



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:16 PM UTC

PDB ID : 9LGJ / pdb_00009lgj
EMDB ID : EMD-63067
Title : Cryo-EM structure of a designed AAV2-based vector
Authors : Luo, S.; Ke, X.; Zheng, Q.
Deposited on : 2025-01-10
Resolution : 2.58 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

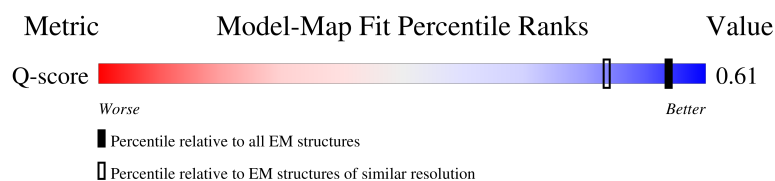
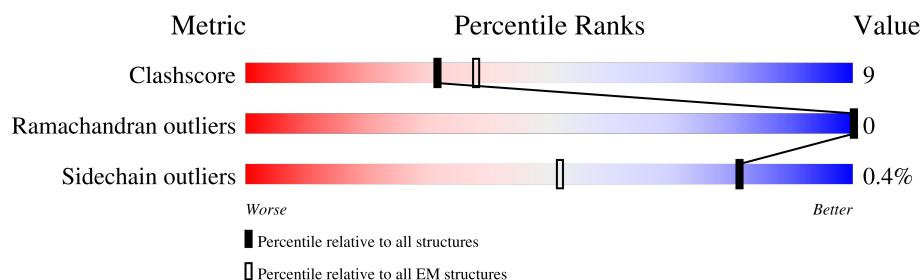
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.58 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.



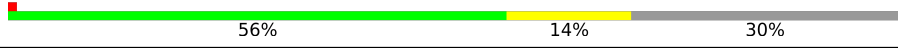
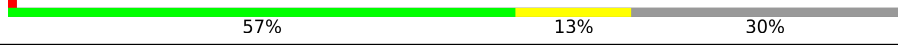
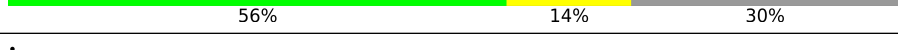
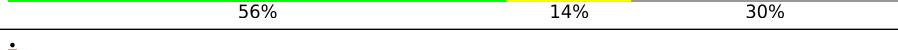
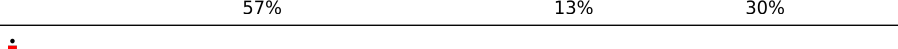
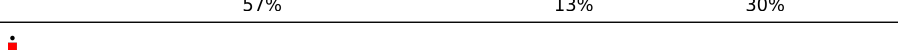
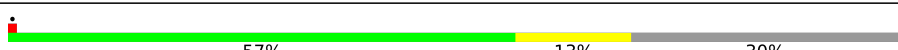
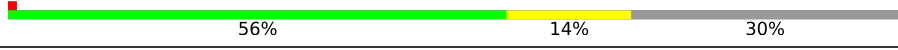
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7675 (2.08 - 3.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	743	
1	AA	743	
1	AB	743	
1	B	743	

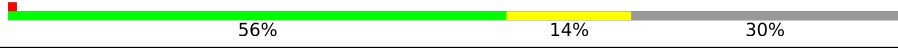
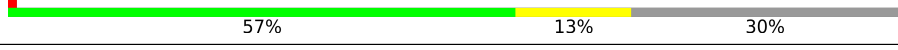
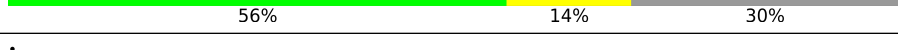
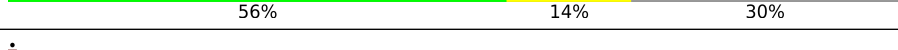
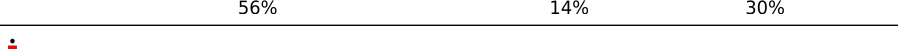
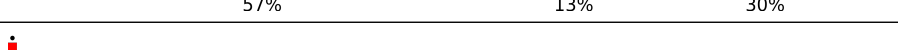
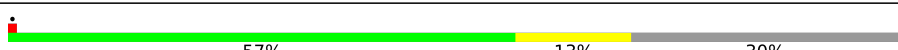
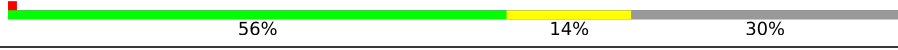
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Mol	Chain	Length	Quality of chain
1	BA	743	
1	BB	743	
1	C	743	
1	CA	743	
1	CB	743	
1	D	743	
1	DA	743	
1	DB	743	
1	E	743	
1	EA	743	
1	EB	743	
1	F	743	
1	FA	743	
1	FB	743	
1	G	743	
1	GA	743	
1	GB	743	
1	H	743	
1	HA	743	
1	HB	743	
1	I	743	
1	IA	743	
1	IB	743	
1	J	743	
1	JA	743	

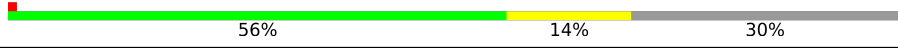
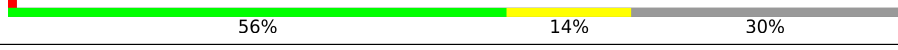
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Mol	Chain	Length	Quality of chain
1	K	743	
1	KA	743	
1	L	743	
1	LA	743	
1	M	743	
1	MA	743	
1	N	743	
1	NA	743	
1	O	743	
1	OA	743	
1	P	743	
1	PA	743	
1	Q	743	
1	QA	743	
1	R	743	
1	RA	743	
1	S	743	
1	SA	743	
1	T	743	
1	TA	743	
1	UA	743	
1	V	743	
1	VA	743	
1	W	743	
1	WA	743	

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Mol	Chain	Length	Quality of chain
1	X	743	
1	XA	743	
1	Y	743	
1	YA	743	
1	Z	743	
1	ZA	743	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 249660 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	B	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	C	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	D	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	E	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	F	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	G	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	H	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	I	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	J	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	K	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	L	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	M	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	N	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	O	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	P	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	Q	520	Total 4161	C 2616	N 726	O 806	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	S	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	T	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	V	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	W	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	X	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	Y	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	Z	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	AA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	BA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	CA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	DA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	EA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	FA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	GA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	HA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	IA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	JA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	KA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	LA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	MA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	NA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	OA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	PA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	QA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	RA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	SA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	TA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	UA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	VA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	WA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	XA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	YA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	ZA	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	AB	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	BB	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	CB	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	DB	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	EB	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	FB	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	GB	520	Total 4161	C 2616	N 726	O 806	S 13	0	0
1	HB	520	Total 4161	C 2616	N 726	O 806	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	IB	520	Total	C	N	O	S	0	0
			4161	2616	726	806	13		

There are 600 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	THR	ILE	engineered mutation	UNP P03135
A	588	ILE	-	insertion	UNP P03135
A	589	ALA	-	insertion	UNP P03135
A	590	ASP	-	insertion	UNP P03135
A	591	SER	-	insertion	UNP P03135
A	592	SER	-	insertion	UNP P03135
A	593	ARG	-	insertion	UNP P03135
A	594	THR	-	insertion	UNP P03135
A	595	SER	-	insertion	UNP P03135
A	716	ILE	VAL	engineered mutation	UNP P03135
B	240	THR	ILE	engineered mutation	UNP P03135
B	588	ILE	-	insertion	UNP P03135
B	589	ALA	-	insertion	UNP P03135
B	590	ASP	-	insertion	UNP P03135
B	591	SER	-	insertion	UNP P03135
B	592	SER	-	insertion	UNP P03135
B	593	ARG	-	insertion	UNP P03135
B	594	THR	-	insertion	UNP P03135
B	595	SER	-	insertion	UNP P03135
B	716	ILE	VAL	engineered mutation	UNP P03135
C	240	THR	ILE	engineered mutation	UNP P03135
C	588	ILE	-	insertion	UNP P03135
C	589	ALA	-	insertion	UNP P03135
C	590	ASP	-	insertion	UNP P03135
C	591	SER	-	insertion	UNP P03135
C	592	SER	-	insertion	UNP P03135
C	593	ARG	-	insertion	UNP P03135
C	594	THR	-	insertion	UNP P03135
C	595	SER	-	insertion	UNP P03135
C	716	ILE	VAL	engineered mutation	UNP P03135
D	240	THR	ILE	engineered mutation	UNP P03135
D	588	ILE	-	insertion	UNP P03135
D	589	ALA	-	insertion	UNP P03135
D	590	ASP	-	insertion	UNP P03135
D	591	SER	-	insertion	UNP P03135
D	592	SER	-	insertion	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
D	593	ARG	-	insertion	UNP P03135
D	594	THR	-	insertion	UNP P03135
D	595	SER	-	insertion	UNP P03135
D	716	ILE	VAL	engineered mutation	UNP P03135
E	240	THR	ILE	engineered mutation	UNP P03135
E	588	ILE	-	insertion	UNP P03135
E	589	ALA	-	insertion	UNP P03135
E	590	ASP	-	insertion	UNP P03135
E	591	SER	-	insertion	UNP P03135
E	592	SER	-	insertion	UNP P03135
E	593	ARG	-	insertion	UNP P03135
E	594	THR	-	insertion	UNP P03135
E	595	SER	-	insertion	UNP P03135
E	716	ILE	VAL	engineered mutation	UNP P03135
F	240	THR	ILE	engineered mutation	UNP P03135
F	588	ILE	-	insertion	UNP P03135
F	589	ALA	-	insertion	UNP P03135
F	590	ASP	-	insertion	UNP P03135
F	591	SER	-	insertion	UNP P03135
F	592	SER	-	insertion	UNP P03135
F	593	ARG	-	insertion	UNP P03135
F	594	THR	-	insertion	UNP P03135
F	595	SER	-	insertion	UNP P03135
F	716	ILE	VAL	engineered mutation	UNP P03135
G	240	THR	ILE	engineered mutation	UNP P03135
G	588	ILE	-	insertion	UNP P03135
G	589	ALA	-	insertion	UNP P03135
G	590	ASP	-	insertion	UNP P03135
G	591	SER	-	insertion	UNP P03135
G	592	SER	-	insertion	UNP P03135
G	593	ARG	-	insertion	UNP P03135
G	594	THR	-	insertion	UNP P03135
G	595	SER	-	insertion	UNP P03135
G	716	ILE	VAL	engineered mutation	UNP P03135
H	240	THR	ILE	engineered mutation	UNP P03135
H	588	ILE	-	insertion	UNP P03135
H	589	ALA	-	insertion	UNP P03135
H	590	ASP	-	insertion	UNP P03135
H	591	SER	-	insertion	UNP P03135
H	592	SER	-	insertion	UNP P03135
H	593	ARG	-	insertion	UNP P03135
H	594	THR	-	insertion	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
H	595	SER	-	insertion	UNP P03135
H	716	ILE	VAL	engineered mutation	UNP P03135
I	240	THR	ILE	engineered mutation	UNP P03135
I	588	ILE	-	insertion	UNP P03135
I	589	ALA	-	insertion	UNP P03135
I	590	ASP	-	insertion	UNP P03135
I	591	SER	-	insertion	UNP P03135
I	592	SER	-	insertion	UNP P03135
I	593	ARG	-	insertion	UNP P03135
I	594	THR	-	insertion	UNP P03135
I	595	SER	-	insertion	UNP P03135
I	716	ILE	VAL	engineered mutation	UNP P03135
J	240	THR	ILE	engineered mutation	UNP P03135
J	588	ILE	-	insertion	UNP P03135
J	589	ALA	-	insertion	UNP P03135
J	590	ASP	-	insertion	UNP P03135
J	591	SER	-	insertion	UNP P03135
J	592	SER	-	insertion	UNP P03135
J	593	ARG	-	insertion	UNP P03135
J	594	THR	-	insertion	UNP P03135
J	595	SER	-	insertion	UNP P03135
J	716	ILE	VAL	engineered mutation	UNP P03135
K	240	THR	ILE	engineered mutation	UNP P03135
K	588	ILE	-	insertion	UNP P03135
K	589	ALA	-	insertion	UNP P03135
K	590	ASP	-	insertion	UNP P03135
K	591	SER	-	insertion	UNP P03135
K	592	SER	-	insertion	UNP P03135
K	593	ARG	-	insertion	UNP P03135
K	594	THR	-	insertion	UNP P03135
K	595	SER	-	insertion	UNP P03135
K	716	ILE	VAL	engineered mutation	UNP P03135
L	240	THR	ILE	engineered mutation	UNP P03135
L	588	ILE	-	insertion	UNP P03135
L	589	ALA	-	insertion	UNP P03135
L	590	ASP	-	insertion	UNP P03135
L	591	SER	-	insertion	UNP P03135
L	592	SER	-	insertion	UNP P03135
L	593	ARG	-	insertion	UNP P03135
L	594	THR	-	insertion	UNP P03135
L	595	SER	-	insertion	UNP P03135
L	716	ILE	VAL	engineered mutation	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
M	240	THR	ILE	engineered mutation	UNP P03135
M	588	ILE	-	insertion	UNP P03135
M	589	ALA	-	insertion	UNP P03135
M	590	ASP	-	insertion	UNP P03135
M	591	SER	-	insertion	UNP P03135
M	592	SER	-	insertion	UNP P03135
M	593	ARG	-	insertion	UNP P03135
M	594	THR	-	insertion	UNP P03135
M	595	SER	-	insertion	UNP P03135
M	716	ILE	VAL	engineered mutation	UNP P03135
N	240	THR	ILE	engineered mutation	UNP P03135
N	588	ILE	-	insertion	UNP P03135
N	589	ALA	-	insertion	UNP P03135
N	590	ASP	-	insertion	UNP P03135
N	591	SER	-	insertion	UNP P03135
N	592	SER	-	insertion	UNP P03135
N	593	ARG	-	insertion	UNP P03135
N	594	THR	-	insertion	UNP P03135
N	595	SER	-	insertion	UNP P03135
N	716	ILE	VAL	engineered mutation	UNP P03135
O	240	THR	ILE	engineered mutation	UNP P03135
O	588	ILE	-	insertion	UNP P03135
O	589	ALA	-	insertion	UNP P03135
O	590	ASP	-	insertion	UNP P03135
O	591	SER	-	insertion	UNP P03135
O	592	SER	-	insertion	UNP P03135
O	593	ARG	-	insertion	UNP P03135
O	594	THR	-	insertion	UNP P03135
O	595	SER	-	insertion	UNP P03135
O	716	ILE	VAL	engineered mutation	UNP P03135
P	240	THR	ILE	engineered mutation	UNP P03135
P	588	ILE	-	insertion	UNP P03135
P	589	ALA	-	insertion	UNP P03135
P	590	ASP	-	insertion	UNP P03135
P	591	SER	-	insertion	UNP P03135
P	592	SER	-	insertion	UNP P03135
P	593	ARG	-	insertion	UNP P03135
P	594	THR	-	insertion	UNP P03135
P	595	SER	-	insertion	UNP P03135
P	716	ILE	VAL	engineered mutation	UNP P03135
Q	240	THR	ILE	engineered mutation	UNP P03135
Q	588	ILE	-	insertion	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	589	ALA	-	insertion	UNP P03135
Q	590	ASP	-	insertion	UNP P03135
Q	591	SER	-	insertion	UNP P03135
Q	592	SER	-	insertion	UNP P03135
Q	593	ARG	-	insertion	UNP P03135
Q	594	THR	-	insertion	UNP P03135
Q	595	SER	-	insertion	UNP P03135
Q	716	ILE	VAL	engineered mutation	UNP P03135
R	240	THR	ILE	engineered mutation	UNP P03135
R	588	ILE	-	insertion	UNP P03135
R	589	ALA	-	insertion	UNP P03135
R	590	ASP	-	insertion	UNP P03135
R	591	SER	-	insertion	UNP P03135
R	592	SER	-	insertion	UNP P03135
R	593	ARG	-	insertion	UNP P03135
R	594	THR	-	insertion	UNP P03135
R	595	SER	-	insertion	UNP P03135
R	716	ILE	VAL	engineered mutation	UNP P03135
S	240	THR	ILE	engineered mutation	UNP P03135
S	588	ILE	-	insertion	UNP P03135
S	589	ALA	-	insertion	UNP P03135
S	590	ASP	-	insertion	UNP P03135
S	591	SER	-	insertion	UNP P03135
S	592	SER	-	insertion	UNP P03135
S	593	ARG	-	insertion	UNP P03135
S	594	THR	-	insertion	UNP P03135
S	595	SER	-	insertion	UNP P03135
S	716	ILE	VAL	engineered mutation	UNP P03135
T	240	THR	ILE	engineered mutation	UNP P03135
T	588	ILE	-	insertion	UNP P03135
T	589	ALA	-	insertion	UNP P03135
T	590	ASP	-	insertion	UNP P03135
T	591	SER	-	insertion	UNP P03135
T	592	SER	-	insertion	UNP P03135
T	593	ARG	-	insertion	UNP P03135
T	594	THR	-	insertion	UNP P03135
T	595	SER	-	insertion	UNP P03135
T	716	ILE	VAL	engineered mutation	UNP P03135
V	240	THR	ILE	engineered mutation	UNP P03135
V	588	ILE	-	insertion	UNP P03135
V	589	ALA	-	insertion	UNP P03135
V	590	ASP	-	insertion	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
V	591	SER	-	insertion	UNP P03135
V	592	SER	-	insertion	UNP P03135
V	593	ARG	-	insertion	UNP P03135
V	594	THR	-	insertion	UNP P03135
V	595	SER	-	insertion	UNP P03135
V	716	ILE	VAL	engineered mutation	UNP P03135
W	240	THR	ILE	engineered mutation	UNP P03135
W	588	ILE	-	insertion	UNP P03135
W	589	ALA	-	insertion	UNP P03135
W	590	ASP	-	insertion	UNP P03135
W	591	SER	-	insertion	UNP P03135
W	592	SER	-	insertion	UNP P03135
W	593	ARG	-	insertion	UNP P03135
W	594	THR	-	insertion	UNP P03135
W	595	SER	-	insertion	UNP P03135
W	716	ILE	VAL	engineered mutation	UNP P03135
X	240	THR	ILE	engineered mutation	UNP P03135
X	588	ILE	-	insertion	UNP P03135
X	589	ALA	-	insertion	UNP P03135
X	590	ASP	-	insertion	UNP P03135
X	591	SER	-	insertion	UNP P03135
X	592	SER	-	insertion	UNP P03135
X	593	ARG	-	insertion	UNP P03135
X	594	THR	-	insertion	UNP P03135
X	595	SER	-	insertion	UNP P03135
X	716	ILE	VAL	engineered mutation	UNP P03135
Y	240	THR	ILE	engineered mutation	UNP P03135
Y	588	ILE	-	insertion	UNP P03135
Y	589	ALA	-	insertion	UNP P03135
Y	590	ASP	-	insertion	UNP P03135
Y	591	SER	-	insertion	UNP P03135
Y	592	SER	-	insertion	UNP P03135
Y	593	ARG	-	insertion	UNP P03135
Y	594	THR	-	insertion	UNP P03135
Y	595	SER	-	insertion	UNP P03135
Y	716	ILE	VAL	engineered mutation	UNP P03135
Z	240	THR	ILE	engineered mutation	UNP P03135
Z	588	ILE	-	insertion	UNP P03135
Z	589	ALA	-	insertion	UNP P03135
Z	590	ASP	-	insertion	UNP P03135
Z	591	SER	-	insertion	UNP P03135
Z	592	SER	-	insertion	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	593	ARG	-	insertion	UNP P03135
Z	594	THR	-	insertion	UNP P03135
Z	595	SER	-	insertion	UNP P03135
Z	716	ILE	VAL	engineered mutation	UNP P03135
AA	240	THR	ILE	engineered mutation	UNP P03135
AA	588	ILE	-	insertion	UNP P03135
AA	589	ALA	-	insertion	UNP P03135
AA	590	ASP	-	insertion	UNP P03135
AA	591	SER	-	insertion	UNP P03135
AA	592	SER	-	insertion	UNP P03135
AA	593	ARG	-	insertion	UNP P03135
AA	594	THR	-	insertion	UNP P03135
AA	595	SER	-	insertion	UNP P03135
AA	716	ILE	VAL	engineered mutation	UNP P03135
BA	240	THR	ILE	engineered mutation	UNP P03135
BA	588	ILE	-	insertion	UNP P03135
BA	589	ALA	-	insertion	UNP P03135
BA	590	ASP	-	insertion	UNP P03135
BA	591	SER	-	insertion	UNP P03135
BA	592	SER	-	insertion	UNP P03135
BA	593	ARG	-	insertion	UNP P03135
BA	594	THR	-	insertion	UNP P03135
BA	595	SER	-	insertion	UNP P03135
BA	716	ILE	VAL	engineered mutation	UNP P03135
CA	240	THR	ILE	engineered mutation	UNP P03135
CA	588	ILE	-	insertion	UNP P03135
CA	589	ALA	-	insertion	UNP P03135
CA	590	ASP	-	insertion	UNP P03135
CA	591	SER	-	insertion	UNP P03135
CA	592	SER	-	insertion	UNP P03135
CA	593	ARG	-	insertion	UNP P03135
CA	594	THR	-	insertion	UNP P03135
CA	595	SER	-	insertion	UNP P03135
CA	716	ILE	VAL	engineered mutation	UNP P03135
DA	240	THR	ILE	engineered mutation	UNP P03135
DA	588	ILE	-	insertion	UNP P03135
DA	589	ALA	-	insertion	UNP P03135
DA	590	ASP	-	insertion	UNP P03135
DA	591	SER	-	insertion	UNP P03135
DA	592	SER	-	insertion	UNP P03135
DA	593	ARG	-	insertion	UNP P03135
DA	594	THR	-	insertion	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
DA	595	SER	-	insertion	UNP P03135
DA	716	ILE	VAL	engineered mutation	UNP P03135
EA	240	THR	ILE	engineered mutation	UNP P03135
EA	588	ILE	-	insertion	UNP P03135
EA	589	ALA	-	insertion	UNP P03135
EA	590	ASP	-	insertion	UNP P03135
EA	591	SER	-	insertion	UNP P03135
EA	592	SER	-	insertion	UNP P03135
EA	593	ARG	-	insertion	UNP P03135
EA	594	THR	-	insertion	UNP P03135
EA	595	SER	-	insertion	UNP P03135
EA	716	ILE	VAL	engineered mutation	UNP P03135
FA	240	THR	ILE	engineered mutation	UNP P03135
FA	588	ILE	-	insertion	UNP P03135
FA	589	ALA	-	insertion	UNP P03135
FA	590	ASP	-	insertion	UNP P03135
FA	591	SER	-	insertion	UNP P03135
FA	592	SER	-	insertion	UNP P03135
FA	593	ARG	-	insertion	UNP P03135
FA	594	THR	-	insertion	UNP P03135
FA	595	SER	-	insertion	UNP P03135
FA	716	ILE	VAL	engineered mutation	UNP P03135
GA	240	THR	ILE	engineered mutation	UNP P03135
GA	588	ILE	-	insertion	UNP P03135
GA	589	ALA	-	insertion	UNP P03135
GA	590	ASP	-	insertion	UNP P03135
GA	591	SER	-	insertion	UNP P03135
GA	592	SER	-	insertion	UNP P03135
GA	593	ARG	-	insertion	UNP P03135
GA	594	THR	-	insertion	UNP P03135
GA	595	SER	-	insertion	UNP P03135
GA	716	ILE	VAL	engineered mutation	UNP P03135
HA	240	THR	ILE	engineered mutation	UNP P03135
HA	588	ILE	-	insertion	UNP P03135
HA	589	ALA	-	insertion	UNP P03135
HA	590	ASP	-	insertion	UNP P03135
HA	591	SER	-	insertion	UNP P03135
HA	592	SER	-	insertion	UNP P03135
HA	593	ARG	-	insertion	UNP P03135
HA	594	THR	-	insertion	UNP P03135
HA	595	SER	-	insertion	UNP P03135
HA	716	ILE	VAL	engineered mutation	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
IA	240	THR	ILE	engineered mutation	UNP P03135
IA	588	ILE	-	insertion	UNP P03135
IA	589	ALA	-	insertion	UNP P03135
IA	590	ASP	-	insertion	UNP P03135
IA	591	SER	-	insertion	UNP P03135
IA	592	SER	-	insertion	UNP P03135
IA	593	ARG	-	insertion	UNP P03135
IA	594	THR	-	insertion	UNP P03135
IA	595	SER	-	insertion	UNP P03135
IA	716	ILE	VAL	engineered mutation	UNP P03135
JA	240	THR	ILE	engineered mutation	UNP P03135
JA	588	ILE	-	insertion	UNP P03135
JA	589	ALA	-	insertion	UNP P03135
JA	590	ASP	-	insertion	UNP P03135
JA	591	SER	-	insertion	UNP P03135
JA	592	SER	-	insertion	UNP P03135
JA	593	ARG	-	insertion	UNP P03135
JA	594	THR	-	insertion	UNP P03135
JA	595	SER	-	insertion	UNP P03135
JA	716	ILE	VAL	engineered mutation	UNP P03135
KA	240	THR	ILE	engineered mutation	UNP P03135
KA	588	ILE	-	insertion	UNP P03135
KA	589	ALA	-	insertion	UNP P03135
KA	590	ASP	-	insertion	UNP P03135
KA	591	SER	-	insertion	UNP P03135
KA	592	SER	-	insertion	UNP P03135
KA	593	ARG	-	insertion	UNP P03135
KA	594	THR	-	insertion	UNP P03135
KA	595	SER	-	insertion	UNP P03135
KA	716	ILE	VAL	engineered mutation	UNP P03135
LA	240	THR	ILE	engineered mutation	UNP P03135
LA	588	ILE	-	insertion	UNP P03135
LA	589	ALA	-	insertion	UNP P03135
LA	590	ASP	-	insertion	UNP P03135
LA	591	SER	-	insertion	UNP P03135
LA	592	SER	-	insertion	UNP P03135
LA	593	ARG	-	insertion	UNP P03135
LA	594	THR	-	insertion	UNP P03135
LA	595	SER	-	insertion	UNP P03135
LA	716	ILE	VAL	engineered mutation	UNP P03135
MA	240	THR	ILE	engineered mutation	UNP P03135
MA	588	ILE	-	insertion	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
MA	589	ALA	-	insertion	UNP P03135
MA	590	ASP	-	insertion	UNP P03135
MA	591	SER	-	insertion	UNP P03135
MA	592	SER	-	insertion	UNP P03135
MA	593	ARG	-	insertion	UNP P03135
MA	594	THR	-	insertion	UNP P03135
MA	595	SER	-	insertion	UNP P03135
MA	716	ILE	VAL	engineered mutation	UNP P03135
NA	240	THR	ILE	engineered mutation	UNP P03135
NA	588	ILE	-	insertion	UNP P03135
NA	589	ALA	-	insertion	UNP P03135
NA	590	ASP	-	insertion	UNP P03135
NA	591	SER	-	insertion	UNP P03135
NA	592	SER	-	insertion	UNP P03135
NA	593	ARG	-	insertion	UNP P03135
NA	594	THR	-	insertion	UNP P03135
NA	595	SER	-	insertion	UNP P03135
NA	716	ILE	VAL	engineered mutation	UNP P03135
OA	240	THR	ILE	engineered mutation	UNP P03135
OA	588	ILE	-	insertion	UNP P03135
OA	589	ALA	-	insertion	UNP P03135
OA	590	ASP	-	insertion	UNP P03135
OA	591	SER	-	insertion	UNP P03135
OA	592	SER	-	insertion	UNP P03135
OA	593	ARG	-	insertion	UNP P03135
OA	594	THR	-	insertion	UNP P03135
OA	595	SER	-	insertion	UNP P03135
OA	716	ILE	VAL	engineered mutation	UNP P03135
PA	240	THR	ILE	engineered mutation	UNP P03135
PA	588	ILE	-	insertion	UNP P03135
PA	589	ALA	-	insertion	UNP P03135
PA	590	ASP	-	insertion	UNP P03135
PA	591	SER	-	insertion	UNP P03135
PA	592	SER	-	insertion	UNP P03135
PA	593	ARG	-	insertion	UNP P03135
PA	594	THR	-	insertion	UNP P03135
PA	595	SER	-	insertion	UNP P03135
PA	716	ILE	VAL	engineered mutation	UNP P03135
QA	240	THR	ILE	engineered mutation	UNP P03135
QA	588	ILE	-	insertion	UNP P03135
QA	589	ALA	-	insertion	UNP P03135
QA	590	ASP	-	insertion	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
QA	591	SER	-	insertion	UNP P03135
QA	592	SER	-	insertion	UNP P03135
QA	593	ARG	-	insertion	UNP P03135
QA	594	THR	-	insertion	UNP P03135
QA	595	SER	-	insertion	UNP P03135
QA	716	ILE	VAL	engineered mutation	UNP P03135
RA	240	THR	ILE	engineered mutation	UNP P03135
RA	588	ILE	-	insertion	UNP P03135
RA	589	ALA	-	insertion	UNP P03135
RA	590	ASP	-	insertion	UNP P03135
RA	591	SER	-	insertion	UNP P03135
RA	592	SER	-	insertion	UNP P03135
RA	593	ARG	-	insertion	UNP P03135
RA	594	THR	-	insertion	UNP P03135
RA	595	SER	-	insertion	UNP P03135
RA	716	ILE	VAL	engineered mutation	UNP P03135
SA	240	THR	ILE	engineered mutation	UNP P03135
SA	588	ILE	-	insertion	UNP P03135
SA	589	ALA	-	insertion	UNP P03135
SA	590	ASP	-	insertion	UNP P03135
SA	591	SER	-	insertion	UNP P03135
SA	592	SER	-	insertion	UNP P03135
SA	593	ARG	-	insertion	UNP P03135
SA	594	THR	-	insertion	UNP P03135
SA	595	SER	-	insertion	UNP P03135
SA	716	ILE	VAL	engineered mutation	UNP P03135
TA	240	THR	ILE	engineered mutation	UNP P03135
TA	588	ILE	-	insertion	UNP P03135
TA	589	ALA	-	insertion	UNP P03135
TA	590	ASP	-	insertion	UNP P03135
TA	591	SER	-	insertion	UNP P03135
TA	592	SER	-	insertion	UNP P03135
TA	593	ARG	-	insertion	UNP P03135
TA	594	THR	-	insertion	UNP P03135
TA	595	SER	-	insertion	UNP P03135
TA	716	ILE	VAL	engineered mutation	UNP P03135
UA	240	THR	ILE	engineered mutation	UNP P03135
UA	588	ILE	-	insertion	UNP P03135
UA	589	ALA	-	insertion	UNP P03135
UA	590	ASP	-	insertion	UNP P03135
UA	591	SER	-	insertion	UNP P03135
UA	592	SER	-	insertion	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
UA	593	ARG	-	insertion	UNP P03135
UA	594	THR	-	insertion	UNP P03135
UA	595	SER	-	insertion	UNP P03135
UA	716	ILE	VAL	engineered mutation	UNP P03135
VA	240	THR	ILE	engineered mutation	UNP P03135
VA	588	ILE	-	insertion	UNP P03135
VA	589	ALA	-	insertion	UNP P03135
VA	590	ASP	-	insertion	UNP P03135
VA	591	SER	-	insertion	UNP P03135
VA	592	SER	-	insertion	UNP P03135
VA	593	ARG	-	insertion	UNP P03135
VA	594	THR	-	insertion	UNP P03135
VA	595	SER	-	insertion	UNP P03135
VA	716	ILE	VAL	engineered mutation	UNP P03135
WA	240	THR	ILE	engineered mutation	UNP P03135
WA	588	ILE	-	insertion	UNP P03135
WA	589	ALA	-	insertion	UNP P03135
WA	590	ASP	-	insertion	UNP P03135
WA	591	SER	-	insertion	UNP P03135
WA	592	SER	-	insertion	UNP P03135
WA	593	ARG	-	insertion	UNP P03135
WA	594	THR	-	insertion	UNP P03135
WA	595	SER	-	insertion	UNP P03135
WA	716	ILE	VAL	engineered mutation	UNP P03135
XA	240	THR	ILE	engineered mutation	UNP P03135
XA	588	ILE	-	insertion	UNP P03135
XA	589	ALA	-	insertion	UNP P03135
XA	590	ASP	-	insertion	UNP P03135
XA	591	SER	-	insertion	UNP P03135
XA	592	SER	-	insertion	UNP P03135
XA	593	ARG	-	insertion	UNP P03135
XA	594	THR	-	insertion	UNP P03135
XA	595	SER	-	insertion	UNP P03135
XA	716	ILE	VAL	engineered mutation	UNP P03135
YA	240	THR	ILE	engineered mutation	UNP P03135
YA	588	ILE	-	insertion	UNP P03135
YA	589	ALA	-	insertion	UNP P03135
YA	590	ASP	-	insertion	UNP P03135
YA	591	SER	-	insertion	UNP P03135
YA	592	SER	-	insertion	UNP P03135
YA	593	ARG	-	insertion	UNP P03135
YA	594	THR	-	insertion	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
YA	595	SER	-	insertion	UNP P03135
YA	716	ILE	VAL	engineered mutation	UNP P03135
ZA	240	THR	ILE	engineered mutation	UNP P03135
ZA	588	ILE	-	insertion	UNP P03135
ZA	589	ALA	-	insertion	UNP P03135
ZA	590	ASP	-	insertion	UNP P03135
ZA	591	SER	-	insertion	UNP P03135
ZA	592	SER	-	insertion	UNP P03135
ZA	593	ARG	-	insertion	UNP P03135
ZA	594	THR	-	insertion	UNP P03135
ZA	595	SER	-	insertion	UNP P03135
ZA	716	ILE	VAL	engineered mutation	UNP P03135
AB	240	THR	ILE	engineered mutation	UNP P03135
AB	588	ILE	-	insertion	UNP P03135
AB	589	ALA	-	insertion	UNP P03135
AB	590	ASP	-	insertion	UNP P03135
AB	591	SER	-	insertion	UNP P03135
AB	592	SER	-	insertion	UNP P03135
AB	593	ARG	-	insertion	UNP P03135
AB	594	THR	-	insertion	UNP P03135
AB	595	SER	-	insertion	UNP P03135
AB	716	ILE	VAL	engineered mutation	UNP P03135
BB	240	THR	ILE	engineered mutation	UNP P03135
BB	588	ILE	-	insertion	UNP P03135
BB	589	ALA	-	insertion	UNP P03135
BB	590	ASP	-	insertion	UNP P03135
BB	591	SER	-	insertion	UNP P03135
BB	592	SER	-	insertion	UNP P03135
BB	593	ARG	-	insertion	UNP P03135
BB	594	THR	-	insertion	UNP P03135
BB	595	SER	-	insertion	UNP P03135
BB	716	ILE	VAL	engineered mutation	UNP P03135
CB	240	THR	ILE	engineered mutation	UNP P03135
CB	588	ILE	-	insertion	UNP P03135
CB	589	ALA	-	insertion	UNP P03135
CB	590	ASP	-	insertion	UNP P03135
CB	591	SER	-	insertion	UNP P03135
CB	592	SER	-	insertion	UNP P03135
CB	593	ARG	-	insertion	UNP P03135
CB	594	THR	-	insertion	UNP P03135
CB	595	SER	-	insertion	UNP P03135
CB	716	ILE	VAL	engineered mutation	UNP P03135

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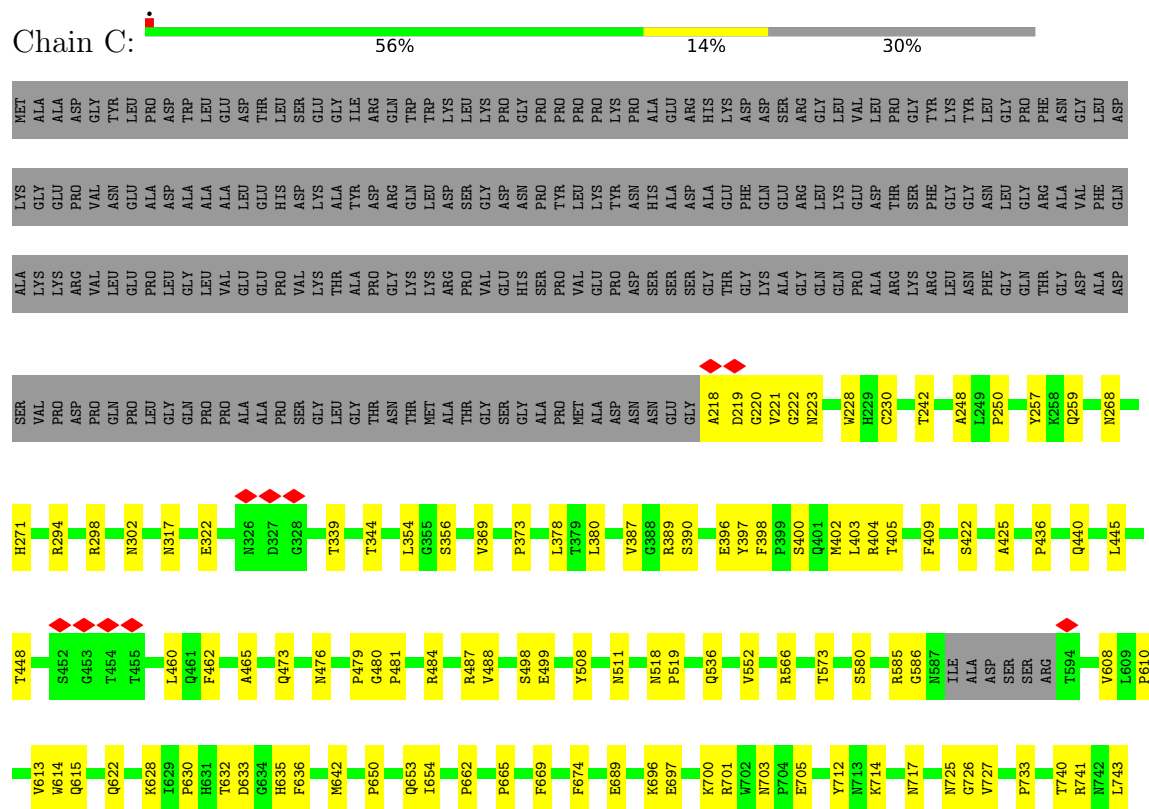
Chain	Residue	Modelled	Actual	Comment	Reference
DB	240	THR	ILE	engineered mutation	UNP P03135
DB	588	ILE	-	insertion	UNP P03135
DB	589	ALA	-	insertion	UNP P03135
DB	590	ASP	-	insertion	UNP P03135
DB	591	SER	-	insertion	UNP P03135
DB	592	SER	-	insertion	UNP P03135
DB	593	ARG	-	insertion	UNP P03135
DB	594	THR	-	insertion	UNP P03135
DB	595	SER	-	insertion	UNP P03135
DB	716	ILE	VAL	engineered mutation	UNP P03135
EB	240	THR	ILE	engineered mutation	UNP P03135
EB	588	ILE	-	insertion	UNP P03135
EB	589	ALA	-	insertion	UNP P03135
EB	590	ASP	-	insertion	UNP P03135
EB	591	SER	-	insertion	UNP P03135
EB	592	SER	-	insertion	UNP P03135
EB	593	ARG	-	insertion	UNP P03135
EB	594	THR	-	insertion	UNP P03135
EB	595	SER	-	insertion	UNP P03135
EB	716	ILE	VAL	engineered mutation	UNP P03135
FB	240	THR	ILE	engineered mutation	UNP P03135
FB	588	ILE	-	insertion	UNP P03135
FB	589	ALA	-	insertion	UNP P03135
FB	590	ASP	-	insertion	UNP P03135
FB	591	SER	-	insertion	UNP P03135
FB	592	SER	-	insertion	UNP P03135
FB	593	ARG	-	insertion	UNP P03135
FB	594	THR	-	insertion	UNP P03135
FB	595	SER	-	insertion	UNP P03135
FB	716	ILE	VAL	engineered mutation	UNP P03135
GB	240	THR	ILE	engineered mutation	UNP P03135
GB	588	ILE	-	insertion	UNP P03135
GB	589	ALA	-	insertion	UNP P03135
GB	590	ASP	-	insertion	UNP P03135
GB	591	SER	-	insertion	UNP P03135
GB	592	SER	-	insertion	UNP P03135
GB	593	ARG	-	insertion	UNP P03135
GB	594	THR	-	insertion	UNP P03135
GB	595	SER	-	insertion	UNP P03135
GB	716	ILE	VAL	engineered mutation	UNP P03135
HB	240	THR	ILE	engineered mutation	UNP P03135
HB	588	ILE	-	insertion	UNP P03135

Continued on next page...

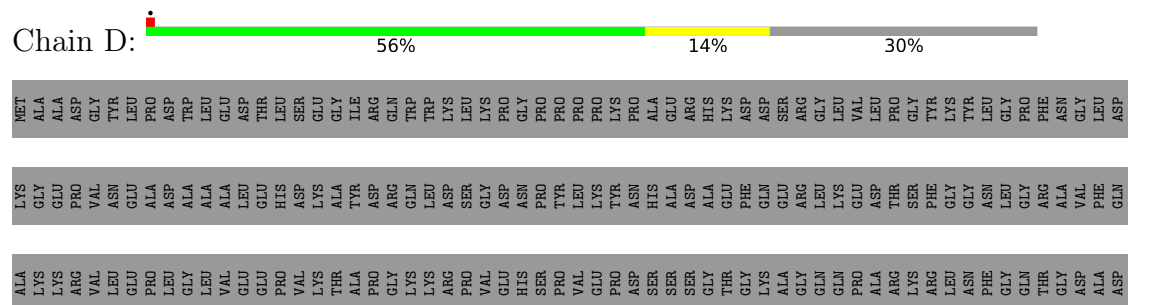
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Chain	Residue	Modelled	Actual	Comment	Reference
HB	589	ALA	-	insertion	UNP P03135
HB	590	ASP	-	insertion	UNP P03135
HB	591	SER	-	insertion	UNP P03135
HB	592	SER	-	insertion	UNP P03135
HB	593	ARG	-	insertion	UNP P03135
HB	594	THR	-	insertion	UNP P03135
HB	595	SER	-	insertion	UNP P03135
HB	716	ILE	VAL	engineered mutation	UNP P03135
IB	240	THR	ILE	engineered mutation	UNP P03135
IB	588	ILE	-	insertion	UNP P03135
IB	589	ALA	-	insertion	UNP P03135
IB	590	ASP	-	insertion	UNP P03135
IB	591	SER	-	insertion	UNP P03135
IB	592	SER	-	insertion	UNP P03135
IB	593	ARG	-	insertion	UNP P03135
IB	594	THR	-	insertion	UNP P03135
IB	595	SER	-	insertion	UNP P03135
IB	716	ILE	VAL	engineered mutation	UNP P03135

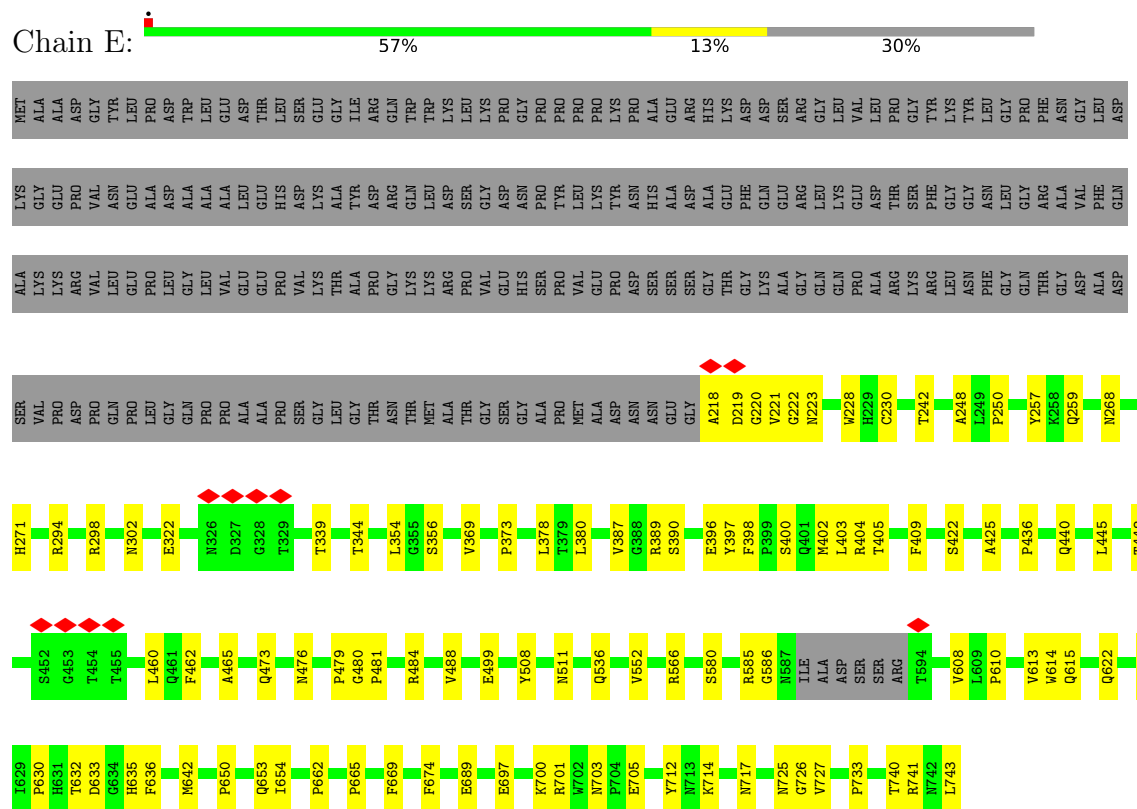
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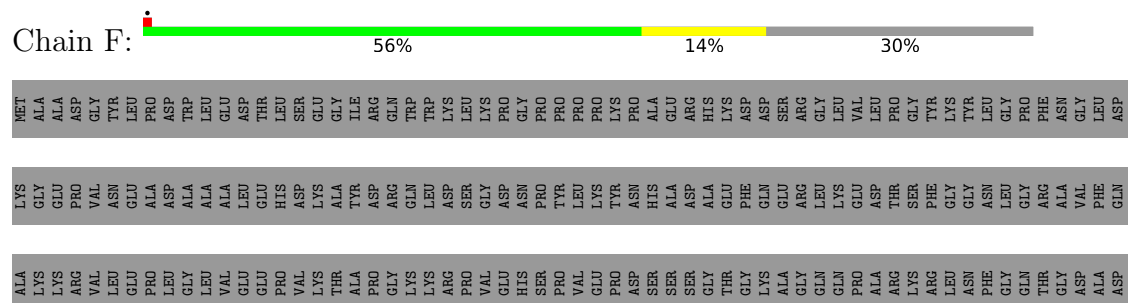
- Molecule 1: Capsid protein VP1



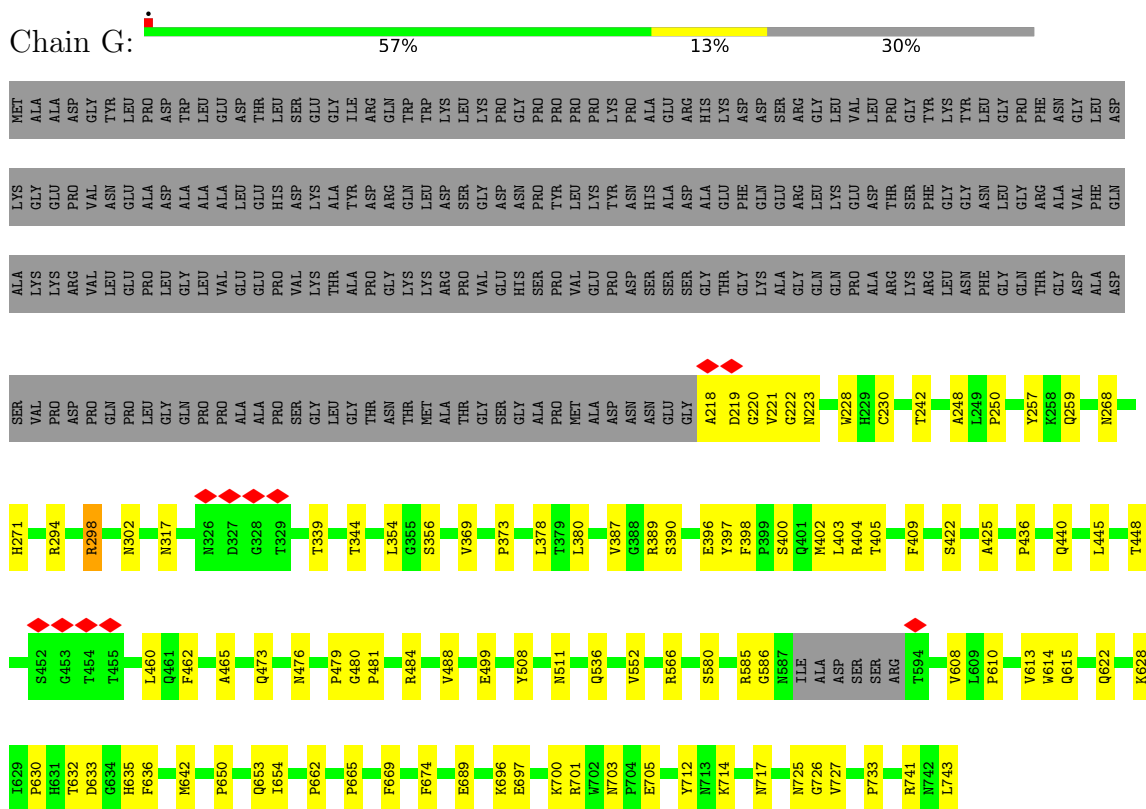
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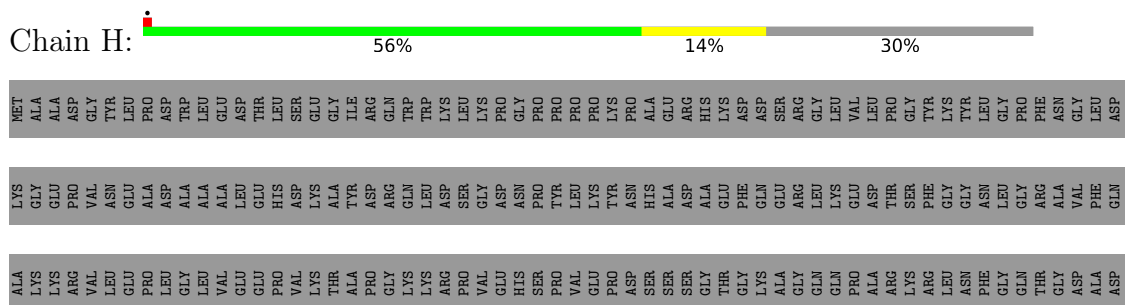
- Molecule 1: Capsid protein VP1



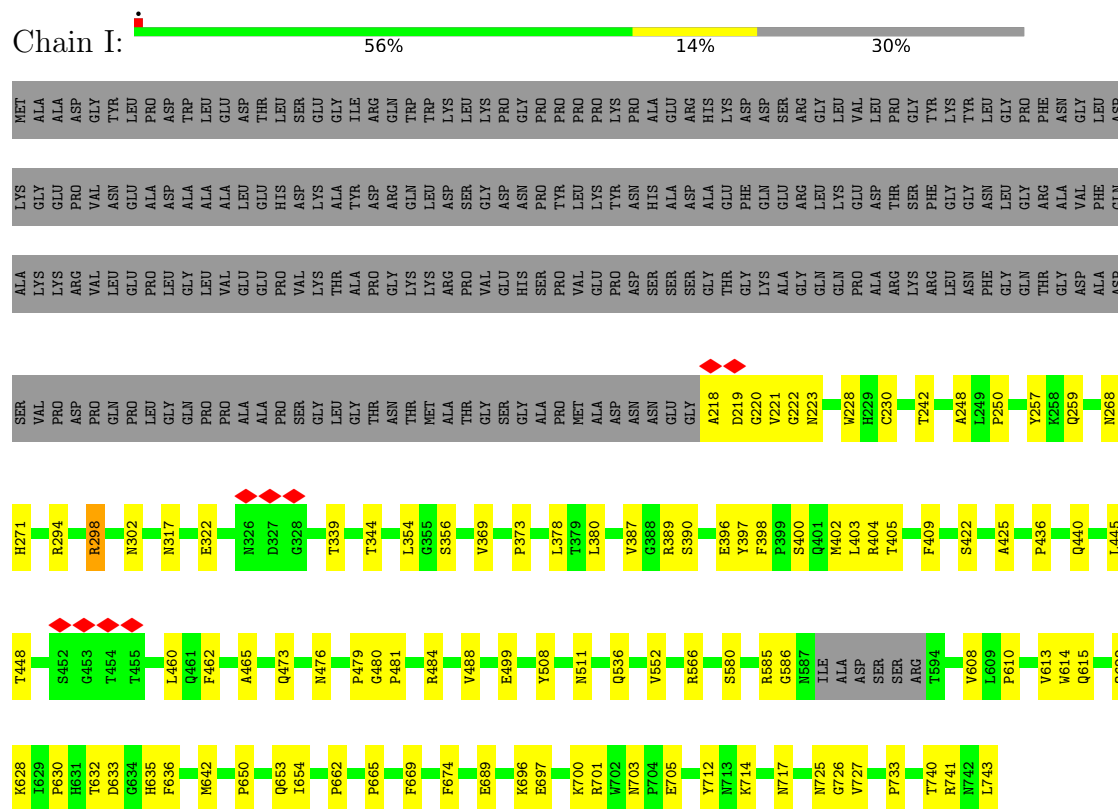
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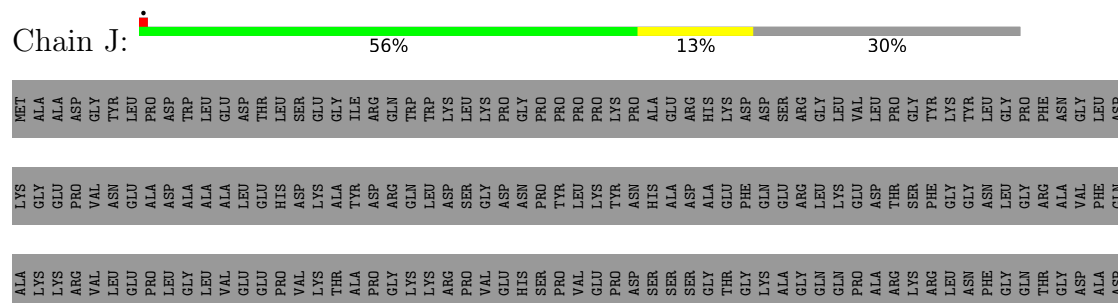
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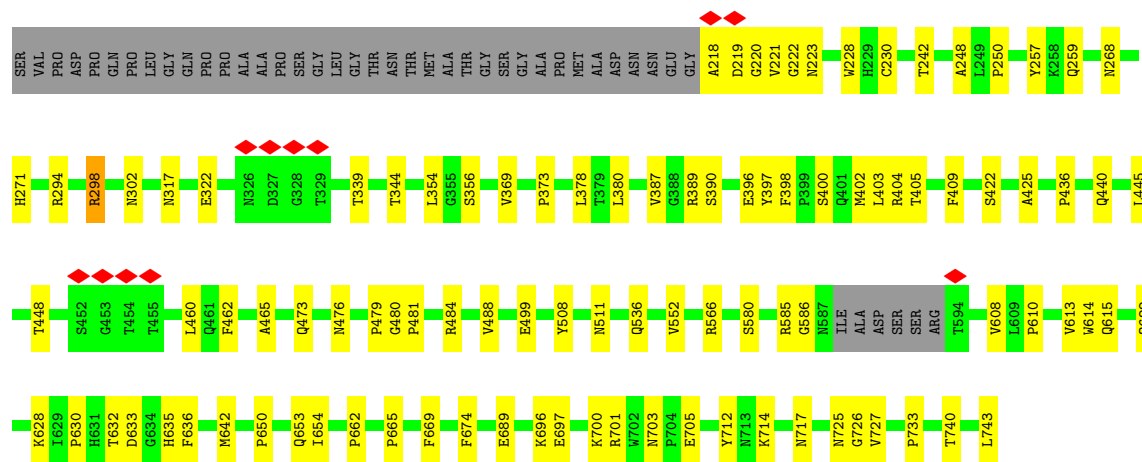


- Molecule 1: Capsid protein VP1



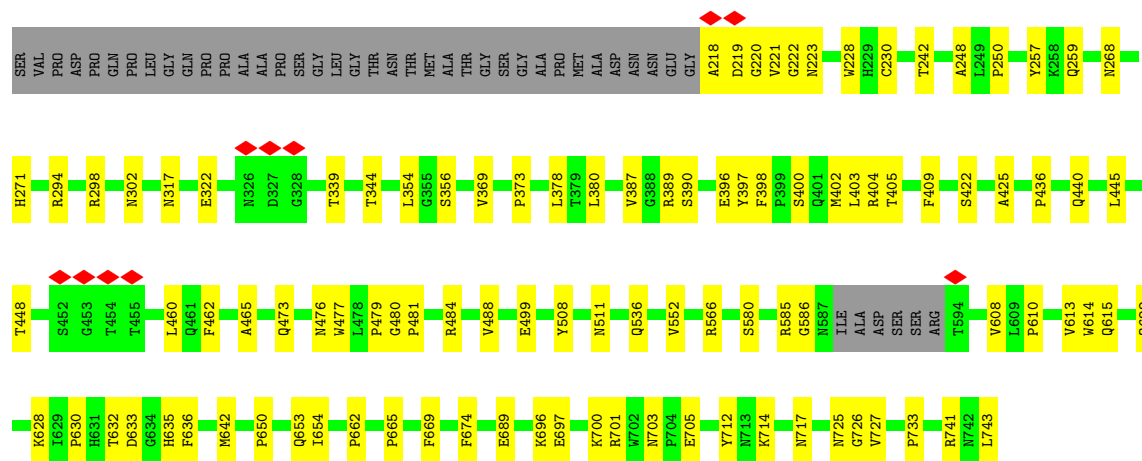
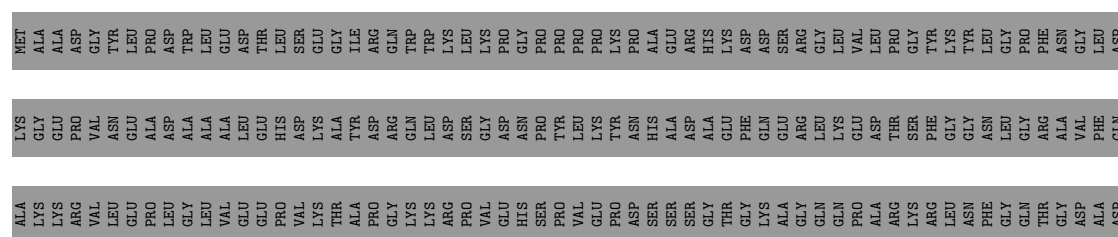
- Molecule 1: Capsid protein VP1





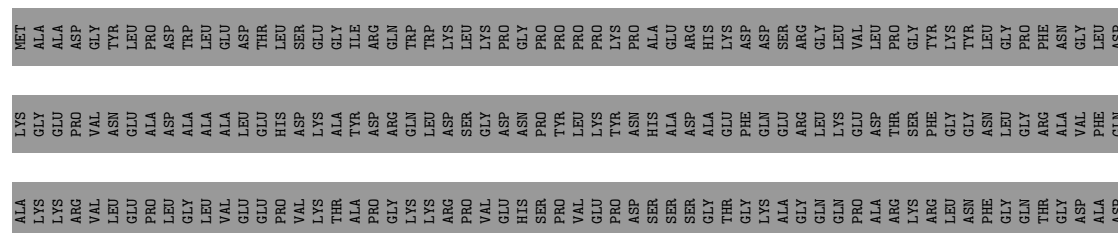
• Molecule 1: Capsid protein VP1

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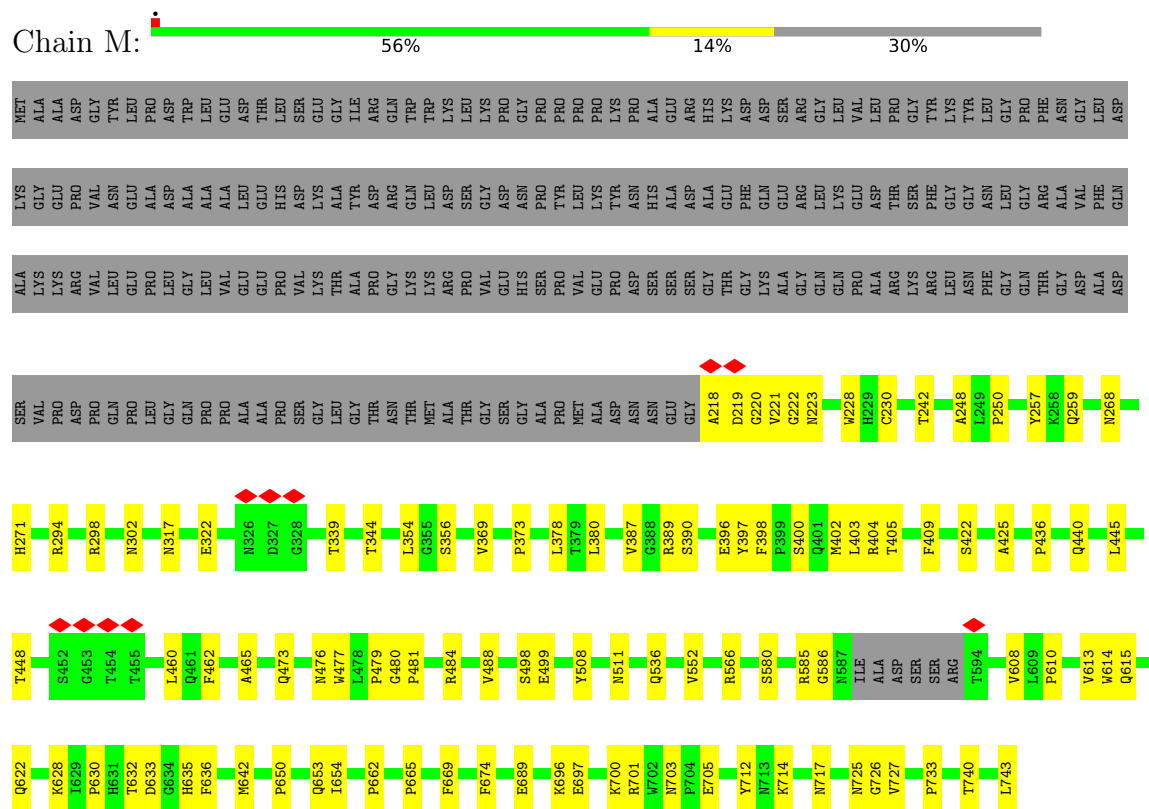


• Molecule 1: Capsid protein VP1

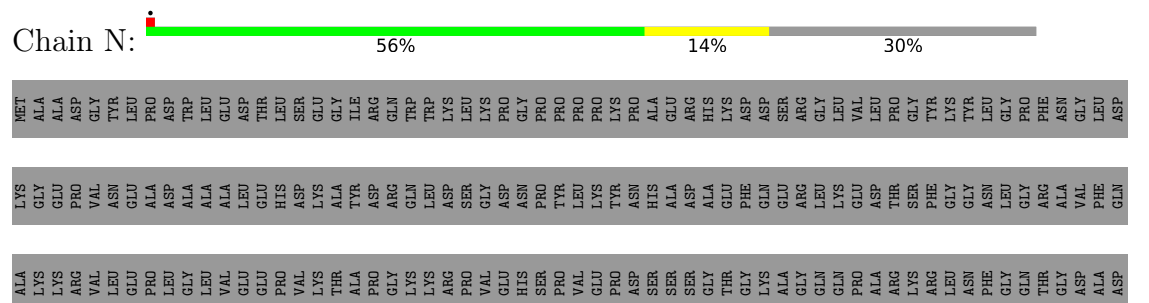
Chain L: 56% 14% 30%

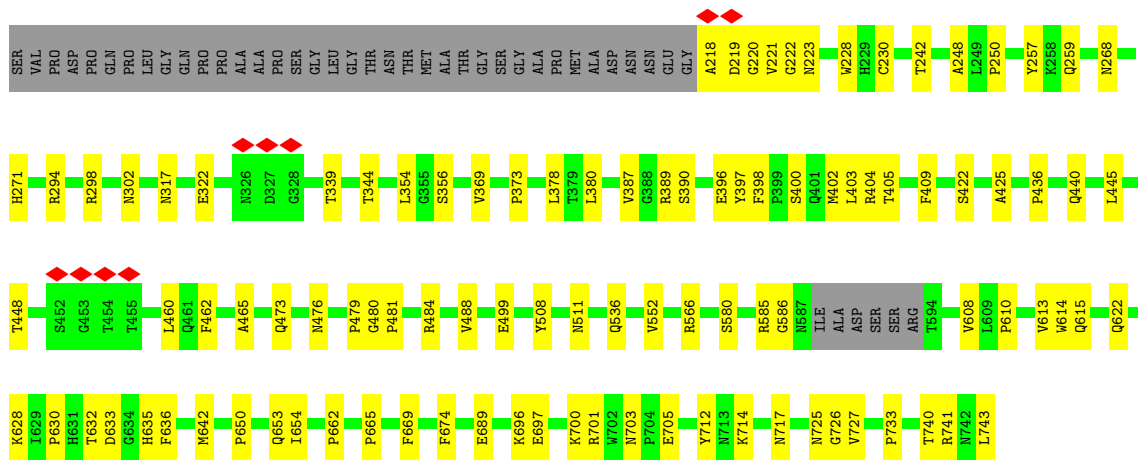


- Molecule 1: Capsid protein VP1

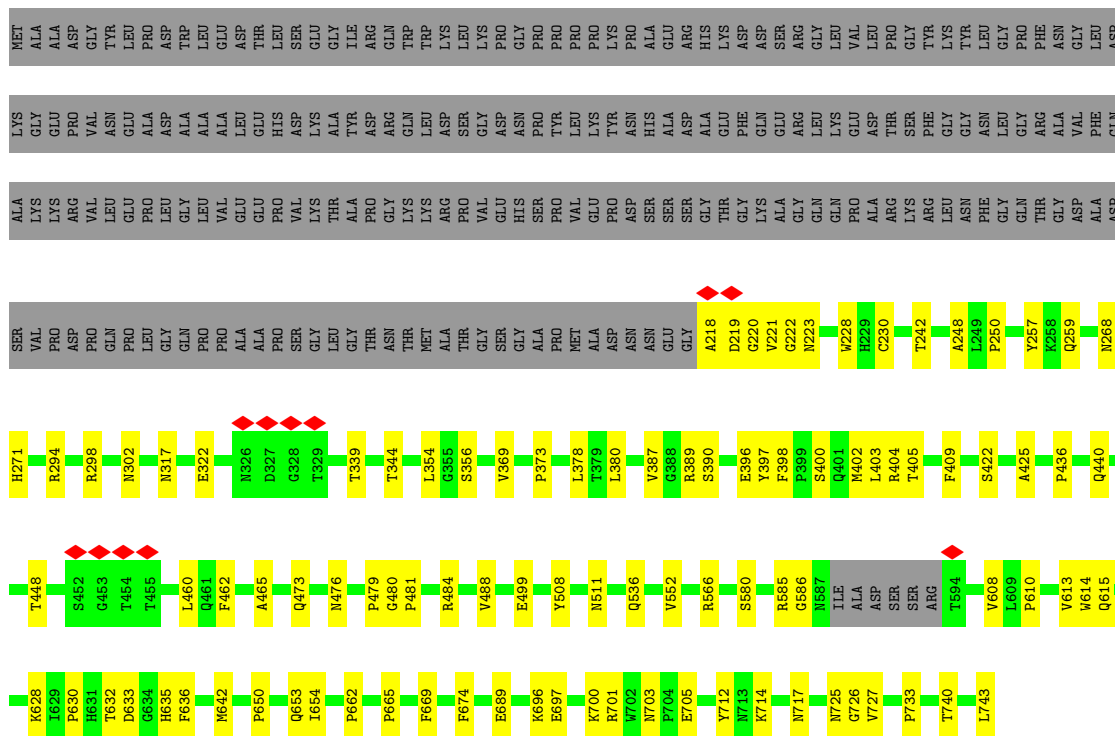


- Molecule 1: Capsid protein VP1

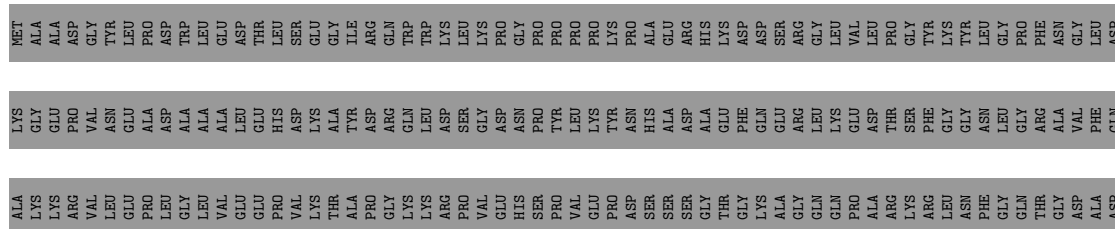


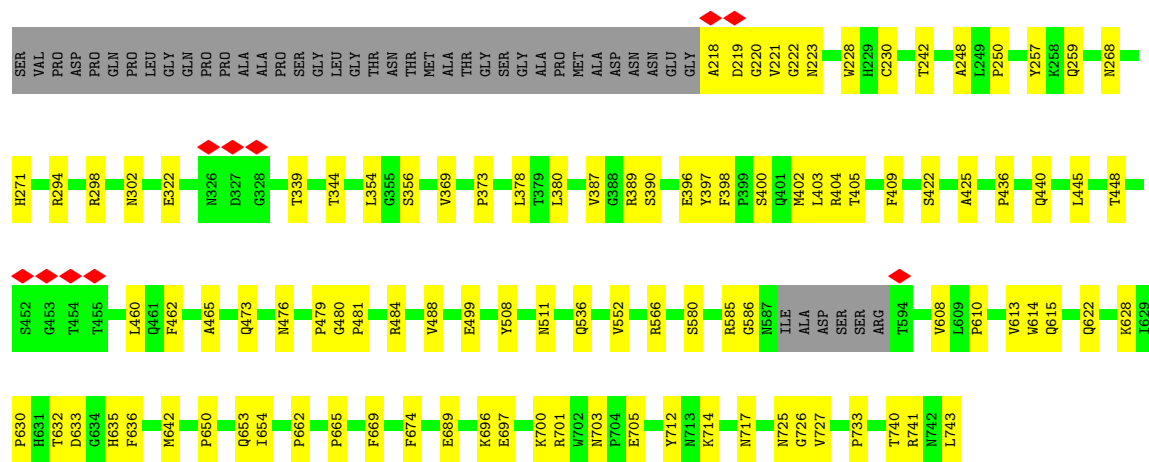


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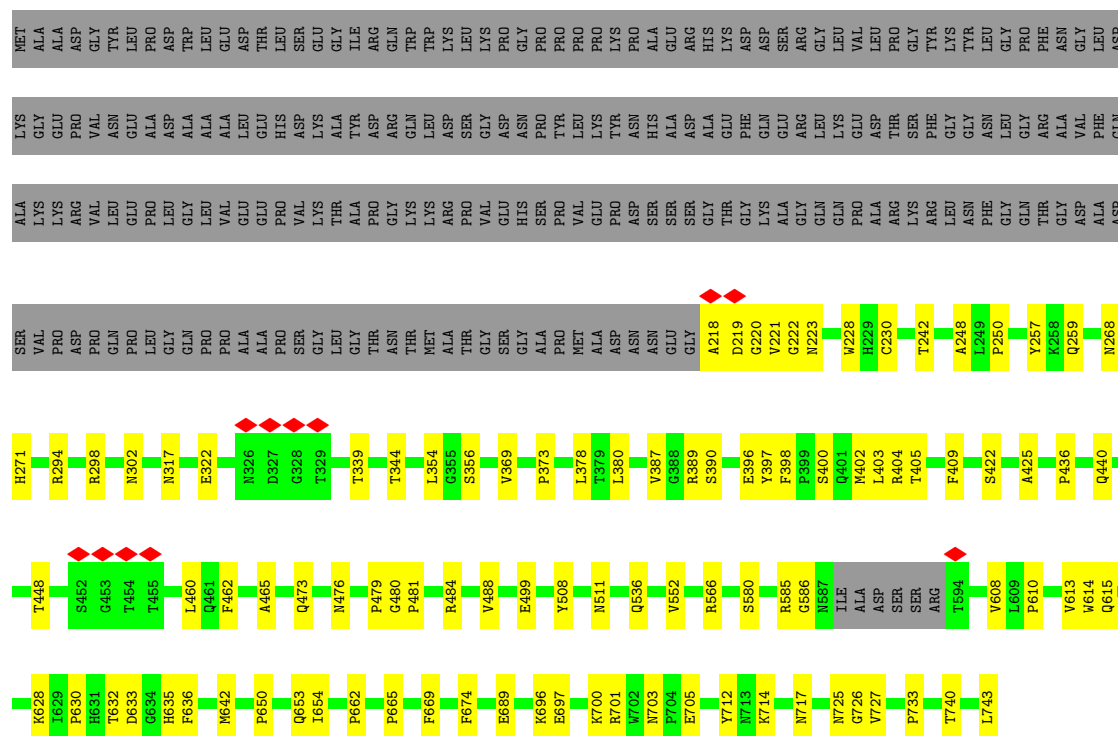


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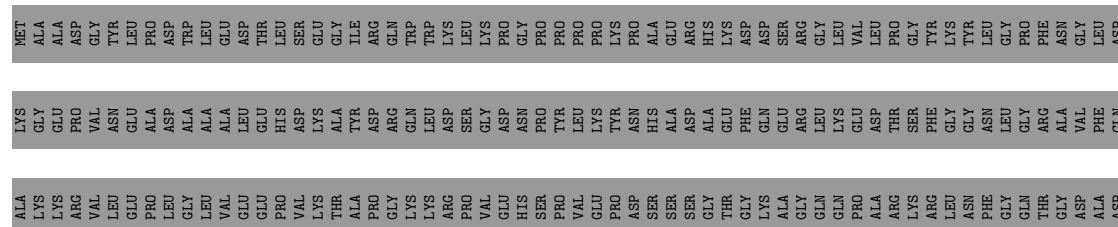




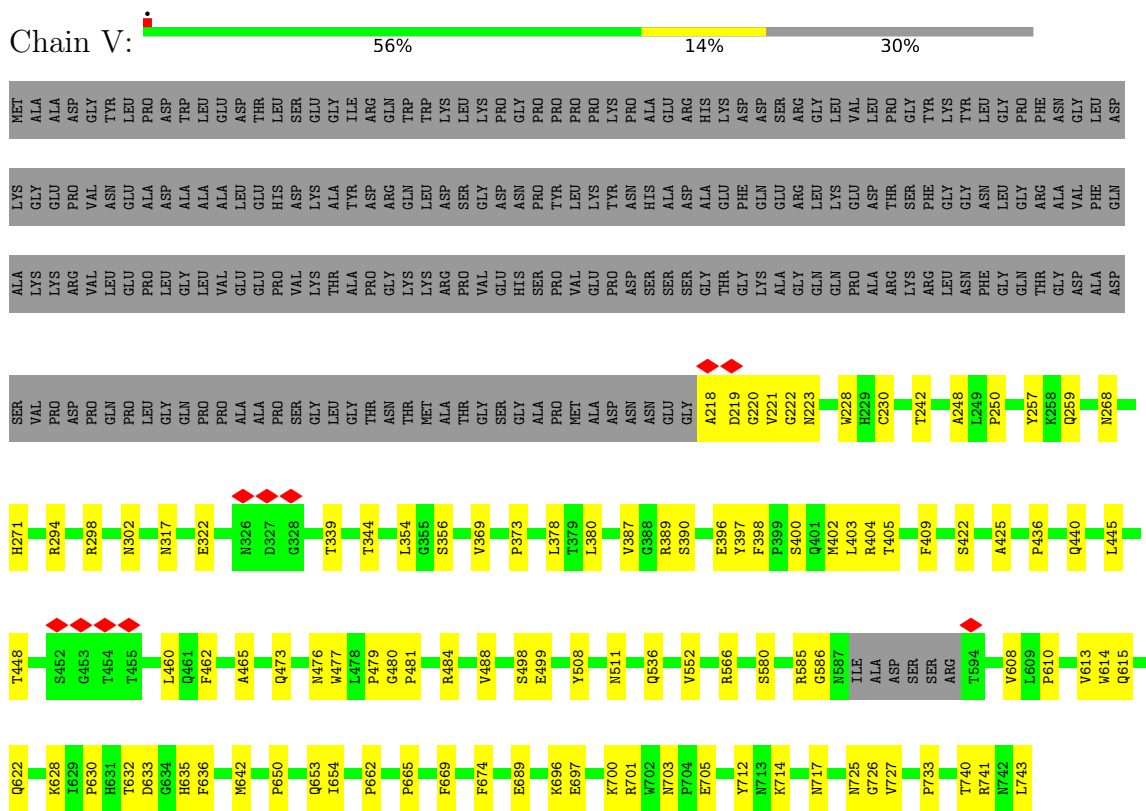
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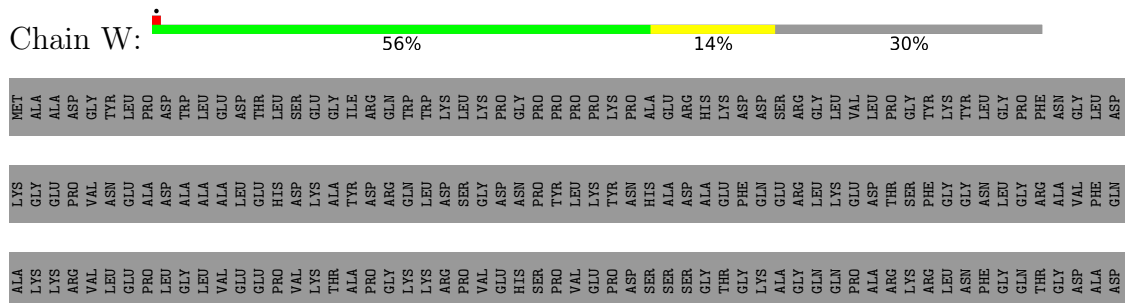
• Molecule 1: Capsid protein VP1



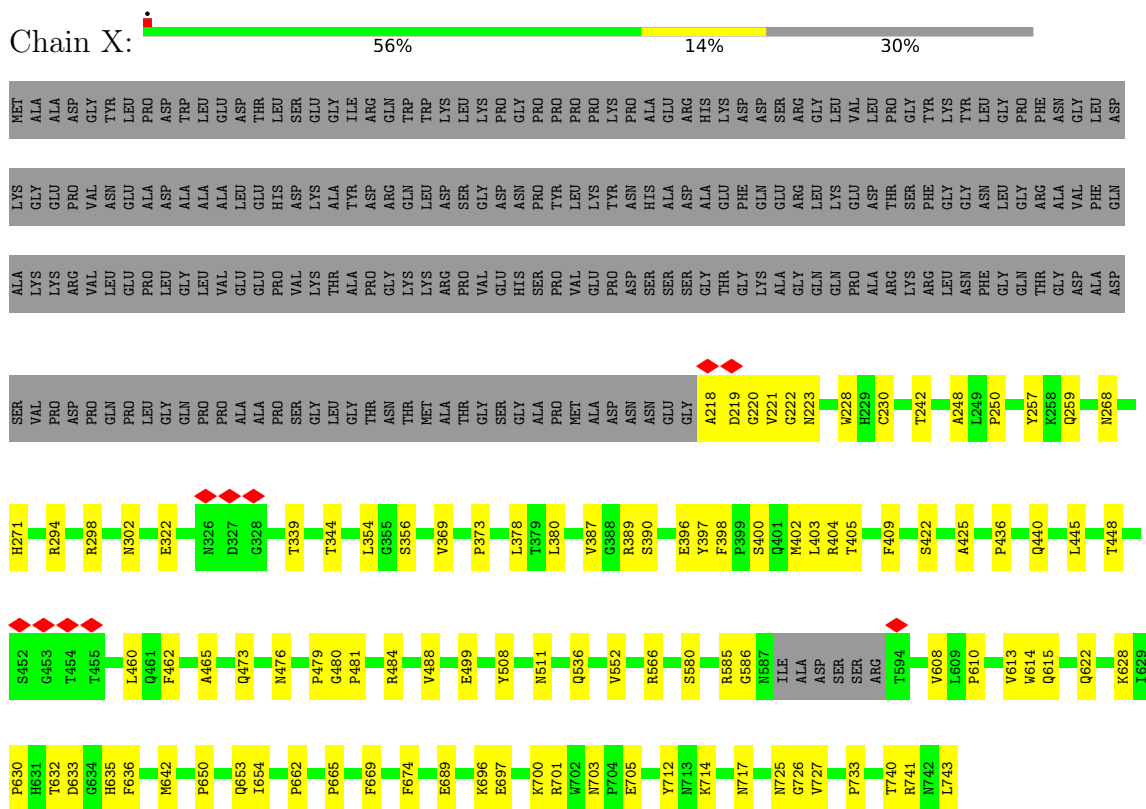
- Molecule 1: Capsid protein VP1



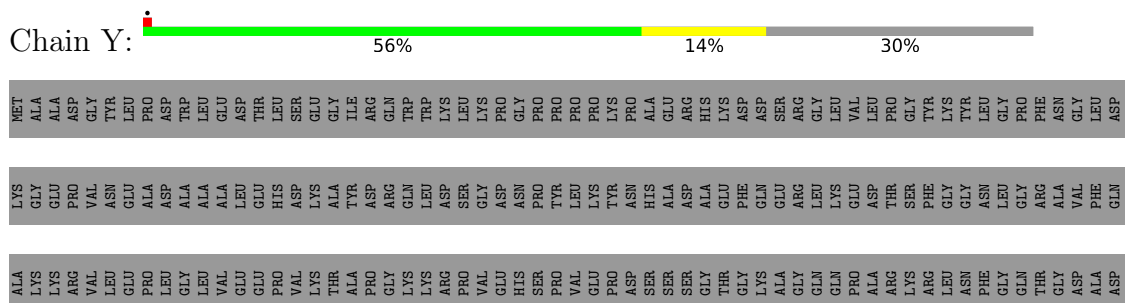
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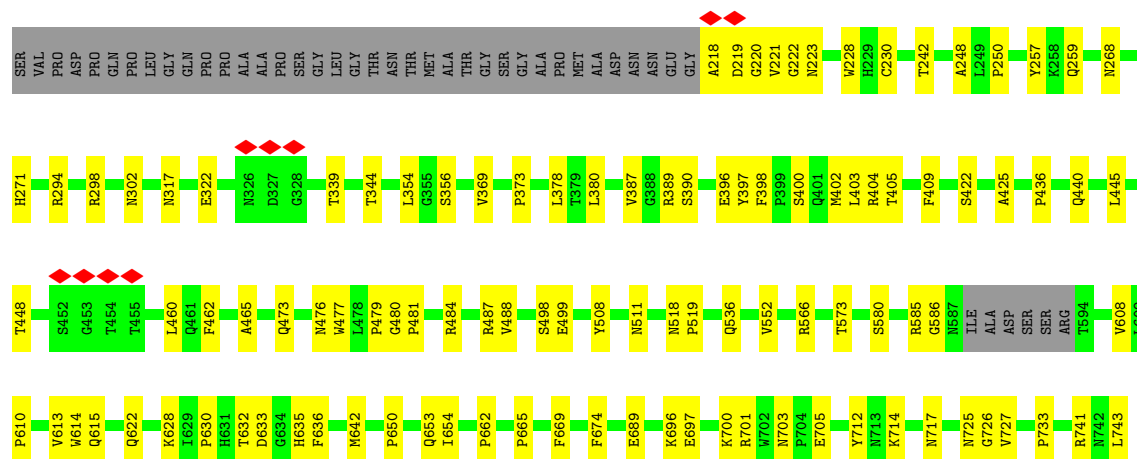


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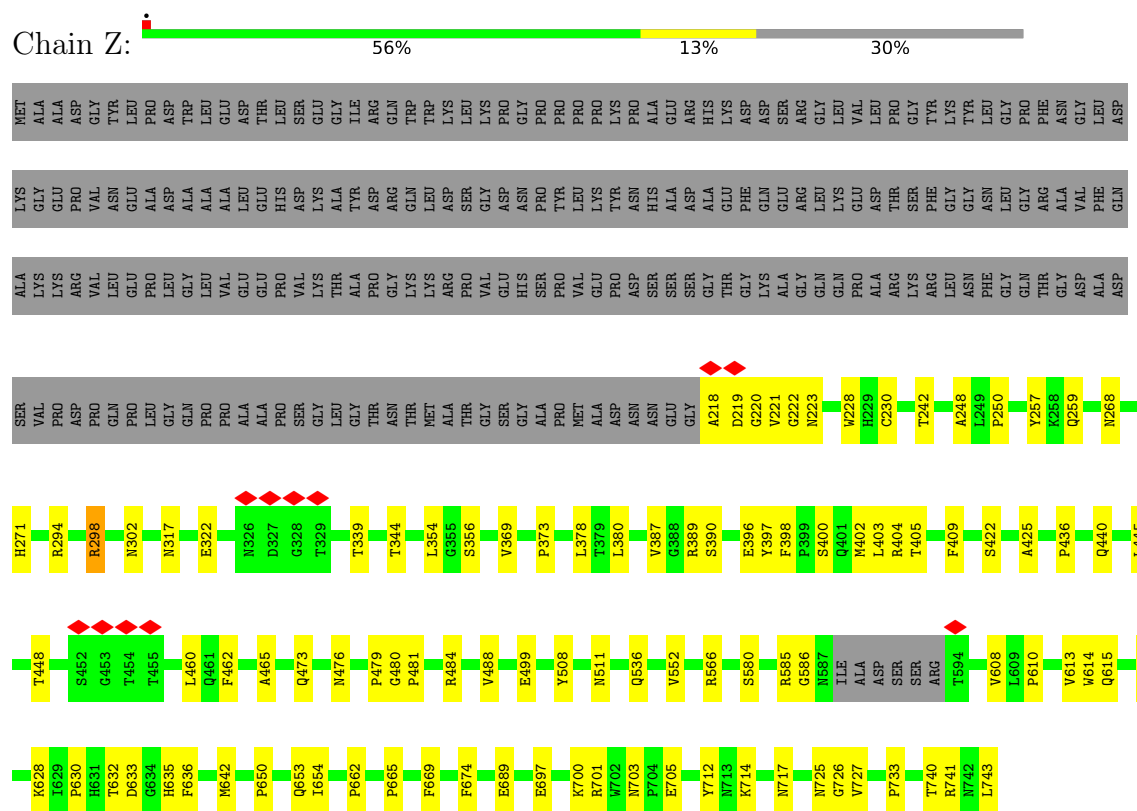


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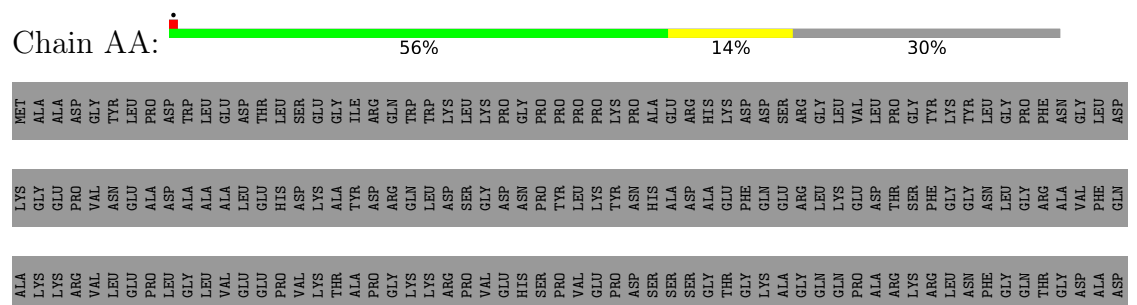




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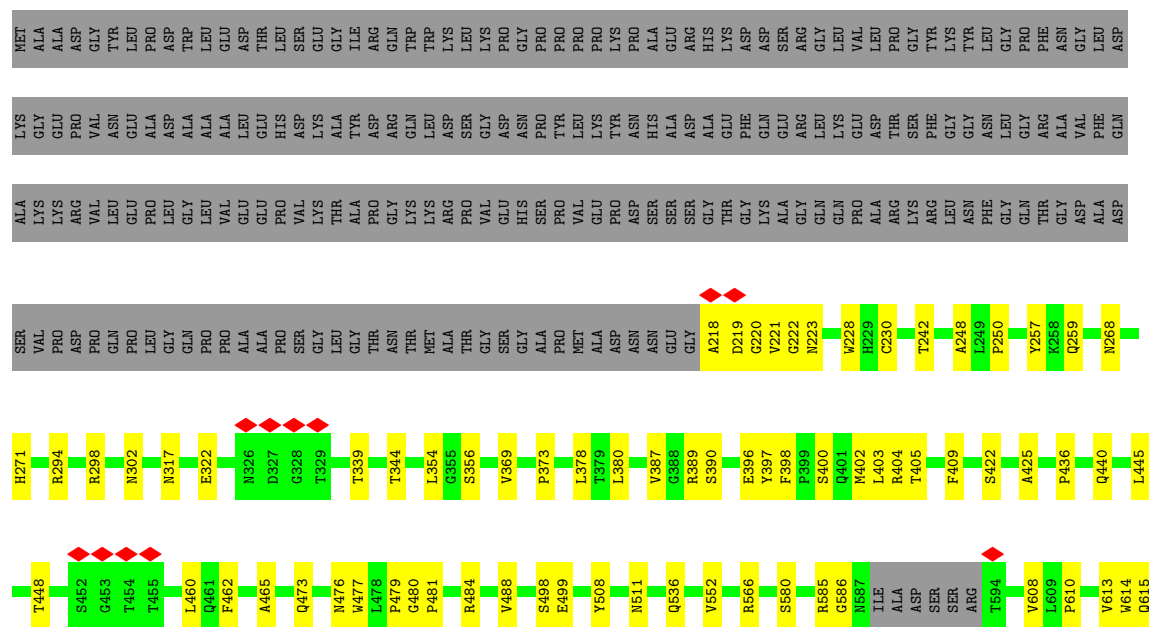


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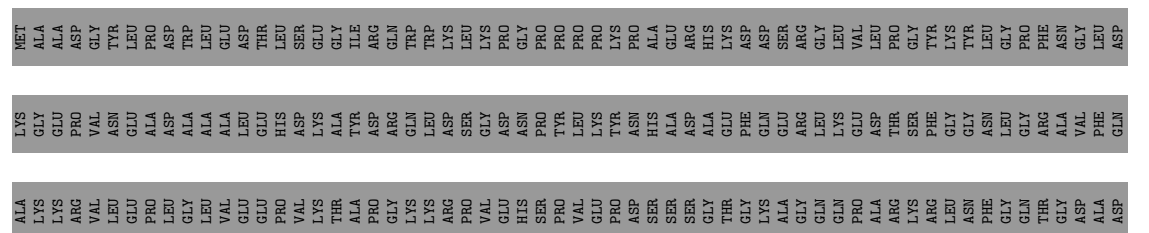
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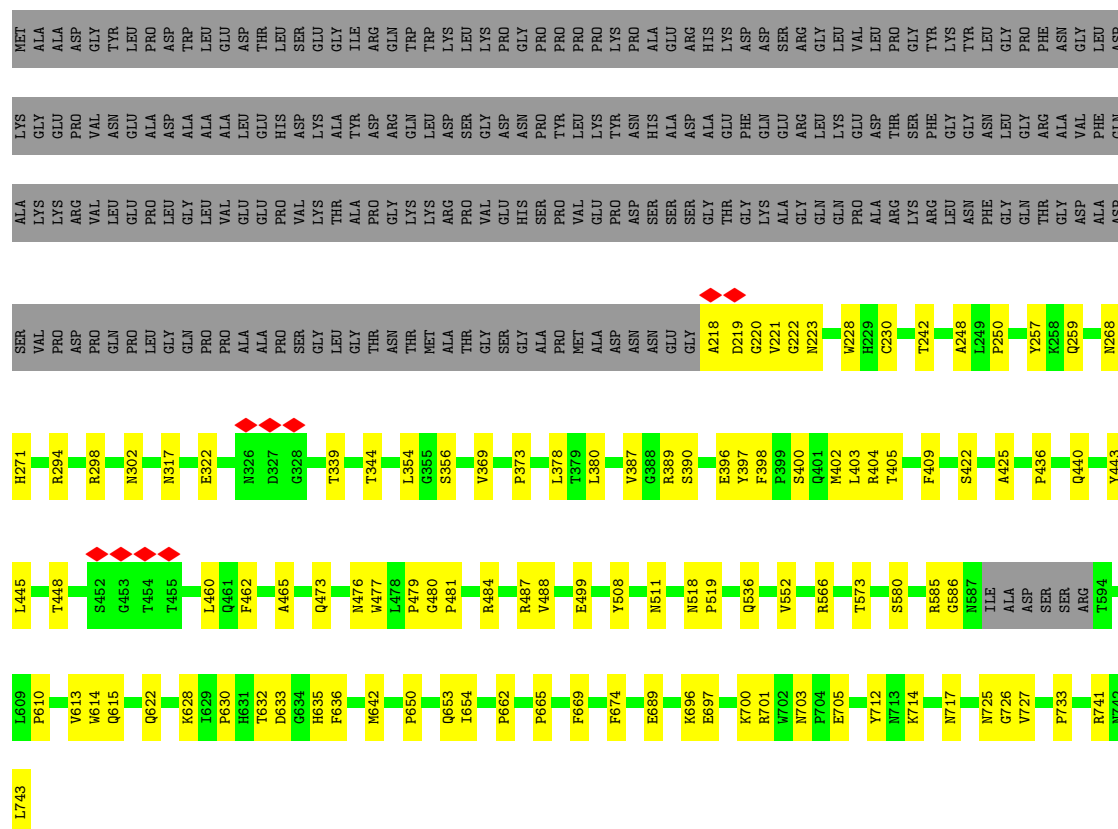


- Molecule 1: Capsid protein VP1

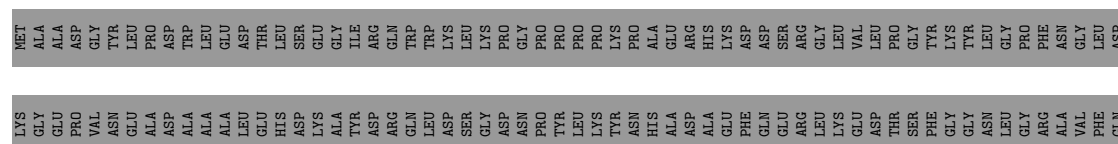
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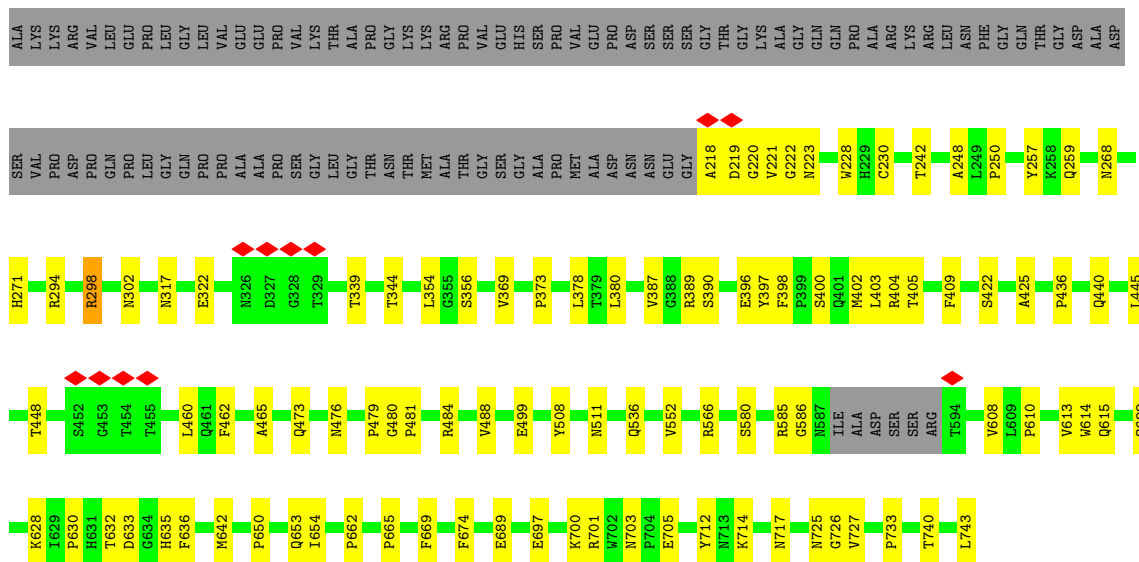


- Molecule 1: Capsid protein VP1

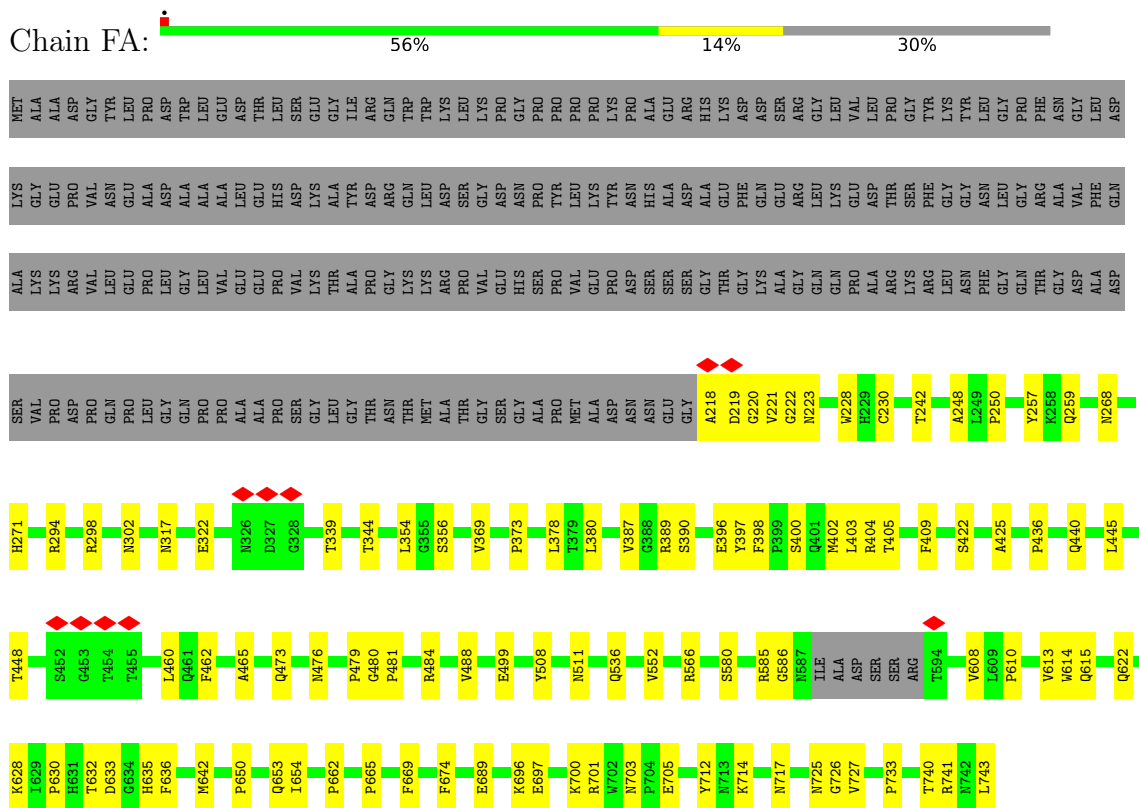


- Molecule 1: Capsid protein VP1

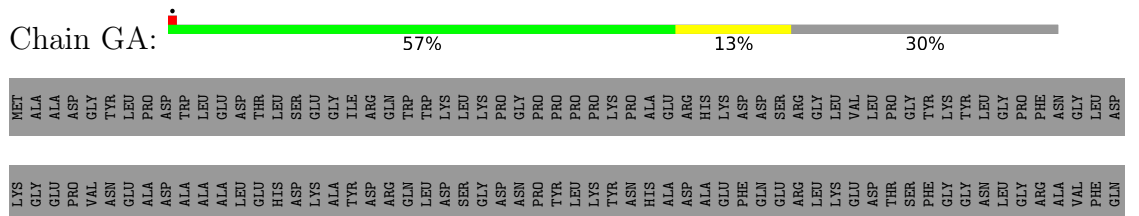


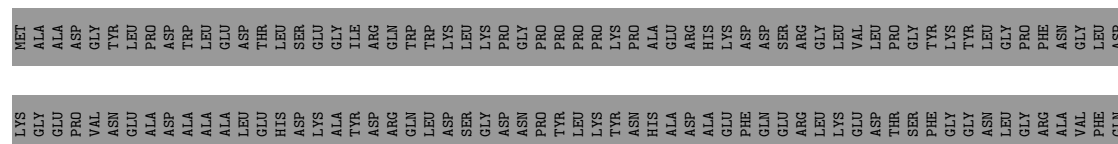


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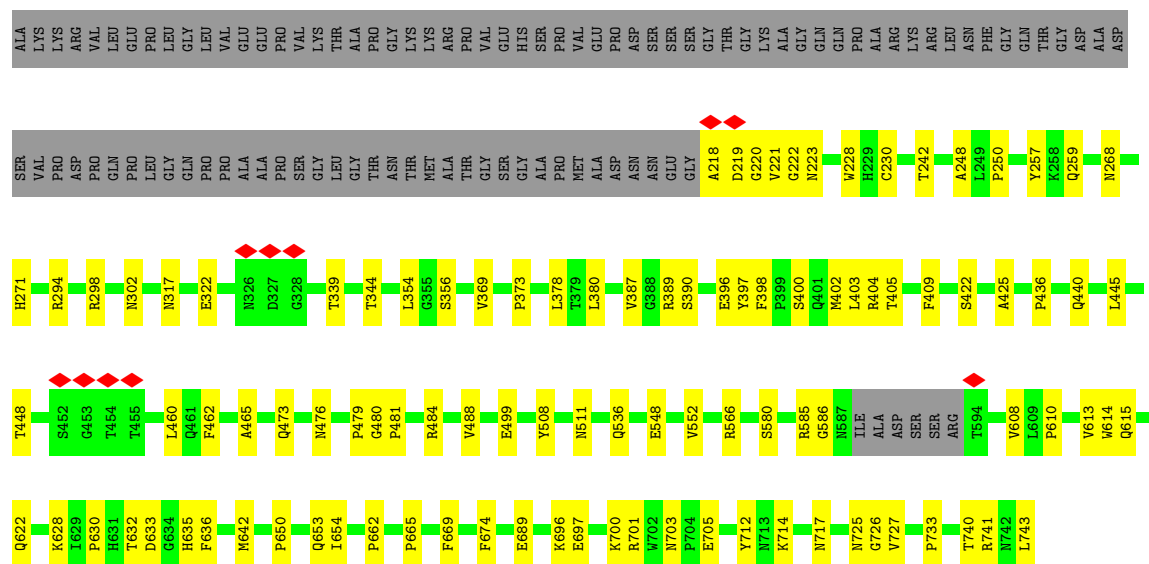


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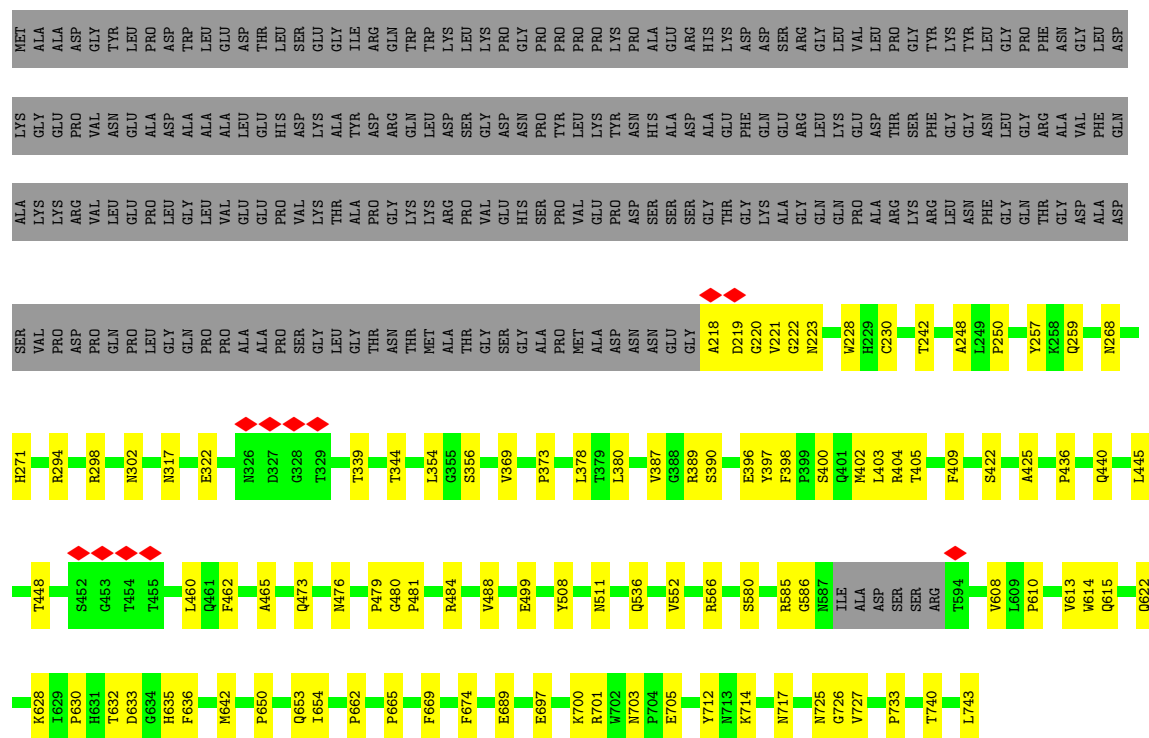




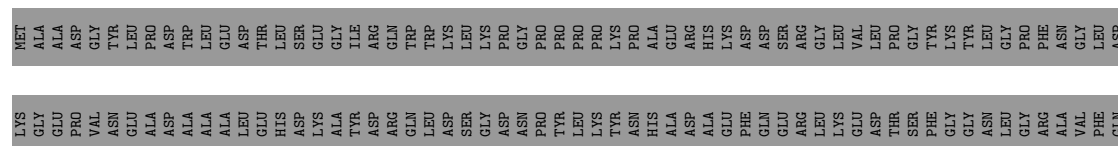


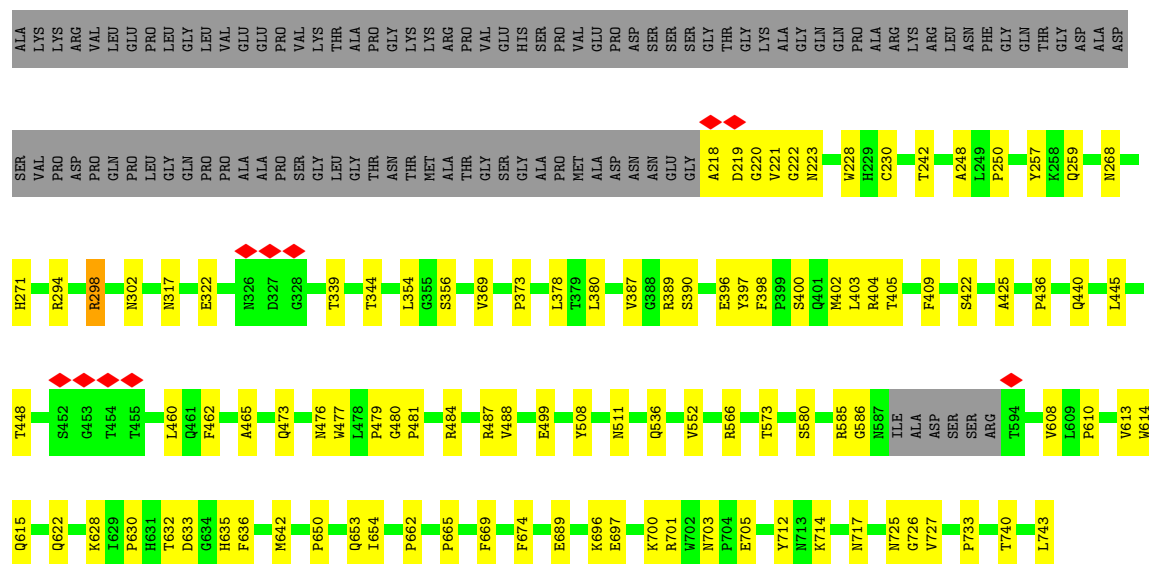


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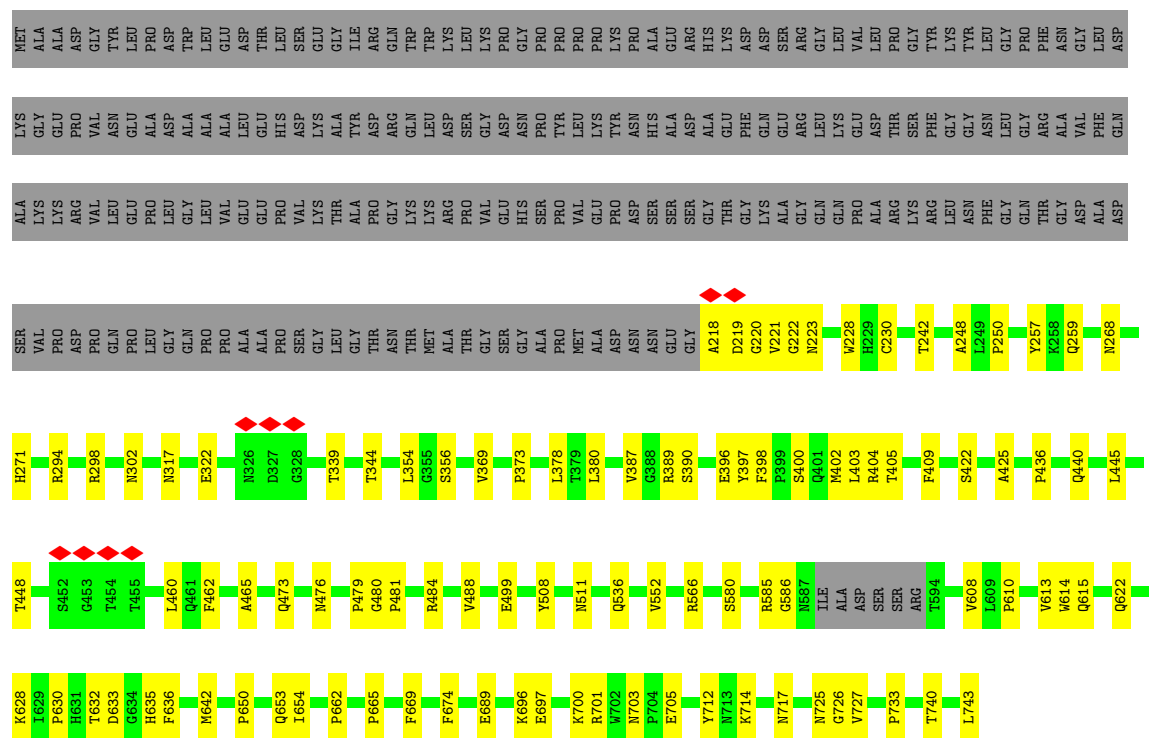


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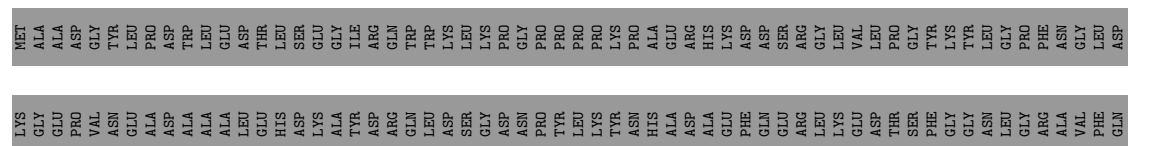


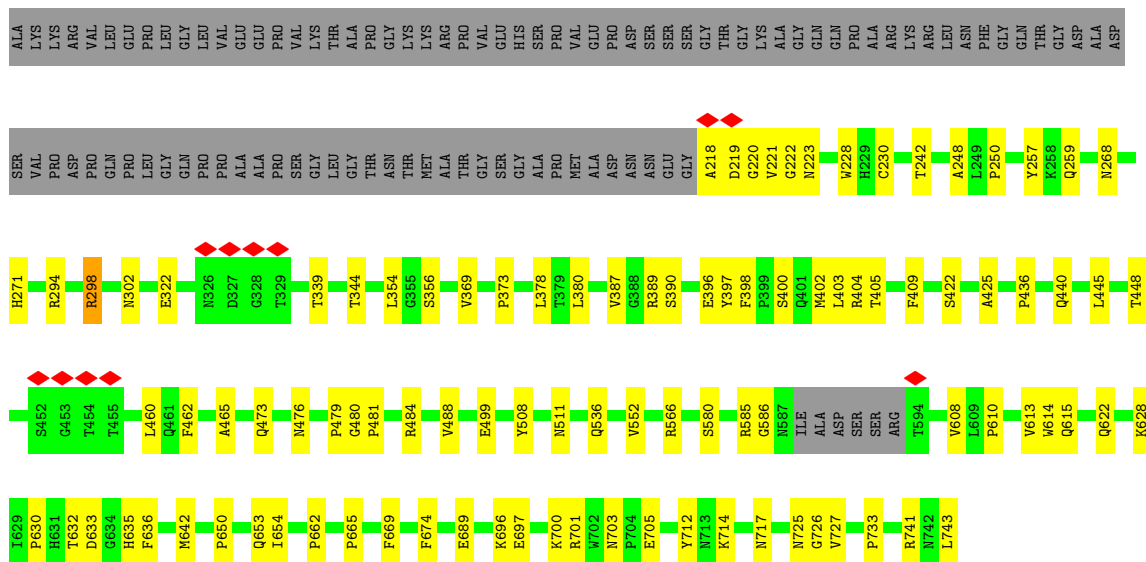


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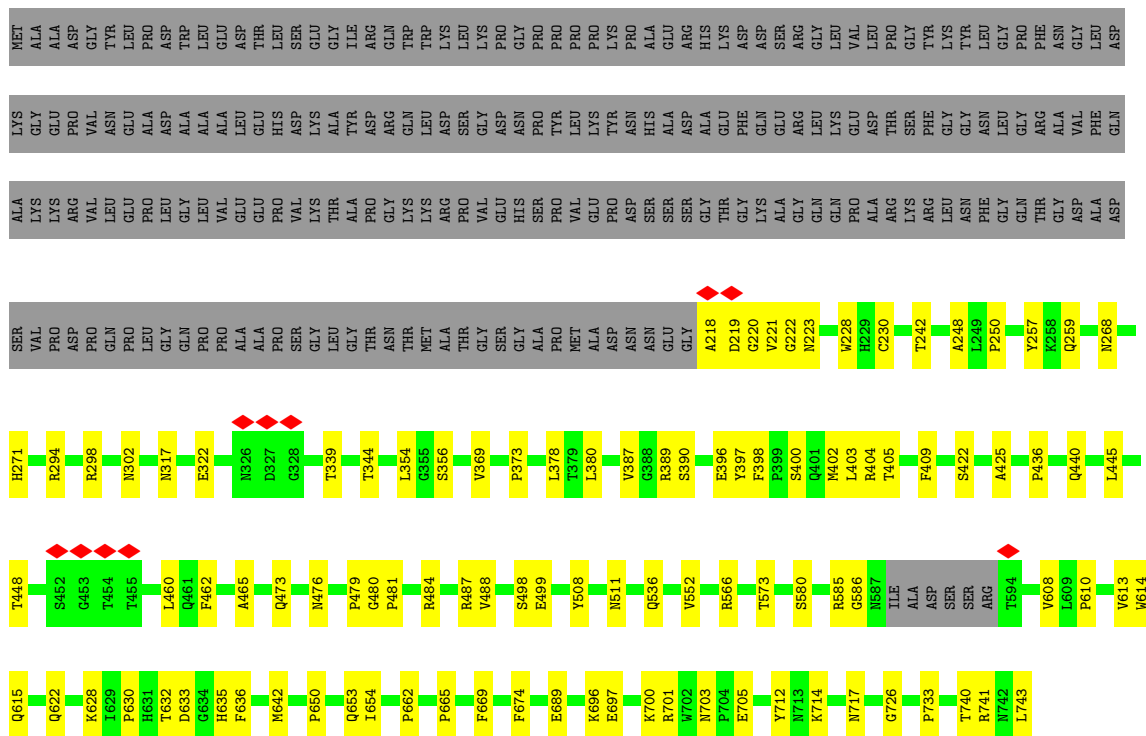


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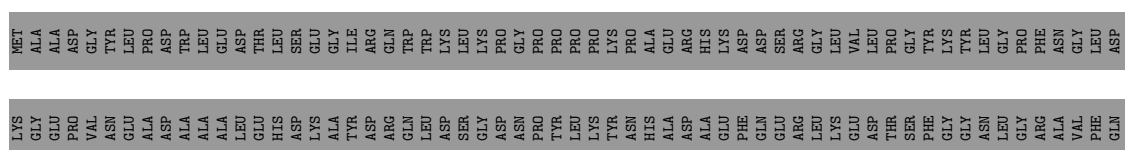


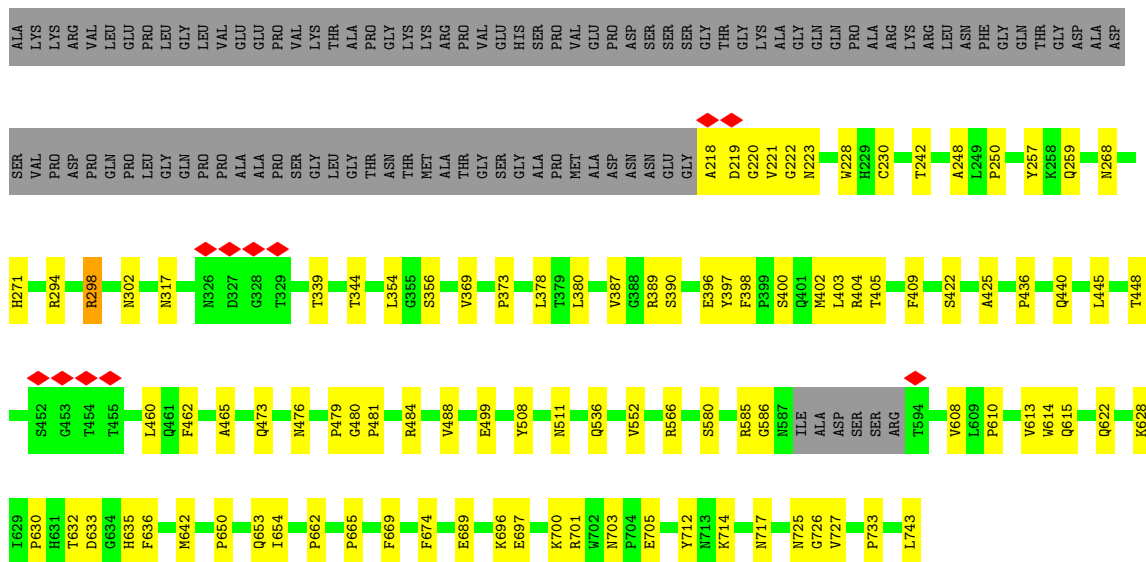


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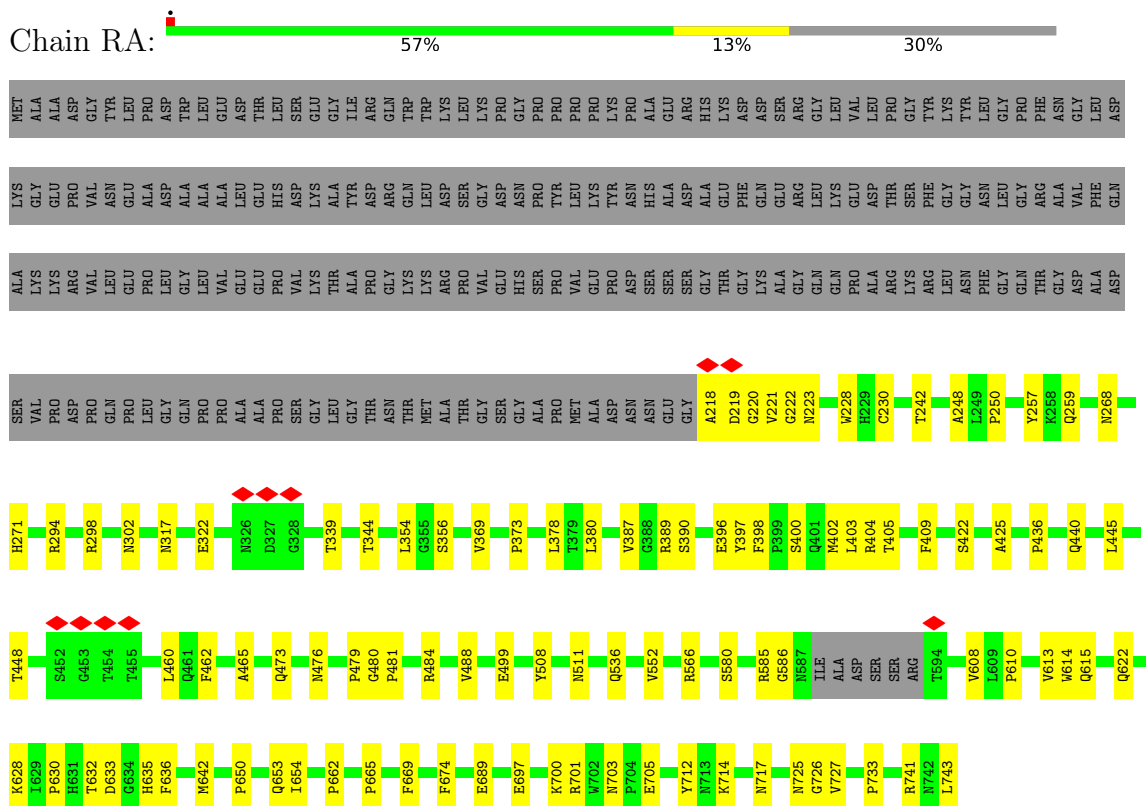


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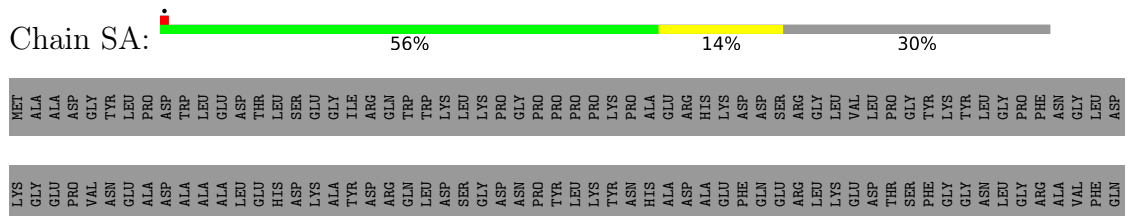


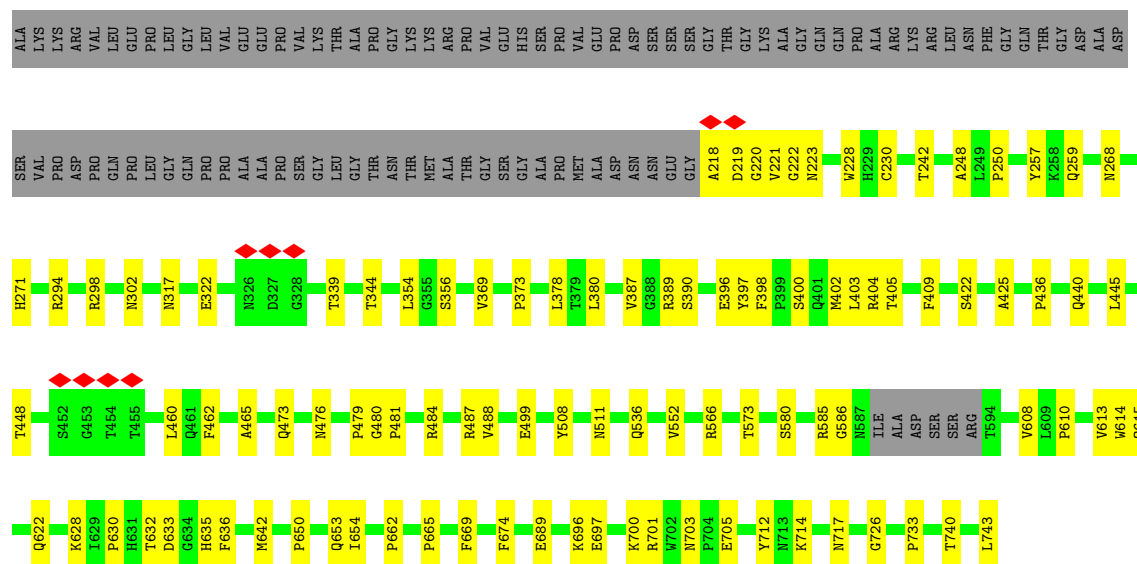


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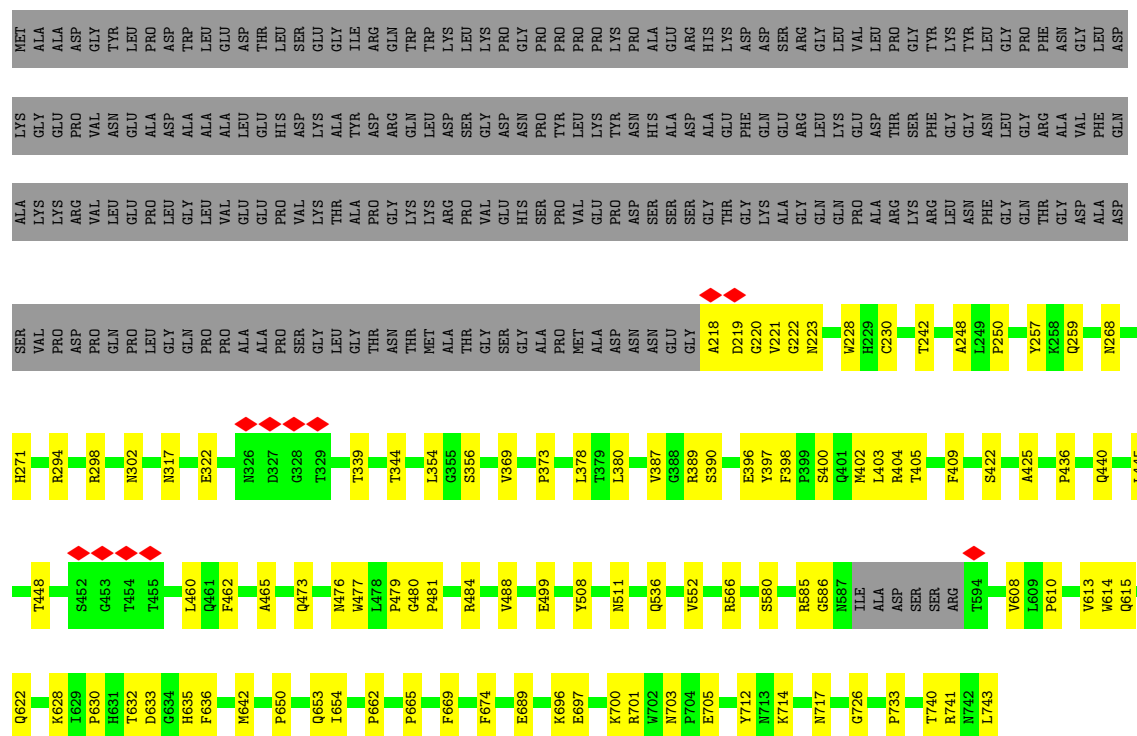


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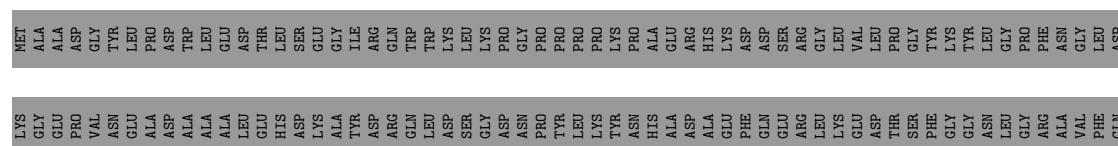


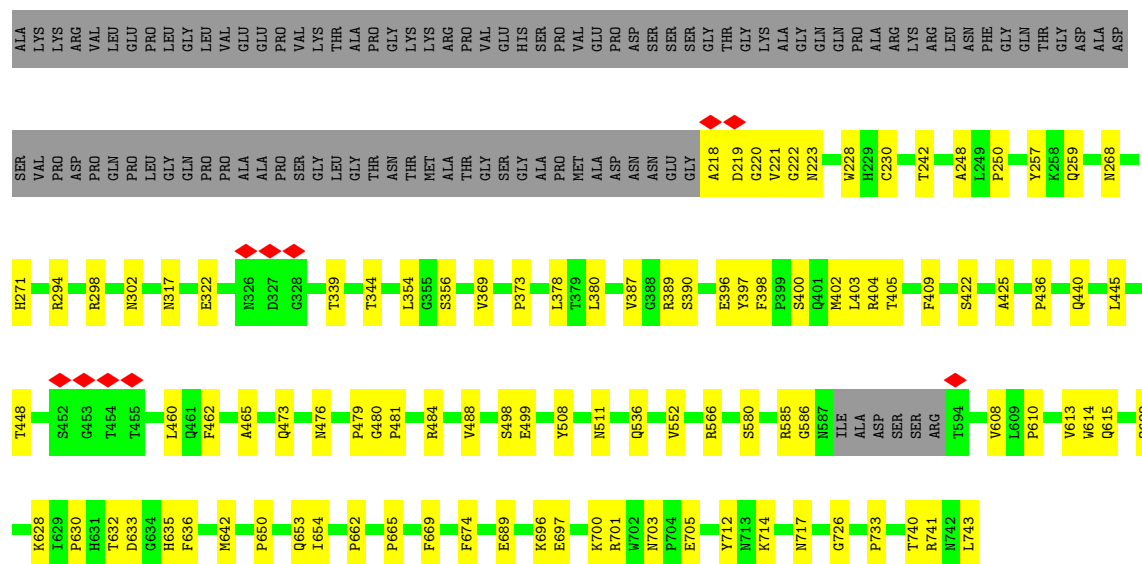


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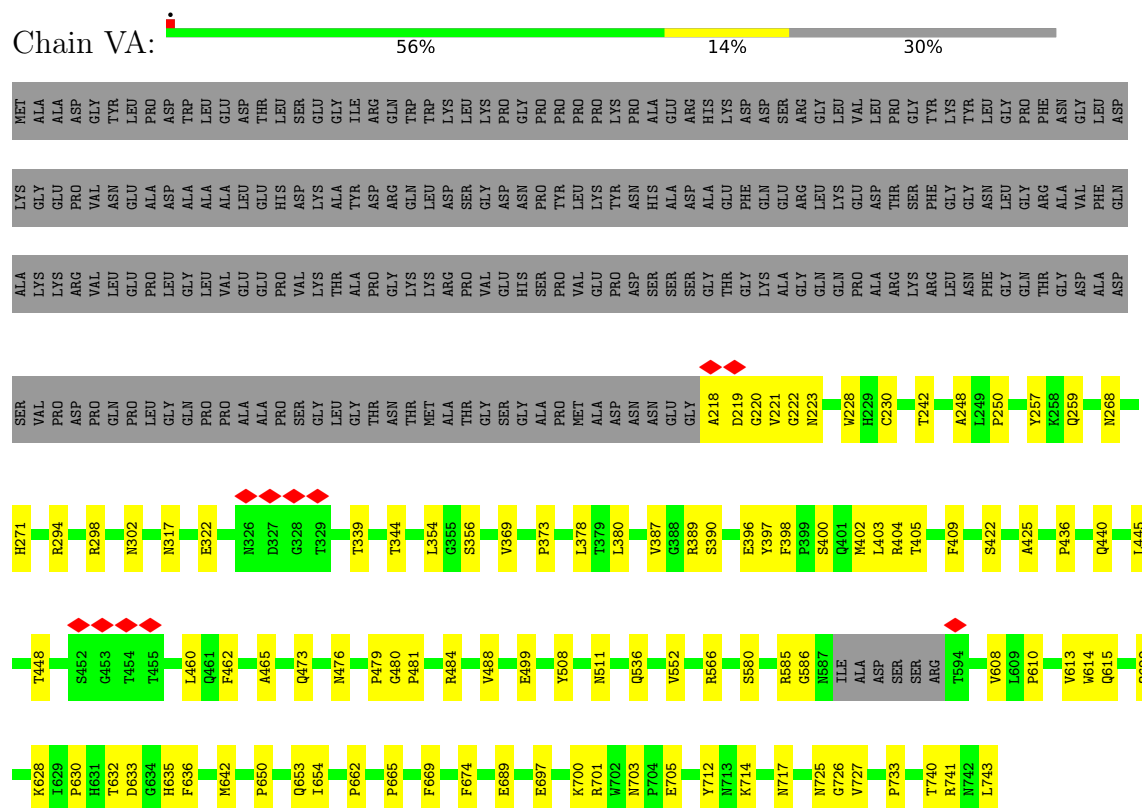


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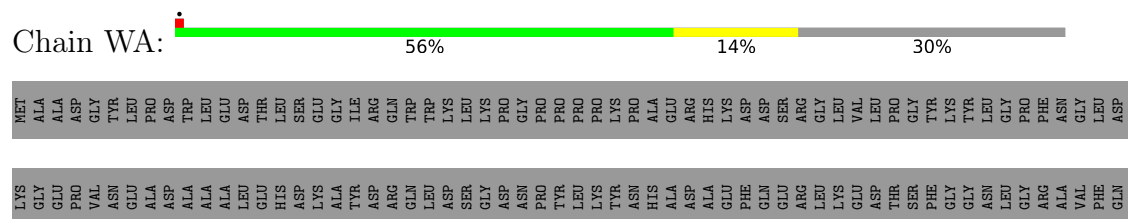


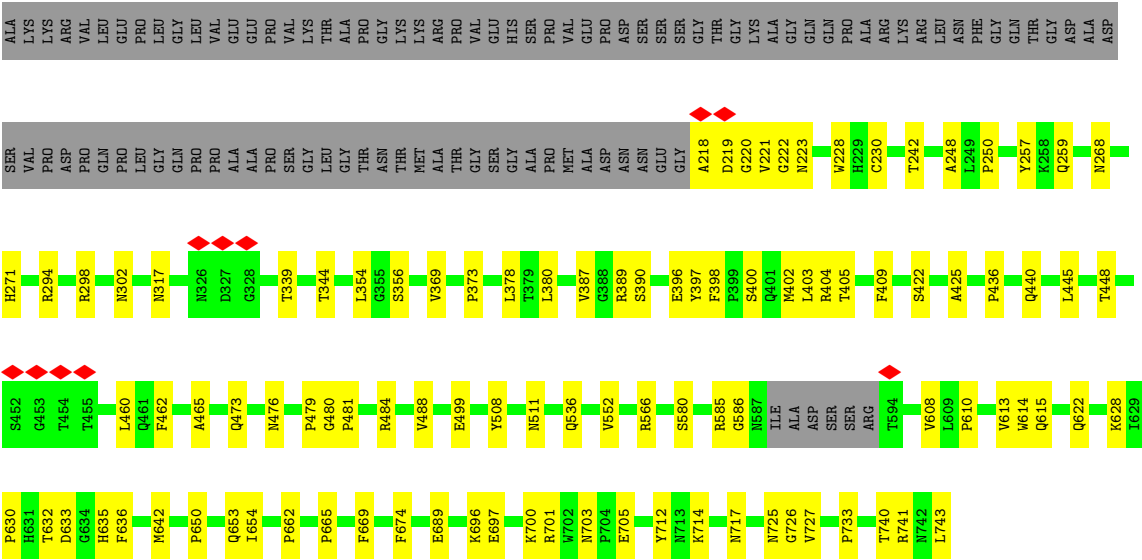


- Molecule 1: Capsid protein VP1

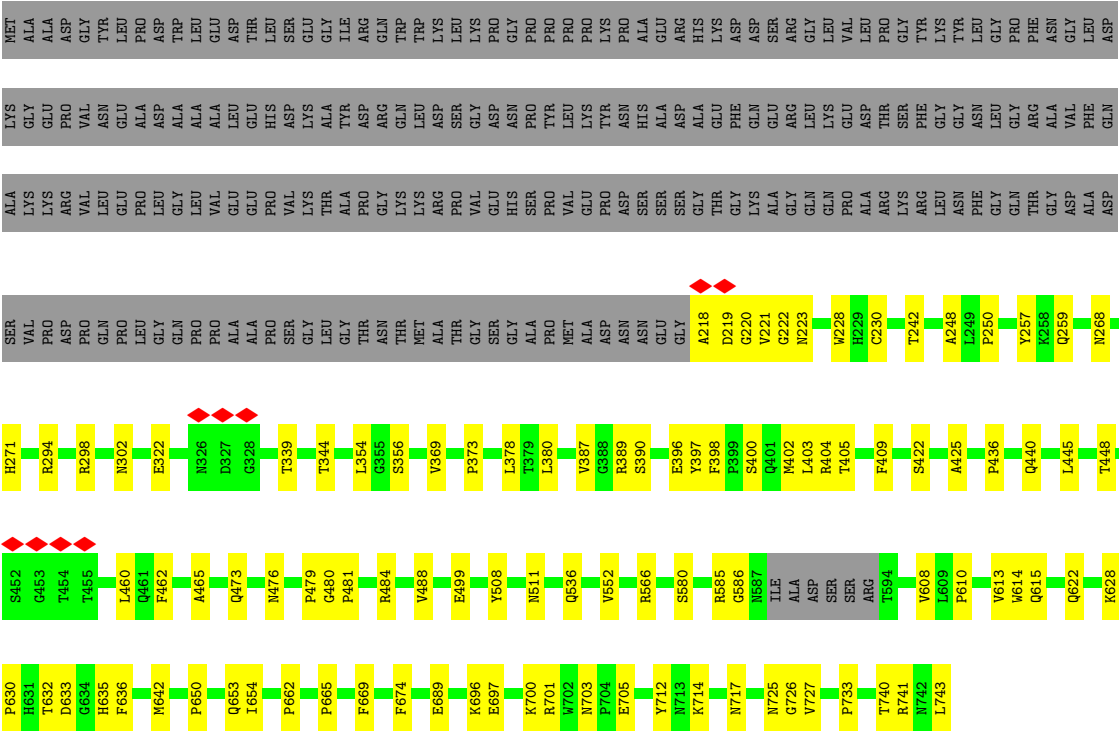


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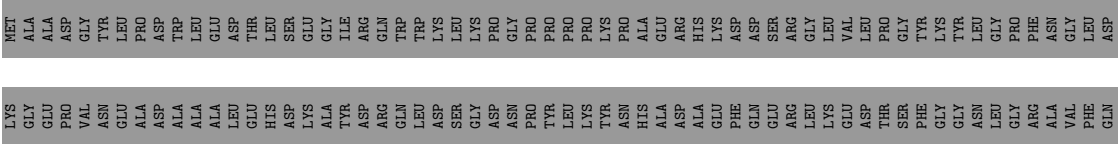


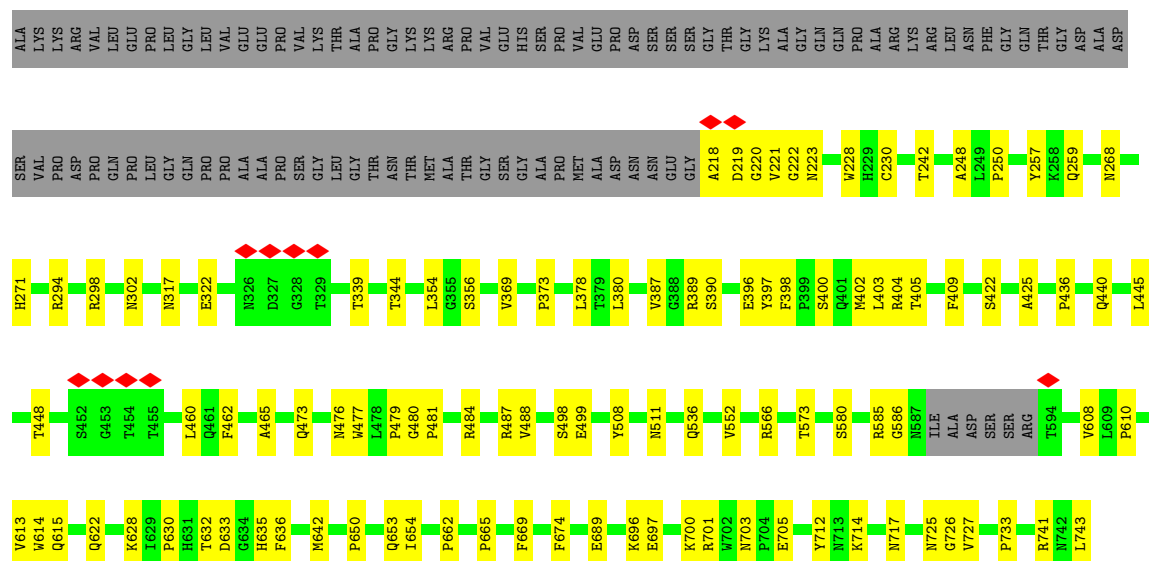


● Molecule 1: Capsid protein VP1

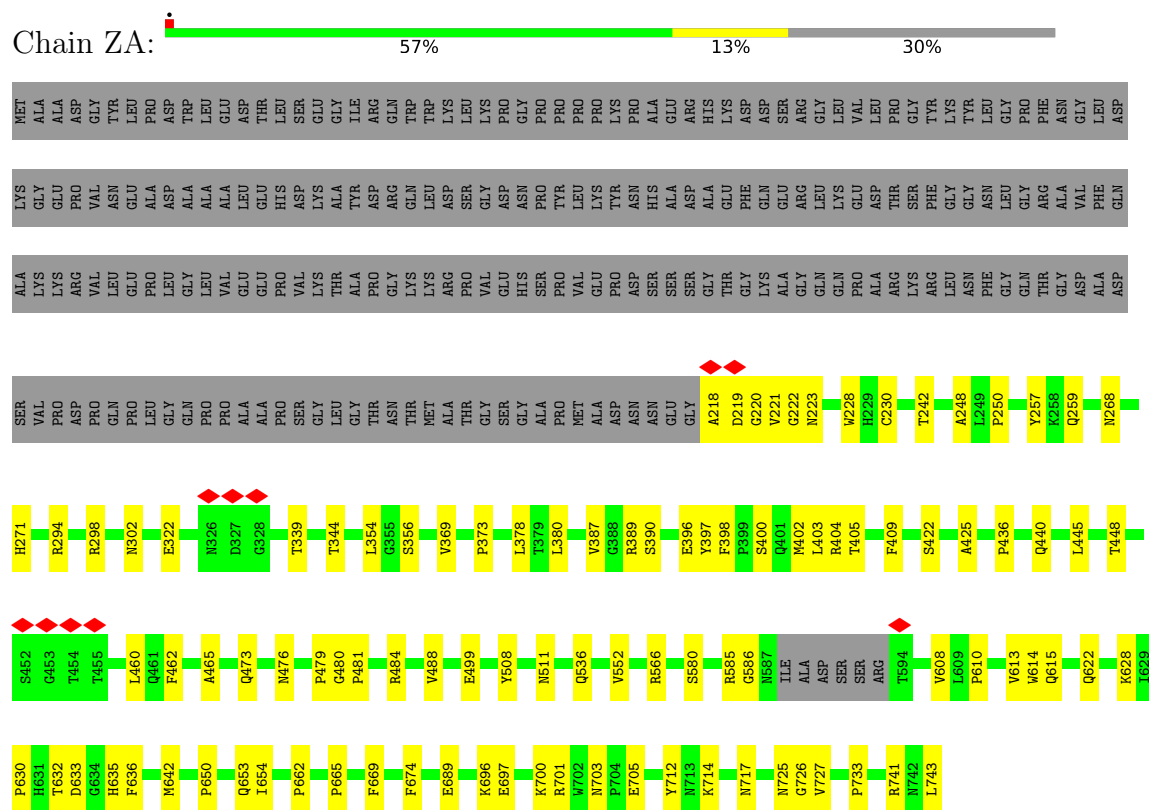


● Molecule 1: Capsid protein VP1

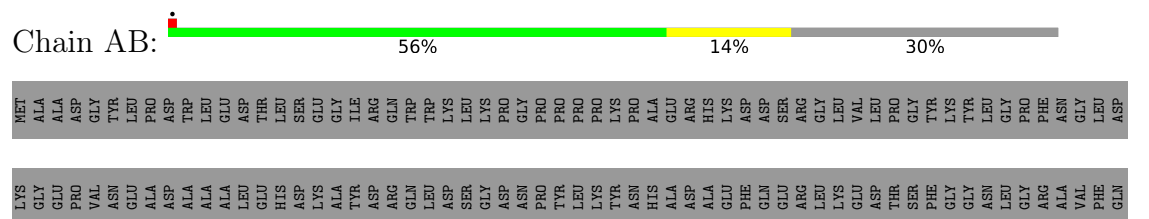


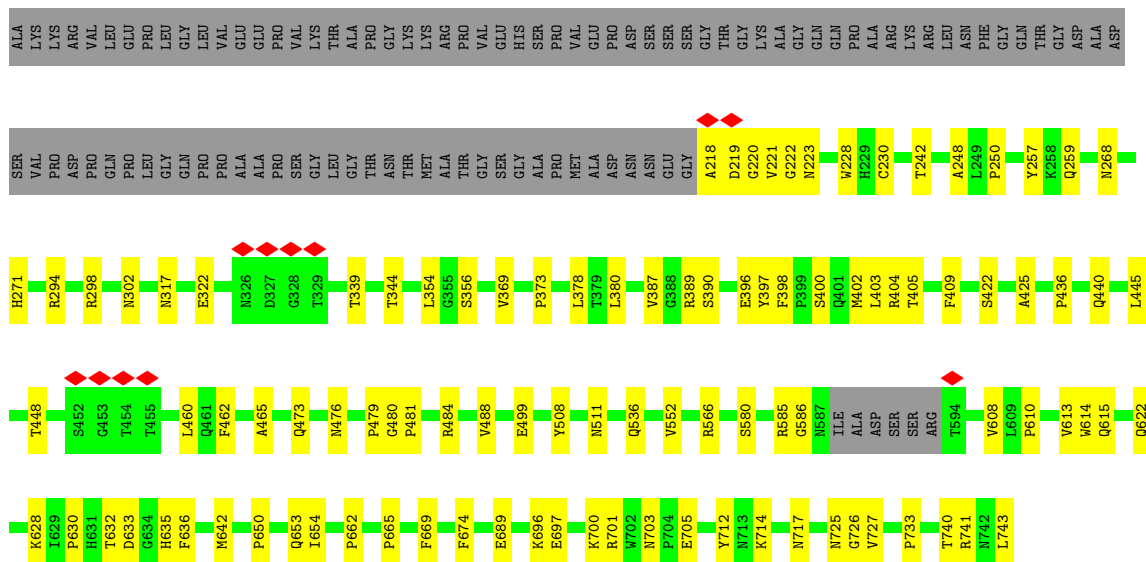


- Molecule 1: Capsid protein VP1

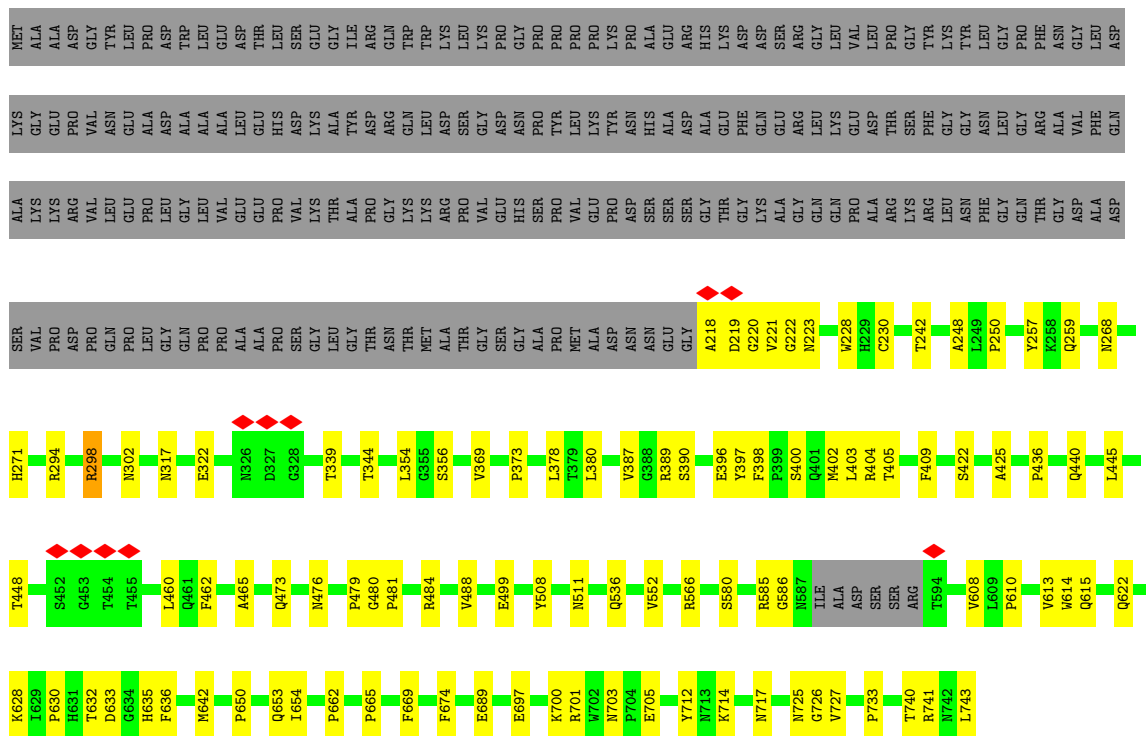


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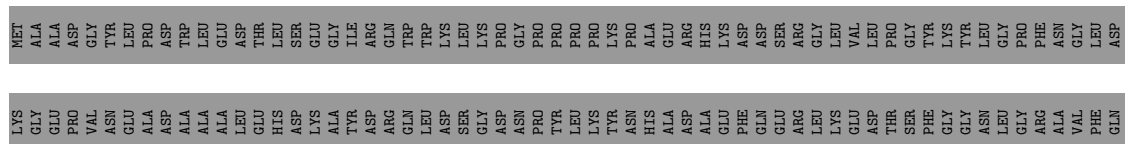


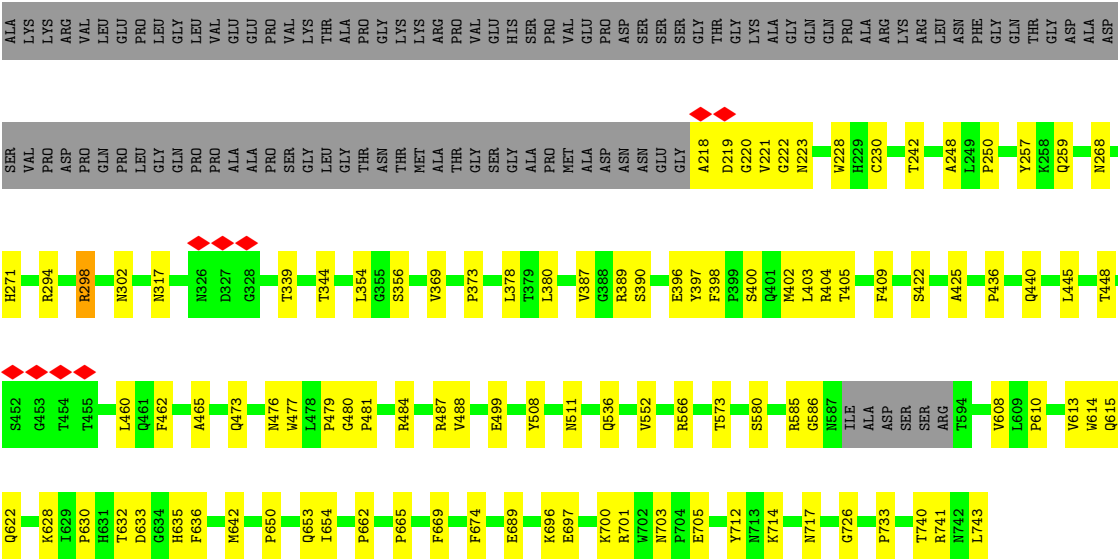


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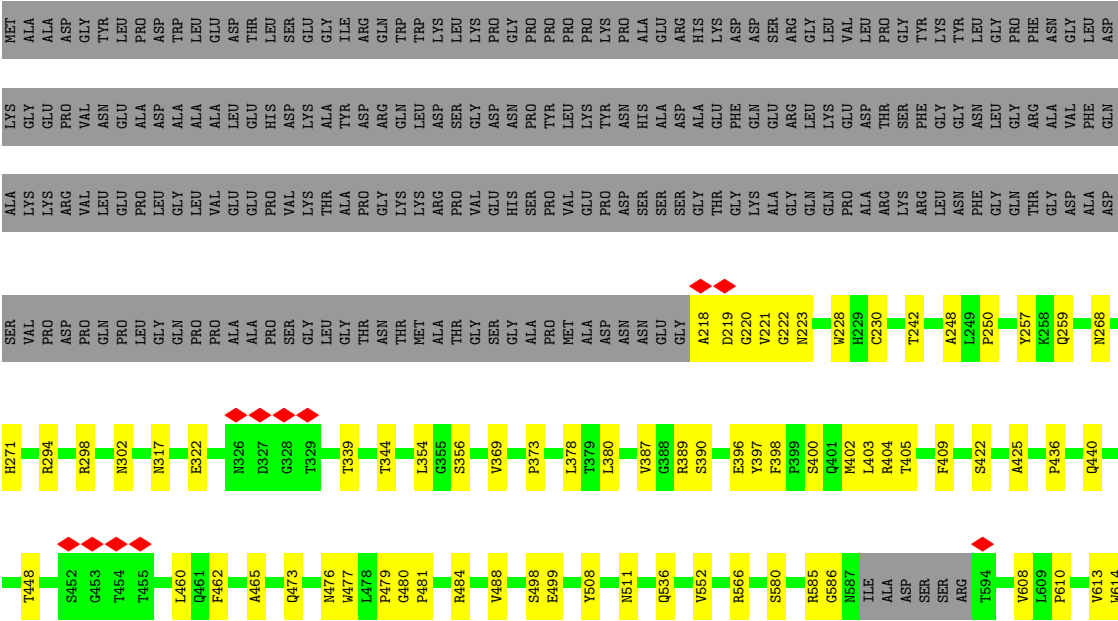


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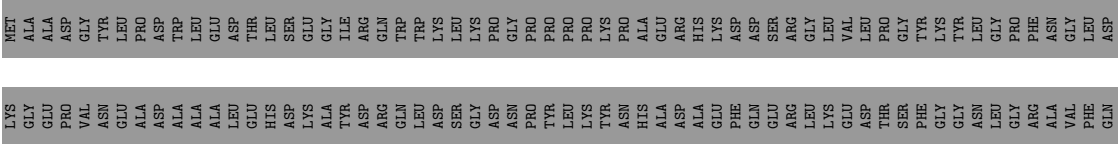


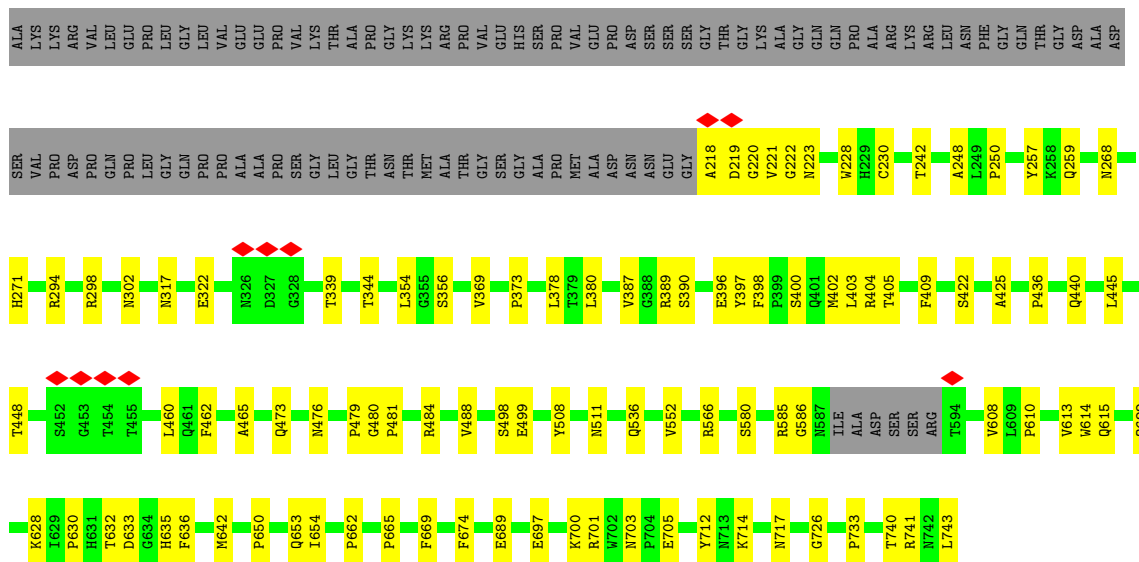


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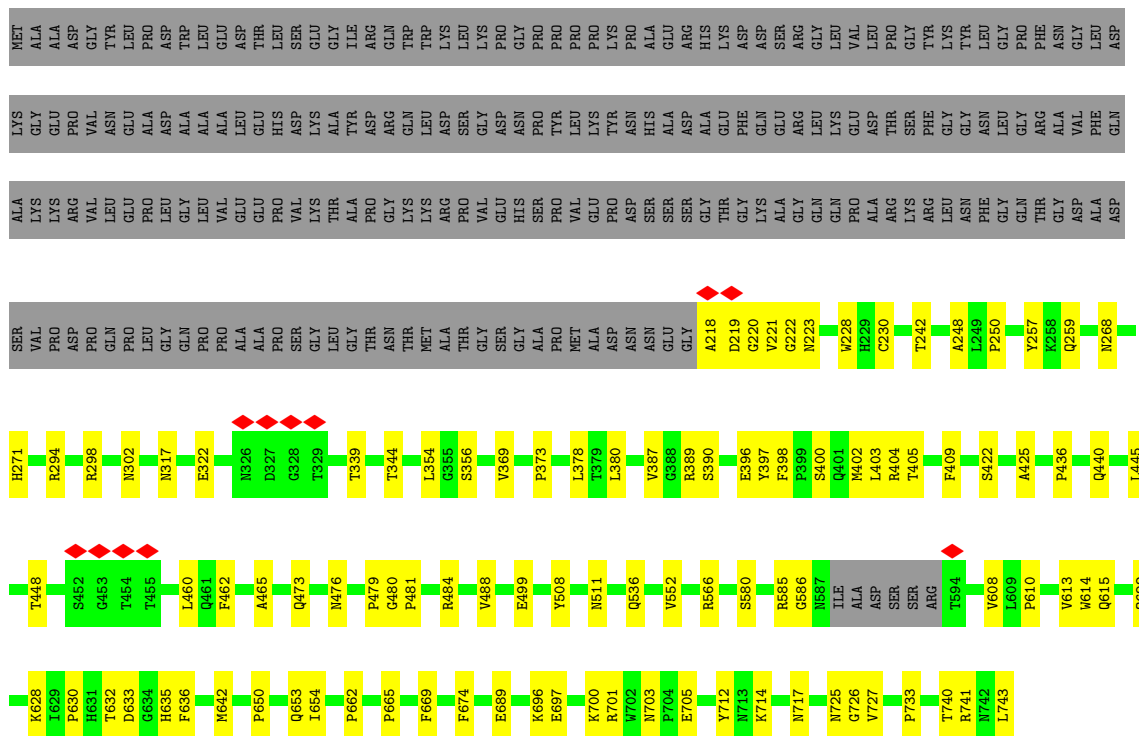


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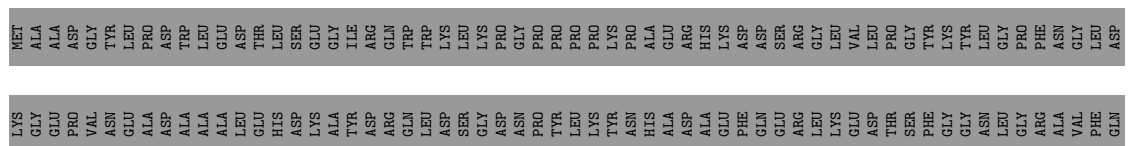


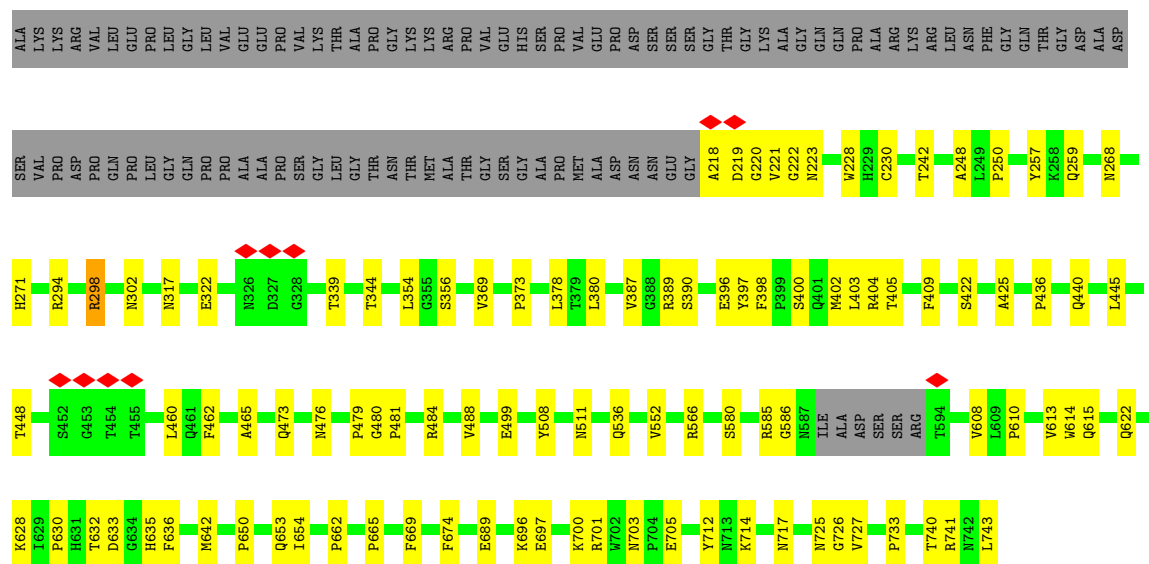


- Molecule 1: Capsid protein VP1

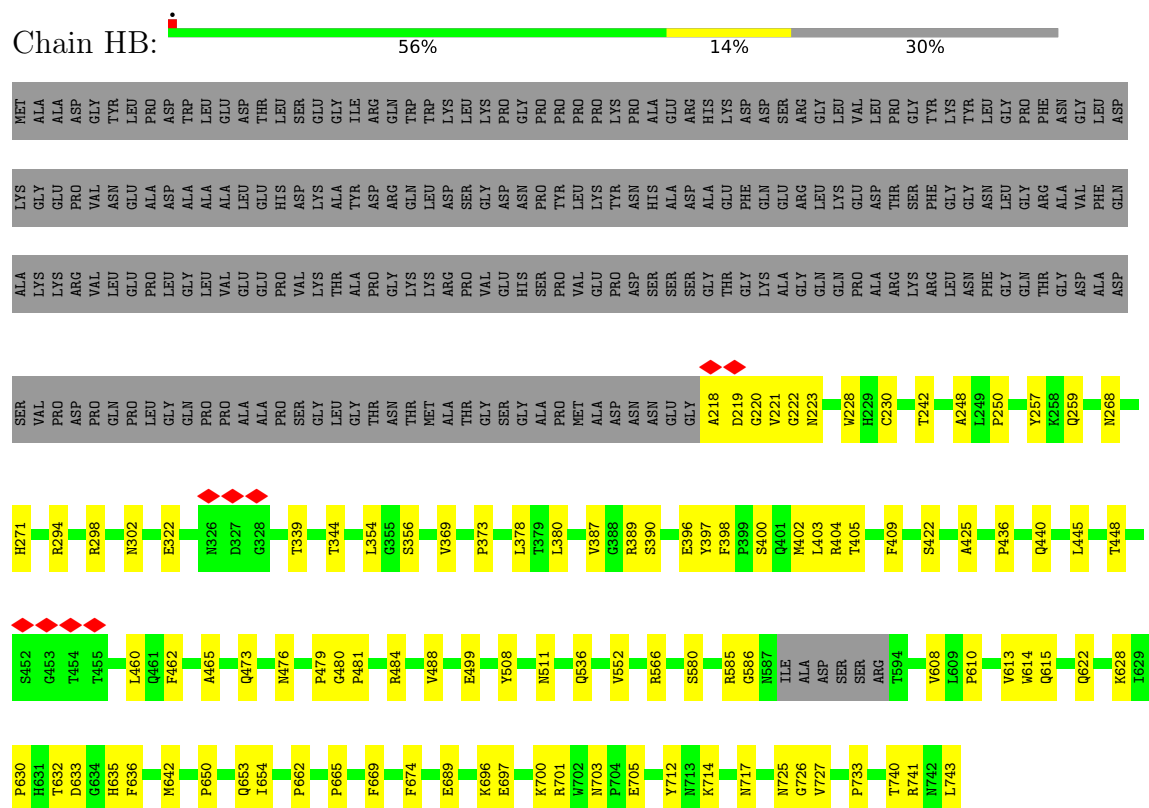


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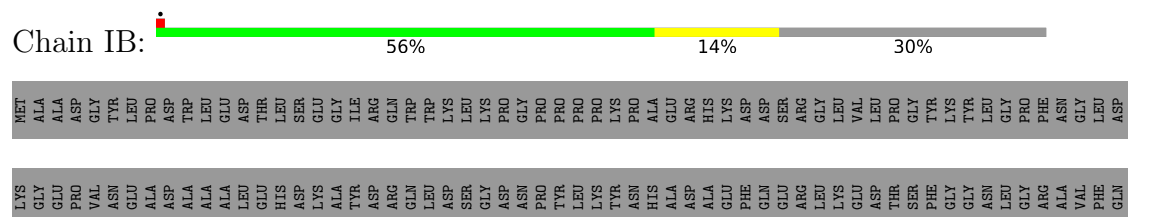


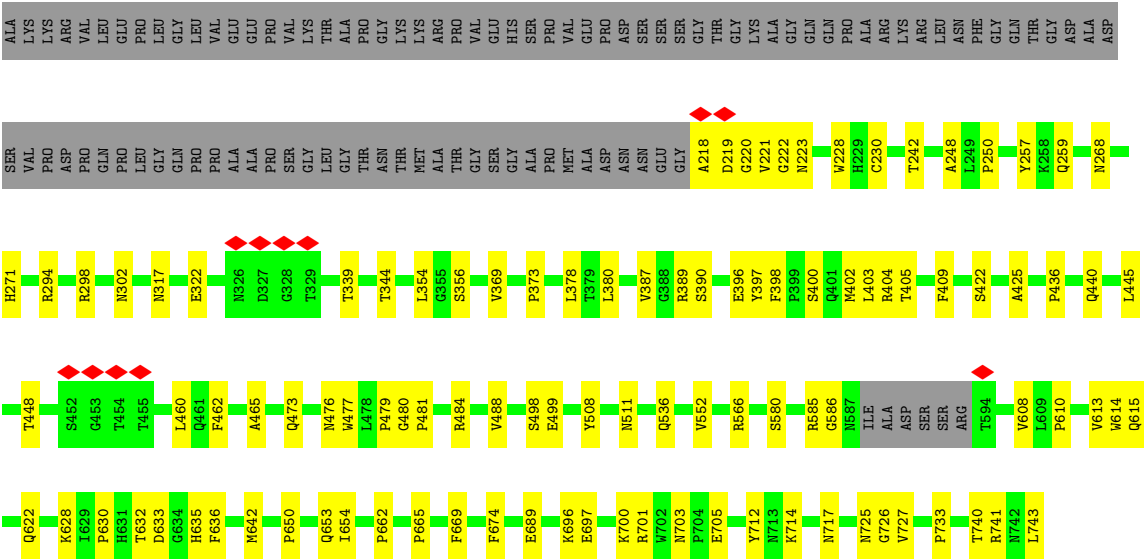


- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19555	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	10000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.387	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	476.16, 476.16, 476.16	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

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	A	0.32	0/4283	0.49	0/5837
1	AA	0.32	0/4283	0.49	0/5837
1	AB	0.32	0/4283	0.49	0/5837
1	B	0.32	0/4283	0.49	0/5837
1	BA	0.32	0/4283	0.49	0/5837
1	BB	0.32	0/4283	0.49	0/5837
1	C	0.32	0/4283	0.49	0/5837
1	CA	0.32	0/4283	0.49	0/5837
1	CB	0.32	0/4283	0.49	0/5837
1	D	0.32	0/4283	0.49	0/5837
1	DA	0.32	0/4283	0.49	0/5837
1	DB	0.32	0/4283	0.49	0/5837
1	E	0.32	0/4283	0.49	0/5837
1	EA	0.32	0/4283	0.49	0/5837
1	EB	0.32	0/4283	0.49	0/5837
1	F	0.32	0/4283	0.49	0/5837
1	FA	0.32	0/4283	0.49	0/5837
1	FB	0.32	0/4283	0.49	0/5837
1	G	0.32	0/4283	0.49	0/5837
1	GA	0.32	0/4283	0.49	0/5837
1	GB	0.32	0/4283	0.49	0/5837
1	H	0.32	0/4283	0.49	0/5837
1	HA	0.32	0/4283	0.49	0/5837
1	HB	0.32	0/4283	0.49	0/5837
1	I	0.32	0/4283	0.49	0/5837
1	IA	0.32	0/4283	0.49	0/5837
1	IB	0.32	0/4283	0.49	0/5837
1	J	0.32	0/4283	0.49	0/5837
1	JA	0.32	0/4283	0.49	0/5837
1	K	0.32	0/4283	0.49	0/5837
1	KA	0.32	0/4283	0.49	0/5837
1	L	0.32	0/4283	0.49	0/5837
1	LA	0.32	0/4283	0.49	0/5837
1	M	0.32	0/4283	0.49	0/5837

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	MA	0.32	0/4283	0.49	0/5837
1	N	0.32	0/4283	0.49	0/5837
1	NA	0.32	0/4283	0.49	0/5837
1	O	0.32	0/4283	0.49	0/5837
1	OA	0.32	0/4283	0.49	0/5837
1	P	0.32	0/4283	0.49	0/5837
1	PA	0.32	0/4283	0.49	0/5837
1	Q	0.32	0/4283	0.49	0/5837
1	QA	0.32	0/4283	0.49	0/5837
1	R	0.32	0/4283	0.49	0/5837
1	RA	0.32	0/4283	0.49	0/5837
1	S	0.32	0/4283	0.49	0/5837
1	SA	0.32	0/4283	0.49	0/5837
1	T	0.32	0/4283	0.49	0/5837
1	TA	0.32	0/4283	0.49	0/5837
1	UA	0.32	0/4283	0.49	0/5837
1	V	0.32	0/4283	0.49	0/5837
1	VA	0.32	0/4283	0.49	0/5837
1	W	0.32	0/4283	0.49	0/5837
1	WA	0.32	0/4283	0.49	0/5837
1	X	0.32	0/4283	0.49	0/5837
1	XA	0.32	0/4283	0.49	0/5837
1	Y	0.32	0/4283	0.49	0/5837
1	YA	0.32	0/4283	0.49	0/5837
1	Z	0.32	0/4283	0.49	0/5837
1	ZA	0.32	0/4283	0.49	0/5837
All	All	0.32	0/256980	0.49	0/350220

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4161	0	3910	118	0
1	AA	4161	0	3910	120	0
1	AB	4161	0	3910	115	0
1	B	4161	0	3910	115	0
1	BA	4161	0	3910	118	0
1	BB	4161	0	3910	117	0
1	C	4161	0	3910	121	0
1	CA	4161	0	3910	115	0
1	CB	4161	0	3910	117	0
1	D	4161	0	3910	119	0
1	DA	4161	0	3910	121	0
1	DB	4161	0	3910	119	0
1	E	4161	0	3910	117	0
1	EA	4161	0	3910	117	0
1	EB	4161	0	3910	117	0
1	F	4161	0	3910	117	0
1	FA	4161	0	3910	117	0
1	FB	4161	0	3910	115	0
1	G	4161	0	3910	116	0
1	GA	4161	0	3910	114	0
1	GB	4161	0	3910	117	0
1	H	4161	0	3910	118	0
1	HA	4161	0	3910	120	0
1	HB	4161	0	3910	118	0
1	I	4161	0	3910	117	0
1	IA	4161	0	3910	118	0
1	IB	4161	0	3910	119	0
1	J	4161	0	3910	118	0
1	JA	4161	0	3910	114	0
1	K	4161	0	3910	119	0
1	KA	4161	0	3910	117	0
1	L	4161	0	3910	116	0
1	LA	4161	0	3910	115	0
1	M	4161	0	3910	119	0
1	MA	4161	0	3910	121	0
1	N	4161	0	3910	120	0
1	NA	4161	0	3910	118	0
1	O	4161	0	3910	119	0
1	OA	4161	0	3910	116	0
1	P	4161	0	3910	116	0
1	PA	4161	0	3910	119	0
1	Q	4161	0	3910	115	0
1	QA	4161	0	3910	116	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	4161	0	3910	119	0
1	RA	4161	0	3910	117	0
1	S	4161	0	3910	118	0
1	SA	4161	0	3910	116	0
1	T	4161	0	3910	117	0
1	TA	4161	0	3910	117	0
1	UA	4161	0	3910	118	0
1	V	4161	0	3910	120	0
1	VA	4161	0	3910	115	0
1	W	4161	0	3910	119	0
1	WA	4161	0	3910	117	0
1	X	4161	0	3910	115	0
1	XA	4161	0	3910	118	0
1	Y	4161	0	3910	121	0
1	YA	4161	0	3910	118	0
1	Z	4161	0	3910	116	0
1	ZA	4161	0	3910	114	0
All	All	249660	0	234600	4220	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (4220) 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:O:642:MET:HB2	1:FA:476:ASN:OD1	1.84	0.78
1:S:642:MET:HB2	1:TA:476:ASN:OD1	1.84	0.78
1:D:642:MET:HB2	1:DB:476:ASN:OD1	1.84	0.78
1:J:642:MET:HB2	1:KA:476:ASN:OD1	1.84	0.78
1:LA:642:MET:HB2	1:AB:476:ASN:OD1	1.84	0.78
1:JA:642:MET:HB2	1:ZA:476:ASN:OD1	1.84	0.78
1:OA:476:ASN:OD1	1:CB:642:MET:HB2	1.84	0.78
1:OA:642:MET:HB2	1:PA:476:ASN:OD1	1.84	0.78
1:I:476:ASN:OD1	1:P:642:MET:HB2	1.84	0.78
1:K:726:GLY:HA2	1:VA:257:TYR:O	1.85	0.78
1:DA:476:ASN:OD1	1:KA:642:MET:HB2	1.84	0.78
1:EA:642:MET:HB2	1:EB:476:ASN:OD1	1.84	0.78
1:GA:642:MET:HB2	1:QA:476:ASN:OD1	1.84	0.78
1:JA:476:ASN:OD1	1:SA:642:MET:HB2	1.84	0.78
1:A:642:MET:HB2	1:N:476:ASN:OD1	1.84	0.77
1:F:726:GLY:HA2	1:FB:257:TYR:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:726:GLY:HA2	1:MA:257:TYR:O	1.85	0.77
1:Y:476:ASN:OD1	1:FA:642:MET:HB2	1.84	0.77
1:MA:726:GLY:HA2	1:HB:257:TYR:O	1.85	0.77
1:J:726:GLY:HA2	1:HA:257:TYR:O	1.85	0.77
1:O:476:ASN:OD1	1:Y:642:MET:HB2	1.84	0.77
1:Z:642:MET:HB2	1:UA:476:ASN:OD1	1.84	0.77
1:HA:726:GLY:HA2	1:XA:257:TYR:O	1.85	0.77
1:MA:476:ASN:OD1	1:RA:642:MET:HB2	1.84	0.77
1:E:476:ASN:OD1	1:NA:642:MET:HB2	1.84	0.77
1:J:476:ASN:OD1	1:DA:642:MET:HB2	1.84	0.77
1:V:642:MET:HB2	1:IA:476:ASN:OD1	1.84	0.77
1:W:257:TYR:O	1:PA:726:GLY:HA2	1.85	0.77
1:Z:476:ASN:OD1	1:HB:642:MET:HB2	1.84	0.77
1:AA:642:MET:HB2	1:NA:476:ASN:OD1	1.84	0.77
1:A:726:GLY:HA2	1:QA:257:TYR:O	1.85	0.77
1:B:642:MET:HB2	1:LA:476:ASN:OD1	1.84	0.77
1:B:726:GLY:HA2	1:YA:257:TYR:O	1.85	0.77
1:P:726:GLY:HA2	1:AB:257:TYR:O	1.85	0.77
1:Q:642:MET:HB2	1:GA:476:ASN:OD1	1.84	0.77
1:BA:257:TYR:O	1:ZA:726:GLY:HA2	1.85	0.77
1:EA:476:ASN:OD1	1:XA:642:MET:HB2	1.84	0.77
1:HA:476:ASN:OD1	1:BB:642:MET:HB2	1.84	0.77
1:C:726:GLY:HA2	1:IA:257:TYR:O	1.85	0.77
1:M:726:GLY:HA2	1:DA:257:TYR:O	1.85	0.77
1:Q:726:GLY:HA2	1:IB:257:TYR:O	1.85	0.77
1:T:476:ASN:OD1	1:IA:642:MET:HB2	1.84	0.77
1:X:726:GLY:HA2	1:CB:257:TYR:O	1.85	0.77
1:CA:476:ASN:OD1	1:GB:642:MET:HB2	1.84	0.77
1:F:476:ASN:OD1	1:TA:642:MET:HB2	1.84	0.77
1:G:726:GLY:HA2	1:DB:257:TYR:O	1.85	0.77
1:H:726:GLY:HA2	1:Y:257:TYR:O	1.85	0.77
1:M:257:TYR:O	1:YA:726:GLY:HA2	1.85	0.77
1:R:257:TYR:O	1:DB:726:GLY:HA2	1.85	0.77
1:R:726:GLY:HA2	1:NA:257:TYR:O	1.85	0.77
1:X:476:ASN:OD1	1:WA:642:MET:HB2	1.84	0.77
1:CA:726:GLY:HA2	1:SA:257:TYR:O	1.85	0.77
1:JA:257:TYR:O	1:VA:726:GLY:HA2	1.85	0.77
1:C:257:TYR:O	1:TA:726:GLY:HA2	1.85	0.77
1:C:476:ASN:OD1	1:CA:642:MET:HB2	1.84	0.77
1:K:476:ASN:OD1	1:DB:642:MET:HB2	1.84	0.77
1:L:726:GLY:HA2	1:TA:257:TYR:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:476:ASN:OD1	1:X:642:MET:HB2	1.84	0.77
1:T:642:MET:HB2	1:V:476:ASN:OD1	1.84	0.77
1:Z:726:GLY:HA2	1:RA:257:TYR:O	1.85	0.77
1:LA:257:TYR:O	1:UA:726:GLY:HA2	1.84	0.77
1:H:257:TYR:O	1:IB:726:GLY:HA2	1.85	0.77
1:OA:257:TYR:O	1:FB:726:GLY:HA2	1.85	0.77
1:ZA:257:TYR:O	1:HB:726:GLY:HA2	1.85	0.77
1:D:726:GLY:HA2	1:F:257:TYR:O	1.85	0.77
1:F:642:MET:HB2	1:S:476:ASN:OD1	1.84	0.77
1:K:257:TYR:O	1:S:726:GLY:HA2	1.85	0.77
1:L:476:ASN:OD1	1:FB:642:MET:HB2	1.84	0.77
1:N:257:TYR:O	1:RA:726:GLY:HA2	1.84	0.77
1:GA:257:TYR:O	1:EB:726:GLY:HA2	1.85	0.77
1:IA:726:GLY:HA2	1:KA:257:TYR:O	1.85	0.77
1:PA:257:TYR:O	1:XA:726:GLY:HA2	1.85	0.77
1:D:476:ASN:OD1	1:K:642:MET:HB2	1.84	0.77
1:E:642:MET:HB2	1:AA:476:ASN:OD1	1.84	0.77
1:H:642:MET:HB2	1:RA:476:ASN:OD1	1.84	0.77
1:I:257:TYR:O	1:BB:726:GLY:HA2	1.85	0.77
1:L:642:MET:HB2	1:W:476:ASN:OD1	1.84	0.77
1:M:642:MET:HB2	1:BB:476:ASN:OD1	1.84	0.77
1:Q:476:ASN:OD1	1:QA:642:MET:HB2	1.84	0.77
1:EA:726:GLY:HA2	1:BB:257:TYR:O	1.85	0.77
1:FA:257:TYR:O	1:NA:726:GLY:HA2	1.85	0.77
1:B:476:ASN:OD1	1:AB:642:MET:HB2	1.84	0.76
1:G:476:ASN:OD1	1:VA:642:MET:HB2	1.84	0.76
1:R:642:MET:HB2	1:WA:476:ASN:OD1	1.84	0.76
1:JA:726:GLY:HA2	1:GB:257:TYR:O	1.85	0.76
1:PA:642:MET:HB2	1:CB:476:ASN:OD1	1.84	0.76
1:C:642:MET:HB2	1:GB:476:ASN:OD1	1.84	0.76
1:M:476:ASN:OD1	1:HA:642:MET:HB2	1.84	0.76
1:Z:257:TYR:O	1:AB:726:GLY:HA2	1.85	0.76
1:SA:476:ASN:OD1	1:ZA:642:MET:HB2	1.84	0.76
1:G:642:MET:HB2	1:BA:476:ASN:OD1	1.84	0.76
1:T:257:TYR:O	1:LA:726:GLY:HA2	1.85	0.76
1:W:642:MET:HB2	1:FB:476:ASN:OD1	1.84	0.76
1:EA:257:TYR:O	1:QA:726:GLY:HA2	1.85	0.76
1:OA:726:GLY:HA2	1:WA:257:TYR:O	1.85	0.76
1:SA:726:GLY:HA2	1:UA:257:TYR:O	1.85	0.76
1:A:476:ASN:OD1	1:IB:642:MET:HB2	1.84	0.76
1:D:257:TYR:O	1:WA:726:GLY:HA2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:257:TYR:O	1:FA:726:GLY:HA2	1.85	0.76
1:H:476:ASN:OD1	1:MA:642:MET:HB2	1.84	0.76
1:L:257:TYR:O	1:KA:726:GLY:HA2	1.84	0.76
1:N:642:MET:HB2	1:IB:476:ASN:OD1	1.84	0.76
1:BA:642:MET:HB2	1:VA:476:ASN:OD1	1.84	0.76
1:UA:642:MET:HB2	1:HB:476:ASN:OD1	1.84	0.76
1:XA:476:ASN:OD1	1:EB:642:MET:HB2	1.84	0.76
1:E:257:TYR:O	1:GA:726:GLY:HA2	1.85	0.76
1:I:642:MET:HB2	1:YA:476:ASN:OD1	1.84	0.76
1:O:257:TYR:O	1:BA:726:GLY:HA2	1.85	0.76
1:P:476:ASN:OD1	1:YA:642:MET:HB2	1.84	0.76
1:S:257:TYR:O	1:GB:726:GLY:HA2	1.85	0.76
1:CB:726:GLY:HA2	1:EB:257:TYR:O	1.85	0.76
1:J:257:TYR:O	1:W:726:GLY:HA2	1.85	0.76
1:N:726:GLY:HA2	1:P:257:TYR:O	1.85	0.76
1:A:257:TYR:O	1:I:726:GLY:HA2	1.85	0.76
1:Q:257:TYR:O	1:AA:726:GLY:HA2	1.85	0.76
1:B:257:TYR:O	1:V:726:GLY:HA2	1.85	0.75
1:V:257:TYR:O	1:DA:726:GLY:HA2	1.85	0.75
1:E:726:GLY:HA2	1:X:257:TYR:O	1.85	0.75
1:Y:726:GLY:HA2	1:AA:257:TYR:O	1.85	0.75
1:T:726:GLY:HA2	1:CA:257:TYR:O	1.85	0.75
1:E:440:GLN:NE2	1:NA:356:SER:O	2.21	0.73
1:T:440:GLN:NE2	1:IA:356:SER:O	2.21	0.73
1:HA:440:GLN:NE2	1:BB:356:SER:O	2.21	0.73
1:MA:440:GLN:NE2	1:RA:356:SER:O	2.21	0.73
1:Z:356:SER:O	1:UA:440:GLN:NE2	2.21	0.72
1:A:440:GLN:NE2	1:IB:356:SER:O	2.20	0.72
1:H:356:SER:O	1:RA:440:GLN:NE2	2.21	0.72
1:M:356:SER:O	1:BB:440:GLN:NE2	2.21	0.72
1:EA:356:SER:O	1:EB:440:GLN:NE2	2.21	0.72
1:K:440:GLN:NE2	1:DB:356:SER:O	2.20	0.72
1:F:440:GLN:NE2	1:TA:356:SER:O	2.21	0.72
1:Y:440:GLN:NE2	1:FA:356:SER:O	2.21	0.72
1:B:356:SER:O	1:LA:440:GLN:NE2	2.21	0.72
1:W:356:SER:O	1:FB:440:GLN:NE2	2.20	0.71
1:I:356:SER:O	1:YA:440:GLN:NE2	2.21	0.71
1:Q:356:SER:O	1:GA:440:GLN:NE2	2.21	0.71
1:R:440:GLN:NE2	1:X:356:SER:O	2.21	0.71
1:OA:440:GLN:NE2	1:CB:356:SER:O	2.21	0.71
1:A:356:SER:O	1:N:440:GLN:NE2	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:440:GLN:NE2	1:QA:356:SER:O	2.21	0.71
1:V:356:SER:O	1:IA:440:GLN:NE2	2.21	0.71
1:DA:440:GLN:NE2	1:KA:356:SER:O	2.21	0.71
1:AA:356:SER:O	1:NA:440:GLN:NE2	2.21	0.71
1:I:440:GLN:NE2	1:P:356:SER:O	2.21	0.71
1:N:356:SER:O	1:IB:440:GLN:NE2	2.21	0.71
1:BA:356:SER:O	1:VA:440:GLN:NE2	2.21	0.71
1:B:440:GLN:NE2	1:AB:356:SER:O	2.21	0.71
1:C:440:GLN:NE2	1:CA:356:SER:O	2.21	0.71
1:JA:440:GLN:NE2	1:SA:356:SER:O	2.21	0.71
1:G:440:GLN:NE2	1:VA:356:SER:O	2.21	0.71
1:L:440:GLN:NE2	1:FB:356:SER:O	2.21	0.71
1:PA:356:SER:O	1:CB:440:GLN:NE2	2.21	0.71
1:G:356:SER:O	1:BA:440:GLN:NE2	2.21	0.71
1:GA:356:SER:O	1:QA:440:GLN:NE2	2.21	0.71
1:SA:440:GLN:NE2	1:ZA:356:SER:O	2.21	0.70
1:LA:356:SER:O	1:AB:440:GLN:NE2	2.21	0.70
1:L:356:SER:O	1:W:440:GLN:NE2	2.21	0.70
1:WA:219:ASP:HB3	1:WA:223:ASN:HB3	1.74	0.70
1:E:356:SER:O	1:AA:440:GLN:NE2	2.21	0.69
1:F:298:ARG:NH1	1:L:697:GLU:OE1	2.26	0.69
1:G:697:GLU:OE1	1:K:298:ARG:NH1	2.25	0.69
1:J:219:ASP:HB3	1:J:223:ASN:HB3	1.74	0.69
1:AA:298:ARG:NH1	1:GA:697:GLU:OE1	2.25	0.69
1:WA:697:GLU:OE1	1:DB:298:ARG:NH1	2.25	0.69
1:H:697:GLU:OE1	1:O:298:ARG:NH1	2.26	0.69
1:J:298:ARG:NH1	1:M:697:GLU:OE1	2.26	0.69
1:T:356:SER:O	1:V:440:GLN:NE2	2.21	0.69
1:V:298:ARG:NH1	1:LA:697:GLU:OE1	2.26	0.69
1:EA:298:ARG:NH1	1:HA:697:GLU:OE1	2.26	0.69
1:UA:219:ASP:HB3	1:UA:223:ASN:HB3	1.74	0.69
1:XA:298:ARG:NH1	1:CB:697:GLU:OE1	2.26	0.69
1:GB:219:ASP:HB3	1:GB:223:ASN:HB3	1.74	0.69
1:C:697:GLU:OE1	1:T:298:ARG:NH1	2.26	0.69
1:E:298:ARG:NH1	1:R:697:GLU:OE1	2.25	0.69
1:J:440:GLN:NE2	1:DA:356:SER:O	2.21	0.69
1:O:219:ASP:HB3	1:O:223:ASN:HB3	1.74	0.69
1:W:697:GLU:OE1	1:KA:298:ARG:NH1	2.25	0.69
1:Z:298:ARG:NH1	1:MA:697:GLU:OE1	2.26	0.69
1:AA:697:GLU:OE1	1:GA:298:ARG:NH1	2.26	0.69
1:SA:298:ARG:NH1	1:HB:697:GLU:OE1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TA:298:ARG:NH1	1:GB:697:GLU:OE1	2.26	0.69
1:VA:697:GLU:OE1	1:ZA:298:ARG:NH1	2.25	0.69
1:XA:697:GLU:OE1	1:CB:298:ARG:NH1	2.26	0.69
1:D:219:ASP:HB3	1:D:223:ASN:HB3	1.74	0.69
1:D:697:GLU:OE1	1:S:298:ARG:NH1	2.26	0.69
1:F:356:SER:O	1:S:440:GLN:NE2	2.21	0.69
1:V:697:GLU:OE1	1:LA:298:ARG:NH1	2.26	0.69
1:X:697:GLU:OE1	1:OA:298:ARG:NH1	2.25	0.69
1:BA:697:GLU:OE1	1:FA:298:ARG:NH1	2.26	0.69
1:PA:298:ARG:NH1	1:FB:697:GLU:OE1	2.26	0.69
1:SA:697:GLU:OE1	1:HB:298:ARG:NH1	2.26	0.69
1:XA:440:GLN:NE2	1:EB:356:SER:O	2.21	0.69
1:EB:219:ASP:HB3	1:EB:223:ASN:HB3	1.74	0.69
1:A:662:PRO:HG3	1:I:369:VAL:HG11	1.75	0.69
1:D:298:ARG:NH1	1:S:697:GLU:OE1	2.26	0.69
1:O:440:GLN:NE2	1:Y:356:SER:O	2.21	0.69
1:S:219:ASP:HB3	1:S:223:ASN:HB3	1.74	0.69
1:Z:369:VAL:HG11	1:RA:662:PRO:HG3	1.75	0.69
1:W:298:ARG:NH1	1:KA:697:GLU:OE1	2.26	0.69
1:CA:369:VAL:HG11	1:SA:662:PRO:HG3	1.75	0.69
1:CA:697:GLU:OE1	1:JA:298:ARG:NH1	2.26	0.69
1:EA:369:VAL:HG11	1:BB:662:PRO:HG3	1.75	0.69
1:LA:662:PRO:HG3	1:UA:369:VAL:HG11	1.75	0.69
1:UA:356:SER:O	1:HB:440:GLN:NE2	2.21	0.69
1:VA:219:ASP:HB3	1:VA:223:ASN:HB3	1.74	0.69
1:ZA:662:PRO:HG3	1:HB:369:VAL:HG11	1.75	0.69
1:F:369:VAL:HG11	1:FB:662:PRO:HG3	1.75	0.69
1:J:662:PRO:HG3	1:W:369:VAL:HG11	1.75	0.69
1:L:369:VAL:HG11	1:TA:662:PRO:HG3	1.75	0.69
1:N:369:VAL:HG11	1:P:662:PRO:HG3	1.75	0.69
1:O:608:VAL:O	1:Y:608:VAL:HG23	1.93	0.69
1:X:369:VAL:HG11	1:CB:662:PRO:HG3	1.75	0.69
1:BA:298:ARG:NH1	1:FA:697:GLU:OE1	2.26	0.69
1:CA:440:GLN:NE2	1:GB:356:SER:O	2.21	0.69
1:HA:369:VAL:HG11	1:XA:662:PRO:HG3	1.75	0.69
1:JA:608:VAL:O	1:SA:608:VAL:HG23	1.93	0.69
1:MA:369:VAL:HG11	1:HB:662:PRO:HG3	1.75	0.69
1:OA:608:VAL:O	1:CB:608:VAL:HG23	1.93	0.69
1:PA:662:PRO:HG3	1:XA:369:VAL:HG11	1.75	0.69
1:D:440:GLN:NE2	1:K:356:SER:O	2.21	0.69
1:E:608:VAL:HG23	1:AA:608:VAL:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:369:VAL:HG11	1:DB:662:PRO:HG3	1.75	0.69
1:I:608:VAL:HG23	1:YA:608:VAL:O	1.93	0.69
1:J:608:VAL:O	1:DA:608:VAL:HG23	1.93	0.69
1:K:369:VAL:HG11	1:VA:662:PRO:HG3	1.75	0.69
1:N:608:VAL:HG23	1:IB:608:VAL:O	1.93	0.69
1:O:662:PRO:HG3	1:BA:369:VAL:HG11	1.75	0.69
1:T:608:VAL:HG23	1:V:608:VAL:O	1.93	0.69
1:X:440:GLN:NE2	1:WA:356:SER:O	2.21	0.69
1:DA:298:ARG:NH1	1:IA:697:GLU:OE1	2.26	0.69
1:GA:662:PRO:HG3	1:EB:369:VAL:HG11	1.75	0.69
1:JA:662:PRO:HG3	1:VA:369:VAL:HG11	1.75	0.69
1:OA:662:PRO:HG3	1:FB:369:VAL:HG11	1.75	0.69
1:QA:219:ASP:HB3	1:QA:223:ASN:HB3	1.74	0.69
1:QA:298:ARG:NH1	1:EB:697:GLU:OE1	2.26	0.69
1:QA:697:GLU:OE1	1:EB:298:ARG:NH1	2.25	0.69
1:UA:697:GLU:OE1	1:AB:298:ARG:NH1	2.26	0.69
1:AB:219:ASP:HB3	1:AB:223:ASN:HB3	1.74	0.69
1:FB:219:ASP:HB3	1:FB:223:ASN:HB3	1.74	0.69
1:A:298:ARG:NH1	1:Q:697:GLU:OE1	2.25	0.69
1:E:697:GLU:OE1	1:R:298:ARG:NH1	2.26	0.69
1:P:440:GLN:NE2	1:YA:356:SER:O	2.21	0.69
1:Y:298:ARG:NH1	1:NA:697:GLU:OE1	2.26	0.69
1:HA:219:ASP:HB3	1:HA:223:ASN:HB3	1.74	0.69
1:MA:219:ASP:HB3	1:MA:223:ASN:HB3	1.74	0.69
1:SA:219:ASP:HB3	1:SA:223:ASN:HB3	1.74	0.69
1:UA:298:ARG:NH1	1:AB:697:GLU:OE1	2.26	0.69
1:F:219:ASP:HB3	1:F:223:ASN:HB3	1.74	0.69
1:I:608:VAL:O	1:P:608:VAL:HG23	1.93	0.69
1:T:219:ASP:HB3	1:T:223:ASN:HB3	1.74	0.69
1:X:298:ARG:NH1	1:OA:697:GLU:OE1	2.26	0.69
1:Y:697:GLU:OE1	1:NA:298:ARG:NH1	2.26	0.69
1:DA:697:GLU:OE1	1:IA:298:ARG:NH1	2.26	0.69
1:RA:697:GLU:OE1	1:IB:298:ARG:NH1	2.26	0.69
1:YA:298:ARG:NH1	1:BB:697:GLU:OE1	2.26	0.69
1:YA:697:GLU:OE1	1:BB:298:ARG:NH1	2.26	0.69
1:A:608:VAL:HG23	1:N:608:VAL:O	1.94	0.68
1:A:697:GLU:OE1	1:Q:298:ARG:NH1	2.26	0.68
1:C:219:ASP:HB3	1:C:223:ASN:HB3	1.74	0.68
1:C:298:ARG:NH1	1:T:697:GLU:OE1	2.26	0.68
1:C:726:GLY:CA	1:IA:257:TYR:O	2.42	0.68
1:D:356:SER:O	1:DB:440:GLN:NE2	2.21	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:608:VAL:O	1:VA:608:VAL:HG23	1.93	0.68
1:K:219:ASP:HB3	1:K:223:ASN:HB3	1.74	0.68
1:L:608:VAL:O	1:FB:608:VAL:HG23	1.93	0.68
1:M:440:GLN:NE2	1:HA:356:SER:O	2.21	0.68
1:R:219:ASP:HB3	1:R:223:ASN:HB3	1.74	0.68
1:R:356:SER:O	1:WA:440:GLN:NE2	2.21	0.68
1:T:608:VAL:O	1:IA:608:VAL:HG23	1.93	0.68
1:V:608:VAL:HG23	1:IA:608:VAL:O	1.94	0.68
1:EA:697:GLU:OE1	1:HA:298:ARG:NH1	2.26	0.68
1:HA:608:VAL:O	1:BB:608:VAL:HG23	1.93	0.68
1:LA:608:VAL:HG23	1:AB:608:VAL:O	1.93	0.68
1:NA:219:ASP:HB3	1:NA:223:ASN:HB3	1.74	0.68
1:OA:219:ASP:HB3	1:OA:223:ASN:HB3	1.74	0.68
1:OA:369:VAL:HG11	1:WA:662:PRO:HG3	1.75	0.68
1:RA:298:ARG:NH1	1:IB:697:GLU:OE1	2.26	0.68
1:SA:369:VAL:HG11	1:UA:662:PRO:HG3	1.75	0.68
1:A:369:VAL:HG11	1:QA:662:PRO:HG3	1.75	0.68
1:B:608:VAL:O	1:AB:608:VAL:HG23	1.93	0.68
1:B:697:GLU:OE1	1:P:298:ARG:NH1	2.26	0.68
1:C:356:SER:O	1:GB:440:GLN:NE2	2.21	0.68
1:C:662:PRO:HG3	1:TA:369:VAL:HG11	1.75	0.68
1:E:219:ASP:HB3	1:E:223:ASN:HB3	1.74	0.68
1:F:697:GLU:OE1	1:L:298:ARG:NH1	2.26	0.68
1:G:608:VAL:HG23	1:BA:608:VAL:O	1.94	0.68
1:K:662:PRO:HG3	1:S:369:VAL:HG11	1.75	0.68
1:L:608:VAL:HG23	1:W:608:VAL:O	1.93	0.68
1:R:726:GLY:CA	1:NA:257:TYR:O	2.42	0.68
1:S:356:SER:O	1:TA:440:GLN:NE2	2.21	0.68
1:T:662:PRO:HG3	1:LA:369:VAL:HG11	1.75	0.68
1:W:662:PRO:HG3	1:PA:369:VAL:HG11	1.75	0.68
1:Y:608:VAL:O	1:FA:608:VAL:HG23	1.93	0.68
1:AA:608:VAL:HG23	1:NA:608:VAL:O	1.94	0.68
1:BA:662:PRO:HG3	1:ZA:369:VAL:HG11	1.75	0.68
1:CA:298:ARG:NH1	1:JA:697:GLU:OE1	2.26	0.68
1:GA:608:VAL:HG23	1:QA:608:VAL:O	1.93	0.68
1:JA:219:ASP:HB3	1:JA:223:ASN:HB3	1.74	0.68
1:JA:369:VAL:HG11	1:GB:662:PRO:HG3	1.75	0.68
1:MA:608:VAL:O	1:RA:608:VAL:HG23	1.93	0.68
1:TA:219:ASP:HB3	1:TA:223:ASN:HB3	1.74	0.68
1:CB:219:ASP:HB3	1:CB:223:ASN:HB3	1.74	0.68
1:CB:369:VAL:HG11	1:EB:662:PRO:HG3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:219:ASP:HB3	1:DB:223:ASN:HB3	1.74	0.68
1:B:298:ARG:NH1	1:P:697:GLU:OE1	2.26	0.68
1:C:608:VAL:O	1:CA:608:VAL:HG23	1.93	0.68
1:D:369:VAL:HG11	1:F:662:PRO:HG3	1.75	0.68
1:E:608:VAL:O	1:NA:608:VAL:HG23	1.93	0.68
1:G:298:ARG:NH1	1:K:697:GLU:OE1	2.26	0.68
1:I:298:ARG:NH1	1:N:697:GLU:OE1	2.26	0.68
1:I:697:GLU:OE1	1:N:298:ARG:NH1	2.26	0.68
1:J:356:SER:O	1:KA:440:GLN:NE2	2.20	0.68
1:M:726:GLY:CA	1:DA:257:TYR:O	2.42	0.68
1:P:369:VAL:HG11	1:AB:662:PRO:HG3	1.75	0.68
1:R:662:PRO:HG3	1:DB:369:VAL:HG11	1.75	0.68
1:Z:697:GLU:OE1	1:MA:298:ARG:NH1	2.26	0.68
1:DA:608:VAL:O	1:KA:608:VAL:HG23	1.94	0.68
1:FA:662:PRO:HG3	1:NA:369:VAL:HG11	1.75	0.68
1:IA:219:ASP:HB3	1:IA:223:ASN:HB3	1.74	0.68
1:IA:369:VAL:HG11	1:KA:662:PRO:HG3	1.75	0.68
1:JA:257:TYR:O	1:VA:726:GLY:CA	2.42	0.68
1:KA:219:ASP:HB3	1:KA:223:ASN:HB3	1.74	0.68
1:PA:697:GLU:OE1	1:FB:298:ARG:NH1	2.26	0.68
1:VA:298:ARG:NH1	1:ZA:697:GLU:OE1	2.26	0.68
1:E:662:PRO:HG3	1:GA:369:VAL:HG11	1.75	0.68
1:H:726:GLY:CA	1:Y:257:TYR:O	2.42	0.68
1:K:608:VAL:O	1:DB:608:VAL:HG23	1.93	0.68
1:L:257:TYR:O	1:KA:726:GLY:CA	2.42	0.68
1:R:608:VAL:O	1:X:608:VAL:HG23	1.94	0.68
1:X:608:VAL:O	1:WA:608:VAL:HG23	1.93	0.68
1:CA:219:ASP:HB3	1:CA:223:ASN:HB3	1.74	0.68
1:CA:608:VAL:O	1:GB:608:VAL:HG23	1.93	0.68
1:FA:219:ASP:HB3	1:FA:223:ASN:HB3	1.74	0.68
1:GA:219:ASP:HB3	1:GA:223:ASN:HB3	1.74	0.68
1:LA:257:TYR:O	1:UA:726:GLY:CA	2.42	0.68
1:OA:257:TYR:O	1:FB:726:GLY:CA	2.42	0.68
1:SA:726:GLY:CA	1:UA:257:TYR:O	2.42	0.68
1:YA:219:ASP:HB3	1:YA:223:ASN:HB3	1.74	0.68
1:ZA:219:ASP:HB3	1:ZA:223:ASN:HB3	1.74	0.68
1:IB:219:ASP:HB3	1:IB:223:ASN:HB3	1.74	0.68
1:H:440:GLN:NE2	1:MA:356:SER:O	2.21	0.68
1:Q:608:VAL:O	1:QA:608:VAL:HG23	1.93	0.68
1:V:219:ASP:HB3	1:V:223:ASN:HB3	1.74	0.68
1:X:219:ASP:HB3	1:X:223:ASN:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:257:TYR:O	1:NA:726:GLY:CA	2.42	0.68
1:GA:257:TYR:O	1:EB:726:GLY:CA	2.42	0.68
1:PA:219:ASP:HB3	1:PA:223:ASN:HB3	1.74	0.68
1:WA:298:ARG:NH1	1:DB:697:GLU:OE1	2.26	0.68
1:ZA:257:TYR:O	1:HB:726:GLY:CA	2.42	0.68
1:BB:219:ASP:HB3	1:BB:223:ASN:HB3	1.74	0.68
1:B:662:PRO:HG3	1:V:369:VAL:HG11	1.75	0.68
1:D:726:GLY:CA	1:F:257:TYR:O	2.42	0.68
1:F:608:VAL:O	1:TA:608:VAL:HG23	1.93	0.68
1:G:257:TYR:O	1:FA:726:GLY:CA	2.42	0.68
1:H:608:VAL:HG23	1:RA:608:VAL:O	1.93	0.68
1:K:257:TYR:O	1:S:726:GLY:CA	2.42	0.68
1:N:257:TYR:O	1:RA:726:GLY:CA	2.42	0.68
1:O:608:VAL:HG23	1:FA:608:VAL:O	1.93	0.68
1:R:369:VAL:HG11	1:NA:662:PRO:HG3	1.75	0.68
1:AA:219:ASP:HB3	1:AA:223:ASN:HB3	1.74	0.68
1:BA:608:VAL:HG23	1:VA:608:VAL:O	1.93	0.68
1:IA:726:GLY:CA	1:KA:257:TYR:O	2.42	0.68
1:LA:219:ASP:HB3	1:LA:223:ASN:HB3	1.74	0.68
1:PA:257:TYR:O	1:XA:726:GLY:CA	2.42	0.68
1:RA:219:ASP:HB3	1:RA:223:ASN:HB3	1.74	0.68
1:CB:726:GLY:CA	1:EB:257:TYR:O	2.42	0.68
1:C:369:VAL:HG11	1:IA:662:PRO:HG3	1.75	0.68
1:J:608:VAL:HG23	1:KA:608:VAL:O	1.93	0.68
1:N:662:PRO:HG3	1:RA:369:VAL:HG11	1.75	0.68
1:Q:662:PRO:HG3	1:AA:369:VAL:HG11	1.75	0.68
1:W:608:VAL:HG23	1:FB:608:VAL:O	1.93	0.68
1:TA:697:GLU:OE1	1:GB:298:ARG:NH1	2.26	0.68
1:A:726:GLY:CA	1:QA:257:TYR:O	2.42	0.68
1:E:369:VAL:HG11	1:X:662:PRO:HG3	1.75	0.68
1:G:219:ASP:HB3	1:G:223:ASN:HB3	1.74	0.68
1:M:608:VAL:HG23	1:BB:608:VAL:O	1.94	0.68
1:O:356:SER:O	1:FA:440:GLN:NE2	2.21	0.68
1:O:726:GLY:CA	1:MA:257:TYR:O	2.42	0.68
1:P:726:GLY:CA	1:AB:257:TYR:O	2.42	0.68
1:BA:219:ASP:HB3	1:BA:223:ASN:HB3	1.74	0.68
1:PA:608:VAL:HG23	1:CB:608:VAL:O	1.94	0.68
1:SA:608:VAL:O	1:ZA:608:VAL:HG23	1.93	0.68
1:XA:608:VAL:O	1:EB:608:VAL:HG23	1.94	0.68
1:E:726:GLY:CA	1:X:257:TYR:O	2.42	0.68
1:H:219:ASP:HB3	1:H:223:ASN:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:257:TYR:O	1:BB:726:GLY:CA	2.42	0.68
1:I:662:PRO:HG3	1:BB:369:VAL:HG11	1.75	0.68
1:J:726:GLY:CA	1:HA:257:TYR:O	2.42	0.68
1:L:219:ASP:HB3	1:L:223:ASN:HB3	1.74	0.68
1:R:257:TYR:O	1:DB:726:GLY:CA	2.42	0.68
1:T:369:VAL:HG11	1:CA:662:PRO:HG3	1.75	0.68
1:W:219:ASP:HB3	1:W:223:ASN:HB3	1.74	0.68
1:CA:726:GLY:CA	1:SA:257:TYR:O	2.42	0.68
1:EA:608:VAL:HG23	1:EB:608:VAL:O	1.93	0.68
1:EA:726:GLY:CA	1:BB:257:TYR:O	2.42	0.68
1:JA:356:SER:O	1:ZA:440:GLN:NE2	2.21	0.68
1:UA:608:VAL:HG23	1:HB:608:VAL:O	1.94	0.68
1:A:219:ASP:HB3	1:A:223:ASN:HB3	1.74	0.68
1:C:257:TYR:O	1:TA:726:GLY:CA	2.42	0.68
1:H:298:ARG:NH1	1:O:697:GLU:OE1	2.26	0.68
1:I:219:ASP:HB3	1:I:223:ASN:HB3	1.74	0.68
1:M:219:ASP:HB3	1:M:223:ASN:HB3	1.74	0.68
1:O:257:TYR:O	1:BA:726:GLY:CA	2.42	0.68
1:P:219:ASP:HB3	1:P:223:ASN:HB3	1.74	0.68
1:Q:219:ASP:HB3	1:Q:223:ASN:HB3	1.74	0.68
1:T:726:GLY:CA	1:CA:257:TYR:O	2.42	0.68
1:X:726:GLY:CA	1:CB:257:TYR:O	2.42	0.68
1:Z:608:VAL:HG23	1:UA:608:VAL:O	1.93	0.68
1:Z:726:GLY:CA	1:RA:257:TYR:O	2.42	0.68
1:OA:356:SER:O	1:PA:440:GLN:NE2	2.21	0.68
1:XA:219:ASP:HB3	1:XA:223:ASN:HB3	1.74	0.68
1:B:219:ASP:HB3	1:B:223:ASN:HB3	1.74	0.67
1:B:369:VAL:HG11	1:YA:662:PRO:HG3	1.75	0.67
1:F:608:VAL:HG23	1:S:608:VAL:O	1.94	0.67
1:F:615:GLN:NE2	1:TA:633:ASP:H	1.93	0.67
1:J:257:TYR:O	1:W:726:GLY:CA	2.42	0.67
1:J:633:ASP:H	1:KA:615:GLN:NE2	1.93	0.67
1:J:697:GLU:OE1	1:M:298:ARG:NH1	2.26	0.67
1:K:615:GLN:NE2	1:DB:633:ASP:H	1.93	0.67
1:L:662:PRO:HG3	1:KA:369:VAL:HG11	1.75	0.67
1:N:219:ASP:HB3	1:N:223:ASN:HB3	1.74	0.67
1:O:633:ASP:H	1:FA:615:GLN:NE2	1.93	0.67
1:V:662:PRO:HG3	1:DA:369:VAL:HG11	1.75	0.67
1:Y:369:VAL:HG11	1:AA:662:PRO:HG3	1.75	0.67
1:Z:615:GLN:NE2	1:HB:633:ASP:H	1.92	0.67
1:Z:662:PRO:HG3	1:AB:369:VAL:HG11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:615:GLN:NE2	1:XA:633:ASP:H	1.92	0.67
1:E:633:ASP:H	1:AA:615:GLN:NE2	1.93	0.67
1:F:633:ASP:H	1:S:615:GLN:NE2	1.93	0.67
1:G:662:PRO:HG3	1:FA:369:VAL:HG11	1.75	0.67
1:J:615:GLN:NE2	1:DA:633:ASP:H	1.92	0.67
1:O:615:GLN:NE2	1:Y:633:ASP:H	1.92	0.67
1:Q:726:GLY:CA	1:IB:257:TYR:O	2.42	0.67
1:T:615:GLN:NE2	1:IA:633:ASP:H	1.92	0.67
1:T:633:ASP:H	1:V:615:GLN:NE2	1.92	0.67
1:DA:219:ASP:HB3	1:DA:223:ASN:HB3	1.74	0.67
1:EA:662:PRO:HG3	1:QA:369:VAL:HG11	1.75	0.67
1:HB:219:ASP:HB3	1:HB:223:ASN:HB3	1.74	0.67
1:B:608:VAL:HG23	1:LA:608:VAL:O	1.93	0.67
1:B:726:GLY:CA	1:YA:257:TYR:O	2.42	0.67
1:D:633:ASP:H	1:DB:615:GLN:NE2	1.92	0.67
1:M:608:VAL:O	1:HA:608:VAL:HG23	1.93	0.67
1:Q:257:TYR:O	1:AA:726:GLY:CA	2.42	0.67
1:Q:369:VAL:HG11	1:IB:662:PRO:HG3	1.75	0.67
1:S:257:TYR:O	1:GB:726:GLY:CA	2.42	0.67
1:Y:219:ASP:HB3	1:Y:223:ASN:HB3	1.74	0.67
1:EA:440:GLN:NE2	1:XA:356:SER:O	2.21	0.67
1:D:257:TYR:O	1:WA:726:GLY:CA	2.42	0.67
1:D:608:VAL:O	1:K:608:VAL:HG23	1.94	0.67
1:D:615:GLN:NE2	1:K:633:ASP:H	1.93	0.67
1:E:615:GLN:NE2	1:NA:633:ASP:H	1.93	0.67
1:K:726:GLY:CA	1:VA:257:TYR:O	2.42	0.67
1:N:726:GLY:CA	1:P:257:TYR:O	2.42	0.67
1:S:608:VAL:HG23	1:TA:608:VAL:O	1.93	0.67
1:S:633:ASP:H	1:TA:615:GLN:NE2	1.93	0.67
1:EA:219:ASP:HB3	1:EA:223:ASN:HB3	1.74	0.67
1:GA:633:ASP:H	1:QA:615:GLN:NE2	1.93	0.67
1:HA:726:GLY:CA	1:XA:257:TYR:O	2.42	0.67
1:JA:615:GLN:NE2	1:SA:633:ASP:H	1.92	0.67
1:JA:633:ASP:H	1:ZA:615:GLN:NE2	1.92	0.67
1:LA:633:ASP:H	1:AB:615:GLN:NE2	1.93	0.67
1:MA:726:GLY:CA	1:HB:257:TYR:O	2.42	0.67
1:B:257:TYR:O	1:V:726:GLY:CA	2.42	0.67
1:B:615:GLN:NE2	1:AB:633:ASP:H	1.93	0.67
1:D:608:VAL:HG23	1:DB:608:VAL:O	1.93	0.67
1:H:608:VAL:O	1:MA:608:VAL:HG23	1.93	0.67
1:Q:608:VAL:HG23	1:GA:608:VAL:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:608:VAL:O	1:HB:608:VAL:HG23	1.93	0.67
1:EA:608:VAL:O	1:XA:608:VAL:HG23	1.93	0.67
1:JA:608:VAL:HG23	1:ZA:608:VAL:O	1.93	0.67
1:OA:608:VAL:HG23	1:PA:608:VAL:O	1.93	0.67
1:OA:615:GLN:NE2	1:CB:633:ASP:H	1.92	0.67
1:A:257:TYR:O	1:I:726:GLY:CA	2.42	0.67
1:E:257:TYR:O	1:GA:726:GLY:CA	2.42	0.67
1:F:726:GLY:CA	1:FB:257:TYR:O	2.42	0.67
1:H:633:ASP:H	1:RA:615:GLN:NE2	1.93	0.67
1:M:633:ASP:H	1:BB:615:GLN:NE2	1.93	0.67
1:P:608:VAL:O	1:YA:608:VAL:HG23	1.93	0.67
1:Q:615:GLN:NE2	1:QA:633:ASP:H	1.93	0.67
1:Z:440:GLN:NE2	1:HB:356:SER:O	2.21	0.67
1:EA:257:TYR:O	1:QA:726:GLY:CA	2.42	0.67
1:OA:633:ASP:H	1:PA:615:GLN:NE2	1.93	0.67
1:A:608:VAL:O	1:IB:608:VAL:HG23	1.93	0.67
1:C:633:ASP:H	1:GB:615:GLN:NE2	1.93	0.67
1:M:257:TYR:O	1:YA:726:GLY:CA	2.42	0.67
1:T:257:TYR:O	1:LA:726:GLY:CA	2.42	0.67
1:Z:219:ASP:HB3	1:Z:223:ASN:HB3	1.74	0.67
1:BA:633:ASP:H	1:VA:615:GLN:NE2	1.93	0.67
1:G:726:GLY:CA	1:DB:257:TYR:O	2.42	0.67
1:H:257:TYR:O	1:IB:726:GLY:CA	2.42	0.67
1:O:369:VAL:HG11	1:MA:662:PRO:HG3	1.75	0.67
1:R:633:ASP:H	1:WA:615:GLN:NE2	1.93	0.67
1:S:662:PRO:HG3	1:GB:369:VAL:HG11	1.75	0.67
1:Z:257:TYR:O	1:AB:726:GLY:CA	2.42	0.67
1:G:633:ASP:H	1:BA:615:GLN:NE2	1.93	0.67
1:H:369:VAL:HG11	1:Y:662:PRO:HG3	1.75	0.67
1:L:726:GLY:CA	1:TA:257:TYR:O	2.42	0.67
1:M:662:PRO:HG3	1:YA:369:VAL:HG11	1.75	0.67
1:W:633:ASP:H	1:FB:615:GLN:NE2	1.93	0.67
1:Y:615:GLN:NE2	1:FA:633:ASP:H	1.93	0.67
1:B:633:ASP:H	1:LA:615:GLN:NE2	1.93	0.67
1:D:662:PRO:HG3	1:WA:369:VAL:HG11	1.75	0.67
1:Q:633:ASP:H	1:GA:615:GLN:NE2	1.93	0.67
1:R:608:VAL:HG23	1:WA:608:VAL:O	1.94	0.67
1:DA:615:GLN:NE2	1:KA:633:ASP:H	1.93	0.67
1:A:633:ASP:H	1:N:615:GLN:NE2	1.93	0.66
1:C:608:VAL:HG23	1:GB:608:VAL:O	1.93	0.66
1:I:633:ASP:H	1:YA:615:GLN:NE2	1.92	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:369:VAL:HG11	1:HA:662:PRO:HG3	1.75	0.66
1:N:633:ASP:H	1:IB:615:GLN:NE2	1.92	0.66
1:UA:633:ASP:H	1:HB:615:GLN:NE2	1.93	0.66
1:XA:615:GLN:NE2	1:EB:633:ASP:H	1.93	0.66
1:H:662:PRO:HG3	1:IB:369:VAL:HG11	1.75	0.66
1:I:615:GLN:NE2	1:P:633:ASP:H	1.93	0.66
1:M:369:VAL:HG11	1:DA:662:PRO:HG3	1.75	0.66
1:M:615:GLN:NE2	1:HA:633:ASP:H	1.93	0.66
1:CA:615:GLN:NE2	1:GB:633:ASP:H	1.93	0.66
1:HA:615:GLN:NE2	1:BB:633:ASP:H	1.93	0.66
1:OA:726:GLY:CA	1:WA:257:TYR:O	2.42	0.66
1:G:615:GLN:NE2	1:VA:633:ASP:H	1.93	0.66
1:L:633:ASP:H	1:W:615:GLN:NE2	1.93	0.66
1:V:633:ASP:H	1:IA:615:GLN:NE2	1.93	0.66
1:BA:257:TYR:O	1:ZA:726:GLY:CA	2.42	0.66
1:JA:726:GLY:CA	1:GB:257:TYR:O	2.42	0.66
1:MA:615:GLN:NE2	1:RA:633:ASP:H	1.93	0.66
1:H:615:GLN:NE2	1:MA:633:ASP:H	1.93	0.66
1:W:257:TYR:O	1:PA:726:GLY:CA	2.42	0.66
1:L:615:GLN:NE2	1:FB:633:ASP:H	1.93	0.66
1:X:615:GLN:NE2	1:WA:633:ASP:H	1.93	0.66
1:AA:633:ASP:H	1:NA:615:GLN:NE2	1.93	0.66
1:A:615:GLN:NE2	1:IB:633:ASP:H	1.93	0.66
1:Y:726:GLY:CA	1:AA:257:TYR:O	2.42	0.66
1:P:615:GLN:NE2	1:YA:633:ASP:H	1.92	0.66
1:R:615:GLN:NE2	1:X:633:ASP:H	1.93	0.66
1:V:257:TYR:O	1:DA:726:GLY:CA	2.42	0.66
1:Z:633:ASP:H	1:UA:615:GLN:NE2	1.93	0.66
1:C:615:GLN:NE2	1:CA:633:ASP:H	1.93	0.66
1:EA:633:ASP:H	1:EB:615:GLN:NE2	1.93	0.66
1:SA:615:GLN:NE2	1:ZA:633:ASP:H	1.93	0.65
1:PA:633:ASP:H	1:CB:615:GLN:NE2	1.93	0.65
1:XA:448:THR:OG1	1:EB:499:GLU:HA	1.97	0.65
1:Q:448:THR:OG1	1:QA:499:GLU:HA	1.97	0.65
1:Z:354:LEU:HD13	1:Z:653:GLN:HG2	1.79	0.65
1:DA:354:LEU:HD13	1:DA:653:GLN:HG2	1.79	0.65
1:DA:448:THR:OG1	1:KA:499:GLU:HA	1.97	0.65
1:UA:499:GLU:HA	1:HB:448:THR:OG1	1.97	0.65
1:CB:354:LEU:HD13	1:CB:653:GLN:HG2	1.80	0.65
1:B:448:THR:OG1	1:AB:499:GLU:HA	1.97	0.64
1:L:499:GLU:HA	1:W:448:THR:OG1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:354:LEU:HD13	1:EA:653:GLN:HG2	1.80	0.64
1:SA:354:LEU:HD13	1:SA:653:GLN:HG2	1.80	0.64
1:TA:354:LEU:HD13	1:TA:653:GLN:HG2	1.80	0.64
1:DB:354:LEU:HD13	1:DB:653:GLN:HG2	1.80	0.64
1:Y:354:LEU:HD13	1:Y:653:GLN:HG2	1.80	0.64
1:Y:448:THR:OG1	1:FA:499:GLU:HA	1.97	0.64
1:BA:354:LEU:HD13	1:BA:653:GLN:HG2	1.79	0.64
1:BB:354:LEU:HD13	1:BB:653:GLN:HG2	1.80	0.64
1:GB:354:LEU:HD13	1:GB:653:GLN:HG2	1.80	0.64
1:B:354:LEU:HD13	1:B:653:GLN:HG2	1.80	0.64
1:G:499:GLU:HA	1:BA:448:THR:OG1	1.98	0.64
1:W:354:LEU:HD13	1:W:653:GLN:HG2	1.80	0.64
1:QA:354:LEU:HD13	1:QA:653:GLN:HG2	1.80	0.64
1:RA:354:LEU:HD13	1:RA:653:GLN:HG2	1.80	0.64
1:WA:354:LEU:HD13	1:WA:653:GLN:HG2	1.80	0.64
1:AB:354:LEU:HD13	1:AB:653:GLN:HG2	1.80	0.64
1:C:448:THR:OG1	1:CA:499:GLU:HA	1.97	0.64
1:Q:354:LEU:HD13	1:Q:653:GLN:HG2	1.79	0.64
1:R:499:GLU:HA	1:WA:448:THR:OG1	1.97	0.64
1:Z:499:GLU:HA	1:UA:448:THR:OG1	1.98	0.64
1:EA:499:GLU:HA	1:EB:448:THR:OG1	1.98	0.64
1:HA:354:LEU:HD13	1:HA:653:GLN:HG2	1.80	0.64
1:JA:448:THR:OG1	1:SA:499:GLU:HA	1.98	0.64
1:MA:354:LEU:HD13	1:MA:653:GLN:HG2	1.79	0.64
1:PA:499:GLU:HA	1:CB:448:THR:OG1	1.97	0.64
1:SA:448:THR:OG1	1:ZA:499:GLU:HA	1.97	0.64
1:EB:354:LEU:HD13	1:EB:653:GLN:HG2	1.80	0.64
1:A:354:LEU:HD13	1:A:653:GLN:HG2	1.80	0.64
1:C:499:GLU:HA	1:GB:448:THR:OG1	1.98	0.64
1:D:448:THR:OG1	1:K:499:GLU:HA	1.97	0.64
1:G:354:LEU:HD13	1:G:653:GLN:HG2	1.80	0.64
1:L:354:LEU:HD13	1:L:653:GLN:HG2	1.79	0.64
1:P:354:LEU:HD13	1:P:653:GLN:HG2	1.80	0.64
1:R:448:THR:OG1	1:X:499:GLU:HA	1.97	0.64
1:BA:499:GLU:HA	1:VA:448:THR:OG1	1.98	0.64
1:PA:354:LEU:HD13	1:PA:653:GLN:HG2	1.80	0.64
1:UA:354:LEU:HD13	1:UA:653:GLN:HG2	1.80	0.64
1:D:499:GLU:HA	1:DB:448:THR:OG1	1.98	0.64
1:S:499:GLU:HA	1:TA:448:THR:OG1	1.98	0.64
1:FA:354:LEU:HD13	1:FA:653:GLN:HG2	1.80	0.64
1:OA:448:THR:OG1	1:CB:499:GLU:HA	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OA:499:GLU:HA	1:PA:448:THR:OG1	1.98	0.64
1:XA:354:LEU:HD13	1:XA:653:GLN:HG2	1.79	0.64
1:ZA:354:LEU:HD13	1:ZA:653:GLN:HG2	1.80	0.64
1:HB:354:LEU:HD13	1:HB:653:GLN:HG2	1.80	0.64
1:E:448:THR:OG1	1:NA:499:GLU:HA	1.98	0.64
1:H:354:LEU:HD13	1:H:653:GLN:HG2	1.79	0.64
1:M:354:LEU:HD13	1:M:653:GLN:HG2	1.80	0.64
1:V:499:GLU:HA	1:IA:448:THR:OG1	1.97	0.64
1:AA:499:GLU:HA	1:NA:448:THR:OG1	1.97	0.64
1:KA:354:LEU:HD13	1:KA:653:GLN:HG2	1.80	0.64
1:YA:354:LEU:HD13	1:YA:653:GLN:HG2	1.80	0.64
1:F:499:GLU:HA	1:S:448:THR:OG1	1.97	0.64
1:P:448:THR:OG1	1:YA:499:GLU:HA	1.98	0.64
1:W:499:GLU:HA	1:FB:448:THR:OG1	1.98	0.64
1:IB:354:LEU:HD13	1:IB:653:GLN:HG2	1.80	0.64
1:A:448:THR:OG1	1:IB:499:GLU:HA	1.98	0.64
1:G:448:THR:OG1	1:VA:499:GLU:HA	1.97	0.64
1:I:499:GLU:HA	1:YA:448:THR:OG1	1.98	0.64
1:T:448:THR:OG1	1:IA:499:GLU:HA	1.98	0.64
1:JA:499:GLU:HA	1:ZA:448:THR:OG1	1.98	0.64
1:E:354:LEU:HD13	1:E:653:GLN:HG2	1.79	0.64
1:F:448:THR:OG1	1:TA:499:GLU:HA	1.98	0.64
1:H:448:THR:OG1	1:MA:499:GLU:HA	1.98	0.64
1:K:448:THR:OG1	1:DB:499:GLU:HA	1.98	0.64
1:HA:448:THR:OG1	1:BB:499:GLU:HA	1.97	0.64
1:J:499:GLU:HA	1:KA:448:THR:OG1	1.98	0.63
1:M:448:THR:OG1	1:HA:499:GLU:HA	1.98	0.63
1:N:499:GLU:HA	1:IB:448:THR:OG1	1.98	0.63
1:L:448:THR:OG1	1:FB:499:GLU:HA	1.98	0.63
1:O:499:GLU:HA	1:FA:448:THR:OG1	1.98	0.63
1:T:354:LEU:HD13	1:T:653:GLN:HG2	1.80	0.63
1:LA:499:GLU:HA	1:AB:448:THR:OG1	1.97	0.63
1:MA:448:THR:OG1	1:RA:499:GLU:HA	1.97	0.63
1:X:354:LEU:HD13	1:X:653:GLN:HG2	1.79	0.63
1:X:448:THR:OG1	1:WA:499:GLU:HA	1.97	0.63
1:CA:448:THR:OG1	1:GB:499:GLU:HA	1.97	0.63
1:I:354:LEU:HD13	1:I:653:GLN:HG2	1.80	0.63
1:V:354:LEU:HD13	1:V:653:GLN:HG2	1.80	0.63
1:AA:354:LEU:HD13	1:AA:653:GLN:HG2	1.80	0.63
1:GA:499:GLU:HA	1:QA:448:THR:OG1	1.98	0.63
1:CA:354:LEU:HD13	1:CA:653:GLN:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:354:LEU:HD13	1:J:653:GLN:HG2	1.80	0.63
1:J:448:THR:OG1	1:DA:499:GLU:HA	1.98	0.63
1:N:354:LEU:HD13	1:N:653:GLN:HG2	1.80	0.63
1:Q:499:GLU:HA	1:GA:448:THR:OG1	1.98	0.63
1:Z:448:THR:OG1	1:HB:499:GLU:HA	1.98	0.63
1:EA:448:THR:OG1	1:XA:499:GLU:HA	1.98	0.63
1:GA:354:LEU:HD13	1:GA:653:GLN:HG2	1.80	0.63
1:LA:354:LEU:HD13	1:LA:653:GLN:HG2	1.80	0.63
1:O:354:LEU:HD13	1:O:653:GLN:HG2	1.80	0.63
1:NA:354:LEU:HD13	1:NA:653:GLN:HG2	1.80	0.63
1:B:499:GLU:HA	1:LA:448:THR:OG1	1.98	0.63
1:O:448:THR:OG1	1:Y:499:GLU:HA	1.98	0.63
1:IA:354:LEU:HD13	1:IA:653:GLN:HG2	1.80	0.63
1:OA:354:LEU:HD13	1:OA:653:GLN:HG2	1.80	0.63
1:K:354:LEU:HD13	1:K:653:GLN:HG2	1.80	0.63
1:M:499:GLU:HA	1:BB:448:THR:OG1	1.97	0.63
1:JA:354:LEU:HD13	1:JA:653:GLN:HG2	1.80	0.63
1:VA:354:LEU:HD13	1:VA:653:GLN:HG2	1.80	0.63
1:FB:354:LEU:HD13	1:FB:653:GLN:HG2	1.80	0.63
1:F:354:LEU:HD13	1:F:653:GLN:HG2	1.80	0.62
1:H:499:GLU:HA	1:RA:448:THR:OG1	1.97	0.62
1:A:499:GLU:HA	1:N:448:THR:OG1	1.97	0.62
1:D:354:LEU:HD13	1:D:653:GLN:HG2	1.80	0.62
1:F:701:ARG:HD3	1:F:705:GLU:HG2	1.82	0.62
1:S:701:ARG:HD3	1:S:705:GLU:HG2	1.81	0.62
1:FA:701:ARG:HD3	1:FA:705:GLU:HG2	1.82	0.62
1:KA:701:ARG:HD3	1:KA:705:GLU:HG2	1.82	0.62
1:TA:701:ARG:HD3	1:TA:705:GLU:HG2	1.81	0.62
1:AB:701:ARG:HD3	1:AB:705:GLU:HG2	1.82	0.62
1:D:701:ARG:HD3	1:D:705:GLU:HG2	1.82	0.62
1:I:448:THR:OG1	1:P:499:GLU:HA	1.98	0.62
1:K:701:ARG:HD3	1:K:705:GLU:HG2	1.82	0.62
1:S:354:LEU:HD13	1:S:653:GLN:HG2	1.80	0.62
1:QA:701:ARG:HD3	1:QA:705:GLU:HG2	1.82	0.62
1:DB:701:ARG:HD3	1:DB:705:GLU:HG2	1.82	0.62
1:AA:701:ARG:HD3	1:AA:705:GLU:HG2	1.82	0.62
1:V:701:ARG:HD3	1:V:705:GLU:HG2	1.82	0.62
1:HB:701:ARG:HD3	1:HB:705:GLU:HG2	1.82	0.62
1:T:499:GLU:HA	1:V:448:THR:OG1	1.98	0.62
1:DA:701:ARG:HD3	1:DA:705:GLU:HG2	1.82	0.62
1:B:701:ARG:HD3	1:B:705:GLU:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:701:ARG:HD3	1:Y:705:GLU:HG2	1.82	0.62
1:WA:701:ARG:HD3	1:WA:705:GLU:HG2	1.82	0.62
1:XA:701:ARG:HD3	1:XA:705:GLU:HG2	1.82	0.62
1:E:499:GLU:HA	1:AA:448:THR:OG1	1.98	0.62
1:Q:701:ARG:HD3	1:Q:705:GLU:HG2	1.82	0.62
1:R:354:LEU:HD13	1:R:653:GLN:HG2	1.80	0.62
1:Z:701:ARG:HD3	1:Z:705:GLU:HG2	1.82	0.62
1:GB:701:ARG:HD3	1:GB:705:GLU:HG2	1.82	0.62
1:C:354:LEU:HD13	1:C:653:GLN:HG2	1.80	0.62
1:O:701:ARG:HD3	1:O:705:GLU:HG2	1.82	0.62
1:EA:701:ARG:HD3	1:EA:705:GLU:HG2	1.82	0.62
1:EB:701:ARG:HD3	1:EB:705:GLU:HG2	1.82	0.62
1:J:701:ARG:HD3	1:J:705:GLU:HG2	1.82	0.62
1:UA:701:ARG:HD3	1:UA:705:GLU:HG2	1.82	0.62
1:L:508:TYR:CD1	1:W:479:PRO:HG2	2.35	0.61
1:GA:508:TYR:CD1	1:QA:479:PRO:HG2	2.35	0.61
1:G:508:TYR:CD1	1:BA:479:PRO:HG2	2.35	0.61
1:P:701:ARG:HD3	1:P:705:GLU:HG2	1.82	0.61
1:W:701:ARG:HD3	1:W:705:GLU:HG2	1.82	0.61
1:LA:508:TYR:CD1	1:AB:479:PRO:HG2	2.35	0.61
1:A:701:ARG:HD3	1:A:705:GLU:HG2	1.82	0.61
1:R:701:ARG:HD3	1:R:705:GLU:HG2	1.82	0.61
1:BA:701:ARG:HD3	1:BA:705:GLU:HG2	1.82	0.61
1:JA:701:ARG:HD3	1:JA:705:GLU:HG2	1.82	0.61
1:E:701:ARG:HD3	1:E:705:GLU:HG2	1.82	0.61
1:I:701:ARG:HD3	1:I:705:GLU:HG2	1.82	0.61
1:J:479:PRO:HG2	1:DA:508:TYR:CD1	2.35	0.61
1:L:701:ARG:HD3	1:L:705:GLU:HG2	1.82	0.61
1:N:701:ARG:HD3	1:N:705:GLU:HG2	1.82	0.61
1:O:479:PRO:HG2	1:Y:508:TYR:CD1	2.36	0.61
1:R:508:TYR:CD1	1:WA:479:PRO:HG2	2.35	0.61
1:DA:479:PRO:HG2	1:KA:508:TYR:CD1	2.36	0.61
1:EA:508:TYR:CD1	1:EB:479:PRO:HG2	2.35	0.61
1:SA:701:ARG:HD3	1:SA:705:GLU:HG2	1.81	0.61
1:VA:701:ARG:HD3	1:VA:705:GLU:HG2	1.82	0.61
1:FB:701:ARG:HD3	1:FB:705:GLU:HG2	1.82	0.61
1:C:508:TYR:CD1	1:GB:479:PRO:HG2	2.36	0.61
1:C:701:ARG:HD3	1:C:705:GLU:HG2	1.82	0.61
1:G:701:ARG:HD3	1:G:705:GLU:HG2	1.82	0.61
1:M:701:ARG:HD3	1:M:705:GLU:HG2	1.82	0.61
1:T:701:ARG:HD3	1:T:705:GLU:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:479:PRO:HG2	1:FA:508:TYR:CD1	2.36	0.61
1:Z:508:TYR:CD1	1:UA:479:PRO:HG2	2.36	0.61
1:PA:508:TYR:CD1	1:CB:479:PRO:HG2	2.35	0.61
1:SA:479:PRO:HG2	1:ZA:508:TYR:CD1	2.36	0.61
1:YA:701:ARG:HD3	1:YA:705:GLU:HG2	1.82	0.61
1:IB:701:ARG:HD3	1:IB:705:GLU:HG2	1.81	0.61
1:A:508:TYR:CD1	1:N:479:PRO:HG2	2.36	0.61
1:I:508:TYR:CD1	1:YA:479:PRO:HG2	2.36	0.61
1:N:508:TYR:CD1	1:IB:479:PRO:HG2	2.36	0.61
1:Q:508:TYR:CD1	1:GA:479:PRO:HG2	2.35	0.61
1:OA:701:ARG:HD3	1:OA:705:GLU:HG2	1.82	0.61
1:A:479:PRO:HG2	1:IB:508:TYR:CD1	2.36	0.61
1:B:508:TYR:CD1	1:LA:479:PRO:HG2	2.35	0.61
1:IA:701:ARG:HD3	1:IA:705:GLU:HG2	1.82	0.61
1:CB:701:ARG:HD3	1:CB:705:GLU:HG2	1.82	0.61
1:E:479:PRO:HG2	1:NA:508:TYR:CD1	2.36	0.61
1:H:701:ARG:HD3	1:H:705:GLU:HG2	1.82	0.61
1:I:479:PRO:HG2	1:P:508:TYR:CD1	2.36	0.61
1:M:508:TYR:CD1	1:BB:479:PRO:HG2	2.35	0.61
1:Q:479:PRO:HG2	1:QA:508:TYR:CD1	2.35	0.61
1:JA:479:PRO:HG2	1:SA:508:TYR:CD1	2.36	0.61
1:NA:701:ARG:HD3	1:NA:705:GLU:HG2	1.82	0.61
1:B:479:PRO:HG2	1:AB:508:TYR:CD1	2.35	0.61
1:E:508:TYR:CD1	1:AA:479:PRO:HG2	2.35	0.61
1:H:479:PRO:HG2	1:MA:508:TYR:CD1	2.35	0.61
1:H:508:TYR:CD1	1:RA:479:PRO:HG2	2.35	0.61
1:M:479:PRO:HG2	1:HA:508:TYR:CD1	2.36	0.61
1:P:479:PRO:HG2	1:YA:508:TYR:CD1	2.36	0.61
1:T:479:PRO:HG2	1:IA:508:TYR:CD1	2.36	0.61
1:AA:508:TYR:CD1	1:NA:479:PRO:HG2	2.35	0.61
1:HA:479:PRO:HG2	1:BB:508:TYR:CD1	2.35	0.61
1:UA:508:TYR:CD1	1:HB:479:PRO:HG2	2.36	0.61
1:XA:479:PRO:HG2	1:EB:508:TYR:CD1	2.36	0.61
1:T:508:TYR:CD1	1:V:479:PRO:HG2	2.35	0.61
1:HA:701:ARG:HD3	1:HA:705:GLU:HG2	1.82	0.61
1:MA:479:PRO:HG2	1:RA:508:TYR:CD1	2.35	0.61
1:MA:701:ARG:HD3	1:MA:705:GLU:HG2	1.82	0.61
1:OA:479:PRO:HG2	1:CB:508:TYR:CD1	2.36	0.61
1:D:479:PRO:HG2	1:K:508:TYR:CD1	2.35	0.60
1:L:479:PRO:HG2	1:FB:508:TYR:CD1	2.35	0.60
1:V:508:TYR:CD1	1:IA:479:PRO:HG2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:479:PRO:HG2	1:XA:508:TYR:CD1	2.36	0.60
1:JA:508:TYR:CD1	1:ZA:479:PRO:HG2	2.36	0.60
1:LA:259:GLN:OE1	1:UA:717:ASN:ND2	2.34	0.60
1:OA:508:TYR:CD1	1:PA:479:PRO:HG2	2.35	0.60
1:F:508:TYR:CD1	1:S:479:PRO:HG2	2.36	0.60
1:G:479:PRO:HG2	1:VA:508:TYR:CD1	2.35	0.60
1:Z:422:SER:HB2	1:HB:633:ASP:OD1	2.01	0.60
1:BA:508:TYR:CD1	1:VA:479:PRO:HG2	2.35	0.60
1:GA:259:GLN:OE1	1:EB:717:ASN:ND2	2.34	0.60
1:JA:259:GLN:OE1	1:VA:717:ASN:ND2	2.34	0.60
1:JA:633:ASP:OD1	1:ZA:422:SER:HB2	2.01	0.60
1:X:479:PRO:HG2	1:WA:508:TYR:CD1	2.35	0.60
1:Z:479:PRO:HG2	1:HB:508:TYR:CD1	2.36	0.60
1:Z:633:ASP:OD1	1:UA:422:SER:HB2	2.02	0.60
1:EA:422:SER:HB2	1:XA:633:ASP:OD1	2.01	0.60
1:OA:259:GLN:OE1	1:FB:717:ASN:ND2	2.34	0.60
1:BB:701:ARG:HD3	1:BB:705:GLU:HG2	1.82	0.60
1:O:508:TYR:CD1	1:FA:479:PRO:HG2	2.36	0.60
1:P:422:SER:HB2	1:YA:633:ASP:OD1	2.01	0.60
1:W:508:TYR:CD1	1:FB:479:PRO:HG2	2.35	0.60
1:GA:701:ARG:HD3	1:GA:705:GLU:HG2	1.82	0.60
1:LA:701:ARG:HD3	1:LA:705:GLU:HG2	1.82	0.60
1:RA:701:ARG:HD3	1:RA:705:GLU:HG2	1.82	0.60
1:C:479:PRO:HG2	1:CA:508:TYR:CD1	2.35	0.60
1:J:508:TYR:CD1	1:KA:479:PRO:HG2	2.36	0.60
1:R:479:PRO:HG2	1:X:508:TYR:CD1	2.35	0.60
1:S:508:TYR:CD1	1:TA:479:PRO:HG2	2.36	0.60
1:EA:633:ASP:OD1	1:EB:422:SER:HB2	2.02	0.60
1:HA:717:ASN:ND2	1:XA:259:GLN:OE1	2.34	0.60
1:OA:633:ASP:OD1	1:PA:422:SER:HB2	2.02	0.60
1:D:508:TYR:CD1	1:DB:479:PRO:HG2	2.36	0.60
1:E:422:SER:HB2	1:NA:633:ASP:OD1	2.02	0.60
1:F:479:PRO:HG2	1:TA:508:TYR:CD1	2.35	0.60
1:H:259:GLN:OE1	1:IB:717:ASN:ND2	2.34	0.60
1:M:259:GLN:OE1	1:YA:717:ASN:ND2	2.34	0.60
1:T:422:SER:HB2	1:IA:633:ASP:OD1	2.01	0.60
1:X:701:ARG:HD3	1:X:705:GLU:HG2	1.82	0.60
1:CA:479:PRO:HG2	1:GB:508:TYR:CD1	2.35	0.60
1:JA:422:SER:HB2	1:SA:633:ASP:OD1	2.01	0.60
1:MA:717:ASN:ND2	1:HB:259:GLN:OE1	2.34	0.60
1:A:422:SER:HB2	1:IB:633:ASP:OD1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:717:ASN:ND2	1:F:259:GLN:OE1	2.34	0.60
1:K:479:PRO:HG2	1:DB:508:TYR:CD1	2.36	0.60
1:T:633:ASP:OD1	1:V:422:SER:HB2	2.01	0.60
1:E:633:ASP:OD1	1:AA:422:SER:HB2	2.02	0.60
1:G:633:ASP:OD1	1:BA:422:SER:HB2	2.02	0.60
1:K:259:GLN:OE1	1:S:717:ASN:ND2	2.34	0.60
1:S:633:ASP:OD1	1:TA:422:SER:HB2	2.01	0.60
1:CA:701:ARG:HD3	1:CA:705:GLU:HG2	1.82	0.60
1:OA:422:SER:HB2	1:CB:633:ASP:OD1	2.02	0.60
1:SA:717:ASN:ND2	1:UA:259:GLN:OE1	2.34	0.60
1:ZA:259:GLN:OE1	1:HB:717:ASN:ND2	2.34	0.60
1:D:633:ASP:OD1	1:DB:422:SER:HB2	2.02	0.60
1:I:259:GLN:OE1	1:BB:717:ASN:ND2	2.34	0.60
1:L:633:ASP:OD1	1:W:422:SER:HB2	2.02	0.60
1:M:633:ASP:OD1	1:BB:422:SER:HB2	2.02	0.60
1:N:259:GLN:OE1	1:RA:717:ASN:ND2	2.34	0.60
1:PA:259:GLN:OE1	1:XA:717:ASN:ND2	2.34	0.60
1:C:633:ASP:OD1	1:GB:422:SER:HB2	2.02	0.60
1:F:633:ASP:OD1	1:S:422:SER:HB2	2.02	0.60
1:CA:422:SER:HB2	1:GB:633:ASP:OD1	2.02	0.60
1:UA:633:ASP:OD1	1:HB:422:SER:HB2	2.02	0.60
1:CB:717:ASN:ND2	1:EB:259:GLN:OE1	2.34	0.60
1:D:422:SER:HB2	1:K:633:ASP:OD1	2.02	0.59
1:H:633:ASP:OD1	1:RA:422:SER:HB2	2.02	0.59
1:I:633:ASP:OD1	1:YA:422:SER:HB2	2.01	0.59
1:R:633:ASP:OD1	1:WA:422:SER:HB2	2.02	0.59
1:X:422:SER:HB2	1:WA:633:ASP:OD1	2.02	0.59
1:AA:633:ASP:OD1	1:NA:422:SER:HB2	2.02	0.59
1:GA:633:ASP:OD1	1:QA:422:SER:HB2	2.02	0.59
1:LA:633:ASP:OD1	1:AB:422:SER:HB2	2.02	0.59
1:PA:701:ARG:HD3	1:PA:705:GLU:HG2	1.82	0.59
1:XA:422:SER:HB2	1:EB:633:ASP:OD1	2.02	0.59
1:G:422:SER:HB2	1:VA:633:ASP:OD1	2.02	0.59
1:J:259:GLN:OE1	1:W:717:ASN:ND2	2.34	0.59
1:L:422:SER:HB2	1:FB:633:ASP:OD1	2.02	0.59
1:N:633:ASP:OD1	1:IB:422:SER:HB2	2.01	0.59
1:O:259:GLN:OE1	1:BA:717:ASN:ND2	2.34	0.59
1:O:422:SER:HB2	1:Y:633:ASP:OD1	2.01	0.59
1:V:633:ASP:OD1	1:IA:422:SER:HB2	2.02	0.59
1:ZA:701:ARG:HD3	1:ZA:705:GLU:HG2	1.82	0.59
1:E:717:ASN:ND2	1:X:259:GLN:OE1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:633:ASP:OD1	1:FB:422:SER:HB2	2.02	0.59
1:A:259:GLN:OE1	1:I:717:ASN:ND2	2.34	0.59
1:J:422:SER:HB2	1:DA:633:ASP:OD1	2.02	0.59
1:K:422:SER:HB2	1:DB:633:ASP:OD1	2.02	0.59
1:T:717:ASN:ND2	1:CA:259:GLN:OE1	2.34	0.59
1:BA:633:ASP:OD1	1:VA:422:SER:HB2	2.02	0.59
1:PA:633:ASP:OD1	1:CB:422:SER:HB2	2.02	0.59
1:B:422:SER:HB2	1:AB:633:ASP:OD1	2.02	0.59
1:F:422:SER:HB2	1:TA:633:ASP:OD1	2.02	0.59
1:M:422:SER:HB2	1:HA:633:ASP:OD1	2.02	0.59
1:N:717:ASN:ND2	1:P:259:GLN:OE1	2.34	0.59
1:Q:422:SER:HB2	1:QA:633:ASP:OD1	2.02	0.59
1:Q:717:ASN:ND2	1:IB:259:GLN:OE1	2.34	0.59
1:EA:259:GLN:OE1	1:QA:717:ASN:ND2	2.34	0.59
1:SA:422:SER:HB2	1:ZA:633:ASP:OD1	2.02	0.59
1:B:633:ASP:OD1	1:LA:422:SER:HB2	2.02	0.59
1:B:717:ASN:ND2	1:YA:259:GLN:OE1	2.34	0.59
1:H:422:SER:HB2	1:MA:633:ASP:OD1	2.02	0.59
1:V:259:GLN:OE1	1:DA:717:ASN:ND2	2.34	0.59
1:Z:259:GLN:OE1	1:AB:717:ASN:ND2	2.34	0.59
1:G:259:GLN:OE1	1:FA:717:ASN:ND2	2.34	0.59
1:L:259:GLN:OE1	1:KA:717:ASN:ND2	2.34	0.59
1:Q:633:ASP:OD1	1:GA:422:SER:HB2	2.02	0.59
1:Y:717:ASN:ND2	1:AA:259:GLN:OE1	2.34	0.59
1:A:633:ASP:OD1	1:N:422:SER:HB2	2.02	0.58
1:I:422:SER:HB2	1:P:633:ASP:OD1	2.02	0.58
1:JA:717:ASN:ND2	1:GB:259:GLN:OE1	2.34	0.58
1:H:717:ASN:ND2	1:Y:259:GLN:OE1	2.34	0.58
1:O:633:ASP:OD1	1:FA:422:SER:HB2	2.02	0.58
1:MA:422:SER:HB2	1:RA:633:ASP:OD1	2.02	0.58
1:C:422:SER:HB2	1:CA:633:ASP:OD1	2.02	0.58
1:DA:422:SER:HB2	1:KA:633:ASP:OD1	2.02	0.58
1:FA:259:GLN:OE1	1:NA:717:ASN:ND2	2.34	0.58
1:HA:422:SER:HB2	1:BB:633:ASP:OD1	2.02	0.58
1:OA:717:ASN:ND2	1:WA:259:GLN:OE1	2.34	0.58
1:J:633:ASP:OD1	1:KA:422:SER:HB2	2.02	0.58
1:M:717:ASN:ND2	1:DA:259:GLN:OE1	2.34	0.58
1:R:422:SER:HB2	1:X:633:ASP:OD1	2.02	0.58
1:D:488:VAL:CG1	1:DB:460:LEU:HD11	2.34	0.58
1:Y:422:SER:HB2	1:FA:633:ASP:OD1	2.02	0.58
1:IA:717:ASN:ND2	1:KA:259:GLN:OE1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:GLN:OE1	1:GA:717:ASN:ND2	2.34	0.58
1:S:488:VAL:CG1	1:TA:460:LEU:HD11	2.34	0.58
1:Y:460:LEU:HD11	1:FA:488:VAL:CG1	2.34	0.58
1:DA:460:LEU:HD11	1:KA:488:VAL:CG1	2.34	0.58
1:HA:250:PRO:HB3	1:XA:665:PRO:HG2	1.86	0.58
1:UA:488:VAL:CG1	1:HB:460:LEU:HD11	2.34	0.58
1:C:250:PRO:HB3	1:IA:665:PRO:HG2	1.86	0.58
1:J:488:VAL:CG1	1:KA:460:LEU:HD11	2.34	0.58
1:K:717:ASN:ND2	1:VA:259:GLN:OE1	2.34	0.58
1:R:250:PRO:HB3	1:NA:665:PRO:HG2	1.86	0.58
1:T:259:GLN:OE1	1:LA:717:ASN:ND2	2.34	0.58
1:MA:250:PRO:HB3	1:HB:665:PRO:HG2	1.86	0.58
1:XA:460:LEU:HD11	1:EB:488:VAL:CG1	2.34	0.58
1:A:665:PRO:HG2	1:I:250:PRO:HB3	1.86	0.58
1:F:717:ASN:ND2	1:FB:259:GLN:OE1	2.34	0.58
1:H:488:VAL:CG1	1:RA:460:LEU:HD11	2.34	0.58
1:M:488:VAL:CG1	1:BB:460:LEU:HD11	2.34	0.58
1:V:665:PRO:HG2	1:DA:250:PRO:HB3	1.86	0.58
1:Y:250:PRO:HB3	1:AA:665:PRO:HG2	1.86	0.58
1:Z:717:ASN:ND2	1:RA:259:GLN:OE1	2.34	0.58
1:LA:665:PRO:HG2	1:UA:250:PRO:HB3	1.86	0.58
1:D:259:GLN:OE1	1:WA:717:ASN:ND2	2.34	0.58
1:N:250:PRO:HB3	1:P:665:PRO:HG2	1.86	0.58
1:O:488:VAL:CG1	1:FA:460:LEU:HD11	2.34	0.58
1:JA:665:PRO:HG2	1:VA:250:PRO:HB3	1.86	0.58
1:A:488:VAL:CG1	1:N:460:LEU:HD11	2.34	0.58
1:B:250:PRO:HB3	1:YA:665:PRO:HG2	1.86	0.58
1:C:460:LEU:HD11	1:CA:488:VAL:CG1	2.34	0.58
1:D:460:LEU:HD11	1:K:488:VAL:CG1	2.34	0.58
1:G:488:VAL:CG1	1:BA:460:LEU:HD11	2.34	0.58
1:I:460:LEU:HD11	1:P:488:VAL:CG1	2.34	0.58
1:L:665:PRO:HG2	1:KA:250:PRO:HB3	1.86	0.58
1:O:665:PRO:HG2	1:BA:250:PRO:HB3	1.86	0.58
1:Q:250:PRO:HB3	1:IB:665:PRO:HG2	1.86	0.58
1:W:259:GLN:OE1	1:PA:717:ASN:ND2	2.34	0.58
1:Z:460:LEU:HD11	1:HB:488:VAL:CG1	2.34	0.58
1:GA:665:PRO:HG2	1:EB:250:PRO:HB3	1.86	0.58
1:LA:488:VAL:CG1	1:AB:460:LEU:HD11	2.34	0.58
1:F:460:LEU:HD11	1:TA:488:VAL:CG1	2.34	0.57
1:F:488:VAL:CG1	1:S:460:LEU:HD11	2.34	0.57
1:G:665:PRO:HG2	1:FA:250:PRO:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:250:PRO:HB3	1:Y:665:PRO:HG2	1.86	0.57
1:J:665:PRO:HG2	1:W:250:PRO:HB3	1.86	0.57
1:K:460:LEU:HD11	1:DB:488:VAL:CG1	2.34	0.57
1:M:250:PRO:HB3	1:DA:665:PRO:HG2	1.86	0.57
1:R:460:LEU:HD11	1:X:488:VAL:CG1	2.34	0.57
1:X:460:LEU:HD11	1:WA:488:VAL:CG1	2.34	0.57
1:CA:250:PRO:HB3	1:SA:665:PRO:HG2	1.86	0.57
1:CA:717:ASN:ND2	1:SA:259:GLN:OE1	2.34	0.57
1:EA:460:LEU:HD11	1:XA:488:VAL:CG1	2.34	0.57
1:EA:717:ASN:ND2	1:BB:259:GLN:OE1	2.34	0.57
1:GA:488:VAL:CG1	1:QA:460:LEU:HD11	2.34	0.57
1:HA:460:LEU:HD11	1:BB:488:VAL:CG1	2.34	0.57
1:OA:665:PRO:HG2	1:FB:250:PRO:HB3	1.86	0.57
1:E:488:VAL:CG1	1:AA:460:LEU:HD11	2.34	0.57
1:G:250:PRO:HB3	1:DB:665:PRO:HG2	1.86	0.57
1:L:488:VAL:CG1	1:W:460:LEU:HD11	2.34	0.57
1:P:460:LEU:HD11	1:YA:488:VAL:CG1	2.34	0.57
1:S:259:GLN:OE1	1:GB:717:ASN:ND2	2.34	0.57
1:T:488:VAL:CG1	1:V:460:LEU:HD11	2.34	0.57
1:X:250:PRO:HB3	1:CB:665:PRO:HG2	1.86	0.57
1:BA:259:GLN:OE1	1:ZA:717:ASN:ND2	2.34	0.57
1:CA:460:LEU:HD11	1:GB:488:VAL:CG1	2.34	0.57
1:A:460:LEU:HD11	1:IB:488:VAL:CG1	2.34	0.57
1:B:488:VAL:CG1	1:LA:460:LEU:HD11	2.34	0.57
1:D:665:PRO:HG2	1:WA:250:PRO:HB3	1.86	0.57
1:M:665:PRO:HG2	1:YA:250:PRO:HB3	1.86	0.57
1:X:717:ASN:ND2	1:CB:259:GLN:OE1	2.34	0.57
1:MA:460:LEU:HD11	1:RA:488:VAL:CG1	2.34	0.57
1:B:259:GLN:OE1	1:V:717:ASN:ND2	2.34	0.57
1:B:460:LEU:HD11	1:AB:488:VAL:CG1	2.34	0.57
1:C:511:ASN:OD1	1:GB:566:ARG:HD2	2.05	0.57
1:C:665:PRO:HG2	1:TA:250:PRO:HB3	1.86	0.57
1:E:400:SER:OG	1:GA:228:TRP:HB3	2.05	0.57
1:H:665:PRO:HG2	1:IB:250:PRO:HB3	1.86	0.57
1:J:566:ARG:HD2	1:DA:511:ASN:OD1	2.05	0.57
1:L:250:PRO:HB3	1:TA:665:PRO:HG2	1.86	0.57
1:M:566:ARG:HD2	1:HA:511:ASN:OD1	2.05	0.57
1:N:488:VAL:CG1	1:IB:460:LEU:HD11	2.34	0.57
1:O:566:ARG:HD2	1:Y:511:ASN:OD1	2.05	0.57
1:S:665:PRO:HG2	1:GB:250:PRO:HB3	1.86	0.57
1:T:400:SER:OG	1:LA:228:TRP:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:488:VAL:CG1	1:IA:460:LEU:HD11	2.34	0.57
1:Z:400:SER:OG	1:AB:228:TRP:HB3	2.05	0.57
1:Z:665:PRO:HG2	1:AB:250:PRO:HB3	1.86	0.57
1:EA:400:SER:OG	1:QA:228:TRP:HB3	2.05	0.57
1:EA:511:ASN:OD1	1:EB:566:ARG:HD2	2.05	0.57
1:EA:665:PRO:HG2	1:QA:250:PRO:HB3	1.86	0.57
1:HA:228:TRP:HB3	1:XA:400:SER:OG	2.05	0.57
1:B:665:PRO:HG2	1:V:250:PRO:HB3	1.86	0.57
1:C:259:GLN:OE1	1:TA:717:ASN:ND2	2.34	0.57
1:C:488:VAL:CG1	1:GB:460:LEU:HD11	2.34	0.57
1:G:460:LEU:HD11	1:VA:488:VAL:CG1	2.34	0.57
1:H:566:ARG:HD2	1:MA:511:ASN:OD1	2.05	0.57
1:I:488:VAL:CG1	1:YA:460:LEU:HD11	2.34	0.57
1:L:460:LEU:HD11	1:FB:488:VAL:CG1	2.34	0.57
1:Q:460:LEU:HD11	1:QA:488:VAL:CG1	2.34	0.57
1:Q:488:VAL:CG1	1:GA:460:LEU:HD11	2.34	0.57
1:R:511:ASN:OD1	1:WA:566:ARG:HD2	2.05	0.57
1:Z:511:ASN:OD1	1:UA:566:ARG:HD2	2.05	0.57
1:EA:566:ARG:HD2	1:XA:511:ASN:OD1	2.05	0.57
1:MA:228:TRP:HB3	1:HB:400:SER:OG	2.05	0.57
1:PA:665:PRO:HG2	1:XA:250:PRO:HB3	1.86	0.57
1:SA:250:PRO:HB3	1:UA:665:PRO:HG2	1.86	0.57
1:CB:250:PRO:HB3	1:EB:665:PRO:HG2	1.86	0.57
1:D:400:SER:OG	1:WA:228:TRP:HB3	2.05	0.57
1:I:400:SER:OG	1:BB:228:TRP:HB3	2.05	0.57
1:L:566:ARG:HD2	1:FB:511:ASN:OD1	2.05	0.57
1:Q:665:PRO:HG2	1:AA:250:PRO:HB3	1.86	0.57
1:R:488:VAL:CG1	1:WA:460:LEU:HD11	2.34	0.57
1:R:665:PRO:HG2	1:DB:250:PRO:HB3	1.86	0.57
1:Z:566:ARG:HD2	1:HB:511:ASN:OD1	2.05	0.57
1:AA:488:VAL:CG1	1:NA:460:LEU:HD11	2.34	0.57
1:BA:488:VAL:CG1	1:VA:460:LEU:HD11	2.34	0.57
1:DA:566:ARG:HD2	1:KA:511:ASN:OD1	2.05	0.57
1:EA:250:PRO:HB3	1:BB:665:PRO:HG2	1.86	0.57
1:LA:511:ASN:OD1	1:AB:566:ARG:HD2	2.05	0.57
1:OA:400:SER:OG	1:FB:228:TRP:HB3	2.05	0.57
1:PA:511:ASN:OD1	1:CB:566:ARG:HD2	2.05	0.57
1:SA:566:ARG:HD2	1:ZA:511:ASN:OD1	2.05	0.57
1:ZA:665:PRO:HG2	1:HB:250:PRO:HB3	1.86	0.57
1:G:566:ARG:HD2	1:VA:511:ASN:OD1	2.05	0.57
1:N:400:SER:OG	1:RA:228:TRP:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:259:GLN:OE1	1:AA:717:ASN:ND2	2.34	0.57
1:R:259:GLN:OE1	1:DB:717:ASN:ND2	2.34	0.57
1:S:400:SER:OG	1:GB:228:TRP:HB3	2.05	0.57
1:T:511:ASN:OD1	1:V:566:ARG:HD2	2.05	0.57
1:BA:511:ASN:OD1	1:VA:566:ARG:HD2	2.05	0.57
1:GA:511:ASN:OD1	1:QA:566:ARG:HD2	2.05	0.57
1:JA:400:SER:OG	1:VA:228:TRP:HB3	2.05	0.57
1:JA:488:VAL:CG1	1:ZA:460:LEU:HD11	2.34	0.57
1:OA:488:VAL:CG1	1:PA:460:LEU:HD11	2.34	0.57
1:ZA:400:SER:OG	1:HB:228:TRP:HB3	2.05	0.57
1:B:566:ARG:HD2	1:AB:511:ASN:OD1	2.05	0.57
1:E:511:ASN:OD1	1:AA:566:ARG:HD2	2.05	0.57
1:F:228:TRP:HB3	1:FB:400:SER:OG	2.05	0.57
1:K:228:TRP:HB3	1:VA:400:SER:OG	2.05	0.57
1:Q:566:ARG:HD2	1:QA:511:ASN:OD1	2.05	0.57
1:T:228:TRP:HB3	1:CA:400:SER:OG	2.05	0.57
1:W:488:VAL:CG1	1:FB:460:LEU:HD11	2.34	0.57
1:Z:250:PRO:HB3	1:RA:665:PRO:HG2	1.86	0.57
1:Z:488:VAL:CG1	1:UA:460:LEU:HD11	2.34	0.57
1:JA:460:LEU:HD11	1:SA:488:VAL:CG1	2.34	0.57
1:MA:566:ARG:HD2	1:RA:511:ASN:OD1	2.05	0.57
1:OA:460:LEU:HD11	1:CB:488:VAL:CG1	2.34	0.57
1:PA:400:SER:OG	1:XA:228:TRP:HB3	2.05	0.57
1:A:400:SER:OG	1:I:228:TRP:HB3	2.05	0.57
1:C:717:ASN:ND2	1:IA:259:GLN:OE1	2.34	0.57
1:D:228:TRP:HB3	1:F:400:SER:OG	2.05	0.57
1:H:400:SER:OG	1:IB:228:TRP:HB3	2.05	0.57
1:H:460:LEU:HD11	1:MA:488:VAL:CG1	2.34	0.57
1:J:228:TRP:HB3	1:HA:400:SER:OG	2.05	0.57
1:K:400:SER:OG	1:S:228:TRP:HB3	2.05	0.57
1:K:566:ARG:HD2	1:DB:511:ASN:OD1	2.05	0.57
1:M:460:LEU:HD11	1:HA:488:VAL:CG1	2.34	0.57
1:T:250:PRO:HB3	1:CA:665:PRO:HG2	1.86	0.57
1:W:511:ASN:OD1	1:FB:566:ARG:HD2	2.05	0.57
1:W:665:PRO:HG2	1:PA:250:PRO:HB3	1.86	0.57
1:Y:566:ARG:HD2	1:FA:511:ASN:OD1	2.05	0.57
1:AA:511:ASN:OD1	1:NA:566:ARG:HD2	2.05	0.57
1:BA:665:PRO:HG2	1:ZA:250:PRO:HB3	1.86	0.57
1:CA:228:TRP:HB3	1:SA:400:SER:OG	2.05	0.57
1:SA:460:LEU:HD11	1:ZA:488:VAL:CG1	2.34	0.57
1:E:228:TRP:HB3	1:X:400:SER:OG	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:PRO:HB3	1:X:665:PRO:HG2	1.86	0.57
1:E:460:LEU:HD11	1:NA:488:VAL:CG1	2.34	0.57
1:F:566:ARG:HD2	1:TA:511:ASN:OD1	2.05	0.57
1:J:460:LEU:HD11	1:DA:488:VAL:CG1	2.34	0.57
1:M:400:SER:OG	1:YA:228:TRP:HB3	2.05	0.57
1:R:228:TRP:HB3	1:NA:400:SER:OG	2.05	0.57
1:X:230:CYS:O	1:CB:397:TYR:O	2.23	0.57
1:EA:488:VAL:CG1	1:EB:460:LEU:HD11	2.34	0.57
1:A:228:TRP:HB3	1:QA:400:SER:OG	2.05	0.56
1:C:228:TRP:HB3	1:IA:400:SER:OG	2.05	0.56
1:D:397:TYR:O	1:WA:230:CYS:O	2.23	0.56
1:D:511:ASN:OD1	1:DB:566:ARG:HD2	2.05	0.56
1:G:400:SER:OG	1:FA:228:TRP:HB3	2.05	0.56
1:J:400:SER:OG	1:W:228:TRP:HB3	2.05	0.56
1:L:400:SER:OG	1:KA:228:TRP:HB3	2.05	0.56
1:N:228:TRP:HB3	1:P:400:SER:OG	2.05	0.56
1:O:228:TRP:HB3	1:MA:400:SER:OG	2.05	0.56
1:O:400:SER:OG	1:BA:228:TRP:HB3	2.05	0.56
1:S:397:TYR:O	1:GB:230:CYS:O	2.23	0.56
1:T:460:LEU:HD11	1:IA:488:VAL:CG1	2.34	0.56
1:V:511:ASN:OD1	1:IA:566:ARG:HD2	2.05	0.56
1:X:228:TRP:HB3	1:CB:400:SER:OG	2.05	0.56
1:CA:230:CYS:O	1:SA:397:TYR:O	2.23	0.56
1:HA:566:ARG:HD2	1:BB:511:ASN:OD1	2.05	0.56
1:IA:230:CYS:O	1:KA:397:TYR:O	2.23	0.56
1:OA:511:ASN:OD1	1:PA:566:ARG:HD2	2.05	0.56
1:PA:488:VAL:CG1	1:CB:460:LEU:HD11	2.34	0.56
1:E:397:TYR:O	1:GA:230:CYS:O	2.23	0.56
1:H:228:TRP:HB3	1:Y:400:SER:OG	2.05	0.56
1:L:228:TRP:HB3	1:TA:400:SER:OG	2.05	0.56
1:P:228:TRP:HB3	1:AB:400:SER:OG	2.05	0.56
1:P:717:ASN:ND2	1:AB:259:GLN:OE1	2.34	0.56
1:S:511:ASN:OD1	1:TA:566:ARG:HD2	2.05	0.56
1:T:397:TYR:O	1:LA:230:CYS:O	2.23	0.56
1:T:665:PRO:HG2	1:LA:250:PRO:HB3	1.86	0.56
1:FA:397:TYR:O	1:NA:230:CYS:O	2.24	0.56
1:FA:665:PRO:HG2	1:NA:250:PRO:HB3	1.86	0.56
1:IA:250:PRO:HB3	1:KA:665:PRO:HG2	1.86	0.56
1:JA:511:ASN:OD1	1:ZA:566:ARG:HD2	2.05	0.56
1:LA:400:SER:OG	1:UA:228:TRP:HB3	2.05	0.56
1:SA:230:CYS:O	1:UA:397:TYR:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CB:230:CYS:O	1:EB:397:TYR:O	2.24	0.56
1:A:717:ASN:ND2	1:QA:259:GLN:OE1	2.34	0.56
1:E:566:ARG:HD2	1:NA:511:ASN:OD1	2.05	0.56
1:E:665:PRO:HG2	1:GA:250:PRO:HB3	1.86	0.56
1:F:511:ASN:OD1	1:S:566:ARG:HD2	2.05	0.56
1:G:228:TRP:HB3	1:DB:400:SER:OG	2.05	0.56
1:M:228:TRP:HB3	1:DA:400:SER:OG	2.05	0.56
1:O:460:LEU:HD11	1:Y:488:VAL:CG1	2.34	0.56
1:O:511:ASN:OD1	1:FA:566:ARG:HD2	2.05	0.56
1:P:250:PRO:HB3	1:AB:665:PRO:HG2	1.86	0.56
1:P:566:ARG:HD2	1:YA:511:ASN:OD1	2.05	0.56
1:R:717:ASN:ND2	1:NA:259:GLN:OE1	2.34	0.56
1:T:566:ARG:HD2	1:IA:511:ASN:OD1	2.05	0.56
1:FA:400:SER:OG	1:NA:228:TRP:HB3	2.05	0.56
1:GA:400:SER:OG	1:EB:228:TRP:HB3	2.05	0.56
1:JA:228:TRP:HB3	1:GB:400:SER:OG	2.05	0.56
1:JA:566:ARG:HD2	1:SA:511:ASN:OD1	2.05	0.56
1:OA:228:TRP:HB3	1:WA:400:SER:OG	2.05	0.56
1:A:250:PRO:HB3	1:QA:665:PRO:HG2	1.86	0.56
1:A:566:ARG:HD2	1:IB:511:ASN:OD1	2.05	0.56
1:D:566:ARG:HD2	1:K:511:ASN:OD1	2.05	0.56
1:H:230:CYS:O	1:Y:397:TYR:O	2.23	0.56
1:M:230:CYS:O	1:DA:397:TYR:O	2.23	0.56
1:M:511:ASN:OD1	1:BB:566:ARG:HD2	2.05	0.56
1:R:566:ARG:HD2	1:X:511:ASN:OD1	2.05	0.56
1:IA:228:TRP:HB3	1:KA:400:SER:OG	2.05	0.56
1:A:397:TYR:O	1:I:230:CYS:O	2.24	0.56
1:B:400:SER:OG	1:V:228:TRP:HB3	2.05	0.56
1:H:511:ASN:OD1	1:RA:566:ARG:HD2	2.05	0.56
1:J:511:ASN:OD1	1:KA:566:ARG:HD2	2.05	0.56
1:K:665:PRO:HG2	1:S:250:PRO:HB3	1.86	0.56
1:L:511:ASN:OD1	1:W:566:ARG:HD2	2.05	0.56
1:Z:230:CYS:O	1:RA:397:TYR:O	2.24	0.56
1:EA:230:CYS:O	1:BB:397:TYR:O	2.24	0.56
1:OA:566:ARG:HD2	1:CB:511:ASN:OD1	2.05	0.56
1:CB:228:TRP:HB3	1:EB:400:SER:OG	2.05	0.56
1:C:566:ARG:HD2	1:CA:511:ASN:OD1	2.05	0.56
1:D:250:PRO:HB3	1:F:665:PRO:HG2	1.86	0.56
1:G:511:ASN:OD1	1:BA:566:ARG:HD2	2.05	0.56
1:J:250:PRO:HB3	1:HA:665:PRO:HG2	1.86	0.56
1:N:230:CYS:O	1:P:397:TYR:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:511:ASN:OD1	1:IB:566:ARG:HD2	2.05	0.56
1:N:665:PRO:HG2	1:RA:250:PRO:HB3	1.86	0.56
1:Q:400:SER:OG	1:AA:228:TRP:HB3	2.05	0.56
1:F:230:CYS:O	1:FB:397:TYR:O	2.24	0.56
1:I:397:TYR:O	1:BB:230:CYS:O	2.23	0.56
1:I:511:ASN:OD1	1:YA:566:ARG:HD2	2.05	0.56
1:I:665:PRO:HG2	1:BB:250:PRO:HB3	1.86	0.56
1:K:230:CYS:O	1:VA:397:TYR:O	2.24	0.56
1:N:397:TYR:O	1:RA:230:CYS:O	2.23	0.56
1:O:250:PRO:HB3	1:MA:665:PRO:HG2	1.86	0.56
1:SA:228:TRP:HB3	1:UA:400:SER:OG	2.05	0.56
1:UA:511:ASN:OD1	1:HB:566:ARG:HD2	2.05	0.56
1:XA:566:ARG:HD2	1:EB:511:ASN:OD1	2.05	0.56
1:B:511:ASN:OD1	1:LA:566:ARG:HD2	2.05	0.56
1:I:566:ARG:HD2	1:P:511:ASN:OD1	2.05	0.56
1:L:397:TYR:O	1:KA:230:CYS:O	2.24	0.56
1:X:566:ARG:HD2	1:WA:511:ASN:OD1	2.05	0.56
1:Y:228:TRP:HB3	1:AA:400:SER:OG	2.05	0.56
1:CA:566:ARG:HD2	1:GB:511:ASN:OD1	2.05	0.56
1:PA:397:TYR:O	1:XA:230:CYS:O	2.24	0.56
1:ZA:397:TYR:O	1:HB:230:CYS:O	2.24	0.56
1:A:511:ASN:OD1	1:N:566:ARG:HD2	2.05	0.56
1:B:397:TYR:O	1:V:230:CYS:O	2.24	0.56
1:G:397:TYR:O	1:FA:230:CYS:O	2.24	0.56
1:R:400:SER:OG	1:DB:228:TRP:HB3	2.05	0.56
1:EA:228:TRP:HB3	1:BB:400:SER:OG	2.05	0.56
1:C:400:SER:OG	1:TA:228:TRP:HB3	2.05	0.56
1:G:230:CYS:O	1:DB:397:TYR:O	2.23	0.56
1:L:230:CYS:O	1:TA:397:TYR:O	2.23	0.56
1:Q:228:TRP:HB3	1:IB:400:SER:OG	2.05	0.56
1:Q:397:TYR:O	1:AA:230:CYS:O	2.24	0.56
1:Q:511:ASN:OD1	1:GA:566:ARG:HD2	2.05	0.56
1:V:400:SER:OG	1:DA:228:TRP:HB3	2.05	0.56
1:Z:228:TRP:HB3	1:RA:400:SER:OG	2.05	0.56
1:I:380:LEU:HD12	1:I:389:ARG:HB3	1.89	0.55
1:C:380:LEU:HD12	1:C:389:ARG:HB3	1.89	0.55
1:F:250:PRO:HB3	1:FB:665:PRO:HG2	1.86	0.55
1:F:380:LEU:HD12	1:F:389:ARG:HB3	1.89	0.55
1:K:380:LEU:HD12	1:K:389:ARG:HB3	1.89	0.55
1:N:380:LEU:HD12	1:N:389:ARG:HB3	1.89	0.55
1:O:717:ASN:ND2	1:MA:259:GLN:OE1	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:380:LEU:HD12	1:R:389:ARG:HB3	1.89	0.55
1:Z:397:TYR:O	1:AB:230:CYS:O	2.23	0.55
1:EA:397:TYR:O	1:QA:230:CYS:O	2.23	0.55
1:MA:230:CYS:O	1:HB:397:TYR:O	2.23	0.55
1:OA:397:TYR:O	1:FB:230:CYS:O	2.23	0.55
1:B:228:TRP:HB3	1:YA:400:SER:OG	2.05	0.55
1:E:380:LEU:HD12	1:E:389:ARG:HB3	1.89	0.55
1:J:397:TYR:O	1:W:230:CYS:O	2.23	0.55
1:K:250:PRO:HB3	1:VA:665:PRO:HG2	1.86	0.55
1:HA:230:CYS:O	1:XA:397:TYR:O	2.23	0.55
1:HA:380:LEU:HD12	1:HA:389:ARG:HB3	1.89	0.55
1:JA:250:PRO:HB3	1:GB:665:PRO:HG2	1.86	0.55
1:B:230:CYS:O	1:YA:397:TYR:O	2.23	0.55
1:J:230:CYS:O	1:HA:397:TYR:O	2.24	0.55
1:J:717:ASN:ND2	1:HA:259:GLN:OE1	2.34	0.55
1:O:230:CYS:O	1:MA:397:TYR:O	2.24	0.55
1:O:397:TYR:O	1:BA:230:CYS:O	2.23	0.55
1:LA:397:TYR:O	1:UA:230:CYS:O	2.24	0.55
1:MA:380:LEU:HD12	1:MA:389:ARG:HB3	1.89	0.55
1:ZA:380:LEU:HD12	1:ZA:389:ARG:HB3	1.89	0.55
1:C:230:CYS:O	1:IA:397:TYR:O	2.23	0.55
1:H:380:LEU:HD12	1:H:389:ARG:HB3	1.89	0.55
1:J:380:LEU:HD12	1:J:389:ARG:HB3	1.89	0.55
1:K:397:TYR:O	1:S:230:CYS:O	2.23	0.55
1:M:380:LEU:HD12	1:M:389:ARG:HB3	1.89	0.55
1:M:397:TYR:O	1:YA:230:CYS:O	2.24	0.55
1:O:380:LEU:HD12	1:O:389:ARG:HB3	1.89	0.55
1:R:230:CYS:O	1:NA:397:TYR:O	2.23	0.55
1:T:380:LEU:HD12	1:T:389:ARG:HB3	1.89	0.55
1:W:397:TYR:O	1:PA:230:CYS:O	2.24	0.55
1:Y:230:CYS:O	1:AA:397:TYR:O	2.24	0.55
1:BA:397:TYR:O	1:ZA:230:CYS:O	2.24	0.55
1:BA:400:SER:OG	1:ZA:228:TRP:HB3	2.05	0.55
1:FA:380:LEU:HD12	1:FA:389:ARG:HB3	1.89	0.55
1:IA:380:LEU:HD12	1:IA:389:ARG:HB3	1.89	0.55
1:JA:397:TYR:O	1:VA:230:CYS:O	2.23	0.55
1:KA:380:LEU:HD12	1:KA:389:ARG:HB3	1.89	0.55
1:NA:380:LEU:HD12	1:NA:389:ARG:HB3	1.89	0.55
1:PA:380:LEU:HD12	1:PA:389:ARG:HB3	1.89	0.55
1:RA:380:LEU:HD12	1:RA:389:ARG:HB3	1.89	0.55
1:TA:380:LEU:HD12	1:TA:389:ARG:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:380:LEU:HD12	1:BB:389:ARG:HB3	1.89	0.55
1:D:230:CYS:O	1:F:397:TYR:O	2.24	0.55
1:H:397:TYR:O	1:IB:230:CYS:O	2.24	0.55
1:L:380:LEU:HD12	1:L:389:ARG:HB3	1.89	0.55
1:Q:230:CYS:O	1:IB:397:TYR:O	2.23	0.55
1:V:397:TYR:O	1:DA:230:CYS:O	2.24	0.55
1:W:400:SER:OG	1:PA:228:TRP:HB3	2.05	0.55
1:X:380:LEU:HD12	1:X:389:ARG:HB3	1.89	0.55
1:GA:397:TYR:O	1:EB:230:CYS:O	2.24	0.55
1:LA:380:LEU:HD12	1:LA:389:ARG:HB3	1.89	0.55
1:OA:250:PRO:HB3	1:WA:665:PRO:HG2	1.86	0.55
1:CB:380:LEU:HD12	1:CB:389:ARG:HB3	1.89	0.55
1:DB:380:LEU:HD12	1:DB:389:ARG:HB3	1.89	0.55
1:C:397:TYR:O	1:TA:230:CYS:O	2.24	0.55
1:G:717:ASN:ND2	1:DB:259:GLN:OE1	2.34	0.55
1:L:717:ASN:ND2	1:TA:259:GLN:OE1	2.34	0.55
1:CA:380:LEU:HD12	1:CA:389:ARG:HB3	1.89	0.55
1:GA:380:LEU:HD12	1:GA:389:ARG:HB3	1.89	0.55
1:OA:230:CYS:O	1:WA:397:TYR:O	2.24	0.55
1:SA:380:LEU:HD12	1:SA:389:ARG:HB3	1.89	0.55
1:AB:380:LEU:HD12	1:AB:389:ARG:HB3	1.89	0.55
1:G:380:LEU:HD12	1:G:389:ARG:HB3	1.89	0.55
1:S:380:LEU:HD12	1:S:389:ARG:HB3	1.89	0.55
1:JA:230:CYS:O	1:GB:397:TYR:O	2.24	0.55
1:QA:380:LEU:HD12	1:QA:389:ARG:HB3	1.89	0.55
1:D:380:LEU:HD12	1:D:389:ARG:HB3	1.89	0.55
1:E:230:CYS:O	1:X:397:TYR:O	2.24	0.55
1:R:397:TYR:O	1:DB:230:CYS:O	2.24	0.55
1:T:230:CYS:O	1:CA:397:TYR:O	2.24	0.55
1:A:230:CYS:O	1:QA:397:TYR:O	2.24	0.54
1:P:230:CYS:O	1:AB:397:TYR:O	2.24	0.54
1:WA:380:LEU:HD12	1:WA:389:ARG:HB3	1.89	0.54
1:B:380:LEU:HD12	1:B:389:ARG:HB3	1.89	0.54
1:Q:380:LEU:HD12	1:Q:389:ARG:HB3	1.89	0.54
1:UA:380:LEU:HD12	1:UA:389:ARG:HB3	1.89	0.54
1:GB:380:LEU:HD12	1:GB:389:ARG:HB3	1.89	0.54
1:EB:380:LEU:HD12	1:EB:389:ARG:HB3	1.89	0.54
1:YA:380:LEU:HD12	1:YA:389:ARG:HB3	1.89	0.54
1:OA:380:LEU:HD12	1:OA:389:ARG:HB3	1.89	0.54
1:V:380:LEU:HD12	1:V:389:ARG:HB3	1.89	0.54
1:BA:380:LEU:HD12	1:BA:389:ARG:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IB:380:LEU:HD12	1:IB:389:ARG:HB3	1.89	0.54
1:L:628:LYS:HB2	1:L:650:PRO:HG3	1.90	0.54
1:JA:380:LEU:HD12	1:JA:389:ARG:HB3	1.89	0.54
1:XA:628:LYS:HB2	1:XA:650:PRO:HG3	1.90	0.54
1:HB:628:LYS:HB2	1:HB:650:PRO:HG3	1.90	0.54
1:D:628:LYS:HB2	1:D:650:PRO:HG3	1.90	0.54
1:G:628:LYS:HB2	1:G:650:PRO:HG3	1.90	0.54
1:P:380:LEU:HD12	1:P:389:ARG:HB3	1.89	0.54
1:S:628:LYS:HB2	1:S:650:PRO:HG3	1.90	0.54
1:AA:380:LEU:HD12	1:AA:389:ARG:HB3	1.89	0.54
1:PA:628:LYS:HB2	1:PA:650:PRO:HG3	1.90	0.54
1:ZA:628:LYS:HB2	1:ZA:650:PRO:HG3	1.90	0.54
1:A:380:LEU:HD12	1:A:389:ARG:HB3	1.89	0.54
1:H:628:LYS:HB2	1:H:650:PRO:HG3	1.90	0.54
1:V:628:LYS:HB2	1:V:650:PRO:HG3	1.90	0.54
1:Y:380:LEU:HD12	1:Y:389:ARG:HB3	1.89	0.54
1:AA:628:LYS:HB2	1:AA:650:PRO:HG3	1.90	0.54
1:JA:628:LYS:HB2	1:JA:650:PRO:HG3	1.90	0.54
1:W:380:LEU:HD12	1:W:389:ARG:HB3	1.89	0.53
1:OA:628:LYS:HB2	1:OA:650:PRO:HG3	1.90	0.53
1:BB:628:LYS:HB2	1:BB:650:PRO:HG3	1.90	0.53
1:F:628:LYS:HB2	1:F:650:PRO:HG3	1.90	0.53
1:K:628:LYS:HB2	1:K:650:PRO:HG3	1.90	0.53
1:M:628:LYS:HB2	1:M:650:PRO:HG3	1.90	0.53
1:R:628:LYS:HB2	1:R:650:PRO:HG3	1.90	0.53
1:DA:380:LEU:HD12	1:DA:389:ARG:HB3	1.89	0.53
1:GA:628:LYS:HB2	1:GA:650:PRO:HG3	1.90	0.53
1:IA:628:LYS:HB2	1:IA:650:PRO:HG3	1.90	0.53
1:JA:405:THR:O	1:VA:222:GLY:O	2.27	0.53
1:LA:628:LYS:HB2	1:LA:650:PRO:HG3	1.90	0.53
1:NA:628:LYS:HB2	1:NA:650:PRO:HG3	1.90	0.53
1:SA:628:LYS:HB2	1:SA:650:PRO:HG3	1.90	0.53
1:VA:380:LEU:HD12	1:VA:389:ARG:HB3	1.89	0.53
1:CB:628:LYS:HB2	1:CB:650:PRO:HG3	1.90	0.53
1:C:628:LYS:HB2	1:C:650:PRO:HG3	1.90	0.53
1:N:628:LYS:HB2	1:N:650:PRO:HG3	1.90	0.53
1:P:628:LYS:HB2	1:P:650:PRO:HG3	1.90	0.53
1:OA:405:THR:O	1:FB:222:GLY:O	2.27	0.53
1:RA:628:LYS:HB2	1:RA:650:PRO:HG3	1.90	0.53
1:A:628:LYS:HB2	1:A:650:PRO:HG3	1.90	0.53
1:FB:380:LEU:HD12	1:FB:389:ARG:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:THR:O	1:I:222:GLY:O	2.27	0.53
1:B:628:LYS:HB2	1:B:650:PRO:HG3	1.90	0.53
1:D:405:THR:O	1:WA:222:GLY:O	2.27	0.53
1:I:628:LYS:HB2	1:I:650:PRO:HG3	1.90	0.53
1:N:222:GLY:O	1:P:405:THR:O	2.27	0.53
1:S:405:THR:O	1:GB:222:GLY:O	2.27	0.53
1:T:405:THR:O	1:LA:222:GLY:O	2.27	0.53
1:FA:628:LYS:HB2	1:FA:650:PRO:HG3	1.90	0.53
1:KA:628:LYS:HB2	1:KA:650:PRO:HG3	1.90	0.53
1:E:405:THR:O	1:GA:222:GLY:O	2.27	0.53
1:E:628:LYS:HB2	1:E:650:PRO:HG3	1.90	0.53
1:Q:628:LYS:HB2	1:Q:650:PRO:HG3	1.90	0.53
1:XA:380:LEU:HD12	1:XA:389:ARG:HB3	1.89	0.53
1:A:222:GLY:O	1:QA:405:THR:O	2.27	0.53
1:C:223:ASN:ND2	1:IA:218:ALA:N	2.57	0.53
1:K:405:THR:O	1:S:222:GLY:O	2.27	0.53
1:M:222:GLY:O	1:DA:405:THR:O	2.27	0.53
1:P:222:GLY:O	1:AB:405:THR:O	2.27	0.53
1:T:218:ALA:N	1:LA:223:ASN:ND2	2.57	0.53
1:UA:628:LYS:HB2	1:UA:650:PRO:HG3	1.90	0.53
1:VA:628:LYS:HB2	1:VA:650:PRO:HG3	1.90	0.53
1:D:222:GLY:O	1:F:405:THR:O	2.27	0.53
1:E:218:ALA:N	1:GA:223:ASN:ND2	2.57	0.53
1:H:222:GLY:O	1:Y:405:THR:O	2.27	0.53
1:H:405:THR:O	1:IB:222:GLY:O	2.27	0.53
1:I:405:THR:O	1:BB:222:GLY:O	2.27	0.53
1:M:405:THR:O	1:YA:222:GLY:O	2.27	0.53
1:N:405:THR:O	1:RA:222:GLY:O	2.27	0.53
1:R:223:ASN:ND2	1:NA:218:ALA:N	2.57	0.53
1:T:628:LYS:HB2	1:T:650:PRO:HG3	1.90	0.53
1:Y:222:GLY:O	1:AA:405:THR:O	2.27	0.53
1:Z:222:GLY:O	1:RA:405:THR:O	2.27	0.53
1:EA:380:LEU:HD12	1:EA:389:ARG:HB3	1.89	0.53
1:HA:628:LYS:HB2	1:HA:650:PRO:HG3	1.91	0.53
1:JA:222:GLY:O	1:GB:405:THR:O	2.27	0.53
1:LA:218:ALA:N	1:UA:223:ASN:ND2	2.57	0.53
1:MA:628:LYS:HB2	1:MA:650:PRO:HG3	1.90	0.53
1:EB:628:LYS:HB2	1:EB:650:PRO:HG3	1.90	0.53
1:HB:380:LEU:HD12	1:HB:389:ARG:HB3	1.89	0.53
1:J:218:ALA:N	1:W:223:ASN:ND2	2.57	0.53
1:O:218:ALA:N	1:BA:223:ASN:ND2	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:405:THR:O	1:DA:222:GLY:O	2.27	0.53
1:Y:628:LYS:HB2	1:Y:650:PRO:HG3	1.90	0.53
1:CA:223:ASN:ND2	1:SA:218:ALA:N	2.57	0.53
1:DA:628:LYS:HB2	1:DA:650:PRO:HG3	1.90	0.53
1:EA:218:ALA:N	1:QA:223:ASN:ND2	2.57	0.53
1:EA:222:GLY:O	1:BB:405:THR:O	2.27	0.53
1:OA:222:GLY:O	1:WA:405:THR:O	2.27	0.53
1:FB:628:LYS:HB2	1:FB:650:PRO:HG3	1.90	0.53
1:A:218:ALA:N	1:I:223:ASN:ND2	2.57	0.53
1:I:218:ALA:N	1:BB:223:ASN:ND2	2.57	0.53
1:N:218:ALA:N	1:RA:223:ASN:ND2	2.57	0.53
1:N:223:ASN:ND2	1:P:218:ALA:N	2.57	0.53
1:T:223:ASN:ND2	1:CA:218:ALA:N	2.57	0.53
1:X:223:ASN:ND2	1:CB:218:ALA:N	2.57	0.53
1:Z:218:ALA:N	1:AB:223:ASN:ND2	2.57	0.53
1:Z:380:LEU:HD12	1:Z:389:ARG:HB3	1.89	0.53
1:CA:222:GLY:O	1:SA:405:THR:O	2.27	0.53
1:MA:223:ASN:ND2	1:HB:218:ALA:N	2.57	0.53
1:WA:628:LYS:HB2	1:WA:650:PRO:HG3	1.90	0.53
1:AB:628:LYS:HB2	1:AB:650:PRO:HG3	1.90	0.53
1:GB:628:LYS:HB2	1:GB:650:PRO:HG3	1.90	0.53
1:IB:628:LYS:HB2	1:IB:650:PRO:HG3	1.90	0.53
1:B:218:ALA:N	1:V:223:ASN:ND2	2.57	0.52
1:E:223:ASN:ND2	1:X:218:ALA:N	2.57	0.52
1:H:218:ALA:N	1:IB:223:ASN:ND2	2.57	0.52
1:H:223:ASN:ND2	1:Y:218:ALA:N	2.57	0.52
1:M:223:ASN:ND2	1:DA:218:ALA:N	2.57	0.52
1:Q:218:ALA:N	1:AA:223:ASN:ND2	2.57	0.52
1:GA:218:ALA:N	1:EB:223:ASN:ND2	2.57	0.52
1:HA:223:ASN:ND2	1:XA:218:ALA:N	2.57	0.52
1:I:610:PRO:HD3	1:P:481:PRO:HG3	1.92	0.52
1:J:481:PRO:HG3	1:KA:610:PRO:HD3	1.92	0.52
1:K:222:GLY:O	1:VA:405:THR:O	2.27	0.52
1:L:223:ASN:ND2	1:TA:218:ALA:N	2.57	0.52
1:M:218:ALA:N	1:YA:223:ASN:ND2	2.57	0.52
1:S:481:PRO:HG3	1:TA:610:PRO:HD3	1.91	0.52
1:X:222:GLY:O	1:CB:405:THR:O	2.27	0.52
1:Z:610:PRO:HD3	1:HB:481:PRO:HG3	1.91	0.52
1:OA:218:ALA:N	1:FB:223:ASN:ND2	2.57	0.52
1:OA:223:ASN:ND2	1:WA:218:ALA:N	2.57	0.52
1:QA:628:LYS:HB2	1:QA:650:PRO:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:628:LYS:HB2	1:YA:650:PRO:HG3	1.90	0.52
1:A:481:PRO:HG3	1:N:610:PRO:HD3	1.92	0.52
1:D:223:ASN:ND2	1:F:218:ALA:N	2.57	0.52
1:F:222:GLY:O	1:FB:405:THR:O	2.27	0.52
1:F:223:ASN:ND2	1:FB:218:ALA:N	2.57	0.52
1:G:223:ASN:ND2	1:DB:218:ALA:N	2.57	0.52
1:I:630:PRO:HA	1:YA:743:LEU:OXT	2.10	0.52
1:J:405:THR:O	1:W:222:GLY:O	2.27	0.52
1:J:743:LEU:OXT	1:DA:630:PRO:HA	2.10	0.52
1:K:218:ALA:N	1:S:223:ASN:ND2	2.57	0.52
1:K:223:ASN:ND2	1:VA:218:ALA:N	2.57	0.52
1:O:481:PRO:HG3	1:FA:610:PRO:HD3	1.92	0.52
1:EA:610:PRO:HD3	1:XA:481:PRO:HG3	1.91	0.52
1:JA:218:ALA:N	1:VA:223:ASN:ND2	2.57	0.52
1:JA:223:ASN:ND2	1:GB:218:ALA:N	2.58	0.52
1:CB:222:GLY:O	1:EB:405:THR:O	2.27	0.52
1:C:405:THR:O	1:TA:222:GLY:O	2.27	0.52
1:J:222:GLY:O	1:HA:405:THR:O	2.27	0.52
1:J:628:LYS:HB2	1:J:650:PRO:HG3	1.90	0.52
1:L:221:VAL:O	1:TA:221:VAL:HG23	2.10	0.52
1:N:630:PRO:HA	1:IB:743:LEU:OXT	2.10	0.52
1:O:222:GLY:O	1:MA:405:THR:O	2.27	0.52
1:O:405:THR:O	1:BA:222:GLY:O	2.27	0.52
1:O:743:LEU:OXT	1:Y:630:PRO:HA	2.10	0.52
1:JA:221:VAL:HG23	1:VA:221:VAL:O	2.10	0.52
1:JA:481:PRO:HG3	1:ZA:610:PRO:HD3	1.92	0.52
1:OA:221:VAL:HG23	1:FB:221:VAL:O	2.10	0.52
1:OA:481:PRO:HG3	1:PA:610:PRO:HD3	1.92	0.52
1:SA:222:GLY:O	1:UA:405:THR:O	2.27	0.52
1:TA:628:LYS:HB2	1:TA:650:PRO:HG3	1.90	0.52
1:A:221:VAL:HG23	1:I:221:VAL:O	2.10	0.52
1:C:610:PRO:HD3	1:CA:481:PRO:HG3	1.92	0.52
1:D:218:ALA:N	1:WA:223:ASN:ND2	2.57	0.52
1:N:481:PRO:HG3	1:IB:610:PRO:HD3	1.91	0.52
1:R:405:THR:O	1:DB:222:GLY:O	2.27	0.52
1:R:610:PRO:HD3	1:X:481:PRO:HG3	1.92	0.52
1:S:218:ALA:N	1:GB:223:ASN:ND2	2.57	0.52
1:S:630:PRO:HA	1:TA:743:LEU:OXT	2.10	0.52
1:FA:405:THR:O	1:NA:222:GLY:O	2.27	0.52
1:IA:222:GLY:O	1:KA:405:THR:O	2.27	0.52
1:SA:610:PRO:HD3	1:ZA:481:PRO:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UA:481:PRO:HG3	1:HB:610:PRO:HD3	1.92	0.52
1:A:223:ASN:ND2	1:QA:218:ALA:N	2.57	0.52
1:D:481:PRO:HG3	1:DB:610:PRO:HD3	1.92	0.52
1:D:610:PRO:HD3	1:K:481:PRO:HG3	1.92	0.52
1:D:630:PRO:HA	1:DB:743:LEU:OXT	2.10	0.52
1:E:743:LEU:OXT	1:NA:630:PRO:HA	2.10	0.52
1:G:221:VAL:O	1:DB:221:VAL:HG23	2.10	0.52
1:I:481:PRO:HG3	1:YA:610:PRO:HD3	1.91	0.52
1:N:221:VAL:O	1:P:221:VAL:HG23	2.10	0.52
1:O:628:LYS:HB2	1:O:650:PRO:HG3	1.90	0.52
1:P:223:ASN:ND2	1:AB:218:ALA:N	2.57	0.52
1:BA:628:LYS:HB2	1:BA:650:PRO:HG3	1.90	0.52
1:CA:628:LYS:HB2	1:CA:650:PRO:HG3	1.90	0.52
1:GA:481:PRO:HG3	1:QA:610:PRO:HD3	1.92	0.52
1:PA:481:PRO:HG3	1:CB:610:PRO:HD3	1.92	0.52
1:SA:223:ASN:ND2	1:UA:218:ALA:N	2.57	0.52
1:XA:610:PRO:HD3	1:EB:481:PRO:HG3	1.92	0.52
1:ZA:218:ALA:N	1:HB:223:ASN:ND2	2.57	0.52
1:DB:628:LYS:HB2	1:DB:650:PRO:HG3	1.90	0.52
1:C:222:GLY:O	1:IA:405:THR:O	2.27	0.52
1:F:481:PRO:HG3	1:S:610:PRO:HD3	1.92	0.52
1:G:222:GLY:O	1:DB:405:THR:O	2.27	0.52
1:L:218:ALA:N	1:KA:223:ASN:ND2	2.57	0.52
1:T:221:VAL:HG23	1:LA:221:VAL:O	2.10	0.52
1:T:743:LEU:OXT	1:IA:630:PRO:HA	2.10	0.52
1:V:221:VAL:HG23	1:DA:221:VAL:O	2.10	0.52
1:W:628:LYS:HB2	1:W:650:PRO:HG3	1.90	0.52
1:X:610:PRO:HD3	1:WA:481:PRO:HG3	1.92	0.52
1:Y:221:VAL:O	1:AA:221:VAL:HG23	2.10	0.52
1:Z:405:THR:O	1:AB:222:GLY:O	2.27	0.52
1:EA:743:LEU:OXT	1:XA:630:PRO:HA	2.10	0.52
1:FA:221:VAL:HG23	1:NA:221:VAL:O	2.10	0.52
1:HA:222:GLY:O	1:XA:405:THR:O	2.27	0.52
1:IA:221:VAL:O	1:KA:221:VAL:HG23	2.10	0.52
1:JA:610:PRO:HD3	1:SA:481:PRO:HG3	1.91	0.52
1:PA:218:ALA:N	1:XA:223:ASN:ND2	2.57	0.52
1:ZA:221:VAL:HG23	1:HB:221:VAL:O	2.10	0.52
1:CB:223:ASN:ND2	1:EB:218:ALA:N	2.57	0.52
1:B:223:ASN:ND2	1:YA:218:ALA:N	2.57	0.52
1:B:630:PRO:HA	1:LA:743:LEU:OXT	2.10	0.52
1:E:221:VAL:HG23	1:GA:221:VAL:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:632:THR:HA	1:AA:615:GLN:NE2	2.25	0.52
1:F:630:PRO:HA	1:S:743:LEU:OXT	2.10	0.52
1:J:610:PRO:HD3	1:DA:481:PRO:HG3	1.91	0.52
1:L:222:GLY:O	1:TA:405:THR:O	2.27	0.52
1:M:221:VAL:O	1:DA:221:VAL:HG23	2.10	0.52
1:Q:223:ASN:ND2	1:IB:218:ALA:N	2.57	0.52
1:R:222:GLY:O	1:NA:405:THR:O	2.27	0.52
1:Z:630:PRO:HA	1:UA:743:LEU:OXT	2.10	0.52
1:Z:743:LEU:OXT	1:HB:630:PRO:HA	2.10	0.52
1:CA:610:PRO:HD3	1:GB:481:PRO:HG3	1.92	0.52
1:EA:630:PRO:HA	1:EB:743:LEU:OXT	2.10	0.52
1:JA:743:LEU:OXT	1:SA:630:PRO:HA	2.10	0.52
1:LA:481:PRO:HG3	1:AB:610:PRO:HD3	1.92	0.52
1:MA:222:GLY:O	1:HB:405:THR:O	2.27	0.52
1:PA:221:VAL:HG23	1:XA:221:VAL:O	2.10	0.52
1:B:222:GLY:O	1:YA:405:THR:O	2.27	0.52
1:D:743:LEU:OXT	1:K:630:PRO:HA	2.10	0.52
1:G:218:ALA:N	1:FA:223:ASN:ND2	2.57	0.52
1:G:610:PRO:HD3	1:VA:481:PRO:HG3	1.92	0.52
1:H:630:PRO:HA	1:RA:743:LEU:OXT	2.10	0.52
1:J:223:ASN:ND2	1:HA:218:ALA:N	2.57	0.52
1:J:445:LEU:HD23	1:DA:536:GLN:HG3	1.92	0.52
1:L:610:PRO:HD3	1:FB:481:PRO:HG3	1.92	0.52
1:M:630:PRO:HA	1:BB:743:LEU:OXT	2.10	0.52
1:O:223:ASN:ND2	1:MA:218:ALA:N	2.57	0.52
1:O:445:LEU:HD23	1:Y:536:GLN:HG3	1.92	0.52
1:O:610:PRO:HD3	1:Y:481:PRO:HG3	1.91	0.52
1:Q:630:PRO:HA	1:GA:743:LEU:OXT	2.10	0.52
1:T:632:THR:HA	1:V:615:GLN:NE2	2.25	0.52
1:X:628:LYS:HB2	1:X:650:PRO:HG3	1.90	0.52
1:Z:628:LYS:HB2	1:Z:650:PRO:HG3	1.90	0.52
1:EA:405:THR:O	1:QA:222:GLY:O	2.27	0.52
1:HA:221:VAL:O	1:XA:221:VAL:HG23	2.10	0.52
1:OA:610:PRO:HD3	1:CB:481:PRO:HG3	1.91	0.52
1:A:610:PRO:HD3	1:IB:481:PRO:HG3	1.92	0.52
1:C:221:VAL:HG23	1:TA:221:VAL:O	2.10	0.52
1:C:630:PRO:HA	1:GB:743:LEU:OXT	2.10	0.52
1:C:743:LEU:OXT	1:CA:630:PRO:HA	2.10	0.52
1:D:221:VAL:O	1:F:221:VAL:HG23	2.10	0.52
1:H:221:VAL:O	1:Y:221:VAL:HG23	2.10	0.52
1:J:632:THR:HA	1:KA:615:GLN:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:221:VAL:HG23	1:S:221:VAL:O	2.10	0.52
1:P:610:PRO:HD3	1:YA:481:PRO:HG3	1.91	0.52
1:P:613:VAL:HG12	1:YA:635:HIS:HB3	1.92	0.52
1:Q:632:THR:HA	1:GA:615:GLN:NE2	2.25	0.52
1:R:630:PRO:HA	1:WA:743:LEU:OXT	2.10	0.52
1:T:222:GLY:O	1:CA:405:THR:O	2.27	0.52
1:T:613:VAL:HG12	1:IA:635:HIS:HB3	1.92	0.52
1:W:481:PRO:HG3	1:FB:610:PRO:HD3	1.92	0.52
1:Y:223:ASN:ND2	1:AA:218:ALA:N	2.57	0.52
1:Z:221:VAL:HG23	1:AB:221:VAL:O	2.10	0.52
1:BA:218:ALA:N	1:ZA:223:ASN:ND2	2.57	0.52
1:BA:632:THR:HA	1:VA:615:GLN:NE2	2.25	0.52
1:IA:223:ASN:ND2	1:KA:218:ALA:N	2.57	0.52
1:JA:615:GLN:NE2	1:SA:632:THR:HA	2.25	0.52
1:LA:405:THR:O	1:UA:222:GLY:O	2.27	0.52
1:LA:630:PRO:HA	1:AB:743:LEU:OXT	2.10	0.52
1:MA:221:VAL:O	1:HB:221:VAL:HG23	2.10	0.52
1:OA:615:GLN:NE2	1:CB:632:THR:HA	2.25	0.52
1:OA:743:LEU:OXT	1:CB:630:PRO:HA	2.10	0.52
1:A:445:LEU:HD23	1:IB:536:GLN:HG3	1.92	0.51
1:A:613:VAL:HG12	1:IB:635:HIS:HB3	1.92	0.51
1:B:221:VAL:O	1:YA:221:VAL:HG23	2.10	0.51
1:C:218:ALA:N	1:TA:223:ASN:ND2	2.57	0.51
1:E:613:VAL:HG12	1:NA:635:HIS:HB3	1.92	0.51
1:G:743:LEU:OXT	1:VA:630:PRO:HA	2.10	0.51
1:H:610:PRO:HD3	1:MA:481:PRO:HG3	1.92	0.51
1:P:445:LEU:HD23	1:YA:536:GLN:HG3	1.92	0.51
1:P:743:LEU:OXT	1:YA:630:PRO:HA	2.10	0.51
1:R:218:ALA:N	1:DB:223:ASN:ND2	2.57	0.51
1:R:221:VAL:HG23	1:DB:221:VAL:O	2.10	0.51
1:T:481:PRO:HG3	1:V:610:PRO:HD3	1.92	0.51
1:W:218:ALA:N	1:PA:223:ASN:ND2	2.57	0.51
1:W:632:THR:HA	1:FB:615:GLN:NE2	2.26	0.51
1:BA:481:PRO:HG3	1:VA:610:PRO:HD3	1.92	0.51
1:EA:221:VAL:HG23	1:QA:221:VAL:O	2.10	0.51
1:EA:615:GLN:NE2	1:XA:632:THR:HA	2.25	0.51
1:FA:218:ALA:N	1:NA:223:ASN:ND2	2.57	0.51
1:JA:445:LEU:HD23	1:SA:536:GLN:HG3	1.92	0.51
1:B:632:THR:HA	1:LA:615:GLN:NE2	2.26	0.51
1:D:615:GLN:NE2	1:K:632:THR:HA	2.26	0.51
1:D:632:THR:HA	1:DB:615:GLN:NE2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:GLY:O	1:X:405:THR:O	2.27	0.51
1:F:632:THR:HA	1:S:615:GLN:NE2	2.26	0.51
1:G:405:THR:O	1:FA:222:GLY:O	2.27	0.51
1:J:615:GLN:NE2	1:DA:632:THR:HA	2.25	0.51
1:M:610:PRO:HD3	1:HA:481:PRO:HG3	1.92	0.51
1:O:632:THR:HA	1:FA:615:GLN:NE2	2.25	0.51
1:R:743:LEU:OXT	1:X:630:PRO:HA	2.10	0.51
1:Z:536:GLN:HG3	1:UA:445:LEU:HD23	1.92	0.51
1:Z:615:GLN:NE2	1:HB:632:THR:HA	2.25	0.51
1:Z:632:THR:HA	1:UA:615:GLN:NE2	2.25	0.51
1:Z:665:PRO:HB3	1:Z:674:PHE:HZ	1.76	0.51
1:BA:405:THR:O	1:ZA:222:GLY:O	2.27	0.51
1:EA:628:LYS:HB2	1:EA:650:PRO:HG3	1.90	0.51
1:EA:632:THR:HA	1:EB:615:GLN:NE2	2.25	0.51
1:EA:665:PRO:HB3	1:EA:674:PHE:HZ	1.76	0.51
1:GA:630:PRO:HA	1:QA:743:LEU:OXT	2.10	0.51
1:GA:632:THR:HA	1:QA:615:GLN:NE2	2.25	0.51
1:KA:665:PRO:HB3	1:KA:674:PHE:HZ	1.76	0.51
1:OA:445:LEU:HD23	1:CB:536:GLN:HG3	1.92	0.51
1:UA:536:GLN:HG3	1:HB:445:LEU:HD23	1.92	0.51
1:UA:630:PRO:HA	1:HB:743:LEU:OXT	2.10	0.51
1:UA:665:PRO:HB3	1:UA:674:PHE:HZ	1.76	0.51
1:A:743:LEU:OXT	1:IB:630:PRO:HA	2.10	0.51
1:E:481:PRO:HG3	1:AA:610:PRO:HD3	1.92	0.51
1:F:536:GLN:HG3	1:S:445:LEU:HD23	1.92	0.51
1:L:405:THR:O	1:KA:222:GLY:O	2.27	0.51
1:L:743:LEU:OXT	1:FB:630:PRO:HA	2.10	0.51
1:Q:222:GLY:O	1:IB:405:THR:O	2.27	0.51
1:V:218:ALA:N	1:DA:223:ASN:ND2	2.57	0.51
1:V:481:PRO:HG3	1:IA:610:PRO:HD3	1.92	0.51
1:W:405:THR:O	1:PA:222:GLY:O	2.27	0.51
1:Y:743:LEU:OXT	1:FA:630:PRO:HA	2.10	0.51
1:Z:221:VAL:O	1:RA:221:VAL:HG23	2.10	0.51
1:Z:613:VAL:HG12	1:HB:635:HIS:HB3	1.92	0.51
1:FA:665:PRO:HB3	1:FA:674:PHE:HZ	1.76	0.51
1:GA:405:THR:O	1:EB:222:GLY:O	2.27	0.51
1:HA:743:LEU:OXT	1:BB:630:PRO:HA	2.10	0.51
1:JA:536:GLN:HG3	1:ZA:445:LEU:HD23	1.92	0.51
1:LA:632:THR:HA	1:AB:615:GLN:NE2	2.25	0.51
1:MA:743:LEU:OXT	1:RA:630:PRO:HA	2.10	0.51
1:RA:665:PRO:HB3	1:RA:674:PHE:HZ	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:743:LEU:OXT	1:EB:630:PRO:HA	2.10	0.51
1:ZA:405:THR:O	1:HB:222:GLY:O	2.27	0.51
1:BB:665:PRO:HB3	1:BB:674:PHE:HZ	1.76	0.51
1:EB:665:PRO:HB3	1:EB:674:PHE:HZ	1.76	0.51
1:A:221:VAL:O	1:QA:221:VAL:HG23	2.10	0.51
1:B:481:PRO:HG3	1:LA:610:PRO:HD3	1.92	0.51
1:F:221:VAL:O	1:FB:221:VAL:HG23	2.10	0.51
1:F:445:LEU:HD23	1:TA:536:GLN:HG3	1.92	0.51
1:F:610:PRO:HD3	1:TA:481:PRO:HG3	1.92	0.51
1:F:665:PRO:HB3	1:F:674:PHE:HZ	1.76	0.51
1:H:481:PRO:HG3	1:RA:610:PRO:HD3	1.92	0.51
1:H:632:THR:HA	1:RA:615:GLN:NE2	2.25	0.51
1:J:221:VAL:HG23	1:W:221:VAL:O	2.10	0.51
1:L:635:HIS:HB3	1:W:613:VAL:HG12	1.93	0.51
1:M:481:PRO:HG3	1:BB:610:PRO:HD3	1.92	0.51
1:P:221:VAL:O	1:AB:221:VAL:HG23	2.10	0.51
1:Q:221:VAL:O	1:IB:221:VAL:HG23	2.10	0.51
1:R:221:VAL:O	1:NA:221:VAL:HG23	2.10	0.51
1:S:632:THR:HA	1:TA:615:GLN:NE2	2.25	0.51
1:X:615:GLN:NE2	1:WA:632:THR:HA	2.25	0.51
1:Z:481:PRO:HG3	1:UA:610:PRO:HD3	1.92	0.51
1:Z:635:HIS:HB3	1:UA:613:VAL:HG12	1.92	0.51
1:AA:481:PRO:HG3	1:NA:610:PRO:HD3	1.92	0.51
1:CA:445:LEU:HD23	1:GB:536:GLN:HG3	1.93	0.51
1:CA:665:PRO:HB3	1:CA:674:PHE:HZ	1.75	0.51
1:DA:743:LEU:OXT	1:KA:630:PRO:HA	2.10	0.51
1:EA:223:ASN:ND2	1:BB:218:ALA:N	2.57	0.51
1:EA:481:PRO:HG3	1:EB:610:PRO:HD3	1.92	0.51
1:EA:536:GLN:HG3	1:EB:445:LEU:HD23	1.93	0.51
1:EA:635:HIS:HB3	1:EB:613:VAL:HG12	1.93	0.51
1:GA:635:HIS:HB3	1:QA:613:VAL:HG12	1.93	0.51
1:HA:613:VAL:HG12	1:BB:635:HIS:HB3	1.93	0.51
1:IA:665:PRO:HB3	1:IA:674:PHE:HZ	1.75	0.51
1:LA:635:HIS:HB3	1:AB:613:VAL:HG12	1.93	0.51
1:NA:665:PRO:HB3	1:NA:674:PHE:HZ	1.76	0.51
1:OA:536:GLN:HG3	1:PA:445:LEU:HD23	1.92	0.51
1:OA:665:PRO:HB3	1:OA:674:PHE:HZ	1.76	0.51
1:B:536:GLN:HG3	1:LA:445:LEU:HD23	1.93	0.51
1:B:610:PRO:HD3	1:AB:481:PRO:HG3	1.92	0.51
1:C:221:VAL:O	1:IA:221:VAL:HG23	2.10	0.51
1:C:481:PRO:HG3	1:GB:610:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:GLN:HG3	1:GB:445:LEU:HD23	1.93	0.51
1:D:665:PRO:HB3	1:D:674:PHE:HZ	1.75	0.51
1:F:743:LEU:OXT	1:TA:630:PRO:HA	2.10	0.51
1:G:635:HIS:HB3	1:BA:613:VAL:HG12	1.93	0.51
1:H:221:VAL:HG23	1:IB:221:VAL:O	2.10	0.51
1:H:615:GLN:NE2	1:MA:632:THR:HA	2.25	0.51
1:I:221:VAL:HG23	1:BB:221:VAL:O	2.10	0.51
1:K:221:VAL:O	1:VA:221:VAL:HG23	2.10	0.51
1:K:445:LEU:HD23	1:DB:536:GLN:HG3	1.93	0.51
1:K:610:PRO:HD3	1:DB:481:PRO:HG3	1.92	0.51
1:K:665:PRO:HB3	1:K:674:PHE:HZ	1.76	0.51
1:M:615:GLN:NE2	1:HA:632:THR:HA	2.25	0.51
1:N:221:VAL:HG23	1:RA:221:VAL:O	2.10	0.51
1:O:615:GLN:NE2	1:Y:632:THR:HA	2.26	0.51
1:Q:481:PRO:HG3	1:GA:610:PRO:HD3	1.92	0.51
1:Q:610:PRO:HD3	1:QA:481:PRO:HG3	1.92	0.51
1:S:665:PRO:HB3	1:S:674:PHE:HZ	1.75	0.51
1:T:630:PRO:HA	1:V:743:LEU:OXT	2.10	0.51
1:X:445:LEU:HD23	1:WA:536:GLN:HG3	1.93	0.51
1:X:665:PRO:HB3	1:X:674:PHE:HZ	1.75	0.51
1:Y:610:PRO:HD3	1:FA:481:PRO:HG3	1.92	0.51
1:Z:223:ASN:ND2	1:RA:218:ALA:N	2.57	0.51
1:AA:665:PRO:HB3	1:AA:674:PHE:HZ	1.76	0.51
1:CA:615:GLN:NE2	1:GB:632:THR:HA	2.25	0.51
1:EA:221:VAL:O	1:BB:221:VAL:HG23	2.10	0.51
1:JA:635:HIS:HB3	1:ZA:613:VAL:HG12	1.92	0.51
1:JA:665:PRO:HB3	1:JA:674:PHE:HZ	1.76	0.51
1:MA:613:VAL:HG12	1:RA:635:HIS:HB3	1.93	0.51
1:PA:405:THR:O	1:XA:222:GLY:O	2.27	0.51
1:XA:445:LEU:HD23	1:EB:536:GLN:HG3	1.93	0.51
1:AB:665:PRO:HB3	1:AB:674:PHE:HZ	1.75	0.51
1:DB:665:PRO:HB3	1:DB:674:PHE:HZ	1.76	0.51
1:B:221:VAL:HG23	1:V:221:VAL:O	2.10	0.51
1:B:405:THR:O	1:V:222:GLY:O	2.27	0.51
1:B:615:GLN:NE2	1:AB:632:THR:HA	2.25	0.51
1:D:221:VAL:HG23	1:WA:221:VAL:O	2.10	0.51
1:D:445:LEU:HD23	1:K:536:GLN:HG3	1.93	0.51
1:E:630:PRO:HA	1:AA:743:LEU:OXT	2.10	0.51
1:I:536:GLN:HG3	1:YA:445:LEU:HD23	1.92	0.51
1:K:743:LEU:OXT	1:DB:630:PRO:HA	2.10	0.51
1:M:221:VAL:HG23	1:YA:221:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:632:THR:HA	1:BB:615:GLN:NE2	2.26	0.51
1:M:665:PRO:HB3	1:M:674:PHE:HZ	1.76	0.51
1:N:536:GLN:HG3	1:IB:445:LEU:HD23	1.92	0.51
1:O:221:VAL:HG23	1:BA:221:VAL:O	2.10	0.51
1:Q:221:VAL:HG23	1:AA:221:VAL:O	2.10	0.51
1:Q:405:THR:O	1:AA:222:GLY:O	2.27	0.51
1:Q:536:GLN:HG3	1:GA:445:LEU:HD23	1.93	0.51
1:R:536:GLN:HG3	1:WA:445:LEU:HD23	1.93	0.51
1:V:665:PRO:HB3	1:V:674:PHE:HZ	1.76	0.51
1:DA:610:PRO:HD3	1:KA:481:PRO:HG3	1.92	0.51
1:EA:613:VAL:HG12	1:XA:635:HIS:HB3	1.92	0.51
1:HA:615:GLN:NE2	1:BB:632:THR:HA	2.25	0.51
1:OA:635:HIS:HB3	1:PA:613:VAL:HG12	1.93	0.51
1:SA:743:LEU:OXT	1:ZA:630:PRO:HA	2.10	0.51
1:TA:665:PRO:HB3	1:TA:674:PHE:HZ	1.76	0.51
1:E:635:HIS:HB3	1:AA:613:VAL:HG12	1.92	0.51
1:H:665:PRO:HB3	1:H:674:PHE:HZ	1.76	0.51
1:I:445:LEU:HD23	1:P:536:GLN:HG3	1.92	0.51
1:M:635:HIS:HB3	1:BB:613:VAL:HG12	1.93	0.51
1:R:481:PRO:HG3	1:WA:610:PRO:HD3	1.92	0.51
1:S:221:VAL:HG23	1:GB:221:VAL:O	2.10	0.51
1:T:221:VAL:O	1:CA:221:VAL:HG23	2.10	0.51
1:V:630:PRO:HA	1:IA:743:LEU:OXT	2.10	0.51
1:V:632:THR:HA	1:IA:615:GLN:NE2	2.26	0.51
1:W:536:GLN:HG3	1:FB:445:LEU:HD23	1.93	0.51
1:AA:632:THR:HA	1:NA:615:GLN:NE2	2.26	0.51
1:BA:536:GLN:HG3	1:VA:445:LEU:HD23	1.93	0.51
1:BA:630:PRO:HA	1:VA:743:LEU:OXT	2.10	0.51
1:MA:610:PRO:HD3	1:RA:481:PRO:HG3	1.92	0.51
1:MA:615:GLN:NE2	1:RA:632:THR:HA	2.25	0.51
1:QA:665:PRO:HB3	1:QA:674:PHE:HZ	1.76	0.51
1:SA:615:GLN:NE2	1:ZA:632:THR:HA	2.26	0.51
1:A:536:GLN:HG3	1:N:445:LEU:HD23	1.92	0.51
1:E:221:VAL:O	1:X:221:VAL:HG23	2.10	0.51
1:G:632:THR:HA	1:BA:615:GLN:NE2	2.26	0.51
1:H:635:HIS:HB3	1:RA:613:VAL:HG12	1.93	0.51
1:I:613:VAL:HG12	1:P:635:HIS:HB3	1.92	0.51
1:J:630:PRO:HA	1:KA:743:LEU:OXT	2.10	0.51
1:L:632:THR:HA	1:W:615:GLN:NE2	2.25	0.51
1:O:630:PRO:HA	1:FA:743:LEU:OXT	2.10	0.51
1:T:445:LEU:HD23	1:IA:536:GLN:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:615:GLN:NE2	1:IA:632:THR:HA	2.25	0.51
1:T:635:HIS:HB3	1:V:613:VAL:HG12	1.92	0.51
1:X:221:VAL:O	1:CB:221:VAL:HG23	2.10	0.51
1:Y:445:LEU:HD23	1:FA:536:GLN:HG3	1.92	0.51
1:AA:630:PRO:HA	1:NA:743:LEU:OXT	2.10	0.51
1:CA:743:LEU:OXT	1:GB:630:PRO:HA	2.10	0.51
1:JA:630:PRO:HA	1:ZA:743:LEU:OXT	2.10	0.51
1:JA:632:THR:HA	1:ZA:615:GLN:NE2	2.25	0.51
1:OA:632:THR:HA	1:PA:615:GLN:NE2	2.25	0.51
1:SA:445:LEU:HD23	1:ZA:536:GLN:HG3	1.92	0.51
1:WA:665:PRO:HB3	1:WA:674:PHE:HZ	1.75	0.51
1:A:630:PRO:HA	1:N:743:LEU:OXT	2.10	0.51
1:A:635:HIS:HB3	1:N:613:VAL:HG12	1.92	0.51
1:E:615:GLN:NE2	1:NA:632:THR:HA	2.25	0.51
1:E:743:LEU:HD22	1:NA:630:PRO:HB3	1.93	0.51
1:J:630:PRO:HB3	1:KA:743:LEU:HD22	1.93	0.51
1:L:221:VAL:HG23	1:KA:221:VAL:O	2.10	0.51
1:Q:615:GLN:NE2	1:QA:632:THR:HA	2.26	0.51
1:T:743:LEU:HD22	1:IA:630:PRO:HB3	1.93	0.51
1:W:630:PRO:HA	1:FB:743:LEU:OXT	2.10	0.51
1:W:635:HIS:HB3	1:FB:613:VAL:HG12	1.93	0.51
1:Y:613:VAL:HG12	1:FA:635:HIS:HB3	1.92	0.51
1:Z:445:LEU:HD23	1:HB:536:GLN:HG3	1.92	0.51
1:CA:221:VAL:O	1:SA:221:VAL:HG23	2.10	0.51
1:DA:445:LEU:HD23	1:KA:536:GLN:HG3	1.92	0.51
1:DA:613:VAL:HG12	1:KA:635:HIS:HB3	1.92	0.51
1:HA:610:PRO:HD3	1:BB:481:PRO:HG3	1.92	0.51
1:PA:536:GLN:HG3	1:CB:445:LEU:HD23	1.93	0.51
1:PA:630:PRO:HA	1:CB:743:LEU:OXT	2.10	0.51
1:PA:632:THR:HA	1:CB:615:GLN:NE2	2.26	0.51
1:SA:221:VAL:O	1:UA:221:VAL:HG23	2.10	0.51
1:B:665:PRO:HB3	1:B:674:PHE:HZ	1.76	0.51
1:C:632:THR:HA	1:GB:615:GLN:NE2	2.25	0.51
1:E:445:LEU:HD23	1:NA:536:GLN:HG3	1.92	0.51
1:F:635:HIS:HB3	1:S:613:VAL:HG12	1.92	0.51
1:G:221:VAL:HG23	1:FA:221:VAL:O	2.10	0.51
1:G:630:PRO:HA	1:BA:743:LEU:OXT	2.10	0.51
1:I:615:GLN:NE2	1:P:632:THR:HA	2.26	0.51
1:I:743:LEU:OXT	1:P:630:PRO:HA	2.10	0.51
1:L:536:GLN:HG3	1:W:445:LEU:HD23	1.93	0.51
1:L:630:PRO:HA	1:W:743:LEU:OXT	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:221:VAL:O	1:MA:221:VAL:HG23	2.10	0.51
1:O:630:PRO:HB3	1:FA:743:LEU:HD22	1.93	0.51
1:R:632:THR:HA	1:WA:615:GLN:NE2	2.26	0.51
1:R:665:PRO:HB3	1:R:674:PHE:HZ	1.75	0.51
1:S:630:PRO:HB3	1:TA:743:LEU:HD22	1.93	0.51
1:T:536:GLN:HG3	1:V:445:LEU:HD23	1.92	0.51
1:V:635:HIS:HB3	1:IA:613:VAL:HG12	1.92	0.51
1:W:221:VAL:HG23	1:PA:221:VAL:O	2.10	0.51
1:X:743:LEU:OXT	1:WA:630:PRO:HA	2.11	0.51
1:BA:221:VAL:HG23	1:ZA:221:VAL:O	2.10	0.51
1:YA:665:PRO:HB3	1:YA:674:PHE:HZ	1.76	0.51
1:CB:665:PRO:HB3	1:CB:674:PHE:HZ	1.76	0.51
1:GB:665:PRO:HB3	1:GB:674:PHE:HZ	1.76	0.51
1:IB:665:PRO:HB3	1:IB:674:PHE:HZ	1.76	0.51
1:A:632:THR:HA	1:N:615:GLN:NE2	2.26	0.50
1:B:445:LEU:HD23	1:AB:536:GLN:HG3	1.93	0.50
1:D:630:PRO:HB3	1:DB:743:LEU:HD22	1.93	0.50
1:E:536:GLN:HG3	1:AA:445:LEU:HD23	1.92	0.50
1:G:536:GLN:HG3	1:BA:445:LEU:HD23	1.93	0.50
1:G:615:GLN:NE2	1:VA:632:THR:HA	2.25	0.50
1:H:445:LEU:HD23	1:MA:536:GLN:HG3	1.93	0.50
1:I:743:LEU:HD22	1:P:630:PRO:HB3	1.94	0.50
1:J:613:VAL:HG12	1:DA:635:HIS:HB3	1.92	0.50
1:M:445:LEU:HD23	1:HA:536:GLN:HG3	1.93	0.50
1:O:613:VAL:HG12	1:Y:635:HIS:HB3	1.92	0.50
1:T:610:PRO:HD3	1:IA:481:PRO:HG3	1.91	0.50
1:AA:635:HIS:HB3	1:NA:613:VAL:HG12	1.92	0.50
1:BA:635:HIS:HB3	1:VA:613:VAL:HG12	1.93	0.50
1:EA:445:LEU:HD23	1:XA:536:GLN:HG3	1.92	0.50
1:HA:445:LEU:HD23	1:BB:536:GLN:HG3	1.93	0.50
1:LA:221:VAL:HG23	1:UA:221:VAL:O	2.10	0.50
1:MA:445:LEU:HD23	1:RA:536:GLN:HG3	1.93	0.50
1:OA:630:PRO:HA	1:PA:743:LEU:OXT	2.10	0.50
1:SA:665:PRO:HB3	1:SA:674:PHE:HZ	1.76	0.50
1:CB:221:VAL:O	1:EB:221:VAL:HG23	2.10	0.50
1:A:630:PRO:HB3	1:N:743:LEU:HD22	1.94	0.50
1:C:613:VAL:HG12	1:CA:635:HIS:HB3	1.93	0.50
1:C:665:PRO:HB3	1:C:674:PHE:HZ	1.75	0.50
1:D:536:GLN:HG3	1:DB:445:LEU:HD23	1.92	0.50
1:D:613:VAL:HG12	1:K:635:HIS:HB3	1.93	0.50
1:E:630:PRO:HB3	1:AA:743:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:615:GLN:NE2	1:TA:632:THR:HA	2.25	0.50
1:H:630:PRO:HB3	1:RA:743:LEU:HD22	1.94	0.50
1:J:221:VAL:O	1:HA:221:VAL:HG23	2.10	0.50
1:P:615:GLN:NE2	1:YA:632:THR:HA	2.25	0.50
1:Q:445:LEU:HD23	1:QA:536:GLN:HG3	1.93	0.50
1:R:630:PRO:HB3	1:WA:743:LEU:HD22	1.94	0.50
1:T:630:PRO:HB3	1:V:743:LEU:HD22	1.93	0.50
1:Y:615:GLN:NE2	1:FA:632:THR:HA	2.26	0.50
1:GA:221:VAL:HG23	1:EB:221:VAL:O	2.10	0.50
1:JA:221:VAL:O	1:GB:221:VAL:HG23	2.10	0.50
1:LA:630:PRO:HB3	1:AB:743:LEU:HD22	1.94	0.50
1:FB:665:PRO:HB3	1:FB:674:PHE:HZ	1.76	0.50
1:A:615:GLN:NE2	1:IB:632:THR:HA	2.25	0.50
1:B:743:LEU:OXT	1:AB:630:PRO:HA	2.10	0.50
1:C:630:PRO:HB3	1:GB:743:LEU:HD22	1.94	0.50
1:G:613:VAL:HG12	1:VA:635:HIS:HB3	1.93	0.50
1:L:613:VAL:HG12	1:FB:635:HIS:HB3	1.93	0.50
1:L:615:GLN:NE2	1:FB:632:THR:HA	2.25	0.50
1:M:630:PRO:HB3	1:BB:743:LEU:HD22	1.94	0.50
1:O:743:LEU:HD22	1:Y:630:PRO:HB3	1.93	0.50
1:Q:665:PRO:HB3	1:Q:674:PHE:HZ	1.76	0.50
1:R:613:VAL:HG12	1:X:635:HIS:HB3	1.93	0.50
1:R:615:GLN:NE2	1:X:632:THR:HA	2.25	0.50
1:S:536:GLN:HG3	1:TA:445:LEU:HD23	1.92	0.50
1:T:665:PRO:HB3	1:T:674:PHE:HZ	1.76	0.50
1:Y:665:PRO:HB3	1:Y:674:PHE:HZ	1.76	0.50
1:CA:613:VAL:HG12	1:GB:635:HIS:HB3	1.93	0.50
1:DA:665:PRO:HB3	1:DA:674:PHE:HZ	1.76	0.50
1:GA:630:PRO:HB3	1:QA:743:LEU:HD22	1.94	0.50
1:MA:665:PRO:HB3	1:MA:674:PHE:HZ	1.76	0.50
1:VA:665:PRO:HB3	1:VA:674:PHE:HZ	1.75	0.50
1:A:665:PRO:HB3	1:A:674:PHE:HZ	1.76	0.50
1:C:615:GLN:NE2	1:CA:632:THR:HA	2.26	0.50
1:G:630:PRO:HB3	1:BA:743:LEU:HD22	1.94	0.50
1:H:536:GLN:HG3	1:RA:445:LEU:HD23	1.93	0.50
1:H:743:LEU:OXT	1:MA:630:PRO:HA	2.10	0.50
1:I:632:THR:HA	1:YA:615:GLN:NE2	2.25	0.50
1:K:615:GLN:NE2	1:DB:632:THR:HA	2.25	0.50
1:M:743:LEU:OXT	1:HA:630:PRO:HA	2.10	0.50
1:R:743:LEU:HD22	1:X:630:PRO:HB3	1.94	0.50
1:S:635:HIS:HB3	1:TA:613:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:613:VAL:HG12	1:WA:635:HIS:HB3	1.93	0.50
1:GA:665:PRO:HB3	1:GA:674:PHE:HZ	1.76	0.50
1:JA:630:PRO:HB3	1:ZA:743:LEU:HD22	1.93	0.50
1:LA:536:GLN:HG3	1:AB:445:LEU:HD23	1.93	0.50
1:OA:221:VAL:O	1:WA:221:VAL:HG23	2.10	0.50
1:B:635:HIS:HB3	1:LA:613:VAL:HG12	1.93	0.50
1:D:635:HIS:HB3	1:DB:613:VAL:HG12	1.92	0.50
1:E:610:PRO:HD3	1:NA:481:PRO:HG3	1.91	0.50
1:E:665:PRO:HB3	1:E:674:PHE:HZ	1.76	0.50
1:J:743:LEU:HD22	1:DA:630:PRO:HB3	1.93	0.50
1:K:613:VAL:HG12	1:DB:635:HIS:HB3	1.93	0.50
1:N:632:THR:HA	1:IB:615:GLN:NE2	2.25	0.50
1:P:665:PRO:HB3	1:P:674:PHE:HZ	1.76	0.50
1:Q:743:LEU:OXT	1:QA:630:PRO:HA	2.10	0.50
1:DA:615:GLN:NE2	1:KA:632:THR:HA	2.26	0.50
1:GA:536:GLN:HG3	1:QA:445:LEU:HD23	1.93	0.50
1:HA:665:PRO:HB3	1:HA:674:PHE:HZ	1.76	0.50
1:LA:665:PRO:HB3	1:LA:674:PHE:HZ	1.76	0.50
1:SA:613:VAL:HG12	1:ZA:635:HIS:HB3	1.92	0.50
1:XA:613:VAL:HG12	1:EB:635:HIS:HB3	1.92	0.50
1:HB:665:PRO:HB3	1:HB:674:PHE:HZ	1.75	0.50
1:B:613:VAL:HG12	1:AB:635:HIS:HB3	1.93	0.50
1:C:445:LEU:HD23	1:CA:536:GLN:HG3	1.93	0.50
1:C:743:LEU:HD22	1:CA:630:PRO:HB3	1.94	0.50
1:J:536:GLN:HG3	1:KA:445:LEU:HD23	1.92	0.50
1:K:743:LEU:HD22	1:DB:630:PRO:HB3	1.93	0.50
1:L:630:PRO:HB3	1:W:743:LEU:HD22	1.94	0.50
1:M:536:GLN:HG3	1:BB:445:LEU:HD23	1.93	0.50
1:N:665:PRO:HB3	1:N:674:PHE:HZ	1.76	0.50
1:O:536:GLN:HG3	1:FA:445:LEU:HD23	1.92	0.50
1:Q:613:VAL:HG12	1:QA:635:HIS:HB3	1.93	0.50
1:Q:635:HIS:HB3	1:GA:613:VAL:HG12	1.93	0.50
1:MA:743:LEU:HD22	1:RA:630:PRO:HB3	1.94	0.50
1:OA:630:PRO:HB3	1:PA:743:LEU:HD22	1.93	0.50
1:UA:635:HIS:HB3	1:HB:613:VAL:HG12	1.92	0.50
1:F:613:VAL:HG12	1:TA:635:HIS:HB3	1.93	0.50
1:F:630:PRO:HB3	1:S:743:LEU:HD22	1.94	0.50
1:F:743:LEU:HD22	1:TA:630:PRO:HB3	1.93	0.50
1:L:481:PRO:HG3	1:W:610:PRO:HD3	1.92	0.50
1:M:743:LEU:HD22	1:HA:630:PRO:HB3	1.93	0.50
1:O:635:HIS:HB3	1:FA:613:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:445:LEU:HD23	1:X:536:GLN:HG3	1.93	0.50
1:HA:743:LEU:HD22	1:BB:630:PRO:HB3	1.94	0.50
1:RA:622:GLN:HE22	1:RA:733:PRO:HA	1.77	0.50
1:XA:615:GLN:NE2	1:EB:632:THR:HA	2.26	0.50
1:BB:622:GLN:HE22	1:BB:733:PRO:HA	1.77	0.50
1:B:622:GLN:HE22	1:B:733:PRO:HA	1.77	0.50
1:B:743:LEU:HD22	1:AB:630:PRO:HB3	1.94	0.50
1:D:743:LEU:HD22	1:K:630:PRO:HB3	1.94	0.50
1:G:481:PRO:HG3	1:BA:610:PRO:HD3	1.92	0.50
1:G:665:PRO:HB3	1:G:674:PHE:HZ	1.76	0.50
1:I:622:GLN:HE22	1:I:733:PRO:HA	1.77	0.50
1:I:665:PRO:HB3	1:I:674:PHE:HZ	1.76	0.50
1:J:635:HIS:HB3	1:KA:613:VAL:HG12	1.93	0.50
1:L:622:GLN:HE22	1:L:733:PRO:HA	1.77	0.50
1:Q:622:GLN:HE22	1:Q:733:PRO:HA	1.77	0.50
1:V:630:PRO:HB3	1:IA:743:LEU:HD22	1.94	0.50
1:AA:630:PRO:HB3	1:NA:743:LEU:HD22	1.94	0.50
1:JA:613:VAL:HG12	1:SA:635:HIS:HB3	1.92	0.50
1:JA:743:LEU:HD22	1:SA:630:PRO:HB3	1.93	0.50
1:OA:613:VAL:HG12	1:CB:635:HIS:HB3	1.92	0.50
1:OA:743:LEU:HD22	1:CB:630:PRO:HB3	1.93	0.50
1:PA:635:HIS:HB3	1:CB:613:VAL:HG12	1.93	0.50
1:XA:665:PRO:HB3	1:XA:674:PHE:HZ	1.76	0.50
1:H:743:LEU:HD22	1:MA:630:PRO:HB3	1.94	0.50
1:I:566:ARG:NH2	1:N:712:TYR:OH	2.45	0.50
1:I:712:TYR:OH	1:N:566:ARG:NH2	2.45	0.50
1:J:622:GLN:HE22	1:J:733:PRO:HA	1.77	0.50
1:N:622:GLN:HE22	1:N:733:PRO:HA	1.77	0.50
1:O:622:GLN:HE22	1:O:733:PRO:HA	1.77	0.50
1:T:622:GLN:HE22	1:T:733:PRO:HA	1.77	0.50
1:W:630:PRO:HB3	1:FB:743:LEU:HD22	1.94	0.50
1:Y:743:LEU:HD22	1:FA:630:PRO:HB3	1.94	0.50
1:SA:712:TYR:OH	1:HB:566:ARG:NH2	2.45	0.50
1:SA:743:LEU:HD22	1:ZA:630:PRO:HB3	1.94	0.50
1:TA:622:GLN:HE22	1:TA:733:PRO:HA	1.77	0.50
1:UA:632:THR:HA	1:HB:615:GLN:NE2	2.26	0.50
1:XA:566:ARG:NH2	1:CB:712:TYR:OH	2.45	0.50
1:DB:622:GLN:HE22	1:DB:733:PRO:HA	1.77	0.50
1:A:622:GLN:HE22	1:A:733:PRO:HA	1.77	0.49
1:E:622:GLN:HE22	1:E:733:PRO:HA	1.77	0.49
1:G:622:GLN:HE22	1:G:733:PRO:HA	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:635:HIS:HB3	1:YA:613:VAL:HG12	1.92	0.49
1:J:665:PRO:HB3	1:J:674:PHE:HZ	1.76	0.49
1:O:665:PRO:HB3	1:O:674:PHE:HZ	1.76	0.49
1:P:622:GLN:HE22	1:P:733:PRO:HA	1.77	0.49
1:Q:743:LEU:HD22	1:QA:630:PRO:HB3	1.94	0.49
1:W:622:GLN:HE22	1:W:733:PRO:HA	1.77	0.49
1:BA:630:PRO:HB3	1:VA:743:LEU:HD22	1.94	0.49
1:DA:743:LEU:HD22	1:KA:630:PRO:HB3	1.94	0.49
1:PA:630:PRO:HB3	1:CB:743:LEU:HD22	1.94	0.49
1:C:635:HIS:HB3	1:GB:613:VAL:HG12	1.93	0.49
1:E:712:TYR:OH	1:R:566:ARG:NH2	2.46	0.49
1:G:566:ARG:NH2	1:K:712:TYR:OH	2.46	0.49
1:I:630:PRO:HB3	1:YA:743:LEU:HD22	1.93	0.49
1:I:662:PRO:HB3	1:I:674:PHE:CD2	2.48	0.49
1:L:665:PRO:HB3	1:L:674:PHE:HZ	1.76	0.49
1:N:484:ARG:HD3	1:IB:580:SER:O	2.12	0.49
1:Q:662:PRO:HB3	1:Q:674:PHE:CD2	2.47	0.49
1:R:635:HIS:HB3	1:WA:613:VAL:HG12	1.93	0.49
1:X:622:GLN:HE22	1:X:733:PRO:HA	1.77	0.49
1:Z:484:ARG:HD3	1:UA:580:SER:O	2.13	0.49
1:BA:622:GLN:HE22	1:BA:733:PRO:HA	1.77	0.49
1:EA:630:PRO:HB3	1:EB:743:LEU:HD22	1.93	0.49
1:IA:622:GLN:HE22	1:IA:733:PRO:HA	1.77	0.49
1:PA:665:PRO:HB3	1:PA:674:PHE:HZ	1.76	0.49
1:A:580:SER:O	1:IB:484:ARG:HD3	2.13	0.49
1:A:743:LEU:HD22	1:IB:630:PRO:HB3	1.93	0.49
1:C:566:ARG:NH2	1:T:712:TYR:OH	2.46	0.49
1:E:662:PRO:HB3	1:E:674:PHE:CD2	2.48	0.49
1:F:662:PRO:HB3	1:F:674:PHE:CD2	2.48	0.49
1:F:712:TYR:OH	1:L:566:ARG:NH2	2.46	0.49
1:H:613:VAL:HG12	1:MA:635:HIS:HB3	1.93	0.49
1:I:484:ARG:HD3	1:YA:580:SER:O	2.12	0.49
1:J:662:PRO:HB3	1:J:674:PHE:CD2	2.48	0.49
1:N:630:PRO:HB3	1:IB:743:LEU:HD22	1.93	0.49
1:N:662:PRO:HB3	1:N:674:PHE:CD2	2.48	0.49
1:P:580:SER:O	1:YA:484:ARG:HD3	2.12	0.49
1:V:536:GLN:HG3	1:IA:445:LEU:HD23	1.92	0.49
1:Z:566:ARG:NH2	1:MA:712:TYR:OH	2.45	0.49
1:DA:662:PRO:HB3	1:DA:674:PHE:CD2	2.48	0.49
1:EA:484:ARG:HD3	1:EB:580:SER:O	2.13	0.49
1:PA:566:ARG:NH2	1:FB:712:TYR:OH	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TA:712:TYR:OH	1:GB:566:ARG:NH2	2.46	0.49
1:WA:566:ARG:NH2	1:DB:712:TYR:OH	2.46	0.49
1:YA:566:ARG:NH2	1:BB:712:TYR:OH	2.45	0.49
1:ZA:665:PRO:HB3	1:ZA:674:PHE:HZ	1.76	0.49
1:B:662:PRO:HB3	1:B:674:PHE:CD2	2.48	0.49
1:K:662:PRO:HB3	1:K:674:PHE:CD2	2.48	0.49
1:N:635:HIS:HB3	1:IB:613:VAL:HG12	1.92	0.49
1:O:662:PRO:HB3	1:O:674:PHE:CD2	2.48	0.49
1:P:743:LEU:HD22	1:YA:630:PRO:HB3	1.93	0.49
1:T:662:PRO:HB3	1:T:674:PHE:CD2	2.48	0.49
1:V:622:GLN:HE22	1:V:733:PRO:HA	1.77	0.49
1:V:662:PRO:HB3	1:V:674:PHE:CD2	2.48	0.49
1:W:712:TYR:OH	1:KA:566:ARG:NH2	2.45	0.49
1:Y:662:PRO:HB3	1:Y:674:PHE:CD2	2.48	0.49
1:Z:630:PRO:HB3	1:UA:743:LEU:HD22	1.93	0.49
1:Z:662:PRO:HB3	1:Z:674:PHE:CD2	2.48	0.49
1:AA:622:GLN:HE22	1:AA:733:PRO:HA	1.77	0.49
1:AA:662:PRO:HB3	1:AA:674:PHE:CD2	2.48	0.49
1:BA:712:TYR:OH	1:FA:566:ARG:NH2	2.45	0.49
1:CA:622:GLN:HE22	1:CA:733:PRO:HA	1.77	0.49
1:EA:566:ARG:NH2	1:HA:712:TYR:OH	2.45	0.49
1:EA:662:PRO:HB3	1:EA:674:PHE:CD2	2.48	0.49
1:QA:712:TYR:OH	1:EB:566:ARG:NH2	2.45	0.49
1:UA:484:ARG:HD3	1:HB:580:SER:O	2.13	0.49
1:UA:566:ARG:NH2	1:AB:712:TYR:OH	2.45	0.49
1:VA:712:TYR:OH	1:ZA:566:ARG:NH2	2.45	0.49
1:WA:712:TYR:OH	1:DB:566:ARG:NH2	2.45	0.49
1:D:622:GLN:HE22	1:D:733:PRO:HA	1.77	0.49
1:G:712:TYR:OH	1:K:566:ARG:NH2	2.45	0.49
1:J:712:TYR:OH	1:M:566:ARG:NH2	2.46	0.49
1:Y:622:GLN:HE22	1:Y:733:PRO:HA	1.77	0.49
1:Z:622:GLN:HE22	1:Z:733:PRO:HA	1.77	0.49
1:Z:712:TYR:OH	1:MA:566:ARG:NH2	2.46	0.49
1:AA:536:GLN:HG3	1:NA:445:LEU:HD23	1.93	0.49
1:BA:662:PRO:HB3	1:BA:674:PHE:CD2	2.48	0.49
1:BA:665:PRO:HB3	1:BA:674:PHE:HZ	1.76	0.49
1:DA:622:GLN:HE22	1:DA:733:PRO:HA	1.77	0.49
1:FA:622:GLN:HE22	1:FA:733:PRO:HA	1.77	0.49
1:NA:622:GLN:HE22	1:NA:733:PRO:HA	1.77	0.49
1:RA:566:ARG:NH2	1:IB:712:TYR:OH	2.46	0.49
1:RA:712:TYR:OH	1:IB:566:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:580:SER:O	1:ZA:484:ARG:HD3	2.13	0.49
1:TA:566:ARG:NH2	1:GB:712:TYR:OH	2.46	0.49
1:VA:662:PRO:HB3	1:VA:674:PHE:CD2	2.48	0.49
1:XA:580:SER:O	1:EB:484:ARG:HD3	2.13	0.49
1:B:630:PRO:HB3	1:LA:743:LEU:HD22	1.94	0.49
1:H:566:ARG:NH2	1:O:712:TYR:OH	2.46	0.49
1:M:613:VAL:HG12	1:HA:635:HIS:HB3	1.93	0.49
1:S:622:GLN:HE22	1:S:733:PRO:HA	1.77	0.49
1:W:662:PRO:HB3	1:W:674:PHE:CD2	2.48	0.49
1:W:665:PRO:HB3	1:W:674:PHE:HZ	1.76	0.49
1:GA:622:GLN:HE22	1:GA:733:PRO:HA	1.77	0.49
1:IA:662:PRO:HB3	1:IA:674:PHE:CD2	2.48	0.49
1:JA:622:GLN:HE22	1:JA:733:PRO:HA	1.77	0.49
1:KA:622:GLN:HE22	1:KA:733:PRO:HA	1.77	0.49
1:NA:662:PRO:HB3	1:NA:674:PHE:CD2	2.48	0.49
1:OA:622:GLN:HE22	1:OA:733:PRO:HA	1.77	0.49
1:YA:712:TYR:OH	1:BB:566:ARG:NH2	2.46	0.49
1:BB:662:PRO:HB3	1:BB:674:PHE:CD2	2.48	0.49
1:FB:662:PRO:HB3	1:FB:674:PHE:CD2	2.48	0.49
1:A:662:PRO:HB3	1:A:674:PHE:CD2	2.48	0.49
1:C:622:GLN:HE22	1:C:733:PRO:HA	1.77	0.49
1:Q:630:PRO:HB3	1:GA:743:LEU:HD22	1.94	0.49
1:X:566:ARG:NH2	1:OA:712:TYR:OH	2.46	0.49
1:X:743:LEU:HD22	1:WA:630:PRO:HB3	1.94	0.49
1:CA:566:ARG:NH2	1:JA:712:TYR:OH	2.46	0.49
1:CA:743:LEU:HD22	1:GB:630:PRO:HB3	1.94	0.49
1:EA:622:GLN:HE22	1:EA:733:PRO:HA	1.77	0.49
1:EA:712:TYR:OH	1:HA:566:ARG:NH2	2.46	0.49
1:HA:662:PRO:HB3	1:HA:674:PHE:CD2	2.48	0.49
1:JA:580:SER:O	1:SA:484:ARG:HD3	2.13	0.49
1:LA:622:GLN:HE22	1:LA:733:PRO:HA	1.77	0.49
1:MA:662:PRO:HB3	1:MA:674:PHE:CD2	2.48	0.49
1:OA:580:SER:O	1:CB:484:ARG:HD3	2.13	0.49
1:PA:484:ARG:HD3	1:CB:580:SER:O	2.13	0.49
1:PA:662:PRO:HB3	1:PA:674:PHE:CD2	2.48	0.49
1:QA:622:GLN:HE22	1:QA:733:PRO:HA	1.77	0.49
1:RA:662:PRO:HB3	1:RA:674:PHE:CD2	2.48	0.49
1:ZA:662:PRO:HB3	1:ZA:674:PHE:CD2	2.48	0.49
1:AB:622:GLN:HE22	1:AB:733:PRO:HA	1.77	0.49
1:A:566:ARG:NH2	1:Q:712:TYR:OH	2.45	0.49
1:F:566:ARG:NH2	1:L:712:TYR:OH	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:445:LEU:HD23	1:VA:536:GLN:HG3	1.93	0.49
1:P:662:PRO:HB3	1:P:674:PHE:CD2	2.48	0.49
1:T:580:SER:O	1:IA:484:ARG:HD3	2.12	0.49
1:V:566:ARG:NH2	1:LA:712:TYR:OH	2.45	0.49
1:BA:566:ARG:NH2	1:FA:712:TYR:OH	2.45	0.49
1:HA:622:GLN:HE22	1:HA:733:PRO:HA	1.77	0.49
1:WA:662:PRO:HB3	1:WA:674:PHE:CD2	2.48	0.49
1:GB:662:PRO:HB3	1:GB:674:PHE:CD2	2.48	0.49
1:A:712:TYR:OH	1:Q:566:ARG:NH2	2.46	0.49
1:B:712:TYR:OH	1:P:566:ARG:NH2	2.45	0.49
1:C:484:ARG:HD3	1:GB:580:SER:O	2.13	0.49
1:C:712:TYR:OH	1:T:566:ARG:NH2	2.45	0.49
1:E:580:SER:O	1:NA:484:ARG:HD3	2.12	0.49
1:G:484:ARG:HD3	1:BA:580:SER:O	2.13	0.49
1:H:662:PRO:HB3	1:H:674:PHE:CD2	2.48	0.49
1:R:622:GLN:HE22	1:R:733:PRO:HA	1.77	0.49
1:V:712:TYR:OH	1:LA:566:ARG:NH2	2.46	0.49
1:Y:712:TYR:OH	1:NA:566:ARG:NH2	2.45	0.49
1:AA:566:ARG:NH2	1:GA:712:TYR:OH	2.45	0.49
1:AA:712:TYR:OH	1:GA:566:ARG:NH2	2.46	0.49
1:FA:662:PRO:HB3	1:FA:674:PHE:CD2	2.48	0.49
1:KA:662:PRO:HB3	1:KA:674:PHE:CD2	2.48	0.49
1:MA:622:GLN:HE22	1:MA:733:PRO:HA	1.77	0.49
1:SA:622:GLN:HE22	1:SA:733:PRO:HA	1.77	0.49
1:VA:566:ARG:NH2	1:ZA:712:TYR:OH	2.46	0.49
1:CB:622:GLN:HE22	1:CB:733:PRO:HA	1.77	0.49
1:B:566:ARG:NH2	1:P:712:TYR:OH	2.46	0.49
1:E:484:ARG:HD3	1:AA:580:SER:O	2.13	0.49
1:E:566:ARG:NH2	1:R:712:TYR:OH	2.45	0.49
1:F:580:SER:O	1:TA:484:ARG:HD3	2.13	0.49
1:H:712:TYR:OH	1:O:566:ARG:NH2	2.45	0.49
1:L:445:LEU:HD23	1:FB:536:GLN:HG3	1.93	0.49
1:M:662:PRO:HB3	1:M:674:PHE:CD2	2.48	0.49
1:O:484:ARG:HD3	1:FA:580:SER:O	2.13	0.49
1:R:662:PRO:HB3	1:R:674:PHE:CD2	2.48	0.49
1:T:484:ARG:HD3	1:V:580:SER:O	2.13	0.49
1:V:484:ARG:HD3	1:IA:580:SER:O	2.13	0.49
1:W:566:ARG:NH2	1:KA:712:TYR:OH	2.46	0.49
1:Y:580:SER:O	1:FA:484:ARG:HD3	2.13	0.49
1:PA:712:TYR:OH	1:FB:566:ARG:NH2	2.46	0.49
1:DB:662:PRO:HB3	1:DB:674:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IB:662:PRO:HB3	1:IB:674:PHE:CD2	2.48	0.49
1:B:484:ARG:HD3	1:LA:580:SER:O	2.13	0.48
1:C:662:PRO:HB3	1:C:674:PHE:CD2	2.48	0.48
1:D:566:ARG:NH2	1:S:712:TYR:OH	2.45	0.48
1:D:712:TYR:OH	1:S:566:ARG:NH2	2.45	0.48
1:F:484:ARG:HD3	1:S:580:SER:O	2.13	0.48
1:G:580:SER:O	1:VA:484:ARG:HD3	2.13	0.48
1:H:580:SER:O	1:MA:484:ARG:HD3	2.13	0.48
1:J:484:ARG:HD3	1:KA:580:SER:O	2.13	0.48
1:J:566:ARG:NH2	1:M:712:TYR:OH	2.45	0.48
1:L:484:ARG:HD3	1:W:580:SER:O	2.13	0.48
1:L:580:SER:O	1:FB:484:ARG:HD3	2.13	0.48
1:O:580:SER:O	1:Y:484:ARG:HD3	2.13	0.48
1:Q:484:ARG:HD3	1:GA:580:SER:O	2.13	0.48
1:R:484:ARG:HD3	1:WA:580:SER:O	2.13	0.48
1:X:712:TYR:OH	1:OA:566:ARG:NH2	2.45	0.48
1:Z:580:SER:O	1:HB:484:ARG:HD3	2.12	0.48
1:AA:484:ARG:HD3	1:NA:580:SER:O	2.13	0.48
1:DA:712:TYR:OH	1:IA:566:ARG:NH2	2.45	0.48
1:TA:662:PRO:HB3	1:TA:674:PHE:CD2	2.48	0.48
1:UA:630:PRO:HB3	1:HB:743:LEU:HD22	1.94	0.48
1:XA:743:LEU:HD22	1:EB:630:PRO:HB3	1.94	0.48
1:YA:662:PRO:HB3	1:YA:674:PHE:CD2	2.48	0.48
1:C:580:SER:O	1:CA:484:ARG:HD3	2.13	0.48
1:D:580:SER:O	1:K:484:ARG:HD3	2.13	0.48
1:J:580:SER:O	1:DA:484:ARG:HD3	2.13	0.48
1:K:580:SER:O	1:DB:484:ARG:HD3	2.13	0.48
1:M:580:SER:O	1:HA:484:ARG:HD3	2.13	0.48
1:R:580:SER:O	1:X:484:ARG:HD3	2.13	0.48
1:Y:566:ARG:NH2	1:NA:712:TYR:OH	2.45	0.48
1:Z:743:LEU:HD22	1:HB:630:PRO:HB3	1.93	0.48
1:CA:712:TYR:OH	1:JA:566:ARG:NH2	2.45	0.48
1:DA:580:SER:O	1:KA:484:ARG:HD3	2.13	0.48
1:EA:580:SER:O	1:XA:484:ARG:HD3	2.12	0.48
1:UA:622:GLN:HE22	1:UA:733:PRO:HA	1.77	0.48
1:WA:622:GLN:HE22	1:WA:733:PRO:HA	1.77	0.48
1:FB:622:GLN:HE22	1:FB:733:PRO:HA	1.77	0.48
1:I:608:VAL:HG21	1:I:636:PHE:CE2	2.49	0.48
1:N:608:VAL:HG21	1:N:636:PHE:CE2	2.49	0.48
1:W:608:VAL:HG21	1:W:636:PHE:CE2	2.49	0.48
1:BA:608:VAL:HG21	1:BA:636:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:662:PRO:HB3	1:CA:674:PHE:CD2	2.48	0.48
1:EA:743:LEU:HD22	1:XA:630:PRO:HB3	1.93	0.48
1:LA:662:PRO:HB3	1:LA:674:PHE:CD2	2.47	0.48
1:VA:622:GLN:HE22	1:VA:733:PRO:HA	1.77	0.48
1:XA:662:PRO:HB3	1:XA:674:PHE:CD2	2.48	0.48
1:YA:608:VAL:HG21	1:YA:636:PHE:CE2	2.49	0.48
1:YA:622:GLN:HE22	1:YA:733:PRO:HA	1.77	0.48
1:EB:622:GLN:HE22	1:EB:733:PRO:HA	1.77	0.48
1:M:622:GLN:HE22	1:M:733:PRO:HA	1.77	0.48
1:V:242:THR:HG23	1:V:689:GLU:HB2	1.96	0.48
1:X:608:VAL:HG21	1:X:636:PHE:CE2	2.49	0.48
1:X:662:PRO:HB3	1:X:674:PHE:CD2	2.48	0.48
1:AA:242:THR:HG23	1:AA:689:GLU:HB2	1.96	0.48
1:CA:608:VAL:HG21	1:CA:636:PHE:CE2	2.49	0.48
1:QA:566:ARG:NH2	1:EB:712:TYR:OH	2.46	0.48
1:SA:566:ARG:NH2	1:HB:712:TYR:OH	2.45	0.48
1:SA:662:PRO:HB3	1:SA:674:PHE:CD2	2.48	0.48
1:UA:608:VAL:HG21	1:UA:636:PHE:CE2	2.49	0.48
1:UA:662:PRO:HB3	1:UA:674:PHE:CD2	2.48	0.48
1:EB:608:VAL:HG21	1:EB:636:PHE:CE2	2.49	0.48
1:EB:662:PRO:HB3	1:EB:674:PHE:CD2	2.48	0.48
1:HB:662:PRO:HB3	1:HB:674:PHE:CD2	2.48	0.48
1:D:242:THR:HG23	1:D:689:GLU:HB2	1.96	0.48
1:F:608:VAL:HG21	1:F:636:PHE:CE2	2.49	0.48
1:H:622:GLN:HE22	1:H:733:PRO:HA	1.77	0.48
1:K:608:VAL:HG21	1:K:636:PHE:CE2	2.49	0.48
1:L:743:LEU:HD22	1:FB:630:PRO:HB3	1.93	0.48
1:O:608:VAL:HG21	1:O:636:PHE:CE2	2.49	0.48
1:S:484:ARG:HD3	1:TA:580:SER:O	2.13	0.48
1:S:608:VAL:HG21	1:S:636:PHE:CE2	2.49	0.48
1:W:242:THR:HG23	1:W:689:GLU:HB2	1.96	0.48
1:BA:242:THR:HG23	1:BA:689:GLU:HB2	1.96	0.48
1:DA:566:ARG:NH2	1:IA:712:TYR:OH	2.45	0.48
1:GA:662:PRO:HB3	1:GA:674:PHE:CD2	2.48	0.48
1:PA:622:GLN:HE22	1:PA:733:PRO:HA	1.77	0.48
1:QA:242:THR:HG23	1:QA:689:GLU:HB2	1.96	0.48
1:UA:712:TYR:OH	1:AB:566:ARG:NH2	2.46	0.48
1:WA:242:THR:HG23	1:WA:689:GLU:HB2	1.96	0.48
1:XA:712:TYR:OH	1:CB:566:ARG:NH2	2.45	0.48
1:CB:662:PRO:HB3	1:CB:674:PHE:CD2	2.48	0.48
1:GB:622:GLN:HE22	1:GB:733:PRO:HA	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IB:608:VAL:HG21	1:IB:636:PHE:CE2	2.49	0.48
1:IB:622:GLN:HE22	1:IB:733:PRO:HA	1.77	0.48
1:D:608:VAL:HG21	1:D:636:PHE:CE2	2.49	0.48
1:G:662:PRO:HB3	1:G:674:PHE:CD2	2.48	0.48
1:G:743:LEU:HD22	1:VA:630:PRO:HB3	1.94	0.48
1:H:608:VAL:HG21	1:H:636:PHE:CE2	2.49	0.48
1:J:608:VAL:HG21	1:J:636:PHE:CE2	2.49	0.48
1:L:662:PRO:HB3	1:L:674:PHE:CD2	2.48	0.48
1:Q:608:VAL:HG21	1:Q:636:PHE:CE2	2.49	0.48
1:S:242:THR:HG23	1:S:689:GLU:HB2	1.96	0.48
1:GA:608:VAL:HG21	1:GA:636:PHE:CE2	2.49	0.48
1:IA:242:THR:HG23	1:IA:689:GLU:HB2	1.96	0.48
1:JA:662:PRO:HB3	1:JA:674:PHE:CD2	2.48	0.48
1:LA:608:VAL:HG21	1:LA:636:PHE:CE2	2.49	0.48
1:NA:242:THR:HG23	1:NA:689:GLU:HB2	1.96	0.48
1:OA:662:PRO:HB3	1:OA:674:PHE:CD2	2.48	0.48
1:XA:608:VAL:HG21	1:XA:636:PHE:CE2	2.49	0.48
1:AB:242:THR:HG23	1:AB:689:GLU:HB2	1.96	0.48
1:AB:662:PRO:HB3	1:AB:674:PHE:CD2	2.48	0.48
1:GB:242:THR:HG23	1:GB:689:GLU:HB2	1.96	0.48
1:HB:608:VAL:HG21	1:HB:636:PHE:CE2	2.49	0.48
1:B:608:VAL:HG21	1:B:636:PHE:CE2	2.49	0.48
1:D:484:ARG:HD3	1:DB:580:SER:O	2.13	0.48
1:D:662:PRO:HB3	1:D:674:PHE:CD2	2.48	0.48
1:M:608:VAL:HG21	1:M:636:PHE:CE2	2.49	0.48
1:S:662:PRO:HB3	1:S:674:PHE:CD2	2.48	0.48
1:KA:242:THR:HG23	1:KA:689:GLU:HB2	1.96	0.48
1:NA:608:VAL:HG21	1:NA:636:PHE:CE2	2.49	0.48
1:QA:662:PRO:HB3	1:QA:674:PHE:CD2	2.48	0.48
1:WA:608:VAL:HG21	1:WA:636:PHE:CE2	2.49	0.48
1:ZA:622:GLN:HE22	1:ZA:733:PRO:HA	1.77	0.48
1:F:622:GLN:HE22	1:F:733:PRO:HA	1.77	0.48
1:Z:608:VAL:HG21	1:Z:636:PHE:CE2	2.49	0.48
1:EA:608:VAL:HG21	1:EA:636:PHE:CE2	2.49	0.48
1:FA:242:THR:HG23	1:FA:689:GLU:HB2	1.96	0.48
1:HA:580:SER:O	1:BB:484:ARG:HD3	2.13	0.48
1:IA:608:VAL:HG21	1:IA:636:PHE:CE2	2.49	0.48
1:KA:608:VAL:HG21	1:KA:636:PHE:CE2	2.49	0.48
1:OA:608:VAL:HG21	1:OA:636:PHE:CE2	2.49	0.48
1:TA:608:VAL:HG21	1:TA:636:PHE:CE2	2.49	0.48
1:VA:608:VAL:HG21	1:VA:636:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZA:242:THR:HG23	1:ZA:689:GLU:HB2	1.96	0.48
1:DB:608:VAL:HG21	1:DB:636:PHE:CE2	2.49	0.48
1:FB:242:THR:HG23	1:FB:689:GLU:HB2	1.96	0.48
1:IB:242:THR:HG23	1:IB:689:GLU:HB2	1.95	0.48
1:B:580:SER:O	1:AB:484:ARG:HD3	2.13	0.48
1:C:242:THR:HG23	1:C:689:GLU:HB2	1.96	0.48
1:C:608:VAL:HG21	1:C:636:PHE:CE2	2.49	0.48
1:F:462:PHE:O	1:TA:552:VAL:HG22	2.14	0.48
1:K:462:PHE:O	1:DB:552:VAL:HG22	2.14	0.48
1:R:608:VAL:HG21	1:R:636:PHE:CE2	2.49	0.48
1:W:484:ARG:HD3	1:FB:580:SER:O	2.13	0.48
1:BA:484:ARG:HD3	1:VA:580:SER:O	2.13	0.48
1:FA:608:VAL:HG21	1:FA:636:PHE:CE2	2.49	0.48
1:GA:484:ARG:HD3	1:QA:580:SER:O	2.13	0.48
1:HA:608:VAL:HG21	1:HA:636:PHE:CE2	2.49	0.48
1:JA:608:VAL:HG21	1:JA:636:PHE:CE2	2.49	0.48
1:LA:484:ARG:HD3	1:AB:580:SER:O	2.13	0.48
1:QA:608:VAL:HG21	1:QA:636:PHE:CE2	2.49	0.48
1:RA:242:THR:HG23	1:RA:689:GLU:HB2	1.96	0.48
1:RA:608:VAL:HG21	1:RA:636:PHE:CE2	2.49	0.48
1:TA:242:THR:HG23	1:TA:689:GLU:HB2	1.95	0.48
1:YA:242:THR:HG23	1:YA:689:GLU:HB2	1.96	0.48
1:AB:608:VAL:HG21	1:AB:636:PHE:CE2	2.49	0.48
1:BB:242:THR:HG23	1:BB:689:GLU:HB2	1.96	0.48
1:FB:608:VAL:HG21	1:FB:636:PHE:CE2	2.49	0.48
1:GB:608:VAL:HG21	1:GB:636:PHE:CE2	2.49	0.48
1:A:608:VAL:HG21	1:A:636:PHE:CE2	2.49	0.48
1:I:580:SER:O	1:P:484:ARG:HD3	2.13	0.48
1:K:622:GLN:HE22	1:K:733:PRO:HA	1.77	0.48
1:L:242:THR:HG23	1:L:689:GLU:HB2	1.95	0.48
1:V:608:VAL:HG21	1:V:636:PHE:CE2	2.49	0.48
1:Z:462:PHE:O	1:HB:552:VAL:HG22	2.14	0.48
1:DA:242:THR:HG23	1:DA:689:GLU:HB2	1.96	0.48
1:EA:462:PHE:O	1:XA:552:VAL:HG22	2.14	0.48
1:MA:608:VAL:HG21	1:MA:636:PHE:CE2	2.49	0.48
1:PA:242:THR:HG23	1:PA:689:GLU:HB2	1.96	0.48
1:XA:622:GLN:HE22	1:XA:733:PRO:HA	1.77	0.48
1:BB:608:VAL:HG21	1:BB:636:PHE:CE2	2.49	0.48
1:DB:242:THR:HG23	1:DB:689:GLU:HB2	1.96	0.48
1:A:242:THR:HG23	1:A:689:GLU:HB2	1.96	0.47
1:E:462:PHE:O	1:NA:552:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:242:THR:HG23	1:P:689:GLU:HB2	1.96	0.47
1:P:608:VAL:HG21	1:P:636:PHE:CE2	2.49	0.47
1:Q:580:SER:O	1:QA:484:ARG:HD3	2.13	0.47
1:T:462:PHE:O	1:IA:552:VAL:HG22	2.14	0.47
1:X:580:SER:O	1:WA:484:ARG:HD3	2.13	0.47
1:Y:242:THR:HG23	1:Y:689:GLU:HB2	1.96	0.47
1:CA:580:SER:O	1:GB:484:ARG:HD3	2.13	0.47
1:MA:580:SER:O	1:RA:484:ARG:HD3	2.13	0.47
1:VA:242:THR:HG23	1:VA:689:GLU:HB2	1.96	0.47
1:HB:242:THR:HG23	1:HB:689:GLU:HB2	1.96	0.47
1:HB:622:GLN:HE22	1:HB:733:PRO:HA	1.77	0.47
1:G:242:THR:HG23	1:G:689:GLU:HB2	1.96	0.47
1:G:462:PHE:O	1:VA:552:VAL:HG22	2.14	0.47
1:G:608:VAL:HG21	1:G:636:PHE:CE2	2.49	0.47
1:H:484:ARG:HD3	1:RA:580:SER:O	2.13	0.47
1:I:552:VAL:HG22	1:YA:462:PHE:O	2.14	0.47
1:L:462:PHE:O	1:FB:552:VAL:HG22	2.14	0.47
1:L:608:VAL:HG21	1:L:636:PHE:CE2	2.49	0.47
1:R:242:THR:HG23	1:R:689:GLU:HB2	1.96	0.47
1:Y:462:PHE:O	1:FA:552:VAL:HG22	2.14	0.47
1:AA:608:VAL:HG21	1:AA:636:PHE:CE2	2.49	0.47
1:DA:462:PHE:O	1:KA:552:VAL:HG22	2.15	0.47
1:XA:242:THR:HG23	1:XA:689:GLU:HB2	1.96	0.47
1:ZA:608:VAL:HG21	1:ZA:636:PHE:CE2	2.49	0.47
1:A:484:ARG:HD3	1:N:580:SER:O	2.13	0.47
1:C:552:VAL:HG22	1:GB:462:PHE:O	2.14	0.47
1:D:552:VAL:HG22	1:DB:462:PHE:O	2.14	0.47
1:P:462:PHE:O	1:YA:552:VAL:HG22	2.14	0.47
1:Q:242:THR:HG23	1:Q:689:GLU:HB2	1.96	0.47
1:R:552:VAL:HG22	1:WA:462:PHE:O	2.14	0.47
1:S:552:VAL:HG22	1:TA:462:PHE:O	2.14	0.47
1:X:462:PHE:O	1:WA:552:VAL:HG22	2.15	0.47
1:Y:608:VAL:HG21	1:Y:636:PHE:CE2	2.49	0.47
1:Z:242:THR:HG23	1:Z:689:GLU:HB2	1.96	0.47
1:CA:462:PHE:O	1:GB:552:VAL:HG22	2.14	0.47
1:DA:608:VAL:HG21	1:DA:636:PHE:CE2	2.49	0.47
1:EA:242:THR:HG23	1:EA:689:GLU:HB2	1.96	0.47
1:PA:608:VAL:HG21	1:PA:636:PHE:CE2	2.49	0.47
1:CB:242:THR:HG23	1:CB:689:GLU:HB2	1.96	0.47
1:A:462:PHE:O	1:IB:552:VAL:HG22	2.14	0.47
1:A:552:VAL:HG22	1:N:462:PHE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:PHE:O	1:AB:552:VAL:HG22	2.14	0.47
1:C:462:PHE:O	1:CA:552:VAL:HG22	2.14	0.47
1:I:462:PHE:O	1:P:552:VAL:HG22	2.14	0.47
1:M:484:ARG:HD3	1:BB:580:SER:O	2.13	0.47
1:N:552:VAL:HG22	1:IB:462:PHE:O	2.14	0.47
1:HA:242:THR:HG23	1:HA:689:GLU:HB2	1.96	0.47
1:JA:484:ARG:HD3	1:ZA:580:SER:O	2.12	0.47
1:MA:242:THR:HG23	1:MA:689:GLU:HB2	1.96	0.47
1:SA:242:THR:HG23	1:SA:689:GLU:HB2	1.96	0.47
1:B:242:THR:HG23	1:B:689:GLU:HB2	1.96	0.47
1:E:633:ASP:N	1:AA:615:GLN:NE2	2.63	0.47
1:F:552:VAL:HG22	1:S:462:PHE:O	2.15	0.47
1:Q:462:PHE:O	1:QA:552:VAL:HG22	2.14	0.47
1:T:633:ASP:N	1:V:615:GLN:NE2	2.63	0.47
1:EA:552:VAL:HG22	1:EB:462:PHE:O	2.14	0.47
1:GA:242:THR:HG23	1:GA:689:GLU:HB2	1.96	0.47
1:JA:242:THR:HG23	1:JA:689:GLU:HB2	1.96	0.47
1:JA:552:VAL:HG22	1:ZA:462:PHE:O	2.14	0.47
1:LA:242:THR:HG23	1:LA:689:GLU:HB2	1.96	0.47
1:OA:242:THR:HG23	1:OA:689:GLU:HB2	1.96	0.47
1:I:242:THR:HG23	1:I:689:GLU:HB2	1.96	0.47
1:M:552:VAL:HG22	1:BB:462:PHE:O	2.15	0.47
1:V:552:VAL:HG22	1:IA:462:PHE:O	2.14	0.47
1:W:552:VAL:HG22	1:FB:462:PHE:O	2.14	0.47
1:Z:669:PHE:CD1	1:AB:373:PRO:HA	2.50	0.47
1:HA:462:PHE:O	1:BB:552:VAL:HG22	2.14	0.47
1:OA:484:ARG:HD3	1:PA:580:SER:O	2.13	0.47
1:OA:552:VAL:HG22	1:PA:462:PHE:O	2.14	0.47
1:XA:462:PHE:O	1:EB:552:VAL:HG22	2.14	0.47
1:D:462:PHE:O	1:K:552:VAL:HG22	2.15	0.47
1:E:552:VAL:HG22	1:AA:462:PHE:O	2.14	0.47
1:E:608:VAL:HG21	1:E:636:PHE:CE2	2.49	0.47
1:H:552:VAL:HG22	1:RA:462:PHE:O	2.15	0.47
1:J:669:PHE:CD1	1:W:373:PRO:HA	2.50	0.47
1:N:242:THR:HG23	1:N:689:GLU:HB2	1.96	0.47
1:O:669:PHE:CD1	1:BA:373:PRO:HA	2.50	0.47
1:R:462:PHE:O	1:X:552:VAL:HG22	2.15	0.47
1:T:552:VAL:HG22	1:V:462:PHE:O	2.14	0.47
1:T:608:VAL:HG21	1:T:636:PHE:CE2	2.49	0.47
1:Z:552:VAL:HG22	1:UA:462:PHE:O	2.14	0.47
1:AA:552:VAL:HG22	1:NA:462:PHE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:552:VAL:HG22	1:VA:462:PHE:O	2.14	0.47
1:EA:669:PHE:CD1	1:QA:373:PRO:HA	2.50	0.47
1:HA:696:LYS:HA	1:HA:696:LYS:HD3	1.73	0.47
1:IA:230:CYS:HB3	1:KA:396:GLU:O	2.15	0.47
1:MA:462:PHE:O	1:RA:552:VAL:HG22	2.15	0.47
1:PA:552:VAL:HG22	1:CB:462:PHE:O	2.15	0.47
1:SA:462:PHE:O	1:ZA:552:VAL:HG22	2.14	0.47
1:SA:608:VAL:HG21	1:SA:636:PHE:CE2	2.49	0.47
1:UA:242:THR:HG23	1:UA:689:GLU:HB2	1.96	0.47
1:UA:552:VAL:HG22	1:HB:462:PHE:O	2.15	0.47
1:CB:608:VAL:HG21	1:CB:636:PHE:CE2	2.49	0.47
1:C:373:PRO:HA	1:IA:669:PHE:CD1	2.50	0.47
1:H:462:PHE:O	1:MA:552:VAL:HG22	2.14	0.47
1:J:552:VAL:HG22	1:KA:462:PHE:O	2.14	0.47
1:Q:552:VAL:HG22	1:GA:462:PHE:O	2.14	0.47
1:W:696:LYS:HD3	1:W:696:LYS:HA	1.73	0.47
1:X:373:PRO:HA	1:CB:669:PHE:CD1	2.50	0.47
1:EB:242:THR:HG23	1:EB:689:GLU:HB2	1.96	0.47
1:B:552:VAL:HG22	1:LA:462:PHE:O	2.14	0.47
1:H:373:PRO:HA	1:Y:669:PHE:CD1	2.50	0.47
1:M:462:PHE:O	1:HA:552:VAL:HG22	2.14	0.47
1:V:669:PHE:CD1	1:DA:373:PRO:HA	2.50	0.47
1:Y:373:PRO:HA	1:AA:669:PHE:CD1	2.50	0.47
1:Z:396:GLU:O	1:AB:230:CYS:HB3	2.15	0.47
1:FA:396:GLU:O	1:NA:230:CYS:HB3	2.15	0.47
1:UA:696:LYS:HA	1:UA:696:LYS:HD3	1.73	0.47
1:FB:696:LYS:HD3	1:FB:696:LYS:HA	1.73	0.47
1:G:230:CYS:HB3	1:DB:396:GLU:O	2.15	0.47
1:H:230:CYS:HB3	1:Y:396:GLU:O	2.15	0.47
1:H:242:THR:HG23	1:H:689:GLU:HB2	1.96	0.47
1:J:230:CYS:HB3	1:HA:396:GLU:O	2.16	0.47
1:M:230:CYS:HB3	1:DA:396:GLU:O	2.15	0.47
1:O:242:THR:HG23	1:O:689:GLU:HB2	1.96	0.47
1:O:552:VAL:HG22	1:FA:462:PHE:O	2.14	0.47
1:R:373:PRO:HA	1:NA:669:PHE:CD1	2.50	0.47
1:Y:230:CYS:HB3	1:AA:396:GLU:O	2.15	0.47
1:CA:373:PRO:HA	1:SA:669:PHE:CD1	2.50	0.47
1:EA:396:GLU:O	1:QA:230:CYS:HB3	2.15	0.47
1:LA:552:VAL:HG22	1:AB:462:PHE:O	2.14	0.47
1:E:242:THR:HG23	1:E:689:GLU:HB2	1.96	0.46
1:I:633:ASP:N	1:YA:615:GLN:NE2	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:242:THR:HG23	1:J:689:GLU:HB2	1.96	0.46
1:L:230:CYS:HB3	1:TA:396:GLU:O	2.15	0.46
1:L:552:VAL:HG22	1:W:462:PHE:O	2.14	0.46
1:M:373:PRO:HA	1:DA:669:PHE:CD1	2.50	0.46
1:O:230:CYS:HB3	1:MA:396:GLU:O	2.16	0.46
1:T:585:ARG:HG2	1:T:586:GLY:O	2.16	0.46
1:V:396:GLU:O	1:DA:230:CYS:HB3	2.15	0.46
1:X:242:THR:HG23	1:X:689:GLU:HB2	1.96	0.46
1:GA:552:VAL:HG22	1:QA:462:PHE:O	2.14	0.46
1:HA:585:ARG:HG2	1:HA:586:GLY:O	2.16	0.46
1:JA:585:ARG:HG2	1:JA:586:GLY:O	2.16	0.46
1:JA:615:GLN:NE2	1:SA:633:ASP:N	2.63	0.46
1:MA:585:ARG:HG2	1:MA:586:GLY:O	2.16	0.46
1:OA:585:ARG:HG2	1:OA:586:GLY:O	2.16	0.46
1:E:585:ARG:HG2	1:E:586:GLY:O	2.16	0.46
1:F:230:CYS:HB3	1:FB:396:GLU:O	2.16	0.46
1:G:552:VAL:HG22	1:BA:462:PHE:O	2.14	0.46
1:I:585:ARG:HG2	1:I:586:GLY:O	2.16	0.46
1:M:242:THR:HG23	1:M:689:GLU:HB2	1.96	0.46
1:N:585:ARG:HG2	1:N:586:GLY:O	2.16	0.46
1:T:242:THR:HG23	1:T:689:GLU:HB2	1.96	0.46
1:Z:373:PRO:HA	1:RA:669:PHE:CD1	2.50	0.46
1:JA:396:GLU:O	1:VA:230:CYS:HB3	2.15	0.46
1:JA:462:PHE:O	1:SA:552:VAL:HG22	2.14	0.46
1:OA:615:GLN:NE2	1:CB:633:ASP:N	2.63	0.46
1:PA:669:PHE:CD1	1:XA:373:PRO:HA	2.50	0.46
1:A:585:ARG:HG2	1:A:586:GLY:O	2.16	0.46
1:B:230:CYS:HB3	1:YA:396:GLU:O	2.15	0.46
1:C:396:GLU:O	1:TA:230:CYS:HB3	2.16	0.46
1:G:373:PRO:HA	1:DB:669:PHE:CD1	2.50	0.46
1:G:585:ARG:HG2	1:G:586:GLY:O	2.16	0.46
1:J:462:PHE:O	1:DA:552:VAL:HG22	2.14	0.46
1:K:230:CYS:HB3	1:VA:396:GLU:O	2.16	0.46
1:K:242:THR:HG23	1:K:689:GLU:HB2	1.96	0.46
1:L:373:PRO:HA	1:TA:669:PHE:CD1	2.50	0.46
1:L:585:ARG:HG2	1:L:586:GLY:O	2.16	0.46
1:N:633:ASP:N	1:IB:615:GLN:NE2	2.63	0.46
1:N:669:PHE:CD1	1:RA:373:PRO:HA	2.50	0.46
1:P:585:ARG:HG2	1:P:586:GLY:O	2.16	0.46
1:Q:230:CYS:HB3	1:IB:396:GLU:O	2.15	0.46
1:V:585:ARG:HG2	1:V:586:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:396:GLU:O	1:PA:230:CYS:HB3	2.16	0.46
1:Z:230:CYS:HB3	1:RA:396:GLU:O	2.16	0.46
1:AA:585:ARG:HG2	1:AA:586:GLY:O	2.16	0.46
1:BA:396:GLU:O	1:ZA:230:CYS:HB3	2.16	0.46
1:BA:696:LYS:HD3	1:BA:696:LYS:HA	1.73	0.46
1:CA:242:THR:HG23	1:CA:689:GLU:HB2	1.96	0.46
1:EA:230:CYS:HB3	1:BB:396:GLU:O	2.16	0.46
1:HA:230:CYS:HB3	1:XA:396:GLU:O	2.15	0.46
1:LA:396:GLU:O	1:UA:230:CYS:HB3	2.16	0.46
1:MA:696:LYS:HA	1:MA:696:LYS:HD3	1.73	0.46
1:OA:396:GLU:O	1:FB:230:CYS:HB3	2.15	0.46
1:OA:462:PHE:O	1:CB:552:VAL:HG22	2.14	0.46
1:OA:669:PHE:CD1	1:FB:373:PRO:HA	2.50	0.46
1:PA:396:GLU:O	1:XA:230:CYS:HB3	2.15	0.46
1:PA:585:ARG:HG2	1:PA:586:GLY:O	2.16	0.46
1:QA:696:LYS:HD3	1:QA:696:LYS:HA	1.73	0.46
1:TA:585:ARG:HG2	1:TA:586:GLY:O	2.16	0.46
1:VA:585:ARG:HG2	1:VA:586:GLY:O	2.16	0.46
1:ZA:396:GLU:O	1:HB:230:CYS:HB3	2.15	0.46
1:ZA:669:PHE:CD1	1:HB:373:PRO:HA	2.50	0.46
1:DB:585:ARG:HG2	1:DB:586:GLY:O	2.16	0.46
1:D:669:PHE:CD1	1:WA:373:PRO:HA	2.50	0.46
1:E:396:GLU:O	1:GA:230:CYS:HB3	2.15	0.46
1:F:373:PRO:HA	1:FB:669:PHE:CD1	2.50	0.46
1:I:669:PHE:CD1	1:BB:373:PRO:HA	2.50	0.46
1:J:373:PRO:HA	1:HA:669:PHE:CD1	2.50	0.46
1:O:373:PRO:HA	1:MA:669:PHE:CD1	2.50	0.46
1:O:462:PHE:O	1:Y:552:VAL:HG22	2.14	0.46
1:Q:373:PRO:HA	1:IB:669:PHE:CD1	2.50	0.46
1:R:396:GLU:O	1:DB:230:CYS:HB3	2.16	0.46
1:S:669:PHE:CD1	1:GB:373:PRO:HA	2.50	0.46
1:T:396:GLU:O	1:LA:230:CYS:HB3	2.15	0.46
1:GA:396:GLU:O	1:EB:230:CYS:HB3	2.16	0.46
1:IA:373:PRO:HA	1:KA:669:PHE:CD1	2.50	0.46
1:IA:585:ARG:HG2	1:IA:586:GLY:O	2.16	0.46
1:MA:230:CYS:HB3	1:HB:396:GLU:O	2.15	0.46
1:MA:373:PRO:HA	1:HB:669:PHE:CD1	2.50	0.46
1:SA:373:PRO:HA	1:UA:669:PHE:CD1	2.50	0.46
1:ZA:585:ARG:HG2	1:ZA:586:GLY:O	2.16	0.46
1:BB:585:ARG:HG2	1:BB:586:GLY:O	2.16	0.46
1:FB:585:ARG:HG2	1:FB:586:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:PHE:CD1	1:I:373:PRO:HA	2.50	0.46
1:A:696:LYS:HD3	1:A:696:LYS:HA	1.73	0.46
1:B:373:PRO:HA	1:YA:669:PHE:CD1	2.50	0.46
1:B:633:ASP:N	1:LA:615:GLN:NE2	2.63	0.46
1:C:230:CYS:HB3	1:IA:396:GLU:O	2.15	0.46
1:F:242:THR:HG23	1:F:689:GLU:HB2	1.96	0.46
1:G:669:PHE:CD1	1:FA:373:PRO:HA	2.50	0.46
1:L:669:PHE:CD1	1:KA:373:PRO:HA	2.50	0.46
1:N:373:PRO:HA	1:P:669:PHE:CD1	2.50	0.46
1:P:696:LYS:HD3	1:P:696:LYS:HA	1.73	0.46
1:R:230:CYS:HB3	1:NA:396:GLU:O	2.15	0.46
1:T:669:PHE:CD1	1:LA:373:PRO:HA	2.50	0.46
1:W:633:ASP:N	1:FB:615:GLN:NE2	2.63	0.46
1:X:585:ARG:HG2	1:X:586:GLY:O	2.16	0.46
1:CA:585:ARG:HG2	1:CA:586:GLY:O	2.16	0.46
1:EA:373:PRO:HA	1:BB:669:PHE:CD1	2.50	0.46
1:FA:669:PHE:CD1	1:NA:373:PRO:HA	2.50	0.46
1:JA:669:PHE:CD1	1:VA:373:PRO:HA	2.50	0.46
1:NA:585:ARG:HG2	1:NA:586:GLY:O	2.16	0.46
1:D:373:PRO:HA	1:F:669:PHE:CD1	2.50	0.46
1:H:669:PHE:CD1	1:IB:373:PRO:HA	2.50	0.46
1:H:726:GLY:HA3	1:Y:257:TYR:O	2.16	0.46
1:K:373:PRO:HA	1:VA:669:PHE:CD1	2.50	0.46
1:M:669:PHE:CD1	1:YA:373:PRO:HA	2.50	0.46
1:M:726:GLY:HA3	1:DA:257:TYR:O	2.16	0.46
1:N:257:TYR:O	1:RA:726:GLY:HA3	2.16	0.46
1:O:585:ARG:HG2	1:O:586:GLY:O	2.16	0.46
1:P:615:GLN:NE2	1:YA:633:ASP:N	2.63	0.46
1:HA:373:PRO:HA	1:XA:669:PHE:CD1	2.50	0.46
1:RA:585:ARG:HG2	1:RA:586:GLY:O	2.16	0.46
1:XA:585:ARG:HG2	1:XA:586:GLY:O	2.16	0.46
1:AB:585:ARG:HG2	1:AB:586:GLY:O	2.16	0.46
1:CB:373:PRO:HA	1:EB:669:PHE:CD1	2.50	0.46
1:A:615:GLN:NE2	1:IB:633:ASP:N	2.63	0.46
1:C:585:ARG:HG2	1:C:586:GLY:O	2.16	0.46
1:D:230:CYS:HB3	1:F:396:GLU:O	2.15	0.46
1:E:669:PHE:CD1	1:GA:373:PRO:HA	2.50	0.46
1:F:378:LEU:CD2	1:S:436:PRO:HG3	2.46	0.46
1:G:396:GLU:O	1:FA:230:CYS:HB3	2.16	0.46
1:G:436:PRO:HG3	1:VA:378:LEU:CD2	2.46	0.46
1:I:257:TYR:O	1:BB:726:GLY:HA3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:436:PRO:HG3	1:P:378:LEU:CD2	2.46	0.46
1:J:585:ARG:HG2	1:J:586:GLY:O	2.16	0.46
1:L:396:GLU:O	1:KA:230:CYS:HB3	2.16	0.46
1:L:436:PRO:HG3	1:FB:378:LEU:CD2	2.46	0.46
1:P:230:CYS:HB3	1:AB:396:GLU:O	2.16	0.46
1:P:373:PRO:HA	1:AB:669:PHE:CD1	2.50	0.46
1:Q:436:PRO:HG3	1:QA:378:LEU:CD2	2.46	0.46
1:Q:633:ASP:N	1:GA:615:GLN:NE2	2.63	0.46
1:Q:696:LYS:HD3	1:Q:696:LYS:HA	1.73	0.46
1:R:585:ARG:HG2	1:R:586:GLY:O	2.16	0.46
1:V:378:LEU:CD2	1:IA:436:PRO:HG3	2.46	0.46
1:X:726:GLY:HA3	1:CB:257:TYR:O	2.16	0.46
1:Z:726:GLY:HA3	1:RA:257:TYR:O	2.16	0.46
1:BA:633:ASP:N	1:VA:615:GLN:NE2	2.63	0.46
1:CA:726:GLY:HA3	1:SA:257:TYR:O	2.16	0.46
1:MA:615:GLN:NE2	1:RA:633:ASP:N	2.63	0.46
1:OA:436:PRO:HG3	1:CB:378:LEU:CD2	2.46	0.46
1:QA:585:ARG:HG2	1:QA:586:GLY:O	2.16	0.46
1:A:378:LEU:CD2	1:N:436:PRO:HG3	2.46	0.46
1:B:436:PRO:HG3	1:AB:378:LEU:CD2	2.46	0.46
1:C:669:PHE:CD1	1:TA:373:PRO:HA	2.50	0.46
1:D:436:PRO:HG3	1:K:378:LEU:CD2	2.46	0.46
1:E:436:PRO:HG3	1:NA:378:LEU:CD2	2.46	0.46
1:F:436:PRO:HG3	1:TA:378:LEU:CD2	2.46	0.46
1:H:378:LEU:CD2	1:RA:436:PRO:HG3	2.46	0.46
1:I:378:LEU:CD2	1:YA:436:PRO:HG3	2.46	0.46
1:K:396:GLU:O	1:S:230:CYS:HB3	2.15	0.46
1:K:669:PHE:CD1	1:S:373:PRO:HA	2.50	0.46
1:N:378:LEU:CD2	1:IB:436:PRO:HG3	2.46	0.46
1:O:396:GLU:O	1:BA:230:CYS:HB3	2.15	0.46
1:R:669:PHE:CD1	1:DB:373:PRO:HA	2.50	0.46
1:S:585:ARG:HG2	1:S:586:GLY:O	2.16	0.46
1:X:230:CYS:HB3	1:CB:396:GLU:O	2.15	0.46
1:Y:696:LYS:HA	1:Y:696:LYS:HD3	1.73	0.46
1:Z:378:LEU:CD2	1:UA:436:PRO:HG3	2.46	0.46
1:AA:378:LEU:CD2	1:NA:436:PRO:HG3	2.46	0.46
1:BA:585:ARG:HG2	1:BA:586:GLY:O	2.16	0.46
1:CA:230:CYS:HB3	1:SA:396:GLU:O	2.15	0.46
1:DA:696:LYS:HA	1:DA:696:LYS:HD3	1.73	0.46
1:EA:585:ARG:HG2	1:EA:586:GLY:O	2.16	0.46
1:EA:726:GLY:HA3	1:BB:257:TYR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:373:PRO:HA	1:GB:669:PHE:CD1	2.50	0.46
1:JA:436:PRO:HG3	1:SA:378:LEU:CD2	2.46	0.46
1:SA:585:ARG:HG2	1:SA:586:GLY:O	2.16	0.46
1:WA:585:ARG:HG2	1:WA:586:GLY:O	2.16	0.46
1:GB:585:ARG:HG2	1:GB:586:GLY:O	2.16	0.46
1:HB:585:ARG:HG2	1:HB:586:GLY:O	2.16	0.46
1:A:230:CYS:HB3	1:QA:396:GLU:O	2.16	0.46
1:A:373:PRO:HA	1:QA:669:PHE:CD1	2.50	0.46
1:B:669:PHE:CD1	1:V:373:PRO:HA	2.50	0.46
1:H:633:ASP:N	1:RA:615:GLN:NE2	2.63	0.46
1:J:396:GLU:O	1:W:230:CYS:HB3	2.15	0.46
1:J:436:PRO:HG3	1:DA:378:LEU:CD2	2.46	0.46
1:K:436:PRO:HG3	1:DB:378:LEU:CD2	2.46	0.46
1:M:378:LEU:CD2	1:BB:436:PRO:HG3	2.46	0.46
1:M:633:ASP:N	1:BB:615:GLN:NE2	2.63	0.46
1:Q:669:PHE:CD1	1:AA:373:PRO:HA	2.51	0.46
1:T:436:PRO:HG3	1:IA:378:LEU:CD2	2.46	0.46
1:W:585:ARG:HG2	1:W:586:GLY:O	2.16	0.46
1:Z:585:ARG:HG2	1:Z:586:GLY:O	2.16	0.46
1:EA:378:LEU:CD2	1:EB:436:PRO:HG3	2.46	0.46
1:FA:585:ARG:HG2	1:FA:586:GLY:O	2.16	0.46
1:GA:669:PHE:CD1	1:EB:373:PRO:HA	2.50	0.46
1:HA:615:GLN:NE2	1:BB:633:ASP:N	2.63	0.46
1:LA:669:PHE:CD1	1:UA:373:PRO:HA	2.50	0.46
1:OA:373:PRO:HA	1:WA:669:PHE:CD1	2.50	0.46
1:WA:696:LYS:HD3	1:WA:696:LYS:HA	1.73	0.46
1:XA:696:LYS:HD3	1:XA:696:LYS:HA	1.73	0.46
1:AB:696:LYS:HA	1:AB:696:LYS:HD3	1.73	0.46
1:CB:585:ARG:HG2	1:CB:586:GLY:O	2.16	0.46
1:C:257:TYR:O	1:TA:726:GLY:HA3	2.16	0.46
1:D:398:PHE:CZ	1:DB:700:LYS:HG2	2.51	0.46
1:D:585:ARG:HG2	1:D:586:GLY:O	2.16	0.46
1:J:615:GLN:NE2	1:DA:633:ASP:N	2.62	0.46
1:K:585:ARG:HG2	1:K:586:GLY:O	2.16	0.46
1:L:615:GLN:NE2	1:FB:633:ASP:N	2.63	0.46
1:M:615:GLN:NE2	1:HA:633:ASP:N	2.63	0.46
1:O:436:PRO:HG3	1:Y:378:LEU:CD2	2.46	0.46
1:R:257:TYR:O	1:DB:726:GLY:HA3	2.16	0.46
1:T:615:GLN:NE2	1:IA:633:ASP:N	2.62	0.46
1:JA:230:CYS:HB3	1:GB:396:GLU:O	2.15	0.46
1:KA:585:ARG:HG2	1:KA:586:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OA:230:CYS:HB3	1:WA:396:GLU:O	2.16	0.46
1:SA:436:PRO:HG3	1:ZA:378:LEU:CD2	2.46	0.46
1:D:396:GLU:O	1:WA:230:CYS:HB3	2.15	0.45
1:E:230:CYS:HB3	1:X:396:GLU:O	2.16	0.45
1:E:373:PRO:HA	1:X:669:PHE:CD1	2.50	0.45
1:F:585:ARG:HG2	1:F:586:GLY:O	2.16	0.45
1:F:633:ASP:N	1:S:615:GLN:NE2	2.63	0.45
1:G:615:GLN:NE2	1:VA:633:ASP:N	2.63	0.45
1:M:436:PRO:HG3	1:HA:378:LEU:CD2	2.46	0.45
1:O:700:LYS:HG2	1:Y:398:PHE:CZ	2.51	0.45
1:S:396:GLU:O	1:GB:230:CYS:HB3	2.15	0.45
1:S:398:PHE:CZ	1:TA:700:LYS:HG2	2.52	0.45
1:T:230:CYS:HB3	1:CA:396:GLU:O	2.15	0.45
1:T:700:LYS:HG2	1:IA:398:PHE:CZ	2.51	0.45
1:X:436:PRO:HG3	1:WA:378:LEU:CD2	2.46	0.45
1:X:479:PRO:CG	1:WA:508:TYR:CD1	3.00	0.45
1:CA:436:PRO:HG3	1:GB:378:LEU:CD2	2.46	0.45
1:EA:436:PRO:HG3	1:XA:378:LEU:CD2	2.46	0.45
1:PA:378:LEU:CD2	1:CB:436:PRO:HG3	2.46	0.45
1:A:396:GLU:O	1:I:230:CYS:HB3	2.15	0.45
1:A:436:PRO:HG3	1:IB:378:LEU:CD2	2.46	0.45
1:B:585:ARG:HG2	1:B:586:GLY:O	2.16	0.45
1:B:696:LYS:HD3	1:B:696:LYS:HA	1.73	0.45
1:C:436:PRO:HG3	1:CA:378:LEU:CD2	2.46	0.45
1:E:700:LYS:HG2	1:NA:398:PHE:CZ	2.52	0.45
1:G:339:THR:HG22	1:G:404:ARG:HG3	1.99	0.45
1:G:403:LEU:HD11	1:G:409:PHE:HB2	1.99	0.45
1:H:436:PRO:HG3	1:MA:378:LEU:CD2	2.46	0.45
1:H:615:GLN:NE2	1:MA:633:ASP:N	2.63	0.45
1:J:403:LEU:HD11	1:J:409:PHE:HB2	1.99	0.45
1:L:403:LEU:HD11	1:L:409:PHE:HB2	1.99	0.45
1:O:615:GLN:NE2	1:Y:633:ASP:N	2.63	0.45
1:P:436:PRO:HG3	1:YA:378:LEU:CD2	2.46	0.45
1:T:373:PRO:HA	1:CA:669:PHE:CD1	2.50	0.45
1:T:460:LEU:HD11	1:IA:488:VAL:HG12	1.98	0.45
1:V:257:TYR:O	1:DA:726:GLY:HA3	2.16	0.45
1:Y:726:GLY:HA3	1:AA:257:TYR:O	2.16	0.45
1:BA:669:PHE:CD1	1:ZA:373:PRO:HA	2.50	0.45
1:GA:585:ARG:HG2	1:GA:586:GLY:O	2.16	0.45
1:JA:460:LEU:HD11	1:SA:488:VAL:HG12	1.99	0.45
1:LA:257:TYR:O	1:UA:726:GLY:HA3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:585:ARG:HG2	1:LA:586:GLY:O	2.16	0.45
1:SA:403:LEU:HD11	1:SA:409:PHE:HB2	1.99	0.45
1:WA:294:ARG:NE	1:DB:705:GLU:HG3	2.32	0.45
1:WA:339:THR:HG22	1:WA:404:ARG:HG3	1.99	0.45
1:CB:403:LEU:HD11	1:CB:409:PHE:HB2	1.99	0.45
1:EB:585:ARG:HG2	1:EB:586:GLY:O	2.16	0.45
1:B:378:LEU:CD2	1:LA:436:PRO:HG3	2.46	0.45
1:G:378:LEU:CD2	1:BA:436:PRO:HG3	2.46	0.45
1:J:479:PRO:CG	1:DA:508:TYR:CD1	3.00	0.45
1:J:700:LYS:HG2	1:DA:398:PHE:CZ	2.52	0.45
1:K:726:GLY:HA3	1:VA:257:TYR:O	2.16	0.45
1:L:339:THR:HG22	1:L:404:ARG:HG3	1.99	0.45
1:L:378:LEU:CD2	1:W:436:PRO:HG3	2.46	0.45
1:N:396:GLU:O	1:RA:230:CYS:HB3	2.15	0.45
1:O:403:LEU:HD11	1:O:409:PHE:HB2	1.99	0.45
1:O:479:PRO:CG	1:Y:508:TYR:CD1	3.00	0.45
1:Q:700:LYS:HG2	1:QA:398:PHE:CZ	2.52	0.45
1:R:436:PRO:HG3	1:X:378:LEU:CD2	2.46	0.45
1:R:508:TYR:CD1	1:WA:479:PRO:CG	3.00	0.45
1:S:378:LEU:CD2	1:TA:436:PRO:HG3	2.46	0.45
1:W:669:PHE:CD1	1:PA:373:PRO:HA	2.50	0.45
1:Y:436:PRO:HG3	1:FA:378:LEU:CD2	2.46	0.45
1:Z:436:PRO:HG3	1:HB:378:LEU:CD2	2.46	0.45
1:CA:479:PRO:CG	1:GB:508:TYR:CD1	3.00	0.45
1:CA:700:LYS:HG2	1:GB:398:PHE:CZ	2.52	0.45
1:EA:508:TYR:CD1	1:EB:479:PRO:CG	3.00	0.45
1:GA:257:TYR:O	1:EB:726:GLY:HA3	2.16	0.45
1:GA:508:TYR:CD1	1:QA:479:PRO:CG	3.00	0.45
1:JA:398:PHE:CZ	1:ZA:700:LYS:HG2	2.52	0.45
1:LA:508:TYR:CD1	1:AB:479:PRO:CG	3.00	0.45
1:OA:460:LEU:HD11	1:CB:488:VAL:HG12	1.99	0.45
1:PA:508:TYR:CD1	1:CB:479:PRO:CG	3.00	0.45
1:SA:230:CYS:HB3	1:UA:396:GLU:O	2.15	0.45
1:SA:479:PRO:CG	1:ZA:508:TYR:CD1	3.00	0.45
1:UA:398:PHE:CZ	1:HB:700:LYS:HG2	2.52	0.45
1:XA:700:LYS:HG2	1:EB:398:PHE:CZ	2.52	0.45
1:ZA:339:THR:HG22	1:ZA:404:ARG:HG3	1.99	0.45
1:B:700:LYS:HG2	1:AB:398:PHE:CZ	2.52	0.45
1:C:488:VAL:HG12	1:GB:460:LEU:HD11	1.99	0.45
1:D:615:GLN:NE2	1:K:633:ASP:N	2.63	0.45
1:E:460:LEU:HD11	1:NA:488:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:615:GLN:NE2	1:NA:633:ASP:N	2.63	0.45
1:G:700:LYS:HG2	1:VA:398:PHE:CZ	2.52	0.45
1:I:396:GLU:O	1:BB:230:CYS:HB3	2.15	0.45
1:N:230:CYS:HB3	1:P:396:GLU:O	2.15	0.45
1:Q:378:LEU:CD2	1:GA:436:PRO:HG3	2.46	0.45
1:Q:585:ARG:HG2	1:Q:586:GLY:O	2.16	0.45
1:R:488:VAL:HG12	1:WA:460:LEU:HD11	1.99	0.45
1:V:508:TYR:CD1	1:IA:479:PRO:CG	3.00	0.45
1:Z:508:TYR:CD1	1:UA:479:PRO:CG	3.00	0.45
1:AA:508:TYR:CD1	1:NA:479:PRO:CG	3.00	0.45
1:AA:705:GLU:HG3	1:GA:294:ARG:NE	2.32	0.45
1:DA:436:PRO:HG3	1:KA:378:LEU:CD2	2.46	0.45
1:JA:339:THR:HG22	1:JA:404:ARG:HG3	1.99	0.45
1:JA:633:ASP:N	1:ZA:615:GLN:NE2	2.62	0.45
1:MA:726:GLY:HA3	1:HB:257:TYR:O	2.16	0.45
1:OA:339:THR:HG22	1:OA:404:ARG:HG3	1.99	0.45
1:OA:398:PHE:CZ	1:PA:700:LYS:HG2	2.52	0.45
1:PA:339:THR:HG22	1:PA:404:ARG:HG3	1.99	0.45
1:TA:705:GLU:HG3	1:GB:294:ARG:NE	2.32	0.45
1:UA:378:LEU:HD21	1:HB:436:PRO:HG3	1.99	0.45
1:UA:585:ARG:HG2	1:UA:586:GLY:O	2.16	0.45
1:YA:403:LEU:HD11	1:YA:409:PHE:HB2	1.99	0.45
1:GB:339:THR:HG22	1:GB:404:ARG:HG3	1.99	0.45
1:A:398:PHE:CZ	1:N:700:LYS:HG2	2.52	0.45
1:C:508:TYR:CD1	1:GB:479:PRO:CG	3.00	0.45
1:D:378:LEU:CD2	1:DB:436:PRO:HG3	2.46	0.45
1:D:508:TYR:CD1	1:DB:479:PRO:CG	3.00	0.45
1:F:339:THR:HG22	1:F:404:ARG:HG3	1.99	0.45
1:F:403:LEU:HD11	1:F:409:PHE:HB2	1.99	0.45
1:F:460:LEU:HD11	1:TA:488:VAL:HG12	1.99	0.45
1:F:726:GLY:HA3	1:FB:257:TYR:O	2.16	0.45
1:G:436:PRO:HG3	1:VA:378:LEU:HD21	1.99	0.45
1:H:339:THR:HG22	1:H:404:ARG:HG3	1.99	0.45
1:I:700:LYS:HG2	1:P:398:PHE:CZ	2.52	0.45
1:J:257:TYR:O	1:W:726:GLY:HA3	2.16	0.45
1:J:378:LEU:CD2	1:KA:436:PRO:HG3	2.46	0.45
1:K:339:THR:HG22	1:K:404:ARG:HG3	1.99	0.45
1:K:615:GLN:NE2	1:DB:633:ASP:N	2.63	0.45
1:L:508:TYR:CD1	1:W:479:PRO:CG	3.00	0.45
1:M:339:THR:HG22	1:M:404:ARG:HG3	1.99	0.45
1:M:403:LEU:HD11	1:M:409:PHE:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:257:TYR:O	1:BA:726:GLY:HA3	2.16	0.45
1:O:378:LEU:CD2	1:FA:436:PRO:HG3	2.46	0.45
1:P:339:THR:HG22	1:P:404:ARG:HG3	1.99	0.45
1:Q:398:PHE:CZ	1:GA:700:LYS:HG2	2.52	0.45
1:S:508:TYR:CD1	1:TA:479:PRO:CG	3.00	0.45
1:T:339:THR:HG22	1:T:404:ARG:HG3	1.99	0.45
1:T:403:LEU:HD11	1:T:409:PHE:HB2	1.99	0.45
1:V:705:GLU:HG3	1:LA:294:ARG:NE	2.32	0.45
1:X:403:LEU:HD11	1:X:409:PHE:HB2	1.99	0.45
1:X:700:LYS:HG2	1:WA:398:PHE:CZ	2.52	0.45
1:Y:294:ARG:NE	1:NA:705:GLU:HG3	2.32	0.45
1:Y:700:LYS:HG2	1:FA:398:PHE:CZ	2.52	0.45
1:AA:398:PHE:CZ	1:NA:700:LYS:HG2	2.52	0.45
1:BA:398:PHE:CZ	1:VA:700:LYS:HG2	2.52	0.45
1:DA:700:LYS:HG2	1:KA:398:PHE:CZ	2.52	0.45
1:HA:726:GLY:HA3	1:XA:257:TYR:O	2.16	0.45
1:XA:436:PRO:HG3	1:EB:378:LEU:HD21	1.99	0.45
1:GB:696:LYS:HD3	1:GB:696:LYS:HA	1.73	0.45
1:IB:403:LEU:HD11	1:IB:409:PHE:HB2	1.99	0.45
1:A:339:THR:HG22	1:A:404:ARG:HG3	1.99	0.45
1:B:378:LEU:HD21	1:LA:436:PRO:HG3	1.99	0.45
1:B:398:PHE:CZ	1:LA:700:LYS:HG2	2.52	0.45
1:D:339:THR:HG22	1:D:404:ARG:HG3	1.99	0.45
1:H:396:GLU:O	1:IB:230:CYS:HB3	2.16	0.45
1:H:398:PHE:CZ	1:RA:700:LYS:HG2	2.52	0.45
1:H:403:LEU:HD11	1:H:409:PHE:HB2	1.99	0.45
1:I:403:LEU:HD11	1:I:409:PHE:HB2	1.99	0.45
1:K:403:LEU:HD11	1:K:409:PHE:HB2	1.99	0.45
1:L:700:LYS:HG2	1:FB:398:PHE:CZ	2.52	0.45
1:L:726:GLY:HA3	1:TA:257:TYR:O	2.16	0.45
1:M:398:PHE:CZ	1:BB:700:LYS:HG2	2.52	0.45
1:M:436:PRO:HG3	1:HA:378:LEU:HD21	1.99	0.45
1:M:508:TYR:CD1	1:BB:479:PRO:CG	3.00	0.45
1:M:585:ARG:HG2	1:M:586:GLY:O	2.16	0.45
1:N:403:LEU:HD11	1:N:409:PHE:HB2	1.99	0.45
1:N:508:TYR:CD1	1:IB:479:PRO:CG	3.00	0.45
1:P:700:LYS:HG2	1:YA:398:PHE:CZ	2.51	0.45
1:V:398:PHE:CZ	1:IA:700:LYS:HG2	2.52	0.45
1:Y:705:GLU:HG3	1:NA:294:ARG:NE	2.32	0.45
1:Z:339:THR:HG22	1:Z:404:ARG:HG3	1.99	0.45
1:CA:403:LEU:HD11	1:CA:409:PHE:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:294:ARG:NE	1:IA:705:GLU:HG3	2.32	0.45
1:DA:339:THR:HG22	1:DA:404:ARG:HG3	1.99	0.45
1:JA:700:LYS:HG2	1:SA:398:PHE:CZ	2.51	0.45
1:MA:700:LYS:HG2	1:RA:398:PHE:CZ	2.52	0.45
1:OA:508:TYR:CD1	1:PA:479:PRO:CG	3.00	0.45
1:CB:230:CYS:HB3	1:EB:396:GLU:O	2.15	0.45
1:A:700:LYS:HG2	1:IB:398:PHE:CZ	2.52	0.45
1:B:396:GLU:O	1:V:230:CYS:HB3	2.16	0.45
1:C:339:THR:HG22	1:C:404:ARG:HG3	1.99	0.45
1:C:378:LEU:HD21	1:GB:436:PRO:HG3	1.99	0.45
1:D:700:LYS:HG2	1:K:398:PHE:CZ	2.52	0.45
1:E:436:PRO:HG3	1:NA:378:LEU:HD21	1.99	0.45
1:E:488:VAL:HG12	1:AA:460:LEU:HD11	1.99	0.45
1:F:615:GLN:NE2	1:TA:633:ASP:N	2.63	0.45
1:G:294:ARG:NE	1:K:705:GLU:HG3	2.32	0.45
1:G:508:TYR:CD1	1:BA:479:PRO:CG	3.00	0.45
1:G:726:GLY:HA3	1:DB:257:TYR:O	2.16	0.45
1:H:294:ARG:NE	1:O:705:GLU:HG3	2.32	0.45
1:H:436:PRO:HG3	1:MA:378:LEU:HD21	1.99	0.45
1:I:508:TYR:CD1	1:YA:479:PRO:CG	3.00	0.45
1:I:615:GLN:NE2	1:P:633:ASP:N	2.63	0.45
1:J:705:GLU:HG3	1:M:294:ARG:NE	2.32	0.45
1:K:460:LEU:HD11	1:DB:488:VAL:HG12	1.99	0.45
1:L:398:PHE:CZ	1:W:700:LYS:HG2	2.52	0.45
1:L:436:PRO:HG3	1:FB:378:LEU:HD21	1.99	0.45
1:M:396:GLU:O	1:YA:230:CYS:HB3	2.16	0.45
1:Q:396:GLU:O	1:AA:230:CYS:HB3	2.16	0.45
1:S:339:THR:HG22	1:S:404:ARG:HG3	1.99	0.45
1:W:398:PHE:CZ	1:FB:700:LYS:HG2	2.52	0.45
1:X:294:ARG:NE	1:OA:705:GLU:HG3	2.32	0.45
1:Y:339:THR:HG22	1:Y:404:ARG:HG3	1.99	0.45
1:CA:705:GLU:HG3	1:JA:294:ARG:NE	2.32	0.45
1:DA:403:LEU:HD11	1:DA:409:PHE:HB2	1.98	0.45
1:DA:705:GLU:HG3	1:IA:294:ARG:NE	2.32	0.45
1:EA:339:THR:HG22	1:EA:404:ARG:HG3	1.99	0.45
1:GA:398:PHE:CZ	1:QA:700:LYS:HG2	2.52	0.45
1:IA:339:THR:HG22	1:IA:404:ARG:HG3	1.99	0.45
1:JA:508:TYR:CD1	1:ZA:479:PRO:CG	3.00	0.45
1:OA:633:ASP:N	1:PA:615:GLN:NE2	2.63	0.45
1:SA:700:LYS:HG2	1:ZA:398:PHE:CZ	2.52	0.45
1:XA:705:GLU:HG3	1:CB:294:ARG:NE	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:585:ARG:HG2	1:YA:586:GLY:O	2.16	0.45
1:CB:696:LYS:HD3	1:CB:696:LYS:HA	1.73	0.45
1:HB:696:LYS:HD3	1:HB:696:LYS:HA	1.73	0.45
1:A:508:TYR:CD1	1:N:479:PRO:CG	3.00	0.45
1:A:633:ASP:N	1:N:615:GLN:NE2	2.63	0.45
1:E:339:THR:HG22	1:E:404:ARG:HG3	1.99	0.45
1:E:403:LEU:HD11	1:E:409:PHE:HB2	1.99	0.45
1:F:398:PHE:CZ	1:S:700:LYS:HG2	2.52	0.45
1:F:705:GLU:HG3	1:L:294:ARG:NE	2.32	0.45
1:G:398:PHE:CZ	1:BA:700:LYS:HG2	2.52	0.45
1:H:508:TYR:CD1	1:RA:479:PRO:CG	3.00	0.45
1:H:585:ARG:HG2	1:H:586:GLY:O	2.16	0.45
1:H:700:LYS:HG2	1:MA:398:PHE:CZ	2.52	0.45
1:I:294:ARG:NE	1:N:705:GLU:HG3	2.32	0.45
1:I:479:PRO:CG	1:P:508:TYR:CD1	3.00	0.45
1:J:398:PHE:CZ	1:KA:700:LYS:HG2	2.51	0.45
1:J:436:PRO:HG3	1:DA:378:LEU:HD21	1.99	0.45
1:O:436:PRO:HG3	1:Y:378:LEU:HD21	1.99	0.45
1:P:726:GLY:HA3	1:AB:257:TYR:O	2.16	0.45
1:Q:378:LEU:HD21	1:GA:436:PRO:HG3	1.99	0.45
1:R:339:THR:HG22	1:R:404:ARG:HG3	1.99	0.45
1:R:378:LEU:HD21	1:WA:436:PRO:HG3	1.99	0.45
1:R:398:PHE:CZ	1:WA:700:LYS:HG2	2.52	0.45
1:T:436:PRO:HG3	1:IA:378:LEU:HD21	1.99	0.45
1:T:488:VAL:HG12	1:V:460:LEU:HD11	1.99	0.45
1:X:705:GLU:HG3	1:OA:294:ARG:NE	2.32	0.45
1:DA:436:PRO:HG3	1:KA:378:LEU:HD21	1.99	0.45
1:EA:398:PHE:CZ	1:EB:700:LYS:HG2	2.51	0.45
1:EA:700:LYS:HG2	1:XA:398:PHE:CZ	2.52	0.45
1:JA:257:TYR:O	1:VA:726:GLY:HA3	2.16	0.45
1:JA:436:PRO:HG3	1:SA:378:LEU:HD21	1.99	0.45
1:LA:398:PHE:CZ	1:AB:700:LYS:HG2	2.52	0.45
1:NA:339:THR:HG22	1:NA:404:ARG:HG3	1.99	0.45
1:PA:398:PHE:CZ	1:CB:700:LYS:HG2	2.52	0.45
1:QA:339:THR:HG22	1:QA:404:ARG:HG3	1.99	0.45
1:SA:294:ARG:NE	1:HB:705:GLU:HG3	2.32	0.45
1:AB:339:THR:HG22	1:AB:404:ARG:HG3	1.99	0.45
1:A:726:GLY:HA3	1:QA:257:TYR:O	2.16	0.45
1:B:403:LEU:HD11	1:B:409:PHE:HB2	1.99	0.45
1:C:479:PRO:CG	1:CA:508:TYR:CD1	3.00	0.45
1:C:633:ASP:N	1:GB:615:GLN:NE2	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:ARG:NE	1:S:705:GLU:HG3	2.32	0.45
1:I:705:GLU:HG3	1:N:294:ARG:NE	2.32	0.45
1:M:700:LYS:HG2	1:HA:398:PHE:CZ	2.52	0.45
1:N:398:PHE:CZ	1:IB:700:LYS:HG2	2.52	0.45
1:Q:403:LEU:HD11	1:Q:409:PHE:HB2	1.99	0.45
1:R:479:PRO:CG	1:X:508:TYR:CD1	3.00	0.45
1:W:378:LEU:CD2	1:FB:436:PRO:HG3	2.46	0.45
1:Y:403:LEU:HD11	1:Y:409:PHE:HB2	1.99	0.45
1:Y:436:PRO:HG3	1:FA:378:LEU:HD21	1.99	0.45
1:Z:398:PHE:CZ	1:UA:700:LYS:HG2	2.51	0.45
1:Z:700:LYS:HG2	1:HB:398:PHE:CZ	2.52	0.45
1:Z:705:GLU:HG3	1:MA:294:ARG:NE	2.32	0.45
1:BA:339:THR:HG22	1:BA:404:ARG:HG3	1.99	0.45
1:EA:633:ASP:N	1:EB:615:GLN:NE2	2.63	0.45
1:HA:700:LYS:HG2	1:BB:398:PHE:CZ	2.52	0.45
1:OA:257:TYR:O	1:FB:726:GLY:HA3	2.16	0.45
1:OA:378:LEU:CD2	1:PA:436:PRO:HG3	2.46	0.45
1:OA:700:LYS:HG2	1:CB:398:PHE:CZ	2.52	0.45
1:SA:339:THR:HG22	1:SA:404:ARG:HG3	1.99	0.45
1:TA:696:LYS:HD3	1:TA:696:LYS:HA	1.73	0.45
1:VA:339:THR:HG22	1:VA:404:ARG:HG3	1.99	0.45
1:XA:436:PRO:HG3	1:EB:378:LEU:CD2	2.46	0.45
1:CB:339:THR:HG22	1:CB:404:ARG:HG3	1.99	0.45
1:FB:339:THR:HG22	1:FB:404:ARG:HG3	1.99	0.45
1:FB:403:LEU:HD11	1:FB:409:PHE:HB2	1.99	0.45
1:IB:339:THR:HG22	1:IB:404:ARG:HG3	1.99	0.45
1:IB:585:ARG:HG2	1:IB:586:GLY:O	2.16	0.45
1:A:705:GLU:HG3	1:Q:294:ARG:NE	2.32	0.45
1:B:294:ARG:NE	1:P:705:GLU:HG3	2.32	0.45
1:C:378:LEU:CD2	1:GB:436:PRO:HG3	2.46	0.45
1:C:398:PHE:CZ	1:GB:700:LYS:HG2	2.52	0.45
1:E:294:ARG:NE	1:R:705:GLU:HG3	2.32	0.45
1:G:480:GLY:HA3	1:G:614:TRP:HB3	1.99	0.45
1:H:378:LEU:HD21	1:RA:436:PRO:HG3	1.99	0.45
1:I:398:PHE:CZ	1:YA:700:LYS:HG2	2.52	0.45
1:L:480:GLY:HA3	1:L:614:TRP:HB3	1.99	0.45
1:M:378:LEU:HD21	1:BB:436:PRO:HG3	1.99	0.45
1:N:726:GLY:HA3	1:P:257:TYR:O	2.16	0.45
1:O:398:PHE:CZ	1:FA:700:LYS:HG2	2.52	0.45
1:T:378:LEU:CD2	1:V:436:PRO:HG3	2.46	0.45
1:W:294:ARG:NE	1:KA:705:GLU:HG3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:460:LEU:HD11	1:FA:488:VAL:HG12	1.99	0.45
1:Z:633:ASP:N	1:UA:615:GLN:NE2	2.63	0.45
1:BA:378:LEU:CD2	1:VA:436:PRO:HG3	2.46	0.45
1:CA:294:ARG:NE	1:JA:705:GLU:HG3	2.32	0.45
1:DA:460:LEU:HD11	1:KA:488:VAL:HG12	1.99	0.45
1:DA:585:ARG:HG2	1:DA:586:GLY:O	2.16	0.45
1:EA:615:GLN:NE2	1:XA:633:ASP:N	2.62	0.45
1:EA:705:GLU:HG3	1:HA:294:ARG:NE	2.32	0.45
1:GA:339:THR:HG22	1:GA:404:ARG:HG3	1.99	0.45
1:GA:403:LEU:HD11	1:GA:409:PHE:HB2	1.98	0.45
1:HA:480:GLY:HA3	1:HA:614:TRP:HB3	1.99	0.45
1:JA:378:LEU:CD2	1:ZA:436:PRO:HG3	2.46	0.45
1:LA:339:THR:HG22	1:LA:404:ARG:HG3	1.99	0.45
1:MA:436:PRO:HG3	1:RA:378:LEU:CD2	2.46	0.45
1:OA:436:PRO:HG3	1:CB:378:LEU:HD21	1.99	0.45
1:PA:294:ARG:NE	1:FB:705:GLU:HG3	2.32	0.45
1:PA:705:GLU:HG3	1:FB:294:ARG:NE	2.32	0.45
1:RA:480:GLY:HA3	1:RA:614:TRP:HB3	1.99	0.45
1:UA:378:LEU:CD2	1:HB:436:PRO:HG3	2.46	0.45
1:VA:294:ARG:NE	1:ZA:705:GLU:HG3	2.32	0.45
1:VA:403:LEU:HD11	1:VA:409:PHE:HB2	1.99	0.45
1:VA:705:GLU:HG3	1:ZA:294:ARG:NE	2.32	0.45
1:WA:403:LEU:HD11	1:WA:409:PHE:HB2	1.98	0.45
1:XA:480:GLY:HA3	1:XA:614:TRP:HB3	1.99	0.45
1:YA:705:GLU:HG3	1:BB:294:ARG:NE	2.32	0.45
1:BB:480:GLY:HA3	1:BB:614:TRP:HB3	1.99	0.45
1:HB:480:GLY:HA3	1:HB:614:TRP:HB3	1.99	0.45
1:A:257:TYR:O	1:I:726:GLY:HA3	2.16	0.44
1:C:294:ARG:NE	1:T:705:GLU:HG3	2.32	0.44
1:C:700:LYS:HG2	1:CA:398:PHE:CZ	2.52	0.44
1:C:705:GLU:HG3	1:T:294:ARG:NE	2.32	0.44
1:E:378:LEU:CD2	1:AA:436:PRO:HG3	2.46	0.44
1:F:294:ARG:NE	1:L:705:GLU:HG3	2.32	0.44
1:F:480:GLY:HA3	1:F:614:TRP:HB3	1.99	0.44
1:G:378:LEU:HD21	1:BA:436:PRO:HG3	1.99	0.44
1:G:705:GLU:HG3	1:K:294:ARG:NE	2.32	0.44
1:L:378:LEU:HD21	1:W:436:PRO:HG3	1.99	0.44
1:N:378:LEU:HD21	1:IB:436:PRO:HG3	1.99	0.44
1:N:696:LYS:HA	1:N:696:LYS:HD3	1.73	0.44
1:O:508:TYR:CD1	1:FA:479:PRO:CG	3.00	0.44
1:Q:339:THR:HG22	1:Q:404:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:436:PRO:HG3	1:QA:378:LEU:HD21	1.99	0.44
1:R:378:LEU:CD2	1:WA:436:PRO:HG3	2.46	0.44
1:R:633:ASP:N	1:WA:615:GLN:NE2	2.63	0.44
1:T:508:TYR:CD1	1:V:479:PRO:CG	3.00	0.44
1:W:339:THR:HG22	1:W:404:ARG:HG3	1.99	0.44
1:W:402:MET:HE3	1:PA:228:TRP:HE3	1.83	0.44
1:Z:402:MET:HE3	1:AB:228:TRP:HE3	1.82	0.44
1:Z:480:GLY:HA3	1:Z:614:TRP:HB3	1.99	0.44
1:AA:403:LEU:HD11	1:AA:409:PHE:HB2	1.99	0.44
1:BA:402:MET:HE3	1:ZA:228:TRP:HE3	1.82	0.44
1:CA:228:TRP:HE3	1:SA:402:MET:HE3	1.82	0.44
1:EA:402:MET:HE3	1:QA:228:TRP:HE3	1.82	0.44
1:EA:480:GLY:HA3	1:EA:614:TRP:HB3	1.99	0.44
1:GA:378:LEU:HD21	1:QA:436:PRO:HG3	1.99	0.44
1:HA:436:PRO:HG3	1:BB:378:LEU:CD2	2.46	0.44
1:HA:436:PRO:HG3	1:BB:378:LEU:HD21	1.99	0.44
1:KA:403:LEU:HD11	1:KA:409:PHE:HB2	1.99	0.44
1:LA:378:LEU:CD2	1:AB:436:PRO:HG3	2.46	0.44
1:LA:378:LEU:HD21	1:AB:436:PRO:HG3	1.99	0.44
1:LA:403:LEU:HD11	1:LA:409:PHE:HB2	1.99	0.44
1:MA:436:PRO:HG3	1:RA:378:LEU:HD21	1.99	0.44
1:PA:378:LEU:HD21	1:CB:436:PRO:HG3	1.99	0.44
1:QA:705:GLU:HG3	1:EB:294:ARG:NE	2.32	0.44
1:SA:436:PRO:HG3	1:ZA:378:LEU:HD21	1.99	0.44
1:UA:403:LEU:HD11	1:UA:409:PHE:HB2	1.99	0.44
1:XA:615:GLN:NE2	1:EB:633:ASP:N	2.63	0.44
1:YA:480:GLY:HA3	1:YA:614:TRP:HB3	1.99	0.44
1:DB:480:GLY:HA3	1:DB:614:TRP:HB3	1.99	0.44
1:EB:403:LEU:HD11	1:EB:409:PHE:HB2	1.99	0.44
1:HB:339:THR:HG22	1:HB:404:ARG:HG3	1.99	0.44
1:IB:480:GLY:HA3	1:IB:614:TRP:HB3	1.99	0.44
1:B:339:THR:HG22	1:B:404:ARG:HG3	1.99	0.44
1:B:436:PRO:HG3	1:AB:378:LEU:HD21	1.99	0.44
1:D:403:LEU:HD11	1:D:409:PHE:HB2	1.99	0.44
1:D:705:GLU:HG3	1:S:294:ARG:NE	2.32	0.44
1:E:508:TYR:CD1	1:AA:479:PRO:CG	3.00	0.44
1:E:705:GLU:HG3	1:R:294:ARG:NE	2.32	0.44
1:I:378:LEU:HD21	1:YA:436:PRO:HG3	1.99	0.44
1:J:339:THR:HG22	1:J:404:ARG:HG3	1.99	0.44
1:K:480:GLY:HA3	1:K:614:TRP:HB3	1.99	0.44
1:K:700:LYS:HG2	1:DB:398:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:228:TRP:HE3	1:TA:402:MET:HE3	1.82	0.44
1:R:700:LYS:HG2	1:X:398:PHE:CZ	2.52	0.44
1:T:398:PHE:CZ	1:V:700:LYS:HG2	2.51	0.44
1:V:403:LEU:HD11	1:V:409:PHE:HB2	1.99	0.44
1:W:378:LEU:HD21	1:FB:436:PRO:HG3	1.99	0.44
1:X:480:GLY:HA3	1:X:614:TRP:HB3	1.99	0.44
1:Y:585:ARG:HG2	1:Y:586:GLY:O	2.16	0.44
1:Z:615:GLN:NE2	1:HB:633:ASP:N	2.62	0.44
1:BA:294:ARG:NE	1:FA:705:GLU:HG3	2.32	0.44
1:FA:403:LEU:HD11	1:FA:409:PHE:HB2	1.99	0.44
1:IA:480:GLY:HA3	1:IA:614:TRP:HB3	1.99	0.44
1:JA:402:MET:HE3	1:VA:228:TRP:HE3	1.82	0.44
1:JA:479:PRO:CG	1:SA:508:TYR:CD1	3.00	0.44
1:MA:228:TRP:HE3	1:HB:402:MET:HE3	1.83	0.44
1:MA:339:THR:HG22	1:MA:404:ARG:HG3	1.99	0.44
1:MA:479:PRO:CG	1:RA:508:TYR:CD1	3.00	0.44
1:MA:480:GLY:HA3	1:MA:614:TRP:HB3	1.99	0.44
1:NA:480:GLY:HA3	1:NA:614:TRP:HB3	1.99	0.44
1:OA:402:MET:HE3	1:FB:228:TRP:HE3	1.82	0.44
1:OA:696:LYS:HD3	1:OA:696:LYS:HA	1.73	0.44
1:PA:696:LYS:HD3	1:PA:696:LYS:HA	1.73	0.44
1:RA:294:ARG:NE	1:IB:705:GLU:HG3	2.32	0.44
1:SA:705:GLU:HG3	1:HB:294:ARG:NE	2.32	0.44
1:TA:339:THR:HG22	1:TA:404:ARG:HG3	1.99	0.44
1:TA:480:GLY:HA3	1:TA:614:TRP:HB3	1.99	0.44
1:UA:294:ARG:NE	1:AB:705:GLU:HG3	2.32	0.44
1:UA:508:TYR:CD1	1:HB:479:PRO:CG	3.00	0.44
1:UA:633:ASP:N	1:HB:615:GLN:NE2	2.63	0.44
1:YA:339:THR:HG22	1:YA:404:ARG:HG3	1.99	0.44
1:YA:701:ARG:HH21	1:YA:703:ASN:ND2	2.16	0.44
1:BB:339:THR:HG22	1:BB:404:ARG:HG3	1.99	0.44
1:DB:465:ALA:HB1	1:DB:473:GLN:HG2	2.00	0.44
1:GB:403:LEU:HD11	1:GB:409:PHE:HB2	1.99	0.44
1:A:402:MET:HE3	1:I:228:TRP:HE3	1.82	0.44
1:A:480:GLY:HA3	1:A:614:TRP:HB3	1.99	0.44
1:F:465:ALA:HB1	1:F:473:GLN:HG2	2.00	0.44
1:F:700:LYS:HG2	1:TA:398:PHE:CZ	2.51	0.44
1:G:257:TYR:O	1:FA:726:GLY:HA3	2.16	0.44
1:G:402:MET:HE3	1:FA:228:TRP:HE3	1.83	0.44
1:G:488:VAL:HG12	1:BA:460:LEU:HD11	1.99	0.44
1:I:488:VAL:HG12	1:YA:460:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:460:LEU:HD11	1:DA:488:VAL:HG12	1.98	0.44
1:J:508:TYR:CD1	1:KA:479:PRO:CG	3.00	0.44
1:K:402:MET:HE3	1:S:228:TRP:HE3	1.82	0.44
1:K:436:PRO:HG3	1:DB:378:LEU:HD21	1.99	0.44
1:L:488:VAL:HG12	1:W:460:LEU:HD11	1.99	0.44
1:N:228:TRP:HE3	1:P:402:MET:HE3	1.82	0.44
1:N:339:THR:HG22	1:N:404:ARG:HG3	1.99	0.44
1:O:480:GLY:HA3	1:O:614:TRP:HB3	1.99	0.44
1:T:257:TYR:O	1:LA:726:GLY:HA3	2.16	0.44
1:T:479:PRO:CG	1:IA:508:TYR:CD1	3.00	0.44
1:X:228:TRP:HE3	1:CB:402:MET:HE3	1.83	0.44
1:BA:378:LEU:HD21	1:VA:436:PRO:HG3	1.99	0.44
1:BA:705:GLU:HG3	1:FA:294:ARG:NE	2.32	0.44
1:CA:480:GLY:HA3	1:CA:614:TRP:HB3	1.99	0.44
1:EA:436:PRO:HG3	1:XA:378:LEU:HD21	1.99	0.44
1:GA:378:LEU:CD2	1:QA:436:PRO:HG3	2.46	0.44
1:HA:228:TRP:HE3	1:XA:402:MET:HE3	1.83	0.44
1:HA:465:ALA:HB1	1:HA:473:GLN:HG2	2.00	0.44
1:OA:403:LEU:HD11	1:OA:409:PHE:HB2	1.99	0.44
1:OA:479:PRO:CG	1:CB:508:TYR:CD1	3.00	0.44
1:SA:480:GLY:HA3	1:SA:614:TRP:HB3	2.00	0.44
1:SA:696:LYS:HD3	1:SA:696:LYS:HA	1.73	0.44
1:TA:465:ALA:HB1	1:TA:473:GLN:HG2	2.00	0.44
1:UA:339:THR:HG22	1:UA:404:ARG:HG3	1.99	0.44
1:XA:479:PRO:CG	1:EB:508:TYR:CD1	3.00	0.44
1:CB:465:ALA:HB1	1:CB:473:GLN:HG2	2.00	0.44
1:CB:480:GLY:HA3	1:CB:614:TRP:HB3	1.99	0.44
1:DB:339:THR:HG22	1:DB:404:ARG:HG3	1.99	0.44
1:EB:339:THR:HG22	1:EB:404:ARG:HG3	1.99	0.44
1:IB:701:ARG:HH21	1:IB:703:ASN:ND2	2.16	0.44
1:A:403:LEU:HD11	1:A:409:PHE:HB2	1.99	0.44
1:B:465:ALA:HB1	1:B:473:GLN:HG2	2.00	0.44
1:C:436:PRO:HG3	1:CA:378:LEU:HD21	1.99	0.44
1:C:696:LYS:HD3	1:C:696:LYS:HA	1.73	0.44
1:D:228:TRP:HE3	1:F:402:MET:HE3	1.83	0.44
1:E:257:TYR:O	1:GA:726:GLY:HA3	2.16	0.44
1:E:398:PHE:CZ	1:AA:700:LYS:HG2	2.51	0.44
1:E:479:PRO:CG	1:NA:508:TYR:CD1	3.00	0.44
1:F:378:LEU:HD21	1:S:436:PRO:HG3	1.99	0.44
1:F:436:PRO:HG3	1:TA:378:LEU:HD21	1.99	0.44
1:F:701:ARG:HH21	1:F:703:ASN:ND2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:TRP:HE3	1:DB:402:MET:HE3	1.83	0.44
1:H:402:MET:HE3	1:IB:228:TRP:HE3	1.82	0.44
1:I:460:LEU:HD11	1:P:488:VAL:HG12	1.99	0.44
1:I:480:GLY:HA3	1:I:614:TRP:HB3	1.99	0.44
1:J:488:VAL:HG12	1:KA:460:LEU:HD11	1.99	0.44
1:K:465:ALA:HB1	1:K:473:GLN:HG2	2.00	0.44
1:K:701:ARG:HH21	1:K:703:ASN:ND2	2.16	0.44
1:L:257:TYR:O	1:KA:726:GLY:HA3	2.16	0.44
1:L:402:MET:HE3	1:KA:228:TRP:HE3	1.82	0.44
1:M:402:MET:HE3	1:YA:228:TRP:HE3	1.82	0.44
1:N:480:GLY:HA3	1:N:614:TRP:HB3	1.99	0.44
1:O:339:THR:HG22	1:O:404:ARG:HG3	1.99	0.44
1:O:488:VAL:HG12	1:FA:460:LEU:HD11	1.99	0.44
1:P:403:LEU:HD11	1:P:409:PHE:HB2	1.99	0.44
1:P:480:GLY:HA3	1:P:614:TRP:HB3	1.99	0.44
1:R:696:LYS:HD3	1:R:696:LYS:HA	1.73	0.44
1:R:701:ARG:HH21	1:R:703:ASN:ND2	2.16	0.44
1:S:403:LEU:HD11	1:S:409:PHE:HB2	1.99	0.44
1:V:339:THR:HG22	1:V:404:ARG:HG3	1.99	0.44
1:X:436:PRO:HG3	1:WA:378:LEU:HD21	1.99	0.44
1:Y:228:TRP:HE3	1:AA:402:MET:HE3	1.82	0.44
1:Y:701:ARG:HH21	1:Y:703:ASN:ND2	2.16	0.44
1:Z:294:ARG:NE	1:MA:705:GLU:HG3	2.32	0.44
1:Z:436:PRO:HG3	1:HB:378:LEU:HD21	1.99	0.44
1:AA:389:ARG:HD3	1:NA:425:ALA:HB3	2.00	0.44
1:BA:389:ARG:HD3	1:VA:425:ALA:HB3	2.00	0.44
1:CA:436:PRO:HG3	1:GB:378:LEU:HD21	1.99	0.44
1:DA:479:PRO:CG	1:KA:508:TYR:CD1	3.00	0.44
1:DA:701:ARG:HH21	1:DA:703:ASN:ND2	2.16	0.44
1:EA:294:ARG:NE	1:HA:705:GLU:HG3	2.32	0.44
1:FA:402:MET:HE3	1:NA:228:TRP:HE3	1.83	0.44
1:FA:465:ALA:HB1	1:FA:473:GLN:HG2	2.00	0.44
1:GA:701:ARG:HH21	1:GA:703:ASN:ND2	2.16	0.44
1:HA:339:THR:HG22	1:HA:404:ARG:HG3	1.99	0.44
1:HA:460:LEU:HD11	1:BB:488:VAL:HG12	1.99	0.44
1:HA:479:PRO:CG	1:BB:508:TYR:CD1	3.00	0.44
1:IA:228:TRP:HE3	1:KA:402:MET:HE3	1.82	0.44
1:JA:403:LEU:HD11	1:JA:409:PHE:HB2	1.99	0.44
1:JA:701:ARG:HH21	1:JA:703:ASN:ND2	2.16	0.44
1:LA:701:ARG:HH21	1:LA:703:ASN:ND2	2.16	0.44
1:MA:460:LEU:HD11	1:RA:488:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:294:ARG:NE	1:EB:705:GLU:HG3	2.32	0.44
1:RA:339:THR:HG22	1:RA:404:ARG:HG3	1.99	0.44
1:SA:465:ALA:HB1	1:SA:473:GLN:HG2	2.00	0.44
1:UA:488:VAL:HG12	1:HB:460:LEU:HD11	1.99	0.44
1:XA:339:THR:HG22	1:XA:404:ARG:HG3	1.99	0.44
1:XA:460:LEU:HD11	1:EB:488:VAL:HG12	1.99	0.44
1:XA:701:ARG:HH21	1:XA:703:ASN:ND2	2.16	0.44
1:DB:403:LEU:HD11	1:DB:409:PHE:HB2	1.99	0.44
1:HB:403:LEU:HD11	1:HB:409:PHE:HB2	1.99	0.44
1:HB:701:ARG:HH21	1:HB:703:ASN:ND2	2.16	0.44
1:B:228:TRP:HE3	1:YA:402:MET:HE3	1.82	0.44
1:C:425:ALA:HB3	1:CA:389:ARG:HD3	2.00	0.44
1:C:701:ARG:HH21	1:C:703:ASN:ND2	2.16	0.44
1:D:436:PRO:HG3	1:K:378:LEU:HD21	1.99	0.44
1:F:228:TRP:HE3	1:FB:402:MET:HE3	1.82	0.44
1:I:339:THR:HG22	1:I:404:ARG:HG3	1.99	0.44
1:I:436:PRO:HG3	1:P:378:LEU:HD21	1.99	0.44
1:I:696:LYS:HA	1:I:696:LYS:HD3	1.73	0.44
1:J:402:MET:HE3	1:W:228:TRP:HE3	1.82	0.44
1:J:480:GLY:HA3	1:J:614:TRP:HB3	2.00	0.44
1:L:425:ALA:HB3	1:FB:389:ARG:HD3	2.00	0.44
1:O:460:LEU:HD11	1:Y:488:VAL:HG12	1.99	0.44
1:Q:465:ALA:HB1	1:Q:473:GLN:HG2	2.00	0.44
1:V:402:MET:HE3	1:DA:228:TRP:HE3	1.82	0.44
1:W:705:GLU:HG3	1:KA:294:ARG:NE	2.32	0.44
1:AA:339:THR:HG22	1:AA:404:ARG:HG3	1.99	0.44
1:BA:403:LEU:HD11	1:BA:409:PHE:HB2	1.99	0.44
1:DA:615:GLN:NE2	1:KA:633:ASP:N	2.63	0.44
1:IA:701:ARG:HH21	1:IA:703:ASN:ND2	2.16	0.44
1:KA:465:ALA:HB1	1:KA:473:GLN:HG2	2.00	0.44
1:MA:465:ALA:HB1	1:MA:473:GLN:HG2	2.00	0.44
1:NA:403:LEU:HD11	1:NA:409:PHE:HB2	1.99	0.44
1:NA:701:ARG:HH21	1:NA:703:ASN:ND2	2.16	0.44
1:OA:378:LEU:HD21	1:PA:436:PRO:HG3	1.99	0.44
1:PA:488:VAL:HG12	1:CB:460:LEU:HD11	1.99	0.44
1:SA:460:LEU:HD11	1:ZA:488:VAL:HG12	1.99	0.44
1:UA:705:GLU:HG3	1:AB:294:ARG:NE	2.32	0.44
1:XA:294:ARG:NE	1:CB:705:GLU:HG3	2.32	0.44
1:YA:465:ALA:HB1	1:YA:473:GLN:HG2	2.00	0.44
1:EB:480:GLY:HA3	1:EB:614:TRP:HB3	1.99	0.44
1:FB:465:ALA:HB1	1:FB:473:GLN:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IB:465:ALA:HB1	1:IB:473:GLN:HG2	2.00	0.44
1:A:378:LEU:HD21	1:N:436:PRO:HG3	1.99	0.44
1:B:402:MET:HE3	1:V:228:TRP:HE3	1.83	0.44
1:B:705:GLU:HG3	1:P:294:ARG:NE	2.32	0.44
1:D:460:LEU:HD11	1:K:488:VAL:HG12	1.99	0.44
1:D:633:ASP:N	1:DB:615:GLN:NE2	2.63	0.44
1:F:488:VAL:HG12	1:S:460:LEU:HD11	1.99	0.44
1:J:294:ARG:NE	1:M:705:GLU:HG3	2.32	0.44
1:K:228:TRP:HE3	1:VA:402:MET:HE3	1.83	0.44
1:L:701:ARG:HH21	1:L:703:ASN:ND2	2.16	0.44
1:O:402:MET:HE3	1:BA:228:TRP:HE3	1.82	0.44
1:P:479:PRO:CG	1:YA:508:TYR:CD1	3.00	0.44
1:Q:228:TRP:HE3	1:IB:402:MET:HE3	1.82	0.44
1:Q:402:MET:HE3	1:AA:228:TRP:HE3	1.83	0.44
1:R:436:PRO:HG3	1:X:378:LEU:HD21	1.99	0.44
1:T:701:ARG:HH21	1:T:703:ASN:ND2	2.16	0.44
1:V:389:ARG:HD3	1:IA:425:ALA:HB3	2.00	0.44
1:W:389:ARG:HD3	1:FB:425:ALA:HB3	2.00	0.44
1:Y:465:ALA:HB1	1:Y:473:GLN:HG2	2.00	0.44
1:Y:479:PRO:CG	1:FA:508:TYR:CD1	3.00	0.44
1:AA:378:LEU:HD21	1:NA:436:PRO:HG3	1.99	0.44
1:CA:339:THR:HG22	1:CA:404:ARG:HG3	1.99	0.44
1:DA:465:ALA:HB1	1:DA:473:GLN:HG2	2.00	0.44
1:EA:228:TRP:HE3	1:BB:402:MET:HE3	1.82	0.44
1:FA:339:THR:HG22	1:FA:404:ARG:HG3	1.99	0.44
1:HA:425:ALA:HB3	1:BB:389:ARG:HD3	2.00	0.44
1:IA:403:LEU:HD11	1:IA:409:PHE:HB2	1.99	0.44
1:JA:378:LEU:HD21	1:ZA:436:PRO:HG3	1.99	0.44
1:JA:488:VAL:HG12	1:ZA:460:LEU:HD11	1.99	0.44
1:JA:696:LYS:HA	1:JA:696:LYS:HD3	1.73	0.44
1:JA:726:GLY:HA3	1:GB:257:TYR:O	2.16	0.44
1:LA:488:VAL:HG12	1:AB:460:LEU:HD11	1.99	0.44
1:MA:425:ALA:HB3	1:RA:389:ARG:HD3	2.00	0.44
1:MA:701:ARG:HH21	1:MA:703:ASN:ND2	2.16	0.44
1:OA:488:VAL:HG12	1:PA:460:LEU:HD11	1.99	0.44
1:OA:701:ARG:HH21	1:OA:703:ASN:ND2	2.16	0.44
1:OA:726:GLY:HA3	1:WA:257:TYR:O	2.16	0.44
1:PA:701:ARG:HH21	1:PA:703:ASN:ND2	2.16	0.44
1:TA:403:LEU:HD11	1:TA:409:PHE:HB2	1.99	0.44
1:UA:480:GLY:HA3	1:UA:614:TRP:HB3	1.99	0.44
1:VA:465:ALA:HB1	1:VA:473:GLN:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:403:LEU:HD11	1:XA:409:PHE:HB2	1.99	0.44
1:ZA:696:LYS:HD3	1:ZA:696:LYS:HA	1.73	0.44
1:ZA:701:ARG:HH21	1:ZA:703:ASN:ND2	2.16	0.44
1:CB:701:ARG:HH21	1:CB:703:ASN:ND2	2.16	0.44
1:DB:696:LYS:HD3	1:DB:696:LYS:HA	1.73	0.44
1:A:488:VAL:HG12	1:N:460:LEU:HD11	1.99	0.44
1:C:480:GLY:HA3	1:C:614:TRP:HB3	1.99	0.44
1:D:257:TYR:O	1:WA:726:GLY:HA3	2.16	0.44
1:D:479:PRO:CG	1:K:508:TYR:CD1	3.00	0.44
1:E:701:ARG:HH21	1:E:703:ASN:ND2	2.16	0.44
1:G:425:ALA:HB3	1:VA:389:ARG:HD3	2.00	0.44
1:G:701:ARG:HH21	1:G:703:ASN:ND2	2.16	0.44
1:H:425:ALA:HB3	1:MA:389:ARG:HD3	2.00	0.44
1:L:460:LEU:HD11	1:FB:488:VAL:HG12	1.99	0.44
1:L:465:ALA:HB1	1:L:473:GLN:HG2	2.00	0.44
1:L:701:ARG:HH21	1:L:703:ASN:HD21	1.66	0.44
1:M:389:ARG:HD3	1:BB:425:ALA:HB3	2.00	0.44
1:M:425:ALA:HB3	1:HA:389:ARG:HD3	2.00	0.44
1:M:701:ARG:HH21	1:M:703:ASN:ND2	2.16	0.44
1:N:488:VAL:HG12	1:IB:460:LEU:HD11	1.99	0.44
1:R:402:MET:HE3	1:DB:228:TRP:HE3	1.82	0.44
1:R:425:ALA:HB3	1:X:389:ARG:HD3	2.00	0.44
1:R:480:GLY:HA3	1:R:614:TRP:HB3	1.99	0.44
1:S:402:MET:HE3	1:GB:228:TRP:HE3	1.83	0.44
1:W:403:LEU:HD11	1:W:409:PHE:HB2	1.99	0.44
1:W:480:GLY:HA3	1:W:614:TRP:HB3	1.99	0.44
1:W:488:VAL:HG12	1:FB:460:LEU:HD11	1.99	0.44
1:W:701:ARG:HH21	1:W:703:ASN:ND2	2.16	0.44
1:X:339:THR:HG22	1:X:404:ARG:HG3	1.99	0.44
1:X:465:ALA:HB1	1:X:473:GLN:HG2	2.00	0.44
1:X:696:LYS:HD3	1:X:696:LYS:HA	1.73	0.44
1:Y:615:GLN:NE2	1:FA:633:ASP:N	2.63	0.44
1:Z:228:TRP:HE3	1:RA:402:MET:HE3	1.82	0.44
1:BA:480:GLY:HA3	1:BA:614:TRP:HB3	1.99	0.44
1:BA:701:ARG:HH21	1:BA:703:ASN:ND2	2.16	0.44
1:CA:465:ALA:HB1	1:CA:473:GLN:HG2	2.00	0.44
1:GA:488:VAL:HG12	1:QA:460:LEU:HD11	1.99	0.44
1:HA:701:ARG:HH21	1:HA:703:ASN:ND2	2.16	0.44
1:JA:228:TRP:HE3	1:GB:402:MET:HE3	1.82	0.44
1:NA:465:ALA:HB1	1:NA:473:GLN:HG2	2.00	0.44
1:OA:228:TRP:HE3	1:WA:402:MET:HE3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:403:LEU:HD11	1:QA:409:PHE:HB2	1.99	0.44
1:RA:403:LEU:HD11	1:RA:409:PHE:HB2	1.99	0.44
1:SA:701:ARG:HH21	1:SA:703:ASN:ND2	2.16	0.44
1:TA:294:ARG:NE	1:GB:705:GLU:HG3	2.32	0.44
1:UA:701:ARG:HH21	1:UA:703:ASN:HD21	1.66	0.44
1:VA:480:GLY:HA3	1:VA:614:TRP:HB3	1.99	0.44
1:WA:705:GLU:HG3	1:DB:294:ARG:NE	2.32	0.44
1:AB:403:LEU:HD11	1:AB:409:PHE:HB2	1.99	0.44
1:BB:403:LEU:HD11	1:BB:409:PHE:HB2	1.98	0.44
1:EB:701:ARG:HH21	1:EB:703:ASN:HD21	1.66	0.44
1:FB:480:GLY:HA3	1:FB:614:TRP:HB3	1.99	0.44
1:A:294:ARG:NE	1:Q:705:GLU:HG3	2.32	0.44
1:A:479:PRO:CG	1:IB:508:TYR:CD1	3.00	0.44
1:B:480:GLY:HA3	1:B:614:TRP:HB3	1.99	0.44
1:B:701:ARG:HH21	1:B:703:ASN:HD21	1.66	0.44
1:D:701:ARG:HH21	1:D:703:ASN:ND2	2.16	0.44
1:F:425:ALA:HB3	1:TA:389:ARG:HD3	2.00	0.44
1:G:460:LEU:HD11	1:VA:488:VAL:HG12	1.99	0.44
1:G:465:ALA:HB1	1:G:473:GLN:HG2	2.00	0.44
1:G:633:ASP:N	1:BA:615:GLN:NE2	2.63	0.44
1:G:701:ARG:HH21	1:G:703:ASN:HD21	1.66	0.44
1:H:705:GLU:HG3	1:O:294:ARG:NE	2.32	0.44
1:L:479:PRO:CG	1:FB:508:TYR:CD1	3.00	0.44
1:Q:480:GLY:HA3	1:Q:614:TRP:HB3	1.99	0.44
1:Q:615:GLN:NE2	1:QA:633:ASP:N	2.63	0.44
1:Q:701:ARG:HH21	1:Q:703:ASN:HD21	1.66	0.44
1:S:701:ARG:HH21	1:S:703:ASN:ND2	2.16	0.44
1:T:480:GLY:HA3	1:T:614:TRP:HB3	1.99	0.44
1:V:378:LEU:HD21	1:IA:436:PRO:HG3	1.99	0.44
1:V:633:ASP:N	1:IA:615:GLN:NE2	2.63	0.44
1:X:425:ALA:HB3	1:WA:389:ARG:HD3	2.00	0.44
1:Z:701:ARG:HH21	1:Z:703:ASN:ND2	2.16	0.44
1:AA:633:ASP:N	1:NA:615:GLN:NE2	2.63	0.44
1:BA:257:TYR:O	1:ZA:726:GLY:HA3	2.16	0.44
1:BA:488:VAL:HG12	1:VA:460:LEU:HD11	1.99	0.44
1:CA:460:LEU:HD11	1:GB:488:VAL:HG12	1.99	0.44
1:EA:701:ARG:HH21	1:EA:703:ASN:ND2	2.16	0.44
1:IA:465:ALA:HB1	1:IA:473:GLN:HG2	2.00	0.44
1:IA:696:LYS:HA	1:IA:696:LYS:HD3	1.73	0.44
1:KA:339:THR:HG22	1:KA:404:ARG:HG3	1.99	0.44
1:LA:402:MET:HE3	1:UA:228:TRP:HE3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MA:403:LEU:HD11	1:MA:409:PHE:HB2	1.99	0.44
1:PA:633:ASP:N	1:CB:615:GLN:NE2	2.63	0.44
1:BB:701:ARG:HH21	1:BB:703:ASN:ND2	2.16	0.44
1:GB:701:ARG:HH21	1:GB:703:ASN:ND2	2.16	0.44
1:B:615:GLN:NE2	1:AB:633:ASP:N	2.63	0.44
1:C:402:MET:HE3	1:TA:228:TRP:HE3	1.82	0.44
1:D:402:MET:HE3	1:WA:228:TRP:HE3	1.83	0.44
1:E:480:GLY:HA3	1:E:614:TRP:HB3	1.99	0.44
1:F:479:PRO:CG	1:TA:508:TYR:CD1	3.00	0.44
1:H:389:ARG:HD3	1:RA:425:ALA:HB3	2.00	0.44
1:H:696:LYS:HD3	1:H:696:LYS:HA	1.73	0.44
1:H:701:ARG:HH21	1:H:703:ASN:ND2	2.16	0.44
1:K:425:ALA:HB3	1:DB:389:ARG:HD3	2.00	0.44
1:K:479:PRO:CG	1:DB:508:TYR:CD1	3.00	0.44
1:M:228:TRP:HE3	1:DA:402:MET:HE3	1.83	0.44
1:O:465:ALA:HB1	1:O:473:GLN:HG2	2.00	0.44
1:O:726:GLY:HA3	1:MA:257:TYR:O	2.16	0.44
1:Q:508:TYR:CD1	1:GA:479:PRO:CG	3.00	0.44
1:S:257:TYR:O	1:GB:726:GLY:HA3	2.16	0.44
1:S:633:ASP:N	1:TA:615:GLN:NE2	2.63	0.44
1:V:488:VAL:HG12	1:IA:460:LEU:HD11	1.99	0.44
1:X:460:LEU:HD11	1:WA:488:VAL:HG12	1.99	0.44
1:Z:257:TYR:O	1:AB:726:GLY:HA3	2.16	0.44
1:Z:488:VAL:HG12	1:UA:460:LEU:HD11	1.99	0.44
1:CA:696:LYS:HD3	1:CA:696:LYS:HA	1.73	0.44
1:EA:257:TYR:O	1:QA:726:GLY:HA3	2.16	0.44
1:HA:403:LEU:HD11	1:HA:409:PHE:HB2	1.99	0.44
1:JA:701:ARG:HH21	1:JA:703:ASN:HD21	1.66	0.44
1:LA:389:ARG:HD3	1:AB:425:ALA:HB3	2.00	0.44
1:NA:696:LYS:HA	1:NA:696:LYS:HD3	1.73	0.44
1:OA:701:ARG:HH21	1:OA:703:ASN:HD21	1.66	0.44
1:PA:390:SER:O	1:CB:701:ARG:NH2	2.51	0.44
1:RA:465:ALA:HB1	1:RA:473:GLN:HG2	2.00	0.44
1:SA:701:ARG:NH2	1:ZA:390:SER:O	2.51	0.44
1:TA:701:ARG:HH21	1:TA:703:ASN:HD21	1.66	0.44
1:XA:425:ALA:HB3	1:EB:389:ARG:HD3	2.00	0.44
1:ZA:257:TYR:O	1:HB:726:GLY:HA3	2.16	0.44
1:ZA:465:ALA:HB1	1:ZA:473:GLN:HG2	2.00	0.44
1:CB:228:TRP:HE3	1:EB:402:MET:HE3	1.82	0.44
1:DB:701:ARG:HH21	1:DB:703:ASN:HD21	1.66	0.44
1:A:465:ALA:HB1	1:A:473:GLN:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:TYR:CD1	1:LA:479:PRO:CG	3.00	0.43
1:C:228:TRP:HE3	1:IA:402:MET:HE3	1.83	0.43
1:D:701:ARG:HH21	1:D:703:ASN:HD21	1.66	0.43
1:F:508:TYR:CD1	1:S:479:PRO:CG	3.00	0.43
1:G:479:PRO:CG	1:VA:508:TYR:CD1	3.00	0.43
1:H:257:TYR:O	1:IB:726:GLY:HA3	2.16	0.43
1:I:701:ARG:HH21	1:I:703:ASN:ND2	2.16	0.43
1:L:696:LYS:HD3	1:L:696:LYS:HA	1.73	0.43
1:N:701:ARG:HH21	1:N:703:ASN:ND2	2.16	0.43
1:O:378:LEU:HD21	1:FA:436:PRO:HG3	1.99	0.43
1:O:701:ARG:NH2	1:Y:390:SER:O	2.51	0.43
1:P:436:PRO:HG3	1:YA:378:LEU:HD21	1.99	0.43
1:P:465:ALA:HB1	1:P:473:GLN:HG2	2.00	0.43
1:P:701:ARG:NH2	1:YA:390:SER:O	2.51	0.43
1:Q:390:SER:O	1:GA:701:ARG:NH2	2.51	0.43
1:S:389:ARG:HD3	1:TA:425:ALA:HB3	2.00	0.43
1:V:294:ARG:NE	1:LA:705:GLU:HG3	2.32	0.43
1:V:390:SER:O	1:IA:701:ARG:NH2	2.51	0.43
1:W:257:TYR:O	1:PA:726:GLY:HA3	2.16	0.43
1:AA:390:SER:O	1:NA:701:ARG:NH2	2.51	0.43
1:CA:425:ALA:HB3	1:GB:389:ARG:HD3	2.00	0.43
1:EA:403:LEU:HD11	1:EA:409:PHE:HB2	1.99	0.43
1:GA:389:ARG:HD3	1:QA:425:ALA:HB3	2.00	0.43
1:GA:402:MET:HE3	1:EB:228:TRP:HE3	1.83	0.43
1:MA:701:ARG:NH2	1:RA:390:SER:O	2.51	0.43
1:PA:465:ALA:HB1	1:PA:473:GLN:HG2	2.00	0.43
1:RA:701:ARG:HH21	1:RA:703:ASN:ND2	2.16	0.43
1:SA:228:TRP:HE3	1:UA:402:MET:HE3	1.82	0.43
1:SA:615:GLN:NE2	1:ZA:633:ASP:N	2.63	0.43
1:WA:701:ARG:HH21	1:WA:703:ASN:ND2	2.16	0.43
1:YA:701:ARG:HH21	1:YA:703:ASN:HD21	1.66	0.43
1:A:701:ARG:NH2	1:IB:390:SER:O	2.52	0.43
1:A:701:ARG:HH21	1:A:703:ASN:ND2	2.16	0.43
1:B:390:SER:O	1:LA:701:ARG:NH2	2.52	0.43
1:B:488:VAL:HG12	1:LA:460:LEU:HD11	1.99	0.43
1:C:403:LEU:HD11	1:C:409:PHE:HB2	1.99	0.43
1:C:460:LEU:HD11	1:CA:488:VAL:HG12	1.99	0.43
1:D:378:LEU:HD21	1:DB:436:PRO:HG3	1.99	0.43
1:D:389:ARG:HD3	1:DB:425:ALA:HB3	2.00	0.43
1:E:425:ALA:HB3	1:NA:389:ARG:HD3	2.00	0.43
1:G:390:SER:O	1:BA:701:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:701:ARG:NH2	1:DA:390:SER:O	2.51	0.43
1:L:390:SER:O	1:W:701:ARG:NH2	2.51	0.43
1:L:633:ASP:N	1:W:615:GLN:NE2	2.63	0.43
1:Q:425:ALA:HB3	1:QA:389:ARG:HD3	2.00	0.43
1:R:615:GLN:NE2	1:X:633:ASP:N	2.63	0.43
1:S:378:LEU:HD21	1:TA:436:PRO:HG3	1.99	0.43
1:T:228:TRP:HE3	1:CA:402:MET:HE3	1.83	0.43
1:V:696:LYS:HD3	1:V:696:LYS:HA	1.73	0.43
1:Z:403:LEU:HD11	1:Z:409:PHE:HB2	1.99	0.43
1:AA:294:ARG:NE	1:GA:705:GLU:HG3	2.32	0.43
1:AA:488:VAL:HG12	1:NA:460:LEU:HD11	1.99	0.43
1:EA:479:PRO:CG	1:XA:508:TYR:CD1	3.00	0.43
1:GA:465:ALA:HB1	1:GA:473:GLN:HG2	2.00	0.43
1:HA:701:ARG:NH2	1:BB:390:SER:O	2.51	0.43
1:LA:465:ALA:HB1	1:LA:473:GLN:HG2	2.00	0.43
1:PA:257:TYR:O	1:XA:726:GLY:HA3	2.16	0.43
1:QA:480:GLY:HA3	1:QA:614:TRP:HB3	1.99	0.43
1:QA:701:ARG:HH21	1:QA:703:ASN:ND2	2.16	0.43
1:UA:389:ARG:HD3	1:HB:425:ALA:HB3	2.00	0.43
1:VA:701:ARG:HH21	1:VA:703:ASN:HD21	1.66	0.43
1:AB:701:ARG:HH21	1:AB:703:ASN:ND2	2.16	0.43
1:FB:701:ARG:HH21	1:FB:703:ASN:HD21	1.66	0.43
1:GB:465:ALA:HB1	1:GB:473:GLN:HG2	2.00	0.43
1:IB:701:ARG:HH21	1:IB:703:ASN:HD21	1.66	0.43
1:A:425:ALA:HB3	1:IB:389:ARG:HD3	2.00	0.43
1:B:389:ARG:HD3	1:LA:425:ALA:HB3	2.00	0.43
1:B:425:ALA:HB3	1:AB:389:ARG:HD3	2.00	0.43
1:C:615:GLN:NE2	1:CA:633:ASP:N	2.63	0.43
1:H:228:TRP:HE3	1:Y:402:MET:HE3	1.83	0.43
1:I:701:ARG:HH21	1:I:703:ASN:HD21	1.66	0.43
1:M:257:TYR:O	1:YA:726:GLY:HA3	2.16	0.43
1:M:390:SER:O	1:BB:701:ARG:NH2	2.51	0.43
1:O:228:TRP:HE3	1:MA:402:MET:HE3	1.83	0.43
1:O:390:SER:O	1:FA:701:ARG:NH2	2.51	0.43
1:P:460:LEU:HD11	1:YA:488:VAL:HG12	1.99	0.43
1:P:701:ARG:HH21	1:P:703:ASN:ND2	2.16	0.43
1:Q:479:PRO:CG	1:QA:508:TYR:CD1	3.00	0.43
1:Q:488:VAL:HG12	1:GA:460:LEU:HD11	1.99	0.43
1:R:228:TRP:HE3	1:NA:402:MET:HE3	1.83	0.43
1:R:403:LEU:HD11	1:R:409:PHE:HB2	1.99	0.43
1:R:460:LEU:HD11	1:X:488:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:701:ARG:HH21	1:R:703:ASN:HD21	1.66	0.43
1:S:701:ARG:HH21	1:S:703:ASN:HD21	1.66	0.43
1:T:425:ALA:HB3	1:IA:389:ARG:HD3	2.00	0.43
1:V:465:ALA:HB1	1:V:473:GLN:HG2	2.00	0.43
1:Z:701:ARG:HH21	1:Z:703:ASN:HD21	1.66	0.43
1:AA:465:ALA:HB1	1:AA:473:GLN:HG2	2.00	0.43
1:EA:460:LEU:HD11	1:XA:488:VAL:HG12	1.99	0.43
1:FA:701:ARG:HH21	1:FA:703:ASN:ND2	2.16	0.43
1:KA:701:ARG:HH21	1:KA:703:ASN:ND2	2.16	0.43
1:PA:389:ARG:HD3	1:CB:425:ALA:HB3	2.00	0.43
1:PA:701:ARG:HH21	1:PA:703:ASN:HD21	1.66	0.43
1:RA:268:ASN:HA	1:RA:271:HIS:CD2	2.54	0.43
1:WA:465:ALA:HB1	1:WA:473:GLN:HG2	2.00	0.43
1:ZA:403:LEU:HD11	1:ZA:409:PHE:HB2	1.99	0.43
1:AB:480:GLY:HA3	1:AB:614:TRP:HB3	1.99	0.43
1:BB:268:ASN:HA	1:BB:271:HIS:CD2	2.54	0.43
1:BB:465:ALA:HB1	1:BB:473:GLN:HG2	2.00	0.43
1:A:436:PRO:HG3	1:IB:378:LEU:HD21	1.99	0.43
1:A:460:LEU:HD11	1:IB:488:VAL:HG12	1.99	0.43
1:C:390:SER:O	1:GB:701:ARG:NH2	2.51	0.43
1:E:228:TRP:HE3	1:X:402:MET:HE3	1.83	0.43
1:F:701:ARG:NH2	1:TA:390:SER:O	2.51	0.43
1:G:696:LYS:HD3	1:G:696:LYS:HA	1.73	0.43
1:H:701:ARG:HH21	1:H:703:ASN:HD21	1.66	0.43
1:J:228:TRP:HE3	1:HA:402:MET:HE3	1.83	0.43
1:J:465:ALA:HB1	1:J:473:GLN:HG2	2.00	0.43
1:K:701:ARG:NH2	1:DB:390:SER:O	2.51	0.43
1:M:701:ARG:HH21	1:M:703:ASN:HD21	1.66	0.43
1:Q:389:ARG:HD3	1:GA:425:ALA:HB3	2.00	0.43
1:R:390:SER:O	1:WA:701:ARG:NH2	2.51	0.43
1:T:378:LEU:HD21	1:V:436:PRO:HG3	1.99	0.43
1:V:480:GLY:HA3	1:V:614:TRP:HB3	1.99	0.43
1:W:390:SER:O	1:FB:701:ARG:NH2	2.51	0.43
1:W:701:ARG:HH21	1:W:703:ASN:HD21	1.66	0.43
1:X:302:ASN:OD1	1:OA:302:ASN:OD1	2.37	0.43
1:Z:465:ALA:HB1	1:Z:473:GLN:HG2	2.00	0.43
1:BA:390:SER:O	1:VA:701:ARG:NH2	2.51	0.43
1:BA:508:TYR:CD1	1:VA:479:PRO:CG	3.00	0.43
1:BA:701:ARG:HH21	1:BA:703:ASN:HD21	1.66	0.43
1:EA:701:ARG:HH21	1:EA:703:ASN:HD21	1.66	0.43
1:PA:402:MET:HE3	1:XA:228:TRP:HE3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WA:268:ASN:HA	1:WA:271:HIS:CD2	2.54	0.43
1:XA:268:ASN:HA	1:XA:271:HIS:CD2	2.54	0.43
1:ZA:701:ARG:HH21	1:ZA:703:ASN:HD21	1.66	0.43
1:HB:268:ASN:HA	1:HB:271:HIS:CD2	2.54	0.43
1:B:479:PRO:CG	1:AB:508:TYR:CD1	3.00	0.43
1:C:701:ARG:HH21	1:C:703:ASN:HD21	1.66	0.43
1:E:268:ASN:HA	1:E:271:HIS:CD2	2.54	0.43
1:F:268:ASN:HA	1:F:271:HIS:CD2	2.54	0.43
1:H:390:SER:O	1:RA:701:ARG:NH2	2.51	0.43
1:H:479:PRO:CG	1:MA:508:TYR:CD1	3.00	0.43
1:J:378:LEU:HD21	1:KA:436:PRO:HG3	1.99	0.43
1:J:390:SER:O	1:KA:701:ARG:NH2	2.52	0.43
1:J:726:GLY:HA3	1:HA:257:TYR:O	2.16	0.43
1:K:268:ASN:HA	1:K:271:HIS:CD2	2.54	0.43
1:M:696:LYS:HD3	1:M:696:LYS:HA	1.73	0.43
1:N:465:ALA:HB1	1:N:473:GLN:HG2	2.00	0.43
1:P:425:ALA:HB3	1:YA:389:ARG:HD3	2.00	0.43
1:S:488:VAL:HG12	1:TA:460:LEU:HD11	1.99	0.43
1:Z:268:ASN:HA	1:Z:271:HIS:CD2	2.54	0.43
1:Z:425:ALA:HB3	1:HB:389:ARG:HD3	2.00	0.43
1:Z:460:LEU:HD11	1:HB:488:VAL:HG12	1.98	0.43
1:CA:302:ASN:OD1	1:JA:302:ASN:OD1	2.37	0.43
1:EA:268:ASN:HA	1:EA:271:HIS:CD2	2.54	0.43
1:FA:268:ASN:HA	1:FA:271:HIS:CD2	2.54	0.43
1:GA:390:SER:O	1:QA:701:ARG:NH2	2.51	0.43
1:GA:480:GLY:HA3	1:GA:614:TRP:HB3	1.99	0.43
1:JA:465:ALA:HB1	1:JA:473:GLN:HG2	2.00	0.43
1:KA:268:ASN:HA	1:KA:271:HIS:CD2	2.54	0.43
1:LA:390:SER:O	1:AB:701:ARG:NH2	2.51	0.43
1:MA:701:ARG:HH21	1:MA:703:ASN:HD21	1.66	0.43
1:OA:390:SER:O	1:PA:701:ARG:NH2	2.51	0.43
1:OA:465:ALA:HB1	1:OA:473:GLN:HG2	2.00	0.43
1:PA:403:LEU:HD11	1:PA:409:PHE:HB2	1.99	0.43
1:PA:480:GLY:HA3	1:PA:614:TRP:HB3	1.99	0.43
1:QA:465:ALA:HB1	1:QA:473:GLN:HG2	2.00	0.43
1:SA:425:ALA:HB3	1:ZA:389:ARG:HD3	2.00	0.43
1:ZA:402:MET:HE3	1:HB:228:TRP:HE3	1.82	0.43
1:ZA:480:GLY:HA3	1:ZA:614:TRP:HB3	1.99	0.43
1:CB:701:ARG:HH21	1:CB:703:ASN:HD21	1.66	0.43
1:GB:268:ASN:HA	1:GB:271:HIS:CD2	2.54	0.43
1:D:488:VAL:HG12	1:DB:460:LEU:HD11	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:701:ARG:NH2	1:NA:390:SER:O	2.52	0.43
1:H:302:ASN:OD1	1:O:302:ASN:OD1	2.37	0.43
1:I:302:ASN:OD1	1:N:302:ASN:OD1	2.37	0.43
1:I:465:ALA:HB1	1:I:473:GLN:HG2	2.00	0.43
1:J:302:ASN:OD1	1:M:302:ASN:OD1	2.37	0.43
1:M:479:PRO:CG	1:HA:508:TYR:CD1	3.00	0.43
1:N:701:ARG:HH21	1:N:703:ASN:HD21	1.66	0.43
1:T:402:MET:HE3	1:LA:228:TRP:HE3	1.82	0.43
1:T:701:ARG:NH2	1:IA:390:SER:O	2.52	0.43
1:V:701:ARG:HH21	1:V:703:ASN:ND2	2.16	0.43
1:W:508:TYR:CD1	1:FB:479:PRO:CG	3.00	0.43
1:X:701:ARG:NH2	1:WA:390:SER:O	2.52	0.43
1:X:701:ARG:HH21	1:X:703:ASN:HD21	1.66	0.43
1:Z:479:PRO:CG	1:HB:508:TYR:CD1	3.00	0.43
1:AA:480:GLY:HA3	1:AA:614:TRP:HB3	1.99	0.43
1:CA:701:ARG:HH21	1:CA:703:ASN:HD21	1.66	0.43
1:CA:701:ARG:NH2	1:GB:390:SER:O	2.51	0.43
1:DA:425:ALA:HB3	1:KA:389:ARG:HD3	2.00	0.43
1:EA:425:ALA:HB3	1:XA:389:ARG:HD3	2.00	0.43
1:EA:465:ALA:HB1	1:EA:473:GLN:HG2	2.00	0.43
1:FA:480:GLY:HA3	1:FA:614:TRP:HB3	1.99	0.43
1:HA:701:ARG:HH21	1:HA:703:ASN:HD21	1.66	0.43
1:JA:390:SER:O	1:ZA:701:ARG:NH2	2.52	0.43
1:LA:480:GLY:HA3	1:LA:614:TRP:HB3	1.99	0.43
1:PA:302:ASN:OD1	1:FB:302:ASN:OD1	2.37	0.43
1:SA:701:ARG:HH21	1:SA:703:ASN:HD21	1.66	0.43
1:TA:302:ASN:OD1	1:GB:302:ASN:OD1	2.37	0.43
1:UA:390:SER:O	1:HB:701:ARG:NH2	2.51	0.43
1:VA:701:ARG:HH21	1:VA:703:ASN:ND2	2.16	0.43
1:WA:302:ASN:OD1	1:DB:302:ASN:OD1	2.37	0.43
1:AB:465:ALA:HB1	1:AB:473:GLN:HG2	2.00	0.43
1:FB:701:ARG:HH21	1:FB:703:ASN:ND2	2.16	0.43
1:D:268:ASN:HA	1:D:271:HIS:CD2	2.54	0.43
1:D:465:ALA:HB1	1:D:473:GLN:HG2	2.00	0.43
1:E:378:LEU:HD21	1:AA:436:PRO:HG3	1.99	0.43
1:F:302:ASN:OD1	1:L:302:ASN:OD1	2.37	0.43
1:G:302:ASN:OD1	1:K:302:ASN:OD1	2.37	0.43
1:G:701:ARG:NH2	1:VA:390:SER:O	2.51	0.43
1:O:389:ARG:HD3	1:FA:425:ALA:HB3	2.00	0.43
1:P:228:TRP:HE3	1:AB:402:MET:HE3	1.82	0.43
1:S:268:ASN:HA	1:S:271:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:268:ASN:HA	1:T:271:HIS:CD2	2.54	0.43
1:T:726:GLY:HA3	1:CA:257:TYR:O	2.16	0.43
1:Y:701:ARG:NH2	1:FA:390:SER:O	2.51	0.43
1:AA:701:ARG:HH21	1:AA:703:ASN:ND2	2.16	0.43
1:CA:701:ARG:HH21	1:CA:703:ASN:ND2	2.16	0.43
1:DA:480:GLY:HA3	1:DA:614:TRP:HB3	1.99	0.43
1:DA:701:ARG:NH2	1:KA:390:SER:O	2.51	0.43
1:KA:480:GLY:HA3	1:KA:614:TRP:HB3	1.99	0.43
1:RA:705:GLU:HG3	1:IB:294:ARG:NE	2.32	0.43
1:VA:302:ASN:OD1	1:ZA:302:ASN:OD1	2.37	0.43
1:XA:701:ARG:NH2	1:EB:390:SER:O	2.51	0.43
1:YA:268:ASN:HA	1:YA:271:HIS:CD2	2.54	0.43
1:IB:268:ASN:HA	1:IB:271:HIS:CD2	2.54	0.43
1:J:389:ARG:HD3	1:KA:425:ALA:HB3	2.00	0.43
1:L:701:ARG:NH2	1:FB:390:SER:O	2.52	0.43
1:M:488:VAL:HG12	1:BB:460:LEU:HD11	1.99	0.43
1:M:701:ARG:NH2	1:HA:390:SER:O	2.51	0.43
1:N:389:ARG:HD3	1:IB:425:ALA:HB3	2.00	0.43
1:Q:701:ARG:NH2	1:QA:390:SER:O	2.51	0.43
1:R:701:ARG:NH2	1:X:390:SER:O	2.51	0.43
1:S:465:ALA:HB1	1:S:473:GLN:HG2	2.00	0.43
1:T:465:ALA:HB1	1:T:473:GLN:HG2	2.00	0.43
1:X:701:ARG:HH21	1:X:703:ASN:ND2	2.16	0.43
1:Y:480:GLY:HA3	1:Y:614:TRP:HB3	1.99	0.43
1:AA:268:ASN:HA	1:AA:271:HIS:CD2	2.54	0.43
1:BA:465:ALA:HB1	1:BA:473:GLN:HG2	2.00	0.43
1:EA:302:ASN:OD1	1:HA:302:ASN:OD1	2.37	0.43
1:JA:480:GLY:HA3	1:JA:614:TRP:HB3	1.99	0.43
1:OA:480:GLY:HA3	1:OA:614:TRP:HB3	1.99	0.43
1:WA:480:GLY:HA3	1:WA:614:TRP:HB3	1.99	0.43
1:XA:465:ALA:HB1	1:XA:473:GLN:HG2	2.00	0.43
1:YA:294:ARG:NE	1:BB:705:GLU:HG3	2.32	0.43
1:AB:268:ASN:HA	1:AB:271:HIS:CD2	2.54	0.43
1:CB:268:ASN:HA	1:CB:271:HIS:CD2	2.54	0.43
1:DB:701:ARG:HH21	1:DB:703:ASN:ND2	2.16	0.43
1:EB:701:ARG:HH21	1:EB:703:ASN:ND2	2.16	0.43
1:HB:465:ALA:HB1	1:HB:473:GLN:HG2	2.00	0.43
1:A:389:ARG:HD3	1:N:425:ALA:HB3	2.00	0.43
1:B:701:ARG:NH2	1:AB:390:SER:O	2.51	0.43
1:C:701:ARG:NH2	1:CA:390:SER:O	2.51	0.43
1:E:402:MET:HE3	1:GA:228:TRP:HE3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:701:ARG:NH2	1:MA:390:SER:O	2.51	0.43
1:I:425:ALA:HB3	1:P:389:ARG:HD3	2.00	0.43
1:P:448:THR:OG1	1:YA:498:SER:O	2.35	0.43
1:Q:701:ARG:HH21	1:Q:703:ASN:ND2	2.16	0.43
1:S:480:GLY:HA3	1:S:614:TRP:HB3	1.99	0.43
1:V:268:ASN:HA	1:V:271:HIS:CD2	2.54	0.43
1:V:302:ASN:OD1	1:LA:302:ASN:OD1	2.37	0.43
1:W:465:ALA:HB1	1:W:473:GLN:HG2	2.00	0.43
1:Y:425:ALA:HB3	1:FA:389:ARG:HD3	2.00	0.43
1:Z:302:ASN:OD1	1:MA:302:ASN:OD1	2.37	0.43
1:AA:696:LYS:HD3	1:AA:696:LYS:HA	1.73	0.43
1:DA:268:ASN:HA	1:DA:271:HIS:CD2	2.54	0.43
1:JA:389:ARG:HD3	1:ZA:425:ALA:HB3	2.00	0.43
1:OA:389:ARG:HD3	1:PA:425:ALA:HB3	2.00	0.43
1:QA:268:ASN:HA	1:QA:271:HIS:CD2	2.54	0.43
1:SA:268:ASN:HA	1:SA:271:HIS:CD2	2.54	0.43
1:UA:498:SER:O	1:HB:448:THR:OG1	2.35	0.43
1:UA:701:ARG:HH21	1:UA:703:ASN:ND2	2.16	0.43
1:GB:480:GLY:HA3	1:GB:614:TRP:HB3	1.99	0.43
1:A:228:TRP:HE3	1:QA:402:MET:HE3	1.82	0.43
1:A:390:SER:O	1:N:701:ARG:NH2	2.51	0.43
1:B:701:ARG:HH21	1:B:703:ASN:ND2	2.16	0.43
1:C:268:ASN:HA	1:C:271:HIS:CD2	2.54	0.43
1:D:302:ASN:OD1	1:S:302:ASN:OD1	2.37	0.43
1:D:480:GLY:HA3	1:D:614:TRP:HB3	1.99	0.43
1:E:389:ARG:HD3	1:AA:425:ALA:HB3	2.00	0.43
1:E:465:ALA:HB1	1:E:473:GLN:HG2	2.00	0.43
1:E:726:GLY:HA3	1:X:257:TYR:O	2.16	0.43
1:I:268:ASN:HA	1:I:271:HIS:CD2	2.54	0.43
1:X:219:ASP:O	1:X:220:GLY:C	2.62	0.43
1:Y:268:ASN:HA	1:Y:271:HIS:CD2	2.54	0.43
1:AA:302:ASN:OD1	1:GA:302:ASN:OD1	2.37	0.43
1:CA:219:ASP:O	1:CA:220:GLY:C	2.62	0.43
1:CA:615:GLN:NE2	1:GB:633:ASP:N	2.63	0.43
1:EA:389:ARG:HD3	1:EB:425:ALA:HB3	2.00	0.43
1:JA:268:ASN:HA	1:JA:271:HIS:CD2	2.54	0.43
1:B:268:ASN:HA	1:B:271:HIS:CD2	2.54	0.42
1:D:701:ARG:NH2	1:K:390:SER:O	2.51	0.42
1:H:488:VAL:HG12	1:RA:460:LEU:HD11	1.99	0.42
1:I:389:ARG:HD3	1:YA:425:ALA:HB3	2.00	0.42
1:M:480:GLY:HA3	1:M:614:TRP:HB3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:390:SER:O	1:IB:701:ARG:NH2	2.51	0.42
1:P:714:LYS:HA	1:AB:387:VAL:HA	2.01	0.42
1:Q:726:GLY:HA3	1:IB:257:TYR:O	2.16	0.42
1:R:268:ASN:HA	1:R:271:HIS:CD2	2.54	0.42
1:R:389:ARG:HD3	1:WA:425:ALA:HB3	2.00	0.42
1:T:389:ARG:HD3	1:V:425:ALA:HB3	2.00	0.42
1:V:701:ARG:HH21	1:V:703:ASN:HD21	1.66	0.42
1:AA:701:ARG:HH21	1:AA:703:ASN:HD21	1.66	0.42
1:BA:302:ASN:OD1	1:FA:302:ASN:OD1	2.37	0.42
1:GA:701:ARG:HH21	1:GA:703:ASN:HD21	1.66	0.42
1:JA:425:ALA:HB3	1:SA:389:ARG:HD3	2.00	0.42
1:OA:268:ASN:HA	1:OA:271:HIS:CD2	2.54	0.42
1:BB:701:ARG:HH21	1:BB:703:ASN:HD21	1.66	0.42
1:A:714:LYS:HA	1:QA:387:VAL:HA	2.01	0.42
1:C:387:VAL:HA	1:TA:714:LYS:HA	2.02	0.42
1:C:465:ALA:HB1	1:C:473:GLN:HG2	2.00	0.42
1:H:465:ALA:HB1	1:H:473:GLN:HG2	2.00	0.42
1:I:390:SER:O	1:YA:701:ARG:NH2	2.52	0.42
1:I:701:ARG:NH2	1:P:390:SER:O	2.51	0.42
1:L:714:LYS:HA	1:TA:387:VAL:HA	2.02	0.42
1:M:465:ALA:HB1	1:M:473:GLN:HG2	2.00	0.42
1:P:701:ARG:HH21	1:P:703:ASN:HD21	1.66	0.42
1:R:387:VAL:HA	1:DB:714:LYS:HA	2.01	0.42
1:T:390:SER:O	1:V:701:ARG:NH2	2.51	0.42
1:W:302:ASN:OD1	1:KA:302:ASN:OD1	2.37	0.42
1:Z:378:LEU:HD21	1:UA:436:PRO:HG3	1.99	0.42
1:Z:389:ARG:HD3	1:UA:425:ALA:HB3	2.00	0.42
1:Z:390:SER:O	1:UA:701:ARG:NH2	2.51	0.42
1:AA:498:SER:O	1:NA:448:THR:OG1	2.35	0.42
1:DA:302:ASN:OD1	1:IA:302:ASN:OD1	2.37	0.42
1:DA:701:ARG:HH21	1:DA:703:ASN:HD21	1.66	0.42
1:EA:378:LEU:HD21	1:EB:436:PRO:HG3	1.99	0.42
1:EA:701:ARG:NH2	1:XA:390:SER:O	2.51	0.42
1:GA:219:ASP:O	1:GA:220:GLY:C	2.62	0.42
1:JA:701:ARG:NH2	1:SA:390:SER:O	2.51	0.42
1:LA:219:ASP:O	1:LA:220:GLY:C	2.62	0.42
1:LA:701:ARG:HH21	1:LA:703:ASN:HD21	1.66	0.42
1:MA:268:ASN:HA	1:MA:271:HIS:CD2	2.54	0.42
1:TA:268:ASN:HA	1:TA:271:HIS:CD2	2.54	0.42
1:TA:701:ARG:HH21	1:TA:703:ASN:ND2	2.16	0.42
1:UA:268:ASN:HA	1:UA:271:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:448:THR:OG1	1:EB:498:SER:O	2.35	0.42
1:DB:268:ASN:HA	1:DB:271:HIS:CD2	2.54	0.42
1:A:448:THR:OG1	1:IB:498:SER:O	2.35	0.42
1:G:387:VAL:HA	1:FA:714:LYS:HA	2.01	0.42
1:H:460:LEU:HD11	1:MA:488:VAL:HG12	1.99	0.42
1:H:480:GLY:HA3	1:H:614:TRP:HB3	2.00	0.42
1:I:387:VAL:HA	1:BB:714:LYS:HA	2.02	0.42
1:K:714:LYS:HA	1:VA:387:VAL:HA	2.01	0.42
1:N:268:ASN:HA	1:N:271:HIS:CD2	2.54	0.42
1:N:402:MET:HE3	1:RA:228:TRP:HE3	1.82	0.42
1:O:701:ARG:HH21	1:O:703:ASN:ND2	2.16	0.42
1:Q:268:ASN:HA	1:Q:271:HIS:CD2	2.54	0.42
1:R:714:LYS:HA	1:NA:387:VAL:HA	2.02	0.42
1:W:219:ASP:O	1:W:220:GLY:C	2.62	0.42
1:X:615:GLN:NE2	1:WA:633:ASP:N	2.63	0.42
1:Y:302:ASN:OD1	1:NA:302:ASN:OD1	2.36	0.42
1:Z:701:ARG:NH2	1:HB:390:SER:O	2.51	0.42
1:BA:219:ASP:O	1:BA:220:GLY:C	2.62	0.42
1:EA:488:VAL:HG12	1:EB:460:LEU:HD11	1.99	0.42
1:FA:701:ARG:HH21	1:FA:703:ASN:HD21	1.66	0.42
1:OA:425:ALA:HB3	1:CB:389:ARG:HD3	2.00	0.42
1:EB:268:ASN:HA	1:EB:271:HIS:CD2	2.54	0.42
1:EB:465:ALA:HB1	1:EB:473:GLN:HG2	2.00	0.42
1:EB:701:ARG:HD3	1:EB:705:GLU:CG	2.49	0.42
1:A:268:ASN:HA	1:A:271:HIS:CD2	2.54	0.42
1:A:701:ARG:HH21	1:A:703:ASN:HD21	1.66	0.42
1:B:257:TYR:O	1:V:726:GLY:HA3	2.16	0.42
1:B:726:GLY:HA3	1:YA:257:TYR:O	2.16	0.42
1:C:219:ASP:O	1:C:220:GLY:C	2.62	0.42
1:C:389:ARG:HD3	1:GB:425:ALA:HB3	2.00	0.42
1:C:714:LYS:HA	1:IA:387:VAL:HA	2.02	0.42
1:E:390:SER:O	1:AA:701:ARG:NH2	2.51	0.42
1:E:701:ARG:HD3	1:E:705:GLU:CG	2.49	0.42
1:F:390:SER:O	1:S:701:ARG:NH2	2.51	0.42
1:H:268:ASN:HA	1:H:271:HIS:CD2	2.54	0.42
1:H:615:GLN:HE21	1:MA:633:ASP:H	1.67	0.42
1:I:701:ARG:HD3	1:I:705:GLU:CG	2.49	0.42
1:J:425:ALA:HB3	1:DA:389:ARG:HD3	2.00	0.42
1:L:387:VAL:HA	1:KA:714:LYS:HA	2.01	0.42
1:M:268:ASN:HA	1:M:271:HIS:CD2	2.54	0.42
1:M:344:THR:HG22	1:M:654:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:460:LEU:HD11	1:HA:488:VAL:HG12	1.99	0.42
1:N:387:VAL:HA	1:RA:714:LYS:HA	2.02	0.42
1:O:425:ALA:HB3	1:Y:389:ARG:HD3	2.00	0.42
1:O:714:LYS:HA	1:MA:387:VAL:HA	2.01	0.42
1:P:268:ASN:HA	1:P:271:HIS:CD2	2.54	0.42
1:Q:460:LEU:HD11	1:QA:488:VAL:HG12	1.99	0.42
1:R:465:ALA:HB1	1:R:473:GLN:HG2	2.00	0.42
1:T:387:VAL:HA	1:LA:714:LYS:HA	2.02	0.42
1:Y:701:ARG:HH21	1:Y:703:ASN:HD21	1.66	0.42
1:EA:390:SER:O	1:EB:701:ARG:NH2	2.51	0.42
1:FA:344:THR:HG22	1:FA:654:ILE:HG12	2.02	0.42
1:GA:633:ASP:N	1:QA:615:GLN:NE2	2.63	0.42
1:HA:268:ASN:HA	1:HA:271:HIS:CD2	2.54	0.42
1:HA:701:ARG:HD3	1:HA:705:GLU:CG	2.49	0.42
1:KA:344:THR:HG22	1:KA:654:ILE:HG12	2.02	0.42
1:KA:696:LYS:HD3	1:KA:696:LYS:HA	1.73	0.42
1:LA:268:ASN:HA	1:LA:271:HIS:CD2	2.54	0.42
1:QA:302:ASN:OD1	1:EB:302:ASN:OD1	2.37	0.42
1:RA:302:ASN:OD1	1:IB:302:ASN:OD1	2.37	0.42
1:RA:701:ARG:HH21	1:RA:703:ASN:HD21	1.66	0.42
1:UA:302:ASN:OD1	1:AB:302:ASN:OD1	2.37	0.42
1:UA:701:ARG:HD3	1:UA:705:GLU:CG	2.49	0.42
1:E:344:THR:HG22	1:E:654:ILE:HG12	2.02	0.42
1:E:387:VAL:HA	1:GA:714:LYS:HA	2.02	0.42
1:F:389:ARG:HD3	1:S:425:ALA:HB3	2.00	0.42
1:F:714:LYS:HA	1:FB:387:VAL:HA	2.02	0.42
1:G:268:ASN:HA	1:G:271:HIS:CD2	2.54	0.42
1:G:714:LYS:HA	1:DB:387:VAL:HA	2.02	0.42
1:H:344:THR:HG22	1:H:654:ILE:HG12	2.02	0.42
1:I:402:MET:HE3	1:BB:228:TRP:HE3	1.83	0.42
1:J:714:LYS:HA	1:HA:387:VAL:HA	2.01	0.42
1:M:387:VAL:HA	1:YA:714:LYS:HA	2.01	0.42
1:M:615:GLN:HE21	1:HA:633:ASP:H	1.67	0.42
1:N:701:ARG:HD3	1:N:705:GLU:CG	2.49	0.42
1:O:268:ASN:HA	1:O:271:HIS:CD2	2.54	0.42
1:O:344:THR:HG22	1:O:654:ILE:HG12	2.02	0.42
1:P:344:THR:HG22	1:P:654:ILE:HG12	2.02	0.42
1:Q:257:TYR:O	1:AA:726:GLY:HA3	2.16	0.42
1:T:701:ARG:HD3	1:T:705:GLU:CG	2.49	0.42
1:V:498:SER:O	1:IA:448:THR:OG1	2.35	0.42
1:W:268:ASN:HA	1:W:271:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:219:ASP:O	1:FA:220:GLY:C	2.62	0.42
1:GA:268:ASN:HA	1:GA:271:HIS:CD2	2.54	0.42
1:HA:344:THR:HG22	1:HA:654:ILE:HG12	2.02	0.42
1:KA:219:ASP:O	1:KA:220:GLY:C	2.62	0.42
1:KA:701:ARG:HH21	1:KA:703:ASN:HD21	1.66	0.42
1:MA:344:THR:HG22	1:MA:654:ILE:HG12	2.02	0.42
1:MA:701:ARG:HD3	1:MA:705:GLU:CG	2.49	0.42
1:NA:219:ASP:O	1:NA:220:GLY:C	2.62	0.42
1:OA:701:ARG:NH2	1:CB:390:SER:O	2.52	0.42
1:UA:465:ALA:HB1	1:UA:473:GLN:HG2	2.00	0.42
1:XA:665:PRO:HB3	1:XA:674:PHE:CZ	2.55	0.42
1:YA:302:ASN:OD1	1:BB:302:ASN:OD1	2.37	0.42
1:HB:665:PRO:HB3	1:HB:674:PHE:CZ	2.55	0.42
1:A:344:THR:HG22	1:A:654:ILE:HG12	2.02	0.42
1:B:302:ASN:OD1	1:P:302:ASN:OD1	2.37	0.42
1:D:344:THR:HG22	1:D:654:ILE:HG12	2.02	0.42
1:D:425:ALA:HB3	1:K:389:ARG:HD3	2.00	0.42
1:H:387:VAL:HA	1:IB:714:LYS:HA	2.02	0.42
1:J:268:ASN:HA	1:J:271:HIS:CD2	2.54	0.42
1:J:344:THR:HG22	1:J:654:ILE:HG12	2.02	0.42
1:J:701:ARG:HH21	1:J:703:ASN:ND2	2.16	0.42
1:L:268:ASN:HA	1:L:271:HIS:CD2	2.54	0.42
1:L:389:ARG:HD3	1:W:425:ALA:HB3	2.00	0.42
1:L:701:ARG:HD3	1:L:705:GLU:CG	2.49	0.42
1:M:498:SER:O	1:BB:448:THR:OG1	2.35	0.42
1:R:219:ASP:O	1:R:220:GLY:C	2.62	0.42
1:S:344:THR:HG22	1:S:654:ILE:HG12	2.02	0.42
1:T:344:THR:HG22	1:T:654:ILE:HG12	2.02	0.42
1:BA:498:SER:O	1:VA:448:THR:OG1	2.35	0.42
1:BA:633:ASP:H	1:VA:615:GLN:HE21	1.67	0.42
1:CA:268:ASN:HA	1:CA:271:HIS:CD2	2.54	0.42
1:GA:344:THR:HG22	1:GA:654:ILE:HG12	2.02	0.42
1:JA:665:PRO:HB3	1:JA:674:PHE:CZ	2.55	0.42
1:LA:344:THR:HG22	1:LA:654:ILE:HG12	2.02	0.42
1:OA:219:ASP:O	1:OA:220:GLY:C	2.62	0.42
1:PA:498:SER:O	1:CB:448:THR:OG1	2.35	0.42
1:FB:268:ASN:HA	1:FB:271:HIS:CD2	2.54	0.42
1:A:302:ASN:OD1	1:Q:302:ASN:OD1	2.37	0.42
1:B:460:LEU:HD11	1:AB:488:VAL:HG12	1.99	0.42
1:G:389:ARG:HD3	1:BA:425:ALA:HB3	2.00	0.42
1:I:344:THR:HG22	1:I:654:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:665:PRO:HB3	1:I:674:PHE:CZ	2.55	0.42
1:J:701:ARG:HH21	1:J:703:ASN:HD21	1.66	0.42
1:N:665:PRO:HB3	1:N:674:PHE:CZ	2.55	0.42
1:X:268:ASN:HA	1:X:271:HIS:CD2	2.54	0.42
1:BA:268:ASN:HA	1:BA:271:HIS:CD2	2.54	0.42
1:EA:665:PRO:HB3	1:EA:674:PHE:CZ	2.55	0.42
1:LA:633:ASP:N	1:AB:615:GLN:NE2	2.63	0.42
1:NA:701:ARG:HD3	1:NA:705:GLU:CG	2.49	0.42
1:OA:665:PRO:HB3	1:OA:674:PHE:CZ	2.55	0.42
1:SA:714:LYS:HA	1:UA:387:VAL:HA	2.02	0.42
1:TA:344:THR:HG22	1:TA:654:ILE:HG12	2.02	0.42
1:VA:268:ASN:HA	1:VA:271:HIS:CD2	2.54	0.42
1:ZA:387:VAL:HA	1:HB:714:LYS:HA	2.02	0.42
1:CB:714:LYS:HA	1:EB:387:VAL:HA	2.02	0.42
1:B:219:ASP:O	1:B:220:GLY:C	2.62	0.42
1:C:726:GLY:HA3	1:IA:257:TYR:O	2.16	0.42
1:D:219:ASP:O	1:D:220:GLY:C	2.62	0.42
1:J:633:ASP:N	1:KA:615:GLN:NE2	2.63	0.42
1:L:344:THR:HG22	1:L:654:ILE:HG12	2.02	0.42
1:N:344:THR:HG22	1:N:654:ILE:HG12	2.02	0.42
1:O:701:ARG:HH21	1:O:703:ASN:HD21	1.66	0.42
1:S:219:ASP:O	1:S:220:GLY:C	2.62	0.42
1:W:633:ASP:H	1:FB:615:GLN:HE21	1.67	0.42
1:Y:219:ASP:O	1:Y:220:GLY:C	2.62	0.42
1:Z:344:THR:HG22	1:Z:654:ILE:HG12	2.02	0.42
1:Z:665:PRO:HB3	1:Z:674:PHE:CZ	2.55	0.42
1:DA:344:THR:HG22	1:DA:654:ILE:HG12	2.02	0.42
1:IA:701:ARG:HD3	1:IA:705:GLU:CG	2.49	0.42
1:JA:714:LYS:HA	1:GB:387:VAL:HA	2.01	0.42
1:NA:268:ASN:HA	1:NA:271:HIS:CD2	2.54	0.42
1:PA:387:VAL:HA	1:XA:714:LYS:HA	2.02	0.42
1:QA:344:THR:HG22	1:QA:654:ILE:HG12	2.02	0.42
1:QA:701:ARG:HH21	1:QA:703:ASN:HD21	1.66	0.42
1:XA:302:ASN:OD1	1:CB:302:ASN:OD1	2.37	0.42
1:AB:344:THR:HG22	1:AB:654:ILE:HG12	2.02	0.42
1:AB:701:ARG:HH21	1:AB:703:ASN:HD21	1.66	0.42
1:A:665:PRO:HB3	1:A:674:PHE:CZ	2.55	0.42
1:C:302:ASN:OD1	1:T:302:ASN:OD1	2.37	0.42
1:C:498:SER:O	1:GB:448:THR:OG1	2.35	0.42
1:G:344:THR:HG22	1:G:654:ILE:HG12	2.02	0.42
1:G:701:ARG:HD3	1:G:705:GLU:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:665:PRO:HB3	1:P:674:PHE:CZ	2.55	0.42
1:R:498:SER:O	1:WA:448:THR:OG1	2.35	0.42
1:R:726:GLY:HA3	1:NA:257:TYR:O	2.16	0.42
1:S:390:SER:O	1:TA:701:ARG:NH2	2.51	0.42
1:X:344:THR:HG22	1:X:654:ILE:HG12	2.02	0.42
1:Y:344:THR:HG22	1:Y:654:ILE:HG12	2.02	0.42
1:AA:344:THR:HG22	1:AA:654:ILE:HG12	2.02	0.42
1:DA:219:ASP:O	1:DA:220:GLY:C	2.62	0.42
1:EA:344:THR:HG22	1:EA:654:ILE:HG12	2.02	0.42
1:IA:268:ASN:HA	1:IA:271:HIS:CD2	2.54	0.42
1:OA:633:ASP:H	1:PA:615:GLN:HE21	1.67	0.42
1:RA:219:ASP:O	1:RA:220:GLY:C	2.62	0.42
1:SA:302:ASN:OD1	1:HB:302:ASN:OD1	2.36	0.42
1:UA:633:ASP:H	1:HB:615:GLN:HE21	1.67	0.42
1:WA:701:ARG:HH21	1:WA:703:ASN:HD21	1.66	0.42
1:DB:344:THR:HG22	1:DB:654:ILE:HG12	2.02	0.42
1:EB:219:ASP:O	1:EB:220:GLY:C	2.62	0.42
1:GB:219:ASP:O	1:GB:220:GLY:C	2.62	0.42
1:GB:701:ARG:HH21	1:GB:703:ASN:HD21	1.66	0.42
1:A:674:PHE:CZ	1:I:248:ALA:HB3	2.55	0.42
1:B:344:THR:HG22	1:B:654:ILE:HG12	2.02	0.42
1:E:302:ASN:OD1	1:R:302:ASN:OD1	2.37	0.42
1:E:665:PRO:HB3	1:E:674:PHE:CZ	2.55	0.42
1:F:219:ASP:O	1:F:220:GLY:C	2.62	0.42
1:Q:219:ASP:O	1:Q:220:GLY:C	2.62	0.42
1:Q:344:THR:HG22	1:Q:654:ILE:HG12	2.02	0.42
1:V:344:THR:HG22	1:V:654:ILE:HG12	2.02	0.42
1:CA:344:THR:HG22	1:CA:654:ILE:HG12	2.02	0.42
1:HA:615:GLN:HE21	1:BB:633:ASP:H	1.67	0.42
1:MA:615:GLN:HE21	1:RA:633:ASP:H	1.68	0.42
1:OA:714:LYS:HA	1:WA:387:VAL:HA	2.02	0.42
1:PA:268:ASN:HA	1:PA:271:HIS:CD2	2.54	0.42
1:XA:701:ARG:HH21	1:XA:703:ASN:HD21	1.66	0.42
1:AB:725:ASN:HB2	1:AB:727:VAL:HG23	2.02	0.42
1:BB:219:ASP:O	1:BB:220:GLY:C	2.62	0.42
1:HB:219:ASP:O	1:HB:220:GLY:C	2.62	0.42
1:B:714:LYS:HA	1:YA:387:VAL:HA	2.02	0.41
1:D:390:SER:O	1:DB:701:ARG:NH2	2.51	0.41
1:F:701:ARG:HH21	1:F:703:ASN:HD21	1.66	0.41
1:H:498:SER:O	1:RA:448:THR:OG1	2.35	0.41
1:K:219:ASP:O	1:K:220:GLY:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:633:ASP:N	1:FA:615:GLN:NE2	2.63	0.41
1:P:725:ASN:HB2	1:P:727:VAL:HG23	2.02	0.41
1:S:725:ASN:HB2	1:S:727:VAL:HG23	2.02	0.41
1:T:665:PRO:HB3	1:T:674:PHE:CZ	2.55	0.41
1:V:387:VAL:HA	1:DA:714:LYS:HA	2.02	0.41
1:Y:714:LYS:HA	1:AA:387:VAL:HA	2.02	0.41
1:AA:219:ASP:O	1:AA:220:GLY:C	2.62	0.41
1:DA:701:ARG:HD3	1:DA:705:GLU:CG	2.49	0.41
1:FA:725:ASN:HB2	1:FA:727:VAL:HG23	2.02	0.41
1:HA:714:LYS:HA	1:XA:387:VAL:HA	2.02	0.41
1:KA:725:ASN:HB2	1:KA:727:VAL:HG23	2.02	0.41
1:QA:725:ASN:HB2	1:QA:727:VAL:HG23	2.02	0.41
1:SA:344:THR:HG22	1:SA:654:ILE:HG12	2.02	0.41
1:WA:219:ASP:O	1:WA:220:GLY:C	2.62	0.41
1:WA:665:PRO:HB3	1:WA:674:PHE:CZ	2.55	0.41
1:XA:615:GLN:HE21	1:EB:633:ASP:H	1.67	0.41
1:ZA:268:ASN:HA	1:ZA:271:HIS:CD2	2.54	0.41
1:CB:344:THR:HG22	1:CB:654:ILE:HG12	2.02	0.41
1:CB:726:GLY:HA3	1:EB:257:TYR:O	2.17	0.41
1:HB:701:ARG:HH21	1:HB:703:ASN:HD21	1.66	0.41
1:A:725:ASN:HB2	1:A:727:VAL:HG23	2.02	0.41
1:D:725:ASN:HB2	1:D:727:VAL:HG23	2.02	0.41
1:G:248:ALA:HB3	1:DB:674:PHE:CZ	2.55	0.41
1:I:674:PHE:CZ	1:BB:248:ALA:HB3	2.56	0.41
1:K:701:ARG:HH21	1:K:703:ASN:HD21	1.66	0.41
1:O:674:PHE:CZ	1:BA:248:ALA:HB3	2.55	0.41
1:T:701:ARG:HH21	1:T:703:ASN:HD21	1.66	0.41
1:Y:701:ARG:HD3	1:Y:705:GLU:CG	2.49	0.41
1:FA:696:LYS:HA	1:FA:696:LYS:HD3	1.73	0.41
1:GA:387:VAL:HA	1:EB:714:LYS:HA	2.01	0.41
1:KA:701:ARG:HD3	1:KA:705:GLU:CG	2.49	0.41
1:LA:387:VAL:HA	1:UA:714:LYS:HA	2.01	0.41
1:MA:714:LYS:HA	1:HB:387:VAL:HA	2.02	0.41
1:PA:674:PHE:CZ	1:XA:248:ALA:HB3	2.55	0.41
1:SA:726:GLY:HA3	1:UA:257:TYR:O	2.16	0.41
1:TA:665:PRO:HB3	1:TA:674:PHE:CZ	2.55	0.41
1:XA:219:ASP:O	1:XA:220:GLY:C	2.62	0.41
1:YA:219:ASP:O	1:YA:220:GLY:C	2.62	0.41
1:ZA:674:PHE:CZ	1:HB:248:ALA:HB3	2.55	0.41
1:GB:665:PRO:HB3	1:GB:674:PHE:CZ	2.55	0.41
1:D:387:VAL:HA	1:WA:714:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:674:PHE:CZ	1:WA:248:ALA:HB3	2.56	0.41
1:E:633:ASP:H	1:AA:615:GLN:HE21	1.67	0.41
1:E:674:PHE:CZ	1:GA:248:ALA:HB3	2.55	0.41
1:G:219:ASP:O	1:G:220:GLY:C	2.62	0.41
1:L:248:ALA:HB3	1:TA:674:PHE:CZ	2.55	0.41
1:N:248:ALA:HB3	1:P:674:PHE:CZ	2.55	0.41
1:Q:714:LYS:HA	1:IB:387:VAL:HA	2.02	0.41
1:S:387:VAL:HA	1:GB:714:LYS:HA	2.02	0.41
1:S:674:PHE:CZ	1:GB:248:ALA:HB3	2.56	0.41
1:T:674:PHE:CZ	1:LA:248:ALA:HB3	2.55	0.41
1:V:219:ASP:O	1:V:220:GLY:C	2.62	0.41
1:V:725:ASN:HB2	1:V:727:VAL:HG23	2.02	0.41
1:Z:219:ASP:O	1:Z:220:GLY:C	2.62	0.41
1:DA:725:ASN:HB2	1:DA:727:VAL:HG23	2.03	0.41
1:EA:387:VAL:HA	1:QA:714:LYS:HA	2.02	0.41
1:FA:257:TYR:O	1:NA:726:GLY:HA3	2.16	0.41
1:FA:387:VAL:HA	1:NA:714:LYS:HA	2.02	0.41
1:FA:701:ARG:HD3	1:FA:705:GLU:CG	2.49	0.41
1:HA:219:ASP:O	1:HA:220:GLY:C	2.62	0.41
1:MA:219:ASP:O	1:MA:220:GLY:C	2.62	0.41
1:VA:219:ASP:O	1:VA:220:GLY:C	2.62	0.41
1:DB:665:PRO:HB3	1:DB:674:PHE:CZ	2.55	0.41
1:FB:219:ASP:O	1:FB:220:GLY:C	2.62	0.41
1:IB:219:ASP:O	1:IB:220:GLY:C	2.62	0.41
1:IB:725:ASN:HB2	1:IB:727:VAL:HG23	2.02	0.41
1:A:219:ASP:O	1:A:220:GLY:C	2.62	0.41
1:E:701:ARG:HH21	1:E:703:ASN:HD21	1.66	0.41
1:J:674:PHE:CZ	1:W:248:ALA:HB3	2.55	0.41
1:K:696:LYS:HD3	1:K:696:LYS:HA	1.73	0.41
1:L:219:ASP:O	1:L:220:GLY:C	2.62	0.41
1:N:674:PHE:CZ	1:RA:248:ALA:HB3	2.56	0.41
1:R:674:PHE:CZ	1:DB:248:ALA:HB3	2.56	0.41
1:T:633:ASP:H	1:V:615:GLN:HE21	1.67	0.41
1:V:674:PHE:CZ	1:DA:248:ALA:HB3	2.55	0.41
1:Y:248:ALA:HB3	1:AA:674:PHE:CZ	2.55	0.41
1:Y:725:ASN:HB2	1:Y:727:VAL:HG23	2.03	0.41
1:Z:387:VAL:HA	1:AB:714:LYS:HA	2.02	0.41
1:AA:725:ASN:HB2	1:AA:727:VAL:HG23	2.02	0.41
1:BA:387:VAL:HA	1:ZA:714:LYS:HA	2.01	0.41
1:CA:248:ALA:HB3	1:SA:674:PHE:CZ	2.56	0.41
1:EA:219:ASP:O	1:EA:220:GLY:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:714:LYS:HA	1:KA:387:VAL:HA	2.02	0.41
1:XA:701:ARG:HD3	1:XA:705:GLU:CG	2.50	0.41
1:YA:725:ASN:HB2	1:YA:727:VAL:HG23	2.02	0.41
1:AB:665:PRO:HB3	1:AB:674:PHE:CZ	2.55	0.41
1:CB:219:ASP:O	1:CB:220:GLY:C	2.62	0.41
1:C:674:PHE:CZ	1:TA:248:ALA:HB3	2.56	0.41
1:E:248:ALA:HB3	1:X:674:PHE:CZ	2.56	0.41
1:H:674:PHE:CZ	1:IB:248:ALA:HB3	2.56	0.41
1:P:219:ASP:O	1:P:220:GLY:C	2.62	0.41
1:P:248:ALA:HB3	1:AB:674:PHE:CZ	2.56	0.41
1:T:219:ASP:O	1:T:220:GLY:C	2.62	0.41
1:T:248:ALA:HB3	1:CA:674:PHE:CZ	2.56	0.41
1:W:387:VAL:HA	1:PA:714:LYS:HA	2.01	0.41
1:X:248:ALA:HB3	1:CB:674:PHE:CZ	2.56	0.41
1:X:701:ARG:HD3	1:X:705:GLU:CG	2.49	0.41
1:Z:248:ALA:HB3	1:RA:674:PHE:CZ	2.56	0.41
1:CA:714:LYS:HA	1:SA:387:VAL:HA	2.02	0.41
1:EA:248:ALA:HB3	1:BB:674:PHE:CZ	2.56	0.41
1:EA:714:LYS:HA	1:BB:387:VAL:HA	2.01	0.41
1:GA:725:ASN:HB2	1:GA:727:VAL:HG23	2.02	0.41
1:IA:248:ALA:HB3	1:KA:674:PHE:CZ	2.55	0.41
1:IA:701:ARG:HH21	1:IA:703:ASN:HD21	1.66	0.41
1:JA:219:ASP:O	1:JA:220:GLY:C	2.62	0.41
1:JA:701:ARG:HD3	1:JA:705:GLU:CG	2.49	0.41
1:LA:725:ASN:HB2	1:LA:727:VAL:HG23	2.02	0.41
1:NA:701:ARG:HH21	1:NA:703:ASN:HD21	1.66	0.41
1:OA:701:ARG:HD3	1:OA:705:GLU:CG	2.50	0.41
1:QA:665:PRO:HB3	1:QA:674:PHE:CZ	2.55	0.41
1:QA:701:ARG:HD3	1:QA:705:GLU:CG	2.50	0.41
1:RA:344:THR:HG22	1:RA:654:ILE:HG12	2.02	0.41
1:SA:219:ASP:O	1:SA:220:GLY:C	2.62	0.41
1:SA:248:ALA:HB3	1:UA:674:PHE:CZ	2.55	0.41
1:BB:344:THR:HG22	1:BB:654:ILE:HG12	2.02	0.41
1:A:248:ALA:HB3	1:QA:674:PHE:CZ	2.56	0.41
1:E:219:ASP:O	1:E:220:GLY:C	2.62	0.41
1:E:714:LYS:HA	1:X:387:VAL:HA	2.02	0.41
1:F:344:THR:HG22	1:F:654:ILE:HG12	2.02	0.41
1:F:725:ASN:HB2	1:F:727:VAL:HG23	2.02	0.41
1:H:725:ASN:HB2	1:H:727:VAL:HG23	2.03	0.41
1:I:219:ASP:O	1:I:220:GLY:C	2.62	0.41
1:J:696:LYS:HA	1:J:696:LYS:HD3	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:344:THR:HG22	1:K:654:ILE:HG12	2.02	0.41
1:K:725:ASN:HB2	1:K:727:VAL:HG23	2.02	0.41
1:M:674:PHE:CZ	1:YA:248:ALA:HB3	2.56	0.41
1:O:219:ASP:O	1:O:220:GLY:C	2.62	0.41
1:O:725:ASN:HB2	1:O:727:VAL:HG23	2.02	0.41
1:Z:633:ASP:H	1:UA:615:GLN:HE21	1.67	0.41
1:FA:674:PHE:CZ	1:NA:248:ALA:HB3	2.56	0.41
1:HA:317:ASN:ND2	1:XA:402:MET:SD	2.94	0.41
1:JA:725:ASN:HB2	1:JA:727:VAL:HG23	2.02	0.41
1:OA:725:ASN:HB2	1:OA:727:VAL:HG23	2.02	0.41
1:WA:725:ASN:HB2	1:WA:727:VAL:HG23	2.02	0.41
1:XA:344:THR:HG22	1:XA:654:ILE:HG12	2.02	0.41
1:AB:701:ARG:HD3	1:AB:705:GLU:CG	2.49	0.41
1:CB:248:ALA:HB3	1:EB:674:PHE:CZ	2.55	0.41
1:HB:701:ARG:HD3	1:HB:705:GLU:CG	2.49	0.41
1:HB:725:ASN:HB2	1:HB:727:VAL:HG23	2.02	0.41
1:C:344:THR:HG22	1:C:654:ILE:HG12	2.02	0.41
1:D:402:MET:SD	1:WA:317:ASN:ND2	2.94	0.41
1:D:714:LYS:HA	1:F:387:VAL:HA	2.02	0.41
1:E:725:ASN:HB2	1:E:727:VAL:HG23	2.02	0.41
1:F:696:LYS:HD3	1:F:696:LYS:HA	1.73	0.41
1:G:633:ASP:H	1:BA:615:GLN:HE21	1.67	0.41
1:G:674:PHE:CZ	1:FA:248:ALA:HB3	2.56	0.41
1:J:219:ASP:O	1:J:220:GLY:C	2.62	0.41
1:J:402:MET:SD	1:W:317:ASN:ND2	2.94	0.41
1:K:387:VAL:HA	1:S:714:LYS:HA	2.02	0.41
1:L:317:ASN:ND2	1:TA:402:MET:SD	2.94	0.41
1:M:725:ASN:HB2	1:M:727:VAL:HG23	2.03	0.41
1:O:402:MET:SD	1:BA:317:ASN:ND2	2.94	0.41
1:R:344:THR:HG22	1:R:654:ILE:HG12	2.02	0.41
1:S:402:MET:SD	1:GB:317:ASN:ND2	2.94	0.41
1:T:714:LYS:HA	1:CA:387:VAL:HA	2.02	0.41
1:Z:714:LYS:HA	1:RA:387:VAL:HA	2.01	0.41
1:EA:633:ASP:H	1:EB:615:GLN:HE21	1.67	0.41
1:IA:344:THR:HG22	1:IA:654:ILE:HG12	2.02	0.41
1:JA:387:VAL:HA	1:VA:714:LYS:HA	2.02	0.41
1:JA:674:PHE:CZ	1:VA:248:ALA:HB3	2.55	0.41
1:MA:317:ASN:ND2	1:HB:402:MET:SD	2.94	0.41
1:PA:344:THR:HG22	1:PA:654:ILE:HG12	2.02	0.41
1:SA:317:ASN:ND2	1:UA:402:MET:SD	2.94	0.41
1:SA:701:ARG:HD3	1:SA:705:GLU:CG	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TA:219:ASP:O	1:TA:220:GLY:C	2.62	0.41
1:XA:725:ASN:HB2	1:XA:727:VAL:HG23	2.02	0.41
1:YA:344:THR:HG22	1:YA:654:ILE:HG12	2.02	0.41
1:GB:725:ASN:HB2	1:GB:727:VAL:HG23	2.02	0.41
1:IB:344:THR:HG22	1:IB:654:ILE:HG12	2.02	0.41
1:C:665:PRO:HB3	1:C:674:PHE:CZ	2.55	0.41
1:G:317:ASN:ND2	1:DB:402:MET:SD	2.94	0.41
1:H:219:ASP:O	1:H:220:GLY:C	2.62	0.41
1:J:248:ALA:HB3	1:HA:674:PHE:CZ	2.56	0.41
1:J:387:VAL:HA	1:W:714:LYS:HA	2.02	0.41
1:J:725:ASN:HB2	1:J:727:VAL:HG23	2.03	0.41
1:L:674:PHE:CZ	1:KA:248:ALA:HB3	2.56	0.41
1:N:219:ASP:O	1:N:220:GLY:C	2.62	0.41
1:N:725:ASN:HB2	1:N:727:VAL:HG23	2.03	0.41
1:T:725:ASN:HB2	1:T:727:VAL:HG23	2.03	0.41
1:W:674:PHE:CZ	1:PA:248:ALA:HB3	2.56	0.41
1:W:701:ARG:HD3	1:W:705:GLU:CG	2.50	0.41
1:X:714:LYS:HA	1:CB:387:VAL:HA	2.02	0.41
1:Y:518:ASN:HA	1:Y:519:PRO:HA	1.96	0.41
1:Z:674:PHE:CZ	1:AB:248:ALA:HB3	2.55	0.41
1:AA:701:ARG:HD3	1:AA:705:GLU:CG	2.49	0.41
1:BA:674:PHE:CZ	1:ZA:248:ALA:HB3	2.56	0.41
1:CA:701:ARG:HD3	1:CA:705:GLU:CG	2.49	0.41
1:DA:443:TYR:OH	1:KA:548:GLU:O	2.32	0.41
1:GA:402:MET:SD	1:EB:317:ASN:ND2	2.94	0.41
1:GA:665:PRO:HB3	1:GA:674:PHE:CZ	2.55	0.41
1:NA:344:THR:HG22	1:NA:654:ILE:HG12	2.02	0.41
1:OA:387:VAL:HA	1:FB:714:LYS:HA	2.02	0.41
1:OA:674:PHE:CZ	1:FB:248:ALA:HB3	2.55	0.41
1:QA:219:ASP:O	1:QA:220:GLY:C	2.62	0.41
1:TA:701:ARG:HD3	1:TA:705:GLU:CG	2.49	0.41
1:UA:219:ASP:O	1:UA:220:GLY:C	2.62	0.41
1:CB:317:ASN:ND2	1:EB:402:MET:SD	2.94	0.41
1:CB:701:ARG:HD3	1:CB:705:GLU:CG	2.49	0.41
1:DB:219:ASP:O	1:DB:220:GLY:C	2.62	0.41
1:FB:344:THR:HG22	1:FB:654:ILE:HG12	2.02	0.41
1:HB:344:THR:HG22	1:HB:654:ILE:HG12	2.02	0.41
1:A:389:ARG:HG2	1:N:740:THR:CG2	2.51	0.41
1:B:248:ALA:HB3	1:YA:674:PHE:CZ	2.55	0.41
1:B:387:VAL:HA	1:V:714:LYS:HA	2.01	0.41
1:B:389:ARG:HG2	1:LA:740:THR:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:ARG:HG2	1:GB:740:THR:CG2	2.51	0.41
1:D:665:PRO:HB3	1:D:674:PHE:CZ	2.55	0.41
1:D:726:GLY:HA3	1:F:257:TYR:O	2.16	0.41
1:D:740:THR:CG2	1:K:389:ARG:HG2	2.51	0.41
1:G:402:MET:SD	1:FA:317:ASN:ND2	2.94	0.41
1:G:725:ASN:HB2	1:G:727:VAL:HG23	2.02	0.41
1:H:248:ALA:HB3	1:Y:674:PHE:CZ	2.56	0.41
1:H:317:ASN:ND2	1:Y:402:MET:SD	2.94	0.41
1:I:725:ASN:HB2	1:I:727:VAL:HG23	2.03	0.41
1:J:740:THR:CG2	1:DA:389:ARG:HG2	2.51	0.41
1:K:674:PHE:CZ	1:S:248:ALA:HB3	2.55	0.41
1:L:725:ASN:HB2	1:L:727:VAL:HG23	2.02	0.41
1:M:248:ALA:HB3	1:DA:674:PHE:CZ	2.56	0.41
1:M:665:PRO:HB3	1:M:674:PHE:CZ	2.55	0.41
1:N:714:LYS:HA	1:P:387:VAL:HA	2.02	0.41
1:O:248:ALA:HB3	1:MA:674:PHE:CZ	2.56	0.41
1:O:387:VAL:HA	1:BA:714:LYS:HA	2.02	0.41
1:O:696:LYS:HA	1:O:696:LYS:HD3	1.73	0.41
1:O:740:THR:CG2	1:Y:389:ARG:HG2	2.51	0.41
1:Q:248:ALA:HB3	1:IB:674:PHE:CZ	2.55	0.41
1:Q:387:VAL:HA	1:AA:714:LYS:HA	2.01	0.41
1:R:389:ARG:HG2	1:WA:740:THR:CG2	2.51	0.41
1:V:701:ARG:HD3	1:V:705:GLU:CG	2.49	0.41
1:W:344:THR:HG22	1:W:654:ILE:HG12	2.02	0.41
1:Z:317:ASN:ND2	1:RA:402:MET:SD	2.94	0.41
1:Z:389:ARG:HG2	1:UA:740:THR:CG2	2.51	0.41
1:Z:402:MET:SD	1:AB:317:ASN:ND2	2.94	0.41
1:Z:740:THR:CG2	1:HB:389:ARG:HG2	2.51	0.41
1:BA:344:THR:HG22	1:BA:654:ILE:HG12	2.02	0.41
1:BA:701:ARG:HD3	1:BA:705:GLU:CG	2.50	0.41
1:EA:317:ASN:ND2	1:BB:402:MET:SD	2.94	0.41
1:EA:402:MET:SD	1:QA:317:ASN:ND2	2.94	0.41
1:EA:674:PHE:CZ	1:QA:248:ALA:HB3	2.55	0.41
1:EA:740:THR:CG2	1:XA:389:ARG:HG2	2.51	0.41
1:IA:219:ASP:O	1:IA:220:GLY:C	2.62	0.41
1:IA:726:GLY:HA3	1:KA:257:TYR:O	2.17	0.41
1:JA:402:MET:SD	1:VA:317:ASN:ND2	2.94	0.41
1:LA:402:MET:SD	1:UA:317:ASN:ND2	2.94	0.41
1:LA:665:PRO:HB3	1:LA:674:PHE:CZ	2.55	0.41
1:MA:248:ALA:HB3	1:HB:674:PHE:CZ	2.56	0.41
1:OA:402:MET:SD	1:FB:317:ASN:ND2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PA:219:ASP:O	1:PA:220:GLY:C	2.62	0.41
1:PA:665:PRO:HB3	1:PA:674:PHE:CZ	2.55	0.41
1:VA:344:THR:HG22	1:VA:654:ILE:HG12	2.02	0.41
1:VA:725:ASN:HB2	1:VA:727:VAL:HG23	2.02	0.41
1:WA:344:THR:HG22	1:WA:654:ILE:HG12	2.02	0.41
1:ZA:344:THR:HG22	1:ZA:654:ILE:HG12	2.02	0.41
1:AB:219:ASP:O	1:AB:220:GLY:C	2.62	0.41
1:BB:725:ASN:HB2	1:BB:727:VAL:HG23	2.02	0.41
1:DB:701:ARG:HD3	1:DB:705:GLU:CG	2.49	0.41
1:FB:725:ASN:HB2	1:FB:727:VAL:HG23	2.02	0.41
1:GB:344:THR:HG22	1:GB:654:ILE:HG12	2.02	0.41
1:IB:696:LYS:HD3	1:IB:696:LYS:HA	1.73	0.41
1:C:725:ASN:HB2	1:C:727:VAL:HG23	2.02	0.41
1:D:248:ALA:HB3	1:F:674:PHE:CZ	2.55	0.41
1:E:402:MET:SD	1:GA:317:ASN:ND2	2.94	0.41
1:H:665:PRO:HB3	1:H:674:PHE:CZ	2.55	0.41
1:I:740:THR:CG2	1:P:389:ARG:HG2	2.51	0.41
1:K:701:ARG:HD3	1:K:705:GLU:CG	2.49	0.41
1:L:402:MET:SD	1:KA:317:ASN:ND2	2.94	0.41
1:L:633:ASP:H	1:W:615:GLN:HE21	1.68	0.41
1:M:219:ASP:O	1:M:220:GLY:C	2.62	0.41
1:M:317:ASN:ND2	1:DA:402:MET:SD	2.94	0.41
1:M:714:LYS:HA	1:DA:387:VAL:HA	2.02	0.41
1:Q:317:ASN:ND2	1:IB:402:MET:SD	2.94	0.41
1:Q:389:ARG:HG2	1:GA:740:THR:CG2	2.51	0.41
1:Q:665:PRO:HB3	1:Q:674:PHE:CZ	2.55	0.41
1:R:665:PRO:HB3	1:R:674:PHE:CZ	2.55	0.41
1:BA:389:ARG:HG2	1:VA:740:THR:CG2	2.51	0.41
1:DA:518:ASN:HA	1:DA:519:PRO:HA	1.96	0.41
1:EA:389:ARG:HG2	1:EB:740:THR:CG2	2.51	0.41
1:HA:248:ALA:HB3	1:XA:674:PHE:CZ	2.56	0.41
1:A:387:VAL:HA	1:I:714:LYS:HA	2.02	0.40
1:A:402:MET:SD	1:I:317:ASN:ND2	2.94	0.40
1:C:740:THR:CG2	1:CA:389:ARG:HG2	2.51	0.40
1:F:317:ASN:ND2	1:FB:402:MET:SD	2.94	0.40
1:F:389:ARG:HG2	1:S:740:THR:CG2	2.51	0.40
1:F:701:ARG:HD3	1:F:705:GLU:CG	2.49	0.40
1:H:714:LYS:HA	1:Y:387:VAL:HA	2.02	0.40
1:I:402:MET:SD	1:BB:317:ASN:ND2	2.94	0.40
1:K:317:ASN:ND2	1:VA:402:MET:SD	2.94	0.40
1:M:740:THR:CG2	1:HA:389:ARG:HG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:665:PRO:HB3	1:O:674:PHE:CZ	2.55	0.40
1:R:317:ASN:ND2	1:NA:402:MET:SD	2.94	0.40
1:R:725:ASN:HB2	1:R:727:VAL:HG23	2.03	0.40
1:R:740:THR:CG2	1:X:389:ARG:HG2	2.51	0.40
1:S:665:PRO:HB3	1:S:674:PHE:CZ	2.55	0.40
1:Z:725:ASN:HB2	1:Z:727:VAL:HG23	2.02	0.40
1:AA:389:ARG:HG2	1:NA:740:THR:CG2	2.51	0.40
1:DA:487:ARG:HB2	1:DA:573:THR:HB	2.03	0.40
1:EA:725:ASN:HB2	1:EA:727:VAL:HG23	2.02	0.40
1:GA:674:PHE:CZ	1:EB:248:ALA:HB3	2.56	0.40
1:HA:725:ASN:HB2	1:HA:727:VAL:HG23	2.02	0.40
1:JA:248:ALA:HB3	1:GB:674:PHE:CZ	2.56	0.40
1:LA:674:PHE:CZ	1:UA:248:ALA:HB3	2.56	0.40
1:PA:389:ARG:HG2	1:CB:740:THR:CG2	2.51	0.40
1:SA:487:ARG:HB2	1:SA:573:THR:HB	2.04	0.40
1:UA:389:ARG:HG2	1:HB:740:THR:HG21	2.04	0.40
1:WA:701:ARG:HD3	1:WA:705:GLU:CG	2.49	0.40
1:YA:696:LYS:HD3	1:YA:696:LYS:HA	1.73	0.40
1:ZA:665:PRO:HB3	1:ZA:674:PHE:CZ	2.55	0.40
1:CB:487:ARG:HB2	1:CB:573:THR:HB	2.04	0.40
1:IB:665:PRO:HB3	1:IB:674:PHE:CZ	2.55	0.40
1:B:317:ASN:ND2	1:YA:402:MET:SD	2.94	0.40
1:B:665:PRO:HB3	1:B:674:PHE:CZ	2.55	0.40
1:D:633:ASP:H	1:DB:615:GLN:HE21	1.67	0.40
1:E:740:THR:CG2	1:NA:389:ARG:HG2	2.51	0.40
1:H:740:THR:CG2	1:MA:389:ARG:HG2	2.51	0.40
1:K:257:TYR:O	1:S:726:GLY:HA3	2.17	0.40
1:N:317:ASN:ND2	1:P:402:MET:SD	2.94	0.40
1:S:389:ARG:HG2	1:TA:740:THR:HG21	2.04	0.40
1:T:402:MET:SD	1:LA:317:ASN:ND2	2.94	0.40
1:AA:389:ARG:HG2	1:NA:740:THR:HG21	2.04	0.40
1:BA:725:ASN:HB2	1:BA:727:VAL:HG23	2.02	0.40
1:DA:665:PRO:HB3	1:DA:674:PHE:CZ	2.55	0.40
1:HA:477:TRP:CE2	1:BB:630:PRO:HD3	2.57	0.40
1:MA:740:THR:HG21	1:RA:389:ARG:HG2	2.04	0.40
1:RA:725:ASN:HB2	1:RA:727:VAL:HG23	2.02	0.40
1:SA:740:THR:CG2	1:ZA:389:ARG:HG2	2.51	0.40
1:EB:344:THR:HG22	1:EB:654:ILE:HG12	2.02	0.40
1:A:498:SER:O	1:N:448:THR:OG1	2.35	0.40
1:B:402:MET:SD	1:V:317:ASN:ND2	2.94	0.40
1:C:317:ASN:ND2	1:IA:402:MET:SD	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:ARG:HG2	1:DB:740:THR:HG21	2.04	0.40
1:D:477:TRP:CE2	1:K:630:PRO:HD3	2.57	0.40
1:D:630:PRO:HD3	1:DB:477:TRP:CE2	2.57	0.40
1:F:630:PRO:HD3	1:S:477:TRP:CE2	2.57	0.40
1:G:630:PRO:HD3	1:BA:477:TRP:CE2	2.57	0.40
1:H:402:MET:SD	1:IB:317:ASN:ND2	2.94	0.40
1:J:665:PRO:HB3	1:J:674:PHE:CZ	2.55	0.40
1:J:740:THR:HG21	1:DA:389:ARG:HG2	2.04	0.40
1:L:630:PRO:HD3	1:W:477:TRP:CE2	2.57	0.40
1:M:477:TRP:CE2	1:HA:630:PRO:HD3	2.57	0.40
1:N:402:MET:SD	1:RA:317:ASN:ND2	2.94	0.40
1:O:389:ARG:HG2	1:FA:740:THR:HG21	2.04	0.40
1:R:487:ARG:HB2	1:R:573:THR:HB	2.03	0.40
1:R:701:ARG:HD3	1:R:705:GLU:CG	2.49	0.40
1:T:740:THR:CG2	1:IA:389:ARG:HG2	2.51	0.40
1:V:389:ARG:HG2	1:IA:740:THR:HG21	2.04	0.40
1:V:389:ARG:HG2	1:IA:740:THR:CG2	2.51	0.40
1:W:389:ARG:HG2	1:FB:740:THR:CG2	2.51	0.40
1:W:725:ASN:HB2	1:W:727:VAL:HG23	2.03	0.40
1:Y:317:ASN:ND2	1:AA:402:MET:SD	2.94	0.40
1:Y:487:ARG:HB2	1:Y:573:THR:HB	2.04	0.40
1:FA:402:MET:SD	1:NA:317:ASN:ND2	2.94	0.40
1:MA:477:TRP:CE2	1:RA:630:PRO:HD3	2.57	0.40
1:XA:740:THR:HG21	1:EB:389:ARG:HG2	2.04	0.40
1:YA:665:PRO:HB3	1:YA:674:PHE:CZ	2.55	0.40
1:ZA:219:ASP:O	1:ZA:220:GLY:C	2.62	0.40
1:GB:701:ARG:HD3	1:GB:705:GLU:CG	2.49	0.40
1:B:674:PHE:CZ	1:V:248:ALA:HB3	2.56	0.40
1:C:248:ALA:HB3	1:IA:674:PHE:CZ	2.56	0.40
1:C:402:MET:SD	1:TA:317:ASN:ND2	2.94	0.40
1:C:487:ARG:HB2	1:C:573:THR:HB	2.04	0.40
1:C:701:ARG:HD3	1:C:705:GLU:CG	2.49	0.40
1:D:487:ARG:HB2	1:D:573:THR:HB	2.03	0.40
1:E:630:PRO:HD3	1:AA:477:TRP:CE2	2.57	0.40
1:F:477:TRP:CE2	1:TA:630:PRO:HD3	2.57	0.40
1:H:477:TRP:CE2	1:MA:630:PRO:HD3	2.57	0.40
1:K:248:ALA:HB3	1:VA:674:PHE:CZ	2.56	0.40
1:K:477:TRP:CE2	1:DB:630:PRO:HD3	2.57	0.40
1:K:665:PRO:HB3	1:K:674:PHE:CZ	2.55	0.40
1:O:317:ASN:ND2	1:MA:402:MET:SD	2.94	0.40
1:O:389:ARG:HG2	1:FA:740:THR:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:448:THR:OG1	1:Y:498:SER:O	2.35	0.40
1:O:740:THR:HG21	1:Y:389:ARG:HG2	2.04	0.40
1:P:740:THR:CG2	1:YA:389:ARG:HG2	2.51	0.40
1:Q:402:MET:SD	1:AA:317:ASN:ND2	2.94	0.40
1:Q:725:ASN:HB2	1:Q:727:VAL:HG23	2.02	0.40
1:R:248:ALA:HB3	1:NA:674:PHE:CZ	2.56	0.40
1:T:389:ARG:HG2	1:V:740:THR:CG2	2.51	0.40
1:Y:665:PRO:HB3	1:Y:674:PHE:CZ	2.55	0.40
1:CA:725:ASN:HB2	1:CA:727:VAL:HG23	2.02	0.40
1:HA:740:THR:HG21	1:BB:389:ARG:HG2	2.04	0.40
1:IA:317:ASN:ND2	1:KA:402:MET:SD	2.94	0.40
1:IA:725:ASN:HB2	1:IA:727:VAL:HG23	2.02	0.40
1:JA:344:THR:HG22	1:JA:654:ILE:HG12	2.02	0.40
1:LA:389:ARG:HG2	1:AB:740:THR:HG21	2.04	0.40
1:MA:725:ASN:HB2	1:MA:727:VAL:HG23	2.03	0.40
1:NA:725:ASN:HB2	1:NA:727:VAL:HG23	2.03	0.40
1:OA:248:ALA:HB3	1:WA:674:PHE:CZ	2.56	0.40
1:SA:740:THR:HG21	1:ZA:389:ARG:HG2	2.04	0.40
1:UA:344:THR:HG22	1:UA:654:ILE:HG12	2.02	0.40
1:A:615:GLN:HE21	1:IB:633:ASP:H	1.67	0.40
1:A:740:THR:CG2	1:IB:389:ARG:HG2	2.52	0.40
1:B:725:ASN:HB2	1:B:727:VAL:HG23	2.03	0.40
1:C:389:ARG:HG2	1:GB:740:THR:HG21	2.04	0.40
1:C:518:ASN:HA	1:C:519:PRO:HA	1.97	0.40
1:D:317:ASN:ND2	1:F:402:MET:SD	2.94	0.40
1:E:389:ARG:HG2	1:AA:740:THR:CG2	2.51	0.40
1:F:248:ALA:HB3	1:FB:674:PHE:CZ	2.56	0.40
1:I:630:PRO:HD3	1:YA:477:TRP:CE2	2.57	0.40
1:J:317:ASN:ND2	1:HA:402:MET:SD	2.94	0.40
1:J:389:ARG:HG2	1:KA:740:THR:HG21	2.04	0.40
1:J:701:ARG:HD3	1:J:705:GLU:CG	2.49	0.40
1:K:397:TYR:C	1:S:230:CYS:O	2.65	0.40
1:K:448:THR:OG1	1:DB:498:SER:O	2.35	0.40
1:M:389:ARG:HG2	1:BB:740:THR:HG21	2.04	0.40
1:M:402:MET:SD	1:YA:317:ASN:ND2	2.94	0.40
1:N:389:ARG:HG2	1:IB:740:THR:HG21	2.04	0.40
1:N:397:TYR:C	1:RA:230:CYS:O	2.65	0.40
1:N:630:PRO:HD3	1:IB:477:TRP:CE2	2.57	0.40
1:Q:740:THR:HG21	1:QA:389:ARG:HG2	2.04	0.40
1:R:402:MET:SD	1:DB:317:ASN:ND2	2.94	0.40
1:S:487:ARG:HB2	1:S:573:THR:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:630:PRO:HD3	1:TA:477:TRP:CE2	2.57	0.40
1:T:630:PRO:HD3	1:V:477:TRP:CE2	2.57	0.40
1:V:402:MET:SD	1:DA:317:ASN:ND2	2.94	0.40
1:W:402:MET:SD	1:PA:317:ASN:ND2	2.94	0.40
1:W:518:ASN:HA	1:W:519:PRO:HA	1.96	0.40
1:X:665:PRO:HB3	1:X:674:PHE:CZ	2.55	0.40
1:X:725:ASN:HB2	1:X:727:VAL:HG23	2.02	0.40
1:X:740:THR:CG2	1:WA:389:ARG:HG2	2.51	0.40
1:Y:477:TRP:CE2	1:FA:630:PRO:HD3	2.57	0.40
1:AA:487:ARG:HB2	1:AA:573:THR:HB	2.04	0.40
1:CA:317:ASN:ND2	1:SA:402:MET:SD	2.94	0.40
1:CA:665:PRO:HB3	1:CA:674:PHE:CZ	2.55	0.40
1:DA:477:TRP:CE2	1:KA:630:PRO:HD3	2.57	0.40
1:EA:397:TYR:C	1:QA:230:CYS:O	2.65	0.40
1:MA:487:ARG:HB2	1:MA:573:THR:HB	2.03	0.40
1:OA:344:THR:HG22	1:OA:654:ILE:HG12	2.02	0.40
1:OA:389:ARG:HG2	1:PA:740:THR:CG2	2.51	0.40
1:PA:389:ARG:HG2	1:CB:740:THR:HG21	2.04	0.40
1:PA:487:ARG:HB2	1:PA:573:THR:HB	2.04	0.40
1:PA:630:PRO:HD3	1:CB:477:TRP:CE2	2.57	0.40
1:YA:487:ARG:HB2	1:YA:573:THR:HB	2.04	0.40
1:ZA:725:ASN:HB2	1:ZA:727:VAL:HG23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	A	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	AA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	AB	516/743 (69%)	507 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	BA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	BB	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	C	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	CA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	CB	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	D	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	DA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	DB	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	E	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	EA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	EB	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	F	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	FA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	FB	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	G	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	GA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	GB	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	H	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	HA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	HB	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	I	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	IA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	IB	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	J	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	JA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	K	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	KA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	L	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	LA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	M	516/743 (69%)	507 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	MA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	N	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	NA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	O	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	OA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	P	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	PA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	Q	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	QA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	R	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	RA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	S	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	SA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	T	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	TA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	UA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	V	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	VA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	W	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	WA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	X	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	XA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	Y	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	YA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	Z	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
1	ZA	516/743 (69%)	507 (98%)	9 (2%)	0	100	100
All	All	30960/44580 (69%)	30420 (98%)	540 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	A	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	AA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	AB	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	B	461/637 (72%)	458 (99%)	3 (1%)	76	88
1	BA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	BB	461/637 (72%)	458 (99%)	3 (1%)	76	88
1	C	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	CA	461/637 (72%)	460 (100%)	1 (0%)	87	95
1	CB	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	D	461/637 (72%)	460 (100%)	1 (0%)	87	95
1	DA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	DB	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	E	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	EA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	EB	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	F	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	FA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	FB	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	G	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	GA	461/637 (72%)	460 (100%)	1 (0%)	87	95
1	GB	461/637 (72%)	458 (99%)	3 (1%)	76	88
1	H	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	HA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	HB	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	I	461/637 (72%)	458 (99%)	3 (1%)	76	88
1	IA	461/637 (72%)	460 (100%)	1 (0%)	87	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	IB	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	J	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	JA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	K	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	KA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	L	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	LA	461/637 (72%)	460 (100%)	1 (0%)	87	95
1	M	461/637 (72%)	460 (100%)	1 (0%)	87	95
1	MA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	N	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	NA	461/637 (72%)	460 (100%)	1 (0%)	87	95
1	O	461/637 (72%)	460 (100%)	1 (0%)	87	95
1	OA	461/637 (72%)	458 (99%)	3 (1%)	76	88
1	P	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	PA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	Q	461/637 (72%)	460 (100%)	1 (0%)	87	95
1	QA	461/637 (72%)	460 (100%)	1 (0%)	87	95
1	R	461/637 (72%)	460 (100%)	1 (0%)	87	95
1	RA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	S	461/637 (72%)	458 (99%)	3 (1%)	76	88
1	SA	461/637 (72%)	460 (100%)	1 (0%)	87	95
1	T	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	TA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	UA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	V	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	VA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	W	461/637 (72%)	458 (99%)	3 (1%)	76	88
1	WA	461/637 (72%)	460 (100%)	1 (0%)	87	95
1	X	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	XA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	Y	461/637 (72%)	459 (100%)	2 (0%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	YA	461/637 (72%)	459 (100%)	2 (0%)	84	92
1	Z	461/637 (72%)	458 (99%)	3 (1%)	76	88
1	ZA	461/637 (72%)	459 (100%)	2 (0%)	84	92
All	All	27660/38220 (72%)	27545 (100%)	115 (0%)	81	92

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	GLU
1	A	741	ARG
1	B	298	ARG
1	B	322	GLU
1	B	741	ARG
1	C	322	GLU
1	C	741	ARG
1	D	322	GLU
1	E	322	GLU
1	E	741	ARG
1	F	322	GLU
1	F	741	ARG
1	G	298	ARG
1	G	741	ARG
1	H	322	GLU
1	H	741	ARG
1	I	298	ARG
1	I	322	GLU
1	I	741	ARG
1	J	298	ARG
1	J	322	GLU
1	K	322	GLU
1	K	741	ARG
1	L	322	GLU
1	L	741	ARG
1	M	322	GLU
1	N	322	GLU
1	N	741	ARG
1	O	322	GLU
1	P	322	GLU
1	P	741	ARG
1	Q	322	GLU
1	R	322	GLU

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Mol	Chain	Res	Type
1	S	298	ARG
1	S	322	GLU
1	S	741	ARG
1	T	298	ARG
1	T	322	GLU
1	V	322	GLU
1	V	741	ARG
1	W	298	ARG
1	W	322	GLU
1	W	741	ARG
1	X	322	GLU
1	X	741	ARG
1	Y	322	GLU
1	Y	741	ARG
1	Z	298	ARG
1	Z	322	GLU
1	Z	741	ARG
1	AA	322	GLU
1	AA	741	ARG
1	BA	322	GLU
1	BA	741	ARG
1	CA	741	ARG
1	DA	322	GLU
1	DA	741	ARG
1	EA	298	ARG
1	EA	322	GLU
1	FA	322	GLU
1	FA	741	ARG
1	GA	322	GLU
1	HA	322	GLU
1	HA	741	ARG
1	IA	322	GLU
1	JA	322	GLU
1	JA	741	ARG
1	KA	322	GLU
1	KA	741	ARG
1	LA	322	GLU
1	MA	298	ARG
1	MA	322	GLU
1	NA	322	GLU
1	OA	298	ARG
1	OA	322	GLU

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Mol	Chain	Res	Type
1	OA	741	ARG
1	PA	322	GLU
1	PA	741	ARG
1	QA	298	ARG
1	RA	322	GLU
1	RA	741	ARG
1	SA	322	GLU
1	TA	322	GLU
1	TA	741	ARG
1	UA	322	GLU
1	UA	741	ARG
1	VA	322	GLU
1	VA	741	ARG
1	WA	741	ARG
1	XA	322	GLU
1	XA	741	ARG
1	YA	322	GLU
1	YA	741	ARG
1	ZA	322	GLU
1	ZA	741	ARG
1	AB	322	GLU
1	AB	741	ARG
1	BB	298	ARG
1	BB	322	GLU
1	BB	741	ARG
1	CB	298	ARG
1	CB	741	ARG
1	DB	322	GLU
1	DB	741	ARG
1	EB	322	GLU
1	EB	741	ARG
1	FB	322	GLU
1	FB	741	ARG
1	GB	298	ARG
1	GB	322	GLU
1	GB	741	ARG
1	HB	322	GLU
1	HB	741	ARG
1	IB	322	GLU
1	IB	741	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (486) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	HIS
1	A	259	GLN
1	A	312	ASN
1	A	428	GLN
1	A	461	GLN
1	A	464	GLN
1	A	497	ASN
1	A	615	GLN
1	A	717	ASN
1	B	259	GLN
1	B	312	ASN
1	B	385	GLN
1	B	428	GLN
1	B	464	GLN
1	B	497	ASN
1	B	615	GLN
1	B	717	ASN
1	C	229	HIS
1	C	259	GLN
1	C	312	ASN
1	C	428	GLN
1	C	464	GLN
1	C	497	ASN
1	C	615	GLN
1	C	717	ASN
1	D	259	GLN
1	D	312	ASN
1	D	385	GLN
1	D	428	GLN
1	D	461	GLN
1	D	464	GLN
1	D	497	ASN
1	D	615	GLN
1	D	717	ASN
1	E	259	GLN
1	E	312	ASN
1	E	385	GLN
1	E	428	GLN
1	E	461	GLN
1	E	464	GLN
1	E	497	ASN
1	E	615	GLN
1	E	717	ASN

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Mol	Chain	Res	Type
1	F	229	HIS
1	F	259	GLN
1	F	312	ASN
1	F	428	GLN
1	F	461	GLN
1	F	464	GLN
1	F	497	ASN
1	F	615	GLN
1	F	717	ASN
1	G	312	ASN
1	G	428	GLN
1	G	461	GLN
1	G	464	GLN
1	G	497	ASN
1	G	615	GLN
1	H	259	GLN
1	H	312	ASN
1	H	385	GLN
1	H	428	GLN
1	H	461	GLN
1	H	464	GLN
1	H	497	ASN
1	H	615	GLN
1	I	312	ASN
1	I	428	GLN
1	I	461	GLN
1	I	464	GLN
1	I	497	ASN
1	I	615	GLN
1	I	717	ASN
1	J	229	HIS
1	J	259	GLN
1	J	312	ASN
1	J	428	GLN
1	J	461	GLN
1	J	464	GLN
1	J	497	ASN
1	J	615	GLN
1	K	229	HIS
1	K	259	GLN
1	K	312	ASN
1	K	428	GLN

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Mol	Chain	Res	Type
1	K	461	GLN
1	K	464	GLN
1	K	497	ASN
1	K	615	GLN
1	K	717	ASN
1	L	312	ASN
1	L	428	GLN
1	L	461	GLN
1	L	464	GLN
1	L	497	ASN
1	L	615	GLN
1	M	229	HIS
1	M	259	GLN
1	M	312	ASN
1	M	428	GLN
1	M	461	GLN
1	M	464	GLN
1	M	497	ASN
1	M	615	GLN
1	N	312	ASN
1	N	385	GLN
1	N	428	GLN
1	N	461	GLN
1	N	464	GLN
1	N	497	ASN
1	N	615	GLN
1	O	229	HIS
1	O	259	GLN
1	O	312	ASN
1	O	385	GLN
1	O	428	GLN
1	O	461	GLN
1	O	464	GLN
1	O	497	ASN
1	O	615	GLN
1	P	229	HIS
1	P	312	ASN
1	P	428	GLN
1	P	464	GLN
1	P	497	ASN
1	P	615	GLN
1	P	717	ASN

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Mol	Chain	Res	Type
1	Q	259	GLN
1	Q	312	ASN
1	Q	385	GLN
1	Q	428	GLN
1	Q	464	GLN
1	Q	497	ASN
1	Q	615	GLN
1	Q	717	ASN
1	R	229	HIS
1	R	259	GLN
1	R	312	ASN
1	R	428	GLN
1	R	464	GLN
1	R	497	ASN
1	R	615	GLN
1	R	717	ASN
1	S	259	GLN
1	S	312	ASN
1	S	385	GLN
1	S	428	GLN
1	S	461	GLN
1	S	464	GLN
1	S	497	ASN
1	S	615	GLN
1	S	717	ASN
1	T	259	GLN
1	T	312	ASN
1	T	385	GLN
1	T	428	GLN
1	T	461	GLN
1	T	464	GLN
1	T	497	ASN
1	T	615	GLN
1	T	717	ASN
1	V	229	HIS
1	V	259	GLN
1	V	312	ASN
1	V	385	GLN
1	V	428	GLN
1	V	461	GLN
1	V	464	GLN
1	V	497	ASN

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Mol	Chain	Res	Type
1	V	615	GLN
1	V	717	ASN
1	W	312	ASN
1	W	428	GLN
1	W	461	GLN
1	W	464	GLN
1	W	497	ASN
1	W	615	GLN
1	W	717	ASN
1	X	259	GLN
1	X	312	ASN
1	X	385	GLN
1	X	428	GLN
1	X	464	GLN
1	X	497	ASN
1	X	615	GLN
1	X	717	ASN
1	Y	312	ASN
1	Y	428	GLN
1	Y	461	GLN
1	Y	464	GLN
1	Y	497	ASN
1	Y	615	GLN
1	Y	717	ASN
1	Z	229	HIS
1	Z	259	GLN
1	Z	312	ASN
1	Z	385	GLN
1	Z	428	GLN
1	Z	461	GLN
1	Z	464	GLN
1	Z	497	ASN
1	Z	615	GLN
1	Z	717	ASN
1	AA	259	GLN
1	AA	312	ASN
1	AA	385	GLN
1	AA	428	GLN
1	AA	461	GLN
1	AA	464	GLN
1	AA	497	ASN
1	AA	615	GLN

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Mol	Chain	Res	Type
1	AA	717	ASN
1	BA	312	ASN
1	BA	428	GLN
1	BA	461	GLN
1	BA	464	GLN
1	BA	497	ASN
1	BA	615	GLN
1	BA	717	ASN
1	CA	259	GLN
1	CA	312	ASN
1	CA	385	GLN
1	CA	428	GLN
1	CA	461	GLN
1	CA	464	GLN
1	CA	497	ASN
1	CA	615	GLN
1	CA	717	ASN
1	DA	312	ASN
1	DA	428	GLN
1	DA	461	GLN
1	DA	464	GLN
1	DA	497	ASN
1	DA	615	GLN
1	DA	717	ASN
1	EA	229	HIS
1	EA	259	GLN
1	EA	312	ASN
1	EA	385	GLN
1	EA	428	GLN
1	EA	461	GLN
1	EA	464	GLN
1	EA	497	ASN
1	EA	615	GLN
1	EA	717	ASN
1	FA	229	HIS
1	FA	312	ASN
1	FA	385	GLN
1	FA	428	GLN
1	FA	461	GLN
1	FA	464	GLN
1	FA	497	ASN
1	FA	615	GLN

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Mol	Chain	Res	Type
1	GA	229	HIS
1	GA	259	GLN
1	GA	312	ASN
1	GA	428	GLN
1	GA	461	GLN
1	GA	464	GLN
1	GA	497	ASN
1	GA	615	GLN
1	GA	717	ASN
1	HA	229	HIS
1	HA	312	ASN
1	HA	428	GLN
1	HA	464	GLN
1	HA	497	ASN
1	HA	615	GLN
1	HA	717	ASN
1	IA	229	HIS
1	IA	259	GLN
1	IA	312	ASN
1	IA	385	GLN
1	IA	428	GLN
1	IA	464	GLN
1	IA	497	ASN
1	IA	615	GLN
1	JA	259	GLN
1	JA	312	ASN
1	JA	428	GLN
1	JA	461	GLN
1	JA	464	GLN
1	JA	497	ASN
1	JA	615	GLN
1	JA	717	ASN
1	KA	229	HIS
1	KA	312	ASN
1	KA	428	GLN
1	KA	461	GLN
1	KA	464	GLN
1	KA	497	ASN
1	KA	615	GLN
1	LA	259	GLN
1	LA	312	ASN
1	LA	428	GLN

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Mol	Chain	Res	Type
1	LA	461	GLN
1	LA	464	GLN
1	LA	497	ASN
1	LA	615	GLN
1	LA	717	ASN
1	MA	312	ASN
1	MA	428	GLN
1	MA	464	GLN
1	MA	497	ASN
1	MA	615	GLN
1	MA	717	ASN
1	MA	725	ASN
1	NA	259	GLN
1	NA	312	ASN
1	NA	385	GLN
1	NA	428	GLN
1	NA	464	GLN
1	NA	497	ASN
1	NA	615	GLN
1	OA	229	HIS
1	OA	259	GLN
1	OA	312	ASN
1	OA	428	GLN
1	OA	461	GLN
1	OA	464	GLN
1	OA	497	ASN
1	OA	615	GLN
1	OA	717	ASN
1	PA	312	ASN
1	PA	385	GLN
1	PA	428	GLN
1	PA	461	GLN
1	PA	464	GLN
1	PA	497	ASN
1	PA	615	GLN
1	QA	229	HIS
1	QA	259	GLN
1	QA	312	ASN
1	QA	428	GLN
1	QA	461	GLN
1	QA	464	GLN
1	QA	497	ASN

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Mol	Chain	Res	Type
1	QA	615	GLN
1	QA	717	ASN
1	RA	259	GLN
1	RA	312	ASN
1	RA	385	GLN
1	RA	428	GLN
1	RA	461	GLN
1	RA	464	GLN
1	RA	497	ASN
1	RA	615	GLN
1	SA	259	GLN
1	SA	312	ASN
1	SA	385	GLN
1	SA	428	GLN
1	SA	461	GLN
1	SA	464	GLN
1	SA	497	ASN
1	SA	615	GLN
1	SA	717	ASN
1	TA	312	ASN
1	TA	428	GLN
1	TA	464	GLN
1	TA	497	ASN
1	TA	615	GLN
1	TA	717	ASN
1	UA	229	HIS
1	UA	259	GLN
1	UA	312	ASN
1	UA	428	GLN
1	UA	464	GLN
1	UA	497	ASN
1	UA	615	GLN
1	UA	717	ASN
1	VA	259	GLN
1	VA	312	ASN
1	VA	428	GLN
1	VA	461	GLN
1	VA	464	GLN
1	VA	497	ASN
1	VA	615	GLN
1	VA	717	ASN
1	WA	259	GLN

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Mol	Chain	Res	Type
1	WA	312	ASN
1	WA	428	GLN
1	WA	461	GLN
1	WA	464	GLN
1	WA	497	ASN
1	WA	615	GLN
1	WA	717	ASN
1	XA	259	GLN
1	XA	312	ASN
1	XA	385	GLN
1	XA	428	GLN
1	XA	461	GLN
1	XA	464	GLN
1	XA	497	ASN
1	XA	615	GLN
1	YA	259	GLN
1	YA	312	ASN
1	YA	385	GLN
1	YA	428	GLN
1	YA	461	GLN
1	YA	464	GLN
1	YA	497	ASN
1	YA	615	GLN
1	YA	717	ASN
1	ZA	312	ASN
1	ZA	385	GLN
1	ZA	428	GLN
1	ZA	461	GLN
1	ZA	464	GLN
1	ZA	497	ASN
1	ZA	615	GLN
1	AB	229	HIS
1	AB	259	GLN
1	AB	312	ASN
1	AB	428	GLN
1	AB	461	GLN
1	AB	464	GLN
1	AB	497	ASN
1	AB	615	GLN
1	AB	717	ASN
1	BB	259	GLN
1	BB	312	ASN

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Mol	Chain	Res	Type
1	BB	385	GLN
1	BB	428	GLN
1	BB	461	GLN
1	BB	464	GLN
1	BB	497	ASN
1	BB	615	GLN
1	CB	229	HIS
1	CB	259	GLN
1	CB	312	ASN
1	CB	385	GLN
1	CB	428	GLN
1	CB	461	GLN
1	CB	464	GLN
1	CB	497	ASN
1	CB	615	GLN
1	CB	717	ASN
1	DB	312	ASN
1	DB	428	GLN
1	DB	461	GLN
1	DB	464	GLN
1	DB	497	ASN
1	DB	615	GLN
1	DB	717	ASN
1	EB	229	HIS
1	EB	259	GLN
1	EB	312	ASN
1	EB	428	GLN
1	EB	464	GLN
1	EB	497	ASN
1	EB	615	GLN
1	EB	717	ASN
1	FB	259	GLN
1	FB	312	ASN
1	FB	428	GLN
1	FB	461	GLN
1	FB	464	GLN
1	FB	497	ASN
1	FB	615	GLN
1	FB	717	ASN
1	GB	229	HIS
1	GB	259	GLN
1	GB	312	ASN

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Mol	Chain	Res	Type
1	GB	428	GLN
1	GB	461	GLN
1	GB	464	GLN
1	GB	497	ASN
1	GB	615	GLN
1	GB	717	ASN
1	HB	259	GLN
1	HB	312	ASN
1	HB	385	GLN
1	HB	428	GLN
1	HB	464	GLN
1	HB	496	ASN
1	HB	497	ASN
1	HB	615	GLN
1	IB	259	GLN
1	IB	312	ASN
1	IB	385	GLN
1	IB	428	GLN
1	IB	461	GLN
1	IB	464	GLN
1	IB	497	ASN
1	IB	615	GLN
1	IB	717	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

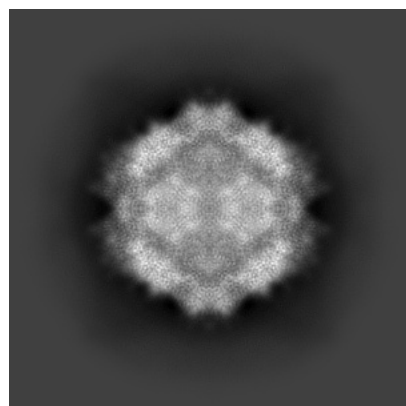
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63067. These allow visual inspection of the internal detail of the map and identification of artifacts.

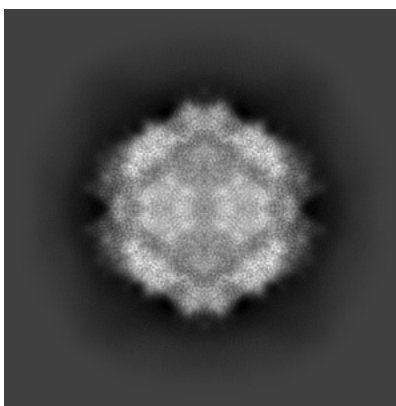
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

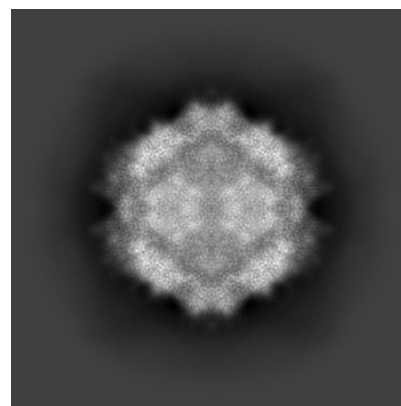
6.1.1 Primary map



X

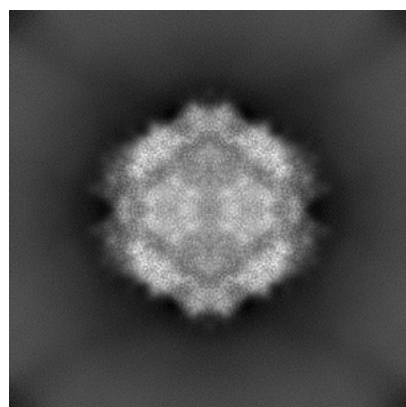


Y

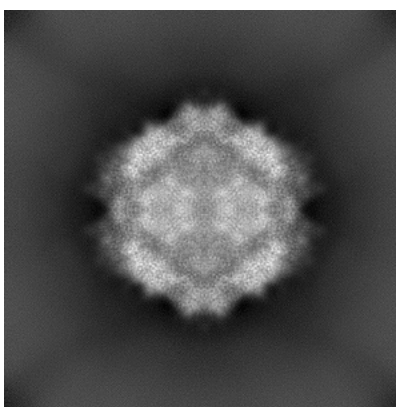


Z

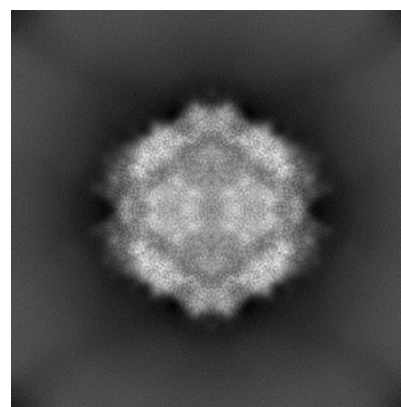
6.1.2 Raw map



X



Y

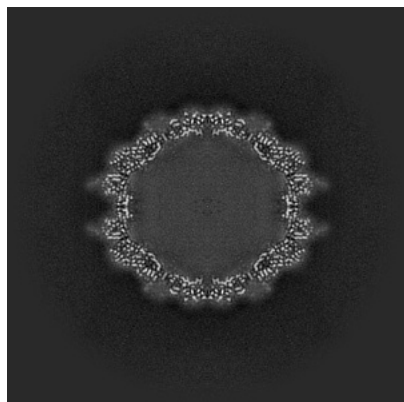


Z

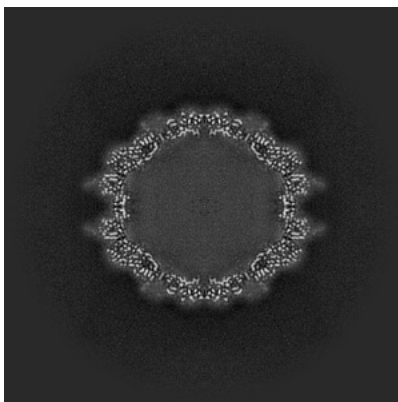
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

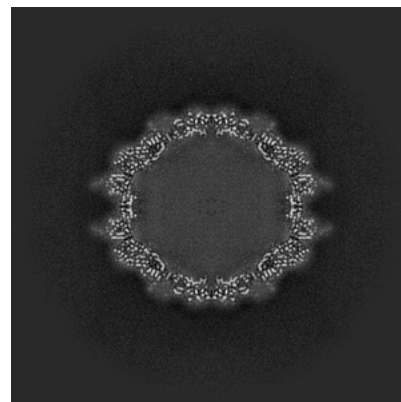
6.2.1 Primary map



X Index: 256

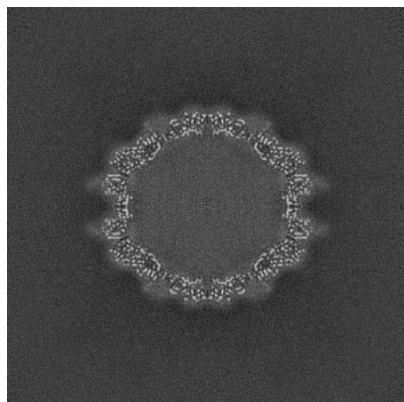


Y Index: 256

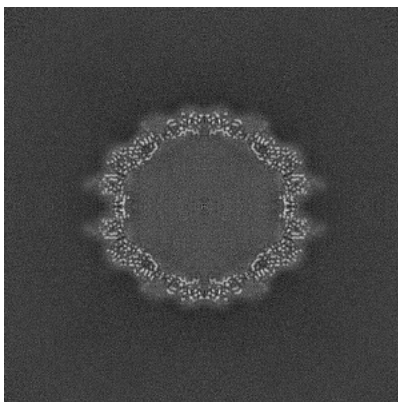


Z Index: 256

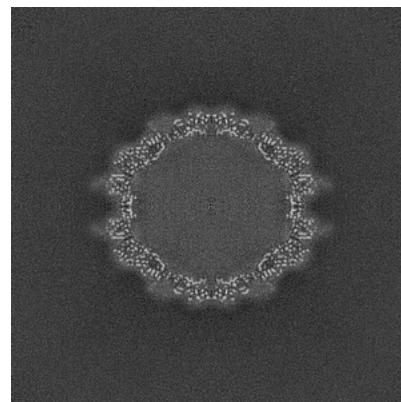
6.2.2 Raw map



X Index: 256



Y Index: 256

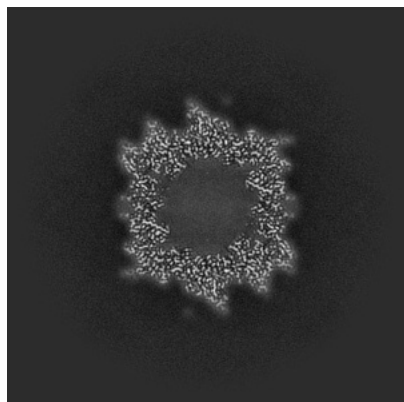


Z Index: 256

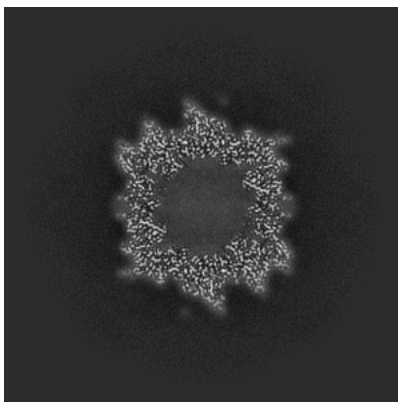
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

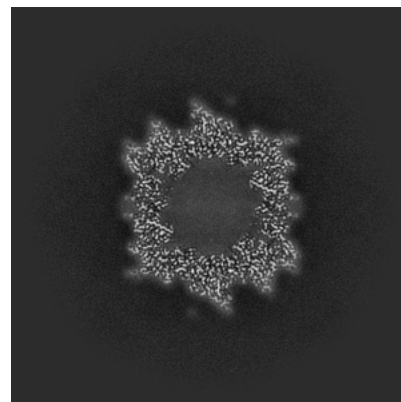
6.3.1 Primary map



X Index: 186

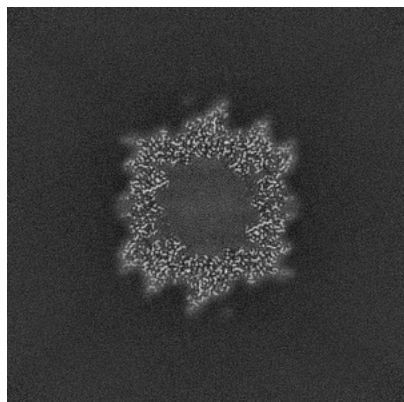


Y Index: 186

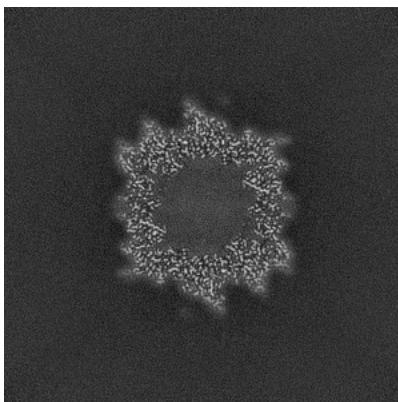


Z Index: 186

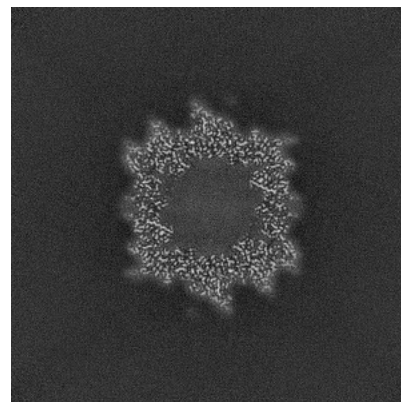
6.3.2 Raw map



X Index: 326



Y Index: 186

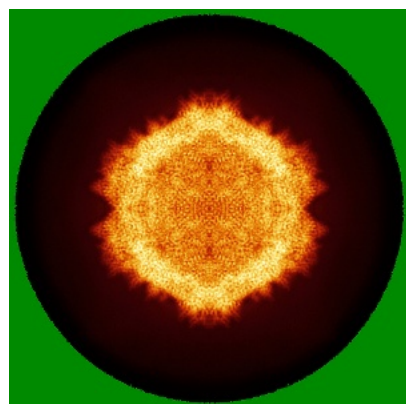


Z Index: 186

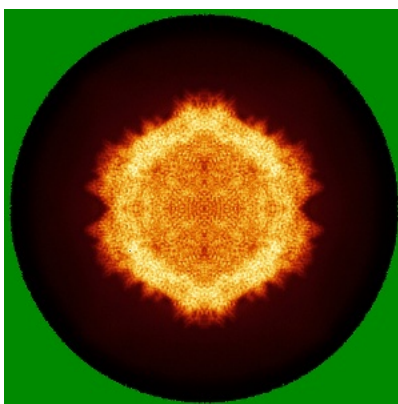
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

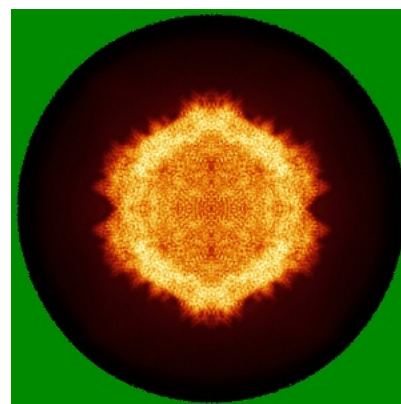
6.4.1 Primary map



X

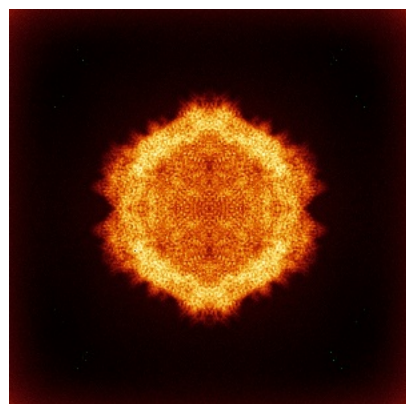


Y

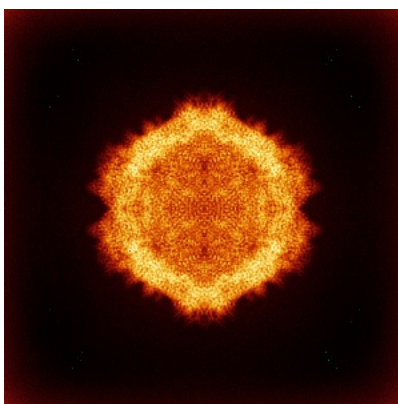


Z

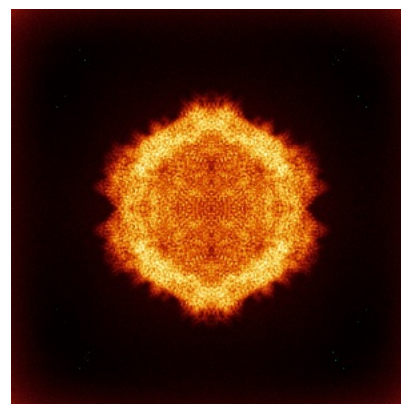
6.4.2 Raw map



X



Y

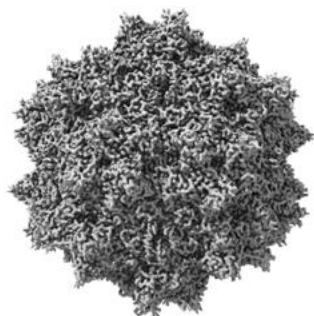


Z

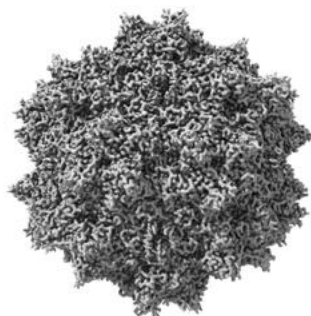
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

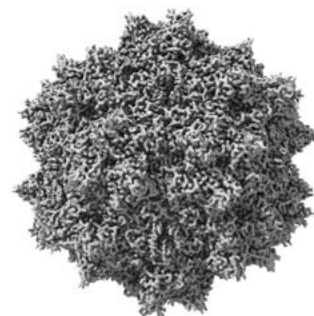
6.5.1 Primary map



X



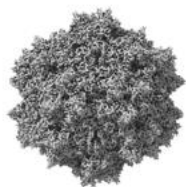
Y



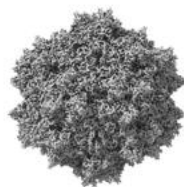
Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

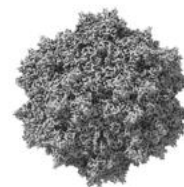
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

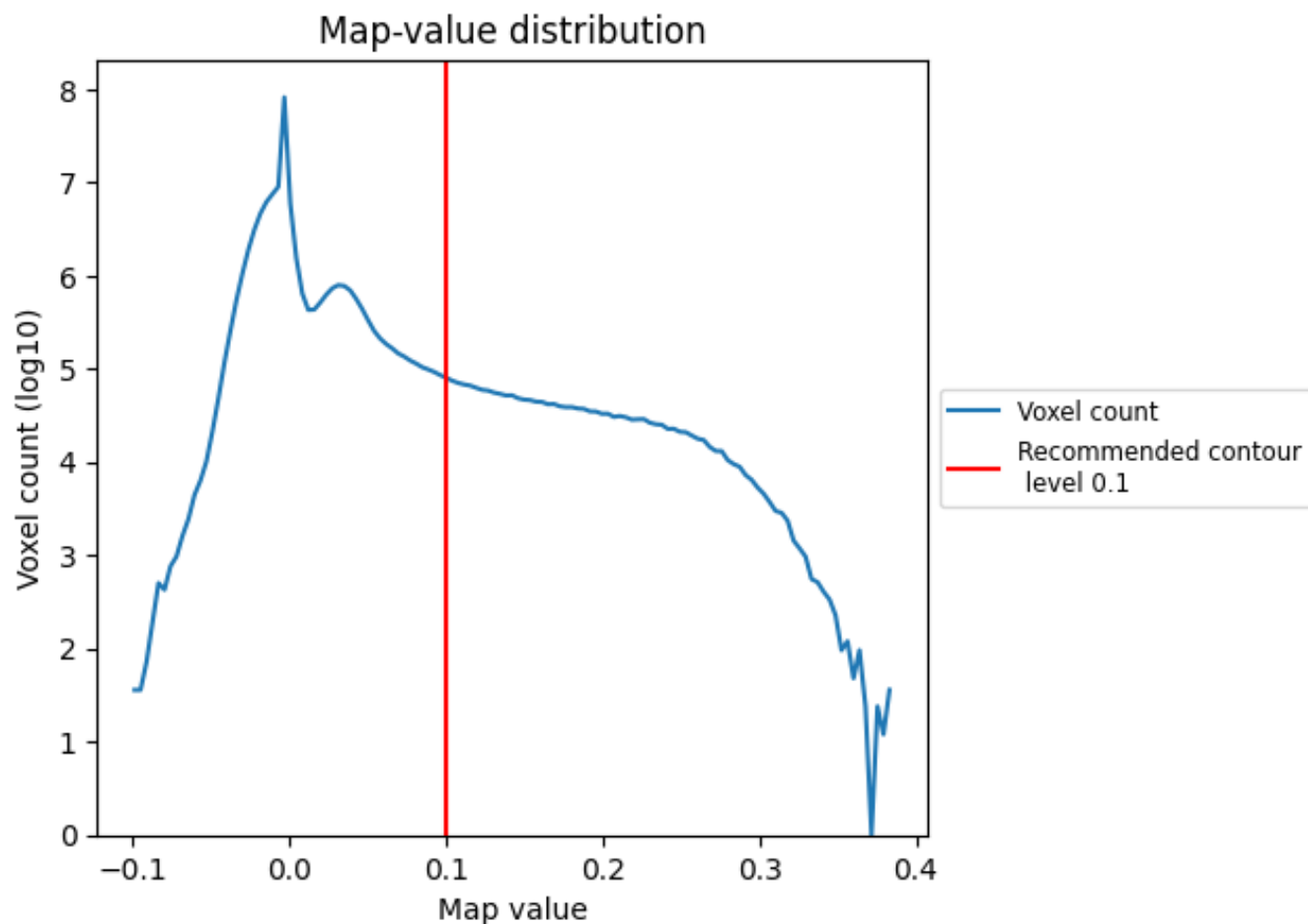
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

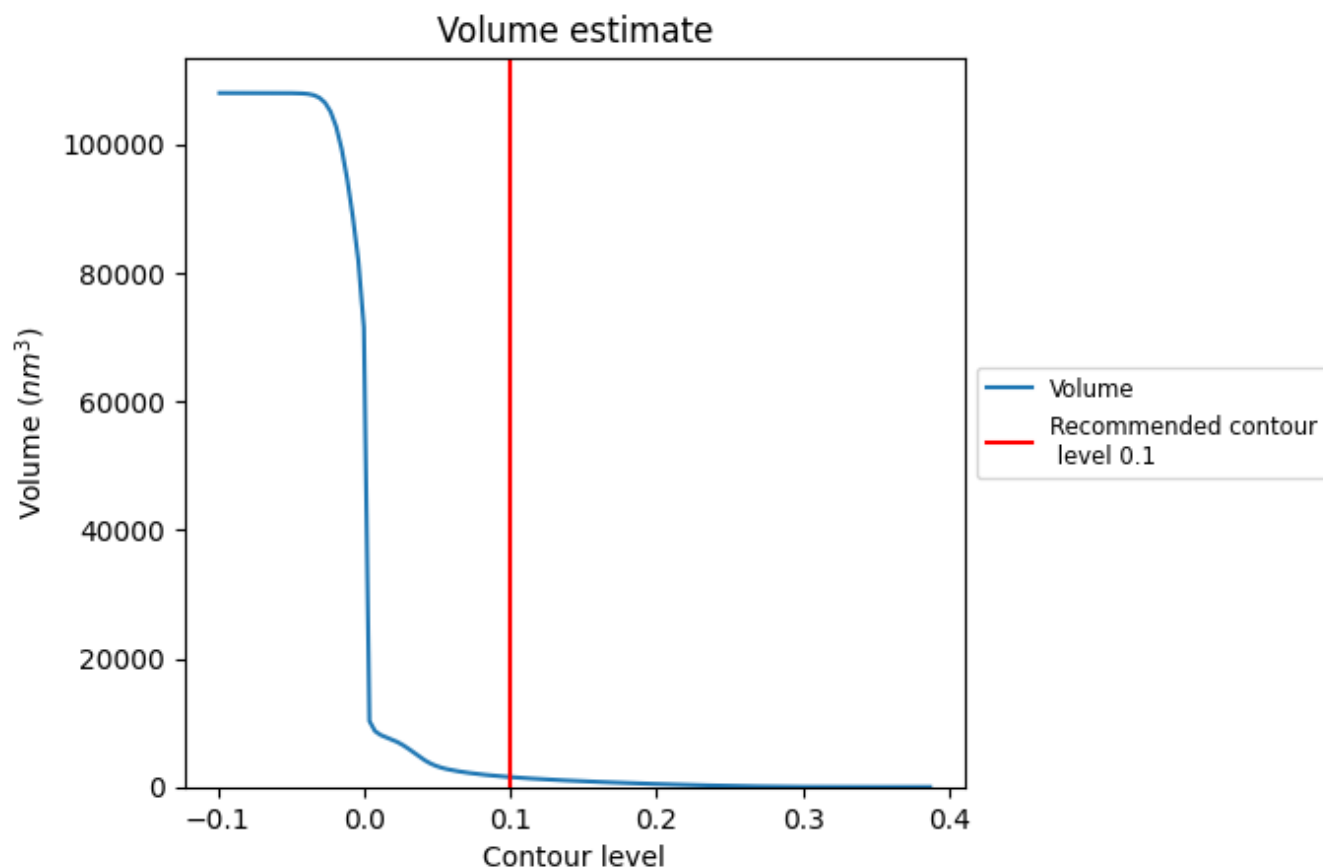
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

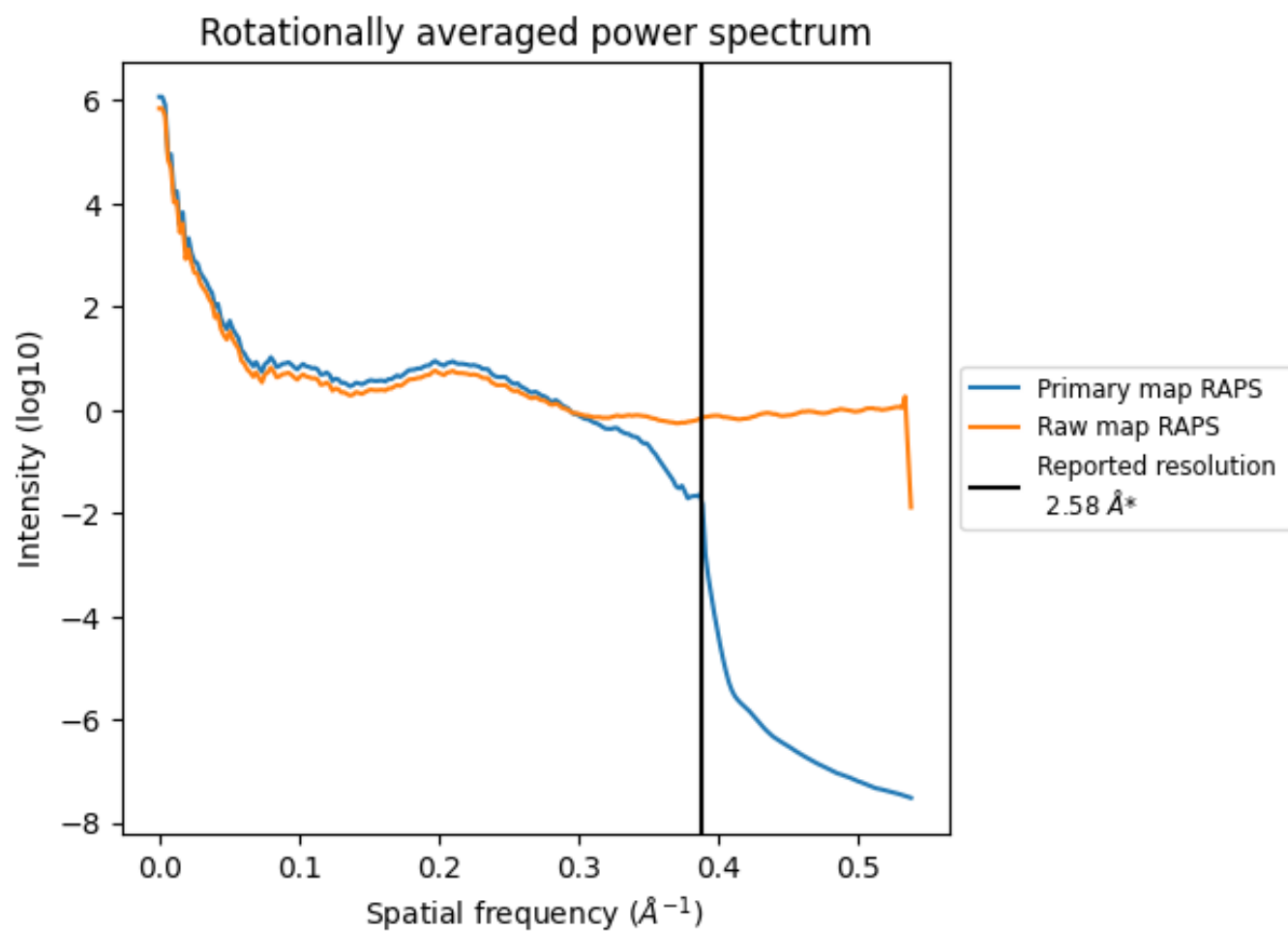
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1532 nm^3 ; this corresponds to an approximate mass of 1384 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

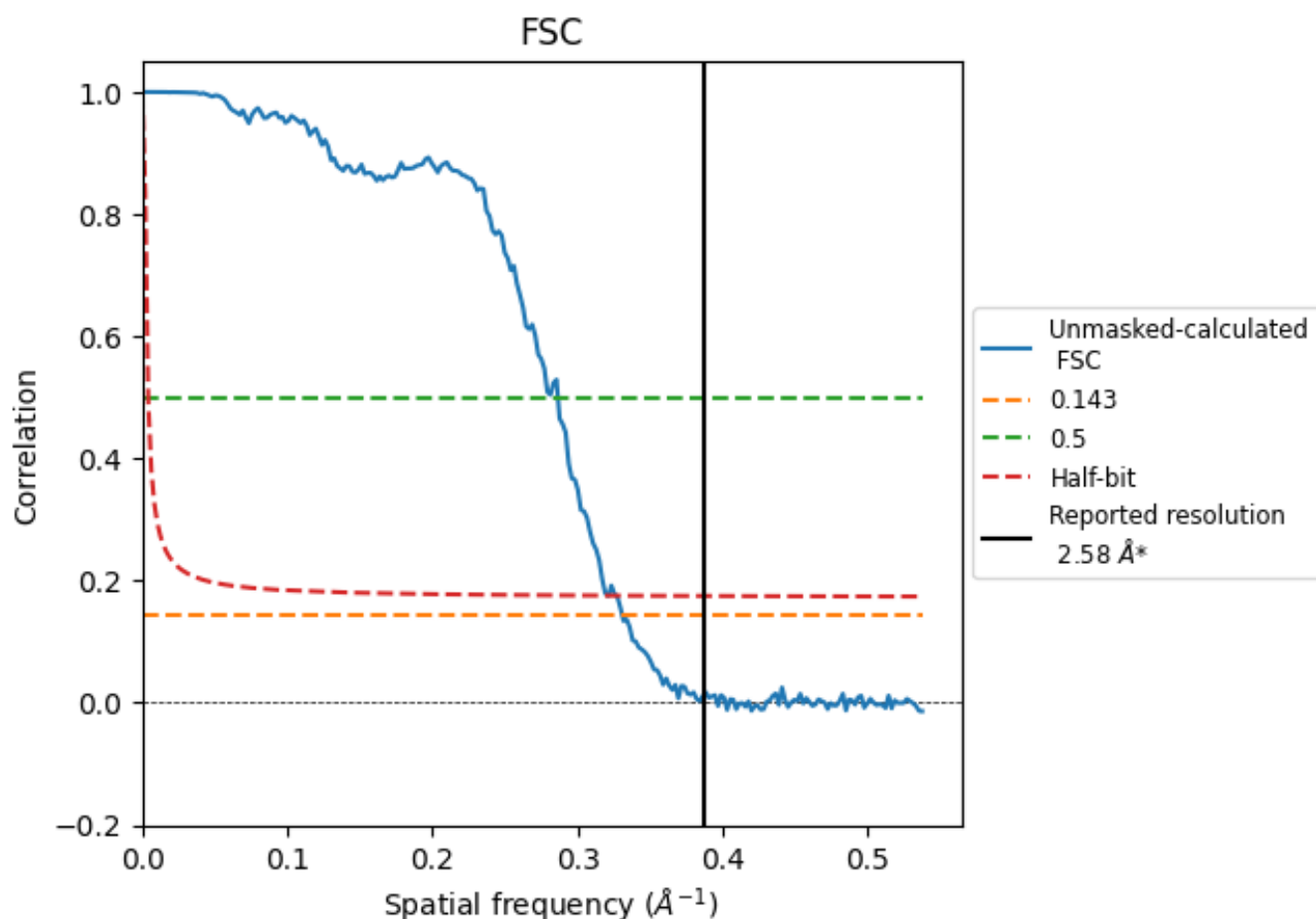


*Reported resolution corresponds to spatial frequency of 0.388 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.388 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.02	3.49	3.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.02 differs from the reported value 2.58 by more than 10 %

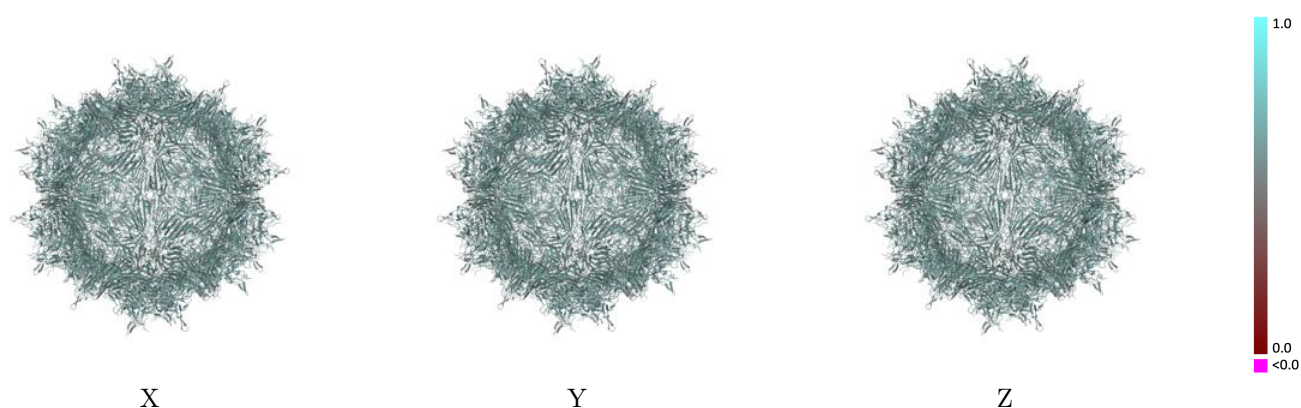
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63067 and PDB model 9LGJ. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay [i](#)

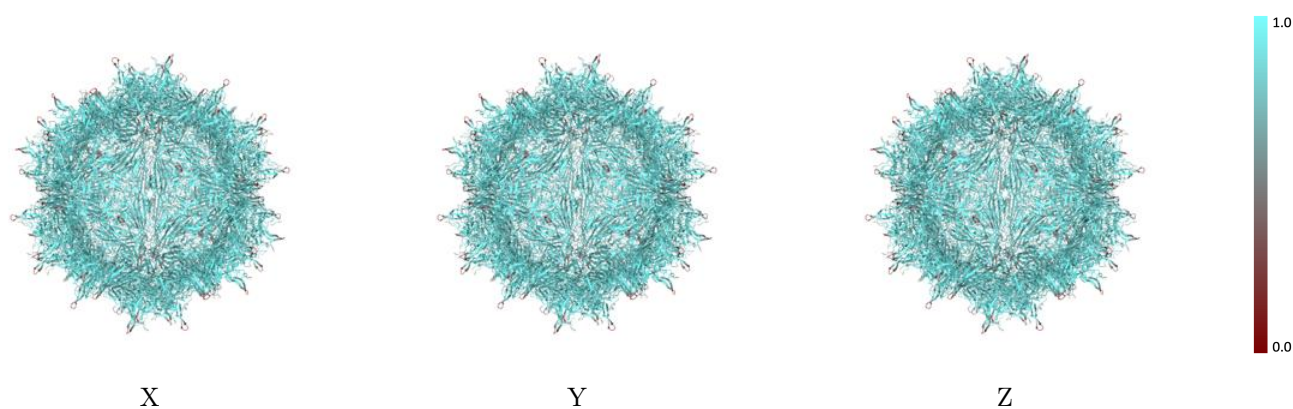
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



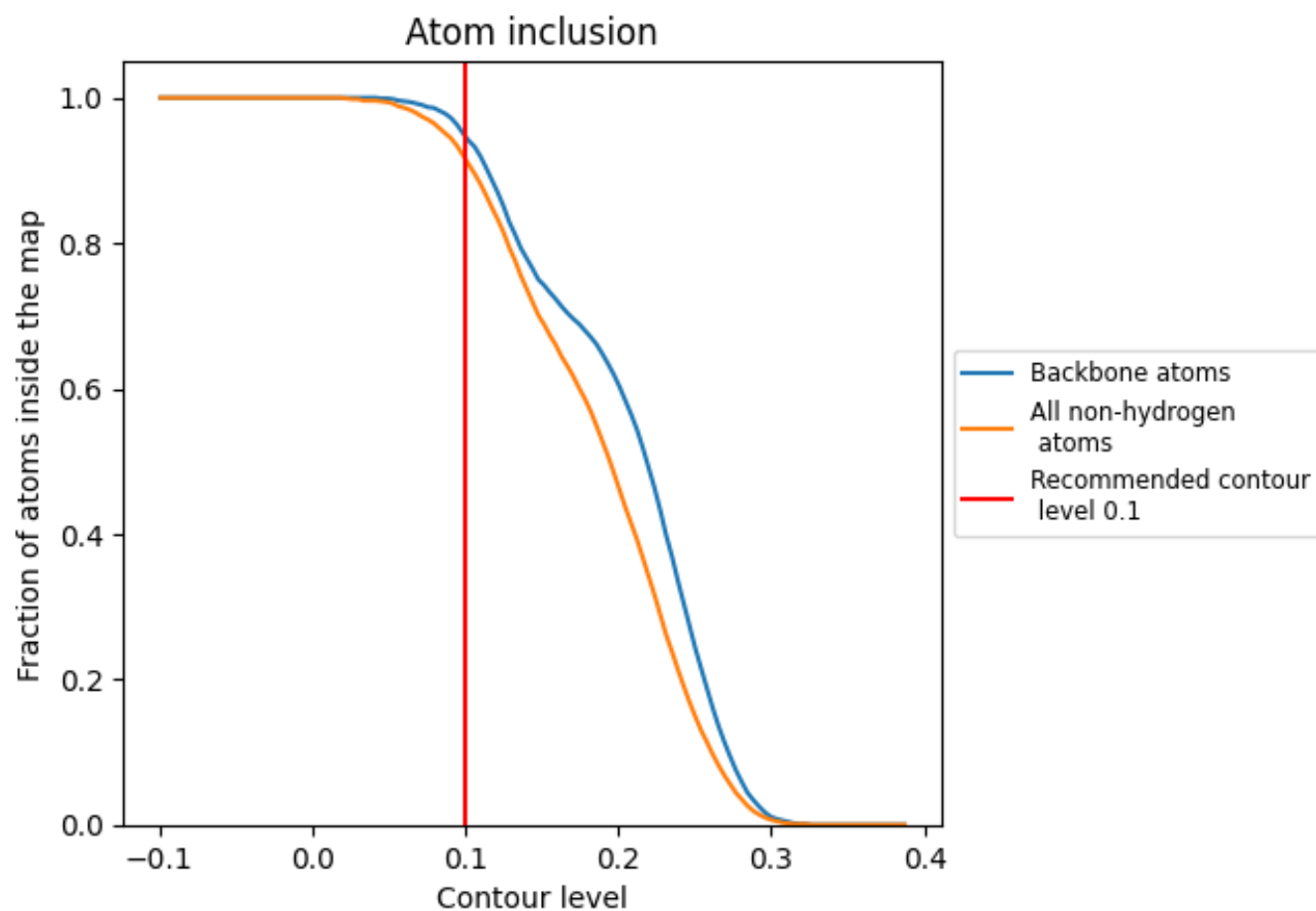
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.6100
A	 0.9170	 0.6120
AA	 0.9170	 0.6110
AB	 0.9150	 0.6090
B	 0.9150	 0.6100
BA	 0.9150	 0.6090
BB	 0.9170	 0.6100
C	 0.9170	 0.6100
CA	 0.9170	 0.6110
CB	 0.9160	 0.6090
D	 0.9150	 0.6100
DA	 0.9160	 0.6100
DB	 0.9160	 0.6100
E	 0.9160	 0.6100
EA	 0.9160	 0.6100
EB	 0.9180	 0.6110
F	 0.9170	 0.6120
FA	 0.9170	 0.6110
FB	 0.9150	 0.6090
G	 0.9150	 0.6090
GA	 0.9150	 0.6080
GB	 0.9170	 0.6090
H	 0.9170	 0.6090
HA	 0.9170	 0.6100
HB	 0.9160	 0.6100
I	 0.9160	 0.6110
IA	 0.9160	 0.6110
IB	 0.9160	 0.6110
J	 0.9160	 0.6090
JA	 0.9160	 0.6100
K	 0.9170	 0.6120
KA	 0.9170	 0.6110
L	 0.9150	 0.6090
LA	 0.9150	 0.6090
M	 0.9170	 0.6090



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Chain	Atom inclusion	Q-score
MA	 0.9170	 0.6100
N	 0.9160	 0.6100
NA	 0.9160	 0.6110
O	 0.9160	 0.6100
OA	 0.9160	 0.6090
P	 0.9170	 0.6120
PA	 0.9170	 0.6110
Q	 0.9150	 0.6090
QA	 0.9150	 0.6080
R	 0.9170	 0.6100
RA	 0.9170	 0.6100
S	 0.9150	 0.6100
SA	 0.9150	 0.6100
T	 0.9160	 0.6090
TA	 0.9160	 0.6110
UA	 0.9170	 0.6110
V	 0.9170	 0.6120
VA	 0.9150	 0.6100
W	 0.9150	 0.6090
WA	 0.9170	 0.6090
X	 0.9170	 0.6090
XA	 0.9160	 0.6100
Y	 0.9160	 0.6110
YA	 0.9160	 0.6100
Z	 0.9160	 0.6090
ZA	 0.9170	 0.6120