Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:34 PM GMT

PDB ID	:	4RFT
Title	:	T=1 subviral particle of Grouper nervous necrosis virus capsid protein deletion mutant (delta 1-34 & 218-338)
Authors	:	Chen, N.C.; Chen, C.J.; Yoshimura, M.; Guan, H.H.; Chen, T.Y.
Deposited on	:	2014-09-27
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

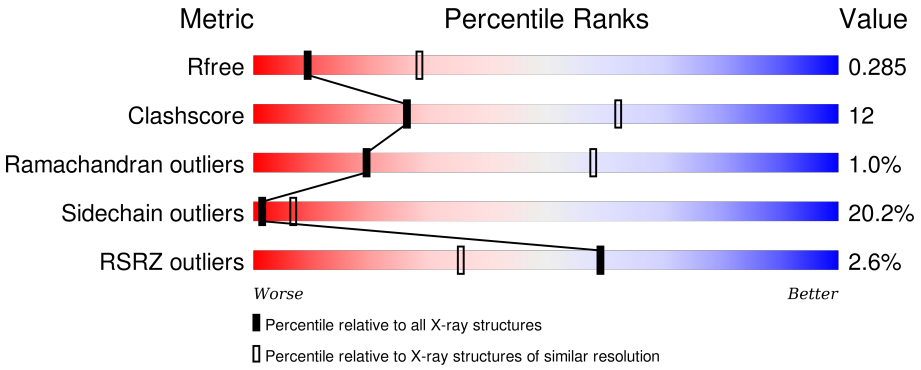
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	0	183	% 60% 23% 5% • 11%
1	1	183	5% 54% 28% 7% • 11%
1	2	183	3% 52% 31% 7% 11%
1	3	183	3% 61% 23% 5% • 11%
1	4	183	4% 54% 26% 9% 11%

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Mol	Chain	Length	Quality of chain
1	5	183	3% 55% 28% 7% 11%
1	6	183	5% 62% 21% 6% 11%
1	7	183	% 50% 32% 7% 11%
1	8	183	2% 53% 27% 9% 11%
1	9	183	% 58% 23% 7% 11%
1	A	183	% 43% 37% 9% 11%
1	B	183	4% 39% 40% 10% 11%
1	C	183	6% 59% 23% 7% 11%
1	D	183	% 47% 33% 9% 11%
1	E	183	42% 34% 11% 11%
1	F	183	2% 57% 26% 5% 11%
1	G	183	% 47% 31% 11% 11%
1	H	183	40% 37% 11% 11%
1	I	183	% 56% 25% 7% 11%
1	J	183	3% 44% 38% 7% 11%
1	K	183	3% 43% 37% 9% 11%
1	L	183	5% 58% 25% 5% 11%
1	M	183	% 41% 37% 11% 11%
1	N	183	% 46% 34% 8% 11%
1	O	183	% 55% 26% 7% 11%
1	P	183	3% 45% 34% 8% 11%
1	Q	183	3% 41% 39% 8% 11%
1	R	183	7% 57% 24% 8% 11%
1	S	183	% 47% 34% 7% 11%
1	T	183	% 44% 37% 8% 11%

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Mol	Chain	Length	Quality of chain
1	U	183	3% 56% 26% 6% • 11%
1	V	183	5% 44% 36% 9% • 11%
1	W	183	3% 49% 33% 8% 11%
1	X	183	6% 58% 25% 6% • 11%
1	Y	183	% 52% 29% 7% • 11%
1	Z	183	% 51% 29% 9% • 11%
1	a	183	% 75% 14% • 11%
1	b	183	4% 74% 15% • 11%
1	c	183	3% 74% 15% • 11%
1	d	183	3% 73% 16% • 11%
1	e	183	3% 72% 16% • 11%
1	f	183	5% 74% 15% • 11%
1	g	183	% 71% 17% • 11%
1	h	183	% 73% 16% • 11%
1	i	183	% 74% 14% • 11%
1	j	183	2% 72% 16% • 11%
1	k	183	2% 74% 14% • 11%
1	l	183	7% 74% 15% • 11%
1	m	183	% 72% 16% • 11%
1	n	183	% 72% 16% • 11%
1	o	183	% 74% 14% • 11%
1	p	183	% 71% 17% • 11%
1	q	183	74% 15% • 11%
1	r	183	2% 74% 15% • 11%
1	s	183	4% 73% 15% • 11%

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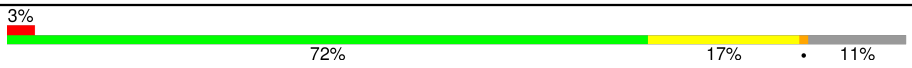
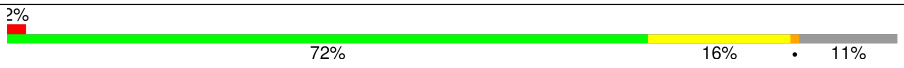
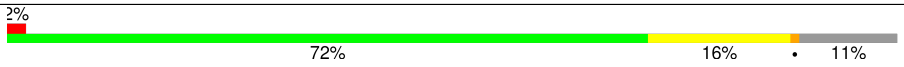
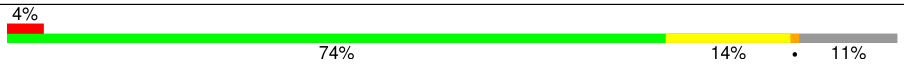
Mol	Chain	Length	Quality of chain
1	t	183	
1	u	183	
1	v	183	
1	w	183	
1	x	183	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 75180 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 Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	B	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	C	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	D	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	E	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	F	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	G	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	H	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	I	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	J	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	K	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	L	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	M	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	N	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	O	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	P	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	R	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	S	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	T	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	U	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	V	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	W	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	X	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	Y	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	Z	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	0	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	1	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	2	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	3	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	4	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	5	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	6	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	7	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	8	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	9	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	a	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	b	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	c	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	d	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	e	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	f	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	g	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	h	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	i	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	j	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	k	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	l	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	m	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	n	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	o	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	p	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	q	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	r	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	s	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	t	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	u	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	v	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	w	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	x	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
B	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
C	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
D	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
E	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
F	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
G	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
H	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
I	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
J	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
K	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
L	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
M	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
N	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
O	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
P	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
Q	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
R	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
S	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
T	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
U	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
V	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
W	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
X	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
Y	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
Z	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
0	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
1	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
2	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
3	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
4	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
5	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
6	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
7	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5

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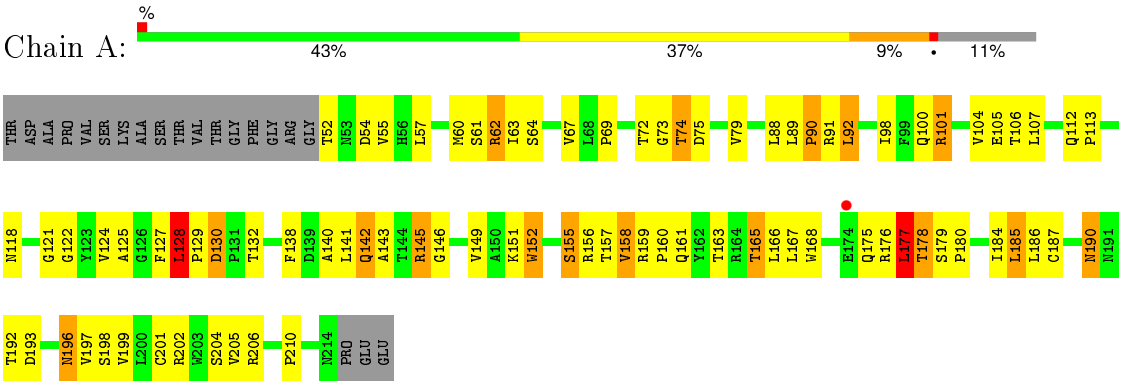
Chain	Residue	Modelled	Actual	Comment	Reference
8	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
9	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
a	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
b	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
c	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
d	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
e	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
f	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
g	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
h	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
i	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
j	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
k	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
l	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
m	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
n	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
o	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
p	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
q	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
r	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
s	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
t	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
u	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
v	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
w	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
x	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5

3 Residue-property plots (i)

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

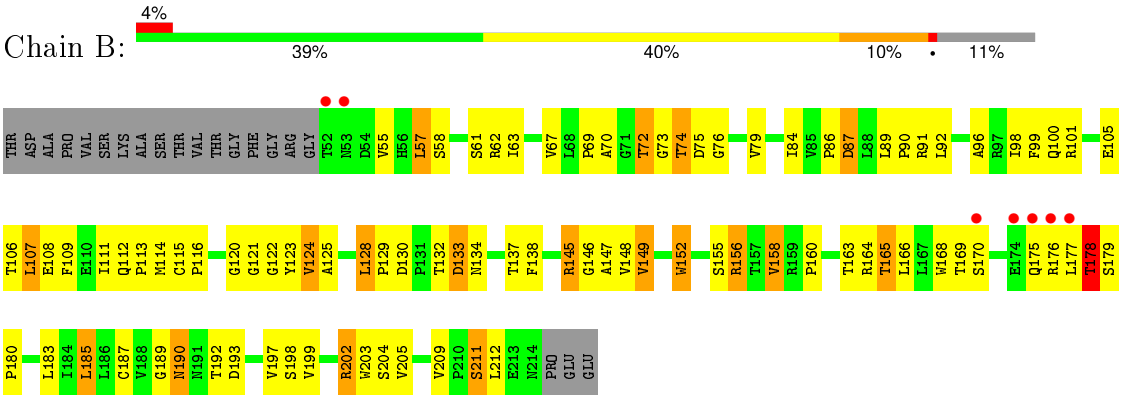
- Molecule 1: Coat protein

Chain A:



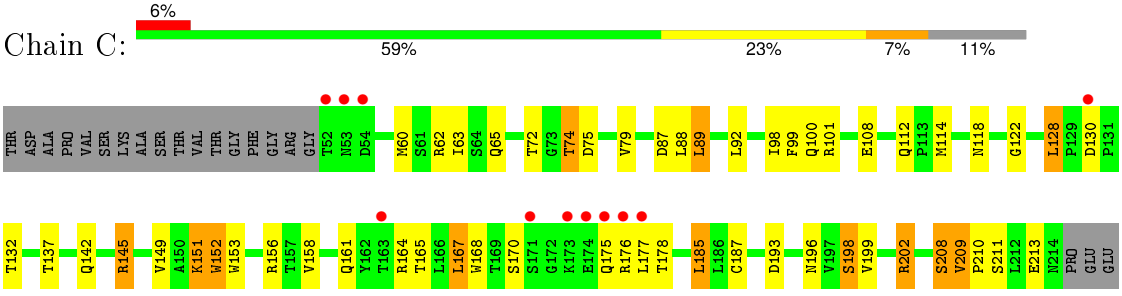
- Molecule 1: Coat protein

Chain B:



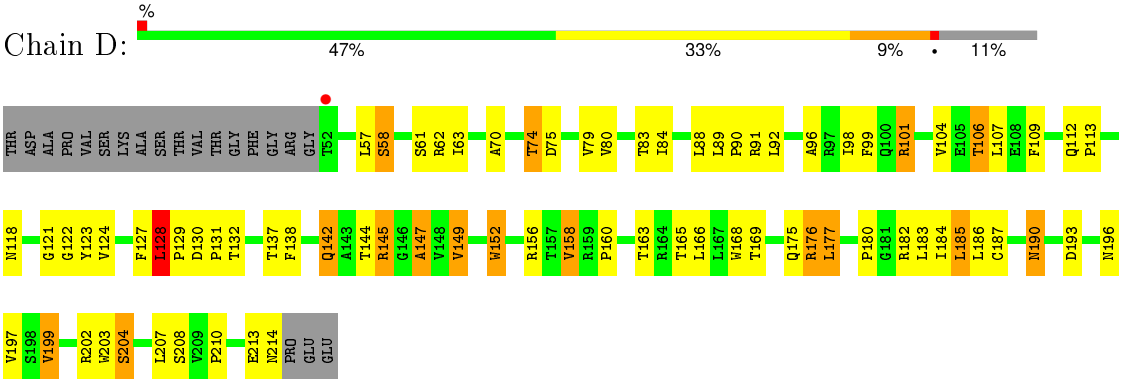
- Molecule 1: Coat protein

Chain C:



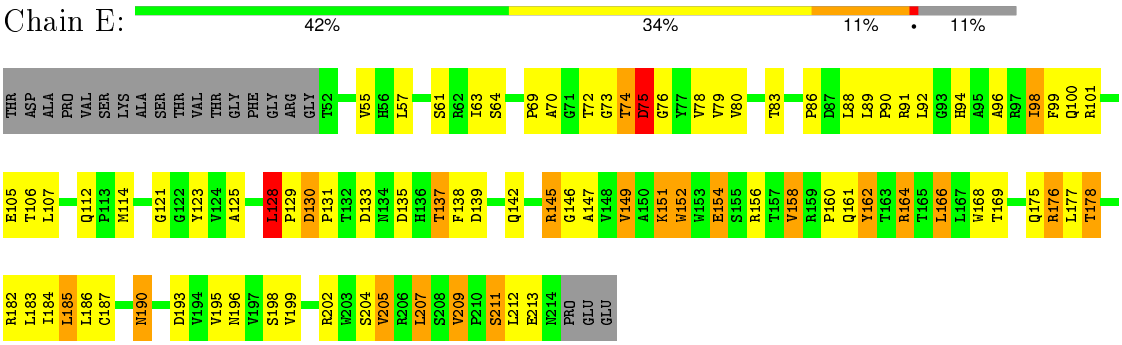
- Molecule 1: Coat protein

Chain D:



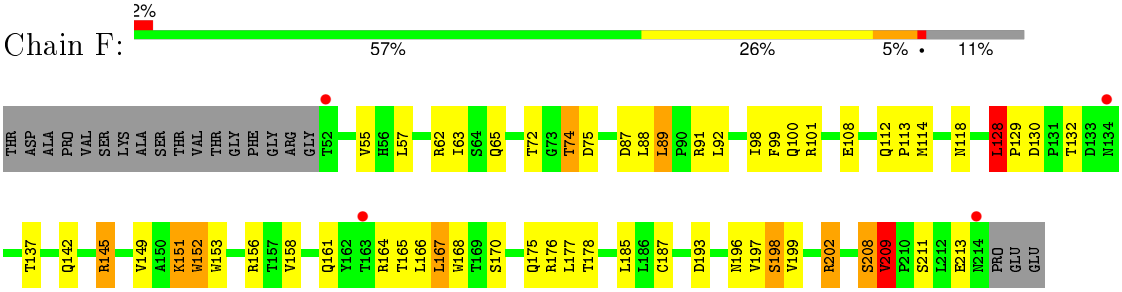
• Molecule 1: Coat protein

Chain E:



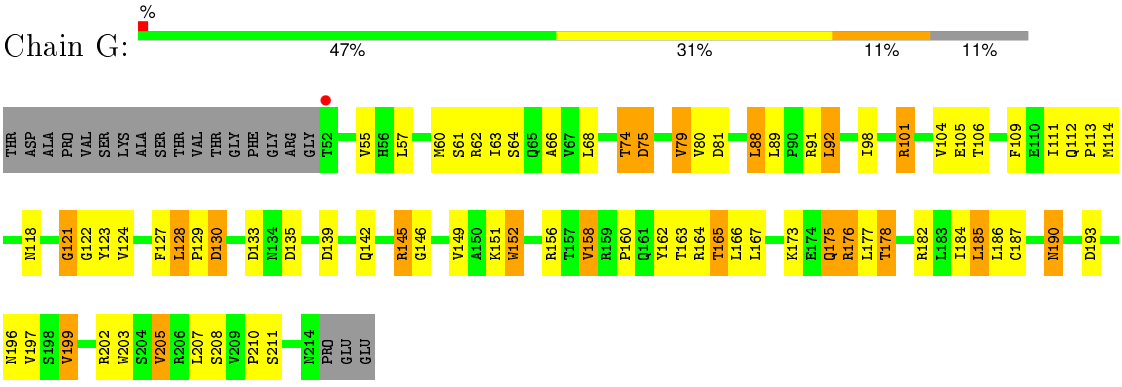
• Molecule 1: Coat protein

Chain F:



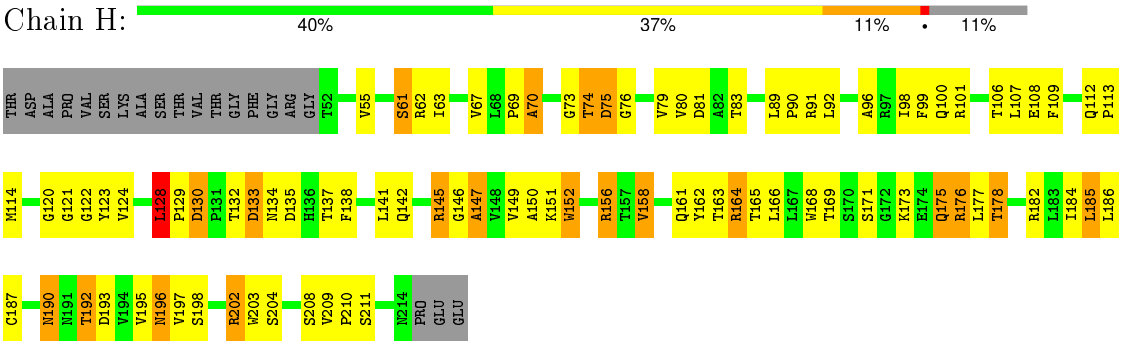
• Molecule 1: Coat protein

Chain G:



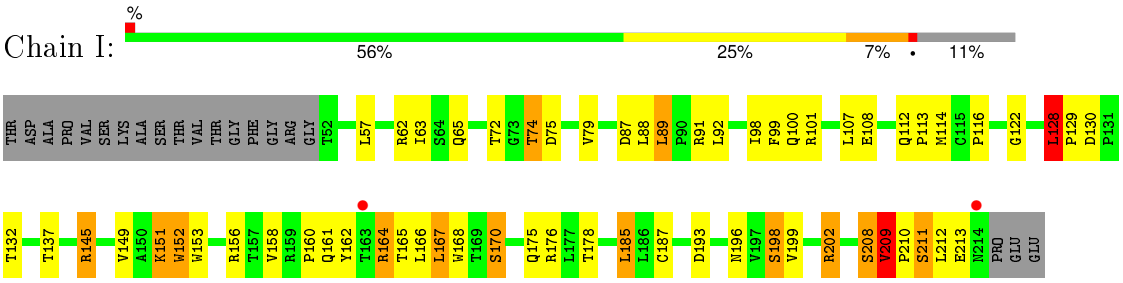
• Molecule 1: Coat protein

Chain H:



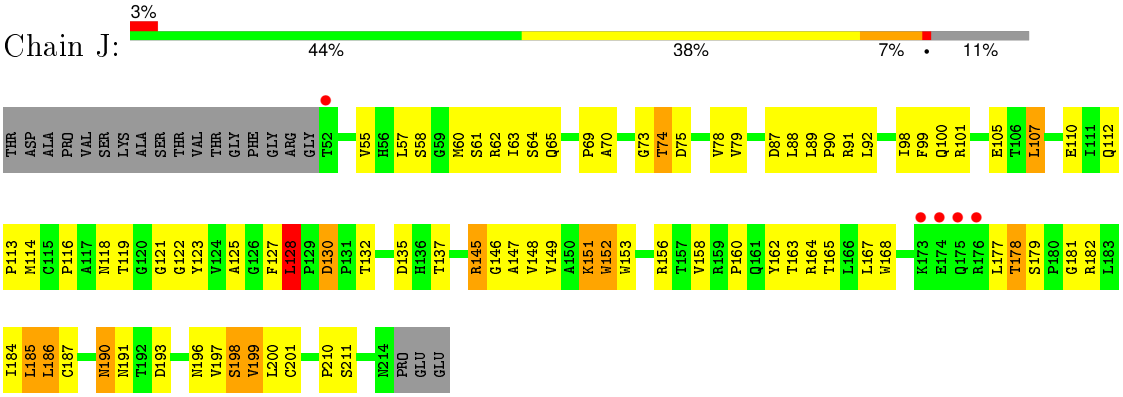
• Molecule 1: Coat protein

Chain I:



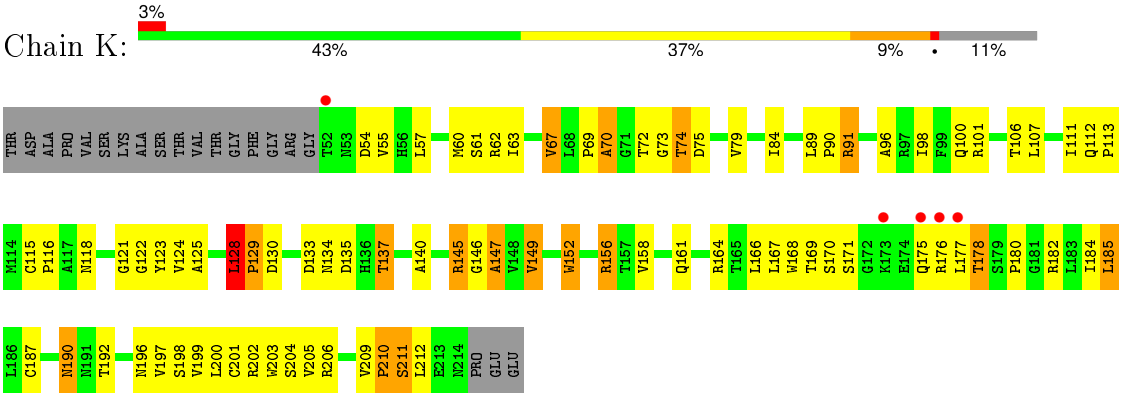
• Molecule 1: Coat protein

Chain J:



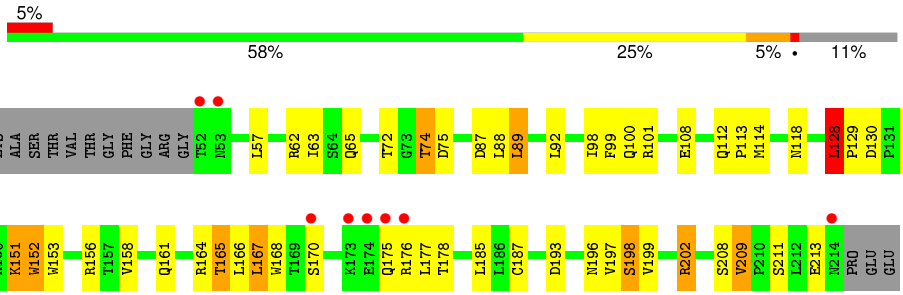
• Molecule 1: Coat protein

Chain K:



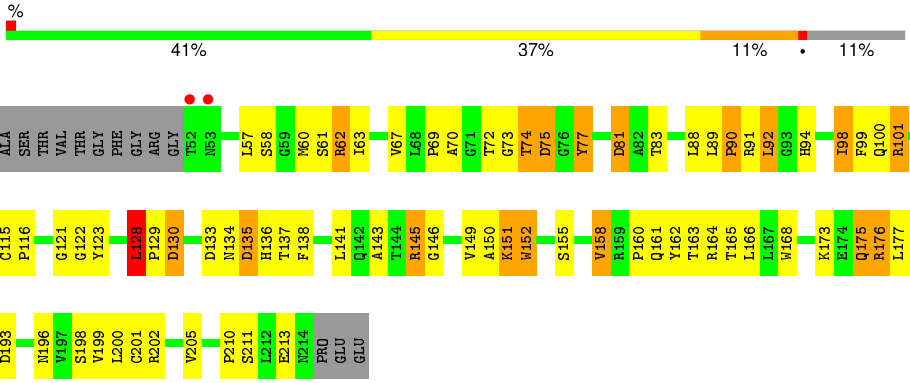
• Molecule 1: Coat protein

Chain L:



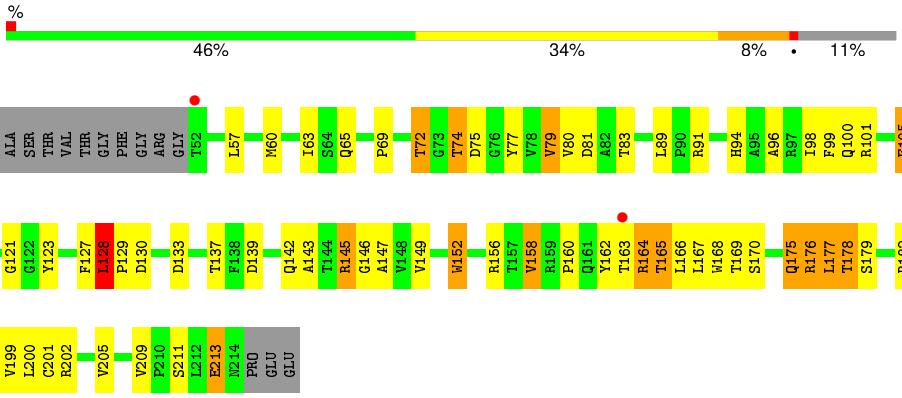
• Molecule 1: Coat protein

Chain M:



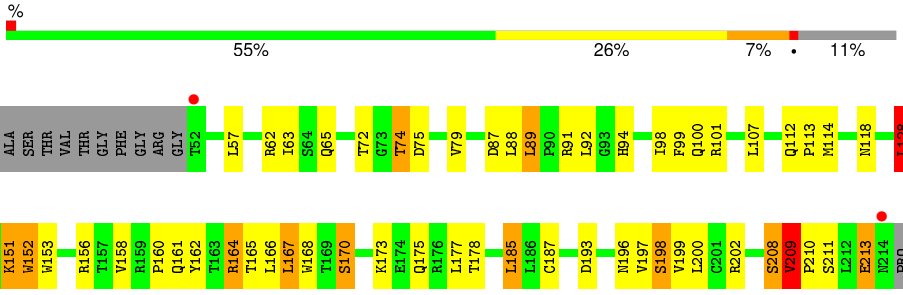
• Molecule 1: Coat protein

Chain N:



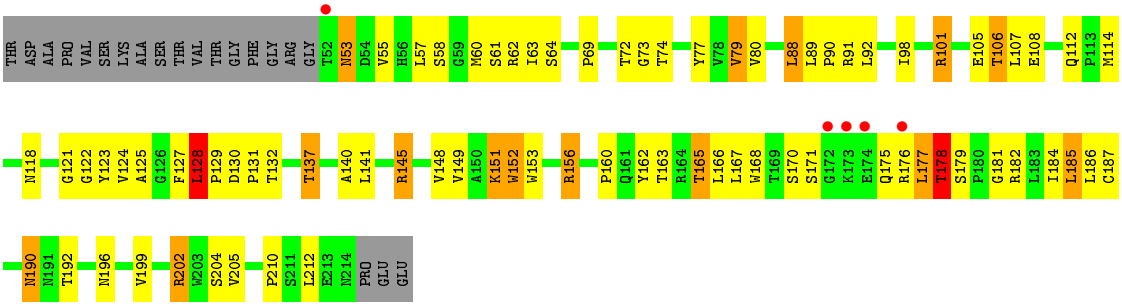
• Molecule 1: Coat protein

Chain O:



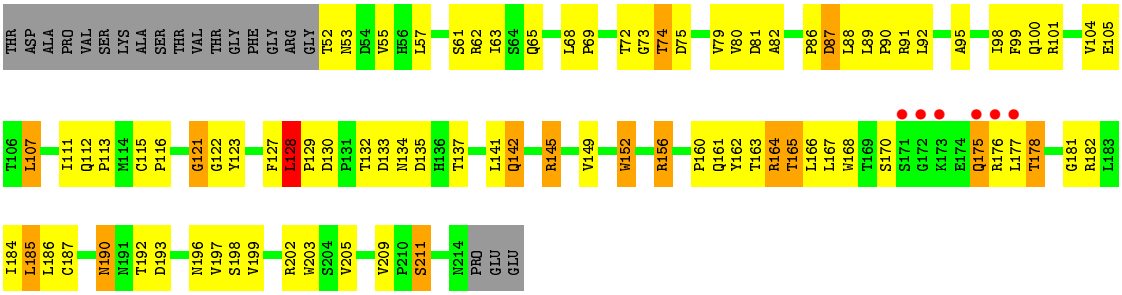
• Molecule 1: Coat protein

Chain P:



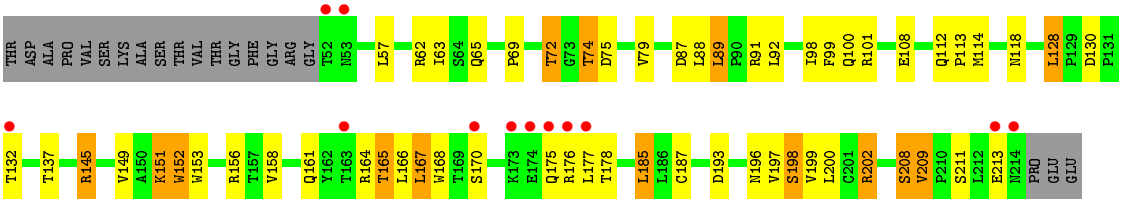
• Molecule 1: Coat protein

Chain Q:



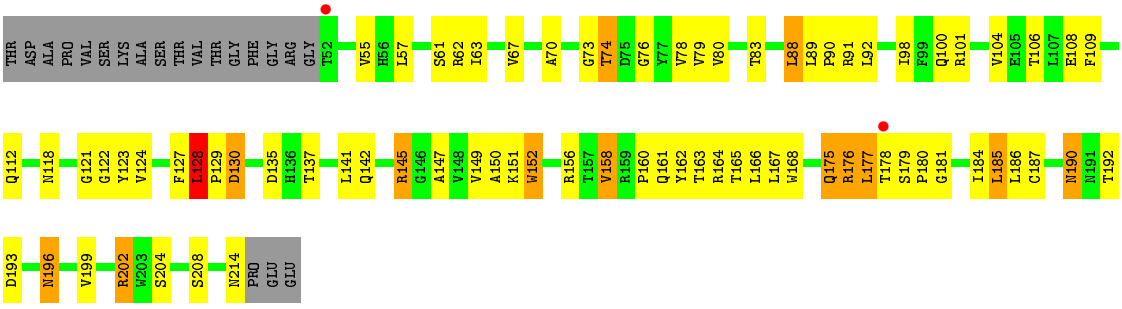
• Molecule 1: Coat protein

Chain R:



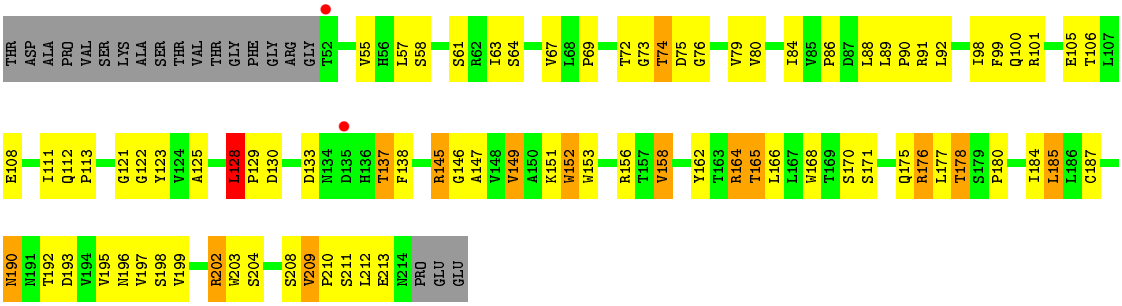
• Molecule 1: Coat protein

Chain S:

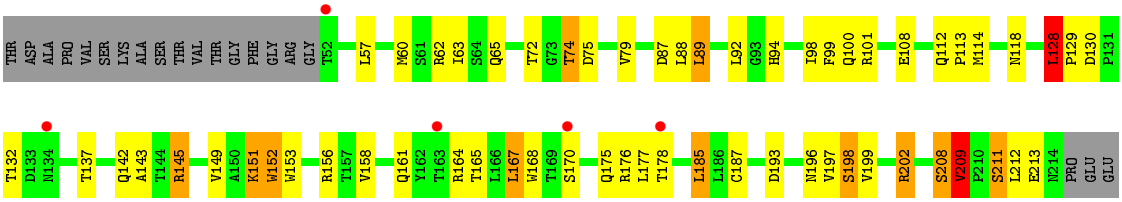


• Molecule 1: Coat protein

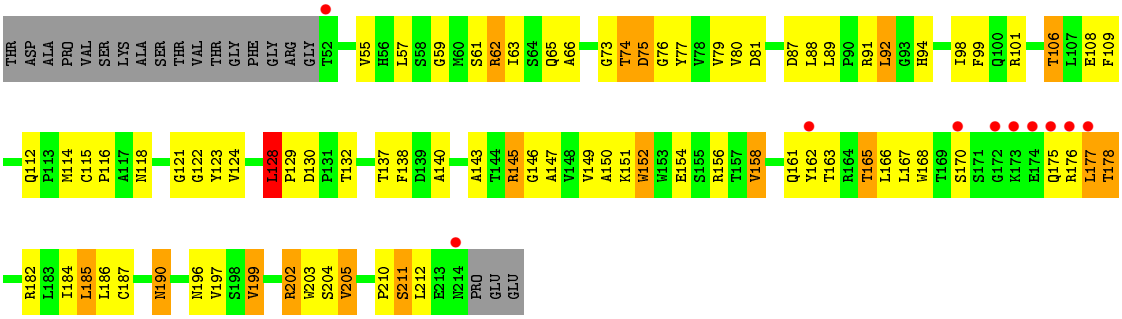
Chain T:



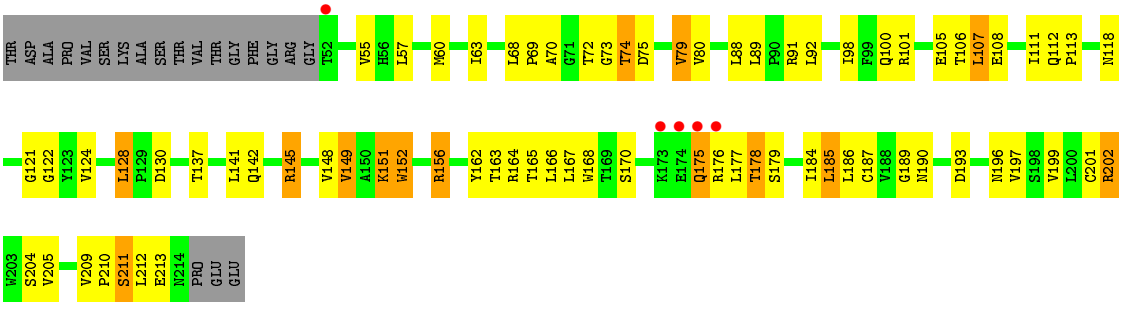
• Molecule 1: Coat protein



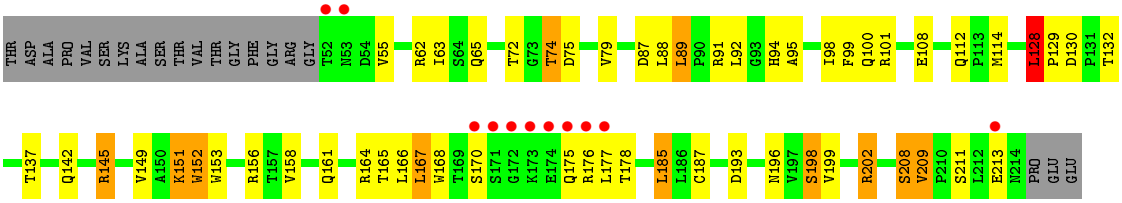
• Molecule 1: Coat protein



• Molecule 1: Coat protein

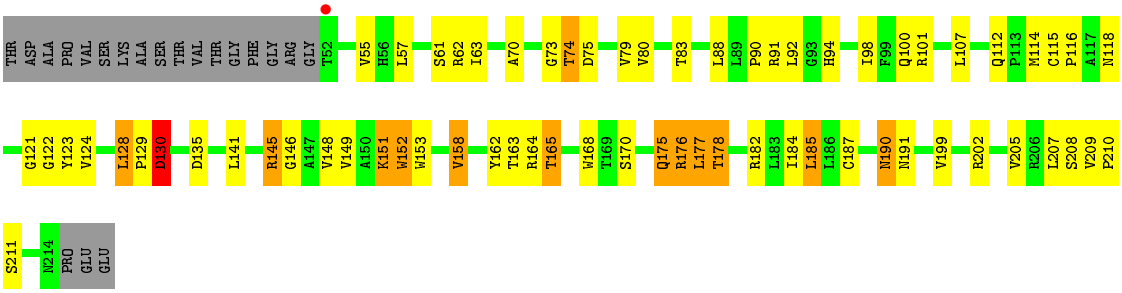


• Molecule 1: Coat protein



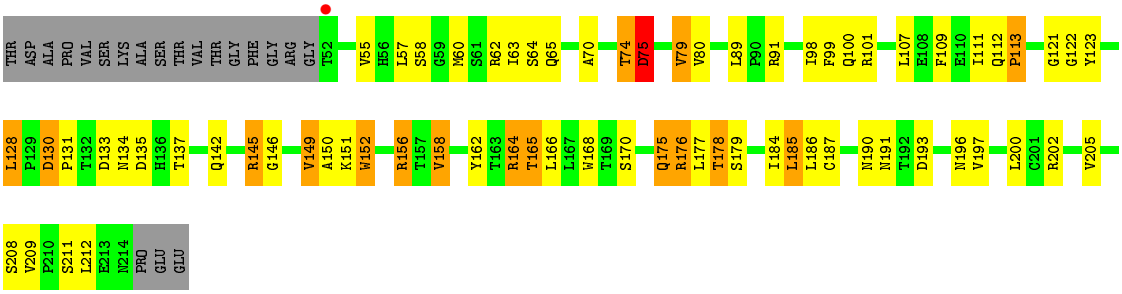
• Molecule 1: Coat protein

Chain Y:



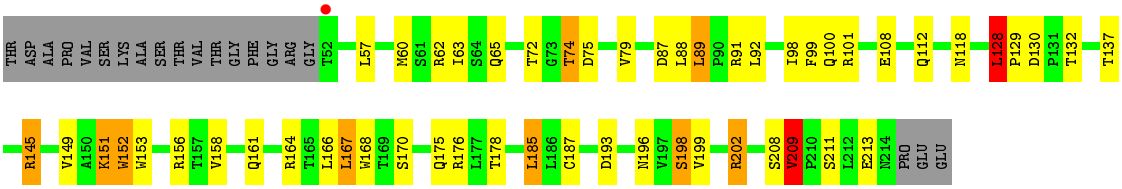
• Molecule 1: Coat protein

Chain Z:



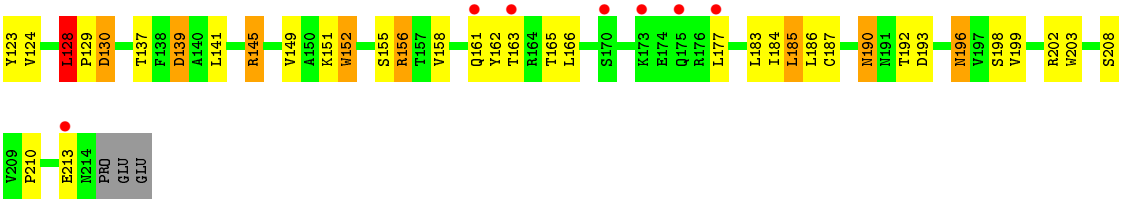
• Molecule 1: Coat protein

Chain 0:



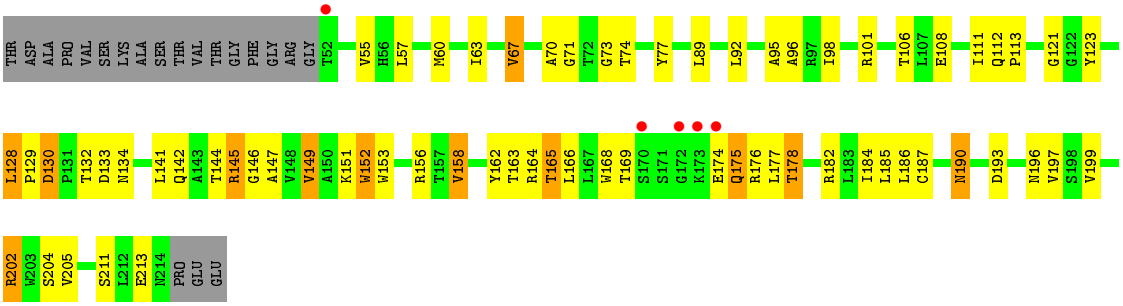
• Molecule 1: Coat protein

Chain 1:



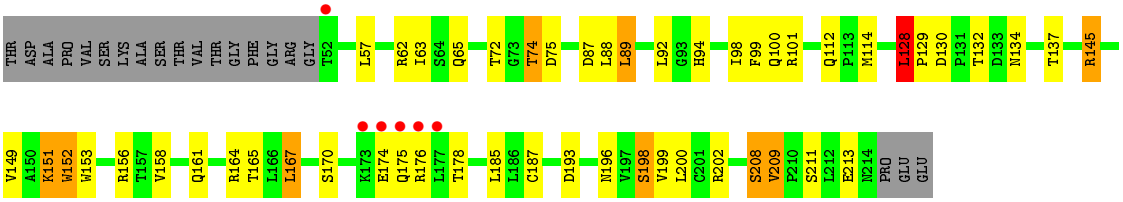
• Molecule 1: Coat protein

Chain 2:



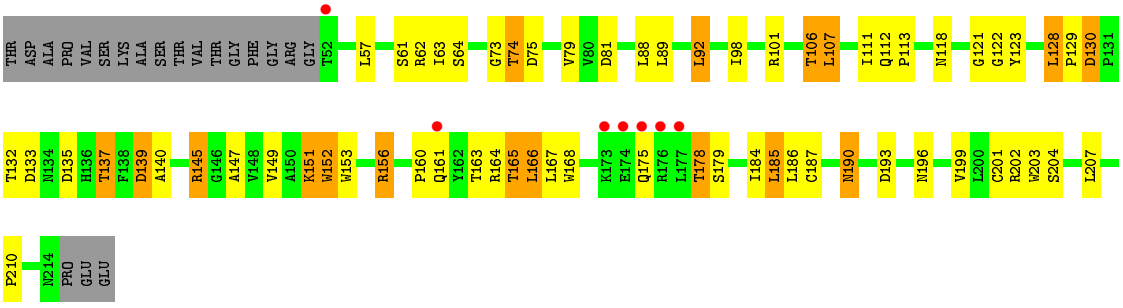
• Molecule 1: Coat protein

Chain 3:



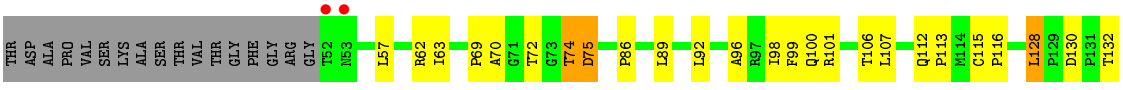
• Molecule 1: Coat protein

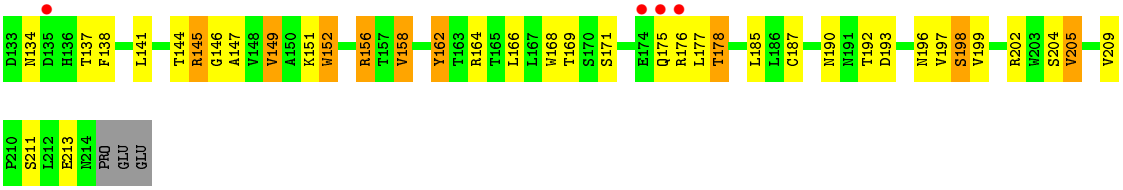
Chain 4:



• Molecule 1: Coat protein

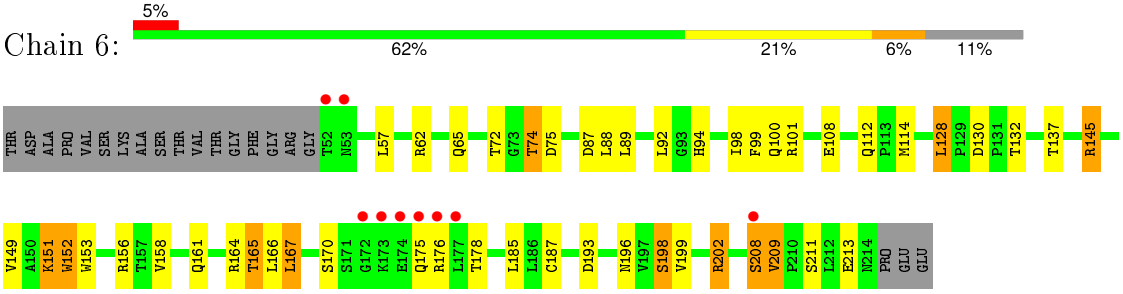
Chain 5:





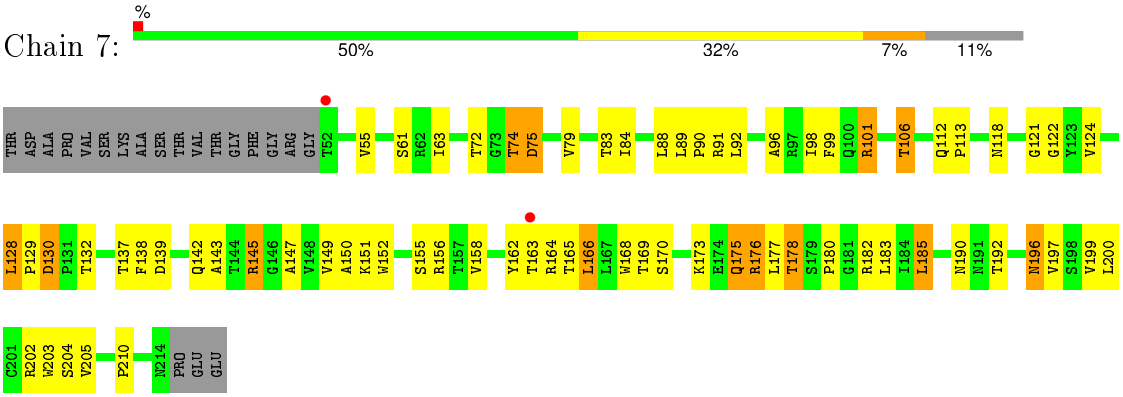
• Molecule 1: Coat protein

Chain 6:



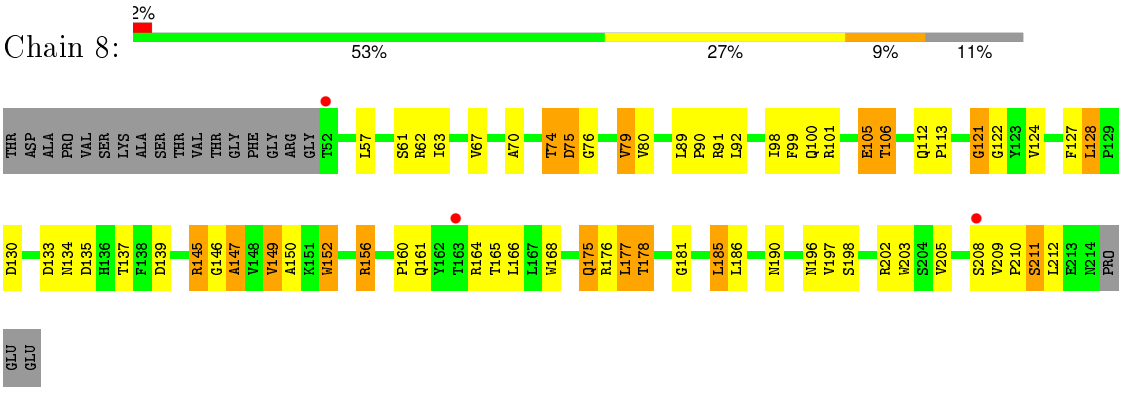
• Molecule 1: Coat protein

Chain 7:



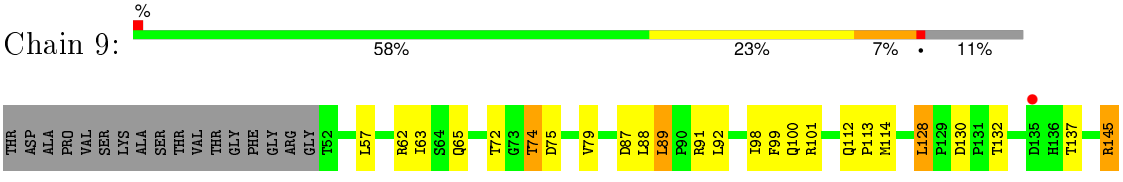
• Molecule 1: Coat protein

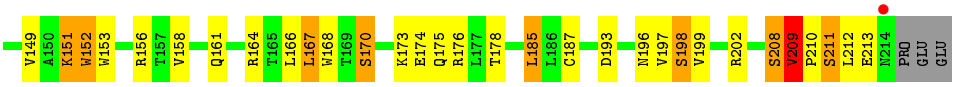
Chain 8:



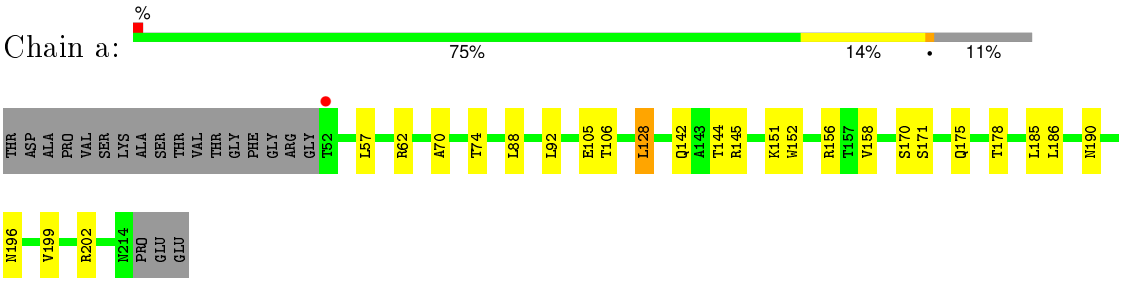
• Molecule 1: Coat protein

Chain 9:

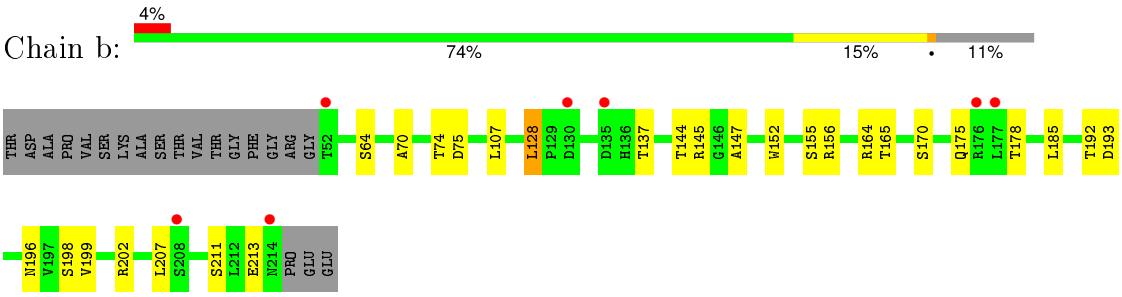




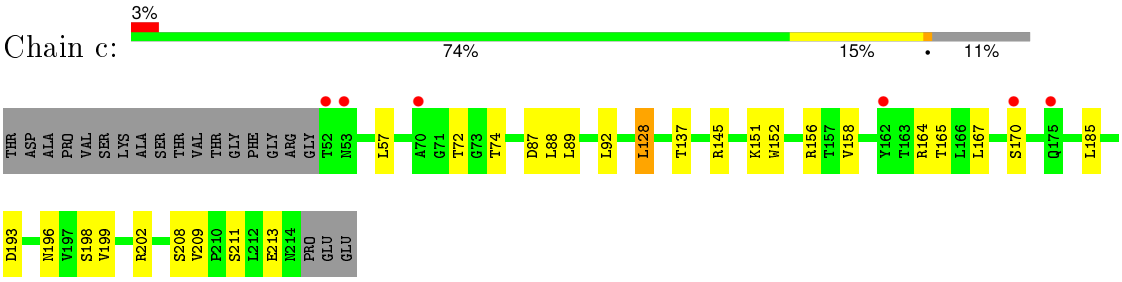
• Molecule 1: Coat protein



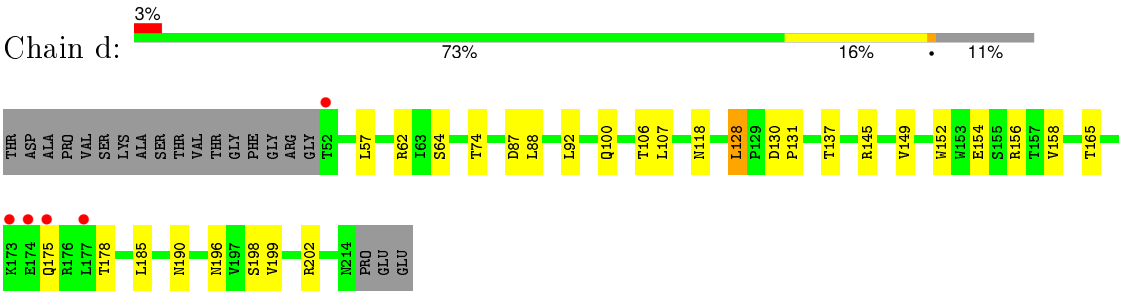
• Molecule 1: Coat protein



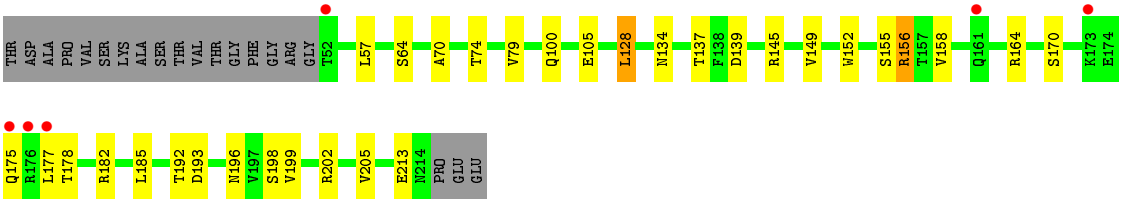
• Molecule 1: Coat protein



• Molecule 1: Coat protein

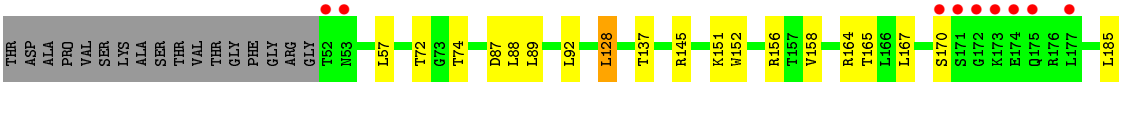


• Molecule 1: Coat protein



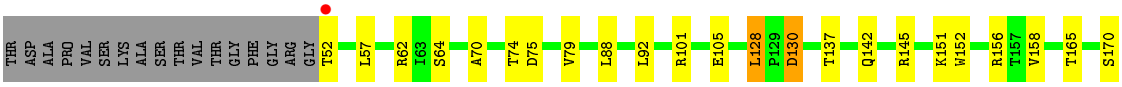
• Molecule 1: Coat protein

Chain f:



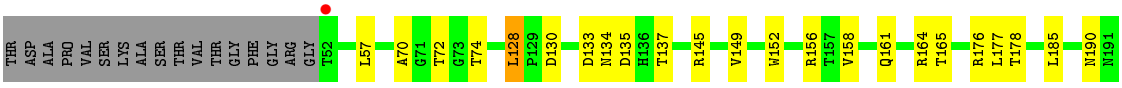
• Molecule 1: Coat protein

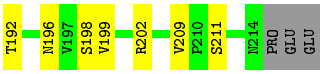
Chain g:



• Molecule 1: Coat protein

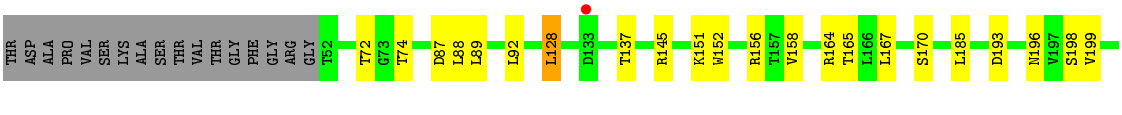
Chain h:





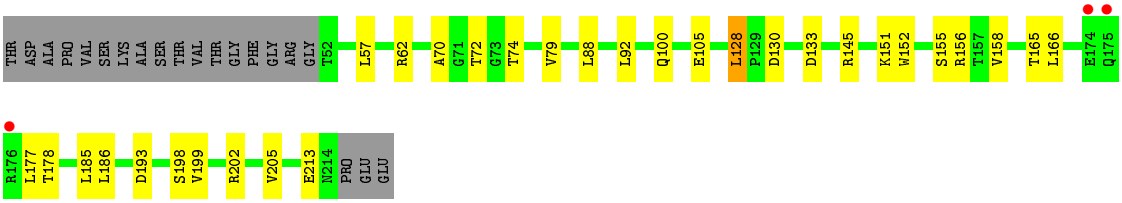
• Molecule 1: Coat protein

Chain i:



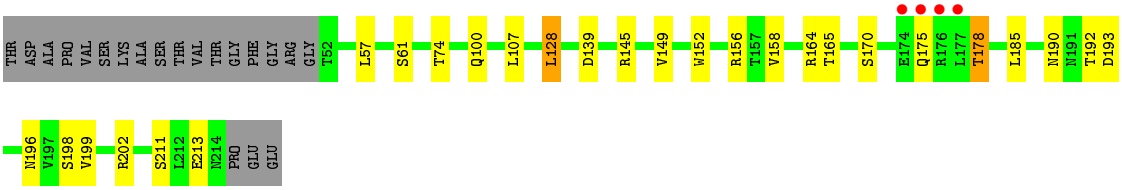
• Molecule 1: Coat protein

Chain j:



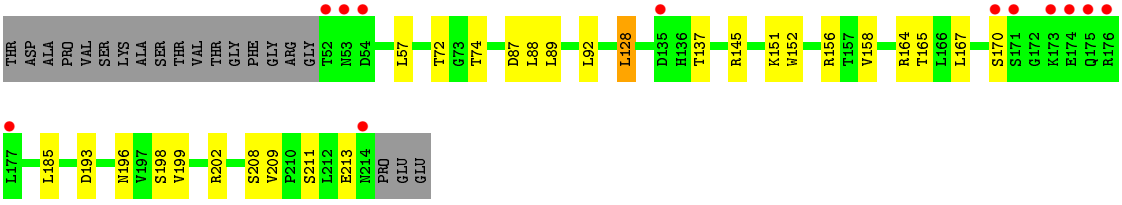
• Molecule 1: Coat protein

Chain k:



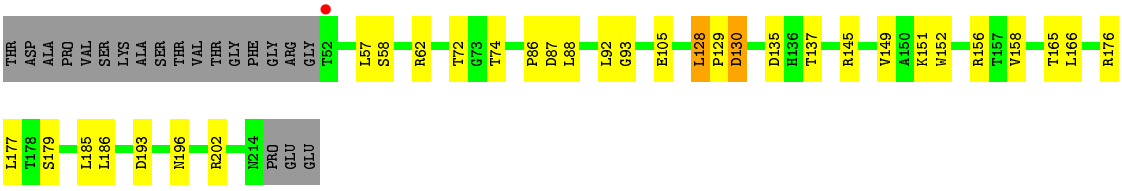
• Molecule 1: Coat protein

Chain l:



• Molecule 1: Coat protein

Chain m:

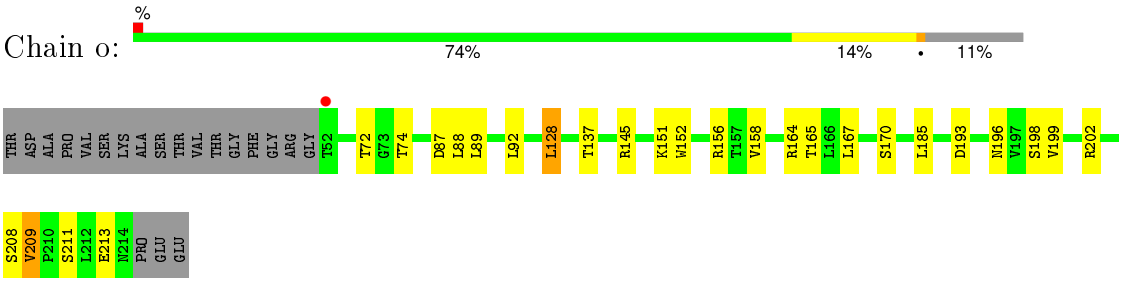


• Molecule 1: Coat protein

Chain n:

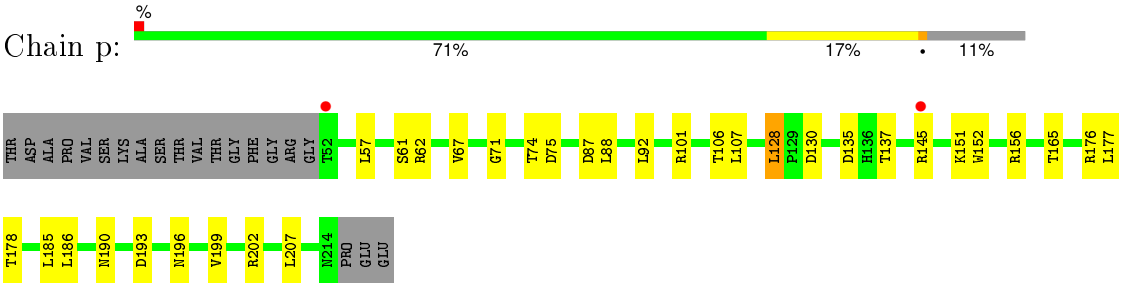
• Molecule 1: Coat protein

Chain o:



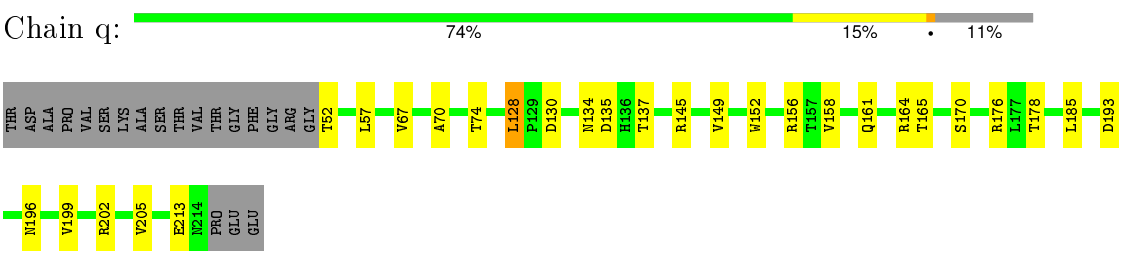
- Molecule 1: Coat protein

Chain p:



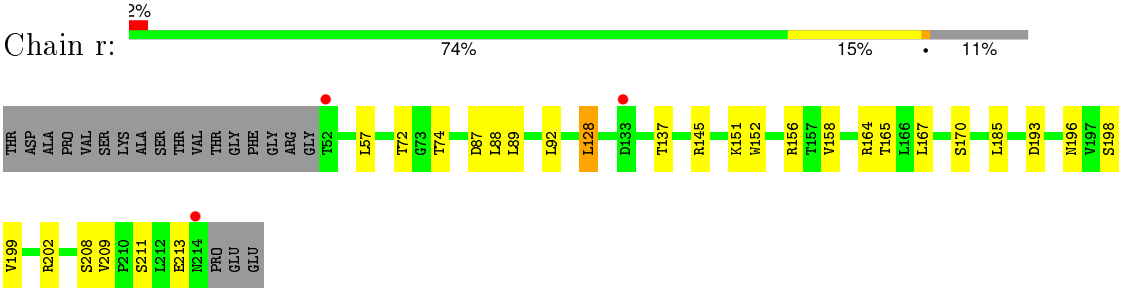
- Molecule 1: Coat protein

Chain q:



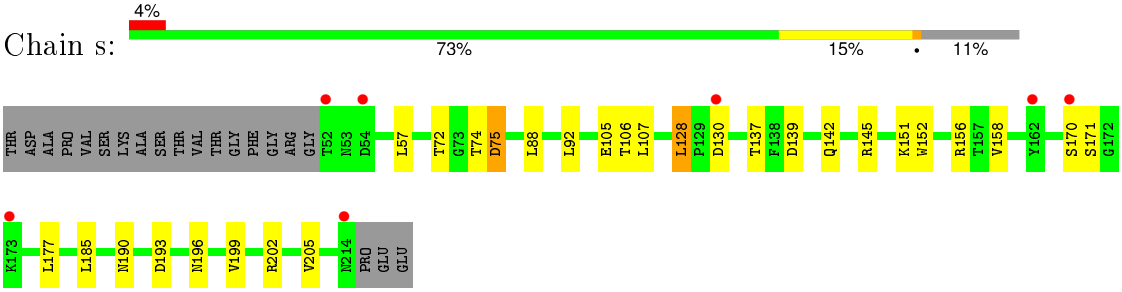
- Molecule 1: Coat protein

Chain r:



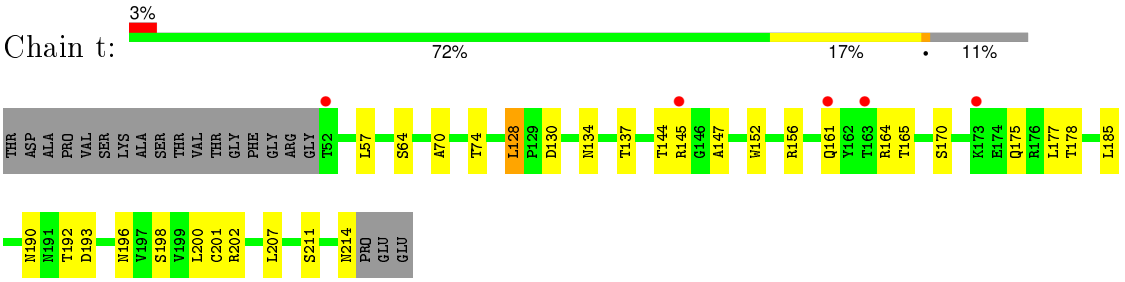
- Molecule 1: Coat protein

Chain s:



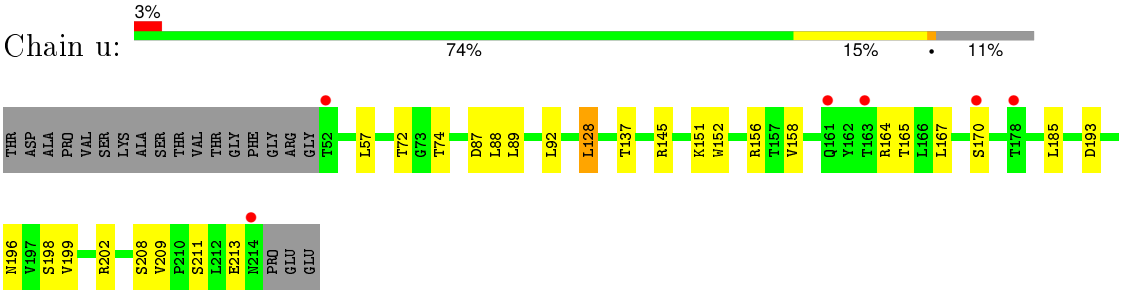
- Molecule 1: Coat protein

Chain t:



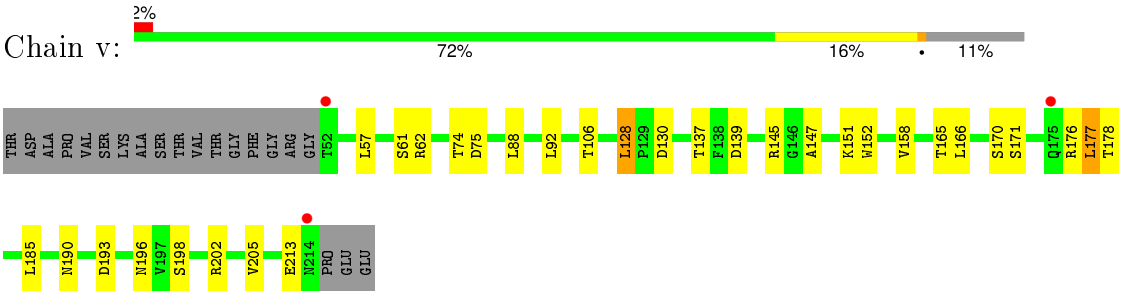
- Molecule 1: Coat protein

Chain u:



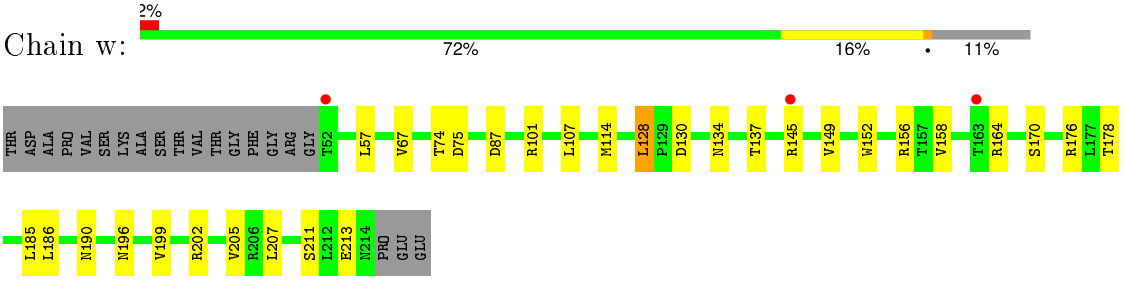
- Molecule 1: Coat protein

Chain v:



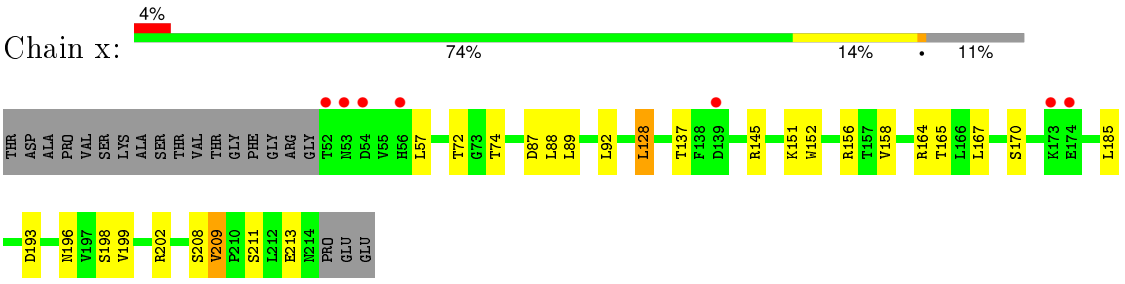
- Molecule 1: Coat protein

Chain w:



- Molecule 1: Coat protein

Chain x:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α, β, γ	288.95Å 288.95Å 175.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.37 – 3.10 26.37 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.1 (26.37-3.10) 98.3 (26.37-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.238 , 0.288 0.238 , 0.285	Depositor DCC
R_{free} test set	12823 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	51.5	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 9.5	EDS
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 255488 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	75180	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.53	0/1281	0.75	1/1753 (0.1%)
1	1	0.55	0/1281	0.80	2/1753 (0.1%)
1	2	0.52	0/1281	0.78	0/1753
1	3	0.53	0/1281	0.74	1/1753 (0.1%)
1	4	0.54	0/1281	0.79	1/1753 (0.1%)
1	5	0.54	0/1281	0.77	1/1753 (0.1%)
1	6	0.49	0/1281	0.74	1/1753 (0.1%)
1	7	0.61	0/1281	0.86	0/1753
1	8	0.59	0/1281	0.85	1/1753 (0.1%)
1	9	0.54	0/1281	0.76	1/1753 (0.1%)
1	A	0.55	0/1281	0.82	2/1753 (0.1%)
1	B	0.54	0/1281	0.78	0/1753
1	C	0.51	0/1281	0.75	1/1753 (0.1%)
1	D	0.55	0/1281	0.83	1/1753 (0.1%)
1	E	0.55	0/1281	0.84	1/1753 (0.1%)
1	F	0.51	0/1281	0.74	1/1753 (0.1%)
1	G	0.60	0/1281	0.85	0/1753
1	H	0.58	0/1281	0.82	1/1753 (0.1%)
1	I	0.55	0/1281	0.77	1/1753 (0.1%)
1	J	0.53	0/1281	0.81	1/1753 (0.1%)
1	K	0.53	0/1281	0.78	1/1753 (0.1%)
1	L	0.50	0/1281	0.72	1/1753 (0.1%)
1	M	0.62	0/1281	0.85	1/1753 (0.1%)
1	N	0.60	0/1281	0.84	1/1753 (0.1%)
1	O	0.53	0/1281	0.75	1/1753 (0.1%)
1	P	0.56	0/1281	0.82	1/1753 (0.1%)
1	Q	0.57	0/1281	0.81	1/1753 (0.1%)
1	R	0.50	0/1281	0.73	1/1753 (0.1%)
1	S	0.56	0/1281	0.84	1/1753 (0.1%)
1	T	0.57	0/1281	0.82	1/1753 (0.1%)
1	U	0.50	0/1281	0.74	1/1753 (0.1%)
1	V	0.56	0/1281	0.80	1/1753 (0.1%)
1	W	0.57	0/1281	0.79	1/1753 (0.1%)
1	X	0.52	0/1281	0.74	1/1753 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	Y	0.58	0/1281	0.84	2/1753 (0.1%)
1	Z	0.53	0/1281	0.77	1/1753 (0.1%)
1	a	0.50	0/1281	0.76	1/1753 (0.1%)
1	b	0.53	0/1281	0.77	1/1753 (0.1%)
1	c	0.47	0/1281	0.72	1/1753 (0.1%)
1	d	0.59	0/1281	0.81	1/1753 (0.1%)
1	e	0.54	0/1281	0.78	3/1753 (0.2%)
1	f	0.46	0/1281	0.72	1/1753 (0.1%)
1	g	0.55	0/1281	0.79	2/1753 (0.1%)
1	h	0.57	0/1281	0.83	1/1753 (0.1%)
1	i	0.55	0/1281	0.76	1/1753 (0.1%)
1	j	0.56	0/1281	0.86	2/1753 (0.1%)
1	k	0.56	0/1281	0.79	1/1753 (0.1%)
1	l	0.50	0/1281	0.73	1/1753 (0.1%)
1	m	0.63	0/1281	0.85	2/1753 (0.1%)
1	n	0.58	0/1281	0.83	1/1753 (0.1%)
1	o	0.56	0/1281	0.76	1/1753 (0.1%)
1	p	0.57	0/1281	0.82	1/1753 (0.1%)
1	q	0.55	0/1281	0.78	1/1753 (0.1%)
1	r	0.49	0/1281	0.73	1/1753 (0.1%)
1	s	0.48	0/1281	0.79	1/1753 (0.1%)
1	t	0.54	0/1281	0.78	1/1753 (0.1%)
1	u	0.46	0/1281	0.72	1/1753 (0.1%)
1	v	0.53	0/1281	0.78	2/1753 (0.1%)
1	w	0.52	0/1281	0.81	1/1753 (0.1%)
1	x	0.51	0/1281	0.74	1/1753 (0.1%)
All	All	0.54	0/76860	0.79	65/105180 (0.1%)

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	4	0	1
1	E	0	1
1	Y	0	2
1	b	0	1
1	m	0	1
1	t	0	1
1	w	0	1
All	All	0	8

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	b	128	LEU	CA-CB-CG	8.91	135.78	115.30
1	t	128	LEU	CA-CB-CG	8.16	134.06	115.30
1	N	128	LEU	CA-CB-CG	7.52	132.60	115.30
1	S	128	LEU	CA-CB-CG	7.37	132.25	115.30
1	4	128	LEU	CA-CB-CG	7.32	132.14	115.30
1	m	128	LEU	CA-CB-CG	7.28	132.05	115.30
1	K	128	LEU	CA-CB-CG	7.27	132.02	115.30
1	k	128	LEU	CA-CB-CG	7.14	131.72	115.30
1	Z	128	LEU	CA-CB-CG	7.07	131.57	115.30
1	h	128	LEU	CA-CB-CG	6.80	130.95	115.30
1	E	128	LEU	CA-CB-CG	6.70	130.71	115.30
1	M	128	LEU	CA-CB-CG	6.59	130.46	115.30
1	o	128	LEU	CA-CB-CG	6.56	130.38	115.30
1	H	128	LEU	CA-CB-CG	6.54	130.35	115.30
1	Q	128	LEU	CA-CB-CG	6.54	130.35	115.30
1	O	128	LEU	CA-CB-CG	6.53	130.32	115.30
1	p	128	LEU	CA-CB-CG	6.52	130.30	115.30
1	g	128	LEU	CA-CB-CG	6.48	130.21	115.30
1	D	128	LEU	CA-CB-CG	6.45	130.12	115.30
1	n	128	LEU	CA-CB-CG	6.38	129.97	115.30
1	L	128	LEU	CA-CB-CG	6.33	129.87	115.30
1	q	128	LEU	CA-CB-CG	6.33	129.86	115.30
1	9	128	LEU	CA-CB-CG	6.32	129.84	115.30
1	T	128	LEU	CA-CB-CG	6.22	129.61	115.30
1	I	128	LEU	CA-CB-CG	6.20	129.56	115.30
1	R	128	LEU	CA-CB-CG	6.20	129.56	115.30
1	x	128	LEU	CA-CB-CG	6.18	129.52	115.30
1	F	128	LEU	CA-CB-CG	6.17	129.49	115.30
1	0	128	LEU	CA-CB-CG	6.16	129.46	115.30
1	u	128	LEU	CA-CB-CG	6.14	129.42	115.30
1	U	128	LEU	CA-CB-CG	6.14	129.41	115.30
1	r	128	LEU	CA-CB-CG	6.13	129.39	115.30
1	Y	130	ASP	N-CA-CB	6.12	121.62	110.60
1	i	128	LEU	CA-CB-CG	6.11	129.35	115.30
1	Y	128	LEU	CA-CB-CG	6.11	129.34	115.30
1	5	128	LEU	CA-CB-CG	6.11	129.34	115.30
1	C	128	LEU	CA-CB-CG	6.09	129.32	115.30
1	3	128	LEU	CA-CB-CG	6.09	129.31	115.30
1	c	128	LEU	CA-CB-CG	6.07	129.27	115.30
1	6	128	LEU	CA-CB-CG	6.07	129.25	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	128	LEU	CA-CB-CG	6.04	129.18	115.30
1	W	128	LEU	CA-CB-CG	6.00	129.10	115.30
1	l	128	LEU	CA-CB-CG	5.97	129.04	115.30
1	V	128	LEU	CA-CB-CG	5.97	129.02	115.30
1	1	177	LEU	CA-CB-CG	5.96	129.02	115.30
1	j	128	LEU	CA-CB-CG	5.89	128.85	115.30
1	J	128	LEU	CA-CB-CG	5.84	128.72	115.30
1	1	128	LEU	CA-CB-CG	5.80	128.65	115.30
1	f	128	LEU	CA-CB-CG	5.80	128.63	115.30
1	m	130	ASP	N-CA-CB	5.75	120.96	110.60
1	A	128	LEU	CA-CB-CG	5.71	128.44	115.30
1	8	128	LEU	CA-CB-CG	5.68	128.37	115.30
1	v	128	LEU	CA-CB-CG	5.68	128.36	115.30
1	d	128	LEU	CA-CB-CG	5.60	128.17	115.30
1	P	128	LEU	CA-CB-CG	5.57	128.11	115.30
1	a	128	LEU	CA-CB-CG	5.56	128.09	115.30
1	v	177	LEU	CA-CB-CG	5.30	127.50	115.30
1	w	128	LEU	CA-CB-CG	5.30	127.50	115.30
1	g	130	ASP	N-CA-CB	5.26	120.07	110.60
1	e	128	LEU	CA-CB-CG	5.16	127.18	115.30
1	s	128	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	177	LEU	CA-CB-CG	5.14	127.13	115.30
1	j	177	LEU	CA-CB-CG	5.14	127.12	115.30
1	e	177	LEU	CA-CB-CG	5.14	127.11	115.30
1	e	156	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	4	207	LEU	Peptide
1	E	207	LEU	Peptide
1	Y	129	PRO	Peptide
1	Y	207	LEU	Peptide
1	b	207	LEU	Peptide
1	m	129	PRO	Peptide
1	t	207	LEU	Peptide
1	w	207	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1253	0	1242	41	0
1	1	1253	0	1242	39	0
1	2	1253	0	1242	42	0
1	3	1253	0	1242	31	1
1	4	1253	0	1242	42	0
1	5	1253	0	1242	41	0
1	6	1253	0	1242	32	0
1	7	1253	0	1242	62	0
1	8	1253	0	1242	49	0
1	9	1253	0	1242	54	0
1	A	1253	0	1242	74	0
1	B	1253	0	1242	84	0
1	C	1253	0	1242	44	0
1	D	1253	0	1242	77	0
1	E	1253	0	1242	84	0
1	F	1253	0	1242	51	0
1	G	1253	0	1242	85	0
1	H	1253	0	1242	98	0
1	I	1253	0	1242	76	0
1	J	1253	0	1242	77	0
1	K	1253	0	1242	79	0
1	L	1253	0	1242	46	0
1	M	1253	0	1242	96	0
1	N	1253	0	1242	72	1
1	O	1253	0	1242	66	0
1	P	1253	0	1242	73	0
1	Q	1253	0	1242	84	0
1	R	1253	0	1242	48	0
1	S	1253	0	1242	73	0
1	T	1253	0	1242	84	0
1	U	1253	0	1242	59	0
1	V	1253	0	1242	86	0
1	W	1253	0	1242	75	0
1	X	1253	0	1242	49	0
1	Y	1253	0	1242	58	0
1	Z	1253	0	1242	56	0
1	a	1253	0	1242	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b	1253	0	1242	0	0
1	c	1253	0	1242	0	0
1	d	1253	0	1242	0	0
1	e	1253	0	1242	0	0
1	f	1253	0	1242	0	0
1	g	1253	0	1242	0	0
1	h	1253	0	1242	0	0
1	i	1253	0	1242	0	0
1	j	1253	0	1242	0	0
1	k	1253	0	1242	0	0
1	l	1253	0	1242	0	0
1	m	1253	0	1242	0	0
1	n	1253	0	1242	0	0
1	o	1253	0	1242	0	0
1	p	1253	0	1242	0	0
1	q	1253	0	1242	0	0
1	r	1253	0	1242	0	0
1	s	1253	0	1242	0	0
1	t	1253	0	1242	0	0
1	u	1253	0	1242	0	0
1	v	1253	0	1242	0	0
1	w	1253	0	1242	0	0
1	x	1253	0	1242	0	0
All	All	75180	0	74520	1835	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 12.

All (1835) 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:N:101:ARG:HE	1:N:166:LEU:HD21	1.02	1.07
1:T:101:ARG:HE	1:T:166:LEU:HD21	1.23	1.03
1:Q:101:ARG:HE	1:Q:166:LEU:HD21	1.21	1.02
1:H:91:ARG:O	1:M:98:ILE:HD11	1.61	1.00
1:V:163:THR:HA	1:X:101:ARG:HH22	1.64	1.00
1:Y:163:THR:HA	1:0:101:ARG:HH22	1.26	0.99
1:1:152:TRP:HH2	1:1:187:CYS:HG	1.04	0.98
1:M:163:THR:HA	1:O:101:ARG:HH22	1.50	0.97
1:E:101:ARG:HE	1:E:166:LEU:HD21	1.30	0.96
1:F:112:GLN:HG2	1:S:149:VAL:HG23	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:112:GLN:HG2	1:Y:149:VAL:HG23	1.48	0.94
1:H:121:GLY:HA3	1:H:152:TRP:HE3	1.33	0.93
1:J:149:VAL:HG23	1:6:112:GLN:HG2	151.79	0.92
1:H:101:ARG:HE	1:H:166:LEU:HD21	1.38	0.89
1:N:101:ARG:NE	1:N:166:LEU:HD21	1.88	0.89
1:T:101:ARG:NE	1:T:166:LEU:HD21	1.88	0.89
1:D:168:TRP:HZ3	1:E:130:ASP:OD1	1.53	0.89
1:I:112:GLN:HG2	1:P:149:VAL:HG23	125.19	0.88
1:S:101:ARG:HE	1:S:166:LEU:HD21	1.38	0.88
1:K:152:TRP:HH2	1:K:187:CYS:HG	1.62	0.88
1:V:101:ARG:HE	1:V:166:LEU:HD21	1.81	0.87
1:W:73:GLY:O	1:W:190:ASN:HB3	2.16	0.87
1:5:101:ARG:HE	1:5:166:LEU:HD21	1.40	0.86
1:7:145:ARG:N	1:7:145:ARG:HE	1.74	0.86
1:P:152:TRP:HH2	1:P:187:CYS:HG	1.44	0.86
1:P:210:PRO:HG2	1:Q:145:ARG:CD	2.08	0.85
1:E:152:TRP:HH2	1:E:187:CYS:HG	1.33	0.85
1:T:112:GLN:HG2	1:0:149:VAL:HG23	150.28	0.85
1:D:101:ARG:HE	1:D:166:LEU:HD21	1.41	0.84
1:O:149:VAL:HG23	1:Q:112:GLN:HG2	122.62	0.84
1:B:152:TRP:HH2	1:B:187:CYS:HG	1.25	0.83
1:G:163:THR:HA	1:I:101:ARG:HH22	1.67	0.83
1:H:120:GLY:N	1:H:192:THR:OG1	2.11	0.83
1:P:121:GLY:HA3	1:P:152:TRP:HE3	1.43	0.83
1:A:149:VAL:HG23	1:U:112:GLN:HG2	78.40	0.82
1:J:152:TRP:HH2	1:J:187:CYS:SG	2.36	0.82
1:J:152:TRP:HH2	1:J:187:CYS:HG	1.55	0.82
1:O:94:HIS:HB2	1:X:98:ILE:HD11	1.60	0.82
1:D:168:TRP:CZ3	1:E:130:ASP:OD1	2.33	0.82
1:7:101:ARG:HE	1:7:166:LEU:HD21	1.44	0.82
1:D:130:ASP:OD1	1:F:168:TRP:CH2	2.33	0.81
1:W:121:GLY:HA3	1:W:152:TRP:HE3	1.44	0.81
1:Z:101:ARG:HE	1:Z:166:LEU:HD21	1.44	0.81
1:8:121:GLY:HA3	1:8:152:TRP:HE3	1.46	0.81
1:1:152:TRP:HH2	1:1:187:CYS:SG	2.04	0.81
1:4:210:PRO:HG2	1:5:145:ARG:HD2	1.63	0.80
1:I:149:VAL:HG23	1:M:112:GLN:HG2	1.62	0.80
1:S:163:THR:OG1	1:S:165:THR:HG22	1.82	0.80
1:D:130:ASP:OD1	1:F:168:TRP:HH2	1.64	0.80
1:7:145:ARG:HD3	1:9:210:PRO:HB2	1.64	0.79
1:D:149:VAL:HG23	1:X:112:GLN:HG2	78.60	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:152:TRP:HH2	1:W:187:CYS:HG	1.54	0.79
1:V:210:PRO:HG2	1:W:145:ARG:CD	2.57	0.79
1:T:73:GLY:O	1:T:190:ASN:HB3	2.08	0.79
1:N:162:TYR:O	1:N:164:ARG:HG3	1.83	0.79
1:P:152:TRP:HH2	1:P:187:CYS:SG	2.19	0.79
1:Q:73:GLY:O	1:Q:190:ASN:HB3	1.82	0.79
1:7:163:THR:HA	1:9:101:ARG:HH22	1.47	0.78
1:A:91:ARG:O	1:E:98:ILE:HD11	1.81	0.78
1:C:112:GLN:HG2	1:S:149:VAL:HG23	78.53	0.78
1:4:101:ARG:HE	1:4:166:LEU:HD21	1.46	0.78
1:2:73:GLY:O	1:2:190:ASN:HB3	1.84	0.78
1:M:101:ARG:HE	1:M:166:LEU:HD21	1.66	0.77
1:M:149:VAL:HG23	1:X:112:GLN:HG2	1.67	0.77
1:O:118:ASN:HB2	1:7:118:ASN:HD21	149.85	0.77
1:D:112:GLN:HG2	1:6:149:VAL:HG23	101.23	0.77
1:E:101:ARG:NE	1:E:166:LEU:HD21	1.99	0.76
1:O:112:GLN:HG2	1:V:149:VAL:HG23	1.68	0.76
1:P:210:PRO:HG2	1:Q:145:ARG:HD2	1.65	0.76
1:H:101:ARG:HE	1:H:166:LEU:CD2	1.98	0.76
1:K:101:ARG:HE	1:K:166:LEU:HD21	1.51	0.76
1:N:112:GLN:HG2	1:R:149:VAL:HG23	89.03	0.75
1:S:168:TRP:HZ3	1:T:130:ASP:OD1	1.69	0.75
1:2:168:TRP:HB2	1:2:177:LEU:O	1.86	0.75
1:W:112:GLN:HG2	1:X:149:VAL:HG23	50.93	0.75
1:E:152:TRP:HH2	1:E:187:CYS:SG	2.15	0.75
1:5:149:VAL:HG23	1:8:112:GLN:HG2	1.69	0.75
1:B:152:TRP:HH2	1:B:187:CYS:SG	2.09	0.74
1:P:163:THR:HA	1:R:101:ARG:HH22	1.90	0.74
1:B:112:GLN:HG2	1:H:149:VAL:CG2	20.55	0.74
1:K:91:ARG:O	1:T:98:ILE:HD11	119.96	0.74
1:L:152:TRP:HH2	1:L:187:CYS:HG	1.54	0.74
1:C:112:GLN:HG2	1:P:149:VAL:HG23	1.69	0.74
1:S:168:TRP:CZ3	1:T:130:ASP:OD1	2.39	0.74
1:G:74:THR:O	1:G:75:ASP:C	2.24	0.74
1:B:121:GLY:HA3	1:B:152:TRP:HE3	1.53	0.73
1:S:163:THR:HA	1:U:101:ARG:HH22	1.53	0.73
1:M:149:VAL:HG23	1:9:112:GLN:HG2	128.86	0.73
1:G:149:VAL:HG23	1:0:112:GLN:HG2	1.70	0.73
1:J:98:ILE:HG22	1:J:99:PHE:CD1	2.23	0.73
1:7:145:ARG:CD	1:9:210:PRO:HB2	2.18	0.73
1:S:121:GLY:HA3	1:S:152:TRP:HE3	1.63	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:VAL:HG23	1:R:112:GLN:HG2	125.85	0.73
1:G:118:ASN:HD21	1:R:118:ASN:HB2	151.38	0.73
1:W:149:VAL:HG23	1:Y:112:GLN:HG2	76.71	0.72
1:V:73:GLY:O	1:V:190:ASN:HB3	2.38	0.72
1:H:100:GLN:HB2	1:H:209:VAL:HG22	1.72	0.72
1:O:149:VAL:CG2	1:Q:112:GLN:HG2	122.52	0.72
1:M:176:ARG:HD2	1:O:168:TRP:CZ2	2.45	0.72
1:K:152:TRP:HH2	1:K:187:CYS:SG	2.40	0.72
1:H:73:GLY:O	1:H:190:ASN:HB3	3.00	0.72
1:8:101:ARG:HE	1:8:166:LEU:HD21	1.55	0.72
1:Q:112:GLN:HG2	1:3:149:VAL:HG23	74.27	0.72
1:L:152:TRP:HH2	1:L:187:CYS:SG	2.32	0.72
1:G:175:GLN:HA	1:G:178:THR:HG22	2.24	0.72
1:C:114:MET:SD	1:P:122:GLY:HA3	2.30	0.72
1:Y:152:TRP:HH2	1:Y:187:CYS:HG	1.35	0.71
1:J:210:PRO:HG2	1:K:145:ARG:CD	2.37	0.71
1:H:98:ILE:HD11	1:M:91:ARG:O	1.90	0.71
1:Q:121:GLY:HA3	1:Q:152:TRP:HE3	1.70	0.71
1:H:121:GLY:HA3	1:H:152:TRP:CE3	2.20	0.71
1:J:63:ILE:HB	1:J:199:VAL:HG22	2.18	0.71
1:E:100:GLN:HB2	1:E:209:VAL:HG22	1.73	0.71
1:E:149:VAL:CG2	1:N:112:GLN:HG2	2.21	0.71
1:P:112:GLN:HG2	1:Q:149:VAL:HG23	51.58	0.71
1:2:101:ARG:HE	1:2:166:LEU:HD21	1.55	0.71
1:Q:168:TRP:HB2	1:Q:177:LEU:O	1.90	0.70
1:C:149:VAL:HG23	1:G:112:GLN:HG2	71.29	0.70
1:B:55:VAL:HG13	1:G:55:VAL:HG13	40.08	0.70
1:M:145:ARG:HE	1:M:145:ARG:N	2.16	0.70
1:N:130:ASP:OD2	1:N:176:ARG:NH2	2.45	0.70
1:J:149:VAL:HG23	1:3:112:GLN:HG2	1.71	0.70
1:K:145:ARG:HE	1:K:145:ARG:N	1.89	0.70
1:L:145:ARG:HE	1:L:145:ARG:N	1.94	0.70
1:H:175:GLN:HA	1:H:178:THR:HG23	1.72	0.70
1:K:55:VAL:HG13	1:T:55:VAL:HG13	107.93	0.70
1:D:163:THR:HA	1:F:101:ARG:HH22	1.56	0.70
1:8:133:ASP:OD2	1:8:135:ASP:HB2	1.92	0.70
1:D:130:ASP:HB2	1:D:132:THR:OG1	3.68	0.69
1:W:101:ARG:HE	1:W:166:LEU:HD21	1.60	0.69
1:D:145:ARG:HE	1:D:145:ARG:N	1.90	0.69
1:4:130:ASP:HB2	1:4:132:THR:OG1	1.92	0.69
1:F:112:GLN:HG2	1:V:149:VAL:HG23	78.01	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:175:GLN:HA	1:N:178:THR:HG23	1.74	0.69
1:L:98:ILE:HD11	1:3:94:HIS:HB2	1.74	0.69
1:8:74:THR:O	1:8:75:ASP:C	2.31	0.69
1:G:176:ARG:HD2	1:I:168:TRP:CZ2	2.28	0.69
1:A:141:LEU:HD21	1:A:184:ILE:HB	2.20	0.69
1:U:149:VAL:HG23	1:Z:112:GLN:HG2	134.93	0.69
1:O:145:ARG:HE	1:O:145:ARG:N	1.94	0.68
1:W:63:ILE:HD11	1:W:89:LEU:CD2	2.24	0.68
1:H:106:THR:OG1	1:H:204:SER:HB3	1.93	0.68
1:Q:145:ARG:N	1:Q:145:ARG:HE	1.92	0.68
1:W:152:TRP:HH2	1:W:187:CYS:SG	2.40	0.68
1:7:168:TRP:HZ3	1:8:130:ASP:OD1	1.76	0.68
1:M:63:ILE:HB	1:M:199:VAL:HG22	1.74	0.68
1:P:121:GLY:HA3	1:P:152:TRP:CE3	2.29	0.68
1:G:112:GLN:HG2	1:L:149:VAL:HG23	1.75	0.68
1:3:145:ARG:HE	1:3:145:ARG:N	1.92	0.68
1:4:163:THR:HA	1:6:101:ARG:HH22	1.59	0.68
1:L:112:GLN:HG2	1:1:149:VAL:HG23	1.76	0.68
1:R:152:TRP:HH2	1:R:187:CYS:SG	2.17	0.68
1:7:74:THR:O	1:7:75:ASP:C	2.32	0.67
1:D:118:ASN:HD21	1:U:118:ASN:HB2	1.59	0.67
1:Z:101:ARG:HE	1:Z:166:LEU:CD2	2.07	0.67
1:W:118:ASN:HD21	1:Y:118:ASN:HB2	94.97	0.67
1:S:130:ASP:OD1	1:U:100:GLN:CD	2.33	0.67
1:D:98:ILE:HG22	1:D:99:PHE:CD1	2.96	0.67
1:I:145:ARG:HE	1:I:145:ARG:N	1.91	0.67
1:T:74:THR:O	1:T:75:ASP:C	2.33	0.67
1:X:145:ARG:HE	1:X:145:ARG:N	1.93	0.67
1:6:145:ARG:N	1:6:145:ARG:HE	1.93	0.67
1:M:122:GLY:HA3	1:9:114:MET:SD	139.64	0.67
1:C:145:ARG:N	1:C:145:ARG:HE	1.92	0.67
1:Q:152:TRP:HH2	1:Q:187:CYS:HG	1.40	0.67
1:Z:175:GLN:HA	1:Z:178:THR:HG23	1.75	0.67
1:N:121:GLY:HA3	1:N:152:TRP:HE3	1.86	0.67
1:G:145:ARG:N	1:G:145:ARG:HE	1.92	0.67
1:H:62:ARG:HD2	1:H:198:SER:HB3	2.10	0.67
1:L:112:GLN:HG2	1:4:149:VAL:HG23	151.85	0.67
1:A:130:ASP:HB3	1:A:132:THR:OG1	2.30	0.67
1:A:60:MET:O	1:F:142:GLN:NE2	2.28	0.67
1:C:118:ASN:HB2	1:S:118:ASN:HD21	92.95	0.67
1:B:100:GLN:OE1	1:C:130:ASP:OD1	2.63	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:VAL:HG23	1:J:112:GLN:HG2	1.76	0.66
1:L:149:VAL:HG23	1:T:112:GLN:HG2	148.24	0.66
1:A:121:GLY:HA3	1:A:152:TRP:HE3	1.67	0.66
1:4:112:GLN:HG2	1:9:149:VAL:HG23	1.76	0.66
1:R:145:ARG:HE	1:R:145:ARG:N	1.96	0.66
1:T:100:GLN:HB2	1:T:209:VAL:HG22	1.90	0.66
1:B:91:ARG:O	1:J:98:ILE:HD11	1.96	0.66
1:P:168:TRP:HZ3	1:Q:130:ASP:OD1	2.31	0.66
1:U:152:TRP:HH2	1:U:187:CYS:HG	1.59	0.66
1:A:112:GLN:HG2	1:F:149:VAL:HG23	1.85	0.66
1:9:145:ARG:N	1:9:145:ARG:HE	1.93	0.66
1:K:121:GLY:HA3	1:K:152:TRP:HE3	1.61	0.66
1:7:145:ARG:NE	1:7:145:ARG:N	2.42	0.66
1:M:112:GLN:HG2	1:T:149:VAL:HG23	129.69	0.66
1:N:100:GLN:HB2	1:N:209:VAL:HG22	1.77	0.66
1:U:145:ARG:HE	1:U:145:ARG:N	1.97	0.66
1:S:176:ARG:O	1:S:177:LEU:HD13	2.64	0.66
1:T:121:GLY:HA3	1:T:152:TRP:HE3	1.74	0.65
1:F:145:ARG:HE	1:F:145:ARG:N	1.94	0.65
1:0:145:ARG:HE	1:0:145:ARG:N	1.94	0.65
1:V:112:GLN:HG2	1:Z:149:VAL:HG23	114.77	0.65
1:H:98:ILE:HD11	1:7:91:ARG:O	139.84	0.65
1:B:101:ARG:HE	1:B:166:LEU:HD21	2.00	0.65
1:I:152:TRP:HH2	1:I:187:CYS:HG	1.45	0.65
1:J:149:VAL:CG2	1:6:112:GLN:HG2	151.68	0.65
1:H:101:ARG:NE	1:H:166:LEU:HD21	2.10	0.65
1:W:149:VAL:CG2	1:Y:112:GLN:HG2	76.50	0.65
1:W:121:GLY:CA	1:W:152:TRP:HE3	2.15	0.65
1:H:112:GLN:HG2	1:8:149:VAL:HG23	149.92	0.65
1:1:210:PRO:HG2	1:2:145:ARG:CD	2.26	0.64
1:J:118:ASN:HB2	1:W:118:ASN:HD21	177.48	0.64
1:D:74:THR:HG23	1:D:190:ASN:OD1	2.39	0.64
1:T:98:ILE:HG22	1:T:99:PHE:CD1	2.39	0.64
1:B:61:SER:OG	1:B:90:PRO:HD2	1.98	0.64
1:P:106:THR:HG23	1:P:204:SER:HB3	1.79	0.64
1:I:91:ARG:NE	1:0:98:ILE:HG23	2.13	0.64
1:T:101:ARG:HE	1:T:166:LEU:CD2	2.05	0.64
1:A:101:ARG:HE	1:A:166:LEU:HD21	2.48	0.64
1:M:145:ARG:NE	1:M:145:ARG:N	2.65	0.64
1:V:146:GLY:HA3	1:V:158:VAL:HG23	1.80	0.64
1:1:190:ASN:OD1	1:1:190:ASN:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:GLY:HA3	1:G:152:TRP:HE3	1.62	0.64
1:G:122:GLY:HA3	1:R:114:MET:SD	133.56	0.64
1:M:122:GLY:HA3	1:X:114:MET:SD	2.38	0.64
1:A:167:LEU:HD23	1:A:179:SER:N	2.47	0.64
1:J:60:MET:HG2	1:W:142:GLN:HE22	137.33	0.64
1:S:145:ARG:N	1:S:145:ARG:HE	1.96	0.64
1:0:152:TRP:HH2	1:0:187:CYS:HG	1.46	0.63
1:B:100:GLN:HB2	1:B:209:VAL:HG22	2.08	0.63
1:C:152:TRP:HH2	1:C:187:CYS:HG	1.47	0.63
1:A:210:PRO:HG2	1:B:145:ARG:CD	2.27	0.63
1:J:210:PRO:HG2	1:K:145:ARG:HD2	2.10	0.63
1:D:122:GLY:HA3	1:U:114:MET:SD	2.38	0.63
1:N:145:ARG:N	1:N:145:ARG:HE	1.98	0.63
1:Y:210:PRO:HG2	1:Z:145:ARG:HD2	1.81	0.63
1:A:69:PRO:HD2	1:A:72:THR:OG1	1.99	0.63
1:H:55:VAL:HG13	1:7:55:VAL:HG13	122.14	0.63
1:A:122:GLY:HA3	1:U:114:MET:SD	82.35	0.63
1:M:130:ASP:OD1	1:O:100:GLN:NE2	2.45	0.63
1:O:62:ARG:HD2	1:O:198:SER:HB3	1.84	0.63
1:A:104:VAL:HG21	1:A:180:PRO:HG3	2.53	0.63
1:T:112:GLN:HG2	1:0:149:VAL:CG2	149.92	0.63
1:D:122:GLY:HA3	1:X:114:MET:SD	81.90	0.63
1:S:112:GLN:HG2	1:2:149:VAL:HG23	135.60	0.63
1:L:114:MET:SD	1:1:122:GLY:HA3	2.37	0.63
1:K:60:MET:O	1:U:142:GLN:NE2	106.78	0.63
1:P:58:SER:O	1:P:91:ARG:NH1	2.92	0.63
1:O:94:HIS:CB	1:X:98:ILE:HD11	2.29	0.63
1:Y:175:GLN:HA	1:Y:178:THR:HG22	1.81	0.63
1:I:98:ILE:HG23	1:0:91:ARG:NE	2.14	0.63
1:W:92:LEU:HD11	1:W:205:VAL:HG11	1.81	0.63
1:Z:121:GLY:HA3	1:Z:152:TRP:HE3	1.64	0.63
1:M:98:ILE:HG22	1:M:99:PHE:CD1	2.33	0.63
1:Q:79:VAL:CG2	1:Q:185:LEU:HD13	2.52	0.63
1:Y:210:PRO:HG2	1:Z:145:ARG:CD	2.28	0.62
1:T:69:PRO:HD2	1:T:72:THR:OG1	2.14	0.62
1:R:152:TRP:HH2	1:R:187:CYS:HG	1.44	0.62
1:K:74:THR:O	1:K:75:ASP:C	2.38	0.62
1:A:149:VAL:HG23	1:R:112:GLN:HG2	1.81	0.62
1:Z:146:GLY:HA3	1:Z:158:VAL:HG23	1.81	0.62
1:M:130:ASP:OD1	1:M:130:ASP:N	2.31	0.62
1:Z:152:TRP:HH2	1:Z:187:CYS:HG	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:149:VAL:HG23	1:7:112:GLN:HG2	150.48	0.62
1:Y:152:TRP:HH2	1:Y:187:CYS:SG	2.22	0.62
1:S:55:VAL:HG13	1:1:55:VAL:HG13	118.09	0.62
1:N:100:GLN:HG2	1:N:211:SER:CB	2.49	0.62
1:H:91:ARG:NH1	1:M:98:ILE:HG23	2.15	0.62
1:V:98:ILE:HD11	1:Y:91:ARG:O	82.67	0.62
1:L:114:MET:SD	1:4:122:GLY:HA3	162.83	0.62
1:5:152:TRP:HH2	1:5:187:CYS:HG	1.47	0.62
1:A:127:PHE:HB3	1:A:160:PRO:HB3	2.21	0.62
1:B:113:PRO:HA	1:B:197:VAL:HA	2.09	0.62
1:D:130:ASP:OD1	1:D:130:ASP:N	3.10	0.62
1:V:98:ILE:HG22	1:V:99:PHE:CD1	2.34	0.62
1:V:211:SER:OG	1:V:212:LEU:N	2.30	0.62
1:C:62:ARG:HD2	1:C:198:SER:HB3	1.88	0.62
1:S:127:PHE:HB3	1:S:160:PRO:HB3	2.33	0.62
1:Q:73:GLY:O	1:Q:190:ASN:CB	2.76	0.62
1:P:63:ILE:HD11	1:P:89:LEU:HD21	1.82	0.62
1:W:100:GLN:HB2	1:W:209:VAL:HG23	2.25	0.61
1:A:168:TRP:CH2	1:B:176:ARG:HD2	3.29	0.61
1:N:74:THR:O	1:N:75:ASP:C	2.78	0.61
1:S:121:GLY:HA3	1:S:152:TRP:CE3	2.51	0.61
1:H:112:GLN:HG2	1:8:149:VAL:CG2	149.49	0.61
1:B:149:VAL:CG2	1:E:112:GLN:HG2	2.37	0.61
1:4:210:PRO:HG2	1:5:145:ARG:CD	2.30	0.61
1:N:149:VAL:HG23	1:S:112:GLN:HG2	98.68	0.61
1:B:121:GLY:HA3	1:B:152:TRP:CE3	2.35	0.61
1:A:145:ARG:N	1:A:145:ARG:HE	2.11	0.61
1:H:108:GLU:HB2	1:H:202:ARG:HG2	2.37	0.61
1:D:112:GLN:HG2	1:O:149:VAL:HG23	1.83	0.61
1:Z:109:PHE:HB2	1:Z:158:VAL:HG13	1.83	0.61
1:N:152:TRP:HH2	1:N:187:CYS:HG	1.59	0.61
1:V:91:ARG:O	1:Y:98:ILE:HD11	86.95	0.61
1:4:145:ARG:N	1:4:145:ARG:HE	1.98	0.61
1:V:63:ILE:HD11	1:V:89:LEU:HD21	1.81	0.61
1:W:121:GLY:HA3	1:W:152:TRP:CE3	2.32	0.61
1:W:63:ILE:HD11	1:W:89:LEU:HD21	1.82	0.61
1:1:98:ILE:HG22	1:1:99:PHE:CD1	2.34	0.61
1:G:63:ILE:HD11	1:G:89:LEU:HD21	1.82	0.61
1:H:163:THR:OG1	1:H:165:THR:HG22	2.26	0.61
1:K:112:GLN:HG2	1:U:149:VAL:HG23	101.46	0.61
1:T:79:VAL:HG23	1:T:80:VAL:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:98:ILE:HG22	1:H:99:PHE:CD1	2.44	0.61
1:I:91:ARG:O	1:0:98:ILE:HD11	2.01	0.61
1:C:152:TRP:HH2	1:C:187:CYS:SG	2.24	0.61
1:K:149:VAL:HG23	1:V:112:GLN:HG2	102.00	0.61
1:G:79:VAL:HG23	1:G:80:VAL:HG23	1.83	0.61
1:N:101:ARG:HE	1:N:166:LEU:CD2	1.95	0.60
1:Y:175:GLN:HA	1:Y:178:THR:CG2	2.29	0.60
1:M:184:ILE:HG22	1:M:186:LEU:HD13	1.96	0.60
1:Z:74:THR:O	1:Z:75:ASP:C	2.40	0.60
1:V:168:TRP:HZ3	1:W:130:ASP:OD1	2.38	0.60
1:N:100:GLN:HB2	1:N:209:VAL:CG2	2.31	0.60
1:3:152:TRP:HH2	1:3:187:CYS:HG	1.49	0.60
1:7:101:ARG:NE	1:7:166:LEU:HD21	2.14	0.60
1:Z:168:TRP:HZ3	1:0:130:ASP:OD1	1.83	0.60
1:V:55:VAL:HG13	1:Y:55:VAL:HG13	74.13	0.60
1:8:101:ARG:NE	1:8:166:LEU:HD21	2.16	0.60
1:D:210:PRO:HG2	1:E:145:ARG:CD	2.51	0.60
1:5:101:ARG:HE	1:5:166:LEU:CD2	2.13	0.60
1:E:74:THR:O	1:E:75:ASP:C	2.40	0.60
1:M:98:ILE:HD11	1:S:91:ARG:O	110.09	0.60
1:M:69:PRO:HD2	1:M:72:THR:OG1	2.01	0.60
1:2:182:ARG:HG3	1:2:184:ILE:HD11	1.84	0.60
1:D:149:VAL:CG2	1:X:112:GLN:HG2	78.99	0.60
1:E:98:ILE:HG22	1:E:99:PHE:CD1	2.37	0.60
1:2:73:GLY:O	1:2:190:ASN:CB	2.49	0.60
1:Q:61:SER:OG	1:Q:90:PRO:HD2	2.00	0.60
1:1:196:ASN:C	1:1:196:ASN:HD22	2.05	0.60
1:9:62:ARG:HD2	1:9:198:SER:HB3	1.84	0.60
1:N:63:ILE:HD11	1:N:89:LEU:HD21	1.82	0.60
1:D:152:TRP:HH2	1:D:187:CYS:SG	2.52	0.60
1:1:130:ASP:OD1	1:1:130:ASP:N	2.35	0.60
1:X:62:ARG:HD2	1:X:198:SER:HB3	1.90	0.59
1:O:152:TRP:HH2	1:O:187:CYS:SG	2.25	0.59
1:Y:145:ARG:N	1:Y:145:ARG:HE	2.00	0.59
1:U:62:ARG:HD2	1:U:198:SER:HB3	1.84	0.59
1:1:210:PRO:HG2	1:2:145:ARG:HD2	1.84	0.59
1:B:145:ARG:N	1:B:145:ARG:HE	2.00	0.59
1:P:73:GLY:O	1:P:190:ASN:HB3	2.03	0.59
1:8:168:TRP:HZ3	1:9:130:ASP:OD1	1.84	0.59
1:R:149:VAL:HG23	1:2:112:GLN:HG2	114.81	0.59
1:6:62:ARG:HD2	1:6:198:SER:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:GLY:HA3	1:H:158:VAL:HG23	2.37	0.59
1:L:145:ARG:NE	1:L:145:ARG:N	2.54	0.59
1:4:163:THR:OG1	1:4:165:THR:HG22	2.03	0.59
1:G:121:GLY:CA	1:G:152:TRP:HE3	2.15	0.59
1:B:74:THR:O	1:B:76:GLY:N	2.91	0.59
1:N:166:LEU:O	1:N:166:LEU:HD23	2.03	0.59
1:7:89:LEU:HD13	1:7:203:TRP:CD1	2.38	0.59
1:M:149:VAL:CG2	1:X:112:GLN:HG2	2.33	0.59
1:H:202:ARG:HG3	1:H:202:ARG:O	2.03	0.59
1:I:62:ARG:HD2	1:I:198:SER:HB3	1.86	0.59
1:9:152:TRP:HH2	1:9:187:CYS:HG	1.51	0.59
1:T:101:ARG:HB2	1:T:208:SER:HB2	1.92	0.59
1:6:152:TRP:HH2	1:6:187:CYS:HG	1.50	0.59
1:G:176:ARG:CZ	1:I:168:TRP:CE3	2.86	0.59
1:B:132:THR:OG1	1:B:176:ARG:NH2	2.35	0.59
1:N:145:ARG:N	1:N:145:ARG:NE	2.53	0.58
1:V:152:TRP:HH2	1:V:187:CYS:HG	1.51	0.58
1:P:130:ASP:HB3	1:P:132:THR:OG1	2.03	0.58
1:Z:121:GLY:HA3	1:Z:152:TRP:CE3	2.38	0.58
1:H:79:VAL:HG23	1:H:80:VAL:HG23	1.84	0.58
1:D:130:ASP:O	1:D:132:THR:N	2.85	0.58
1:D:176:ARG:NH1	1:F:168:TRP:CE3	2.71	0.58
1:V:98:ILE:HD11	1:Y:94:HIS:HB2	83.40	0.58
1:3:152:TRP:HH2	1:3:187:CYS:SG	2.25	0.58
1:D:152:TRP:HH2	1:D:187:CYS:HG	1.80	0.58
1:F:62:ARG:HD2	1:F:198:SER:HB3	1.85	0.58
1:R:62:ARG:HD2	1:R:198:SER:HB3	1.85	0.58
1:5:98:ILE:HG22	1:5:99:PHE:CD1	2.38	0.58
1:O:114:MET:HB3	1:7:121:GLY:O	141.93	0.58
1:5:74:THR:O	1:5:75:ASP:C	2.42	0.58
1:M:63:ILE:HD11	1:M:89:LEU:HD21	2.01	0.58
1:V:106:THR:HA	1:V:162:TYR:OH	2.56	0.58
1:J:122:GLY:HA3	1:6:114:MET:SD	163.42	0.58
1:N:100:GLN:HB2	1:N:209:VAL:HG23	2.08	0.58
1:5:168:TRP:CZ3	1:6:176:ARG:NH2	2.71	0.58
1:2:152:TRP:HH2	1:2:187:CYS:SG	2.26	0.58
1:Q:87:ASP:OD1	1:Q:87:ASP:N	2.34	0.58
1:G:176:ARG:NH2	1:I:168:TRP:CZ3	2.81	0.58
1:Q:130:ASP:OD2	1:Q:176:ARG:NH2	3.12	0.58
1:7:63:ILE:HD11	1:7:89:LEU:CD2	2.34	0.58
1:S:175:GLN:HA	1:S:178:THR:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ASP:HB3	1:C:132:THR:OG1	2.04	0.58
1:4:73:GLY:O	1:4:190:ASN:HB3	2.04	0.58
1:G:145:ARG:N	1:G:145:ARG:NE	2.51	0.58
1:0:62:ARG:HD2	1:0:198:SER:HB3	1.85	0.58
1:S:192:THR:HG22	1:S:192:THR:O	2.29	0.58
1:T:63:ILE:HD11	1:T:89:LEU:CD2	2.49	0.57
1:P:55:VAL:HG13	1:P:55:VAL:HG13	0.00	0.57
1:W:111:ILE:HG22	1:W:113:PRO:HD3	1.87	0.57
1:W:124:VAL:HG13	1:W:186:LEU:HB2	2.17	0.57
1:L:62:ARG:HD2	1:L:198:SER:HB3	1.86	0.57
1:Q:92:LEU:HD11	1:Q:205:VAL:HG11	2.29	0.57
1:5:62:ARG:HD2	1:5:198:SER:HB3	1.84	0.57
1:8:100:GLN:OE1	1:9:130:ASP:OD1	2.22	0.57
1:X:152:TRP:HH2	1:X:187:CYS:HG	1.54	0.57
1:E:130:ASP:HB2	1:E:133:ASP:HB2	2.14	0.57
1:V:114:MET:SD	1:Z:122:GLY:HA3	125.85	0.57
1:S:167:LEU:HD23	1:S:179:SER:N	2.54	0.57
1:A:63:ILE:HB	1:A:199:VAL:HG22	1.85	0.57
1:T:106:THR:HA	1:T:162:TYR:OH	2.04	0.57
1:E:73:GLY:O	1:E:190:ASN:HB3	2.18	0.57
1:P:91:ARG:NH2	1:P:210:PRO:HB3	16.26	0.57
1:K:100:GLN:HB2	1:K:209:VAL:HG23	1.86	0.57
1:H:210:PRO:HG2	1:I:145:ARG:HD2	1.86	0.57
1:I:145:ARG:NE	1:I:145:ARG:N	2.52	0.57
1:T:98:ILE:HD11	1:Z:91:ARG:O	133.81	0.57
1:M:152:TRP:HH2	1:M:187:CYS:SG	2.55	0.57
1:D:210:PRO:HG2	1:E:145:ARG:HD2	1.86	0.57
1:B:74:THR:O	1:B:75:ASP:C	2.56	0.57
1:S:83:THR:O	1:S:88:LEU:HD12	2.62	0.57
1:3:62:ARG:HD2	1:3:198:SER:HB3	1.85	0.57
1:Z:184:ILE:HG22	1:Z:186:LEU:HD13	1.85	0.57
1:N:79:VAL:HG23	1:N:80:VAL:HG23	1.88	0.57
1:Y:79:VAL:HG23	1:Y:80:VAL:HG23	1.85	0.57
1:A:152:TRP:HH2	1:A:187:CYS:SG	2.28	0.57
1:J:113:PRO:HA	1:J:197:VAL:HA	2.17	0.57
1:O:152:TRP:HH2	1:O:187:CYS:HG	1.56	0.57
1:H:83:THR:HA	1:H:182:ARG:HB3	2.34	0.57
1:C:145:ARG:N	1:C:145:ARG:NE	2.53	0.56
1:I:62:ARG:NH1	1:I:65:GLN:NE2	2.53	0.56
1:X:145:ARG:NE	1:X:145:ARG:N	2.54	0.56
1:2:145:ARG:N	1:2:145:ARG:HE	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:62:ARG:NH1	1:O:65:GLN:NE2	2.53	0.56
1:S:141:LEU:HD21	1:S:184:ILE:HB	2.01	0.56
1:P:210:PRO:HG2	1:Q:145:ARG:HD3	1.93	0.56
1:3:130:ASP:HB3	1:3:132:THR:OG1	2.05	0.56
1:R:145:ARG:NE	1:R:145:ARG:N	2.56	0.56
1:D:91:ARG:O	1:5:98:ILE:HD11	119.50	0.56
1:H:89:LEU:HD13	1:H:203:TRP:CD1	2.77	0.56
1:F:152:TRP:HH2	1:F:187:CYS:HG	1.61	0.56
1:B:111:ILE:HG21	1:B:123:TYR:CE2	2.70	0.56
1:O:112:GLN:HG2	1:7:149:VAL:HG23	129.25	0.56
1:H:121:GLY:CA	1:H:152:TRP:HE3	2.17	0.56
1:E:121:GLY:HA3	1:E:152:TRP:HB2	1.91	0.56
1:3:145:ARG:NE	1:3:145:ARG:N	2.53	0.56
1:B:149:VAL:HG22	1:E:112:GLN:HG2	2.32	0.56
1:L:62:ARG:NH1	1:L:65:GLN:NE2	2.56	0.56
1:P:125:ALA:HB2	1:P:185:LEU:HD23	1.88	0.56
1:M:146:GLY:HA3	1:M:158:VAL:HG23	1.88	0.56
1:A:125:ALA:HB2	1:A:185:LEU:HD23	1.87	0.56
1:T:100:GLN:OE1	1:U:130:ASP:OD1	2.47	0.56
1:H:145:ARG:N	1:H:145:ARG:HE	2.04	0.56
1:T:175:GLN:HA	1:T:178:THR:HG22	2.48	0.56
1:7:192:THR:HG22	1:7:192:THR:O	2.06	0.56
1:O:145:ARG:N	1:O:145:ARG:NE	2.54	0.56
1:T:152:TRP:HH2	1:T:187:CYS:SG	2.29	0.56
1:B:145:ARG:N	1:B:145:ARG:NE	2.53	0.56
1:2:130:ASP:OD2	1:2:132:THR:OG1	2.23	0.56
1:L:149:VAL:CG2	1:T:112:GLN:HG2	147.82	0.56
1:V:210:PRO:HG2	1:W:145:ARG:NE	3.00	0.56
1:K:145:ARG:NE	1:K:145:ARG:N	2.54	0.56
1:A:121:GLY:HA3	1:A:152:TRP:CE3	2.53	0.56
1:P:101:ARG:HE	1:P:166:LEU:HD21	2.32	0.56
1:E:166:LEU:O	1:E:166:LEU:HD23	2.06	0.56
1:E:149:VAL:HG23	1:N:112:GLN:HG2	1.87	0.56
1:L:98:ILE:HD11	1:6:94:HIS:HB2	146.42	0.56
1:6:145:ARG:N	1:6:145:ARG:NE	2.53	0.56
1:E:69:PRO:HD2	1:E:72:THR:OG1	2.05	0.56
1:1:145:ARG:HE	1:1:145:ARG:N	2.04	0.56
1:E:168:TRP:CZ3	1:F:176:ARG:NH2	3.77	0.56
1:F:112:GLN:HG2	1:S:149:VAL:CG2	2.27	0.56
1:K:168:TRP:CZ3	1:L:176:ARG:NH2	2.74	0.56
1:O:114:MET:SD	1:7:122:GLY:HA3	139.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:ARG:NE	1:F:145:ARG:N	2.54	0.56
1:1:163:THR:HA	1:3:101:ARG:HH22	1.71	0.56
1:T:86:PRO:HA	1:T:92:LEU:HD23	2.16	0.56
1:8:175:GLN:HA	1:8:178:THR:HG23	1.87	0.56
1:H:196:ASN:HD22	1:H:196:ASN:C	2.08	0.56
1:O:130:ASP:HB3	1:O:132:THR:OG1	2.12	0.55
1:E:168:TRP:CH2	1:F:176:ARG:HD2	2.93	0.55
1:Q:152:TRP:HH2	1:Q:187:CYS:SG	2.29	0.55
1:0:152:TRP:HH2	1:0:187:CYS:SG	2.28	0.55
1:H:145:ARG:N	1:H:145:ARG:NE	2.62	0.55
1:E:106:THR:HA	1:E:162:TYR:OH	2.06	0.55
1:M:58:SER:O	1:M:91:ARG:NH1	3.46	0.55
1:2:152:TRP:HH2	1:2:187:CYS:HG	1.52	0.55
1:X:152:TRP:HH2	1:X:187:CYS:SG	2.28	0.55
1:B:108:GLU:OE1	1:B:202:ARG:NH1	2.39	0.55
1:B:109:PHE:HB2	1:B:158:VAL:HG13	1.88	0.55
1:J:98:ILE:HG22	1:J:99:PHE:CE1	2.41	0.55
1:T:152:TRP:HH2	1:T:187:CYS:HG	1.55	0.55
1:K:111:ILE:HG22	1:K:113:PRO:HD3	1.89	0.55
1:Q:145:ARG:N	1:Q:145:ARG:NE	2.54	0.55
1:M:166:LEU:HD23	1:M:166:LEU:O	2.37	0.55
1:P:63:ILE:HD11	1:P:89:LEU:CD2	2.37	0.55
1:A:176:ARG:O	1:A:177:LEU:HD13	2.13	0.55
1:Z:130:ASP:OD1	1:Z:176:ARG:NH2	2.39	0.55
1:U:175:GLN:HA	1:U:178:THR:HG22	1.91	0.55
1:I:175:GLN:HA	1:I:178:THR:HG22	1.88	0.55
1:H:190:ASN:OD1	1:H:190:ASN:N	2.39	0.55
1:U:152:TRP:HH2	1:U:187:CYS:SG	2.29	0.55
1:N:79:VAL:CG2	1:N:185:LEU:HD13	2.59	0.55
1:Q:63:ILE:HD11	1:Q:89:LEU:HD21	1.88	0.55
1:D:101:ARG:NE	1:D:166:LEU:HD21	2.17	0.55
1:G:55:VAL:HG13	1:K:55:VAL:HG13	1.89	0.55
1:B:79:VAL:CG2	1:B:185:LEU:HD13	2.35	0.55
1:N:146:GLY:HA3	1:N:158:VAL:HG23	2.11	0.55
1:W:106:THR:OG1	1:W:204:SER:HB3	2.45	0.55
1:T:168:TRP:CZ3	1:U:176:ARG:NH2	3.25	0.55
1:7:210:PRO:HG2	1:8:145:ARG:CD	2.37	0.55
1:P:176:ARG:O	1:P:177:LEU:HD13	2.07	0.55
1:H:67:VAL:HG13	1:H:67:VAL:O	2.18	0.55
1:M:176:ARG:CZ	1:O:168:TRP:CE3	2.97	0.55
1:U:145:ARG:N	1:U:145:ARG:NE	2.57	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:125:ALA:HB2	1:J:185:LEU:HD23	1.89	0.55
1:I:130:ASP:HB3	1:I:132:THR:OG1	2.10	0.55
1:Z:149:VAL:O	1:Z:156:ARG:NH2	2.40	0.55
1:S:100:GLN:OE1	1:T:130:ASP:OD1	3.33	0.54
1:A:112:GLN:HG2	1:F:149:VAL:CG2	2.68	0.54
1:0:145:ARG:N	1:0:145:ARG:NE	2.54	0.54
1:S:112:GLN:HG2	1:2:149:VAL:CG2	135.34	0.54
1:9:175:GLN:HA	1:9:178:THR:HG22	1.89	0.54
1:B:86:PRO:HA	1:B:92:LEU:HD23	2.12	0.54
1:C:175:GLN:HA	1:C:178:THR:HG22	1.92	0.54
1:G:190:ASN:OD1	1:G:190:ASN:N	2.97	0.54
1:4:98:ILE:HG23	1:8:91:ARG:HD2	1.89	0.54
1:7:145:ARG:NE	1:7:145:ARG:H	2.06	0.54
1:N:63:ILE:HD11	1:N:89:LEU:CD2	2.37	0.54
1:X:175:GLN:HA	1:X:178:THR:HG22	1.92	0.54
1:7:145:ARG:HD3	1:9:210:PRO:CB	2.36	0.54
1:J:114:MET:SD	1:W:122:GLY:HA3	161.03	0.54
1:F:118:ASN:HB2	1:V:118:ASN:HD21	91.47	0.54
1:H:100:GLN:HB2	1:H:209:VAL:CG2	2.36	0.54
1:9:145:ARG:NE	1:9:145:ARG:N	2.55	0.54
1:Z:152:TRP:HH2	1:Z:187:CYS:SG	2.30	0.54
1:5:152:TRP:HH2	1:5:187:CYS:SG	2.29	0.54
1:J:62:ARG:NH1	1:J:65:GLN:HE21	2.06	0.54
1:A:55:VAL:HG13	1:E:55:VAL:HG13	1.89	0.54
1:B:163:THR:OG1	1:B:165:THR:HG22	2.42	0.54
1:6:62:ARG:NH1	1:6:65:GLN:NE2	2.54	0.54
1:4:133:ASP:OD2	1:4:135:ASP:HB2	2.06	0.54
1:K:73:GLY:O	1:K:190:ASN:HB3	2.07	0.54
1:E:100:GLN:OE1	1:F:130:ASP:OD1	2.24	0.54
1:K:121:GLY:HA3	1:K:152:TRP:CE3	2.42	0.54
1:7:145:ARG:HE	1:7:145:ARG:H	1.52	0.54
1:0:130:ASP:HB3	1:0:132:THR:OG1	2.08	0.54
1:K:113:PRO:HA	1:K:197:VAL:HA	1.96	0.54
1:H:74:THR:O	1:H:75:ASP:C	2.54	0.54
1:B:122:GLY:HA3	1:E:114:MET:SD	2.56	0.54
1:L:100:GLN:HB3	1:L:209:VAL:CG2	2.39	0.54
1:4:111:ILE:HG22	1:4:113:PRO:HD3	1.88	0.54
1:E:146:GLY:HA3	1:E:158:VAL:HG23	1.90	0.54
1:M:74:THR:O	1:M:75:ASP:C	2.46	0.54
1:Y:163:THR:OG1	1:Y:165:THR:HG22	2.06	0.54
1:W:168:TRP:CZ3	1:X:176:ARG:NH2	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:121:GLY:CA	1:P:152:TRP:HE3	2.34	0.54
1:F:175:GLN:HA	1:F:178:THR:HG22	1.89	0.54
1:W:108:GLU:OE1	1:W:202:ARG:NH1	2.46	0.54
1:B:175:GLN:HA	1:B:178:THR:CG2	2.68	0.54
1:J:112:GLN:HG2	1:W:149:VAL:CG2	150.24	0.54
1:M:149:VAL:CG2	1:9:112:GLN:HG2	128.38	0.54
1:E:175:GLN:HA	1:E:178:THR:HG23	1.87	0.54
1:4:79:VAL:CG2	1:4:185:LEU:HD13	2.38	0.54
1:X:74:THR:O	1:X:75:ASP:C	2.49	0.54
1:7:63:ILE:HD11	1:7:89:LEU:HD23	1.90	0.54
1:H:133:ASP:OD2	1:H:135:ASP:HB2	2.71	0.54
1:G:124:VAL:HG13	1:G:186:LEU:HB2	2.37	0.54
1:4:74:THR:O	1:4:75:ASP:C	2.47	0.54
1:T:166:LEU:O	1:T:166:LEU:HD23	2.08	0.54
1:E:130:ASP:CB	1:E:133:ASP:HB2	2.60	0.54
1:V:210:PRO:HB3	1:Y:91:ARG:NH2	67.82	0.54
1:P:184:ILE:HG22	1:P:186:LEU:HD13	2.40	0.54
1:L:130:ASP:HB3	1:L:132:THR:OG1	2.09	0.53
1:R:100:GLN:HB3	1:R:209:VAL:CG2	2.39	0.53
1:6:130:ASP:HB3	1:6:132:THR:OG1	2.08	0.53
1:S:124:VAL:HG13	1:S:186:LEU:HB2	2.27	0.53
1:5:63:ILE:HD11	1:5:89:LEU:HD21	1.91	0.53
1:5:100:GLN:HB2	1:5:209:VAL:HG22	1.90	0.53
1:S:104:VAL:HG21	1:S:180:PRO:HG3	2.02	0.53
1:V:145:ARG:HE	1:V:145:ARG:N	2.06	0.53
1:U:62:ARG:NH1	1:U:65:GLN:NE2	2.56	0.53
1:M:145:ARG:CD	1:O:210:PRO:HB2	2.93	0.53
1:E:79:VAL:HG23	1:E:80:VAL:HG23	1.91	0.53
1:4:63:ILE:HD11	1:4:201:CYS:HB3	1.90	0.53
1:T:101:ARG:HB2	1:T:208:SER:CB	2.55	0.53
1:R:130:ASP:HB3	1:R:132:THR:OG1	2.08	0.53
1:D:121:GLY:HA3	1:D:152:TRP:CE3	2.44	0.53
1:E:162:TYR:O	1:E:164:ARG:HG3	2.17	0.53
1:H:96:ALA:HB1	1:H:169:THR:HB	1.91	0.53
1:J:74:THR:O	1:J:75:ASP:C	2.47	0.53
1:Z:162:TYR:O	1:Z:164:ARG:HG3	2.09	0.53
1:Q:62:ARG:NH1	1:Q:65:GLN:HE21	2.06	0.53
1:D:149:VAL:HG23	1:U:112:GLN:HG2	1.89	0.53
1:B:112:GLN:HG2	1:H:149:VAL:HG23	20.14	0.53
1:M:122:GLY:CA	1:9:114:MET:SD	139.68	0.53
1:V:91:ARG:NH2	1:Y:98:ILE:HG23	89.63	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:VAL:HG23	1:E:112:GLN:HG2	1.89	0.53
1:M:69:PRO:HG2	1:M:72:THR:HG21	1.90	0.53
1:C:100:GLN:HB3	1:C:209:VAL:CG2	2.38	0.53
1:L:175:GLN:HA	1:L:178:THR:HG22	1.90	0.53
1:J:135:ASP:OD1	1:J:137:THR:HG22	2.71	0.53
1:B:120:GLY:N	1:B:192:THR:OG1	3.12	0.53
1:2:175:GLN:HA	1:2:178:THR:HG22	1.90	0.53
1:S:121:GLY:CA	1:S:152:TRP:HE3	2.22	0.53
1:Q:121:GLY:HA3	1:Q:152:TRP:CE3	2.60	0.53
1:M:81:ASP:OD1	1:M:81:ASP:C	2.47	0.53
1:H:163:THR:OG1	1:H:165:THR:CG2	2.79	0.53
1:P:114:MET:SD	1:Q:122:GLY:HA3	57.33	0.53
1:V:109:PHE:HB2	1:V:158:VAL:HG13	1.96	0.53
1:D:121:GLY:HA3	1:D:152:TRP:HE3	1.73	0.53
1:Y:145:ARG:NE	1:Y:145:ARG:N	2.55	0.53
1:E:151:LYS:NZ	1:E:154:GLU:OE1	3.46	0.53
1:7:124:VAL:HG23	1:7:149:VAL:HG12	1.90	0.53
1:N:162:TYR:O	1:N:164:ARG:CG	2.56	0.53
1:A:145:ARG:N	1:A:145:ARG:NE	2.63	0.53
1:R:62:ARG:NH1	1:R:65:GLN:NE2	2.57	0.53
1:3:62:ARG:NH1	1:3:65:GLN:NE2	2.56	0.53
1:A:175:GLN:HB2	1:A:178:THR:CG2	2.39	0.53
1:K:89:LEU:HD13	1:K:203:TRP:CD1	2.57	0.53
1:W:100:GLN:OE1	1:X:130:ASP:OD1	2.26	0.53
1:2:130:ASP:HB3	1:2:133:ASP:H	1.74	0.53
1:W:145:ARG:N	1:W:145:ARG:HE	2.07	0.53
1:H:63:ILE:HD11	1:H:89:LEU:CD2	2.55	0.53
1:Y:141:LEU:HD21	1:Y:184:ILE:HB	1.90	0.53
1:6:100:GLN:HB3	1:6:209:VAL:CG2	2.39	0.53
1:A:100:GLN:OE1	1:B:130:ASP:OD1	2.60	0.53
1:B:96:ALA:HB1	1:B:169:THR:HB	1.91	0.53
1:R:175:GLN:HA	1:R:178:THR:HG22	1.91	0.53
1:I:122:GLY:HA3	1:M:114:MET:SD	2.48	0.53
1:O:98:ILE:HG23	1:9:91:ARG:NE	116.88	0.53
1:X:130:ASP:HB3	1:X:132:THR:OG1	2.08	0.52
1:U:130:ASP:HB3	1:U:132:THR:OG1	2.09	0.52
1:2:145:ARG:N	1:2:145:ARG:NE	2.57	0.52
1:I:98:ILE:HD11	1:0:91:ARG:O	2.10	0.52
1:4:145:ARG:N	1:4:145:ARG:NE	2.56	0.52
1:7:130:ASP:OD1	1:9:100:GLN:NE2	2.42	0.52
1:E:211:SER:OG	1:E:212:LEU:N	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:100:GLN:HB2	1:W:209:VAL:CG2	2.56	0.52
1:J:91:ARG:O	1:V:98:ILE:HD11	129.92	0.52
1:F:101:ARG:HG2	1:F:167:LEU:O	2.15	0.52
1:B:100:GLN:HB2	1:B:209:VAL:O	2.10	0.52
1:G:121:GLY:HA3	1:G:152:TRP:CE3	2.49	0.52
1:Z:145:ARG:NE	1:Z:145:ARG:N	2.56	0.52
1:X:100:GLN:HB3	1:X:209:VAL:CG2	2.39	0.52
1:N:107:LEU:HD22	1:N:109:PHE:CZ	2.44	0.52
1:B:67:VAL:HG13	1:B:67:VAL:O	2.09	0.52
1:E:168:TRP:CZ3	1:F:176:ARG:CZ	4.03	0.52
1:A:168:TRP:CZ3	1:B:176:ARG:HD2	3.95	0.52
1:H:109:PHE:HB2	1:H:158:VAL:HG13	1.91	0.52
1:H:63:ILE:HD11	1:H:89:LEU:HD21	2.22	0.52
1:C:114:MET:SD	1:S:122:GLY:HA3	85.18	0.52
1:T:123:TYR:HB2	1:T:185:LEU:HD21	1.92	0.52
1:S:106:THR:HA	1:S:162:TYR:OH	2.10	0.52
1:Q:111:ILE:HG22	1:Q:113:PRO:HD3	2.51	0.52
1:K:61:SER:HB3	1:K:90:PRO:HD2	2.63	0.52
1:A:210:PRO:HB3	1:E:91:ARG:NH1	2.24	0.52
1:V:152:TRP:HH2	1:V:187:CYS:SG	2.32	0.52
1:T:74:THR:O	1:T:76:GLY:N	2.43	0.52
1:O:100:GLN:HB3	1:O:209:VAL:CG2	2.39	0.52
1:X:62:ARG:NH1	1:X:65:GLN:NE2	2.58	0.52
1:4:63:ILE:HD11	1:4:89:LEU:HD21	1.91	0.52
1:F:130:ASP:HB3	1:F:132:THR:OG1	2.11	0.52
1:H:168:TRP:HZ3	1:I:130:ASP:CG	2.12	0.52
1:D:130:ASP:C	1:D:132:THR:N	2.79	0.52
1:K:168:TRP:CE3	1:L:176:ARG:CZ	2.93	0.52
1:G:98:ILE:HG23	1:K:91:ARG:NH1	2.24	0.52
1:G:145:ARG:CD	1:I:210:PRO:HB2	2.39	0.52
1:Q:175:GLN:HA	1:Q:178:THR:CG2	2.74	0.52
1:0:100:GLN:HB3	1:0:209:VAL:CG2	2.40	0.52
1:3:175:GLN:HA	1:3:178:THR:HG22	1.91	0.52
1:F:114:MET:SD	1:V:122:GLY:HA2	83.26	0.52
1:V:91:ARG:NH2	1:Y:210:PRO:HB3	90.82	0.52
1:B:63:ILE:HD11	1:B:89:LEU:HD21	2.01	0.52
1:P:108:GLU:OE1	1:P:202:ARG:NH1	2.88	0.52
1:Y:123:TYR:HB2	1:Y:185:LEU:CD2	2.40	0.52
1:8:89:LEU:HD13	1:8:203:TRP:CD1	2.44	0.52
1:9:74:THR:O	1:9:75:ASP:C	2.49	0.52
1:J:168:TRP:N	1:J:177:LEU:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:209:VAL:HG23	1:U:209:VAL:O	2.09	0.52
1:I:100:GLN:HB3	1:I:209:VAL:CG2	2.42	0.52
1:V:62:ARG:CZ	1:V:65:GLN:HE21	2.23	0.52
1:C:98:ILE:HD11	1:U:94:HIS:HB2	73.58	0.52
1:D:127:PHE:HB3	1:D:160:PRO:HB3	2.22	0.52
1:I:114:MET:SD	1:Y:122:GLY:HA3	2.50	0.52
1:H:210:PRO:HG2	1:I:145:ARG:CD	2.41	0.52
1:H:79:VAL:CG2	1:H:185:LEU:HD13	2.47	0.52
1:3:100:GLN:HB3	1:3:209:VAL:CG2	2.39	0.52
1:N:69:PRO:HD2	1:N:72:THR:HG21	1.90	0.52
1:Q:100:GLN:HB2	1:Q:209:VAL:CG2	2.50	0.52
1:7:143:ALA:CB	1:9:212:LEU:HB2	2.40	0.52
1:9:152:TRP:HH2	1:9:187:CYS:SG	2.33	0.51
1:G:109:PHE:HB2	1:G:158:VAL:HG13	3.05	0.51
1:5:145:ARG:NE	1:5:145:ARG:N	2.58	0.51
1:M:91:ARG:O	1:S:98:ILE:HD11	114.98	0.51
1:U:100:GLN:HB3	1:U:209:VAL:CG2	2.40	0.51
1:T:123:TYR:HB2	1:T:185:LEU:CD2	2.43	0.51
1:E:145:ARG:N	1:E:145:ARG:HE	2.19	0.51
1:P:79:VAL:HG23	1:P:80:VAL:HG23	1.93	0.51
1:G:146:GLY:HA3	1:G:158:VAL:HG23	3.17	0.51
1:W:79:VAL:CG2	1:W:185:LEU:HD13	2.48	0.51
1:Q:121:GLY:CA	1:Q:152:TRP:HE3	2.43	0.51
1:T:121:GLY:HA3	1:T:152:TRP:CE3	2.60	0.51
1:5:168:TRP:CZ3	1:6:176:ARG:CZ	2.93	0.51
1:O:98:ILE:HD11	1:9:91:ARG:O	120.98	0.51
1:V:108:GLU:OE1	1:V:202:ARG:NH1	2.75	0.51
1:M:106:THR:HA	1:M:162:TYR:OH	2.09	0.51
1:H:61:SER:HB3	1:H:90:PRO:HD2	1.92	0.51
1:H:69:PRO:O	1:H:70:ALA:C	2.50	0.51
1:W:100:GLN:HG2	1:W:211:SER:CB	2.41	0.51
1:A:124:VAL:HB	1:A:149:VAL:HG12	1.92	0.51
1:T:146:GLY:O	1:T:147:ALA:O	2.84	0.51
1:F:62:ARG:NH1	1:F:65:GLN:NE2	2.58	0.51
1:8:79:VAL:HG23	1:8:80:VAL:HG23	1.92	0.51
1:G:81:ASP:OD1	1:G:81:ASP:C	2.60	0.51
1:K:100:GLN:HB2	1:K:209:VAL:CG2	2.41	0.51
1:K:63:ILE:HD11	1:K:89:LEU:HD21	1.93	0.51
1:G:101:ARG:HG2	1:G:167:LEU:O	2.14	0.51
1:Y:100:GLN:HG2	1:Y:211:SER:HB3	1.92	0.51
1:S:79:VAL:CG2	1:S:185:LEU:HD13	2.71	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:TRP:HH2	1:G:187:CYS:SG	2.46	0.51
1:A:63:ILE:HD11	1:A:89:LEU:HD21	2.24	0.51
1:4:152:TRP:HH2	1:4:187:CYS:HG	1.57	0.51
1:Q:127:PHE:CZ	1:Q:181:GLY:HA3	2.46	0.51
1:H:101:ARG:NH1	1:H:168:TRP:CZ2	2.79	0.51
1:H:100:GLN:N	1:H:209:VAL:O	2.72	0.51
1:C:62:ARG:NH1	1:C:65:GLN:NE2	2.58	0.51
1:H:130:ASP:OD2	1:H:176:ARG:NH2	2.44	0.51
1:8:63:ILE:HD11	1:8:89:LEU:HD21	1.93	0.51
1:5:146:GLY:HA3	1:5:158:VAL:HG23	1.92	0.51
1:2:111:ILE:HG21	1:2:123:TYR:CE2	2.46	0.51
1:6:175:GLN:HA	1:6:178:THR:HG22	1.91	0.51
1:F:100:GLN:HB3	1:F:209:VAL:CG2	2.40	0.51
1:J:145:ARG:NE	1:J:145:ARG:N	2.59	0.51
1:J:114:MET:SD	1:W:122:GLY:CA	160.67	0.51
1:G:118:ASN:HD21	1:0:118:ASN:HB2	1.75	0.51
1:D:91:ARG:O	1:N:98:ILE:HD11	2.11	0.51
1:9:100:GLN:HB3	1:9:209:VAL:CG2	2.41	0.51
1:N:91:ARG:O	1:Q:98:ILE:HD11	98.88	0.51
1:E:130:ASP:OD2	1:E:176:ARG:NH2	2.43	0.51
1:S:176:ARG:HD2	1:U:168:TRP:CZ2	2.45	0.51
1:I:98:ILE:HG23	1:0:91:ARG:HE	1.76	0.51
1:G:167:LEU:HD12	1:G:167:LEU:N	2.26	0.51
1:E:78:VAL:HG22	1:E:186:LEU:HD11	1.92	0.51
1:4:167:LEU:HD23	1:4:179:SER:N	2.26	0.51
1:4:106:THR:HG23	1:4:204:SER:HB3	1.93	0.51
1:D:131:PRO:HB2	1:D:175:GLN:NE2	2.25	0.51
1:Q:100:GLN:HB2	1:Q:209:VAL:HG22	1.92	0.51
1:E:131:PRO:HA	1:E:182:ARG:HD2	2.20	0.51
1:J:210:PRO:HG2	1:K:145:ARG:NE	2.26	0.50
1:C:101:ARG:HG2	1:C:167:LEU:O	2.13	0.50
1:9:130:ASP:HB3	1:9:132:THR:OG1	2.12	0.50
1:K:62:ARG:HD2	1:K:198:SER:HB3	1.93	0.50
1:2:146:GLY:HA3	1:2:158:VAL:HG23	1.93	0.50
1:J:122:GLY:HA3	1:3:114:MET:SD	2.51	0.50
1:S:145:ARG:N	1:S:145:ARG:NE	2.59	0.50
1:D:142:GLN:HA	1:D:147:ALA:HB1	1.93	0.50
1:K:96:ALA:HB1	1:K:169:THR:HB	2.63	0.50
1:A:124:VAL:O	1:A:185:LEU:HD23	2.80	0.50
1:M:101:ARG:NE	1:M:166:LEU:HD21	2.40	0.50
1:L:114:MET:SD	1:1:122:GLY:CA	2.98	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:91:ARG:NE	1:9:98:ILE:HG23	117.02	0.50
1:G:101:ARG:HE	1:G:166:LEU:HD21	1.76	0.50
1:L:101:ARG:HG2	1:L:167:LEU:O	2.11	0.50
1:D:106:THR:HG23	1:D:204:SER:HB3	2.08	0.50
1:V:74:THR:O	1:V:75:ASP:C	2.49	0.50
1:E:61:SER:HB3	1:E:90:PRO:HD2	1.94	0.50
1:B:69:PRO:HD2	1:B:72:THR:OG1	2.31	0.50
1:H:152:TRP:HH2	1:H:187:CYS:HG	1.65	0.50
1:5:145:ARG:HE	1:5:145:ARG:N	2.08	0.50
1:7:122:GLY:HA2	1:7:150:ALA:O	2.12	0.50
1:G:130:ASP:CG	1:I:168:TRP:CH2	2.84	0.50
1:G:79:VAL:CG2	1:G:185:LEU:HD13	2.86	0.50
1:0:62:ARG:NH1	1:0:65:GLN:NE2	2.59	0.50
1:1:184:ILE:HG22	1:1:186:LEU:HD13	1.92	0.50
1:D:113:PRO:HA	1:D:197:VAL:HA	1.93	0.50
1:6:101:ARG:HG2	1:6:167:LEU:O	2.11	0.50
1:A:130:ASP:OD1	1:C:168:TRP:HH2	2.53	0.50
1:B:124:VAL:HG11	1:B:138:PHE:CD2	2.46	0.50
1:B:114:MET:SD	1:K:122:GLY:HA3	2.52	0.50
1:0:175:GLN:HA	1:0:178:THR:HG22	1.93	0.50
1:J:151:LYS:HD2	1:J:153:TRP:CZ2	2.66	0.50
1:O:175:GLN:HA	1:O:178:THR:HG22	1.92	0.50
1:N:168:TRP:HZ3	1:O:130:ASP:OD1	1.95	0.50
1:A:118:ASN:HD21	1:U:118:ASN:HB2	93.70	0.50
1:S:78:VAL:HG22	1:S:186:LEU:HD11	1.94	0.50
1:P:137:THR:HG23	1:P:140:ALA:HB3	2.36	0.50
1:G:66:ALA:HB3	1:G:197:VAL:CG1	2.99	0.50
1:S:196:ASN:HD22	1:S:196:ASN:C	2.21	0.50
1:D:145:ARG:NE	1:D:145:ARG:N	2.60	0.50
1:D:122:GLY:CA	1:X:114:MET:SD	81.20	0.50
1:9:62:ARG:NH1	1:9:65:GLN:NE2	2.60	0.50
1:J:116:PRO:O	1:J:119:THR:OG1	2.66	0.50
1:V:124:VAL:HG13	1:V:186:LEU:HB2	2.25	0.50
1:Q:101:ARG:NE	1:Q:166:LEU:HD21	2.06	0.50
1:E:100:GLN:CB	1:E:209:VAL:HG22	2.42	0.50
1:D:124:VAL:HG23	1:D:149:VAL:HG12	1.93	0.50
1:Z:113:PRO:HG2	1:Z:152:TRP:O	2.12	0.50
1:E:145:ARG:N	1:E:145:ARG:NE	2.59	0.50
1:V:121:GLY:CA	1:V:152:TRP:HE3	2.24	0.50
1:J:78:VAL:HA	1:J:186:LEU:HD12	2.15	0.50
1:4:89:LEU:HD13	1:4:203:TRP:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:123:TYR:HB2	1:Y:185:LEU:HD21	1.94	0.50
1:Y:130:ASP:CG	1:0:168:TRP:CH2	2.85	0.50
1:T:61:SER:CB	1:T:90:PRO:HD2	2.41	0.50
1:J:118:ASN:HB2	1:W:118:ASN:ND2	177.41	0.50
1:V:121:GLY:HA2	1:V:152:TRP:HE3	1.77	0.50
1:A:89:LEU:O	1:A:90:PRO:C	2.77	0.50
1:E:83:THR:HA	1:E:182:ARG:HB3	1.93	0.50
1:G:60:MET:O	1:L:142:GLN:NE2	2.45	0.50
1:E:133:ASP:OD2	1:E:135:ASP:HB2	2.12	0.49
1:8:211:SER:OG	1:8:212:LEU:N	2.45	0.49
1:6:152:TRP:HH2	1:6:187:CYS:SG	2.33	0.49
1:W:141:LEU:HD21	1:W:184:ILE:HB	2.13	0.49
1:D:176:ARG:CZ	1:F:168:TRP:CE3	2.95	0.49
1:8:121:GLY:HA3	1:8:152:TRP:CE3	2.36	0.49
1:A:163:THR:HA	1:C:101:ARG:HH22	1.78	0.49
1:P:145:ARG:HE	1:P:145:ARG:N	2.12	0.49
1:D:168:TRP:N	1:D:177:LEU:O	2.61	0.49
1:Z:113:PRO:HA	1:Z:197:VAL:HA	1.95	0.49
1:5:100:GLN:HB2	1:5:209:VAL:CG2	2.42	0.49
1:8:62:ARG:HD2	1:8:198:SER:HB3	1.94	0.49
1:K:123:TYR:OH	1:K:156:ARG:HB2	2.12	0.49
1:H:91:ARG:NH1	1:M:98:ILE:O	2.43	0.49
1:J:98:ILE:HD11	1:V:94:HIS:HB2	123.92	0.49
1:N:152:TRP:HH2	1:N:187:CYS:SG	2.39	0.49
1:Y:176:ARG:HD2	1:0:168:TRP:CZ2	2.48	0.49
1:J:73:GLY:O	1:J:190:ASN:HB3	2.72	0.49
1:E:63:ILE:HD12	1:E:88:LEU:HD13	1.94	0.49
1:S:63:ILE:HD11	1:S:89:LEU:HD21	2.13	0.49
1:Y:74:THR:O	1:Y:75:ASP:C	2.51	0.49
1:4:139:ASP:OD1	1:4:139:ASP:N	2.46	0.49
1:Q:112:GLN:HG2	1:3:149:VAL:CG2	74.33	0.49
1:S:123:TYR:CZ	1:S:150:ALA:HB3	2.87	0.49
1:H:210:PRO:CG	1:I:145:ARG:HD2	2.41	0.49
1:8:100:GLN:HB2	1:8:209:VAL:HG23	1.94	0.49
1:A:89:LEU:O	1:A:92:LEU:N	2.56	0.49
1:B:130:ASP:HB3	1:B:133:ASP:H	1.77	0.49
1:Z:111:ILE:HG21	1:Z:123:TYR:CE2	2.47	0.49
1:2:60:MET:SD	1:2:202:ARG:HB2	2.53	0.49
1:V:79:VAL:CG2	1:V:185:LEU:HD13	2.42	0.49
1:B:115:CYS:HB2	1:B:116:PRO:HD2	1.94	0.49
1:O:200:LEU:HD11	1:7:149:VAL:HG22	127.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:101:ARG:HB2	1:H:208:SER:HB2	2.08	0.49
1:2:168:TRP:CZ3	1:3:176:ARG:NH2	2.80	0.49
1:R:101:ARG:HG2	1:R:167:LEU:O	2.13	0.49
1:D:144:THR:HB	1:D:145:ARG:HH21	1.78	0.49
1:Y:210:PRO:HG2	1:Z:145:ARG:NE	2.28	0.49
1:1:98:ILE:HG22	1:1:99:PHE:CE1	2.46	0.49
1:7:63:ILE:HB	1:7:199:VAL:CG2	2.43	0.49
1:W:141:LEU:HD22	1:W:186:LEU:HD22	2.93	0.49
1:B:123:TYR:HB2	1:B:185:LEU:CD2	2.68	0.49
1:B:125:ALA:O	1:B:147:ALA:HA	2.46	0.49
1:S:61:SER:HB3	1:S:90:PRO:HD2	1.95	0.49
1:M:143:ALA:HB1	1:X:91:ARG:HD2	1.95	0.49
1:P:53:ASN:OD1	1:P:53:ASN:N	2.45	0.49
1:Q:130:ASP:OD2	1:Q:132:THR:OG1	2.31	0.49
1:K:176:ARG:O	1:K:177:LEU:HD13	2.13	0.49
1:0:74:THR:O	1:0:75:ASP:C	2.50	0.49
1:K:211:SER:OG	1:K:212:LEU:N	2.45	0.49
1:B:112:GLN:HG2	1:H:149:VAL:HG22	20.01	0.49
1:Q:123:TYR:OH	1:Q:156:ARG:HB2	2.12	0.49
1:N:98:ILE:HG22	1:N:99:PHE:CD1	2.47	0.49
1:E:63:ILE:HD11	1:E:89:LEU:HD21	2.21	0.49
1:N:113:PRO:HA	1:N:197:VAL:HA	2.21	0.49
1:D:130:ASP:C	1:D:132:THR:H	2.33	0.49
1:S:79:VAL:CG1	1:S:187:CYS:SG	3.40	0.49
1:I:114:MET:SD	1:Y:122:GLY:CA	3.01	0.49
1:H:112:GLN:HG2	1:N:149:VAL:CG2	2.43	0.49
1:J:123:TYR:HA	1:J:186:LEU:O	2.13	0.49
1:X:209:VAL:HG23	1:X:209:VAL:O	2.13	0.49
1:O:91:ARG:O	1:9:98:ILE:HD11	120.97	0.49
1:N:163:THR:OG1	1:N:165:THR:HG22	2.40	0.49
1:X:101:ARG:HG2	1:X:167:LEU:O	2.13	0.49
1:O:118:ASN:HB2	1:V:118:ASN:HD21	1.78	0.49
1:F:114:MET:SD	1:S:122:GLY:HA3	2.53	0.49
1:B:165:THR:HG23	1:B:166:LEU:N	2.39	0.49
1:A:175:GLN:HA	1:A:178:THR:HG22	2.18	0.49
1:A:178:THR:OG1	1:A:178:THR:O	2.27	0.49
1:P:192:THR:HG22	1:P:192:THR:O	2.13	0.49
1:H:210:PRO:HD2	1:I:145:ARG:HD2	1.94	0.48
1:8:210:PRO:HG2	1:9:145:ARG:HD2	1.95	0.48
1:T:210:PRO:HD2	1:U:145:ARG:HD2	1.94	0.48
1:I:152:TRP:HH2	1:I:187:CYS:SG	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:175:GLN:HA	1:T:178:THR:HG23	1.94	0.48
1:V:145:ARG:NE	1:V:145:ARG:N	2.61	0.48
1:Q:141:LEU:HD21	1:Q:184:ILE:HB	2.30	0.48
1:2:163:THR:OG1	1:2:165:THR:HG22	2.13	0.48
1:J:69:PRO:O	1:J:70:ALA:C	2.78	0.48
1:2:92:LEU:HD12	1:2:95:ALA:HB3	1.94	0.48
1:5:149:VAL:CG2	1:8:112:GLN:HG2	2.42	0.48
1:W:63:ILE:HD11	1:W:89:LEU:HD23	1.93	0.48
1:I:91:ARG:CZ	1:0:98:ILE:HG23	2.43	0.48
1:G:210:PRO:HG2	1:H:145:ARG:HD2	2.28	0.48
1:T:171:SER:O	1:U:176:ARG:NH1	2.45	0.48
1:G:142:GLN:NE2	1:0:60:MET:O	2.45	0.48
1:O:74:THR:O	1:O:75:ASP:C	2.51	0.48
1:J:100:GLN:HG2	1:J:211:SER:OG	2.14	0.48
1:B:98:ILE:HG22	1:B:99:PHE:CD1	2.48	0.48
1:1:123:TYR:OH	1:1:156:ARG:HB2	2.13	0.48
1:Q:74:THR:O	1:Q:75:ASP:C	2.52	0.48
1:8:150:ALA:HB2	1:8:156:ARG:HE	1.78	0.48
1:N:166:LEU:HD23	1:N:166:LEU:C	2.47	0.48
1:J:112:GLN:HG2	1:W:149:VAL:HG23	150.86	0.48
1:O:149:VAL:HG23	1:Q:112:GLN:CG	123.42	0.48
1:Q:62:ARG:NH1	1:Q:65:GLN:NE2	2.61	0.48
1:M:114:MET:SD	1:T:122:GLY:HA3	139.28	0.48
1:S:63:ILE:HB	1:S:199:VAL:HG22	1.95	0.48
1:M:134:ASN:O	1:M:136:HIS:CG	2.67	0.48
1:V:163:THR:HA	1:X:101:ARG:NH2	2.49	0.48
1:E:168:TRP:CE3	1:F:176:ARG:CZ	3.68	0.48
1:J:121:GLY:O	1:6:114:MET:HB3	166.27	0.48
1:W:145:ARG:N	1:W:145:ARG:NE	2.62	0.48
1:S:130:ASP:CG	1:U:168:TRP:CH2	2.86	0.48
1:M:122:GLY:CA	1:X:114:MET:SD	3.01	0.48
1:V:176:ARG:NH1	1:X:168:TRP:CE3	4.19	0.48
1:8:113:PRO:HA	1:8:197:VAL:HA	1.95	0.48
1:2:113:PRO:HA	1:2:197:VAL:HA	1.95	0.48
1:7:83:THR:HA	1:7:182:ARG:HB3	1.95	0.48
1:5:106:THR:OG1	1:5:204:SER:HB3	2.13	0.48
1:J:178:THR:O	1:J:178:THR:OG1	2.43	0.48
1:S:67:VAL:HG13	1:S:67:VAL:O	2.54	0.48
1:O:101:ARG:HG2	1:O:167:LEU:O	2.12	0.48
1:B:112:GLN:HG2	1:K:149:VAL:CG2	2.43	0.48
1:M:121:GLY:HA3	1:M:152:TRP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:113:PRO:O	1:P:151:LYS:HE3	128.40	0.48
1:O:94:HIS:HB2	1:X:98:ILE:CD1	2.38	0.48
1:T:63:ILE:HD11	1:T:89:LEU:HD23	1.95	0.48
1:T:122:GLY:HA3	1:1:114:MET:SD	161.76	0.48
1:Q:98:ILE:HG22	1:Q:99:PHE:CD1	2.56	0.48
1:Y:100:GLN:HB2	1:Y:209:VAL:HB	1.95	0.48
1:D:104:VAL:HG11	1:D:107:LEU:HG	1.94	0.48
1:N:143:ALA:HB1	1:S:91:ARG:HD2	105.95	0.48
1:H:101:ARG:HB2	1:H:208:SER:CB	2.51	0.48
1:S:130:ASP:CG	1:U:168:TRP:HH2	2.16	0.48
1:5:106:THR:HA	1:5:162:TYR:OH	2.13	0.48
1:Q:55:VAL:HG13	1:2:55:VAL:HG13	72.79	0.48
1:K:67:VAL:O	1:K:69:PRO:HD3	2.13	0.48
1:J:167:LEU:HD23	1:J:179:SER:N	2.29	0.48
1:Z:212:LEU:O	1:Z:212:LEU:HG	2.13	0.48
1:T:165:THR:HG23	1:T:166:LEU:N	2.40	0.48
1:H:91:ARG:NH1	1:7:98:ILE:HG23	134.92	0.48
1:V:163:THR:OG1	1:V:165:THR:HG22	2.21	0.48
1:0:101:ARG:HG2	1:0:167:LEU:O	2.14	0.48
1:H:165:THR:HG23	1:H:166:LEU:N	2.46	0.48
1:U:101:ARG:HG2	1:U:167:LEU:O	2.13	0.48
1:P:114:MET:HB3	1:Q:121:GLY:O	62.18	0.48
1:A:112:GLN:OE1	1:A:155:SER:OG	2.31	0.48
1:L:209:VAL:O	1:L:209:VAL:HG23	2.13	0.48
1:E:182:ARG:HG3	1:E:184:ILE:HD11	2.60	0.48
1:R:74:THR:O	1:R:75:ASP:C	2.52	0.48
1:H:113:PRO:HA	1:H:197:VAL:HA	1.96	0.48
1:F:118:ASN:HB2	1:S:118:ASN:HD21	1.79	0.48
1:V:122:GLY:HA2	1:V:150:ALA:O	2.13	0.48
1:G:127:PHE:HB3	1:G:160:PRO:HB3	1.95	0.48
1:G:162:TYR:O	1:G:164:ARG:HG3	2.14	0.48
1:J:61:SER:HB3	1:J:90:PRO:HD2	2.16	0.48
1:Q:101:ARG:NH1	1:Q:168:TRP:CZ2	3.05	0.48
1:8:100:GLN:HB2	1:8:209:VAL:CG2	2.44	0.48
1:W:113:PRO:HA	1:W:197:VAL:HA	1.95	0.48
1:2:175:GLN:HA	1:2:178:THR:CG2	2.43	0.48
1:A:146:GLY:HA3	1:A:158:VAL:HG23	2.62	0.48
1:2:141:LEU:O	1:2:144:THR:OG1	2.23	0.48
1:I:101:ARG:HG2	1:I:167:LEU:O	2.15	0.47
1:N:106:THR:HA	1:N:162:TYR:OH	2.27	0.47
1:B:55:VAL:HG13	1:J:55:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:121:GLY:HA3	1:N:152:TRP:CE3	2.71	0.47
1:9:98:ILE:HG22	1:9:99:PHE:CD1	2.48	0.47
1:G:113:PRO:HA	1:G:197:VAL:HA	1.95	0.47
1:1:101:ARG:HE	1:1:166:LEU:HD21	1.79	0.47
1:H:106:THR:OG1	1:H:204:SER:CB	2.62	0.47
1:P:176:ARG:HD2	1:R:168:TRP:CZ2	3.14	0.47
1:1:115:CYS:HB2	1:1:116:PRO:HD2	1.96	0.47
1:1:74:THR:O	1:1:75:ASP:C	2.52	0.47
1:D:214:ASN:HD21	1:E:137:THR:HG21	1.80	0.47
1:Y:61:SER:HB3	1:Y:90:PRO:HD2	1.96	0.47
1:E:168:TRP:CZ2	1:F:176:ARG:HD2	3.02	0.47
1:A:149:VAL:CG2	1:R:200:LEU:HD11	2.44	0.47
1:Q:175:GLN:HA	1:Q:178:THR:HG23	2.66	0.47
1:V:80:VAL:HB	1:V:185:LEU:HB2	1.97	0.47
1:I:74:THR:O	1:I:75:ASP:C	2.52	0.47
1:W:168:TRP:HB2	1:W:177:LEU:O	2.14	0.47
1:I:149:VAL:HG22	1:M:200:LEU:HD11	1.97	0.47
1:K:149:VAL:CG2	1:V:112:GLN:HG2	102.28	0.47
1:L:98:ILE:HD11	1:3:94:HIS:CB	2.44	0.47
1:G:176:ARG:CZ	1:I:168:TRP:CZ3	2.98	0.47
1:4:190:ASN:OD1	1:4:190:ASN:N	2.47	0.47
1:1:145:ARG:NH1	1:1:161:GLN:HB3	2.29	0.47
1:J:79:VAL:CG2	1:J:185:LEU:HD13	2.44	0.47
1:V:130:ASP:OD1	1:X:100:GLN:CD	3.03	0.47
1:J:145:ARG:N	1:J:145:ARG:HE	2.13	0.47
1:U:74:THR:O	1:U:75:ASP:C	2.52	0.47
1:D:96:ALA:HB1	1:D:169:THR:HB	2.14	0.47
1:Y:191:ASN:N	1:Y:191:ASN:OD1	2.46	0.47
1:D:124:VAL:HG11	1:D:138:PHE:CD2	2.79	0.47
1:9:101:ARG:HG2	1:9:167:LEU:O	2.14	0.47
1:M:91:ARG:NE	1:S:98:ILE:HG23	114.18	0.47
1:2:77:TYR:HB3	1:2:187:CYS:SG	2.54	0.47
1:4:89:LEU:HD12	1:4:92:LEU:HD12	1.95	0.47
1:8:80:VAL:HB	1:8:185:LEU:HB2	1.97	0.47
1:M:175:GLN:HA	1:M:178:THR:HG22	2.16	0.47
1:8:98:ILE:HG22	1:8:99:PHE:CD1	2.49	0.47
1:T:145:ARG:HE	1:T:145:ARG:N	2.23	0.47
1:B:112:GLN:HG2	1:K:149:VAL:HG23	1.96	0.47
1:J:63:ILE:HD11	1:J:89:LEU:HD21	1.95	0.47
1:8:100:GLN:HB2	1:8:209:VAL:O	2.15	0.47
1:T:63:ILE:HD11	1:T:89:LEU:HD21	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:139:ASP:O	1:9:212:LEU:HD23	2.15	0.47
1:4:151:LYS:HD2	1:4:153:TRP:CZ2	2.50	0.47
1:Y:151:LYS:HD2	1:Y:153:TRP:CZ2	2.49	0.47
1:7:113:PRO:HA	1:7:197:VAL:HA	1.96	0.47
1:B:155:SER:O	1:B:156:ARG:HD3	2.14	0.47
1:4:107:LEU:O	1:4:160:PRO:HD2	2.15	0.47
1:L:74:THR:O	1:L:75:ASP:C	2.51	0.47
1:I:112:GLN:HG2	1:P:149:VAL:CG2	125.37	0.47
1:G:176:ARG:NH1	1:I:168:TRP:CE3	2.83	0.47
1:N:123:TYR:HB2	1:N:185:LEU:CD2	2.45	0.47
1:N:146:GLY:O	1:N:147:ALA:O	3.18	0.47
1:0:209:VAL:HG23	1:0:209:VAL:O	2.14	0.47
1:W:79:VAL:HG23	1:W:80:VAL:HG23	1.97	0.47
1:M:175:GLN:CA	1:M:178:THR:HG22	2.68	0.47
1:G:173:LYS:HD3	1:H:173:LYS:O	2.68	0.47
1:7:175:GLN:HA	1:7:178:THR:CG2	2.44	0.47
1:Y:146:GLY:HA3	1:Y:158:VAL:HG23	1.96	0.47
1:4:123:TYR:OH	1:4:156:ARG:HB2	2.14	0.47
1:P:60:MET:O	1:Q:142:GLN:NE2	32.01	0.47
1:B:106:THR:OG1	1:B:204:SER:HB3	2.15	0.47
1:F:74:THR:O	1:F:75:ASP:C	2.53	0.47
1:Y:115:CYS:HB2	1:Y:116:PRO:HD2	1.97	0.47
1:2:176:ARG:O	1:2:177:LEU:HD13	2.14	0.47
1:P:163:THR:OG1	1:P:165:THR:HG22	2.24	0.47
1:K:69:PRO:HD2	1:K:72:THR:OG1	2.38	0.47
1:1:107:LEU:HD22	1:1:109:PHE:CZ	2.50	0.47
1:3:98:ILE:HG22	1:3:99:PHE:CD1	2.50	0.47
1:W:122:GLY:N	1:W:152:TRP:CE3	2.96	0.47
1:M:101:ARG:HE	1:M:166:LEU:CD2	2.39	0.47
1:I:98:ILE:HG22	1:I:99:PHE:CD1	2.50	0.47
1:7:63:ILE:HB	1:7:199:VAL:HG23	1.96	0.47
1:N:98:ILE:HD11	1:Q:91:ARG:O	103.15	0.47
1:S:184:ILE:HG22	1:S:186:LEU:HD13	1.97	0.47
1:D:84:ILE:HB	1:D:180:PRO:HD2	2.36	0.47
1:K:54:ASP:OD2	1:K:206:ARG:NH1	2.58	0.47
1:V:210:PRO:HG2	1:W:145:ARG:HD3	2.22	0.47
1:1:145:ARG:NE	1:1:145:ARG:N	2.63	0.47
1:T:212:LEU:HB2	1:U:143:ALA:CB	2.55	0.47
1:Y:101:ARG:CZ	1:Y:168:TRP:CZ2	2.98	0.47
1:E:139:ASP:OD1	1:E:139:ASP:N	2.69	0.47
1:D:168:TRP:CH2	1:E:176:ARG:HD2	2.90	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:145:ARG:NE	1:O:210:PRO:HB2	2.33	0.46
1:K:200:LEU:HD11	1:U:149:VAL:CG2	103.13	0.46
1:T:80:VAL:O	1:T:184:ILE:HA	2.70	0.46
1:P:145:ARG:N	1:P:145:ARG:NE	2.63	0.46
1:Y:146:GLY:O	1:Y:148:VAL:HG13	2.16	0.46
1:V:66:ALA:HB3	1:V:197:VAL:HG12	2.38	0.46
1:Z:131:PRO:HB3	1:Z:179:SER:HB3	1.97	0.46
1:3:74:THR:O	1:3:75:ASP:C	2.53	0.46
1:B:62:ARG:HD2	1:B:198:SER:HB3	2.17	0.46
1:M:60:MET:HA	1:M:201:CYS:O	2.52	0.46
1:A:106:THR:HG23	1:A:204:SER:HB3	2.12	0.46
1:C:118:ASN:HB2	1:P:118:ASN:HD21	1.79	0.46
1:K:91:ARG:NH1	1:T:98:ILE:HG23	111.72	0.46
1:3:101:ARG:HG2	1:3:167:LEU:O	2.15	0.46
1:P:141:LEU:HD21	1:P:184:ILE:HB	2.21	0.46
1:B:63:ILE:HD11	1:B:89:LEU:CD2	2.45	0.46
1:O:91:ARG:HD2	1:7:143:ALA:HB1	122.98	0.46
1:P:69:PRO:HD2	1:P:72:THR:OG1	2.14	0.46
1:E:92:LEU:HD11	1:E:205:VAL:HG11	1.97	0.46
1:7:176:ARG:HD2	1:9:168:TRP:CZ2	2.49	0.46
1:D:79:VAL:HG23	1:D:80:VAL:HG23	2.09	0.46
1:A:98:ILE:HD11	1:E:94:HIS:HB2	1.98	0.46
1:Z:123:TYR:CZ	1:Z:150:ALA:HB3	2.50	0.46
1:1:123:TYR:HB2	1:1:185:LEU:CD2	2.45	0.46
1:N:96:ALA:HB1	1:N:169:THR:HB	2.36	0.46
1:G:79:VAL:HG22	1:G:185:LEU:HB3	2.10	0.46
1:2:184:ILE:HG22	1:2:186:LEU:CD1	2.46	0.46
1:W:184:ILE:HG22	1:W:186:LEU:HD13	2.06	0.46
1:E:79:VAL:CG2	1:E:185:LEU:HD13	2.46	0.46
1:Q:81:ASP:OD2	1:Q:182:ARG:NH2	2.49	0.46
1:O:114:MET:SD	1:V:122:GLY:HA3	2.54	0.46
1:M:121:GLY:HA2	1:M:152:TRP:HE3	1.81	0.46
1:H:62:ARG:CD	1:H:198:SER:HB3	2.51	0.46
1:Q:130:ASP:HB3	1:Q:133:ASP:H	1.81	0.46
1:7:175:GLN:HB2	1:7:175:GLN:HE21	1.60	0.46
1:K:106:THR:HG23	1:K:204:SER:HB3	1.97	0.46
1:J:130:ASP:C	1:J:132:THR:H	2.19	0.46
1:W:175:GLN:HA	1:W:178:THR:CG2	2.51	0.46
1:D:176:ARG:HD2	1:F:168:TRP:CZ2	2.50	0.46
1:G:175:GLN:CA	1:G:178:THR:HG22	3.13	0.46
1:P:63:ILE:HB	1:P:199:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:79:VAL:HG21	1:H:185:LEU:HD13	2.19	0.46
1:P:79:VAL:CG2	1:P:185:LEU:HD13	2.68	0.46
1:E:86:PRO:HA	1:E:92:LEU:HD23	1.97	0.46
1:O:128:LEU:HA	1:O:129:PRO:HD3	1.82	0.46
1:C:74:THR:O	1:C:75:ASP:C	2.52	0.46
1:W:91:ARG:NH1	1:W:98:ILE:CG2	12.62	0.46
1:P:127:PHE:HB3	1:P:160:PRO:HB3	1.98	0.46
1:B:73:GLY:O	1:B:190:ASN:HB3	2.20	0.46
1:H:152:TRP:HH2	1:H:187:CYS:SG	2.38	0.46
1:W:121:GLY:CA	1:W:152:TRP:CE3	2.96	0.46
1:K:124:VAL:HG23	1:K:149:VAL:HG12	2.46	0.46
1:M:176:ARG:NH2	1:O:168:TRP:CZ3	2.91	0.46
1:N:123:TYR:HB2	1:N:185:LEU:HD21	2.07	0.46
1:C:99:PHE:HB3	1:C:208:SER:O	2.16	0.46
1:7:176:ARG:NH1	1:9:170:SER:O	2.49	0.46
1:5:141:LEU:O	1:5:144:THR:HG23	2.15	0.46
1:G:92:LEU:HD21	1:G:207:LEU:HD21	2.49	0.46
1:T:108:GLU:HB2	1:T:202:ARG:HG2	2.59	0.46
1:2:67:VAL:HG22	1:2:67:VAL:O	2.16	0.46
1:J:121:GLY:O	1:3:114:MET:HB3	2.15	0.46
1:K:145:ARG:NH1	1:K:161:GLN:HB3	2.34	0.46
1:G:130:ASP:OD1	1:G:130:ASP:N	2.52	0.46
1:I:98:ILE:HG23	1:R:91:ARG:NE	109.79	0.46
1:G:79:VAL:HG21	1:G:185:LEU:HD13	2.53	0.46
1:2:121:GLY:CA	1:2:152:TRP:HE3	2.28	0.46
1:K:175:GLN:HA	1:K:178:THR:HG22	2.36	0.46
1:V:115:CYS:HB2	1:V:116:PRO:HD2	2.05	0.46
1:Q:163:THR:OG1	1:Q:165:THR:HG22	2.19	0.46
1:I:114:MET:HB3	1:Y:121:GLY:O	2.16	0.46
1:W:118:ASN:ND2	1:Y:118:ASN:HB2	94.25	0.46
1:M:184:ILE:HG22	1:M:186:LEU:CD1	2.45	0.46
1:E:138:PHE:CE1	1:E:142:GLN:HG3	2.67	0.46
1:Z:184:ILE:CG2	1:Z:186:LEU:HD13	2.46	0.46
1:F:152:TRP:HH2	1:F:187:CYS:SG	2.40	0.46
1:B:177:LEU:O	1:B:178:THR:HG22	2.16	0.46
1:6:209:VAL:O	1:6:209:VAL:HG23	2.15	0.46
1:K:79:VAL:CG2	1:K:185:LEU:HD13	2.46	0.46
1:Q:184:ILE:HG22	1:Q:186:LEU:HD13	1.98	0.46
1:F:99:PHE:HB3	1:F:208:SER:O	2.16	0.46
1:T:113:PRO:HA	1:T:197:VAL:HA	2.28	0.46
1:V:77:TYR:CD1	1:V:77:TYR:C	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:162:TYR:CD1	1:J:162:TYR:N	2.84	0.46
1:Q:145:ARG:NH1	1:Q:161:GLN:HB3	2.31	0.46
1:B:91:ARG:O	1:G:98:ILE:HD11	41.22	0.46
1:G:98:ILE:HD11	1:K:91:ARG:O	2.16	0.46
1:S:79:VAL:HG23	1:S:80:VAL:HG23	1.98	0.46
1:1:124:VAL:HG23	1:1:149:VAL:HG12	1.97	0.46
1:H:210:PRO:HB2	1:I:145:ARG:NE	2.31	0.46
1:V:121:GLY:HA3	1:V:152:TRP:HB2	1.98	0.46
1:P:130:ASP:OD1	1:R:100:GLN:CD	3.45	0.46
1:A:73:GLY:O	1:A:190:ASN:HB3	2.63	0.46
1:0:151:LYS:HD2	1:0:153:TRP:CZ2	2.52	0.46
1:7:96:ALA:HB1	1:7:169:THR:HB	1.98	0.46
1:N:81:ASP:CG	1:N:81:ASP:O	3.09	0.46
1:P:210:PRO:HG2	1:Q:145:ARG:NE	2.57	0.45
1:D:149:VAL:CG2	1:U:112:GLN:HG2	2.46	0.45
1:8:145:ARG:N	1:8:145:ARG:NE	2.64	0.45
1:M:162:TYR:O	1:M:164:ARG:HG3	2.16	0.45
1:Q:163:THR:OG1	1:Q:165:THR:CG2	2.64	0.45
1:6:74:THR:O	1:6:75:ASP:C	2.53	0.45
1:L:151:LYS:HD2	1:L:153:TRP:CZ2	2.55	0.45
1:7:183:LEU:C	1:7:183:LEU:HD13	2.37	0.45
1:Q:101:ARG:HE	1:Q:166:LEU:CD2	2.12	0.45
1:G:130:ASP:CG	1:I:168:TRP:HH2	2.18	0.45
1:E:79:VAL:HG22	1:E:185:LEU:HB3	1.98	0.45
1:I:122:GLY:CA	1:M:114:MET:SD	3.05	0.45
1:7:61:SER:HB3	1:7:90:PRO:HD2	1.99	0.45
1:D:61:SER:HB3	1:D:90:PRO:HD2	1.98	0.45
1:1:128:LEU:HD22	1:1:128:LEU:H	1.81	0.45
1:H:124:VAL:HG13	1:H:186:LEU:HB2	1.97	0.45
1:D:183:LEU:HD13	1:D:183:LEU:C	2.36	0.45
1:D:83:THR:HA	1:D:182:ARG:HB3	2.18	0.45
1:A:184:ILE:HG22	1:A:186:LEU:CD1	2.59	0.45
1:D:98:ILE:HG22	1:D:99:PHE:CE1	3.05	0.45
1:E:74:THR:O	1:E:76:GLY:N	2.50	0.45
1:T:175:GLN:HA	1:T:178:THR:CG2	2.47	0.45
1:7:176:ARG:CZ	1:9:168:TRP:CE3	3.00	0.45
1:7:173:LYS:O	1:9:173:LYS:HD3	2.16	0.45
1:N:168:TRP:HD1	1:N:177:LEU:HB3	2.24	0.45
1:K:168:TRP:CZ3	1:L:176:ARG:CZ	2.99	0.45
1:8:74:THR:O	1:8:76:GLY:N	2.48	0.45
1:M:121:GLY:CA	1:M:152:TRP:HE3	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:145:ARG:HE	1:Z:145:ARG:N	2.13	0.45
1:T:111:ILE:HG21	1:T:123:TYR:CE2	2.58	0.45
1:P:176:ARG:NH1	1:R:168:TRP:CE3	3.24	0.45
1:G:210:PRO:HG2	1:H:145:ARG:HD3	1.98	0.45
1:E:79:VAL:HG21	1:E:185:LEU:HD13	1.99	0.45
1:O:98:ILE:HG22	1:O:99:PHE:CD1	2.52	0.45
1:G:109:PHE:HB2	1:G:158:VAL:HG22	1.98	0.45
1:8:105:GLU:O	1:8:106:THR:HG23	2.17	0.45
1:N:115:CYS:HB2	1:N:116:PRO:HD2	2.03	0.45
1:S:73:GLY:O	1:S:190:ASN:HA	3.06	0.45
1:5:69:PRO:HD2	1:5:72:THR:OG1	2.15	0.45
1:G:123:TYR:HB2	1:G:185:LEU:CD2	2.73	0.45
1:M:184:ILE:CG2	1:M:186:LEU:HD13	2.81	0.45
1:N:146:GLY:O	1:N:147:ALA:C	2.84	0.45
1:T:212:LEU:HG	1:T:212:LEU:O	2.28	0.45
1:Q:95:ALA:N	1:2:98:ILE:HD11	80.06	0.45
1:J:122:GLY:CA	1:6:114:MET:SD	163.39	0.45
1:F:118:ASN:HB2	1:V:118:ASN:ND2	92.14	0.45
1:B:91:ARG:NH1	1:G:98:ILE:HG23	35.75	0.45
1:R:98:ILE:HG22	1:R:99:PHE:CD1	2.53	0.45
1:V:91:ARG:CZ	1:Y:98:ILE:HG23	90.07	0.45
1:V:59:GLY:HA3	1:V:203:TRP:CZ2	2.52	0.45
1:V:89:LEU:HD13	1:V:203:TRP:CD1	2.52	0.45
1:V:123:TYR:OH	1:V:154:GLU:O	2.30	0.45
1:D:63:ILE:HB	1:D:199:VAL:HG22	1.98	0.45
1:8:127:PHE:CZ	1:8:181:GLY:HA3	2.52	0.45
1:A:192:THR:O	1:A:192:THR:HG22	2.33	0.45
1:K:166:LEU:O	1:K:166:LEU:HD23	2.47	0.45
1:T:130:ASP:OD2	1:T:176:ARG:NH2	2.50	0.45
1:C:132:THR:HG21	1:C:176:ARG:NH2	2.32	0.45
1:C:98:ILE:HG22	1:C:99:PHE:CD1	2.52	0.45
1:C:151:LYS:HD2	1:C:153:TRP:CZ2	2.53	0.45
1:7:106:THR:HA	1:7:162:TYR:OH	2.16	0.45
1:M:62:ARG:HD3	1:M:198:SER:HB3	2.00	0.45
1:2:174:GLU:HB3	1:3:174:GLU:OE2	2.16	0.45
1:Z:101:ARG:HB2	1:Z:208:SER:HB2	1.99	0.45
1:Z:100:GLN:HB2	1:Z:209:VAL:HG22	1.98	0.45
1:M:100:GLN:HG2	1:M:211:SER:OG	2.49	0.45
1:M:101:ARG:CZ	1:M:168:TRP:CZ2	3.00	0.45
1:M:168:TRP:HZ3	1:N:130:ASP:OD1	2.00	0.45
1:S:152:TRP:HH2	1:S:187:CYS:SG	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:98:ILE:HG22	1:L:99:PHE:CD1	2.52	0.45
1:P:63:ILE:HD12	1:P:88:LEU:HD13	2.12	0.45
1:P:130:ASP:OD1	1:R:168:TRP:HH2	2.00	0.45
1:C:209:VAL:HG23	1:C:209:VAL:O	2.17	0.45
1:J:130:ASP:N	1:J:130:ASP:OD1	2.60	0.45
1:7:128:LEU:HD22	1:7:128:LEU:H	1.81	0.45
1:1:89:LEU:HD13	1:1:203:TRP:CD1	2.51	0.45
1:E:128:LEU:HA	1:E:129:PRO:HD3	1.87	0.45
1:W:55:VAL:HG13	1:W:55:VAL:HG13	0.00	0.45
1:X:98:ILE:HG22	1:X:99:PHE:CD1	2.54	0.45
1:M:210:PRO:HG2	1:N:145:ARG:CD	2.47	0.45
1:G:80:VAL:HB	1:G:185:LEU:HB2	1.99	0.45
1:R:209:VAL:O	1:R:209:VAL:HG23	2.16	0.45
1:T:168:TRP:CZ3	1:U:176:ARG:CZ	3.51	0.45
1:9:209:VAL:O	1:9:209:VAL:HG23	2.17	0.45
1:H:138:PHE:CE1	1:H:142:GLN:HG3	2.53	0.45
1:V:184:ILE:HG22	1:V:186:LEU:CD1	2.47	0.45
1:1:128:LEU:HA	1:1:129:PRO:HD3	1.75	0.45
1:7:84:ILE:O	1:7:180:PRO:HD2	2.17	0.45
1:N:83:THR:HA	1:N:182:ARG:HB3	2.32	0.45
1:2:63:ILE:HD11	1:2:89:LEU:HD21	1.99	0.45
1:G:128:LEU:HA	1:G:129:PRO:HD3	1.74	0.45
1:Y:73:GLY:O	1:Y:190:ASN:HB3	2.17	0.45
1:H:171:SER:O	1:I:176:ARG:NH1	2.49	0.45
1:D:98:ILE:HD11	1:N:94:HIS:HB2	1.99	0.45
1:Q:104:VAL:HG11	1:Q:107:LEU:HG	2.10	0.45
1:K:137:THR:HG23	1:K:140:ALA:HB2	1.98	0.45
1:7:138:PHE:C	1:7:138:PHE:CD1	2.90	0.45
1:M:101:ARG:NH1	1:M:168:TRP:CH2	2.86	0.44
1:W:165:THR:HG23	1:W:166:LEU:N	2.32	0.44
1:M:141:LEU:HD21	1:M:184:ILE:HB	1.99	0.44
1:W:91:ARG:NH1	1:W:98:ILE:HG23	13.32	0.44
1:Q:162:TYR:O	1:Q:164:ARG:HG3	2.51	0.44
1:K:115:CYS:HB2	1:K:116:PRO:HD2	2.29	0.44
1:Q:168:TRP:CZ3	1:R:176:ARG:NH2	2.87	0.44
1:W:211:SER:OG	1:W:212:LEU:N	2.63	0.44
1:G:145:ARG:NE	1:I:210:PRO:HB2	2.32	0.44
1:0:98:ILE:HG22	1:0:99:PHE:CD1	2.51	0.44
1:I:91:ARG:O	1:R:98:ILE:HD11	115.33	0.44
1:G:106:THR:HA	1:G:162:TYR:OH	2.17	0.44
1:I:128:LEU:HA	1:I:129:PRO:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:128:LEU:HA	1:V:129:PRO:HD3	1.78	0.44
1:S:74:THR:O	1:S:76:GLY:N	2.84	0.44
1:Z:168:TRP:CZ3	1:0:130:ASP:OD1	2.67	0.44
1:D:74:THR:O	1:D:75:ASP:C	2.55	0.44
1:G:121:GLY:CA	1:G:152:TRP:CE3	2.99	0.44
1:U:142:GLN:NE2	1:Z:60:MET:O	131.11	0.44
1:G:111:ILE:HG21	1:G:123:TYR:CE2	2.52	0.44
1:K:130:ASP:HB3	1:K:133:ASP:H	1.82	0.44
1:T:55:VAL:HG13	1:Z:55:VAL:HG13	118.25	0.44
1:M:176:ARG:NH1	1:O:170:SER:O	2.54	0.44
1:K:210:PRO:HG2	1:L:145:ARG:HD2	2.00	0.44
1:C:142:GLN:NE2	1:G:60:MET:O	60.78	0.44
1:C:60:MET:O	1:S:142:GLN:NE2	71.50	0.44
1:8:61:SER:OG	1:8:90:PRO:HD2	2.16	0.44
1:X:132:THR:HG21	1:X:176:ARG:NH2	2.33	0.44
1:D:176:ARG:CZ	1:F:168:TRP:CZ3	3.00	0.44
1:N:105:GLU:O	1:N:106:THR:HG23	2.73	0.44
1:V:130:ASP:OD1	1:X:168:TRP:HH2	2.00	0.44
1:S:162:TYR:O	1:S:164:ARG:HG3	2.18	0.44
1:V:184:ILE:HG22	1:V:186:LEU:HD13	2.09	0.44
1:1:63:ILE:HD11	1:1:89:LEU:HD21	1.99	0.44
1:K:128:LEU:HA	1:K:129:PRO:HD3	2.00	0.44
1:7:98:ILE:HG22	1:7:99:PHE:CD1	2.53	0.44
1:X:99:PHE:HB3	1:X:208:SER:O	2.18	0.44
1:T:125:ALA:O	1:T:147:ALA:HA	2.25	0.44
1:Q:63:ILE:HD11	1:Q:89:LEU:CD2	2.48	0.44
1:5:63:ILE:HD11	1:5:89:LEU:CD2	2.48	0.44
1:W:162:TYR:O	1:W:164:ARG:HG3	2.17	0.44
1:W:107:LEU:HD21	1:W:201:CYS:SG	2.85	0.44
1:W:60:MET:O	1:X:142:GLN:NE2	32.24	0.44
1:7:196:ASN:HD22	1:7:196:ASN:C	2.20	0.44
1:G:175:GLN:HA	1:G:178:THR:CG2	2.48	0.44
1:O:209:VAL:HG23	1:O:209:VAL:O	2.18	0.44
1:4:79:VAL:HG21	1:4:185:LEU:HD13	1.98	0.44
1:E:123:TYR:HB2	1:E:185:LEU:CD2	2.48	0.44
1:K:63:ILE:HD11	1:K:201:CYS:HB3	1.98	0.44
1:V:66:ALA:HB3	1:V:197:VAL:CG1	2.83	0.44
1:S:109:PHE:HB2	1:S:158:VAL:HG13	2.16	0.44
1:U:98:ILE:HG22	1:U:99:PHE:CD1	2.54	0.44
1:8:92:LEU:HD11	1:8:205:VAL:HG11	2.00	0.44
1:8:177:LEU:HD23	1:9:174:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:81:ASP:OD1	1:H:81:ASP:C	2.56	0.44
1:Q:168:TRP:CZ3	1:R:176:ARG:CZ	3.00	0.44
1:G:98:ILE:HG23	1:K:91:ARG:CZ	2.48	0.44
1:B:100:GLN:HG3	1:B:209:VAL:HG23	2.00	0.44
1:B:168:TRP:CZ2	1:C:176:ARG:HD2	2.53	0.44
1:7:143:ALA:HB3	1:9:212:LEU:HB3	2.00	0.44
1:H:141:LEU:HD21	1:H:184:ILE:HB	2.04	0.44
1:D:89:LEU:HD13	1:D:203:TRP:CD1	2.75	0.44
1:6:98:ILE:HG22	1:6:99:PHE:CD1	2.52	0.44
1:L:118:ASN:HB2	1:4:118:ASN:HD21	176.26	0.44
1:S:108:GLU:HB2	1:S:202:ARG:HG2	2.17	0.44
1:K:146:GLY:O	1:K:147:ALA:C	2.56	0.44
1:Z:63:ILE:HD11	1:Z:89:LEU:HD21	1.99	0.44
1:1:139:ASP:OD1	1:1:139:ASP:N	2.51	0.44
1:H:121:GLY:CA	1:H:152:TRP:CE3	2.96	0.44
1:V:168:TRP:N	1:V:177:LEU:O	2.51	0.44
1:E:121:GLY:HA2	1:E:152:TRP:HE3	2.00	0.44
1:O:118:ASN:HB2	1:V:118:ASN:ND2	2.32	0.44
1:E:149:VAL:CG2	1:5:112:GLN:HG2	147.57	0.44
1:N:100:GLN:HG2	1:N:211:SER:HB2	2.69	0.44
1:4:145:ARG:NH1	1:4:161:GLN:HB3	2.33	0.44
1:D:58:SER:O	1:D:91:ARG:NH1	2.88	0.44
1:Q:89:LEU:HD22	1:Q:203:TRP:CD1	2.52	0.44
1:P:124:VAL:HG13	1:P:186:LEU:HB2	2.00	0.44
1:7:143:ALA:CB	1:9:212:LEU:CB	2.95	0.44
1:E:184:ILE:HG22	1:E:186:LEU:HD13	2.03	0.44
1:M:134:ASN:O	1:M:136:HIS:CD2	2.70	0.44
1:D:184:ILE:HG22	1:D:186:LEU:CD1	2.48	0.44
1:7:128:LEU:HA	1:7:129:PRO:HD3	1.77	0.44
1:Y:83:THR:HA	1:Y:182:ARG:HB3	2.00	0.44
1:1:106:THR:HA	1:1:162:TYR:OH	2.18	0.44
1:4:137:THR:HG23	1:4:140:ALA:CB	2.48	0.44
1:O:130:ASP:N	1:O:130:ASP:OD1	2.57	0.43
1:F:132:THR:HG21	1:F:176:ARG:NH2	2.43	0.43
1:P:91:ARG:CZ	1:P:210:PRO:HB3	16.85	0.43
1:M:100:GLN:OE1	1:N:130:ASP:OD1	2.35	0.43
1:L:98:ILE:HD11	1:6:94:HIS:CB	147.10	0.43
1:R:99:PHE:HB3	1:R:208:SER:O	2.17	0.43
1:A:175:GLN:HB2	1:A:178:THR:HG23	1.99	0.43
1:O:98:ILE:HG23	1:9:91:ARG:CZ	115.88	0.43
1:Z:98:ILE:HG22	1:Z:99:PHE:CD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:THR:O	1:A:75:ASP:C	2.56	0.43
1:D:128:LEU:HA	1:D:129:PRO:HD3	1.89	0.43
1:E:96:ALA:HB1	1:E:169:THR:HB	2.00	0.43
1:8:166:LEU:C	1:8:166:LEU:HD23	2.39	0.43
1:X:145:ARG:NH1	1:X:161:GLN:HB3	2.33	0.43
1:I:91:ARG:NE	1:R:98:ILE:HG23	115.61	0.43
1:G:89:LEU:HD13	1:G:203:TRP:CD1	2.52	0.43
1:T:79:VAL:CG2	1:T:185:LEU:HD13	2.49	0.43
1:Q:63:ILE:HG23	1:Q:88:LEU:HD13	2.00	0.43
1:N:60:MET:HA	1:N:201:CYS:O	2.18	0.43
1:E:183:LEU:C	1:E:184:ILE:HD13	3.05	0.43
1:Y:61:SER:CB	1:Y:90:PRO:HD2	2.48	0.43
1:B:211:SER:OG	1:B:212:LEU:N	2.51	0.43
1:M:128:LEU:HA	1:M:129:PRO:HD3	1.75	0.43
1:N:65:GLN:HE21	1:N:196:ASN:HD21	1.66	0.43
1:5:132:THR:OG1	1:5:176:ARG:NH2	2.51	0.43
1:T:84:ILE:HB	1:T:180:PRO:HD2	2.00	0.43
1:C:118:ASN:HB2	1:P:118:ASN:ND2	2.34	0.43
1:G:118:ASN:ND2	1:R:118:ASN:HB2	150.95	0.43
1:W:91:ARG:O	1:W:98:ILE:HD11	8.14	0.43
1:E:107:LEU:O	1:E:160:PRO:HD2	2.21	0.43
1:O:151:LYS:HD2	1:O:153:TRP:CZ2	2.55	0.43
1:S:128:LEU:HA	1:S:129:PRO:HD3	1.74	0.43
1:M:111:ILE:HG21	1:M:123:TYR:CE2	2.77	0.43
1:E:101:ARG:NH1	1:E:168:TRP:CZ2	3.01	0.43
1:P:112:GLN:HG2	1:Q:149:VAL:CG2	50.63	0.43
1:D:104:VAL:HG21	1:D:180:PRO:HG3	2.00	0.43
1:M:175:GLN:HB2	1:M:178:THR:CG2	2.71	0.43
1:D:80:VAL:HB	1:D:185:LEU:HB2	2.42	0.43
1:Z:63:ILE:HD11	1:Z:89:LEU:CD2	2.48	0.43
1:X:63:ILE:HD11	1:X:89:LEU:HD11	2.02	0.43
1:R:151:LYS:HD2	1:R:153:TRP:CZ2	2.54	0.43
1:K:101:ARG:HG2	1:K:167:LEU:O	3.23	0.43
1:8:165:THR:HG23	1:8:166:LEU:N	2.34	0.43
1:P:167:LEU:C	1:P:168:TRP:CD1	3.03	0.43
1:N:100:GLN:HG2	1:N:211:SER:HB3	1.99	0.43
1:I:99:PHE:HB3	1:I:208:SER:O	2.18	0.43
1:8:168:TRP:CE2	1:9:176:ARG:HD2	2.54	0.43
1:7:79:VAL:HG22	1:7:185:LEU:HB3	2.00	0.43
1:X:128:LEU:HA	1:X:129:PRO:HD3	1.82	0.43
1:H:152:TRP:CD1	1:H:195:VAL:HG11	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:58:SER:O	1:J:91:ARG:NH1	2.51	0.43
1:W:112:GLN:HG2	1:X:149:VAL:CG2	49.98	0.43
1:B:91:ARG:HD2	1:G:211:SER:O	38.38	0.43
1:K:200:LEU:HD11	1:U:149:VAL:HG22	102.57	0.43
1:A:210:PRO:HG2	1:B:145:ARG:HD2	1.98	0.43
1:A:145:ARG:NH1	1:A:161:GLN:HB3	2.43	0.43
1:G:63:ILE:CD1	1:G:88:LEU:HD22	2.87	0.43
1:P:123:TYR:HB2	1:P:185:LEU:CD2	2.73	0.43
1:T:175:GLN:HE21	1:T:175:GLN:HB2	1.96	0.43
1:Q:100:GLN:HG2	1:Q:211:SER:CB	2.48	0.43
1:K:178:THR:OG1	1:K:178:THR:O	2.36	0.43
1:5:130:ASP:C	1:5:132:THR:H	2.21	0.43
1:K:84:ILE:O	1:K:180:PRO:HD2	2.24	0.43
1:A:128:LEU:HA	1:A:129:PRO:HD3	1.85	0.43
1:V:112:GLN:HG2	1:Z:149:VAL:CG2	113.98	0.43
1:H:100:GLN:CB	1:H:209:VAL:HG22	2.43	0.43
1:M:145:ARG:HD2	1:O:210:PRO:HG2	2.16	0.43
1:F:101:ARG:CG	1:F:167:LEU:O	2.70	0.43
1:Z:109:PHE:HA	1:Z:200:LEU:O	2.19	0.43
1:A:165:THR:HG23	1:A:166:LEU:N	2.34	0.43
1:6:132:THR:HG21	1:6:176:ARG:NH2	2.33	0.43
1:T:162:TYR:O	1:T:164:ARG:HG3	2.23	0.43
1:G:166:LEU:C	1:G:167:LEU:HD12	2.39	0.43
1:Q:165:THR:O	1:Q:167:LEU:HD12	2.19	0.43
1:5:130:ASP:C	1:5:132:THR:N	2.71	0.43
1:I:211:SER:OG	1:I:212:LEU:N	2.66	0.43
1:A:142:GLN:NE2	1:U:60:MET:O	70.27	0.43
1:U:63:ILE:HD11	1:U:89:LEU:HD11	2.03	0.43
1:1:69:PRO:HG2	1:1:72:THR:HG21	1.99	0.43
1:4:184:ILE:HG22	1:4:186:LEU:HD13	2.00	0.43
1:A:54:ASP:OD2	1:A:206:ARG:NH1	2.51	0.43
1:J:149:VAL:CG2	1:3:200:LEU:HD11	2.49	0.43
1:L:132:THR:HG21	1:L:176:ARG:NH2	2.34	0.43
1:8:166:LEU:O	1:8:166:LEU:HD23	2.18	0.43
1:K:61:SER:CB	1:K:90:PRO:HD2	3.10	0.43
1:P:106:THR:HA	1:P:162:TYR:OH	2.24	0.43
1:W:124:VAL:CG1	1:W:186:LEU:HB2	2.75	0.43
1:G:184:ILE:HG22	1:G:186:LEU:HD13	2.02	0.43
1:9:99:PHE:HB3	1:9:208:SER:O	2.18	0.43
1:T:91:ARG:NH1	1:Z:98:ILE:HG23	130.62	0.43
1:N:128:LEU:HA	1:N:129:PRO:HD3	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:108:GLU:HB2	1:0:202:ARG:HG2	2.00	0.43
1:N:127:PHE:HB3	1:N:160:PRO:HB3	2.08	0.43
1:G:104:VAL:HA	1:G:205:VAL:HG22	2.01	0.43
1:X:151:LYS:HD2	1:X:153:TRP:CZ2	2.54	0.43
1:P:175:GLN:HA	1:P:178:THR:CG2	3.05	0.43
1:Z:62:ARG:NH1	1:Z:65:GLN:NE2	2.67	0.43
1:1:121:GLY:HA3	1:1:152:TRP:HB2	2.00	0.43
1:A:124:VAL:HG13	1:A:186:LEU:HB2	2.30	0.43
1:W:163:THR:OG1	1:W:165:THR:HG22	2.19	0.43
1:M:63:ILE:HD12	1:M:88:LEU:HD13	2.11	0.43
1:B:61:SER:CB	1:B:90:PRO:HD2	2.47	0.43
1:A:210:PRO:HG2	1:B:145:ARG:NE	2.33	0.43
1:A:145:ARG:HD2	1:C:210:PRO:HG2	2.01	0.43
1:S:106:THR:HG23	1:S:204:SER:HB3	2.60	0.43
1:V:74:THR:O	1:V:76:GLY:N	2.52	0.43
1:Q:163:THR:OG1	1:Q:165:THR:HB	2.19	0.43
1:K:182:ARG:HG3	1:K:184:ILE:HD11	2.94	0.43
1:A:157:THR:HG21	1:A:159:ARG:NH2	2.33	0.43
1:J:128:LEU:HD22	1:J:128:LEU:H	1.83	0.43
1:Q:115:CYS:HB2	1:Q:116:PRO:HD2	2.16	0.43
1:9:151:LYS:HD2	1:9:153:TRP:CZ2	2.53	0.43
1:G:149:VAL:HG22	1:R:200:LEU:HD11	122.46	0.43
1:I:149:VAL:HG22	1:7:200:LEU:HD11	146.83	0.43
1:V:98:ILE:HG22	1:V:99:PHE:CE1	2.54	0.43
1:3:132:THR:HG21	1:3:176:ARG:NH2	2.33	0.43
1:9:145:ARG:NH1	1:9:161:GLN:HB3	2.33	0.43
1:Q:123:TYR:HB2	1:Q:185:LEU:CD2	2.49	0.43
1:T:146:GLY:O	1:T:147:ALA:C	2.64	0.43
1:H:146:GLY:O	1:H:147:ALA:C	2.57	0.43
1:N:91:ARG:HD2	1:Q:98:ILE:HG23	91.75	0.43
1:H:138:PHE:CE1	1:K:62:ARG:HB2	2.54	0.43
1:P:137:THR:HG23	1:P:140:ALA:HB2	2.01	0.43
1:I:63:ILE:HD11	1:I:89:LEU:HD11	2.01	0.43
1:P:212:LEU:O	1:P:212:LEU:HG	2.83	0.43
1:Z:165:THR:HG23	1:Z:166:LEU:N	2.34	0.42
1:K:168:TRP:CH2	1:L:176:ARG:HD2	2.53	0.42
1:5:149:VAL:O	1:5:156:ARG:NH2	2.52	0.42
1:S:123:TYR:CD2	1:S:185:LEU:HD21	2.54	0.42
1:9:211:SER:OG	1:9:212:LEU:N	2.52	0.42
1:T:145:ARG:NE	1:T:145:ARG:N	2.69	0.42
1:F:151:LYS:HD2	1:F:153:TRP:CZ2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:79:VAL:CG2	1:X:185:LEU:HD13	2.53	0.42
1:V:175:GLN:HA	1:V:178:THR:CG2	2.85	0.42
1:1:192:THR:HG22	1:1:192:THR:O	2.19	0.42
1:M:67:VAL:HG13	1:M:67:VAL:O	2.19	0.42
1:E:55:VAL:HG21	1:E:99:PHE:CZ	2.64	0.42
1:U:145:ARG:NH1	1:U:161:GLN:HB3	2.34	0.42
1:H:130:ASP:HB2	1:H:133:ASP:HB2	2.01	0.42
1:X:168:TRP:N	1:X:177:LEU:O	2.52	0.42
1:O:91:ARG:CZ	1:9:98:ILE:HG23	115.96	0.42
1:9:113:PRO:HA	1:9:197:VAL:HA	2.01	0.42
1:C:63:ILE:HD11	1:C:89:LEU:HD11	2.01	0.42
1:R:63:ILE:HD11	1:R:89:LEU:HD11	2.01	0.42
1:A:196:ASN:HD22	1:A:196:ASN:C	2.79	0.42
1:N:101:ARG:NH1	1:N:168:TRP:CZ2	2.90	0.42
1:Q:168:TRP:CH2	1:R:176:ARG:HD2	2.71	0.42
1:V:101:ARG:CZ	1:V:168:TRP:CZ2	4.05	0.42
1:C:118:ASN:HB2	1:S:118:ASN:ND2	93.49	0.42
1:R:165:THR:HG23	1:R:166:LEU:O	2.20	0.42
1:Y:121:GLY:HA3	1:Y:152:TRP:HE3	1.83	0.42
1:M:63:ILE:HB	1:M:199:VAL:CG2	2.47	0.42
1:I:116:PRO:HB3	1:Y:118:ASN:C	2.40	0.42
1:U:209:VAL:CG2	1:U:209:VAL:O	2.67	0.42
1:Q:79:VAL:HG23	1:Q:80:VAL:HG23	2.29	0.42
1:A:168:TRP:N	1:A:177:LEU:O	3.98	0.42
1:V:63:ILE:HD11	1:V:89:LEU:CD2	2.49	0.42
1:J:130:ASP:C	1:J:132:THR:N	2.72	0.42
1:M:92:LEU:HD11	1:M:205:VAL:HG21	2.00	0.42
1:5:115:CYS:HB2	1:5:116:PRO:HD2	2.01	0.42
1:M:173:LYS:O	1:O:173:LYS:HD3	2.43	0.42
1:6:151:LYS:HD2	1:6:153:TRP:CZ2	2.54	0.42
1:R:108:GLU:HB2	1:R:202:ARG:HG2	2.01	0.42
1:3:151:LYS:HD2	1:3:153:TRP:CZ2	2.54	0.42
1:M:107:LEU:O	1:M:160:PRO:HD2	2.20	0.42
1:G:91:ARG:HE	1:K:98:ILE:HG23	1.83	0.42
1:L:128:LEU:HA	1:L:129:PRO:HD3	1.80	0.42
1:N:167:LEU:HB3	1:N:177:LEU:O	2.70	0.42
1:R:132:THR:HG21	1:R:176:ARG:NH2	2.34	0.42
1:E:152:TRP:CD1	1:E:195:VAL:HG11	2.54	0.42
1:G:98:ILE:CG2	1:K:91:ARG:NH1	2.82	0.42
1:C:114:MET:SD	1:P:122:GLY:CA	3.03	0.42
1:L:145:ARG:NH1	1:L:161:GLN:HB3	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:152:TRP:CD1	1:T:195:VAL:HG11	2.53	0.42
1:T:92:LEU:HD13	1:T:203:TRP:CZ3	2.82	0.42
1:J:123:TYR:CD2	1:J:185:LEU:HD21	2.65	0.42
1:E:125:ALA:O	1:E:147:ALA:HA	2.19	0.42
1:B:146:GLY:O	1:B:147:ALA:C	2.72	0.42
1:U:99:PHE:HB3	1:U:208:SER:O	2.27	0.42
1:W:68:LEU:HA	1:W:69:PRO:HD3	1.93	0.42
1:I:162:TYR:O	1:I:164:ARG:HG3	2.19	0.42
1:W:168:TRP:CE3	1:X:176:ARG:CZ	3.02	0.42
1:M:94:HIS:HB2	1:S:98:ILE:HD11	116.83	0.42
1:W:63:ILE:HA	1:W:63:ILE:HD13	1.73	0.42
1:A:130:ASP:OD1	1:C:168:TRP:CH2	3.39	0.42
1:M:109:PHE:HB2	1:M:158:VAL:HG13	2.01	0.42
1:4:203:TRP:O	1:4:203:TRP:CE3	2.72	0.42
1:Q:113:PRO:HA	1:Q:197:VAL:HA	2.07	0.42
1:4:121:GLY:HA3	1:4:152:TRP:CE3	2.55	0.42
1:F:98:ILE:HD11	1:X:94:HIS:HB2	72.54	0.42
1:8:146:GLY:O	1:8:147:ALA:C	2.57	0.42
1:M:163:THR:HA	1:O:101:ARG:NH2	2.32	0.42
1:A:128:LEU:HD21	1:A:184:ILE:HD11	2.01	0.42
1:A:79:VAL:CG2	1:A:185:LEU:HD13	2.49	0.42
1:J:114:MET:SD	1:W:122:GLY:HA2	159.93	0.42
1:M:112:GLN:OE1	1:M:155:SER:OG	2.28	0.42
1:4:101:ARG:CZ	1:4:168:TRP:CZ2	3.03	0.42
1:K:167:LEU:O	1:K:168:TRP:CD1	2.87	0.42
1:B:124:VAL:HG23	1:B:149:VAL:HG12	2.57	0.42
1:D:123:TYR:CD2	1:D:185:LEU:HD21	2.55	0.42
1:T:91:ARG:O	1:Z:98:ILE:HD11	137.55	0.42
1:2:106:THR:HA	1:2:162:TYR:OH	2.19	0.42
1:8:124:VAL:HG13	1:8:186:LEU:HB2	2.01	0.42
1:N:165:THR:HG23	1:N:166:LEU:N	2.37	0.42
1:H:210:PRO:HD2	1:I:145:ARG:HH11	1.84	0.42
1:C:145:ARG:NH1	1:C:161:GLN:HB3	2.36	0.42
1:T:146:GLY:HA3	1:T:158:VAL:HG23	2.02	0.42
1:T:162:TYR:O	1:T:164:ARG:CG	2.67	0.42
1:K:123:TYR:HB2	1:K:185:LEU:CD2	2.49	0.42
1:2:108:GLU:OE1	1:2:202:ARG:NH1	2.53	0.42
1:J:128:LEU:CD2	1:J:182:ARG:HG2	3.15	0.42
1:W:74:THR:O	1:W:75:ASP:C	2.58	0.42
1:O:166:LEU:HG	1:O:167:LEU:N	2.36	0.42
1:O:101:ARG:CG	1:O:167:LEU:O	2.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ASP:O	1:D:131:PRO:C	2.70	0.42
1:U:168:TRP:N	1:U:177:LEU:O	2.56	0.42
1:D:208:SER:O	1:D:210:PRO:HD3	2.33	0.42
1:H:89:LEU:HB2	1:H:92:LEU:HB3	2.48	0.42
1:G:184:ILE:HG22	1:G:186:LEU:CD1	2.61	0.42
1:K:125:ALA:O	1:K:147:ALA:HA	2.19	0.42
1:F:113:PRO:HA	1:F:197:VAL:HA	2.01	0.42
1:X:108:GLU:HB2	1:X:202:ARG:HG2	2.03	0.42
1:Z:79:VAL:CG2	1:Z:185:LEU:HD13	2.50	0.42
1:Z:79:VAL:HG23	1:Z:80:VAL:HG23	2.02	0.42
1:W:148:VAL:HB	1:W:156:ARG:HG2	2.37	0.42
1:Z:191:ASN:N	1:Z:191:ASN:OD1	2.51	0.42
1:I:101:ARG:HE	1:I:166:LEU:HD21	1.86	0.42
1:2:168:TRP:CZ2	1:3:176:ARG:HD2	2.54	0.42
1:4:163:THR:HG23	1:4:164:ARG:H	1.84	0.42
1:0:145:ARG:NH1	1:0:161:GLN:HB3	2.35	0.42
1:1:73:GLY:O	1:1:190:ASN:HB3	2.20	0.42
1:N:145:ARG:H	1:N:145:ARG:NE	2.41	0.42
1:R:168:TRP:N	1:R:177:LEU:O	2.53	0.42
1:B:92:LEU:HD11	1:B:205:VAL:HG11	2.01	0.42
1:B:58:SER:HA	1:B:203:TRP:O	2.36	0.42
1:V:123:TYR:HB2	1:V:185:LEU:CD2	2.50	0.42
1:H:184:ILE:HG22	1:H:186:LEU:HD13	2.12	0.42
1:H:123:TYR:OH	1:H:156:ARG:HB2	2.20	0.42
1:H:128:LEU:HA	1:H:129:PRO:HD3	1.85	0.42
1:I:151:LYS:HD2	1:I:153:TRP:CZ2	2.55	0.42
1:F:108:GLU:HB2	1:F:202:ARG:HG2	2.02	0.42
1:A:113:PRO:HA	1:A:197:VAL:HA	2.02	0.42
1:V:138:PHE:CD1	1:V:138:PHE:C	2.92	0.42
1:Q:168:TRP:CZ2	1:R:176:ARG:HD2	2.75	0.42
1:O:101:ARG:HE	1:O:166:LEU:HD21	1.85	0.42
1:D:131:PRO:HB2	1:D:175:GLN:HE21	1.84	0.42
1:C:101:ARG:CG	1:C:167:LEU:O	2.71	0.42
1:G:63:ILE:HB	1:G:199:VAL:HG22	2.04	0.42
1:P:79:VAL:HG21	1:P:185:LEU:HD13	2.36	0.42
1:I:209:VAL:O	1:I:209:VAL:HG23	2.21	0.42
1:P:137:THR:HG23	1:P:140:ALA:CB	2.57	0.42
1:E:63:ILE:HD11	1:E:89:LEU:CD2	2.53	0.42
1:F:98:ILE:HG22	1:F:99:PHE:CD1	2.55	0.42
1:F:91:ARG:NE	1:U:98:ILE:HG23	2.35	0.42
1:6:99:PHE:HB3	1:6:208:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:63:ILE:HD11	1:0:89:LEU:HD11	2.02	0.42
1:O:63:ILE:HD11	1:O:89:LEU:HD11	2.01	0.42
1:J:146:GLY:O	1:J:148:VAL:HG13	2.36	0.42
1:5:113:PRO:HA	1:5:197:VAL:HA	2.01	0.42
1:M:115:CYS:HB2	1:M:116:PRO:HD2	2.18	0.42
1:M:110:GLU:HB3	1:M:200:LEU:HB2	2.01	0.41
1:I:145:ARG:NH1	1:I:161:GLN:HB3	2.35	0.41
1:M:121:GLY:O	1:9:114:MET:HB3	142.24	0.41
1:S:145:ARG:NH1	1:S:161:GLN:HB3	2.35	0.41
1:M:138:PHE:CE1	1:9:62:ARG:HB2	132.74	0.41
1:V:145:ARG:NH1	1:V:161:GLN:HB3	2.66	0.41
1:P:127:PHE:CZ	1:P:181:GLY:HA3	2.55	0.41
1:4:137:THR:HG23	1:4:140:ALA:HB2	2.02	0.41
1:T:128:LEU:HA	1:T:129:PRO:HD3	1.87	0.41
1:T:137:THR:O	1:T:138:PHE:C	2.58	0.41
1:C:122:GLY:HA3	1:G:114:MET:SD	78.14	0.41
1:P:128:LEU:HA	1:P:129:PRO:HD3	1.85	0.41
1:G:133:ASP:O	1:G:182:ARG:NH1	2.53	0.41
1:Z:170:SER:O	1:0:176:ARG:NH1	2.53	0.41
1:R:166:LEU:HG	1:R:167:LEU:N	2.37	0.41
1:R:145:ARG:NH1	1:R:161:GLN:HB3	2.36	0.41
1:7:130:ASP:N	1:7:130:ASP:OD1	2.54	0.41
1:0:128:LEU:HA	1:0:129:PRO:HD3	1.84	0.41
1:P:61:SER:HB3	1:P:90:PRO:HD2	2.01	0.41
1:Q:52:THR:OG1	1:Q:53:ASN:N	2.51	0.41
1:J:127:PHE:CZ	1:J:181:GLY:HA3	2.55	0.41
1:Y:124:VAL:HG13	1:Y:124:VAL:O	2.20	0.41
1:X:166:LEU:HG	1:X:167:LEU:N	2.38	0.41
1:K:100:GLN:OE1	1:L:130:ASP:OD1	2.38	0.41
1:S:121:GLY:CA	1:S:152:TRP:CE3	3.03	0.41
1:G:63:ILE:HD11	1:G:89:LEU:CD2	2.49	0.41
1:O:98:ILE:CD1	1:X:95:ALA:HB2	2.51	0.41
1:V:130:ASP:HB3	1:V:132:THR:OG1	2.20	0.41
1:8:89:LEU:HD13	1:8:203:TRP:CG	2.55	0.41
1:5:138:PHE:CE2	1:8:62:ARG:NH1	2.88	0.41
1:U:113:PRO:HA	1:U:197:VAL:HA	2.02	0.41
1:C:108:GLU:HB2	1:C:202:ARG:HG2	2.03	0.41
1:O:79:VAL:CG2	1:O:185:LEU:HD13	2.51	0.41
1:J:110:GLU:HB3	1:J:200:LEU:HB2	2.03	0.41
1:H:114:MET:SD	1:8:122:GLY:HA3	161.77	0.41
1:M:61:SER:HB3	1:M:90:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:LEU:HA	1:F:129:PRO:HD3	1.83	0.41
1:G:176:ARG:NH1	1:I:170:SER:O	2.54	0.41
1:F:145:ARG:NH1	1:F:161:GLN:HB3	2.35	0.41
1:A:98:ILE:CG2	1:E:91:ARG:NH1	2.83	0.41
1:V:114:MET:HB3	1:Z:121:GLY:O	129.60	0.41
1:D:121:GLY:CA	1:D:152:TRP:HE3	2.62	0.41
1:E:138:PHE:CE1	1:5:62:ARG:HB2	147.34	0.41
1:B:89:LEU:HD13	1:B:203:TRP:CG	2.56	0.41
1:5:132:THR:HG21	1:5:176:ARG:NH2	2.35	0.41
1:S:214:ASN:HD21	1:T:137:THR:HG21	1.86	0.41
1:1:79:VAL:HG23	1:1:80:VAL:HG23	2.02	0.41
1:5:96:ALA:HB1	1:5:169:THR:HB	2.02	0.41
1:A:62:ARG:HD3	1:A:198:SER:HB3	2.03	0.41
1:C:79:VAL:CG2	1:C:185:LEU:HD13	2.54	0.41
1:U:108:GLU:HB2	1:U:202:ARG:HG2	2.03	0.41
1:G:163:THR:OG1	1:G:165:THR:HG22	2.21	0.41
1:2:168:TRP:CZ3	1:3:176:ARG:CZ	3.04	0.41
1:J:55:VAL:HG21	1:J:99:PHE:CZ	2.72	0.41
1:O:168:TRP:HB2	1:O:177:LEU:O	2.20	0.41
1:O:145:ARG:NH1	1:O:161:GLN:HB3	2.35	0.41
1:V:91:ARG:NH2	1:Y:98:ILE:CG2	89.21	0.41
1:S:192:THR:CG2	1:S:192:THR:O	2.80	0.41
1:O:99:PHE:HB3	1:O:208:SER:O	2.21	0.41
1:Q:100:GLN:HB2	1:Q:209:VAL:O	2.41	0.41
1:J:101:ARG:HG2	1:J:167:LEU:O	2.61	0.41
1:B:148:VAL:HG21	1:B:156:ARG:HB3	2.03	0.41
1:U:79:VAL:CG2	1:U:185:LEU:HD13	2.52	0.41
1:F:63:ILE:HD11	1:F:89:LEU:HD11	2.02	0.41
1:2:96:ALA:HB1	1:2:169:THR:HB	2.03	0.41
1:K:107:LEU:HD23	1:K:107:LEU:HA	1.93	0.41
1:V:167:LEU:HD12	1:V:167:LEU:N	2.69	0.41
1:C:114:MET:HB3	1:S:121:GLY:O	86.59	0.41
1:Q:121:GLY:CA	1:Q:152:TRP:CE3	3.28	0.41
1:K:61:SER:O	1:K:200:LEU:HA	2.21	0.41
1:S:130:ASP:OD1	1:U:100:GLN:OE1	2.38	0.41
1:N:107:LEU:CD2	1:N:201:CYS:SG	3.38	0.41
1:7:79:VAL:CG2	1:7:185:LEU:HD13	2.51	0.41
1:A:140:ALA:O	1:A:143:ALA:HB3	2.20	0.41
1:A:128:LEU:H	1:A:128:LEU:HD22	1.99	0.41
1:J:152:TRP:CZ3	1:J:191:ASN:HB3	2.55	0.41
1:6:145:ARG:NH1	1:6:161:GLN:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:167:LEU:HD23	1:P:179:SER:N	2.37	0.41
1:T:168:TRP:CE3	1:U:176:ARG:CZ	3.46	0.41
1:E:175:GLN:HA	1:E:178:THR:HG22	3.30	0.41
1:H:130:ASP:CB	1:H:133:ASP:HB2	2.51	0.41
1:J:151:LYS:HD2	1:J:153:TRP:CE2	2.55	0.41
1:O:107:LEU:O	1:O:160:PRO:HD2	2.24	0.41
1:4:175:GLN:HB2	1:4:178:THR:HG23	2.03	0.41
1:U:151:LYS:HD2	1:U:153:TRP:CZ2	2.58	0.41
1:9:63:ILE:HD11	1:9:89:LEU:HD11	2.02	0.41
1:V:140:ALA:O	1:V:143:ALA:HB3	2.41	0.41
1:R:79:VAL:CG2	1:R:185:LEU:HD13	2.51	0.41
1:D:138:PHE:CE2	1:U:62:ARG:NH1	2.89	0.41
1:D:163:THR:OG1	1:D:165:THR:HG22	2.20	0.41
1:3:145:ARG:NH1	1:3:161:GLN:HB3	2.35	0.41
1:M:210:PRO:HG2	1:N:145:ARG:HD2	2.03	0.41
1:T:125:ALA:HA	1:T:184:ILE:O	2.51	0.41
1:8:212:LEU:HG	1:8:212:LEU:O	2.21	0.41
1:8:127:PHE:HB3	1:8:160:PRO:HB3	2.02	0.41
1:W:69:PRO:HD2	1:W:72:THR:OG1	2.20	0.41
1:J:107:LEU:O	1:J:160:PRO:HD2	2.26	0.41
1:V:92:LEU:HD11	1:V:205:VAL:HG21	2.25	0.41
1:5:175:GLN:HA	1:5:178:THR:CG2	2.51	0.41
1:P:148:VAL:HB	1:P:156:ARG:HG2	2.34	0.41
1:M:77:TYR:CD1	1:M:77:TYR:C	2.94	0.41
1:M:133:ASP:OD1	1:O:213:GLU:OE1	3.61	0.41
1:1:121:GLY:CA	1:1:152:TRP:HE3	2.34	0.41
1:W:176:ARG:O	1:W:177:LEU:HD13	2.21	0.41
1:W:100:GLN:HG2	1:W:211:SER:HB2	2.02	0.41
1:E:121:GLY:CA	1:E:152:TRP:HE3	2.33	0.41
1:J:121:GLY:HA3	1:J:152:TRP:CE3	2.56	0.41
1:9:101:ARG:HE	1:9:166:LEU:HD21	1.85	0.41
1:E:149:VAL:HG22	1:N:112:GLN:HG2	1.98	0.41
1:J:210:PRO:CG	1:K:145:ARG:HD2	2.64	0.41
1:J:63:ILE:CG1	1:J:201:CYS:HB2	2.51	0.41
1:M:122:GLY:HA2	1:M:150:ALA:O	2.20	0.41
1:B:163:THR:OG1	1:B:165:THR:HB	2.21	0.41
1:I:98:ILE:HG12	1:0:91:ARG:HG2	2.03	0.41
1:V:63:ILE:HB	1:V:199:VAL:HG22	2.15	0.41
1:5:98:ILE:HD13	1:5:98:ILE:HG21	1.86	0.41
1:5:168:TRP:CZ2	1:6:176:ARG:HD2	2.55	0.41
1:H:83:THR:HA	1:H:182:ARG:CB	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:170:SER:O	1:Z:176:ARG:NH1	2.54	0.41
1:J:79:VAL:HG21	1:J:185:LEU:HD13	2.02	0.41
1:M:73:GLY:C	1:M:74:THR:HG1	2.24	0.41
1:E:123:TYR:HB2	1:E:185:LEU:HD21	2.03	0.41
1:1:183:LEU:HD13	1:1:184:ILE:N	2.36	0.41
1:T:61:SER:HB3	1:T:90:PRO:HD2	2.03	0.41
1:7:113:PRO:HB3	1:7:197:VAL:HG23	2.02	0.41
1:T:212:LEU:HB2	1:U:143:ALA:HB2	2.03	0.41
1:Y:168:TRP:N	1:Y:177:LEU:O	2.53	0.41
1:8:61:SER:HB3	1:8:90:PRO:HD3	2.02	0.41
1:I:108:GLU:HB2	1:I:202:ARG:HG2	2.04	0.41
1:U:128:LEU:HA	1:U:129:PRO:HD3	1.83	0.41
1:W:167:LEU:HD23	1:W:179:SER:N	2.49	0.41
1:H:122:GLY:HA2	1:H:150:ALA:O	2.20	0.41
1:L:113:PRO:HA	1:L:197:VAL:HA	2.03	0.41
1:Y:63:ILE:HB	1:Y:199:VAL:HG22	2.03	0.41
1:A:67:VAL:HG13	1:A:67:VAL:O	2.51	0.41
1:B:57:LEU:HA	1:B:57:LEU:HD23	2.31	0.41
1:E:100:GLN:HB2	1:E:209:VAL:CG2	2.60	0.41
1:B:91:ARG:HD2	1:J:98:ILE:HG23	2.02	0.41
1:U:149:VAL:CG2	1:Z:200:LEU:HD11	133.85	0.41
1:6:101:ARG:CG	1:6:167:LEU:O	2.68	0.41
1:T:121:GLY:CA	1:T:152:TRP:HE3	2.34	0.41
1:I:91:ARG:HG2	1:0:98:ILE:HG12	2.03	0.41
1:I:98:ILE:HD11	1:R:91:ARG:O	116.47	0.41
1:5:168:TRP:HB2	1:5:177:LEU:O	2.20	0.41
1:B:108:GLU:HB2	1:B:202:ARG:HG2	2.67	0.41
1:J:184:ILE:HG22	1:J:186:LEU:HD13	2.14	0.41
1:J:62:ARG:HD3	1:J:198:SER:HB3	2.03	0.41
1:E:146:GLY:O	1:E:147:ALA:C	2.60	0.41
1:Y:100:GLN:N	1:Y:209:VAL:O	2.54	0.41
1:V:79:VAL:HG21	1:V:185:LEU:HD13	2.08	0.41
1:3:99:PHE:HB3	1:3:208:SER:O	2.20	0.41
1:L:151:LYS:HE2	1:T:153:TRP:O	155.18	0.41
1:Z:62:ARG:NH1	1:Z:65:GLN:HE21	2.18	0.41
1:5:92:LEU:HD11	1:5:205:VAL:HG11	2.03	0.41
1:Y:162:TYR:O	1:Y:164:ARG:HG3	2.21	0.41
1:F:55:VAL:HG13	1:X:55:VAL:HG13	61.78	0.41
1:M:83:THR:HA	1:M:182:ARG:HB3	2.02	0.41
1:L:63:ILE:HD11	1:L:89:LEU:HD11	2.02	0.41
1:9:79:VAL:CG2	1:9:185:LEU:HD13	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ILE:O	1:B:180:PRO:HD2	2.34	0.41
1:3:128:LEU:HA	1:3:129:PRO:HD3	1.82	0.41
1:0:101:ARG:HE	1:0:166:LEU:HD21	1.86	0.40
1:O:200:LEU:HD11	1:7:149:VAL:CG2	128.64	0.40
1:H:168:TRP:CZ3	1:I:176:ARG:NH2	3.25	0.40
1:0:130:ASP:OD1	1:0:130:ASP:N	2.55	0.40
1:Z:101:ARG:NH1	1:Z:168:TRP:CZ2	2.90	0.40
1:4:101:ARG:NE	1:4:166:LEU:HD21	2.26	0.40
1:K:101:ARG:NE	1:K:166:LEU:HD21	2.34	0.40
1:J:98:ILE:HG21	1:J:98:ILE:HD13	1.76	0.40
1:O:114:MET:SD	1:7:122:GLY:CA	140.09	0.40
1:M:145:ARG:NH1	1:M:161:GLN:HB3	2.58	0.40
1:F:166:LEU:HG	1:F:167:LEU:N	2.36	0.40
1:K:118:ASN:HB2	1:U:118:ASN:HD21	100.12	0.40
1:A:130:ASP:C	1:A:132:THR:N	2.80	0.40
1:J:60:MET:O	1:W:142:GLN:NE2	138.06	0.40
1:P:77:TYR:CD1	1:P:79:VAL:HG12	2.85	0.40
1:4:121:GLY:HA3	1:4:152:TRP:HE3	1.86	0.40
1:L:101:ARG:CG	1:L:167:LEU:O	2.69	0.40
1:L:167:LEU:HB3	1:L:168:TRP:H	1.78	0.40
1:D:182:ARG:HG3	1:D:184:ILE:HD11	2.03	0.40
1:D:63:ILE:HD11	1:D:89:LEU:HD21	2.03	0.40
1:Q:107:LEU:O	1:Q:160:PRO:HD2	2.21	0.40
1:W:107:LEU:HD23	1:W:107:LEU:HA	2.19	0.40
1:G:139:ASP:O	1:I:212:LEU:HD23	2.20	0.40
1:6:108:GLU:HB2	1:6:202:ARG:HG2	2.03	0.40
1:I:79:VAL:CG2	1:I:185:LEU:HD13	2.52	0.40
1:B:107:LEU:O	1:B:160:PRO:HD2	2.35	0.40
1:P:131:PRO:HA	1:P:182:ARG:HD2	2.03	0.40
1:R:113:PRO:HA	1:R:197:VAL:HA	2.03	0.40
1:3:63:ILE:HD11	1:3:89:LEU:HD11	2.02	0.40
1:W:151:LYS:HA	1:Y:114:MET:HG2	78.31	0.40
1:V:168:TRP:CZ3	1:W:176:ARG:CZ	3.04	0.40
1:I:101:ARG:CG	1:I:167:LEU:O	2.70	0.40
1:Z:100:GLN:OE1	1:0:130:ASP:OD1	2.38	0.40
1:9:166:LEU:HG	1:9:167:LEU:N	2.36	0.40
1:H:98:ILE:HG21	1:H:98:ILE:HD13	1.87	0.40
1:C:168:TRP:N	1:C:177:LEU:O	2.54	0.40
1:A:101:ARG:NE	1:A:166:LEU:HD21	2.89	0.40
1:S:127:PHE:CZ	1:S:181:GLY:HA3	2.56	0.40
1:Q:86:PRO:HA	1:Q:92:LEU:HD23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:63:ILE:CG2	1:Q:82:ALA:CB	3.25	0.40
1:F:209:VAL:O	1:F:209:VAL:HG23	2.25	0.40
1:E:63:ILE:HA	1:E:63:ILE:HD13	1.91	0.40
1:V:79:VAL:HG22	1:V:185:LEU:HB3	2.12	0.40
1:D:104:VAL:CG1	1:D:107:LEU:HG	2.51	0.40
1:M:151:LYS:HE3	1:9:113:PRO:O	134.81	0.40
1:2:128:LEU:HA	1:2:129:PRO:HD3	1.79	0.40
1:6:165:THR:HG23	1:6:166:LEU:O	2.22	0.40
1:O:162:TYR:O	1:O:164:ARG:HG3	2.20	0.40
1:W:88:LEU:HA	1:W:88:LEU:HD23	1.91	0.40
1:H:168:TRP:CZ3	1:I:130:ASP:OD1	2.74	0.40
1:S:168:TRP:CZ3	1:T:176:ARG:HD2	3.13	0.40
1:R:101:ARG:CG	1:R:167:LEU:O	2.71	0.40
1:G:98:ILE:HG23	1:K:91:ARG:HD2	2.04	0.40
1:B:91:ARG:NH1	1:J:210:PRO:HB3	2.36	0.40
1:I:114:MET:SD	1:Y:122:GLY:HA2	2.62	0.40
1:T:100:GLN:HB2	1:T:209:VAL:CG2	2.75	0.40
1:N:100:GLN:NE2	1:N:213:GLU:OE2	2.54	0.40
1:T:210:PRO:HB2	1:U:145:ARG:HD3	2.03	0.40
1:B:109:PHE:CD2	1:B:183:LEU:HD23	2.57	0.40
1:M:73:GLY:O	1:M:190:ASN:HB3	2.23	0.40
1:B:212:LEU:HG	1:B:212:LEU:O	2.61	0.40
1:H:162:TYR:O	1:H:164:ARG:HG3	2.21	0.40
1:J:163:THR:HG23	1:J:164:ARG:N	2.37	0.40
1:A:138:PHE:C	1:A:138:PHE:CD1	2.94	0.40
1:V:167:LEU:HB3	1:V:168:TRP:H	1.77	0.40
1:F:168:TRP:HB2	1:F:177:LEU:O	2.22	0.40
1:S:79:VAL:HG21	1:S:185:LEU:HD13	2.24	0.40
1:H:210:PRO:HB2	1:I:145:ARG:CD	2.51	0.40
1:H:112:GLN:HG2	1:N:149:VAL:HG22	2.03	0.40
1:8:100:GLN:HG2	1:8:211:SER:CB	2.52	0.40
1:H:74:THR:O	1:H:76:GLY:N	2.54	0.40
1:H:130:ASP:C	1:H:132:THR:N	2.84	0.40
1:Q:98:ILE:O	1:Q:211:SER:N	2.54	0.40
1:L:168:TRP:N	1:L:177:LEU:O	2.55	0.40
1:K:69:PRO:O	1:K:70:ALA:C	2.59	0.40
1:Y:151:LYS:HD2	1:Y:153:TRP:CE2	2.56	0.40
1:7:132:THR:OG1	1:7:176:ARG:NH2	2.54	0.40
1:I:107:LEU:O	1:I:160:PRO:HD2	2.27	0.40
1:L:165:THR:HG23	1:L:166:LEU:O	2.24	0.40
1:U:211:SER:OG	1:U:212:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:128:LEU:HA	1:Q:129:PRO:HD3	1.78	0.40
1:D:109:PHE:HB2	1:D:158:VAL:HG22	2.04	0.40
1:T:101:ARG:HH21	1:T:166:LEU:HD22	1.87	0.40
1:I:166:LEU:HG	1:I:167:LEU:N	2.37	0.40
1:S:130:ASP:OD1	1:U:100:GLN:NE2	2.54	0.40
1:B:100:GLN:HB2	1:B:209:VAL:CG2	2.52	0.40
1:A:163:THR:HG22	1:A:180:PRO:CB	3.31	0.40
1:N:79:VAL:HG22	1:N:185:LEU:HB3	2.04	0.40
1:L:209:VAL:O	1:L:209:VAL:CG2	2.71	0.40
1:P:151:LYS:HD2	1:P:153:TRP:CE2	2.74	0.40
1:Z:63:ILE:HA	1:Z:63:ILE:HD13	1.83	0.40
1:B:128:LEU:HA	1:B:129:PRO:HD3	1.95	0.40
1:O:113:PRO:HA	1:O:197:VAL:HA	2.03	0.40
1:0:79:VAL:CG2	1:0:185:LEU:HD13	2.52	0.40
1:V:81:ASP:CG	1:V:182:ARG:HH21	2.25	0.40
1:Q:68:LEU:HA	1:Q:69:PRO:HD3	2.07	0.40
1:L:108:GLU:HB2	1:L:202:ARG:HG2	2.05	0.40
1:R:69:PRO:O	1:R:72:THR:HG23	2.22	0.40
1:2:151:LYS:HD2	1:2:153:TRP:CZ2	2.57	0.40
1:B:87:ASP:N	1:B:87:ASP:OD1	2.55	0.40
1:P:98:ILE:HG21	1:P:98:ILE:HD13	1.88	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:77:TYR:OH	1:3:134:ASN:OD1[3_654]	1.87	0.33

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	1	161/183 (88%)	142 (88%)	17 (11%)	2 (1%)	16	52
1	2	161/183 (88%)	136 (84%)	22 (14%)	3 (2%)	10	40
1	3	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	4	161/183 (88%)	141 (88%)	18 (11%)	2 (1%)	16	52
1	5	161/183 (88%)	148 (92%)	9 (6%)	4 (2%)	7	32
1	6	161/183 (88%)	152 (94%)	8 (5%)	1 (1%)	30	68
1	7	161/183 (88%)	141 (88%)	18 (11%)	2 (1%)	16	52
1	8	161/183 (88%)	145 (90%)	12 (8%)	4 (2%)	7	32
1	9	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
1	A	161/183 (88%)	148 (92%)	11 (7%)	2 (1%)	16	52
1	B	161/183 (88%)	142 (88%)	16 (10%)	3 (2%)	10	40
1	C	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	D	161/183 (88%)	149 (92%)	10 (6%)	2 (1%)	16	52
1	E	161/183 (88%)	147 (91%)	12 (8%)	2 (1%)	16	52
1	F	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	G	161/183 (88%)	144 (89%)	16 (10%)	1 (1%)	30	68
1	H	161/183 (88%)	143 (89%)	15 (9%)	3 (2%)	10	40
1	I	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	J	161/183 (88%)	145 (90%)	15 (9%)	1 (1%)	30	68
1	K	161/183 (88%)	142 (88%)	16 (10%)	3 (2%)	10	40
1	L	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	M	161/183 (88%)	141 (88%)	16 (10%)	4 (2%)	7	32
1	N	161/183 (88%)	143 (89%)	18 (11%)	0	100	100
1	O	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
1	P	161/183 (88%)	139 (86%)	20 (12%)	2 (1%)	16	52
1	Q	161/183 (88%)	145 (90%)	15 (9%)	1 (1%)	30	68
1	R	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
1	S	161/183 (88%)	146 (91%)	13 (8%)	2 (1%)	16	52
1	T	161/183 (88%)	146 (91%)	15 (9%)	0	100	100
1	U	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
1	V	161/183 (88%)	145 (90%)	14 (9%)	2 (1%)	16	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	161/183 (88%)	142 (88%)	17 (11%)	2 (1%)	16	52
1	X	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
1	Y	161/183 (88%)	147 (91%)	13 (8%)	1 (1%)	30	68
1	Z	161/183 (88%)	143 (89%)	15 (9%)	3 (2%)	10	40
1	a	161/183 (88%)	140 (87%)	20 (12%)	1 (1%)	30	68
1	b	161/183 (88%)	141 (88%)	17 (11%)	3 (2%)	10	40
1	c	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	d	161/183 (88%)	148 (92%)	12 (8%)	1 (1%)	30	68
1	e	161/183 (88%)	143 (89%)	17 (11%)	1 (1%)	30	68
1	f	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	g	161/183 (88%)	146 (91%)	14 (9%)	1 (1%)	30	68
1	h	161/183 (88%)	145 (90%)	15 (9%)	1 (1%)	30	68
1	i	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
1	j	161/183 (88%)	146 (91%)	13 (8%)	2 (1%)	16	52
1	k	161/183 (88%)	143 (89%)	17 (11%)	1 (1%)	30	68
1	l	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
1	m	161/183 (88%)	144 (89%)	16 (10%)	1 (1%)	30	68
1	n	161/183 (88%)	146 (91%)	13 (8%)	2 (1%)	16	52
1	o	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
1	p	161/183 (88%)	144 (89%)	15 (9%)	2 (1%)	16	52
1	q	161/183 (88%)	145 (90%)	15 (9%)	1 (1%)	30	68
1	r	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	s	161/183 (88%)	134 (83%)	26 (16%)	1 (1%)	30	68
1	t	161/183 (88%)	147 (91%)	12 (8%)	2 (1%)	16	52
1	u	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	v	161/183 (88%)	143 (89%)	16 (10%)	2 (1%)	16	52
1	w	161/183 (88%)	146 (91%)	14 (9%)	1 (1%)	30	68
1	x	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
All	All	9660/10980 (88%)	8763 (91%)	803 (8%)	94 (1%)	19	58

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	THR
1	C	209	VAL
1	H	70	ALA
1	K	70	ALA
1	W	70	ALA
1	Z	70	ALA
1	5	70	ALA
1	7	147	ALA
1	8	121	GLY
1	b	70	ALA
1	b	75	ASP
1	j	70	ALA
1	j	178	THR
1	l	209	VAL
1	n	147	ALA
1	q	70	ALA
1	s	75	ASP
1	t	70	ALA
1	t	147	ALA
1	x	209	VAL
1	B	70	ALA
1	B	178	THR
1	D	147	ALA
1	F	209	VAL
1	G	121	GLY
1	H	75	ASP
1	I	209	VAL
1	J	147	ALA
1	L	209	VAL
1	M	135	ASP
1	O	209	VAL
1	P	171	SER
1	P	178	THR
1	R	209	VAL
1	S	147	ALA
1	U	209	VAL
1	X	209	VAL
1	Y	70	ALA
1	0	209	VAL
1	2	147	ALA
1	3	209	VAL
1	5	147	ALA
1	6	209	VAL

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Mol	Chain	Res	Type
1	9	209	VAL
1	a	70	ALA
1	b	147	ALA
1	c	209	VAL
1	f	209	VAL
1	g	70	ALA
1	i	209	VAL
1	k	178	THR
1	o	209	VAL
1	p	75	ASP
1	r	209	VAL
1	u	209	VAL
1	v	75	ASP
1	w	75	ASP
1	D	70	ALA
1	E	75	ASP
1	M	75	ASP
1	V	75	ASP
1	4	147	ALA
1	8	147	ALA
1	E	70	ALA
1	H	147	ALA
1	K	147	ALA
1	M	70	ALA
1	V	147	ALA
1	Z	75	ASP
1	1	97	ARG
1	2	70	ALA
1	7	75	ASP
1	8	75	ASP
1	K	129	PRO
1	S	70	ALA
1	5	75	ASP
1	8	70	ALA
1	e	70	ALA
1	v	147	ALA
1	4	129	PRO
1	h	70	ALA
1	n	75	ASP
1	5	86	PRO
1	B	189	GLY
1	W	189	GLY

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Mol	Chain	Res	Type
1	A	90	PRO
1	Z	113	PRO
1	d	131	PRO
1	m	93	GLY
1	M	90	PRO
1	Q	121	GLY
1	1	121	GLY
1	2	71	GLY
1	p	71	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	1	138/153 (90%)	109 (79%)	29 (21%)	1 6
1	2	138/153 (90%)	112 (81%)	26 (19%)	2 8
1	3	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	4	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	5	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	6	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	7	138/153 (90%)	108 (78%)	30 (22%)	1 5
1	8	138/153 (90%)	112 (81%)	26 (19%)	2 8
1	9	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	A	138/153 (90%)	109 (79%)	29 (21%)	1 6
1	B	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	C	138/153 (90%)	112 (81%)	26 (19%)	2 8
1	D	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	E	138/153 (90%)	102 (74%)	36 (26%)	0 2
1	F	138/153 (90%)	110 (80%)	28 (20%)	1 6
1	G	138/153 (90%)	105 (76%)	33 (24%)	1 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	138/153 (90%)	112 (81%)	26 (19%)	2 8
1	I	138/153 (90%)	110 (80%)	28 (20%)	1 6
1	J	138/153 (90%)	114 (83%)	24 (17%)	2 11
1	K	138/153 (90%)	112 (81%)	26 (19%)	2 8
1	L	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	M	138/153 (90%)	109 (79%)	29 (21%)	1 6
1	N	138/153 (90%)	106 (77%)	32 (23%)	1 4
1	O	138/153 (90%)	110 (80%)	28 (20%)	1 6
1	P	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	Q	138/153 (90%)	110 (80%)	28 (20%)	1 6
1	R	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	S	138/153 (90%)	115 (83%)	23 (17%)	3 11
1	T	138/153 (90%)	104 (75%)	34 (25%)	1 3
1	U	138/153 (90%)	110 (80%)	28 (20%)	1 6
1	V	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	W	138/153 (90%)	115 (83%)	23 (17%)	3 11
1	X	138/153 (90%)	112 (81%)	26 (19%)	2 8
1	Y	138/153 (90%)	115 (83%)	23 (17%)	3 11
1	Z	138/153 (90%)	105 (76%)	33 (24%)	1 3
1	a	138/153 (90%)	113 (82%)	25 (18%)	2 9
1	b	138/153 (90%)	114 (83%)	24 (17%)	2 11
1	c	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	d	138/153 (90%)	109 (79%)	29 (21%)	1 6
1	e	138/153 (90%)	108 (78%)	30 (22%)	1 5
1	f	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	g	138/153 (90%)	106 (77%)	32 (23%)	1 4
1	h	138/153 (90%)	109 (79%)	29 (21%)	1 6
1	i	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	j	138/153 (90%)	110 (80%)	28 (20%)	1 6
1	k	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	l	138/153 (90%)	111 (80%)	27 (20%)	1 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	m	138/153 (90%)	108 (78%)	30 (22%)	1 5
1	n	138/153 (90%)	108 (78%)	30 (22%)	1 5
1	o	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	p	138/153 (90%)	107 (78%)	31 (22%)	1 4
1	q	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	r	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	s	138/153 (90%)	109 (79%)	29 (21%)	1 6
1	t	138/153 (90%)	109 (79%)	29 (21%)	1 6
1	u	138/153 (90%)	111 (80%)	27 (20%)	1 7
1	v	138/153 (90%)	108 (78%)	30 (22%)	1 5
1	w	138/153 (90%)	109 (79%)	29 (21%)	1 6
1	x	138/153 (90%)	110 (80%)	28 (20%)	1 6
All	All	8280/9180 (90%)	6606 (80%)	1674 (20%)	1 7

All (1674) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	THR
1	A	57	LEU
1	A	61	SER
1	A	62	ARG
1	A	64	SER
1	A	74	THR
1	A	88	LEU
1	A	92	LEU
1	A	101	ARG
1	A	105	GLU
1	A	107	LEU
1	A	128	LEU
1	A	130	ASP
1	A	142	GLN
1	A	145	ARG
1	A	151	LYS
1	A	152	TRP
1	A	155	SER
1	A	156	ARG
1	A	158	VAL
1	A	165	THR

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Mol	Chain	Res	Type
1	A	177	LEU
1	A	185	LEU
1	A	190	ASN
1	A	193	ASP
1	A	196	ASN
1	A	201	CYS
1	A	202	ARG
1	A	205	VAL
1	B	57	LEU
1	B	72	THR
1	B	74	THR
1	B	87	ASP
1	B	105	GLU
1	B	107	LEU
1	B	124	VAL
1	B	128	LEU
1	B	133	ASP
1	B	134	ASN
1	B	137	THR
1	B	145	ARG
1	B	149	VAL
1	B	152	TRP
1	B	156	ARG
1	B	158	VAL
1	B	164	ARG
1	B	165	THR
1	B	170	SER
1	B	178	THR
1	B	179	SER
1	B	185	LEU
1	B	190	ASN
1	B	193	ASP
1	B	199	VAL
1	B	202	ARG
1	B	211	SER
1	C	72	THR
1	C	74	THR
1	C	87	ASP
1	C	88	LEU
1	C	89	LEU
1	C	92	LEU
1	C	128	LEU

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Mol	Chain	Res	Type
1	C	137	THR
1	C	145	ARG
1	C	151	LYS
1	C	152	TRP
1	C	156	ARG
1	C	158	VAL
1	C	164	ARG
1	C	165	THR
1	C	167	LEU
1	C	170	SER
1	C	185	LEU
1	C	193	ASP
1	C	196	ASN
1	C	198	SER
1	C	199	VAL
1	C	202	ARG
1	C	208	SER
1	C	211	SER
1	C	213	GLU
1	D	57	LEU
1	D	58	SER
1	D	62	ARG
1	D	74	THR
1	D	88	LEU
1	D	92	LEU
1	D	101	ARG
1	D	106	THR
1	D	128	LEU
1	D	137	THR
1	D	142	GLN
1	D	145	ARG
1	D	149	VAL
1	D	152	TRP
1	D	156	ARG
1	D	158	VAL
1	D	176	ARG
1	D	177	LEU
1	D	185	LEU
1	D	190	ASN
1	D	193	ASP
1	D	196	ASN
1	D	199	VAL

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Mol	Chain	Res	Type
1	D	202	ARG
1	D	204	SER
1	D	207	LEU
1	D	213	GLU
1	E	57	LEU
1	E	64	SER
1	E	74	THR
1	E	75	ASP
1	E	98	ILE
1	E	105	GLU
1	E	128	LEU
1	E	130	ASP
1	E	137	THR
1	E	145	ARG
1	E	149	VAL
1	E	151	LYS
1	E	152	TRP
1	E	154	GLU
1	E	156	ARG
1	E	158	VAL
1	E	161	GLN
1	E	162	TYR
1	E	164	ARG
1	E	166	LEU
1	E	176	ARG
1	E	177	LEU
1	E	178	THR
1	E	185	LEU
1	E	190	ASN
1	E	193	ASP
1	E	196	ASN
1	E	198	SER
1	E	199	VAL
1	E	202	ARG
1	E	204	SER
1	E	205	VAL
1	E	207	LEU
1	E	209	VAL
1	E	211	SER
1	E	213	GLU
1	F	57	LEU
1	F	72	THR

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Mol	Chain	Res	Type
1	F	74	THR
1	F	87	ASP
1	F	88	LEU
1	F	89	LEU
1	F	92	LEU
1	F	128	LEU
1	F	137	THR
1	F	145	ARG
1	F	151	LYS
1	F	152	TRP
1	F	156	ARG
1	F	158	VAL
1	F	164	ARG
1	F	165	THR
1	F	167	LEU
1	F	170	SER
1	F	185	LEU
1	F	193	ASP
1	F	196	ASN
1	F	198	SER
1	F	199	VAL
1	F	202	ARG
1	F	208	SER
1	F	209	VAL
1	F	211	SER
1	F	213	GLU
1	G	57	LEU
1	G	61	SER
1	G	62	ARG
1	G	64	SER
1	G	68	LEU
1	G	74	THR
1	G	75	ASP
1	G	79	VAL
1	G	88	LEU
1	G	92	LEU
1	G	101	ARG
1	G	105	GLU
1	G	128	LEU
1	G	130	ASP
1	G	135	ASP
1	G	145	ARG

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Mol	Chain	Res	Type
1	G	151	LYS
1	G	152	TRP
1	G	156	ARG
1	G	158	VAL
1	G	165	THR
1	G	175	GLN
1	G	176	ARG
1	G	177	LEU
1	G	178	THR
1	G	185	LEU
1	G	190	ASN
1	G	193	ASP
1	G	196	ASN
1	G	199	VAL
1	G	202	ARG
1	G	205	VAL
1	G	208	SER
1	H	61	SER
1	H	74	THR
1	H	107	LEU
1	H	128	LEU
1	H	130	ASP
1	H	133	ASP
1	H	134	ASN
1	H	137	THR
1	H	145	ARG
1	H	151	LYS
1	H	152	TRP
1	H	156	ARG
1	H	158	VAL
1	H	161	GLN
1	H	164	ARG
1	H	175	GLN
1	H	176	ARG
1	H	177	LEU
1	H	178	THR
1	H	185	LEU
1	H	190	ASN
1	H	192	THR
1	H	193	ASP
1	H	196	ASN
1	H	202	ARG

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Mol	Chain	Res	Type
1	H	211	SER
1	I	57	LEU
1	I	72	THR
1	I	74	THR
1	I	87	ASP
1	I	88	LEU
1	I	89	LEU
1	I	92	LEU
1	I	128	LEU
1	I	137	THR
1	I	145	ARG
1	I	151	LYS
1	I	152	TRP
1	I	156	ARG
1	I	158	VAL
1	I	164	ARG
1	I	165	THR
1	I	167	LEU
1	I	170	SER
1	I	185	LEU
1	I	193	ASP
1	I	196	ASN
1	I	198	SER
1	I	199	VAL
1	I	202	ARG
1	I	208	SER
1	I	209	VAL
1	I	211	SER
1	I	213	GLU
1	J	57	LEU
1	J	64	SER
1	J	74	THR
1	J	87	ASP
1	J	88	LEU
1	J	92	LEU
1	J	105	GLU
1	J	107	LEU
1	J	128	LEU
1	J	130	ASP
1	J	145	ARG
1	J	151	LYS
1	J	152	TRP

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Mol	Chain	Res	Type
1	J	156	ARG
1	J	158	VAL
1	J	165	THR
1	J	178	THR
1	J	185	LEU
1	J	186	LEU
1	J	190	ASN
1	J	193	ASP
1	J	196	ASN
1	J	198	SER
1	J	199	VAL
1	K	57	LEU
1	K	67	VAL
1	K	74	THR
1	K	91	ARG
1	K	128	LEU
1	K	134	ASN
1	K	135	ASP
1	K	137	THR
1	K	145	ARG
1	K	149	VAL
1	K	152	TRP
1	K	156	ARG
1	K	158	VAL
1	K	164	ARG
1	K	170	SER
1	K	171	SER
1	K	178	THR
1	K	185	LEU
1	K	190	ASN
1	K	192	THR
1	K	196	ASN
1	K	199	VAL
1	K	202	ARG
1	K	205	VAL
1	K	210	PRO
1	K	211	SER
1	L	57	LEU
1	L	72	THR
1	L	74	THR
1	L	87	ASP
1	L	88	LEU

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Mol	Chain	Res	Type
1	L	89	LEU
1	L	92	LEU
1	L	128	LEU
1	L	137	THR
1	L	145	ARG
1	L	151	LYS
1	L	152	TRP
1	L	156	ARG
1	L	158	VAL
1	L	164	ARG
1	L	165	THR
1	L	167	LEU
1	L	170	SER
1	L	185	LEU
1	L	193	ASP
1	L	196	ASN
1	L	198	SER
1	L	199	VAL
1	L	202	ARG
1	L	208	SER
1	L	211	SER
1	L	213	GLU
1	M	57	LEU
1	M	62	ARG
1	M	74	THR
1	M	77	TYR
1	M	81	ASP
1	M	92	LEU
1	M	98	ILE
1	M	101	ARG
1	M	105	GLU
1	M	106	THR
1	M	107	LEU
1	M	128	LEU
1	M	130	ASP
1	M	135	ASP
1	M	137	THR
1	M	145	ARG
1	M	151	LYS
1	M	152	TRP
1	M	158	VAL
1	M	165	THR

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Mol	Chain	Res	Type
1	M	175	GLN
1	M	176	ARG
1	M	177	LEU
1	M	185	LEU
1	M	190	ASN
1	M	193	ASP
1	M	196	ASN
1	M	202	ARG
1	M	213	GLU
1	N	57	LEU
1	N	72	THR
1	N	74	THR
1	N	79	VAL
1	N	105	GLU
1	N	128	LEU
1	N	133	ASP
1	N	137	THR
1	N	139	ASP
1	N	142	GLN
1	N	145	ARG
1	N	152	TRP
1	N	156	ARG
1	N	158	VAL
1	N	164	ARG
1	N	165	THR
1	N	170	SER
1	N	175	GLN
1	N	176	ARG
1	N	177	LEU
1	N	178	THR
1	N	179	SER
1	N	185	LEU
1	N	186	LEU
1	N	192	THR
1	N	193	ASP
1	N	198	SER
1	N	199	VAL
1	N	200	LEU
1	N	202	ARG
1	N	205	VAL
1	N	213	GLU
1	O	57	LEU

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Mol	Chain	Res	Type
1	O	72	THR
1	O	74	THR
1	O	87	ASP
1	O	88	LEU
1	O	89	LEU
1	O	92	LEU
1	O	128	LEU
1	O	137	THR
1	O	145	ARG
1	O	151	LYS
1	O	152	TRP
1	O	156	ARG
1	O	158	VAL
1	O	164	ARG
1	O	165	THR
1	O	167	LEU
1	O	170	SER
1	O	185	LEU
1	O	193	ASP
1	O	196	ASN
1	O	198	SER
1	O	199	VAL
1	O	202	ARG
1	O	208	SER
1	O	209	VAL
1	O	211	SER
1	O	213	GLU
1	P	53	ASN
1	P	57	LEU
1	P	62	ARG
1	P	64	SER
1	P	74	THR
1	P	79	VAL
1	P	88	LEU
1	P	92	LEU
1	P	101	ARG
1	P	105	GLU
1	P	106	THR
1	P	107	LEU
1	P	128	LEU
1	P	137	THR
1	P	145	ARG

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Mol	Chain	Res	Type
1	P	151	LYS
1	P	152	TRP
1	P	156	ARG
1	P	165	THR
1	P	170	SER
1	P	177	LEU
1	P	178	THR
1	P	185	LEU
1	P	190	ASN
1	P	196	ASN
1	P	202	ARG
1	P	205	VAL
1	Q	57	LEU
1	Q	72	THR
1	Q	74	THR
1	Q	87	ASP
1	Q	105	GLU
1	Q	107	LEU
1	Q	128	LEU
1	Q	134	ASN
1	Q	135	ASP
1	Q	137	THR
1	Q	142	GLN
1	Q	145	ARG
1	Q	152	TRP
1	Q	156	ARG
1	Q	164	ARG
1	Q	165	THR
1	Q	170	SER
1	Q	175	GLN
1	Q	178	THR
1	Q	185	LEU
1	Q	190	ASN
1	Q	192	THR
1	Q	193	ASP
1	Q	196	ASN
1	Q	198	SER
1	Q	199	VAL
1	Q	202	ARG
1	Q	211	SER
1	R	57	LEU
1	R	72	THR

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Mol	Chain	Res	Type
1	R	74	THR
1	R	87	ASP
1	R	88	LEU
1	R	89	LEU
1	R	92	LEU
1	R	128	LEU
1	R	137	THR
1	R	145	ARG
1	R	151	LYS
1	R	152	TRP
1	R	156	ARG
1	R	158	VAL
1	R	164	ARG
1	R	165	THR
1	R	167	LEU
1	R	170	SER
1	R	185	LEU
1	R	193	ASP
1	R	196	ASN
1	R	198	SER
1	R	199	VAL
1	R	202	ARG
1	R	208	SER
1	R	211	SER
1	R	213	GLU
1	S	57	LEU
1	S	62	ARG
1	S	74	THR
1	S	88	LEU
1	S	92	LEU
1	S	128	LEU
1	S	130	ASP
1	S	135	ASP
1	S	137	THR
1	S	145	ARG
1	S	151	LYS
1	S	152	TRP
1	S	156	ARG
1	S	158	VAL
1	S	175	GLN
1	S	176	ARG
1	S	177	LEU

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Mol	Chain	Res	Type
1	S	185	LEU
1	S	190	ASN
1	S	193	ASP
1	S	196	ASN
1	S	202	ARG
1	S	208	SER
1	T	57	LEU
1	T	58	SER
1	T	64	SER
1	T	67	VAL
1	T	74	THR
1	T	88	LEU
1	T	105	GLU
1	T	128	LEU
1	T	133	ASP
1	T	137	THR
1	T	145	ARG
1	T	149	VAL
1	T	151	LYS
1	T	152	TRP
1	T	156	ARG
1	T	158	VAL
1	T	164	ARG
1	T	165	THR
1	T	170	SER
1	T	176	ARG
1	T	177	LEU
1	T	178	THR
1	T	185	LEU
1	T	190	ASN
1	T	192	THR
1	T	193	ASP
1	T	196	ASN
1	T	198	SER
1	T	199	VAL
1	T	202	ARG
1	T	204	SER
1	T	209	VAL
1	T	211	SER
1	T	213	GLU
1	U	57	LEU
1	U	72	THR

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Mol	Chain	Res	Type
1	U	74	THR
1	U	87	ASP
1	U	88	LEU
1	U	89	LEU
1	U	92	LEU
1	U	128	LEU
1	U	137	THR
1	U	145	ARG
1	U	151	LYS
1	U	152	TRP
1	U	156	ARG
1	U	158	VAL
1	U	164	ARG
1	U	165	THR
1	U	167	LEU
1	U	170	SER
1	U	185	LEU
1	U	193	ASP
1	U	196	ASN
1	U	198	SER
1	U	199	VAL
1	U	202	ARG
1	U	208	SER
1	U	209	VAL
1	U	211	SER
1	U	213	GLU
1	V	57	LEU
1	V	61	SER
1	V	62	ARG
1	V	74	THR
1	V	87	ASP
1	V	88	LEU
1	V	92	LEU
1	V	106	THR
1	V	128	LEU
1	V	137	THR
1	V	145	ARG
1	V	151	LYS
1	V	152	TRP
1	V	156	ARG
1	V	158	VAL
1	V	165	THR

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Mol	Chain	Res	Type
1	V	170	SER
1	V	177	LEU
1	V	178	THR
1	V	185	LEU
1	V	190	ASN
1	V	196	ASN
1	V	199	VAL
1	V	202	ARG
1	V	204	SER
1	V	205	VAL
1	V	211	SER
1	W	57	LEU
1	W	74	THR
1	W	79	VAL
1	W	105	GLU
1	W	107	LEU
1	W	128	LEU
1	W	137	THR
1	W	145	ARG
1	W	149	VAL
1	W	151	LYS
1	W	152	TRP
1	W	156	ARG
1	W	170	SER
1	W	175	GLN
1	W	178	THR
1	W	185	LEU
1	W	193	ASP
1	W	196	ASN
1	W	199	VAL
1	W	202	ARG
1	W	210	PRO
1	W	211	SER
1	W	213	GLU
1	X	72	THR
1	X	74	THR
1	X	87	ASP
1	X	88	LEU
1	X	89	LEU
1	X	92	LEU
1	X	128	LEU
1	X	137	THR

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Mol	Chain	Res	Type
1	X	145	ARG
1	X	151	LYS
1	X	152	TRP
1	X	156	ARG
1	X	158	VAL
1	X	164	ARG
1	X	165	THR
1	X	167	LEU
1	X	170	SER
1	X	185	LEU
1	X	193	ASP
1	X	196	ASN
1	X	198	SER
1	X	199	VAL
1	X	202	ARG
1	X	208	SER
1	X	211	SER
1	X	213	GLU
1	Y	57	LEU
1	Y	62	ARG
1	Y	74	THR
1	Y	88	LEU
1	Y	92	LEU
1	Y	107	LEU
1	Y	128	LEU
1	Y	130	ASP
1	Y	135	ASP
1	Y	145	ARG
1	Y	151	LYS
1	Y	152	TRP
1	Y	158	VAL
1	Y	165	THR
1	Y	175	GLN
1	Y	176	ARG
1	Y	177	LEU
1	Y	178	THR
1	Y	185	LEU
1	Y	190	ASN
1	Y	202	ARG
1	Y	205	VAL
1	Y	208	SER
1	Z	57	LEU

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Mol	Chain	Res	Type
1	Z	58	SER
1	Z	64	SER
1	Z	74	THR
1	Z	75	ASP
1	Z	79	VAL
1	Z	107	LEU
1	Z	128	LEU
1	Z	130	ASP
1	Z	133	ASP
1	Z	134	ASN
1	Z	135	ASP
1	Z	137	THR
1	Z	142	GLN
1	Z	145	ARG
1	Z	149	VAL
1	Z	151	LYS
1	Z	152	TRP
1	Z	156	ARG
1	Z	158	VAL
1	Z	164	ARG
1	Z	165	THR
1	Z	175	GLN
1	Z	176	ARG
1	Z	177	LEU
1	Z	178	THR
1	Z	185	LEU
1	Z	190	ASN
1	Z	193	ASP
1	Z	196	ASN
1	Z	202	ARG
1	Z	205	VAL
1	Z	211	SER
1	0	57	LEU
1	0	72	THR
1	0	74	THR
1	0	87	ASP
1	0	88	LEU
1	0	89	LEU
1	0	92	LEU
1	0	128	LEU
1	0	137	THR
1	0	145	ARG

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Mol	Chain	Res	Type
1	0	151	LYS
1	0	152	TRP
1	0	156	ARG
1	0	158	VAL
1	0	164	ARG
1	0	167	LEU
1	0	170	SER
1	0	185	LEU
1	0	193	ASP
1	0	196	ASN
1	0	198	SER
1	0	199	VAL
1	0	202	ARG
1	0	208	SER
1	0	209	VAL
1	0	211	SER
1	0	213	GLU
1	1	57	LEU
1	1	62	ARG
1	1	64	SER
1	1	72	THR
1	1	74	THR
1	1	79	VAL
1	1	92	LEU
1	1	105	GLU
1	1	128	LEU
1	1	130	ASP
1	1	137	THR
1	1	139	ASP
1	1	141	LEU
1	1	145	ARG
1	1	151	LYS
1	1	152	TRP
1	1	155	SER
1	1	156	ARG
1	1	158	VAL
1	1	165	THR
1	1	185	LEU
1	1	190	ASN
1	1	193	ASP
1	1	196	ASN
1	1	198	SER

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Mol	Chain	Res	Type
1	1	199	VAL
1	1	202	ARG
1	1	208	SER
1	1	213	GLU
1	2	57	LEU
1	2	67	VAL
1	2	74	THR
1	2	128	LEU
1	2	130	ASP
1	2	134	ASN
1	2	142	GLN
1	2	145	ARG
1	2	149	VAL
1	2	152	TRP
1	2	156	ARG
1	2	158	VAL
1	2	164	ARG
1	2	165	THR
1	2	175	GLN
1	2	178	THR
1	2	185	LEU
1	2	190	ASN
1	2	193	ASP
1	2	196	ASN
1	2	199	VAL
1	2	202	ARG
1	2	204	SER
1	2	205	VAL
1	2	211	SER
1	2	213	GLU
1	3	57	LEU
1	3	72	THR
1	3	74	THR
1	3	87	ASP
1	3	88	LEU
1	3	89	LEU
1	3	92	LEU
1	3	128	LEU
1	3	137	THR
1	3	145	ARG
1	3	151	LYS
1	3	152	TRP

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Mol	Chain	Res	Type
1	3	156	ARG
1	3	158	VAL
1	3	164	ARG
1	3	165	THR
1	3	167	LEU
1	3	170	SER
1	3	185	LEU
1	3	193	ASP
1	3	196	ASN
1	3	198	SER
1	3	199	VAL
1	3	202	ARG
1	3	208	SER
1	3	211	SER
1	3	213	GLU
1	4	57	LEU
1	4	61	SER
1	4	62	ARG
1	4	64	SER
1	4	74	THR
1	4	81	ASP
1	4	88	LEU
1	4	92	LEU
1	4	106	THR
1	4	107	LEU
1	4	128	LEU
1	4	130	ASP
1	4	137	THR
1	4	139	ASP
1	4	145	ARG
1	4	151	LYS
1	4	152	TRP
1	4	156	ARG
1	4	165	THR
1	4	166	LEU
1	4	178	THR
1	4	185	LEU
1	4	190	ASN
1	4	193	ASP
1	4	196	ASN
1	4	199	VAL
1	4	202	ARG

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Mol	Chain	Res	Type
1	5	57	LEU
1	5	74	THR
1	5	107	LEU
1	5	128	LEU
1	5	134	ASN
1	5	137	THR
1	5	145	ARG
1	5	149	VAL
1	5	151	LYS
1	5	152	TRP
1	5	156	ARG
1	5	158	VAL
1	5	162	TYR
1	5	164	ARG
1	5	171	SER
1	5	178	THR
1	5	185	LEU
1	5	190	ASN
1	5	192	THR
1	5	193	ASP
1	5	196	ASN
1	5	198	SER
1	5	199	VAL
1	5	202	ARG
1	5	205	VAL
1	5	211	SER
1	5	213	GLU
1	6	57	LEU
1	6	72	THR
1	6	74	THR
1	6	87	ASP
1	6	88	LEU
1	6	89	LEU
1	6	92	LEU
1	6	128	LEU
1	6	137	THR
1	6	145	ARG
1	6	151	LYS
1	6	152	TRP
1	6	156	ARG
1	6	158	VAL
1	6	164	ARG

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Mol	Chain	Res	Type
1	6	165	THR
1	6	167	LEU
1	6	170	SER
1	6	185	LEU
1	6	193	ASP
1	6	196	ASN
1	6	198	SER
1	6	199	VAL
1	6	202	ARG
1	6	208	SER
1	6	211	SER
1	6	213	GLU
1	7	72	THR
1	7	74	THR
1	7	88	LEU
1	7	92	LEU
1	7	101	ARG
1	7	106	THR
1	7	128	LEU
1	7	130	ASP
1	7	137	THR
1	7	142	GLN
1	7	145	ARG
1	7	151	LYS
1	7	152	TRP
1	7	155	SER
1	7	156	ARG
1	7	158	VAL
1	7	164	ARG
1	7	165	THR
1	7	166	LEU
1	7	170	SER
1	7	175	GLN
1	7	176	ARG
1	7	177	LEU
1	7	178	THR
1	7	185	LEU
1	7	190	ASN
1	7	196	ASN
1	7	202	ARG
1	7	204	SER
1	7	205	VAL

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Mol	Chain	Res	Type
1	8	57	LEU
1	8	67	VAL
1	8	74	THR
1	8	79	VAL
1	8	105	GLU
1	8	106	THR
1	8	128	LEU
1	8	134	ASN
1	8	137	THR
1	8	139	ASP
1	8	145	ARG
1	8	149	VAL
1	8	152	TRP
1	8	156	ARG
1	8	161	GLN
1	8	164	ARG
1	8	175	GLN
1	8	176	ARG
1	8	177	LEU
1	8	178	THR
1	8	185	LEU
1	8	190	ASN
1	8	196	ASN
1	8	202	ARG
1	8	208	SER
1	8	211	SER
1	9	57	LEU
1	9	72	THR
1	9	74	THR
1	9	87	ASP
1	9	88	LEU
1	9	89	LEU
1	9	92	LEU
1	9	128	LEU
1	9	137	THR
1	9	145	ARG
1	9	151	LYS
1	9	152	TRP
1	9	156	ARG
1	9	158	VAL
1	9	164	ARG
1	9	167	LEU

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Mol	Chain	Res	Type
1	9	170	SER
1	9	185	LEU
1	9	193	ASP
1	9	196	ASN
1	9	198	SER
1	9	199	VAL
1	9	202	ARG
1	9	208	SER
1	9	209	VAL
1	9	211	SER
1	9	213	GLU
1	a	57	LEU
1	a	62	ARG
1	a	74	THR
1	a	88	LEU
1	a	92	LEU
1	a	105	GLU
1	a	106	THR
1	a	128	LEU
1	a	142	GLN
1	a	144	THR
1	a	145	ARG
1	a	151	LYS
1	a	152	TRP
1	a	156	ARG
1	a	158	VAL
1	a	170	SER
1	a	171	SER
1	a	175	GLN
1	a	178	THR
1	a	185	LEU
1	a	186	LEU
1	a	190	ASN
1	a	196	ASN
1	a	199	VAL
1	a	202	ARG
1	b	64	SER
1	b	74	THR
1	b	107	LEU
1	b	128	LEU
1	b	137	THR
1	b	144	THR

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Mol	Chain	Res	Type
1	b	145	ARG
1	b	152	TRP
1	b	155	SER
1	b	156	ARG
1	b	164	ARG
1	b	165	THR
1	b	170	SER
1	b	175	GLN
1	b	178	THR
1	b	185	LEU
1	b	192	THR
1	b	193	ASP
1	b	196	ASN
1	b	198	SER
1	b	199	VAL
1	b	202	ARG
1	b	211	SER
1	b	213	GLU
1	c	57	LEU
1	c	72	THR
1	c	74	THR
1	c	87	ASP
1	c	88	LEU
1	c	89	LEU
1	c	92	LEU
1	c	128	LEU
1	c	137	THR
1	c	145	ARG
1	c	151	LYS
1	c	152	TRP
1	c	156	ARG
1	c	158	VAL
1	c	164	ARG
1	c	165	THR
1	c	167	LEU
1	c	170	SER
1	c	185	LEU
1	c	193	ASP
1	c	196	ASN
1	c	198	SER
1	c	199	VAL
1	c	202	ARG

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Mol	Chain	Res	Type
1	c	208	SER
1	c	211	SER
1	c	213	GLU
1	d	57	LEU
1	d	62	ARG
1	d	64	SER
1	d	74	THR
1	d	87	ASP
1	d	88	LEU
1	d	92	LEU
1	d	100	GLN
1	d	106	THR
1	d	107	LEU
1	d	118	ASN
1	d	128	LEU
1	d	130	ASP
1	d	137	THR
1	d	145	ARG
1	d	149	VAL
1	d	152	TRP
1	d	154	GLU
1	d	156	ARG
1	d	158	VAL
1	d	165	THR
1	d	175	GLN
1	d	178	THR
1	d	185	LEU
1	d	190	ASN
1	d	196	ASN
1	d	198	SER
1	d	199	VAL
1	d	202	ARG
1	e	57	LEU
1	e	64	SER
1	e	74	THR
1	e	79	VAL
1	e	100	GLN
1	e	105	GLU
1	e	128	LEU
1	e	134	ASN
1	e	137	THR
1	e	139	ASP

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Mol	Chain	Res	Type
1	e	145	ARG
1	e	149	VAL
1	e	152	TRP
1	e	155	SER
1	e	156	ARG
1	e	158	VAL
1	e	164	ARG
1	e	170	SER
1	e	175	GLN
1	e	178	THR
1	e	182	ARG
1	e	185	LEU
1	e	192	THR
1	e	193	ASP
1	e	196	ASN
1	e	198	SER
1	e	199	VAL
1	e	202	ARG
1	e	205	VAL
1	e	213	GLU
1	f	57	LEU
1	f	72	THR
1	f	74	THR
1	f	87	ASP
1	f	88	LEU
1	f	89	LEU
1	f	92	LEU
1	f	128	LEU
1	f	137	THR
1	f	145	ARG
1	f	151	LYS
1	f	152	TRP
1	f	156	ARG
1	f	158	VAL
1	f	164	ARG
1	f	165	THR
1	f	167	LEU
1	f	170	SER
1	f	185	LEU
1	f	193	ASP
1	f	196	ASN
1	f	198	SER

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Mol	Chain	Res	Type
1	f	199	VAL
1	f	202	ARG
1	f	208	SER
1	f	211	SER
1	f	213	GLU
1	g	52	THR
1	g	57	LEU
1	g	62	ARG
1	g	64	SER
1	g	74	THR
1	g	75	ASP
1	g	79	VAL
1	g	88	LEU
1	g	92	LEU
1	g	101	ARG
1	g	105	GLU
1	g	128	LEU
1	g	130	ASP
1	g	137	THR
1	g	142	GLN
1	g	145	ARG
1	g	151	LYS
1	g	152	TRP
1	g	156	ARG
1	g	158	VAL
1	g	165	THR
1	g	170	SER
1	g	175	GLN
1	g	176	ARG
1	g	177	LEU
1	g	185	LEU
1	g	190	ASN
1	g	193	ASP
1	g	196	ASN
1	g	199	VAL
1	g	202	ARG
1	g	205	VAL
1	h	57	LEU
1	h	72	THR
1	h	74	THR
1	h	128	LEU
1	h	130	ASP

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Mol	Chain	Res	Type
1	h	133	ASP
1	h	134	ASN
1	h	135	ASP
1	h	137	THR
1	h	145	ARG
1	h	149	VAL
1	h	152	TRP
1	h	156	ARG
1	h	158	VAL
1	h	161	GLN
1	h	164	ARG
1	h	165	THR
1	h	176	ARG
1	h	177	LEU
1	h	178	THR
1	h	185	LEU
1	h	190	ASN
1	h	192	THR
1	h	196	ASN
1	h	198	SER
1	h	199	VAL
1	h	202	ARG
1	h	209	VAL
1	h	211	SER
1	i	72	THR
1	i	74	THR
1	i	87	ASP
1	i	88	LEU
1	i	89	LEU
1	i	92	LEU
1	i	128	LEU
1	i	137	THR
1	i	145	ARG
1	i	151	LYS
1	i	152	TRP
1	i	156	ARG
1	i	158	VAL
1	i	164	ARG
1	i	165	THR
1	i	167	LEU
1	i	170	SER
1	i	185	LEU

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Mol	Chain	Res	Type
1	i	193	ASP
1	i	196	ASN
1	i	198	SER
1	i	199	VAL
1	i	202	ARG
1	i	208	SER
1	i	209	VAL
1	i	211	SER
1	i	213	GLU
1	j	57	LEU
1	j	62	ARG
1	j	72	THR
1	j	74	THR
1	j	79	VAL
1	j	88	LEU
1	j	92	LEU
1	j	100	GLN
1	j	105	GLU
1	j	128	LEU
1	j	130	ASP
1	j	133	ASP
1	j	145	ARG
1	j	151	LYS
1	j	152	TRP
1	j	155	SER
1	j	156	ARG
1	j	158	VAL
1	j	165	THR
1	j	166	LEU
1	j	185	LEU
1	j	186	LEU
1	j	193	ASP
1	j	198	SER
1	j	199	VAL
1	j	202	ARG
1	j	205	VAL
1	j	213	GLU
1	k	57	LEU
1	k	61	SER
1	k	74	THR
1	k	100	GLN
1	k	107	LEU

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Mol	Chain	Res	Type
1	k	128	LEU
1	k	139	ASP
1	k	145	ARG
1	k	149	VAL
1	k	152	TRP
1	k	156	ARG
1	k	158	VAL
1	k	164	ARG
1	k	165	THR
1	k	170	SER
1	k	175	GLN
1	k	178	THR
1	k	185	LEU
1	k	190	ASN
1	k	192	THR
1	k	193	ASP
1	k	196	ASN
1	k	198	SER
1	k	199	VAL
1	k	202	ARG
1	k	211	SER
1	k	213	GLU
1	l	57	LEU
1	l	72	THR
1	l	74	THR
1	l	87	ASP
1	l	88	LEU
1	l	89	LEU
1	l	92	LEU
1	l	128	LEU
1	l	137	THR
1	l	145	ARG
1	l	151	LYS
1	l	152	TRP
1	l	156	ARG
1	l	158	VAL
1	l	164	ARG
1	l	165	THR
1	l	167	LEU
1	l	170	SER
1	l	185	LEU
1	l	193	ASP

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Mol	Chain	Res	Type
1	l	196	ASN
1	l	198	SER
1	l	199	VAL
1	l	202	ARG
1	l	208	SER
1	l	211	SER
1	l	213	GLU
1	m	57	LEU
1	m	58	SER
1	m	62	ARG
1	m	72	THR
1	m	74	THR
1	m	86	PRO
1	m	87	ASP
1	m	88	LEU
1	m	92	LEU
1	m	105	GLU
1	m	128	LEU
1	m	130	ASP
1	m	135	ASP
1	m	137	THR
1	m	145	ARG
1	m	149	VAL
1	m	151	LYS
1	m	152	TRP
1	m	156	ARG
1	m	158	VAL
1	m	165	THR
1	m	166	LEU
1	m	176	ARG
1	m	177	LEU
1	m	179	SER
1	m	185	LEU
1	m	186	LEU
1	m	193	ASP
1	m	196	ASN
1	m	202	ARG
1	n	57	LEU
1	n	72	THR
1	n	74	THR
1	n	75	ASP
1	n	79	VAL

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Mol	Chain	Res	Type
1	n	91	ARG
1	n	105	GLU
1	n	128	LEU
1	n	130	ASP
1	n	133	ASP
1	n	134	ASN
1	n	137	THR
1	n	145	ARG
1	n	149	VAL
1	n	152	TRP
1	n	156	ARG
1	n	158	VAL
1	n	161	GLN
1	n	164	ARG
1	n	176	ARG
1	n	178	THR
1	n	185	LEU
1	n	190	ASN
1	n	192	THR
1	n	193	ASP
1	n	196	ASN
1	n	199	VAL
1	n	202	ARG
1	n	211	SER
1	n	213	GLU
1	o	72	THR
1	o	74	THR
1	o	87	ASP
1	o	88	LEU
1	o	89	LEU
1	o	92	LEU
1	o	128	LEU
1	o	137	THR
1	o	145	ARG
1	o	151	LYS
1	o	152	TRP
1	o	156	ARG
1	o	158	VAL
1	o	164	ARG
1	o	165	THR
1	o	167	LEU
1	o	170	SER

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Mol	Chain	Res	Type
1	o	185	LEU
1	o	193	ASP
1	o	196	ASN
1	o	198	SER
1	o	199	VAL
1	o	202	ARG
1	o	208	SER
1	o	209	VAL
1	o	211	SER
1	o	213	GLU
1	p	57	LEU
1	p	61	SER
1	p	62	ARG
1	p	67	VAL
1	p	74	THR
1	p	87	ASP
1	p	88	LEU
1	p	92	LEU
1	p	101	ARG
1	p	106	THR
1	p	107	LEU
1	p	128	LEU
1	p	130	ASP
1	p	135	ASP
1	p	137	THR
1	p	145	ARG
1	p	151	LYS
1	p	152	TRP
1	p	156	ARG
1	p	165	THR
1	p	176	ARG
1	p	177	LEU
1	p	178	THR
1	p	185	LEU
1	p	186	LEU
1	p	190	ASN
1	p	193	ASP
1	p	196	ASN
1	p	199	VAL
1	p	202	ARG
1	p	207	LEU
1	q	52	THR

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Mol	Chain	Res	Type
1	q	57	LEU
1	q	67	VAL
1	q	74	THR
1	q	128	LEU
1	q	130	ASP
1	q	134	ASN
1	q	135	ASP
1	q	137	THR
1	q	145	ARG
1	q	149	VAL
1	q	152	TRP
1	q	156	ARG
1	q	158	VAL
1	q	161	GLN
1	q	164	ARG
1	q	165	THR
1	q	170	SER
1	q	176	ARG
1	q	178	THR
1	q	185	LEU
1	q	193	ASP
1	q	196	ASN
1	q	199	VAL
1	q	202	ARG
1	q	205	VAL
1	q	213	GLU
1	r	57	LEU
1	r	72	THR
1	r	74	THR
1	r	87	ASP
1	r	88	LEU
1	r	89	LEU
1	r	92	LEU
1	r	128	LEU
1	r	137	THR
1	r	145	ARG
1	r	151	LYS
1	r	152	TRP
1	r	156	ARG
1	r	158	VAL
1	r	164	ARG
1	r	165	THR

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Mol	Chain	Res	Type
1	r	167	LEU
1	r	170	SER
1	r	185	LEU
1	r	193	ASP
1	r	196	ASN
1	r	198	SER
1	r	199	VAL
1	r	202	ARG
1	r	208	SER
1	r	211	SER
1	r	213	GLU
1	s	57	LEU
1	s	72	THR
1	s	74	THR
1	s	75	ASP
1	s	88	LEU
1	s	92	LEU
1	s	105	GLU
1	s	106	THR
1	s	107	LEU
1	s	128	LEU
1	s	130	ASP
1	s	137	THR
1	s	139	ASP
1	s	142	GLN
1	s	145	ARG
1	s	151	LYS
1	s	152	TRP
1	s	156	ARG
1	s	158	VAL
1	s	170	SER
1	s	171	SER
1	s	177	LEU
1	s	185	LEU
1	s	190	ASN
1	s	193	ASP
1	s	196	ASN
1	s	199	VAL
1	s	202	ARG
1	s	205	VAL
1	t	57	LEU
1	t	64	SER

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Mol	Chain	Res	Type
1	t	74	THR
1	t	128	LEU
1	t	130	ASP
1	t	134	ASN
1	t	137	THR
1	t	144	THR
1	t	145	ARG
1	t	152	TRP
1	t	156	ARG
1	t	161	GLN
1	t	164	ARG
1	t	165	THR
1	t	170	SER
1	t	175	GLN
1	t	177	LEU
1	t	178	THR
1	t	185	LEU
1	t	190	ASN
1	t	192	THR
1	t	193	ASP
1	t	196	ASN
1	t	198	SER
1	t	200	LEU
1	t	201	CYS
1	t	202	ARG
1	t	211	SER
1	t	214	ASN
1	u	57	LEU
1	u	72	THR
1	u	74	THR
1	u	87	ASP
1	u	88	LEU
1	u	89	LEU
1	u	92	LEU
1	u	128	LEU
1	u	137	THR
1	u	145	ARG
1	u	151	LYS
1	u	152	TRP
1	u	156	ARG
1	u	158	VAL
1	u	164	ARG

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Mol	Chain	Res	Type
1	u	165	THR
1	u	167	LEU
1	u	170	SER
1	u	185	LEU
1	u	193	ASP
1	u	196	ASN
1	u	198	SER
1	u	199	VAL
1	u	202	ARG
1	u	208	SER
1	u	211	SER
1	u	213	GLU
1	v	57	LEU
1	v	61	SER
1	v	62	ARG
1	v	74	THR
1	v	88	LEU
1	v	92	LEU
1	v	106	THR
1	v	128	LEU
1	v	130	ASP
1	v	137	THR
1	v	139	ASP
1	v	145	ARG
1	v	151	LYS
1	v	152	TRP
1	v	158	VAL
1	v	165	THR
1	v	166	LEU
1	v	170	SER
1	v	171	SER
1	v	176	ARG
1	v	177	LEU
1	v	178	THR
1	v	185	LEU
1	v	190	ASN
1	v	193	ASP
1	v	196	ASN
1	v	198	SER
1	v	202	ARG
1	v	205	VAL
1	v	213	GLU

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Mol	Chain	Res	Type
1	w	57	LEU
1	w	67	VAL
1	w	74	THR
1	w	87	ASP
1	w	101	ARG
1	w	107	LEU
1	w	114	MET
1	w	128	LEU
1	w	130	ASP
1	w	134	ASN
1	w	137	THR
1	w	145	ARG
1	w	149	VAL
1	w	152	TRP
1	w	156	ARG
1	w	158	VAL
1	w	164	ARG
1	w	170	SER
1	w	176	ARG
1	w	178	THR
1	w	185	LEU
1	w	186	LEU
1	w	190	ASN
1	w	196	ASN
1	w	199	VAL
1	w	202	ARG
1	w	205	VAL
1	w	211	SER
1	w	213	GLU
1	x	57	LEU
1	x	72	THR
1	x	74	THR
1	x	87	ASP
1	x	88	LEU
1	x	89	LEU
1	x	92	LEU
1	x	128	LEU
1	x	137	THR
1	x	145	ARG
1	x	151	LYS
1	x	152	TRP
1	x	156	ARG

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Mol	Chain	Res	Type
1	x	158	VAL
1	x	164	ARG
1	x	165	THR
1	x	167	LEU
1	x	170	SER
1	x	185	LEU
1	x	193	ASP
1	x	196	ASN
1	x	198	SER
1	x	199	VAL
1	x	202	ARG
1	x	208	SER
1	x	209	VAL
1	x	211	SER
1	x	213	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (195) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	100	GLN
1	A	142	GLN
1	A	161	GLN
1	A	175	GLN
1	B	65	GLN
1	B	142	GLN
1	B	161	GLN
1	B	214	ASN
1	C	65	GLN
1	D	65	GLN
1	D	100	GLN
1	D	118	ASN
1	D	136	HIS
1	D	142	GLN
1	D	175	GLN
1	D	196	ASN
1	E	65	GLN
1	E	100	GLN
1	E	134	ASN
1	E	136	HIS
1	E	142	GLN
1	E	175	GLN

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Mol	Chain	Res	Type
1	E	196	ASN
1	F	65	GLN
1	F	118	ASN
1	F	175	GLN
1	G	118	ASN
1	G	175	GLN
1	H	65	GLN
1	H	118	ASN
1	H	175	GLN
1	H	196	ASN
1	I	65	GLN
1	I	94	HIS
1	I	118	ASN
1	I	175	GLN
1	I	196	ASN
1	J	65	GLN
1	J	118	ASN
1	K	65	GLN
1	K	142	GLN
1	K	196	ASN
1	L	65	GLN
1	M	175	GLN
1	M	196	ASN
1	N	134	ASN
1	N	136	HIS
1	N	142	GLN
1	N	175	GLN
1	N	196	ASN
1	O	65	GLN
1	O	175	GLN
1	P	65	GLN
1	P	118	ASN
1	P	196	ASN
1	Q	65	GLN
1	Q	142	GLN
1	Q	161	GLN
1	Q	196	ASN
1	R	65	GLN
1	S	142	GLN
1	S	175	GLN
1	T	65	GLN
1	T	100	GLN

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Mol	Chain	Res	Type
1	T	134	ASN
1	T	142	GLN
1	T	175	GLN
1	T	196	ASN
1	T	214	ASN
1	U	65	GLN
1	U	118	ASN
1	U	175	GLN
1	V	65	GLN
1	V	118	ASN
1	V	196	ASN
1	W	65	GLN
1	W	118	ASN
1	W	142	GLN
1	X	65	GLN
1	Y	65	GLN
1	Y	175	GLN
1	Y	196	ASN
1	Z	65	GLN
1	Z	118	ASN
1	Z	175	GLN
1	Z	214	ASN
1	0	65	GLN
1	0	175	GLN
1	1	65	GLN
1	1	118	ASN
1	1	175	GLN
1	1	196	ASN
1	2	65	GLN
1	2	175	GLN
1	2	196	ASN
1	3	65	GLN
1	4	65	GLN
1	4	100	GLN
1	4	118	ASN
1	4	196	ASN
1	5	65	GLN
1	5	161	GLN
1	5	196	ASN
1	6	65	GLN
1	6	100	GLN
1	6	175	GLN

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Mol	Chain	Res	Type
1	7	65	GLN
1	7	112	GLN
1	7	118	ASN
1	7	175	GLN
1	7	196	ASN
1	8	65	GLN
1	8	142	GLN
1	8	175	GLN
1	8	214	ASN
1	9	65	GLN
1	9	175	GLN
1	9	196	ASN
1	a	65	GLN
1	a	118	ASN
1	a	136	HIS
1	a	175	GLN
1	b	100	GLN
1	b	118	ASN
1	b	175	GLN
1	b	196	ASN
1	c	65	GLN
1	c	175	GLN
1	d	65	GLN
1	d	100	GLN
1	d	161	GLN
1	d	175	GLN
1	d	196	ASN
1	e	65	GLN
1	e	175	GLN
1	e	196	ASN
1	e	214	ASN
1	f	65	GLN
1	f	175	GLN
1	g	65	GLN
1	g	118	ASN
1	g	175	GLN
1	g	196	ASN
1	h	65	GLN
1	h	142	GLN
1	h	175	GLN
1	i	65	GLN
1	i	175	GLN

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Mol	Chain	Res	Type
1	j	65	GLN
1	j	100	GLN
1	k	142	GLN
1	k	161	GLN
1	k	214	ASN
1	l	65	GLN
1	l	175	GLN
1	m	65	GLN
1	m	100	GLN
1	m	175	GLN
1	m	196	ASN
1	n	94	HIS
1	n	142	GLN
1	n	161	GLN
1	n	175	GLN
1	o	65	GLN
1	o	196	ASN
1	p	65	GLN
1	p	142	GLN
1	p	196	ASN
1	q	65	GLN
1	r	65	GLN
1	r	175	GLN
1	s	65	GLN
1	s	100	GLN
1	s	118	ASN
1	s	134	ASN
1	s	175	GLN
1	s	196	ASN
1	t	175	GLN
1	t	196	ASN
1	t	214	ASN
1	u	65	GLN
1	u	175	GLN
1	v	65	GLN
1	v	118	ASN
1	v	175	GLN
1	v	196	ASN
1	w	65	GLN
1	w	94	HIS
1	w	118	ASN
1	w	136	HIS

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Mol	Chain	Res	Type
1	w	161	GLN
1	x	65	GLN
1	x	118	ASN
1	x	175	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	0	163/183 (89%)	0.07	1 (0%) 90 80	28, 44, 82, 144	0
1	1	163/183 (89%)	0.22	10 (6%) 25 10	30, 49, 106, 153	0
1	2	163/183 (89%)	0.19	5 (3%) 52 28	36, 55, 110, 160	0
1	3	163/183 (89%)	0.19	6 (3%) 45 22	26, 45, 109, 163	0
1	4	163/183 (89%)	0.19	7 (4%) 39 18	30, 52, 109, 171	0
1	5	163/183 (89%)	0.13	6 (3%) 45 22	30, 51, 104, 156	0
1	6	163/183 (89%)	0.40	9 (5%) 29 12	32, 56, 122, 194	0
1	7	163/183 (89%)	-0.08	2 (1%) 81 64	26, 41, 72, 127	0
1	8	163/183 (89%)	-0.06	3 (1%) 71 50	26, 42, 76, 120	0
1	9	163/183 (89%)	0.06	2 (1%) 81 64	25, 43, 86, 112	0
1	A	163/183 (89%)	-0.03	1 (0%) 90 80	31, 47, 89, 132	0
1	B	163/183 (89%)	0.15	7 (4%) 39 18	29, 47, 101, 189	0
1	C	163/183 (89%)	0.28	11 (6%) 21 7	26, 50, 111, 183	0
1	D	163/183 (89%)	-0.05	1 (0%) 90 80	32, 46, 81, 112	0
1	E	163/183 (89%)	-0.06	0 100 100	24, 43, 79, 126	0
1	F	163/183 (89%)	0.25	4 (2%) 61 37	32, 53, 101, 137	0
1	G	163/183 (89%)	-0.07	1 (0%) 90 80	25, 43, 74, 114	0
1	H	163/183 (89%)	-0.05	0 100 100	26, 41, 76, 105	0
1	I	163/183 (89%)	0.05	2 (1%) 81 64	27, 44, 81, 118	0
1	J	163/183 (89%)	0.16	5 (3%) 52 28	27, 52, 110, 177	0
1	K	163/183 (89%)	0.17	5 (3%) 52 28	26, 53, 106, 171	0
1	L	163/183 (89%)	0.28	9 (5%) 29 12	27, 54, 123, 169	0
1	M	163/183 (89%)	-0.06	2 (1%) 81 64	23, 38, 71, 137	0
1	N	163/183 (89%)	-0.08	2 (1%) 81 64	23, 37, 74, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	O	163/183 (89%)	0.09	2 (1%) 81 64	28, 46, 84, 129	0
1	P	163/183 (89%)	0.13	5 (3%) 52 28	25, 47, 100, 159	0
1	Q	163/183 (89%)	0.12	6 (3%) 45 22	26, 45, 113, 151	0
1	R	163/183 (89%)	0.35	12 (7%) 17 6	29, 54, 124, 176	0
1	S	163/183 (89%)	-0.05	2 (1%) 81 64	29, 45, 81, 123	0
1	T	163/183 (89%)	0.01	2 (1%) 81 64	26, 44, 81, 120	0
1	U	163/183 (89%)	0.27	5 (3%) 52 28	36, 52, 96, 140	0
1	V	163/183 (89%)	0.24	10 (6%) 25 10	28, 53, 116, 150	0
1	W	163/183 (89%)	0.09	5 (3%) 52 28	27, 47, 104, 156	0
1	X	163/183 (89%)	0.35	11 (6%) 21 7	28, 47, 116, 193	0
1	Y	163/183 (89%)	-0.06	1 (0%) 90 80	25, 42, 79, 121	0
1	Z	163/183 (89%)	-0.02	1 (0%) 90 80	31, 48, 81, 143	0
1	a	163/183 (89%)	0.25	1 (0%) 90 80	36, 62, 110, 149	0
1	b	163/183 (89%)	0.15	7 (4%) 39 18	31, 53, 104, 147	0
1	c	163/183 (89%)	0.41	6 (3%) 45 22	36, 66, 120, 135	0
1	d	163/183 (89%)	0.07	5 (3%) 52 28	25, 43, 103, 156	0
1	e	163/183 (89%)	0.18	6 (3%) 45 22	28, 49, 106, 153	0
1	f	163/183 (89%)	0.34	9 (5%) 29 12	37, 59, 114, 159	0
1	g	163/183 (89%)	-0.09	1 (0%) 90 80	29, 48, 81, 120	0
1	h	163/183 (89%)	-0.04	1 (0%) 90 80	26, 43, 79, 121	0
1	i	163/183 (89%)	0.07	1 (0%) 90 80	26, 45, 87, 114	0
1	j	163/183 (89%)	0.13	3 (1%) 71 50	26, 49, 102, 165	0
1	k	163/183 (89%)	0.07	4 (2%) 61 37	34, 47, 102, 151	0
1	l	163/183 (89%)	0.43	12 (7%) 17 6	31, 52, 115, 265	0
1	m	163/183 (89%)	-0.11	1 (0%) 90 80	25, 36, 71, 115	0
1	n	163/183 (89%)	0.00	1 (0%) 90 80	28, 44, 78, 137	0
1	o	163/183 (89%)	0.04	1 (0%) 90 80	26, 39, 79, 124	0
1	p	163/183 (89%)	-0.05	2 (1%) 81 64	28, 43, 90, 120	0
1	q	163/183 (89%)	0.06	0 100 100	26, 47, 95, 118	0
1	r	163/183 (89%)	0.18	3 (1%) 71 50	38, 57, 99, 128	0
1	s	163/183 (89%)	0.23	7 (4%) 39 18	39, 61, 103, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	t	163/183 (89%)	0.15	5 (3%) 52 28	33, 52, 103, 141	0
1	u	163/183 (89%)	0.44	6 (3%) 45 22	41, 65, 114, 144	0
1	v	163/183 (89%)	0.15	3 (1%) 71 50	35, 55, 93, 129	0
1	w	163/183 (89%)	-0.02	3 (1%) 71 50	29, 44, 93, 117	0
1	x	163/183 (89%)	0.18	7 (4%) 39 18	26, 49, 97, 122	0
All	All	9780/10980 (89%)	0.12	258 (2%) 59 35	23, 48, 102, 265	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	l	174	GLU	12.7
1	l	175	GLN	12.0
1	l	177	LEU	10.3
1	f	52	THR	9.9
1	l	176	ARG	9.7
1	6	174	GLU	8.5
1	C	176	ARG	7.8
1	X	176	ARG	7.8
1	6	52	THR	7.4
1	4	176	ARG	7.2
1	2	52	THR	7.2
1	1	52	THR	7.1
1	B	175	GLN	7.0
1	2	173	LYS	7.0
1	n	52	THR	7.0
1	6	175	GLN	6.9
1	X	172	GLY	6.7
1	0	52	THR	6.7
1	K	175	GLN	6.5
1	3	173	LYS	6.4
1	f	173	LYS	6.3
1	C	177	LEU	6.3
1	C	175	GLN	6.2
1	K	52	THR	6.2
1	U	52	THR	6.2
1	d	52	THR	6.1
1	v	52	THR	6.1
1	e	52	THR	6.0
1	X	52	THR	5.8
1	j	175	GLN	5.8

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Mol	Chain	Res	Type	RSRZ
1	M	52	THR	5.7
1	K	176	ARG	5.7
1	f	172	GLY	5.7
1	4	174	GLU	5.7
1	X	173	LYS	5.6
1	Z	52	THR	5.6
1	X	53	ASN	5.5
1	B	52	THR	5.5
1	T	52	THR	5.1
1	s	52	THR	5.1
1	X	174	GLU	5.1
1	L	170	SER	5.0
1	Q	173	LYS	5.0
1	J	174	GLU	5.0
1	3	176	ARG	4.9
1	o	52	THR	4.9
1	a	52	THR	4.9
1	e	175	GLN	4.8
1	R	174	GLU	4.8
1	W	52	THR	4.8
1	R	170	SER	4.8
1	t	52	THR	4.8
1	J	175	GLN	4.7
1	6	173	LYS	4.7
1	X	175	GLN	4.6
1	p	52	THR	4.6
1	C	173	LYS	4.6
1	O	52	THR	4.6
1	b	52	THR	4.5
1	3	174	GLU	4.5
1	V	52	THR	4.5
1	l	173	LYS	4.5
1	4	52	THR	4.4
1	7	52	THR	4.4
1	u	163	THR	4.3
1	k	174	GLU	4.3
1	L	174	GLU	4.3
1	P	176	ARG	4.3
1	d	173	LYS	4.3
1	4	175	GLN	4.3
1	f	171	SER	4.3
1	R	176	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	x	52	THR	4.2
1	B	174	GLU	4.2
1	e	176	ARG	4.2
1	e	177	LEU	4.1
1	h	52	THR	4.1
1	u	52	THR	4.1
1	u	214	ASN	4.1
1	6	172	GLY	4.1
1	Q	177	LEU	3.9
1	R	52	THR	3.9
1	m	52	THR	3.9
1	K	173	LYS	3.9
1	J	52	THR	3.9
1	P	174	GLU	3.9
1	5	52	THR	3.9
1	Q	175	GLN	3.9
1	6	177	LEU	3.8
1	3	177	LEU	3.8
1	F	52	THR	3.8
1	6	53	ASN	3.8
1	Y	52	THR	3.8
1	N	52	THR	3.7
1	1	175	GLN	3.7
1	Q	172	GLY	3.7
1	B	176	ARG	3.6
1	L	52	THR	3.6
1	5	53	ASN	3.6
1	C	174	GLU	3.5
1	B	177	LEU	3.5
1	R	53	ASN	3.5
1	S	52	THR	3.5
1	c	170	SER	3.5
1	G	52	THR	3.5
1	v	214	ASN	3.4
1	V	175	GLN	3.4
1	r	52	THR	3.4
1	P	173	LYS	3.4
1	X	171	SER	3.4
1	d	175	GLN	3.4
1	J	176	ARG	3.4
1	i	133	ASP	3.4
1	l	170	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	6	176	ARG	3.3
1	c	70	ALA	3.3
1	k	177	LEU	3.3
1	j	174	GLU	3.3
1	2	174	GLU	3.2
1	R	163	THR	3.2
1	R	214	ASN	3.2
1	f	170	SER	3.2
1	s	173	LYS	3.2
1	k	176	ARG	3.2
1	M	53	ASN	3.2
1	Q	176	ARG	3.2
1	L	173	LYS	3.1
1	P	52	THR	3.1
1	8	52	THR	3.1
1	V	172	GLY	3.1
1	1	163	THR	3.1
1	V	176	ARG	3.1
1	l	53	ASN	3.1
1	R	173	LYS	3.1
1	2	170	SER	3.0
1	8	163	THR	3.0
1	2	172	GLY	3.0
1	I	163	THR	3.0
1	V	177	LEU	3.0
1	t	163	THR	3.0
1	1	177	LEU	3.0
1	k	175	GLN	3.0
1	t	173	LYS	3.0
1	U	170	SER	3.0
1	3	175	GLN	3.0
1	V	173	LYS	2.9
1	g	52	THR	2.9
1	d	177	LEU	2.9
1	F	163	THR	2.9
1	L	53	ASN	2.9
1	W	173	LYS	2.8
1	J	173	LYS	2.8
1	V	174	GLU	2.8
1	d	174	GLU	2.8
1	L	214	ASN	2.8
1	1	213	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	52	THR	2.7
1	1	170	SER	2.7
1	K	177	LEU	2.7
1	b	130	ASP	2.7
1	f	177	LEU	2.6
1	j	176	ARG	2.6
1	t	145	ARG	2.6
1	V	170	SER	2.6
1	P	172	GLY	2.6
1	C	53	ASN	2.6
1	l	214	ASN	2.6
1	e	161	GLN	2.6
1	C	54	ASP	2.6
1	Q	171	SER	2.6
1	1	53	ASN	2.6
1	D	52	THR	2.6
1	N	163	THR	2.6
1	X	170	SER	2.6
1	e	173	LYS	2.6
1	1	161	GLN	2.5
1	L	135	ASP	2.5
1	X	177	LEU	2.5
1	A	174	GLU	2.5
1	c	175	GLN	2.5
1	l	52	THR	2.5
1	B	170	SER	2.5
1	s	170	SER	2.5
1	5	175	GLN	2.5
1	f	174	GLU	2.5
1	f	175	GLN	2.5
1	U	134	ASN	2.5
1	r	214	ASN	2.5
1	c	52	THR	2.5
1	4	177	LEU	2.5
1	W	174	GLU	2.5
1	U	178	THR	2.5
1	u	161	GLN	2.4
1	1	54	ASP	2.4
1	s	130	ASP	2.4
1	F	134	ASN	2.4
1	1	173	LYS	2.4
1	s	162	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	3	52	THR	2.4
1	b	208	SER	2.4
1	b	135	ASP	2.4
1	O	214	ASN	2.4
1	R	177	LEU	2.4
1	c	53	ASN	2.3
1	X	213	GLU	2.3
1	l	135	ASP	2.3
1	6	208	SER	2.3
1	W	175	GLN	2.3
1	R	175	GLN	2.3
1	b	214	ASN	2.3
1	x	173	LYS	2.3
1	x	174	GLU	2.3
1	7	163	THR	2.3
1	L	175	GLN	2.3
1	9	214	ASN	2.3
1	l	171	SER	2.3
1	u	170	SER	2.3
1	s	54	ASP	2.2
1	x	139	ASP	2.2
1	V	162	TYR	2.2
1	U	163	THR	2.2
1	L	176	ARG	2.2
1	5	174	GLU	2.2
1	v	175	GLN	2.2
1	C	171	SER	2.2
1	b	177	LEU	2.2
1	s	214	ASN	2.2
1	4	161	GLN	2.2
1	p	145	ARG	2.2
1	f	53	ASN	2.2
1	x	54	ASP	2.1
1	u	178	THR	2.1
1	x	53	ASN	2.1
1	l	54	ASP	2.1
1	F	214	ASN	2.1
1	c	162	TYR	2.1
1	T	135	ASP	2.1
1	t	161	GLN	2.1
1	5	176	ARG	2.1
1	x	56	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	163	THR	2.1
1	R	132	THR	2.1
1	w	52	THR	2.1
1	9	135	ASP	2.1
1	w	145	ARG	2.1
1	5	135	ASP	2.1
1	b	176	ARG	2.0
1	4	173	LYS	2.0
1	W	176	ARG	2.0
1	w	163	THR	2.0
1	B	53	ASN	2.0
1	8	208	SER	2.0
1	r	133	ASP	2.0
1	I	214	ASN	2.0
1	R	213	GLU	2.0
1	C	130	ASP	2.0
1	S	178	THR	2.0
1	V	214	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.