG3	2.02	0.41
1:8:186:ARG:NH1	1:8:188:GLN:HG2	2.34	0.41
1:b:177:ASN:ND2	2:b:307:HOH:O	2.54	0.41
1:k:144:TYR:HA	1:v:224:PHE:O	2.21	0.41
1:p:186:ARG:NH1	1:p:188:GLN:HG2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:230:PRO:O	2:q:301:HOH:O	2.22	0.41
1:t:128:ASN:HB2	1:w:186:ARG:HD2	2.02	0.41
1:x:101:VAL:O	1:x:160:TYR:HA	2.20	0.41
1:F:175:GLN:CD	1:F:183:LEU:HD22	2.46	0.41
1:J:112:THR:HG22	1:Z:112:THR:CG2	2.50	0.41
1:X:165:PRO:HB2	1:X:167:LEU:HD13	2.02	0.41
1:6:186:ARG:HD2	1:i:128:ASN:HB2	2.01	0.41
1:c:103:VAL:O	1:c:158:SER:HA	2.20	0.41
1:i:151:THR:HG22	1:i:155:SER:HB2	2.01	0.41
1:t:203:GLU:OE1	1:v:212:ASN:ND2	2.54	0.41
1:v:116:ARG:HD2	2:v:321:HOH:O	2.18	0.41
1:w:181:ASN:ND2	1:x:181:ASN:ND2	2.68	0.41
1:K:74:PHE:HE2	1:K:197:GLY:HA3	1.85	0.41
1:L:203:GLU:OE1	1:2:212:ASN:ND2	2.52	0.41
1:6:98:ILE:HD12	1:6:195:HIS:CG	2.55	0.41
1:o:101:VAL:CG2	1:o:163:PRO:HG3	2.49	0.41
1:q:101:VAL:HG23	1:q:163:PRO:HG3	2.03	0.41
1:s:212:ASN:ND2	1:u:203:GLU:OE1	2.53	0.41
1:J:224:PHE:O	1:W:144:TYR:HA	2.21	0.41
1:2:44:HIS:CD2	2:2:319:HOH:O	2.74	0.41
1:2:72:MET:HE1	1:2:105:PHE:CZ	2.55	0.41
1:6:89:ARG:HD2	1:6:187:LEU:HD13	2.02	0.41
1:n:80:LEU:HD11	1:n:91:VAL:HG13	2.02	0.41
1:A:116:ARG:HB2	1:E:108:CYS:HA	2.03	0.41
1:K:139:ASP:OD1	1:K:139:ASP:C	2.63	0.41
1:L:139:ASP:OD1	1:L:139:ASP:C	2.64	0.41
1:P:63:LYS:HA	2:P:318:HOH:O	2.20	0.41
1:P:80:LEU:HD23	1:P:187:LEU:HD21	2.02	0.41
1:T:128:ASN:HB2	1:9:186:ARG:HD2	2.01	0.41
1:3:98:ILE:HD12	1:3:195:HIS:CD2	2.56	0.41
1:8:66:SER:HA	1:8:136:LEU:O	2.21	0.41
1:h:61:THR:O	1:h:62:VAL:C	2.63	0.41
1:j:99:ARG:NH2	2:j:301:HOH:O	2.53	0.41
1:m:74:PHE:CE2	1:m:197:GLY:HA3	2.56	0.41
1:t:116:ARG:HD2	2:t:339:HOH:O	2.20	0.41
1:J:121:SER:O	1:J:147:ARG:HA	2.19	0.41
1:Y:99:ARG:O	1:Y:100:LYS:HD2	2.20	0.41
1:9:177:ASN:ND2	2:9:309:HOH:O	2.52	0.41
1:d:121:SER:O	1:d:147:ARG:HA	2.21	0.41
1:l:179:LYS:O	1:l:180:ARG:C	2.64	0.41
1:r:100:LYS:HG2	1:r:160:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:89:ARG:HD3	1:L:188:GLN:C	2.46	0.41
1:7:71:MET:HG2	2:7:352:HOH:O	2.20	0.41
1:7:151:THR:CG2	1:7:155:SER:OG	2.64	0.41
1:7:206:ILE:HG22	1:7:207:TYR:CE2	2.55	0.41
1:8:101:VAL:HG23	1:8:163:PRO:HG3	2.02	0.41
1:9:75:ASN:OD1	1:9:77:ASN:ND2	2.54	0.41
1:9:98:ILE:HD12	1:9:195:HIS:CD2	2.56	0.41
1:b:101:VAL:HG22	1:b:163:PRO:HG3	2.02	0.41
1:c:100:LYS:HG2	1:c:160:TYR:OH	2.21	0.41
1:G:88:PRO:HB2	1:G:189:THR:HG21	2.03	0.41
1:I:46:ASN:OD1	1:I:220:GLN:HG3	2.21	0.41
1:M:165:PRO:HB2	1:M:167:LEU:HD13	2.01	0.41
1:N:80:LEU:HD12	1:N:80:LEU:HA	1.80	0.41
1:O:165:PRO:HB2	1:O:167:LEU:HD13	2.02	0.41
1:S:186:ARG:CZ	1:S:188:GLN:HG2	2.50	0.41
1:T:116:ARG:HD3	1:T:154:PHE:CE2	2.55	0.41
1:W:77:ASN:HD21	1:W:192:ASN:H	1.67	0.41
1:2:101:VAL:HG23	1:2:163:PRO:HG3	2.02	0.41
1:4:144:TYR:HA	1:5:224:PHE:O	2.21	0.41
1:9:165:PRO:HB2	1:9:167:LEU:HD13	2.03	0.41
1:a:58:LYS:HD2	2:a:303:HOH:O	2.21	0.41
1:c:101:VAL:CG2	1:c:163:PRO:HG3	2.51	0.41
1:d:51:ARG:NH2	2:d:303:HOH:O	2.51	0.41
1:f:151:THR:HG22	1:f:155:SER:OG	2.20	0.41
1:i:80:LEU:HD11	1:i:91:VAL:CG1	2.51	0.41
1:j:124:ILE:N	1:j:197:GLY:O	2.42	0.41
1:o:44:HIS:CB	2:o:364:HOH:O	2.55	0.41
1:p:139:ASP:OD1	1:p:139:ASP:C	2.64	0.41
1:p:175:GLN:OE1	1:p:183:LEU:HD22	2.21	0.41
1:v:226:LEU:HD21	1:w:80:LEU:HD12	2.03	0.41
1:x:71:MET:HE3	2:x:329:HOH:O	2.21	0.41
1:x:139:ASP:C	1:x:139:ASP:OD1	2.62	0.41
1:y:167:LEU:HD22	2:y:303:HOH:O	2.21	0.41
1:N:43:SER:HA	2:N:354:HOH:O	2.20	0.41
1:Q:210:GLU:HG3	2:Q:378:HOH:O	2.21	0.41
1:W:162:THR:HB	1:W:177:ASN:HD22	1.85	0.41
1:X:108:CYS:HB2	1:X:210:GLU:HB3	2.03	0.41
1:X:126:ASP:O	1:X:127:ASP:HB3	2.21	0.41
1:r:51:ARG:NH2	2:r:304:HOH:O	2.50	0.41
1:t:142:VAL:HA	1:t:147:ARG:HG3	2.02	0.41
1:A:73:ARG:HG2	1:A:196:VAL:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:107:PRO:HA	1:X:211:TYR:CD2	2.55	0.40
1:5:74:PHE:CE2	1:5:197:GLY:HA3	2.56	0.40
1:a:158:SER:O	1:a:159:ARG:HD2	2.20	0.40
1:h:101:VAL:HG12	1:h:102:LYS:N	2.35	0.40
1:i:74:PHE:CE2	1:i:197:GLY:HA3	2.54	0.40
1:p:49:LEU:HD13	1:p:80:LEU:HD13	2.03	0.40
1:u:74:PHE:HE2	1:u:197:GLY:HA3	1.86	0.40
1:B:186:ARG:HD2	1:G:128:ASN:HB2	2.04	0.40
1:C:101:VAL:CG2	1:C:163:PRO:HG3	2.52	0.40
1:K:168:ASP:OD1	1:K:170:THR:HB	2.21	0.40
1:P:121:SER:O	1:P:147:ARG:HA	2.21	0.40
1:e:186:ARG:HD2	1:r:128:ASN:HB2	2.03	0.40
1:o:176:PRO:O	1:o:177:ASN:C	2.64	0.40
1:q:116:ARG:HD2	2:q:333:HOH:O	2.21	0.40
1:t:131:THR:HG22	1:t:132:LYS:O	2.21	0.40
1:J:111:ILE:HB	1:Z:111:ILE:HD11	2.04	0.40
1:m:80:LEU:HD12	1:m:80:LEU:HA	1.85	0.40
1:x:51:ARG:NH2	2:x:304:HOH:O	2.49	0.40
1:C:74:PHE:HE2	1:C:197:GLY:HA3	1.87	0.40
1:G:101:VAL:CG2	1:G:163:PRO:HG3	2.50	0.40
1:K:72:MET:HE1	1:K:105:PHE:CZ	2.56	0.40
1:Q:106:TRP:HA	1:Q:107:PRO:HD2	1.91	0.40
1:a:143:ASN:OD1	1:r:49:LEU:HA	2.21	0.40
1:b:186:ARG:CZ	1:b:188:GLN:HG2	2.52	0.40
1:h:99:ARG:O	1:h:100:LYS:HD2	2.20	0.40
1:l:136:LEU:HD12	1:l:136:LEU:HA	1.94	0.40
1:l:158:SER:O	1:l:159:ARG:HD2	2.21	0.40
1:s:80:LEU:HD21	1:s:91:VAL:HG22	2.02	0.40
1:N:94:GLU:OE1	1:5:126:ASP:OD2	2.39	0.40
1:3:80:LEU:HD11	1:3:91:VAL:HG13	2.04	0.40
1:f:224:PHE:O	1:v:144:TYR:HA	2.21	0.40
1:i:100:LYS:HG2	1:i:160:TYR:CZ	2.56	0.40
1:q:164:LYS:NZ	1:q:175:GLN:O	2.52	0.40
1:s:88:PRO:C	1:s:89:ARG:HG3	2.47	0.40
1:v:72:MET:CE	1:v:198:LEU:HD23	2.51	0.40
1:y:99:ARG:NH2	2:y:307:HOH:O	2.54	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:385:HOH:O	2:q:376:HOH:O[2_555]	2.13	0.07

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	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	24	55
1	2	187/209 (90%)	174 (93%)	12 (6%)	1 (0%)	24	55
1	3	186/209 (89%)	175 (94%)	9 (5%)	2 (1%)	11	36
1	4	186/209 (89%)	172 (92%)	13 (7%)	1 (0%)	24	55
1	5	186/209 (89%)	179 (96%)	7 (4%)	0	100	100
1	6	186/209 (89%)	178 (96%)	7 (4%)	1 (0%)	24	55
1	7	186/209 (89%)	178 (96%)	6 (3%)	2 (1%)	11	36
1	8	186/209 (89%)	172 (92%)	13 (7%)	1 (0%)	24	55
1	9	187/209 (90%)	177 (95%)	8 (4%)	2 (1%)	11	36
1	A	186/209 (89%)	178 (96%)	7 (4%)	1 (0%)	24	55
1	B	186/209 (89%)	176 (95%)	9 (5%)	1 (0%)	24	55
1	C	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	24	55
1	D	186/209 (89%)	176 (95%)	10 (5%)	0	100	100
1	E	186/209 (89%)	176 (95%)	10 (5%)	0	100	100
1	F	186/209 (89%)	173 (93%)	13 (7%)	0	100	100
1	G	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	24	55
1	H	186/209 (89%)	173 (93%)	12 (6%)	1 (0%)	24	55
1	I	186/209 (89%)	176 (95%)	10 (5%)	0	100	100
1	J	186/209 (89%)	173 (93%)	12 (6%)	1 (0%)	24	55
1	K	186/209 (89%)	172 (92%)	12 (6%)	2 (1%)	11	36
1	L	187/209 (90%)	179 (96%)	7 (4%)	1 (0%)	24	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	186/209 (89%)	176 (95%)	8 (4%)	2 (1%)	11	36
1	N	186/209 (89%)	175 (94%)	11 (6%)	0	100	100
1	O	186/209 (89%)	173 (93%)	12 (6%)	1 (0%)	24	55
1	P	186/209 (89%)	174 (94%)	10 (5%)	2 (1%)	11	36
1	Q	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	24	55
1	R	186/209 (89%)	173 (93%)	11 (6%)	2 (1%)	11	36
1	S	186/209 (89%)	179 (96%)	6 (3%)	1 (0%)	24	55
1	T	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	24	55
1	U	186/209 (89%)	173 (93%)	10 (5%)	3 (2%)	7	27
1	V	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	24	55
1	W	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	24	55
1	X	186/209 (89%)	170 (91%)	15 (8%)	1 (0%)	24	55
1	Y	186/209 (89%)	171 (92%)	12 (6%)	3 (2%)	7	27
1	Z	186/209 (89%)	173 (93%)	13 (7%)	0	100	100
1	a	187/209 (90%)	176 (94%)	9 (5%)	2 (1%)	11	36
1	b	186/209 (89%)	176 (95%)	8 (4%)	2 (1%)	11	36
1	c	186/209 (89%)	175 (94%)	8 (4%)	3 (2%)	7	27
1	d	186/209 (89%)	172 (92%)	12 (6%)	2 (1%)	11	36
1	e	187/209 (90%)	178 (95%)	7 (4%)	2 (1%)	11	36
1	f	186/209 (89%)	175 (94%)	11 (6%)	0	100	100
1	g	186/209 (89%)	174 (94%)	10 (5%)	2 (1%)	11	36
1	h	186/209 (89%)	169 (91%)	16 (9%)	1 (0%)	24	55
1	i	186/209 (89%)	175 (94%)	11 (6%)	0	100	100
1	j	186/209 (89%)	172 (92%)	12 (6%)	2 (1%)	11	36
1	k	187/209 (90%)	172 (92%)	13 (7%)	2 (1%)	11	36
1	l	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	24	55
1	m	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	24	55
1	n	186/209 (89%)	177 (95%)	7 (4%)	2 (1%)	11	36
1	o	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	24	55
1	p	187/209 (90%)	179 (96%)	8 (4%)	0	100	100
1	q	186/209 (89%)	176 (95%)	9 (5%)	1 (0%)	24	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	r	187/209 (90%)	179 (96%)	7 (4%)	1 (0%)	24	55
1	s	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	24	55
1	t	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	24	55
1	u	186/209 (89%)	173 (93%)	11 (6%)	2 (1%)	11	36
1	v	186/209 (89%)	177 (95%)	9 (5%)	0	100	100
1	w	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	24	55
1	x	187/209 (90%)	177 (95%)	8 (4%)	2 (1%)	11	36
1	y	187/209 (90%)	173 (92%)	13 (7%)	1 (0%)	24	55
All	All	11170/12540 (89%)	10499 (94%)	599 (5%)	72 (1%)	21	51

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	62	VAL
1	g	189	THR
1	Y	62	VAL
1	k	59	ARG
1	A	178	ASN
1	K	223	GLU
1	Q	197	GLY
1	R	178	ASN
1	R	197	GLY
1	d	197	GLY
1	h	223	GLU
1	q	190	ALA
1	y	197	GLY
1	L	197	GLY
1	U	197	GLY
1	X	197	GLY
1	2	197	GLY
1	6	197	GLY
1	7	62	VAL
1	7	172	ASP
1	c	197	GLY
1	e	223	GLU
1	n	197	GLY
1	n	223	GLU
1	r	197	GLY
1	u	62	VAL

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Mol	Chain	Res	Type
1	C	197	GLY
1	K	197	GLY
1	P	197	GLY
1	W	197	GLY
1	Y	178	ASN
1	3	223	GLU
1	8	197	GLY
1	9	197	GLY
1	a	197	GLY
1	b	223	GLU
1	c	223	GLU
1	k	230	PRO
1	l	197	GLY
1	t	197	GLY
1	B	197	GLY
1	G	197	GLY
1	H	115	ASP
1	M	197	GLY
1	U	223	GLU
1	3	197	GLY
1	4	197	GLY
1	9	92	PRO
1	a	230	PRO
1	d	223	GLU
1	j	197	GLY
1	J	197	GLY
1	M	62	VAL
1	T	197	GLY
1	U	92	PRO
1	V	197	GLY
1	Y	197	GLY
1	o	197	GLY
1	u	197	GLY
1	x	62	VAL
1	e	197	GLY
1	x	197	GLY
1	O	197	GLY
1	b	197	GLY
1	c	62	VAL
1	j	65	PRO
1	m	62	VAL
1	s	197	GLY

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Mol	Chain	Res	Type
1	S	197	GLY
1	1	62	VAL
1	g	197	GLY
1	w	62	VAL

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	172/190 (90%)	160 (93%)	12 (7%)	14	40
1	2	173/190 (91%)	160 (92%)	13 (8%)	12	37
1	3	172/190 (90%)	155 (90%)	17 (10%)	7	24
1	4	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	5	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	6	172/190 (90%)	161 (94%)	11 (6%)	16	44
1	7	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	8	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	9	173/190 (91%)	158 (91%)	15 (9%)	9	30
1	A	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	B	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	C	172/190 (90%)	153 (89%)	19 (11%)	6	20
1	D	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	E	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	F	172/190 (90%)	159 (92%)	13 (8%)	12	36
1	G	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	H	172/190 (90%)	155 (90%)	17 (10%)	7	24
1	I	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	J	172/190 (90%)	153 (89%)	19 (11%)	6	20
1	K	172/190 (90%)	158 (92%)	14 (8%)	11	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	173/190 (91%)	155 (90%)	18 (10%)	7	22
1	M	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	N	172/190 (90%)	159 (92%)	13 (8%)	12	36
1	O	172/190 (90%)	155 (90%)	17 (10%)	7	24
1	P	172/190 (90%)	159 (92%)	13 (8%)	12	36
1	Q	172/190 (90%)	159 (92%)	13 (8%)	12	36
1	R	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	S	172/190 (90%)	159 (92%)	13 (8%)	12	36
1	T	172/190 (90%)	155 (90%)	17 (10%)	7	24
1	U	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	V	172/190 (90%)	161 (94%)	11 (6%)	16	44
1	W	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	X	172/190 (90%)	154 (90%)	18 (10%)	6	22
1	Y	172/190 (90%)	151 (88%)	21 (12%)	5	16
1	Z	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	a	173/190 (91%)	155 (90%)	18 (10%)	7	22
1	b	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	c	172/190 (90%)	153 (89%)	19 (11%)	6	20
1	d	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	e	173/190 (91%)	156 (90%)	17 (10%)	7	25
1	f	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	g	172/190 (90%)	155 (90%)	17 (10%)	7	24
1	h	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	i	172/190 (90%)	154 (90%)	18 (10%)	6	22
1	j	172/190 (90%)	153 (89%)	19 (11%)	6	20
1	k	173/190 (91%)	158 (91%)	15 (9%)	9	30
1	l	172/190 (90%)	160 (93%)	12 (7%)	14	40
1	m	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	n	172/190 (90%)	160 (93%)	12 (7%)	14	40
1	o	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	p	173/190 (91%)	159 (92%)	14 (8%)	11	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	q	172/190 (90%)	159 (92%)	13 (8%)	12	36
1	r	173/190 (91%)	157 (91%)	16 (9%)	8	27
1	s	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	t	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	u	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	v	172/190 (90%)	159 (92%)	13 (8%)	12	36
1	w	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	x	173/190 (91%)	160 (92%)	13 (8%)	12	37
1	y	173/190 (91%)	157 (91%)	16 (9%)	8	27
All	All	10330/11400 (91%)	9413 (91%)	917 (9%)	9	29

All (917) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	60	THR
1	A	91	VAL
1	A	95	TYR
1	A	99	ARG
1	A	100	LYS
1	A	151	THR
1	A	167	LEU
1	A	178	ASN
1	A	183	LEU
1	A	187	LEU
1	A	189	THR
1	A	196	VAL
1	A	206	ILE
1	A	217	MET
1	B	48	ARG
1	B	59	ARG
1	B	63	LYS
1	B	91	VAL
1	B	99	ARG
1	B	100	LYS
1	B	151	THR
1	B	167	LEU
1	B	180	ARG
1	B	183	LEU

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Mol	Chain	Res	Type
1	B	187	LEU
1	B	189	THR
1	B	196	VAL
1	B	206	ILE
1	B	217	MET
1	C	47	THR
1	C	58	LYS
1	C	59	ARG
1	C	61	THR
1	C	63	LYS
1	C	71	MET
1	C	80	LEU
1	C	91	VAL
1	C	99	ARG
1	C	100	LYS
1	C	101	VAL
1	C	102	LYS
1	C	151	THR
1	C	167	LEU
1	C	183	LEU
1	C	187	LEU
1	C	196	VAL
1	C	206	ILE
1	C	210	GLU
1	D	44	HIS
1	D	58	LYS
1	D	59	ARG
1	D	63	LYS
1	D	72	MET
1	D	91	VAL
1	D	99	ARG
1	D	109	SER
1	D	151	THR
1	D	167	LEU
1	D	179	LYS
1	D	183	LEU
1	D	187	LEU
1	D	196	VAL
1	D	206	ILE
1	E	59	ARG
1	E	61	THR
1	E	63	LYS

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Mol	Chain	Res	Type
1	E	91	VAL
1	E	99	ARG
1	E	151	THR
1	E	167	LEU
1	E	169	SER
1	E	177	ASN
1	E	179	LYS
1	E	180	ARG
1	E	183	LEU
1	E	187	LEU
1	E	196	VAL
1	E	206	ILE
1	F	58	LYS
1	F	59	ARG
1	F	61	THR
1	F	63	LYS
1	F	91	VAL
1	F	99	ARG
1	F	151	THR
1	F	167	LEU
1	F	183	LEU
1	F	187	LEU
1	F	196	VAL
1	F	206	ILE
1	F	210	GLU
1	G	58	LYS
1	G	59	ARG
1	G	61	THR
1	G	63	LYS
1	G	71	MET
1	G	91	VAL
1	G	99	ARG
1	G	151	THR
1	G	167	LEU
1	G	180	ARG
1	G	183	LEU
1	G	187	LEU
1	G	189	THR
1	G	196	VAL
1	G	206	ILE
1	G	210	GLU
1	H	47	THR

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Mol	Chain	Res	Type
1	H	59	ARG
1	H	60	THR
1	H	91	VAL
1	H	99	ARG
1	H	100	LYS
1	H	132	LYS
1	H	134	THR
1	H	151	THR
1	H	167	LEU
1	H	179	LYS
1	H	180	ARG
1	H	183	LEU
1	H	187	LEU
1	H	196	VAL
1	H	206	ILE
1	H	217	MET
1	I	58	LYS
1	I	59	ARG
1	I	61	THR
1	I	63	LYS
1	I	91	VAL
1	I	99	ARG
1	I	136	LEU
1	I	151	THR
1	I	167	LEU
1	I	179	LYS
1	I	180	ARG
1	I	183	LEU
1	I	187	LEU
1	I	189	THR
1	I	196	VAL
1	I	206	ILE
1	J	43	SER
1	J	59	ARG
1	J	61	THR
1	J	63	LYS
1	J	71	MET
1	J	90	SER
1	J	91	VAL
1	J	99	ARG
1	J	100	LYS
1	J	111	ILE

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Mol	Chain	Res	Type
1	J	151	THR
1	J	167	LEU
1	J	176	PRO
1	J	180	ARG
1	J	183	LEU
1	J	187	LEU
1	J	196	VAL
1	J	206	ILE
1	J	226	LEU
1	K	59	ARG
1	K	91	VAL
1	K	99	ARG
1	K	101	VAL
1	K	136	LEU
1	K	153	PRO
1	K	167	LEU
1	K	170	THR
1	K	183	LEU
1	K	187	LEU
1	K	189	THR
1	K	196	VAL
1	K	206	ILE
1	K	210	GLU
1	L	58	LYS
1	L	59	ARG
1	L	61	THR
1	L	63	LYS
1	L	91	VAL
1	L	99	ARG
1	L	109	SER
1	L	151	THR
1	L	153	PRO
1	L	167	LEU
1	L	177	ASN
1	L	179	LYS
1	L	180	ARG
1	L	183	LEU
1	L	187	LEU
1	L	189	THR
1	L	196	VAL
1	L	206	ILE
1	M	58	LYS

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Mol	Chain	Res	Type
1	M	59	ARG
1	M	61	THR
1	M	63	LYS
1	M	91	VAL
1	M	99	ARG
1	M	151	THR
1	M	167	LEU
1	M	169	SER
1	M	183	LEU
1	M	187	LEU
1	M	189	THR
1	M	196	VAL
1	M	206	ILE
1	N	43	SER
1	N	58	LYS
1	N	59	ARG
1	N	63	LYS
1	N	99	ARG
1	N	151	THR
1	N	167	LEU
1	N	179	LYS
1	N	183	LEU
1	N	187	LEU
1	N	196	VAL
1	N	206	ILE
1	N	210	GLU
1	O	59	ARG
1	O	63	LYS
1	O	80	LEU
1	O	91	VAL
1	O	99	ARG
1	O	109	SER
1	O	151	THR
1	O	153	PRO
1	O	167	LEU
1	O	170	THR
1	O	179	LYS
1	O	180	ARG
1	O	183	LEU
1	O	187	LEU
1	O	189	THR
1	O	196	VAL

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Mol	Chain	Res	Type
1	O	206	ILE
1	P	59	ARG
1	P	61	THR
1	P	91	VAL
1	P	99	ARG
1	P	151	THR
1	P	167	LEU
1	P	180	ARG
1	P	183	LEU
1	P	187	LEU
1	P	189	THR
1	P	196	VAL
1	P	206	ILE
1	P	210	GLU
1	Q	59	ARG
1	Q	63	LYS
1	Q	91	VAL
1	Q	99	ARG
1	Q	151	THR
1	Q	167	LEU
1	Q	169	SER
1	Q	183	LEU
1	Q	187	LEU
1	Q	189	THR
1	Q	196	VAL
1	Q	206	ILE
1	Q	210	GLU
1	R	47	THR
1	R	59	ARG
1	R	61	THR
1	R	63	LYS
1	R	80	LEU
1	R	89	ARG
1	R	91	VAL
1	R	99	ARG
1	R	151	THR
1	R	167	LEU
1	R	179	LYS
1	R	183	LEU
1	R	187	LEU
1	R	196	VAL
1	R	206	ILE

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Mol	Chain	Res	Type
1	R	210	GLU
1	S	59	ARG
1	S	61	THR
1	S	63	LYS
1	S	91	VAL
1	S	99	ARG
1	S	151	THR
1	S	167	LEU
1	S	183	LEU
1	S	187	LEU
1	S	189	THR
1	S	196	VAL
1	S	206	ILE
1	S	226	LEU
1	T	43	SER
1	T	44	HIS
1	T	47	THR
1	T	59	ARG
1	T	63	LYS
1	T	80	LEU
1	T	89	ARG
1	T	99	ARG
1	T	100	LYS
1	T	151	THR
1	T	167	LEU
1	T	183	LEU
1	T	187	LEU
1	T	189	THR
1	T	196	VAL
1	T	206	ILE
1	T	210	GLU
1	U	50	SER
1	U	59	ARG
1	U	63	LYS
1	U	80	LEU
1	U	91	VAL
1	U	99	ARG
1	U	111	ILE
1	U	151	THR
1	U	167	LEU
1	U	170	THR
1	U	183	LEU

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Mol	Chain	Res	Type
1	U	187	LEU
1	U	189	THR
1	U	196	VAL
1	U	206	ILE
1	U	210	GLU
1	V	59	ARG
1	V	63	LYS
1	V	91	VAL
1	V	99	ARG
1	V	151	THR
1	V	167	LEU
1	V	183	LEU
1	V	187	LEU
1	V	189	THR
1	V	196	VAL
1	V	206	ILE
1	W	43	SER
1	W	59	ARG
1	W	63	LYS
1	W	70	ASP
1	W	80	LEU
1	W	89	ARG
1	W	90	SER
1	W	99	ARG
1	W	109	SER
1	W	151	THR
1	W	167	LEU
1	W	179	LYS
1	W	183	LEU
1	W	187	LEU
1	W	196	VAL
1	W	206	ILE
1	X	47	THR
1	X	58	LYS
1	X	59	ARG
1	X	63	LYS
1	X	71	MET
1	X	91	VAL
1	X	99	ARG
1	X	136	LEU
1	X	151	THR
1	X	167	LEU

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Mol	Chain	Res	Type
1	X	180	ARG
1	X	183	LEU
1	X	187	LEU
1	X	189	THR
1	X	196	VAL
1	X	198	LEU
1	X	206	ILE
1	X	226	LEU
1	Y	44	HIS
1	Y	47	THR
1	Y	59	ARG
1	Y	61	THR
1	Y	70	ASP
1	Y	80	LEU
1	Y	82	PRO
1	Y	91	VAL
1	Y	95	TYR
1	Y	99	ARG
1	Y	109	SER
1	Y	151	THR
1	Y	153	PRO
1	Y	167	LEU
1	Y	169	SER
1	Y	180	ARG
1	Y	183	LEU
1	Y	187	LEU
1	Y	189	THR
1	Y	196	VAL
1	Y	206	ILE
1	Z	43	SER
1	Z	59	ARG
1	Z	61	THR
1	Z	89	ARG
1	Z	90	SER
1	Z	99	ARG
1	Z	101	VAL
1	Z	151	THR
1	Z	167	LEU
1	Z	180	ARG
1	Z	183	LEU
1	Z	187	LEU
1	Z	196	VAL

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Mol	Chain	Res	Type
1	Z	206	ILE
1	Z	210	GLU
1	1	58	LYS
1	1	59	ARG
1	1	91	VAL
1	1	99	ARG
1	1	111	ILE
1	1	151	THR
1	1	167	LEU
1	1	183	LEU
1	1	187	LEU
1	1	196	VAL
1	1	206	ILE
1	1	210	GLU
1	2	44	HIS
1	2	59	ARG
1	2	63	LYS
1	2	99	ARG
1	2	109	SER
1	2	151	THR
1	2	167	LEU
1	2	180	ARG
1	2	183	LEU
1	2	187	LEU
1	2	189	THR
1	2	196	VAL
1	2	206	ILE
1	3	44	HIS
1	3	59	ARG
1	3	61	THR
1	3	63	LYS
1	3	91	VAL
1	3	99	ARG
1	3	100	LYS
1	3	111	ILE
1	3	151	THR
1	3	167	LEU
1	3	180	ARG
1	3	183	LEU
1	3	187	LEU
1	3	189	THR
1	3	196	VAL

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Mol	Chain	Res	Type
1	3	206	ILE
1	3	210	GLU
1	4	59	ARG
1	4	61	THR
1	4	63	LYS
1	4	80	LEU
1	4	91	VAL
1	4	99	ARG
1	4	111	ILE
1	4	118	VAL
1	4	151	THR
1	4	167	LEU
1	4	183	LEU
1	4	187	LEU
1	4	189	THR
1	4	196	VAL
1	4	206	ILE
1	4	210	GLU
1	5	58	LYS
1	5	59	ARG
1	5	63	LYS
1	5	90	SER
1	5	91	VAL
1	5	99	ARG
1	5	100	LYS
1	5	111	ILE
1	5	151	THR
1	5	167	LEU
1	5	180	ARG
1	5	183	LEU
1	5	187	LEU
1	5	196	VAL
1	5	206	ILE
1	5	210	GLU
1	6	59	ARG
1	6	63	LYS
1	6	91	VAL
1	6	99	ARG
1	6	151	THR
1	6	167	LEU
1	6	183	LEU
1	6	187	LEU

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Mol	Chain	Res	Type
1	6	196	VAL
1	6	206	ILE
1	6	210	GLU
1	7	59	ARG
1	7	61	THR
1	7	71	MET
1	7	91	VAL
1	7	99	ARG
1	7	100	LYS
1	7	151	THR
1	7	167	LEU
1	7	183	LEU
1	7	187	LEU
1	7	189	THR
1	7	196	VAL
1	7	206	ILE
1	7	210	GLU
1	8	58	LYS
1	8	59	ARG
1	8	61	THR
1	8	63	LYS
1	8	89	ARG
1	8	91	VAL
1	8	99	ARG
1	8	151	THR
1	8	167	LEU
1	8	179	LYS
1	8	180	ARG
1	8	183	LEU
1	8	187	LEU
1	8	189	THR
1	8	196	VAL
1	8	206	ILE
1	9	59	ARG
1	9	61	THR
1	9	91	VAL
1	9	99	ARG
1	9	100	LYS
1	9	111	ILE
1	9	151	THR
1	9	167	LEU
1	9	179	LYS

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Mol	Chain	Res	Type
1	9	180	ARG
1	9	183	LEU
1	9	187	LEU
1	9	189	THR
1	9	196	VAL
1	9	206	ILE
1	a	43	SER
1	a	58	LYS
1	a	59	ARG
1	a	61	THR
1	a	63	LYS
1	a	91	VAL
1	a	99	ARG
1	a	100	LYS
1	a	151	THR
1	a	167	LEU
1	a	179	LYS
1	a	180	ARG
1	a	183	LEU
1	a	187	LEU
1	a	189	THR
1	a	196	VAL
1	a	206	ILE
1	a	231	LEU
1	b	43	SER
1	b	58	LYS
1	b	59	ARG
1	b	61	THR
1	b	99	ARG
1	b	101	VAL
1	b	111	ILE
1	b	151	THR
1	b	167	LEU
1	b	169	SER
1	b	177	ASN
1	b	183	LEU
1	b	187	LEU
1	b	196	VAL
1	b	206	ILE
1	c	43	SER
1	c	59	ARG
1	c	61	THR

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Mol	Chain	Res	Type
1	c	63	LYS
1	c	90	SER
1	c	91	VAL
1	c	99	ARG
1	c	102	LYS
1	c	111	ILE
1	c	151	THR
1	c	167	LEU
1	c	168	ASP
1	c	179	LYS
1	c	180	ARG
1	c	183	LEU
1	c	187	LEU
1	c	189	THR
1	c	196	VAL
1	c	206	ILE
1	d	43	SER
1	d	44	HIS
1	d	59	ARG
1	d	63	LYS
1	d	91	VAL
1	d	99	ARG
1	d	101	VAL
1	d	151	THR
1	d	167	LEU
1	d	179	LYS
1	d	183	LEU
1	d	187	LEU
1	d	189	THR
1	d	196	VAL
1	d	206	ILE
1	e	58	LYS
1	e	59	ARG
1	e	63	LYS
1	e	80	LEU
1	e	91	VAL
1	e	99	ARG
1	e	101	VAL
1	e	111	ILE
1	e	151	THR
1	e	167	LEU
1	e	176	PRO

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Mol	Chain	Res	Type
1	e	180	ARG
1	e	183	LEU
1	e	187	LEU
1	e	196	VAL
1	e	206	ILE
1	e	210	GLU
1	f	58	LYS
1	f	59	ARG
1	f	63	LYS
1	f	91	VAL
1	f	99	ARG
1	f	100	LYS
1	f	151	THR
1	f	167	LEU
1	f	179	LYS
1	f	180	ARG
1	f	183	LEU
1	f	187	LEU
1	f	189	THR
1	f	196	VAL
1	f	206	ILE
1	f	210	GLU
1	g	49	LEU
1	g	59	ARG
1	g	63	LYS
1	g	70	ASP
1	g	99	ARG
1	g	109	SER
1	g	111	ILE
1	g	132	LYS
1	g	151	THR
1	g	153	PRO
1	g	167	LEU
1	g	179	LYS
1	g	183	LEU
1	g	187	LEU
1	g	189	THR
1	g	196	VAL
1	g	206	ILE
1	h	59	ARG
1	h	63	LYS
1	h	72	MET

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Mol	Chain	Res	Type
1	h	91	VAL
1	h	99	ARG
1	h	102	LYS
1	h	151	THR
1	h	167	LEU
1	h	179	LYS
1	h	180	ARG
1	h	183	LEU
1	h	187	LEU
1	h	196	VAL
1	h	206	ILE
1	h	226	LEU
1	i	43	SER
1	i	44	HIS
1	i	50	SER
1	i	58	LYS
1	i	59	ARG
1	i	70	ASP
1	i	89	ARG
1	i	91	VAL
1	i	99	ARG
1	i	151	THR
1	i	167	LEU
1	i	179	LYS
1	i	180	ARG
1	i	183	LEU
1	i	187	LEU
1	i	196	VAL
1	i	200	THR
1	i	206	ILE
1	j	43	SER
1	j	44	HIS
1	j	47	THR
1	j	59	ARG
1	j	63	LYS
1	j	66	SER
1	j	91	VAL
1	j	99	ARG
1	j	100	LYS
1	j	101	VAL
1	j	109	SER
1	j	151	THR

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Mol	Chain	Res	Type
1	j	167	LEU
1	j	180	ARG
1	j	183	LEU
1	j	187	LEU
1	j	196	VAL
1	j	206	ILE
1	j	210	GLU
1	k	43	SER
1	k	44	HIS
1	k	91	VAL
1	k	99	ARG
1	k	100	LYS
1	k	151	THR
1	k	167	LEU
1	k	183	LEU
1	k	187	LEU
1	k	189	THR
1	k	196	VAL
1	k	206	ILE
1	k	210	GLU
1	k	214	ARG
1	k	231	LEU
1	l	59	ARG
1	l	63	LYS
1	l	72	MET
1	l	91	VAL
1	l	99	ARG
1	l	151	THR
1	l	167	LEU
1	l	177	ASN
1	l	183	LEU
1	l	187	LEU
1	l	196	VAL
1	l	206	ILE
1	m	59	ARG
1	m	61	THR
1	m	63	LYS
1	m	89	ARG
1	m	91	VAL
1	m	99	ARG
1	m	167	LEU
1	m	180	ARG

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Mol	Chain	Res	Type
1	m	183	LEU
1	m	187	LEU
1	m	189	THR
1	m	196	VAL
1	m	206	ILE
1	m	210	GLU
1	m	226	LEU
1	n	44	HIS
1	n	59	ARG
1	n	91	VAL
1	n	99	ARG
1	n	151	THR
1	n	167	LEU
1	n	179	LYS
1	n	180	ARG
1	n	183	LEU
1	n	187	LEU
1	n	196	VAL
1	n	206	ILE
1	o	44	HIS
1	o	63	LYS
1	o	89	ARG
1	o	91	VAL
1	o	99	ARG
1	o	102	LYS
1	o	132	LYS
1	o	151	THR
1	o	167	LEU
1	o	179	LYS
1	o	180	ARG
1	o	183	LEU
1	o	187	LEU
1	o	196	VAL
1	o	206	ILE
1	o	210	GLU
1	p	47	THR
1	p	59	ARG
1	p	61	THR
1	p	63	LYS
1	p	89	ARG
1	p	91	VAL
1	p	99	ARG

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Mol	Chain	Res	Type
1	p	151	THR
1	p	167	LEU
1	p	183	LEU
1	p	187	LEU
1	p	196	VAL
1	p	206	ILE
1	p	210	GLU
1	q	59	ARG
1	q	63	LYS
1	q	95	TYR
1	q	99	ARG
1	q	100	LYS
1	q	167	LEU
1	q	179	LYS
1	q	180	ARG
1	q	183	LEU
1	q	187	LEU
1	q	189	THR
1	q	196	VAL
1	q	206	ILE
1	r	58	LYS
1	r	59	ARG
1	r	63	LYS
1	r	90	SER
1	r	91	VAL
1	r	99	ARG
1	r	151	THR
1	r	167	LEU
1	r	180	ARG
1	r	183	LEU
1	r	187	LEU
1	r	189	THR
1	r	196	VAL
1	r	206	ILE
1	r	210	GLU
1	r	231	LEU
1	s	59	ARG
1	s	61	THR
1	s	63	LYS
1	s	99	ARG
1	s	111	ILE
1	s	151	THR

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Mol	Chain	Res	Type
1	s	167	LEU
1	s	179	LYS
1	s	180	ARG
1	s	183	LEU
1	s	187	LEU
1	s	196	VAL
1	s	206	ILE
1	s	210	GLU
1	t	59	ARG
1	t	61	THR
1	t	63	LYS
1	t	91	VAL
1	t	99	ARG
1	t	151	THR
1	t	167	LEU
1	t	179	LYS
1	t	183	LEU
1	t	187	LEU
1	t	189	THR
1	t	196	VAL
1	t	206	ILE
1	t	210	GLU
1	u	43	SER
1	u	59	ARG
1	u	61	THR
1	u	63	LYS
1	u	91	VAL
1	u	99	ARG
1	u	100	LYS
1	u	151	THR
1	u	167	LEU
1	u	183	LEU
1	u	187	LEU
1	u	189	THR
1	u	196	VAL
1	u	205	SER
1	u	206	ILE
1	u	210	GLU
1	v	63	LYS
1	v	82	PRO
1	v	91	VAL
1	v	99	ARG

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Mol	Chain	Res	Type
1	v	118	VAL
1	v	151	THR
1	v	167	LEU
1	v	169	SER
1	v	183	LEU
1	v	187	LEU
1	v	196	VAL
1	v	206	ILE
1	v	210	GLU
1	w	44	HIS
1	w	59	ARG
1	w	63	LYS
1	w	71	MET
1	w	91	VAL
1	w	99	ARG
1	w	109	SER
1	w	151	THR
1	w	167	LEU
1	w	183	LEU
1	w	187	LEU
1	w	196	VAL
1	w	206	ILE
1	w	210	GLU
1	x	44	HIS
1	x	59	ARG
1	x	63	LYS
1	x	71	MET
1	x	91	VAL
1	x	99	ARG
1	x	151	THR
1	x	167	LEU
1	x	177	ASN
1	x	183	LEU
1	x	187	LEU
1	x	196	VAL
1	x	206	ILE
1	y	59	ARG
1	y	61	THR
1	y	63	LYS
1	y	91	VAL
1	y	99	ARG
1	y	101	VAL

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Mol	Chain	Res	Type
1	y	151	THR
1	y	167	LEU
1	y	180	ARG
1	y	183	LEU
1	y	185	LEU
1	y	187	LEU
1	y	189	THR
1	y	196	VAL
1	y	206	ILE
1	y	210	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	A	212	ASN
1	B	44	HIS
1	B	177	ASN
1	B	182	GLN
1	B	188	GLN
1	C	128	ASN
1	C	177	ASN
1	C	181	ASN
1	C	212	ASN
1	D	177	ASN
1	D	204	ASN
1	D	212	ASN
1	E	212	ASN
1	F	195	HIS
1	F	212	ASN
1	G	177	ASN
1	G	181	ASN
1	G	204	ASN
1	G	212	ASN
1	H	188	GLN
1	I	181	ASN
1	I	188	GLN
1	I	212	ASN
1	J	212	ASN
1	K	77	ASN
1	K	148	HIS
1	K	188	GLN

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Mol	Chain	Res	Type
1	K	192	ASN
1	K	212	ASN
1	L	181	ASN
1	L	212	ASN
1	M	148	HIS
1	M	182	GLN
1	M	212	ASN
1	N	148	HIS
1	N	212	ASN
1	O	212	ASN
1	P	188	GLN
1	P	212	ASN
1	Q	177	ASN
1	Q	188	GLN
1	Q	204	ASN
1	Q	212	ASN
1	R	177	ASN
1	R	212	ASN
1	S	177	ASN
1	S	188	GLN
1	S	204	ASN
1	S	212	ASN
1	T	204	ASN
1	T	212	ASN
1	U	44	HIS
1	U	188	GLN
1	U	212	ASN
1	V	113	GLN
1	V	181	ASN
1	V	212	ASN
1	W	177	ASN
1	W	204	ASN
1	W	212	ASN
1	X	77	ASN
1	X	177	ASN
1	X	192	ASN
1	X	195	HIS
1	X	212	ASN
1	Y	188	GLN
1	Y	212	ASN
1	Z	181	ASN
1	Z	212	ASN

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Mol	Chain	Res	Type
1	1	181	ASN
1	1	212	ASN
1	2	148	HIS
1	2	212	ASN
1	3	177	ASN
1	3	188	GLN
1	3	212	ASN
1	5	148	HIS
1	5	181	ASN
1	5	188	GLN
1	5	204	ASN
1	6	181	ASN
1	6	188	GLN
1	6	212	ASN
1	7	181	ASN
1	7	188	GLN
1	7	212	ASN
1	8	177	ASN
1	8	181	ASN
1	8	195	HIS
1	8	212	ASN
1	9	177	ASN
1	9	212	ASN
1	9	225	ASN
1	a	44	HIS
1	a	204	ASN
1	a	212	ASN
1	b	44	HIS
1	c	212	ASN
1	d	44	HIS
1	d	188	GLN
1	d	212	ASN
1	e	44	HIS
1	e	177	ASN
1	e	195	HIS
1	f	181	ASN
1	f	188	GLN
1	f	212	ASN
1	g	177	ASN
1	g	212	ASN
1	h	212	ASN
1	i	148	HIS

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Mol	Chain	Res	Type
1	i	181	ASN
1	i	188	GLN
1	j	204	ASN
1	j	212	ASN
1	k	44	HIS
1	k	188	GLN
1	k	204	ASN
1	k	212	ASN
1	l	181	ASN
1	l	212	ASN
1	m	212	ASN
1	n	188	GLN
1	n	212	ASN
1	o	188	GLN
1	o	195	HIS
1	o	212	ASN
1	p	212	ASN
1	q	44	HIS
1	q	188	GLN
1	q	212	ASN
1	r	177	ASN
1	r	204	ASN
1	r	212	ASN
1	s	212	ASN
1	t	178	ASN
1	t	188	GLN
1	u	177	ASN
1	v	148	HIS
1	w	181	ASN
1	w	188	GLN
1	w	212	ASN
1	x	181	ASN
1	x	212	ASN
1	y	204	ASN
1	y	212	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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	188/209 (89%)	-0.40	3 (1%) 70 61	32, 44, 71, 102	0
1	2	189/209 (90%)	-0.38	6 (3%) 50 40	32, 43, 69, 111	0
1	3	188/209 (89%)	-0.58	2 (1%) 78 70	26, 36, 60, 98	0
1	4	188/209 (89%)	-0.59	2 (1%) 78 70	27, 38, 65, 96	0
1	5	188/209 (89%)	-0.52	3 (1%) 70 61	29, 39, 66, 110	0
1	6	188/209 (89%)	-0.54	6 (3%) 50 40	26, 37, 59, 96	0
1	7	188/209 (89%)	-0.61	2 (1%) 78 70	27, 35, 61, 96	0
1	8	188/209 (89%)	-0.56	2 (1%) 78 70	24, 37, 63, 105	0
1	9	189/209 (90%)	-0.51	4 (2%) 63 54	29, 38, 63, 102	0
1	A	188/209 (89%)	-0.62	3 (1%) 70 61	26, 35, 57, 99	0
1	B	188/209 (89%)	-0.46	2 (1%) 78 70	32, 40, 63, 111	0
1	C	188/209 (89%)	-0.49	3 (1%) 70 61	27, 36, 64, 100	0
1	D	188/209 (89%)	-0.61	2 (1%) 78 70	26, 35, 59, 95	0
1	E	188/209 (89%)	-0.59	3 (1%) 70 61	25, 34, 58, 99	0
1	F	188/209 (89%)	-0.57	2 (1%) 78 70	25, 36, 61, 90	0
1	G	188/209 (89%)	-0.49	4 (2%) 63 54	28, 39, 69, 100	0
1	H	188/209 (89%)	-0.41	4 (2%) 63 54	34, 45, 70, 106	0
1	I	188/209 (89%)	-0.43	3 (1%) 70 61	33, 44, 70, 106	0
1	J	188/209 (89%)	-0.36	4 (2%) 63 54	32, 45, 73, 104	0
1	K	188/209 (89%)	-0.48	1 (0%) 87 82	24, 38, 64, 96	0
1	L	189/209 (90%)	-0.38	4 (2%) 63 54	33, 43, 69, 102	0
1	M	188/209 (89%)	-0.51	4 (2%) 63 54	30, 40, 66, 105	0
1	N	188/209 (89%)	-0.55	4 (2%) 63 54	27, 37, 66, 105	0
1	O	188/209 (89%)	-0.59	3 (1%) 70 61	25, 35, 61, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	P	188/209 (89%)	-0.59	3 (1%) 70 61	27, 35, 60, 95	0
1	Q	188/209 (89%)	-0.56	2 (1%) 78 70	28, 38, 62, 99	0
1	R	188/209 (89%)	-0.63	1 (0%) 87 82	27, 35, 63, 94	0
1	S	188/209 (89%)	-0.46	2 (1%) 78 70	29, 41, 69, 99	0
1	T	188/209 (89%)	-0.47	4 (2%) 63 54	30, 41, 69, 108	0
1	U	188/209 (89%)	-0.45	2 (1%) 78 70	29, 45, 69, 100	0
1	V	188/209 (89%)	-0.35	4 (2%) 63 54	35, 46, 73, 108	0
1	W	188/209 (89%)	-0.37	2 (1%) 78 70	35, 44, 73, 120	0
1	X	188/209 (89%)	-0.37	4 (2%) 63 54	35, 46, 71, 106	0
1	Y	188/209 (89%)	-0.36	2 (1%) 78 70	33, 46, 74, 106	0
1	Z	188/209 (89%)	-0.42	2 (1%) 78 70	32, 43, 73, 97	0
1	a	189/209 (90%)	-0.48	6 (3%) 50 40	30, 41, 66, 107	0
1	b	188/209 (89%)	-0.38	4 (2%) 63 54	32, 46, 73, 110	0
1	c	188/209 (89%)	-0.37	1 (0%) 87 82	33, 45, 68, 112	0
1	d	188/209 (89%)	-0.38	4 (2%) 63 54	35, 44, 69, 100	0
1	e	189/209 (90%)	-0.48	4 (2%) 63 54	29, 39, 64, 109	0
1	f	188/209 (89%)	-0.39	2 (1%) 78 70	32, 45, 72, 101	0
1	g	188/209 (89%)	-0.39	4 (2%) 63 54	32, 45, 71, 96	0
1	h	188/209 (89%)	-0.41	3 (1%) 70 61	32, 42, 65, 111	0
1	i	188/209 (89%)	-0.51	3 (1%) 70 61	30, 41, 64, 105	0
1	j	188/209 (89%)	-0.39	3 (1%) 70 61	35, 45, 70, 104	0
1	k	189/209 (90%)	-0.44	5 (2%) 57 47	29, 40, 72, 107	0
1	l	188/209 (89%)	-0.48	2 (1%) 78 70	28, 40, 68, 101	0
1	m	188/209 (89%)	-0.59	3 (1%) 70 61	27, 36, 64, 105	0
1	n	188/209 (89%)	-0.57	3 (1%) 70 61	26, 36, 65, 95	0
1	o	188/209 (89%)	-0.53	5 (2%) 56 46	27, 37, 64, 111	0
1	p	189/209 (90%)	-0.56	3 (1%) 70 61	26, 38, 62, 106	0
1	q	188/209 (89%)	-0.57	3 (1%) 70 61	28, 35, 64, 99	0
1	r	189/209 (90%)	-0.48	3 (1%) 70 61	30, 41, 64, 94	0
1	s	188/209 (89%)	-0.59	3 (1%) 70 61	28, 36, 63, 102	0
1	t	188/209 (89%)	-0.53	2 (1%) 78 70	27, 38, 64, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	u	188/209 (89%)	-0.57	5 (2%) 56 46	25, 36, 60, 98	0
1	v	188/209 (89%)	-0.53	4 (2%) 63 54	31, 40, 64, 102	0
1	w	188/209 (89%)	-0.57	0 100 100	29, 37, 65, 94	0
1	x	189/209 (90%)	-0.54	5 (2%) 57 47	27, 37, 63, 99	0
1	y	189/209 (90%)	-0.51	5 (2%) 57 47	27, 37, 62, 107	0
All	All	11290/12540 (90%)	-0.49	189 (1%) 69 60	24, 40, 67, 120	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	231	LEU	6.4
1	y	231	LEU	5.9
1	e	231	LEU	5.7
1	p	231	LEU	5.5
1	k	231	LEU	5.3
1	L	231	LEU	5.1
1	x	231	LEU	4.8
1	a	231	LEU	4.5
1	Y	44	HIS	4.5
1	9	231	LEU	4.4
1	n	44	HIS	4.4
1	V	44	HIS	4.3
1	3	44	HIS	4.1
1	2	44	HIS	4.0
1	T	44	HIS	3.9
1	j	44	HIS	3.8
1	l	44	HIS	3.8
1	k	44	HIS	3.7
1	W	179	LYS	3.7
1	d	44	HIS	3.6
1	r	231	LEU	3.6
1	J	44	HIS	3.6
1	g	189	THR	3.6
1	a	43	SER	3.5
1	D	44	HIS	3.5
1	U	44	HIS	3.5
1	B	179	LYS	3.5
1	F	44	HIS	3.5
1	Z	44	HIS	3.5
1	y	44	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	Q	44	HIS	3.4
1	h	179	LYS	3.4
1	C	44	HIS	3.3
1	S	44	HIS	3.3
1	X	44	HIS	3.3
1	h	44	HIS	3.3
1	r	44	HIS	3.3
1	v	44	HIS	3.3
1	a	44	HIS	3.3
1	C	179	LYS	3.3
1	G	44	HIS	3.3
1	7	44	HIS	3.3
1	J	179	LYS	3.3
1	u	179	LYS	3.3
1	x	44	HIS	3.3
1	A	178	ASN	3.2
1	8	44	HIS	3.2
1	m	44	HIS	3.2
1	a	179	LYS	3.2
1	s	179	LYS	3.2
1	B	44	HIS	3.2
1	X	179	LYS	3.2
1	9	179	LYS	3.2
1	A	44	HIS	3.1
1	o	44	HIS	3.1
1	P	44	HIS	3.1
1	5	44	HIS	3.1
1	u	44	HIS	3.1
1	A	179	LYS	3.0
1	W	44	HIS	3.0
1	c	44	HIS	3.0
1	p	44	HIS	3.0
1	t	44	HIS	3.0
1	N	179	LYS	3.0
1	M	43	SER	3.0
1	L	44	HIS	2.9
1	f	44	HIS	2.9
1	V	179	LYS	2.9
1	m	179	LYS	2.9
1	i	178	ASN	2.9
1	h	63	LYS	2.9
1	1	44	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	t	179	LYS	2.9
1	K	44	HIS	2.9
1	T	179	LYS	2.9
1	o	179	LYS	2.8
1	y	179	LYS	2.8
1	M	44	HIS	2.8
1	q	43	SER	2.8
1	9	63	LYS	2.8
1	d	63	LYS	2.8
1	Y	179	LYS	2.8
1	R	44	HIS	2.8
1	b	44	HIS	2.8
1	E	44	HIS	2.7
1	4	44	HIS	2.7
1	d	43	SER	2.7
1	L	179	LYS	2.7
1	v	179	LYS	2.7
1	C	43	SER	2.7
1	2	43	SER	2.7
1	y	43	SER	2.7
1	E	179	LYS	2.7
1	6	179	LYS	2.7
1	6	44	HIS	2.7
1	s	44	HIS	2.7
1	m	178	ASN	2.7
1	G	63	LYS	2.6
1	b	178	ASN	2.6
1	j	179	LYS	2.6
1	x	179	LYS	2.6
1	H	44	HIS	2.6
1	9	44	HIS	2.6
1	i	44	HIS	2.6
1	1	179	LYS	2.6
1	M	178	ASN	2.6
1	L	43	SER	2.5
1	n	179	LYS	2.5
1	O	179	LYS	2.5
1	x	63	LYS	2.5
1	g	43	SER	2.5
1	5	179	LYS	2.5
1	N	44	HIS	2.5
1	e	44	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	179	LYS	2.5
1	S	179	LYS	2.5
1	6	63	LYS	2.5
1	a	178	ASN	2.5
1	e	180	ARG	2.4
1	3	179	LYS	2.4
1	u	178	ASN	2.4
1	E	178	ASN	2.4
1	n	177	ASN	2.4
1	8	179	LYS	2.4
1	e	179	LYS	2.4
1	I	43	SER	2.4
1	1	43	SER	2.4
1	6	43	SER	2.4
1	o	190	ALA	2.4
1	F	178	ASN	2.4
1	P	179	LYS	2.3
1	b	63	LYS	2.3
1	J	43	SER	2.3
1	Z	43	SER	2.3
1	s	178	ASN	2.3
1	N	190	ALA	2.3
1	D	86	SER	2.3
1	2	179	LYS	2.3
1	u	43	SER	2.3
1	V	178	ASN	2.3
1	k	63	LYS	2.3
1	5	43	SER	2.3
1	r	86	SER	2.3
1	o	178	ASN	2.2
1	I	63	LYS	2.2
1	X	178	ASN	2.2
1	6	178	ASN	2.2
1	I	44	HIS	2.2
1	G	179	LYS	2.2
1	H	177	ASN	2.2
1	H	178	ASN	2.2
1	J	178	ASN	2.2
1	x	178	ASN	2.2
1	a	63	LYS	2.2
1	d	179	LYS	2.2
1	G	180	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	T	178	ASN	2.2
1	q	44	HIS	2.2
1	Q	179	LYS	2.2
1	f	43	SER	2.2
1	v	180	ARG	2.1
1	6	177	ASN	2.1
1	7	178	ASN	2.1
1	i	179	LYS	2.1
1	T	111	ILE	2.1
1	o	177	ASN	2.1
1	q	178	ASN	2.1
1	M	179	LYS	2.1
1	4	63	LYS	2.1
1	v	63	LYS	2.1
1	P	43	SER	2.1
1	j	43	SER	2.1
1	N	178	ASN	2.1
1	b	62	VAL	2.1
1	g	63	LYS	2.1
1	O	44	HIS	2.1
1	V	63	LYS	2.1
1	p	179	LYS	2.1
1	X	61	THR	2.1
1	k	179	LYS	2.0
1	l	63	LYS	2.0
1	k	180	ARG	2.0
1	u	180	ARG	2.0
1	g	179	LYS	2.0
1	O	177	ASN	2.0
1	2	177	ASN	2.0
1	y	178	ASN	2.0
1	2	61	THR	2.0
1	U	179	LYS	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.