Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:17 PM GMT

PDB ID	:	4QYK
Title	:	Crystal structure of a canine parvovirus variant
Authors	:	Lukk, T.; Organtini, L.J.; Hafenstein, S.U.
Deposited on	:	2014-07-24
Resolution	:	3.50 Å(reported)

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

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

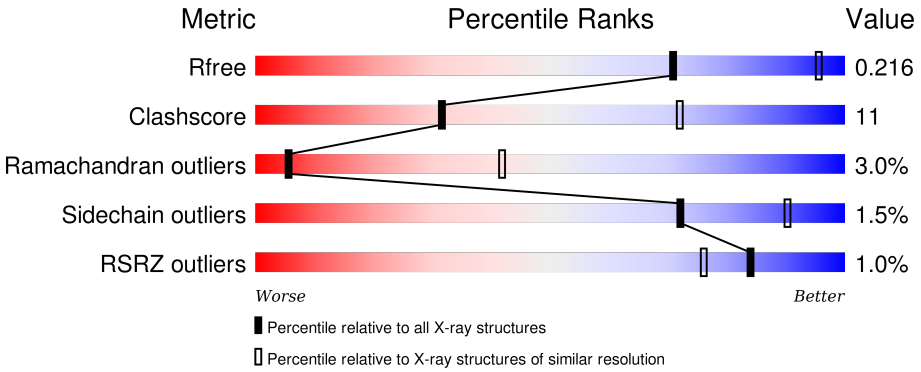
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	584	60% 32% 6%
1	B	584	62% 30% 6%
1	C	584	60% 31% 6%
1	D	584	60% 30% 6%
1	E	584	68% 23% 6%

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Mol	Chain	Length	Quality of chain
1	F	584	66% 25% 6%
1	G	584	68% 23% 6%
1	H	584	69% 22% 6%
1	I	584	67% 24% 6%
1	J	584	73% 19% 6%
1	K	584	70% 21% 6%
1	L	584	67% 25% 6%
1	M	584	70% 21% 6%
1	N	584	70% 21% 6%
1	O	584	71% 21% 6%
1	P	584	72% 20% 6%
1	Q	584	73% 18% 6%
1	R	584	69% 22% 6%
1	S	584	69% 23% 6%
1	T	584	2% 70% 22% 6%
1	U	584	71% 21% 6%
1	V	584	69% 22% 6%
1	W	584	69% 23% 6%
1	X	584	70% 21% 6%
1	Y	584	71% 21% 6%
1	Z	584	70% 22% 6%
1	a	584	90% 6%
1	b	584	90% 6%
1	c	584	89% 6%
1	d	584	89% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	K	800	-	-	-	X
2	MG	Q	800	-	-	-	X
2	MG	T	800	-	-	-	X
2	MG	Y	601	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 130590 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0
1	E	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0
1	J	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0
1	N	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0
1	Q	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0
1	B	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0
1	C	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0
1	D	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0
1	F	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0
1	G	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0
1	H	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0
1	I	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0
1	K	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0
1	L	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0
1	M	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0
1	O	548	Total 4352	C 2767	N 740	O 830	S 15	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	R	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	S	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	T	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	U	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	V	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	W	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	X	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	Y	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	Z	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	a	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	b	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	c	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	d	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	TYR	GLU	CONFLICT	UNP P90456
A	104	GLU	GLN	CONFLICT	UNP P90456
A	426	ASP	ASN	CONFLICT	UNP P90456
A	509	GLN	GLU	CONFLICT	UNP P90456
A	555	VAL	ILE	CONFLICT	UNP P90456
E	60	TYR	GLU	CONFLICT	UNP P90456
E	104	GLU	GLN	CONFLICT	UNP P90456
E	426	ASP	ASN	CONFLICT	UNP P90456
E	509	GLN	GLU	CONFLICT	UNP P90456
E	555	VAL	ILE	CONFLICT	UNP P90456
J	60	TYR	GLU	CONFLICT	UNP P90456

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Chain	Residue	Modelled	Actual	Comment	Reference
J	104	GLU	GLN	CONFLICT	UNP P90456
J	426	ASP	ASN	CONFLICT	UNP P90456
J	509	GLN	GLU	CONFLICT	UNP P90456
J	555	VAL	ILE	CONFLICT	UNP P90456
N	60	TYR	GLU	CONFLICT	UNP P90456
N	104	GLU	GLN	CONFLICT	UNP P90456
N	426	ASP	ASN	CONFLICT	UNP P90456
N	509	GLN	GLU	CONFLICT	UNP P90456
N	555	VAL	ILE	CONFLICT	UNP P90456
Q	60	TYR	GLU	CONFLICT	UNP P90456
Q	104	GLU	GLN	CONFLICT	UNP P90456
Q	426	ASP	ASN	CONFLICT	UNP P90456
Q	509	GLN	GLU	CONFLICT	UNP P90456
Q	555	VAL	ILE	CONFLICT	UNP P90456
B	60	TYR	GLU	CONFLICT	UNP P90456
B	104	GLU	GLN	CONFLICT	UNP P90456
B	426	ASP	ASN	CONFLICT	UNP P90456
B	509	GLN	GLU	CONFLICT	UNP P90456
B	555	VAL	ILE	CONFLICT	UNP P90456
C	60	TYR	GLU	CONFLICT	UNP P90456
C	104	GLU	GLN	CONFLICT	UNP P90456
C	426	ASP	ASN	CONFLICT	UNP P90456
C	509	GLN	GLU	CONFLICT	UNP P90456
C	555	VAL	ILE	CONFLICT	UNP P90456
D	60	TYR	GLU	CONFLICT	UNP P90456
D	104	GLU	GLN	CONFLICT	UNP P90456
D	426	ASP	ASN	CONFLICT	UNP P90456
D	509	GLN	GLU	CONFLICT	UNP P90456
D	555	VAL	ILE	CONFLICT	UNP P90456
F	60	TYR	GLU	CONFLICT	UNP P90456
F	104	GLU	GLN	CONFLICT	UNP P90456
F	426	ASP	ASN	CONFLICT	UNP P90456
F	509	GLN	GLU	CONFLICT	UNP P90456
F	555	VAL	ILE	CONFLICT	UNP P90456
G	60	TYR	GLU	CONFLICT	UNP P90456
G	104	GLU	GLN	CONFLICT	UNP P90456
G	426	ASP	ASN	CONFLICT	UNP P90456
G	509	GLN	GLU	CONFLICT	UNP P90456
G	555	VAL	ILE	CONFLICT	UNP P90456
H	60	TYR	GLU	CONFLICT	UNP P90456
H	104	GLU	GLN	CONFLICT	UNP P90456
H	426	ASP	ASN	CONFLICT	UNP P90456

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Chain	Residue	Modelled	Actual	Comment	Reference
H	509	GLN	GLU	CONFLICT	UNP P90456
H	555	VAL	ILE	CONFLICT	UNP P90456
I	60	TYR	GLU	CONFLICT	UNP P90456
I	104	GLU	GLN	CONFLICT	UNP P90456
I	426	ASP	ASN	CONFLICT	UNP P90456
I	509	GLN	GLU	CONFLICT	UNP P90456
I	555	VAL	ILE	CONFLICT	UNP P90456
K	60	TYR	GLU	CONFLICT	UNP P90456
K	104	GLU	GLN	CONFLICT	UNP P90456
K	426	ASP	ASN	CONFLICT	UNP P90456
K	509	GLN	GLU	CONFLICT	UNP P90456
K	555	VAL	ILE	CONFLICT	UNP P90456
L	60	TYR	GLU	CONFLICT	UNP P90456
L	104	GLU	GLN	CONFLICT	UNP P90456
L	426	ASP	ASN	CONFLICT	UNP P90456
L	509	GLN	GLU	CONFLICT	UNP P90456
L	555	VAL	ILE	CONFLICT	UNP P90456
M	60	TYR	GLU	CONFLICT	UNP P90456
M	104	GLU	GLN	CONFLICT	UNP P90456
M	426	ASP	ASN	CONFLICT	UNP P90456
M	509	GLN	GLU	CONFLICT	UNP P90456
M	555	VAL	ILE	CONFLICT	UNP P90456
O	60	TYR	GLU	CONFLICT	UNP P90456
O	104	GLU	GLN	CONFLICT	UNP P90456
O	426	ASP	ASN	CONFLICT	UNP P90456
O	509	GLN	GLU	CONFLICT	UNP P90456
O	555	VAL	ILE	CONFLICT	UNP P90456
P	60	TYR	GLU	CONFLICT	UNP P90456
P	104	GLU	GLN	CONFLICT	UNP P90456
P	426	ASP	ASN	CONFLICT	UNP P90456
P	509	GLN	GLU	CONFLICT	UNP P90456
P	555	VAL	ILE	CONFLICT	UNP P90456
R	60	TYR	GLU	CONFLICT	UNP P90456
R	104	GLU	GLN	CONFLICT	UNP P90456
R	426	ASP	ASN	CONFLICT	UNP P90456
R	509	GLN	GLU	CONFLICT	UNP P90456
R	555	VAL	ILE	CONFLICT	UNP P90456
S	60	TYR	GLU	CONFLICT	UNP P90456
S	104	GLU	GLN	CONFLICT	UNP P90456
S	426	ASP	ASN	CONFLICT	UNP P90456
S	509	GLN	GLU	CONFLICT	UNP P90456
S	555	VAL	ILE	CONFLICT	UNP P90456

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Chain	Residue	Modelled	Actual	Comment	Reference
T	60	TYR	GLU	CONFLICT	UNP P90456
T	104	GLU	GLN	CONFLICT	UNP P90456
T	426	ASP	ASN	CONFLICT	UNP P90456
T	509	GLN	GLU	CONFLICT	UNP P90456
T	555	VAL	ILE	CONFLICT	UNP P90456
U	60	TYR	GLU	CONFLICT	UNP P90456
U	104	GLU	GLN	CONFLICT	UNP P90456
U	426	ASP	ASN	CONFLICT	UNP P90456
U	509	GLN	GLU	CONFLICT	UNP P90456
U	555	VAL	ILE	CONFLICT	UNP P90456
V	60	TYR	GLU	CONFLICT	UNP P90456
V	104	GLU	GLN	CONFLICT	UNP P90456
V	426	ASP	ASN	CONFLICT	UNP P90456
V	509	GLN	GLU	CONFLICT	UNP P90456
V	555	VAL	ILE	CONFLICT	UNP P90456
W	60	TYR	GLU	CONFLICT	UNP P90456
W	104	GLU	GLN	CONFLICT	UNP P90456
W	426	ASP	ASN	CONFLICT	UNP P90456
W	509	GLN	GLU	CONFLICT	UNP P90456
W	555	VAL	ILE	CONFLICT	UNP P90456
X	60	TYR	GLU	CONFLICT	UNP P90456
X	104	GLU	GLN	CONFLICT	UNP P90456
X	426	ASP	ASN	CONFLICT	UNP P90456
X	509	GLN	GLU	CONFLICT	UNP P90456
X	555	VAL	ILE	CONFLICT	UNP P90456
Y	60	TYR	GLU	CONFLICT	UNP P90456
Y	104	GLU	GLN	CONFLICT	UNP P90456
Y	426	ASP	ASN	CONFLICT	UNP P90456
Y	509	GLN	GLU	CONFLICT	UNP P90456
Y	555	VAL	ILE	CONFLICT	UNP P90456
Z	60	TYR	GLU	CONFLICT	UNP P90456
Z	104	GLU	GLN	CONFLICT	UNP P90456
Z	426	ASP	ASN	CONFLICT	UNP P90456
Z	509	GLN	GLU	CONFLICT	UNP P90456
Z	555	VAL	ILE	CONFLICT	UNP P90456
a	60	TYR	GLU	CONFLICT	UNP P90456
a	104	GLU	GLN	CONFLICT	UNP P90456
a	426	ASP	ASN	CONFLICT	UNP P90456
a	509	GLN	GLU	CONFLICT	UNP P90456
a	555	VAL	ILE	CONFLICT	UNP P90456
b	60	TYR	GLU	CONFLICT	UNP P90456
b	104	GLU	GLN	CONFLICT	UNP P90456

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Chain	Residue	Modelled	Actual	Comment	Reference
b	426	ASP	ASN	CONFLICT	UNP P90456
b	509	GLN	GLU	CONFLICT	UNP P90456
b	555	VAL	ILE	CONFLICT	UNP P90456
c	60	TYR	GLU	CONFLICT	UNP P90456
c	104	GLU	GLN	CONFLICT	UNP P90456
c	426	ASP	ASN	CONFLICT	UNP P90456
c	509	GLN	GLU	CONFLICT	UNP P90456
c	555	VAL	ILE	CONFLICT	UNP P90456
d	60	TYR	GLU	CONFLICT	UNP P90456
d	104	GLU	GLN	CONFLICT	UNP P90456
d	426	ASP	ASN	CONFLICT	UNP P90456
d	509	GLN	GLU	CONFLICT	UNP P90456
d	555	VAL	ILE	CONFLICT	UNP P90456

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	c	1	Total Mg 1 1	0	0
2	W	1	Total Mg 1 1	0	0
2	N	1	Total Mg 1 1	0	0
2	X	1	Total Mg 1 1	0	0
2	S	1	Total Mg 1 1	0	0
2	J	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0
2	A	1	Total Mg 1 1	0	0
2	R	1	Total Mg 1 1	0	0
2	M	1	Total Mg 1 1	0	0

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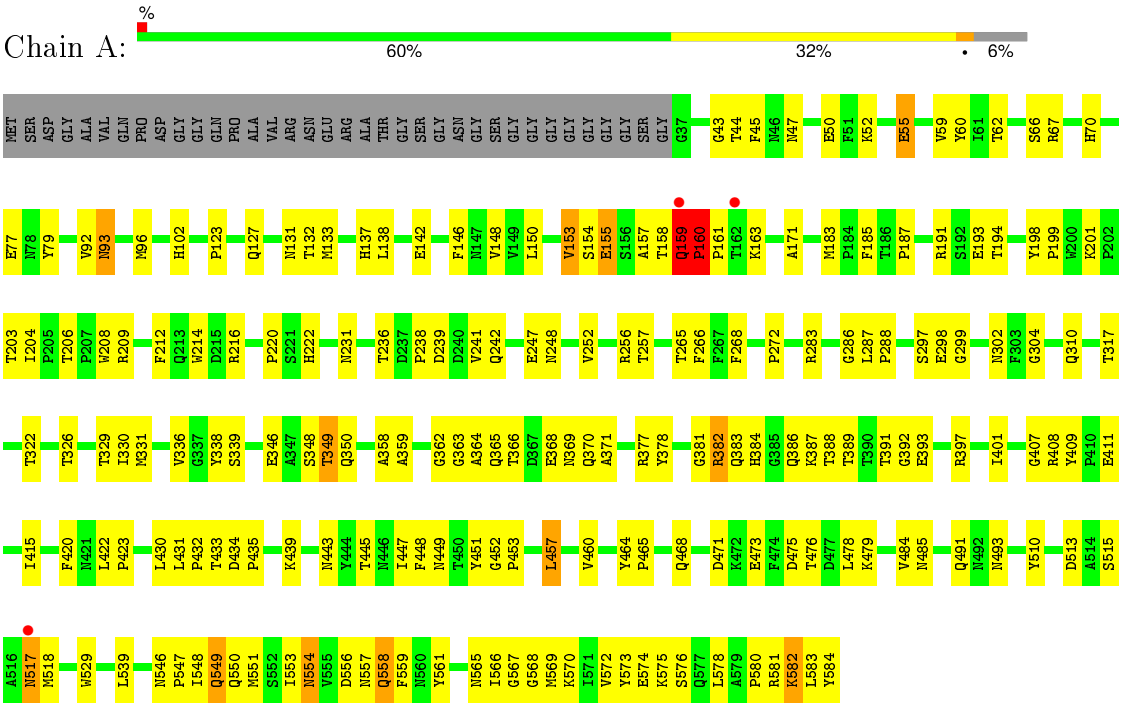
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	Z	1	Total Mg 1 1	0	0
2	L	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	Q	1	Total Mg 1 1	0	0
2	d	2	Total Mg 2 2	0	0
2	H	2	Total Mg 2 2	0	0
2	C	1	Total Mg 1 1	0	0
2	T	1	Total Mg 1 1	0	0
2	O	1	Total Mg 1 1	0	0
2	Y	2	Total Mg 2 2	0	0

3 Residue-property plots (i)

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

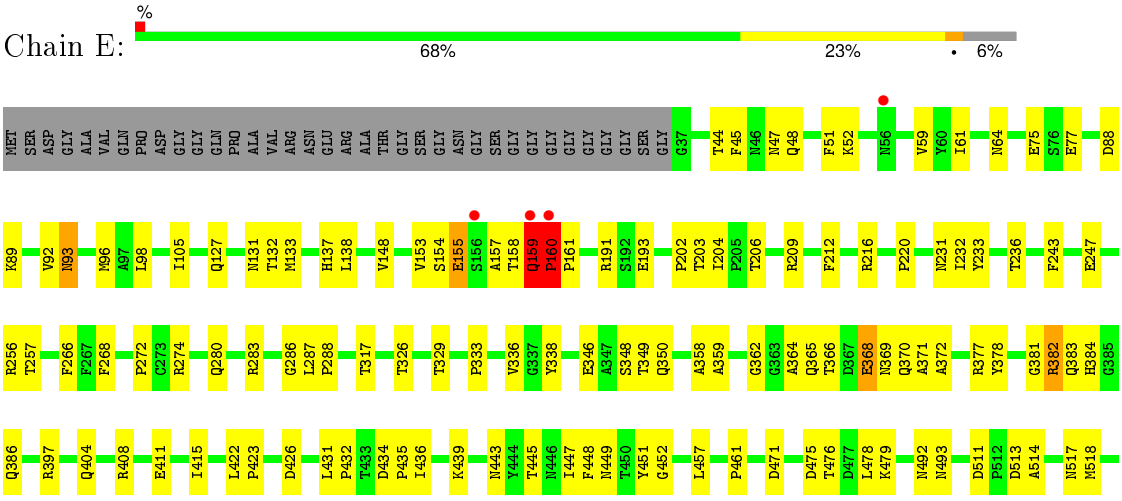
- Molecule 1: Capsid protein VP1

Chain A:



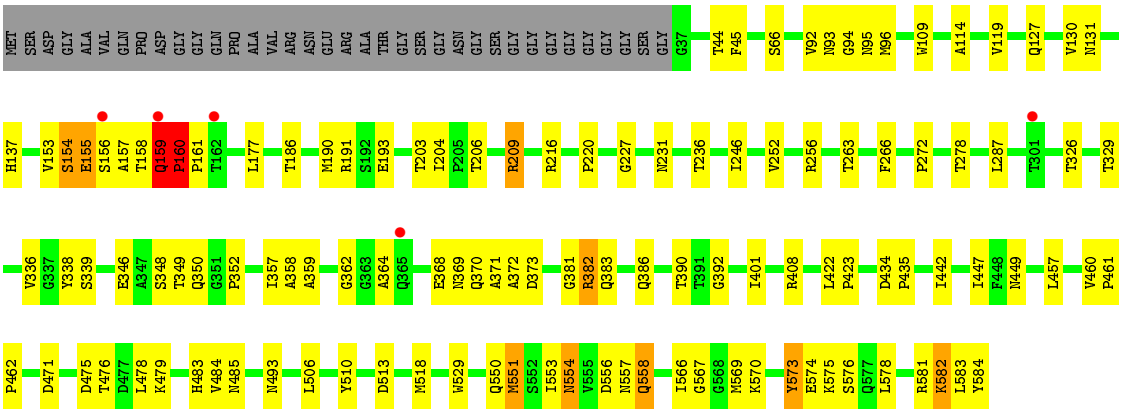
- Molecule 1: Capsid protein VP1

Chain E:



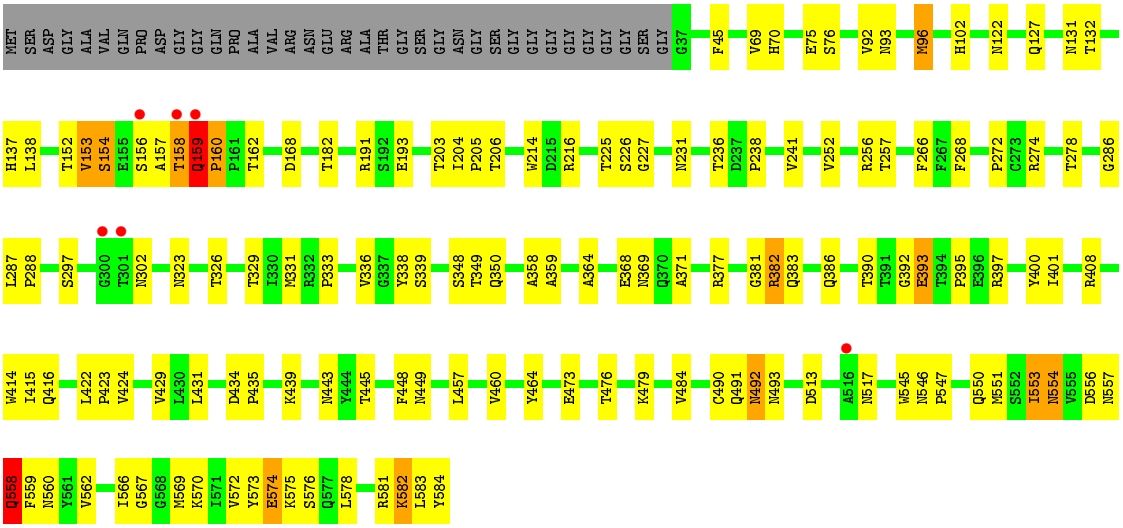
- Molecule 1: Capsid protein VP1

Chain J:



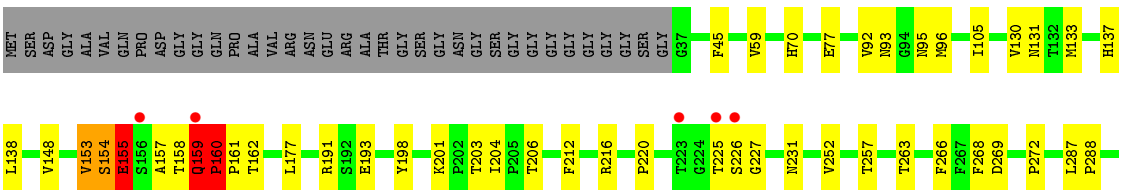
- Molecule 1: Capsid protein VP1

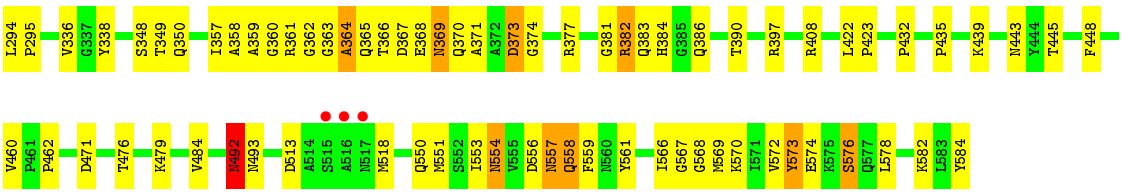
Chain N:



- Molecule 1: Capsid protein VP1

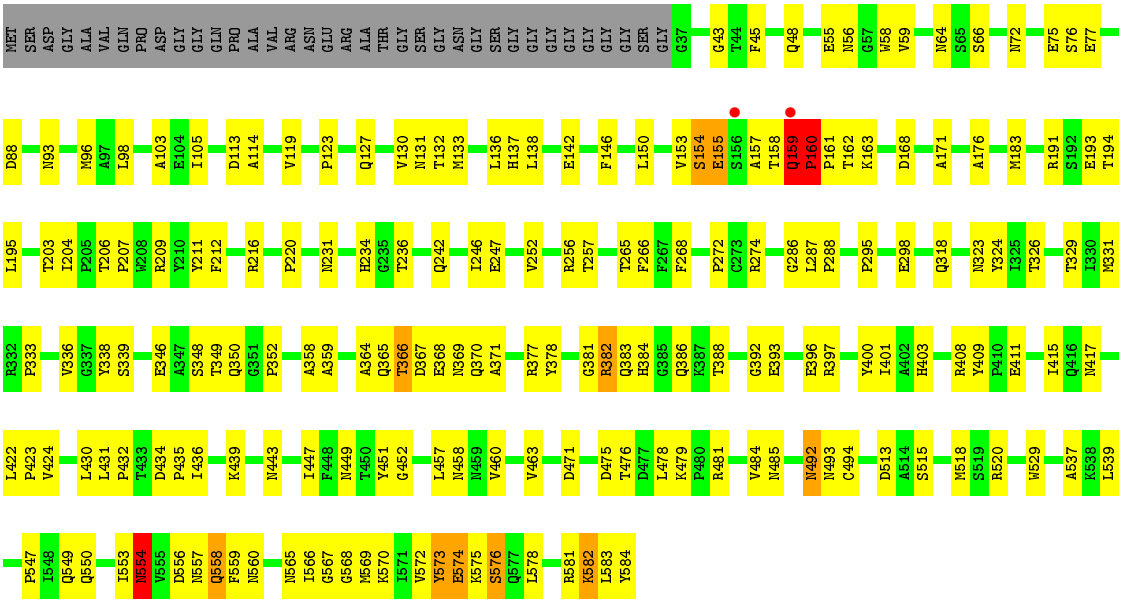
Chain Q:





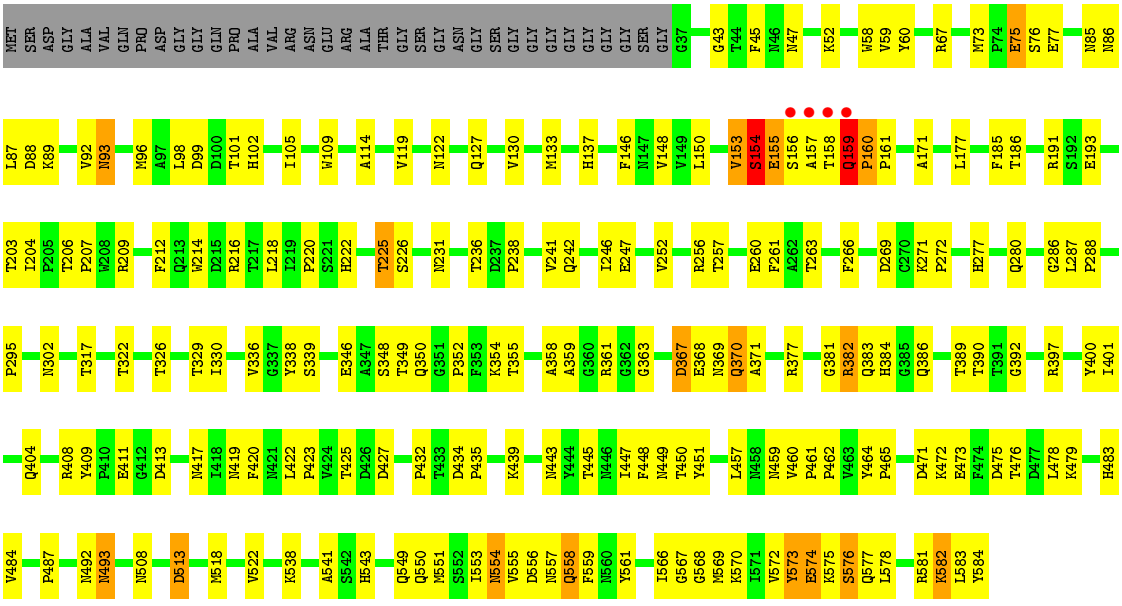
• Molecule 1: Capsid protein VP1

Chain B:



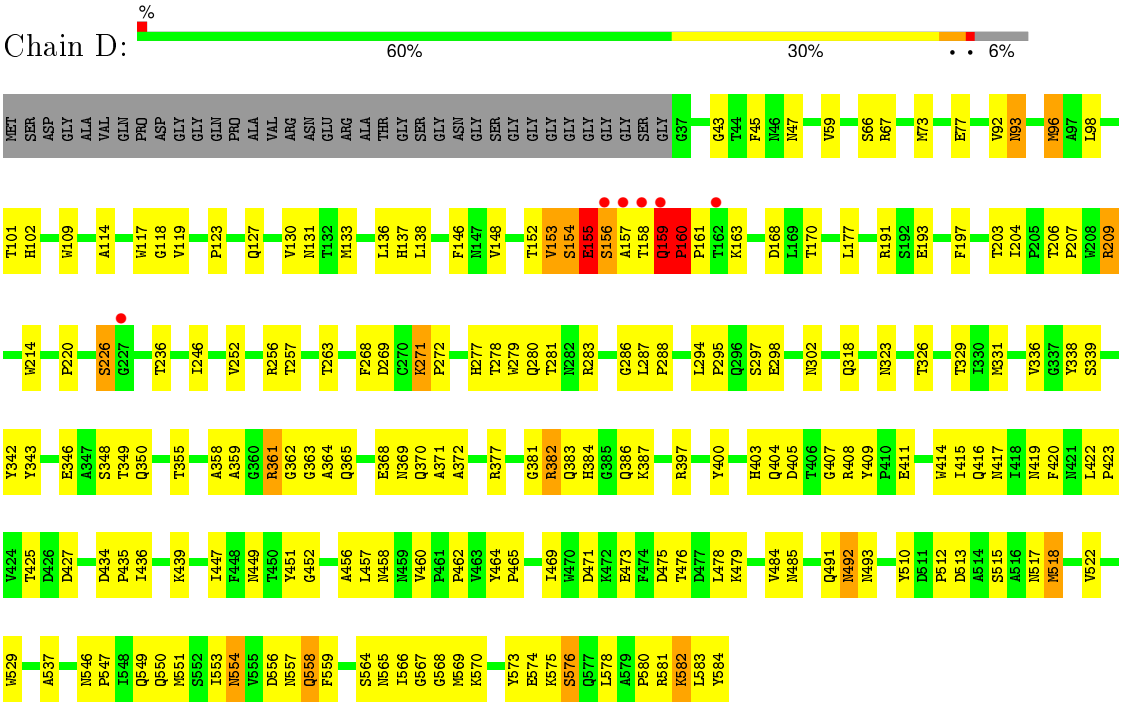
• Molecule 1: Capsid protein VP1

Chain C:



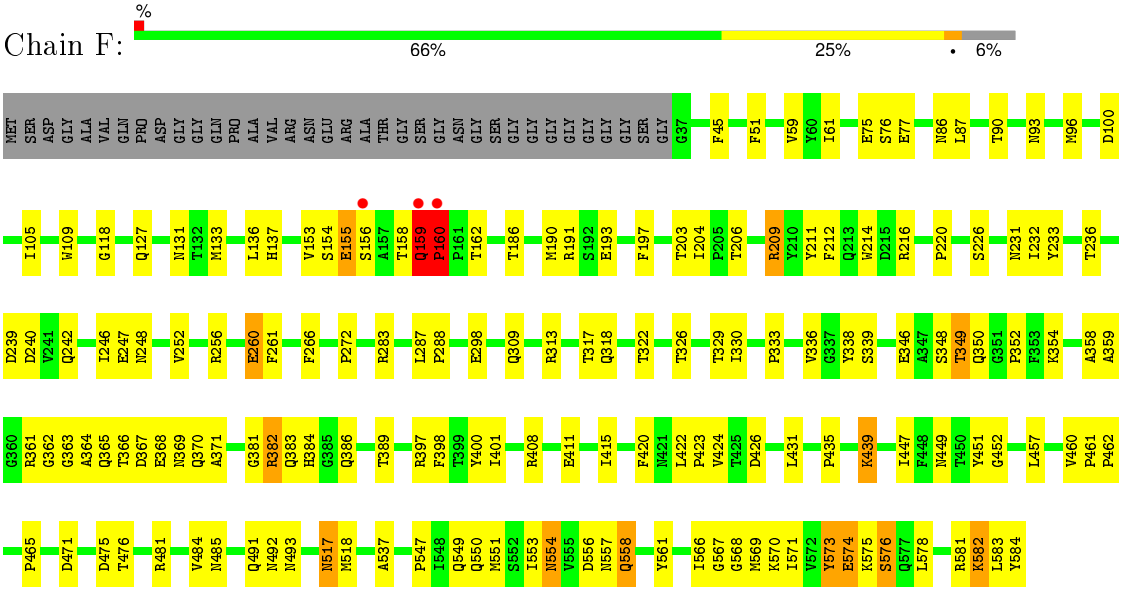
• Molecule 1: Capsid protein VP1

Chain D:



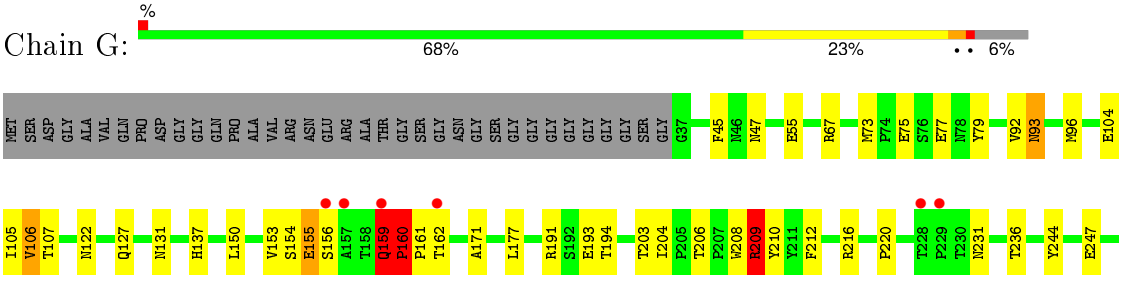
• Molecule 1: Capsid protein VP1

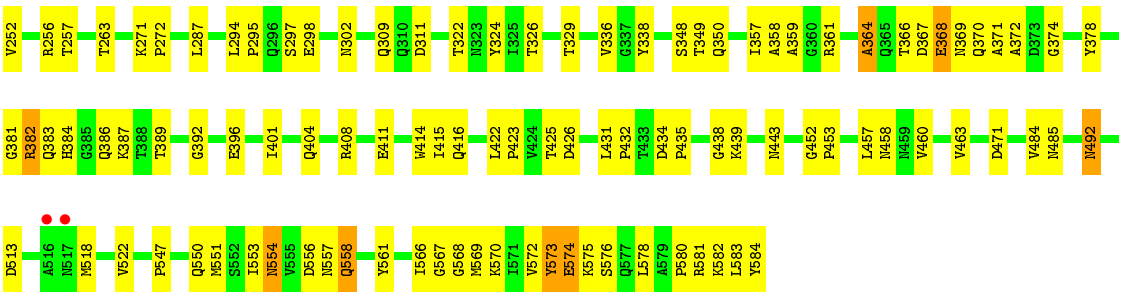
Chain F:



• Molecule 1: Capsid protein VP1

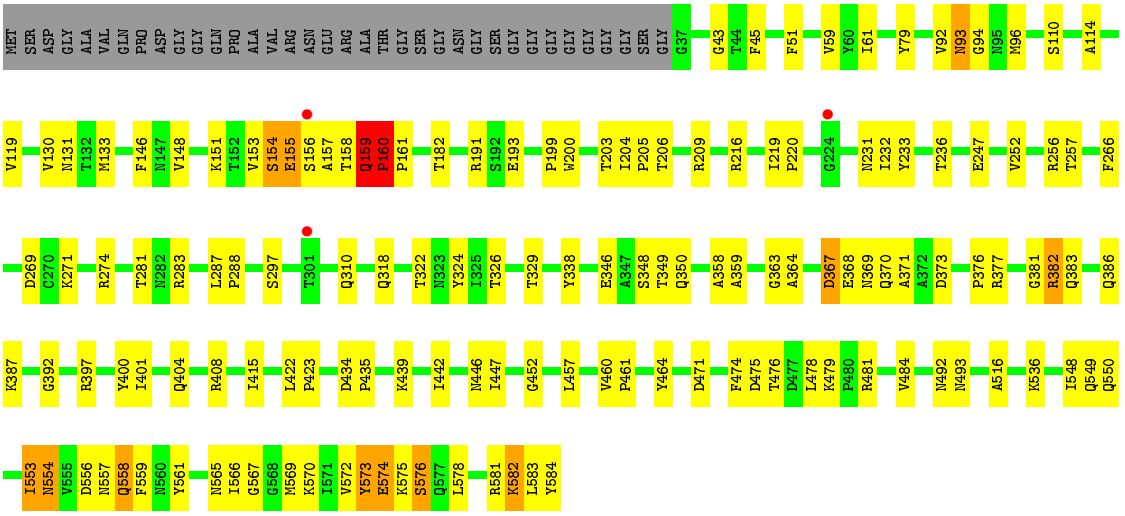
Chain G:





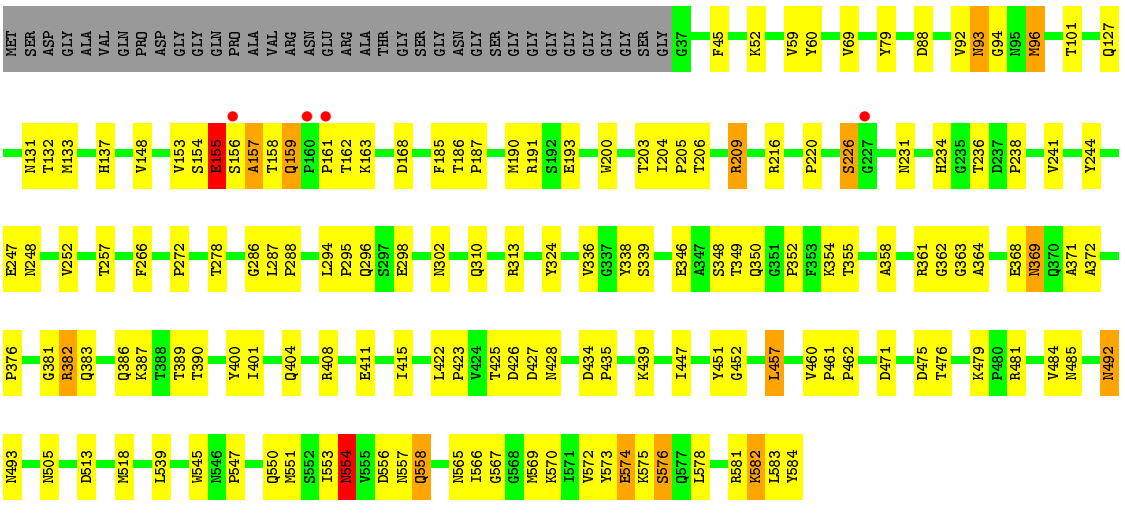
• Molecule 1: Capsid protein VP1

Chain H:



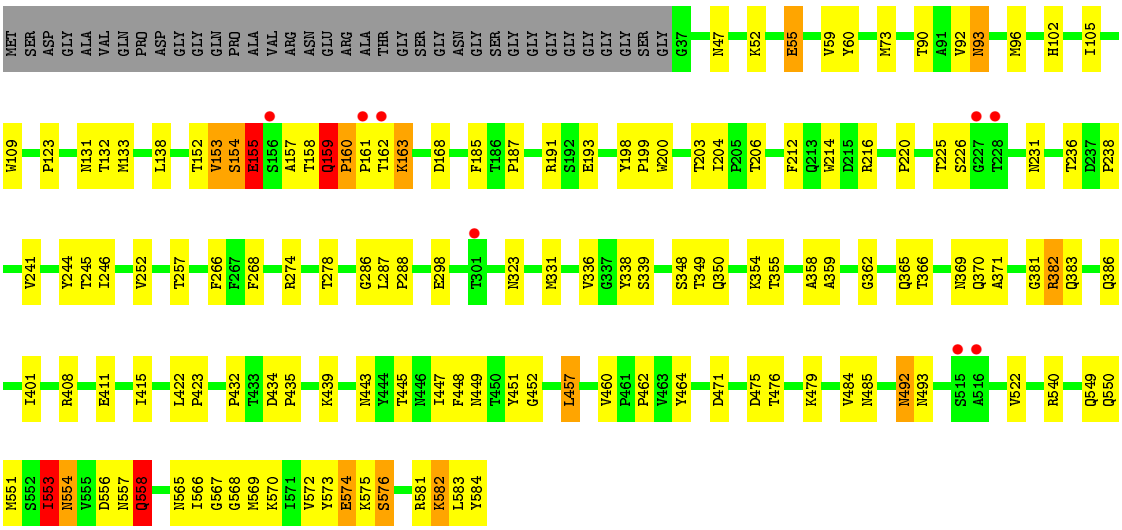
• Molecule 1: Capsid protein VP1

Chain I:



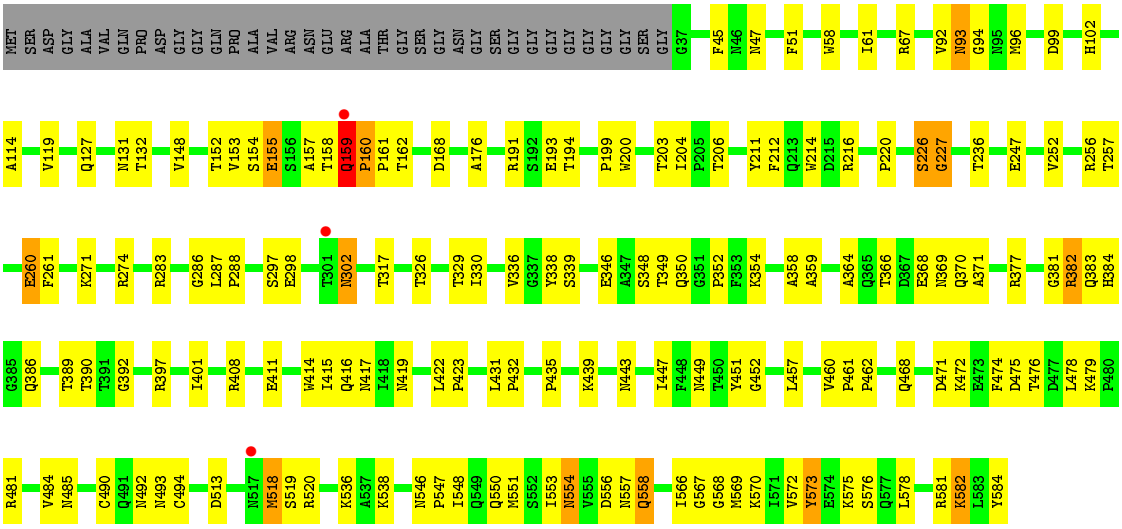
• Molecule 1: Capsid protein VP1

Chain K:



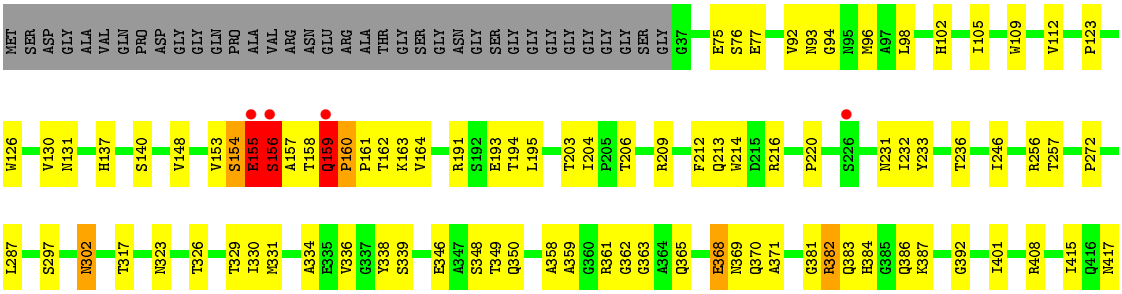
• Molecule 1: Capsid protein VP1

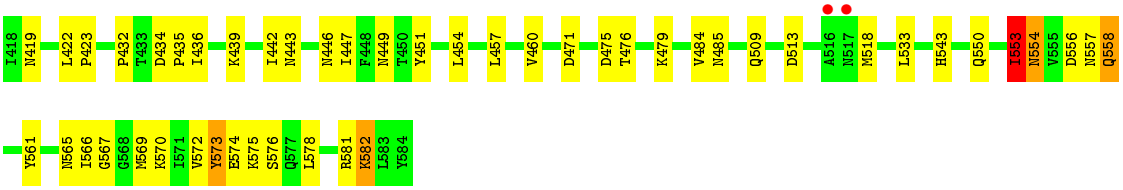
Chain L:



• Molecule 1: Capsid protein VP1

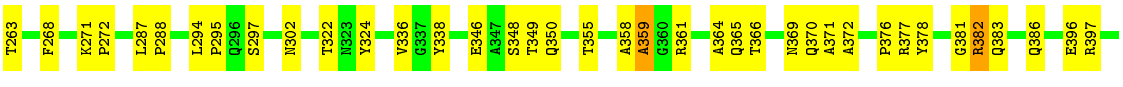
Chain M:

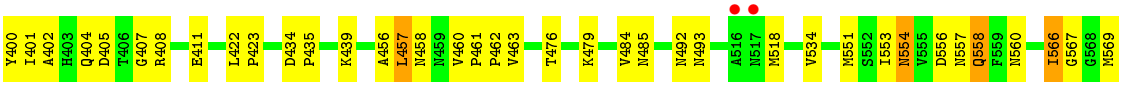




• Molecule 1: Capsid protein VP1

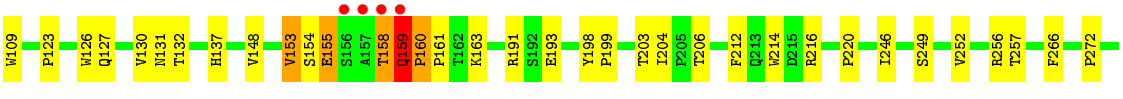
Chain O:

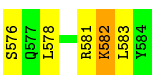




• Molecule 1: Capsid protein VP1

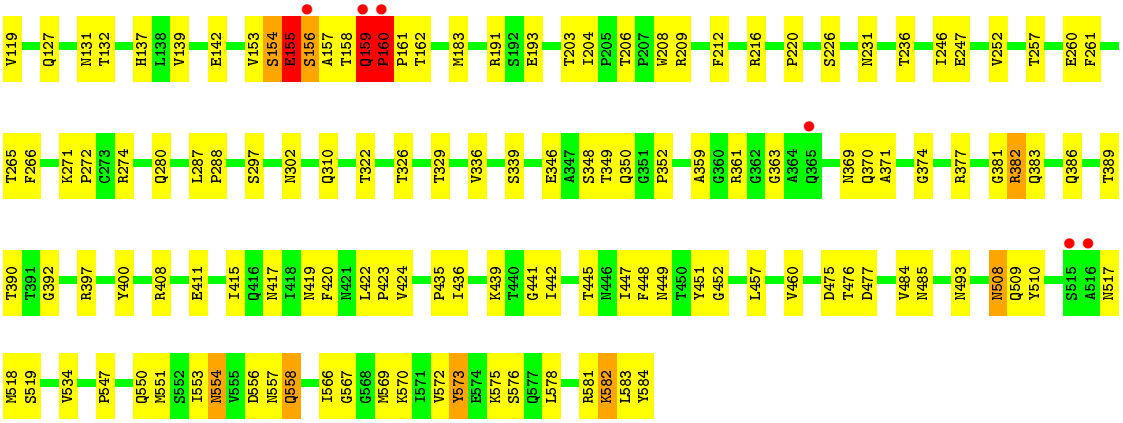
Chain P:



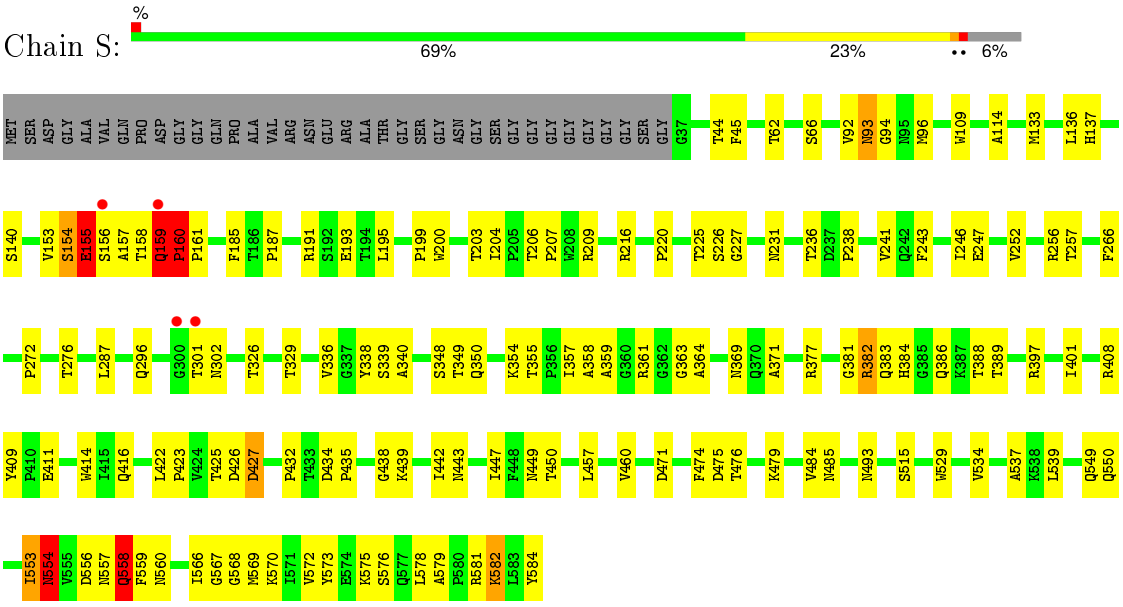


• Molecule 1: Capsid protein VP1

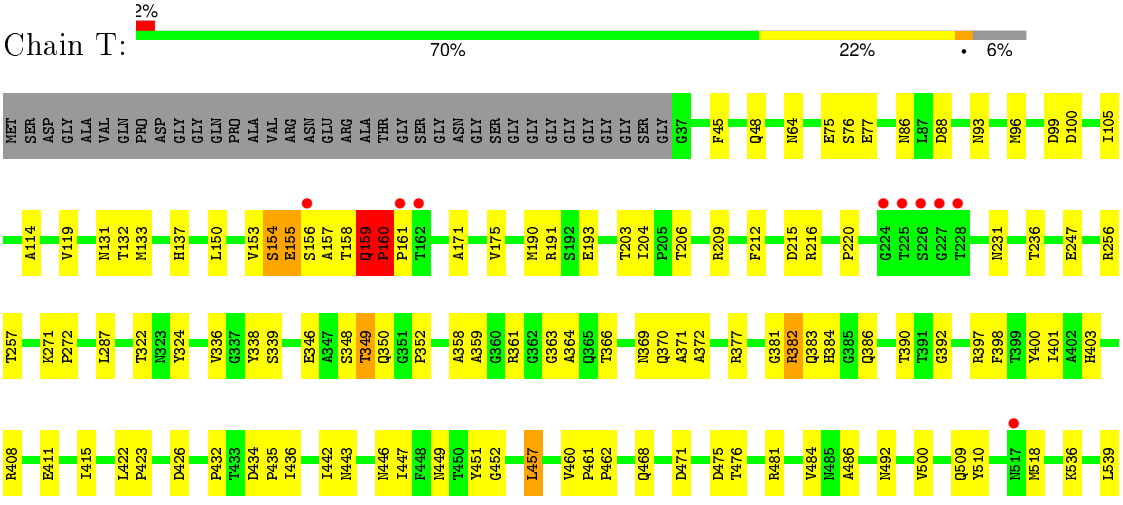
Chain R:

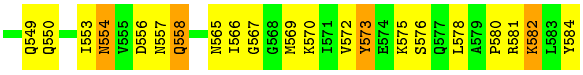


• Molecule 1: Capsid protein VP1

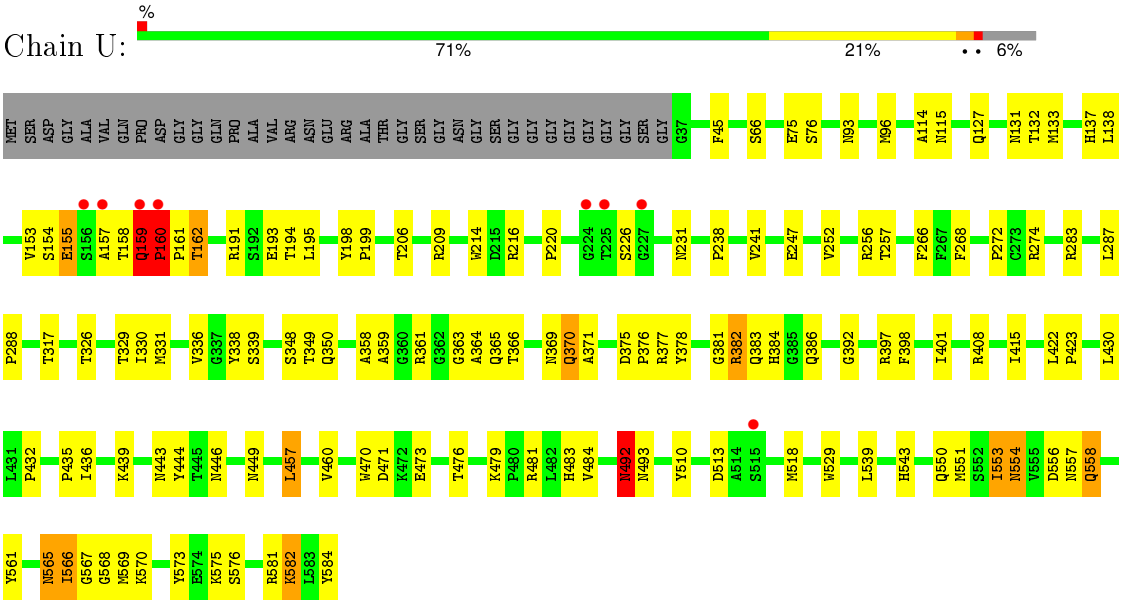


• Molecule 1: Capsid protein VP1

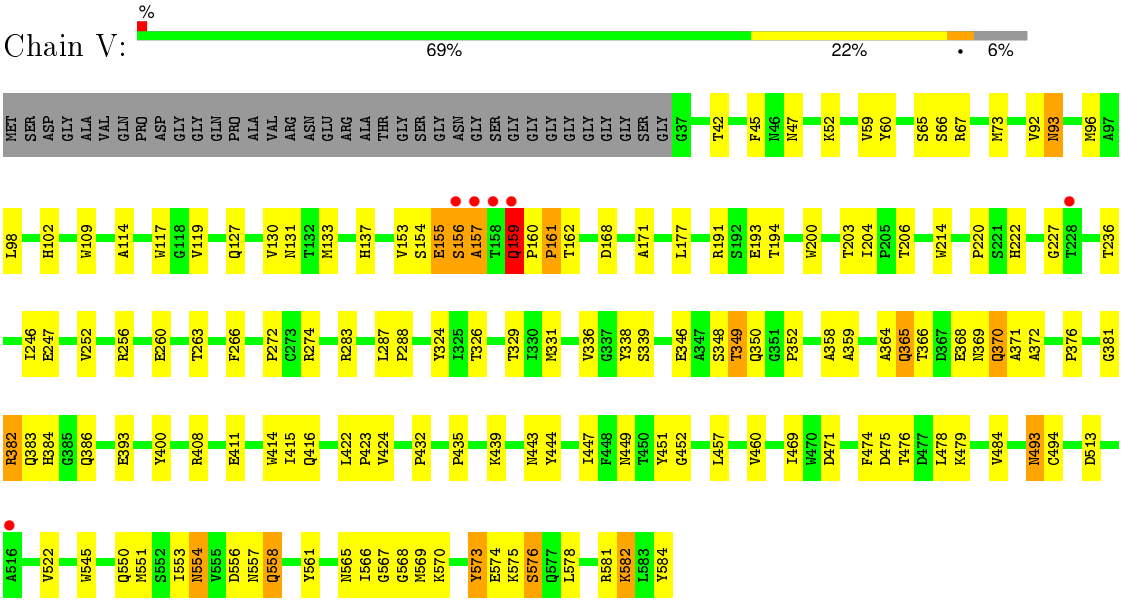




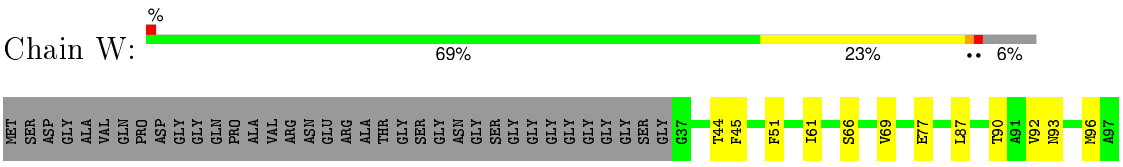
• Molecule 1: Capsid protein VP1

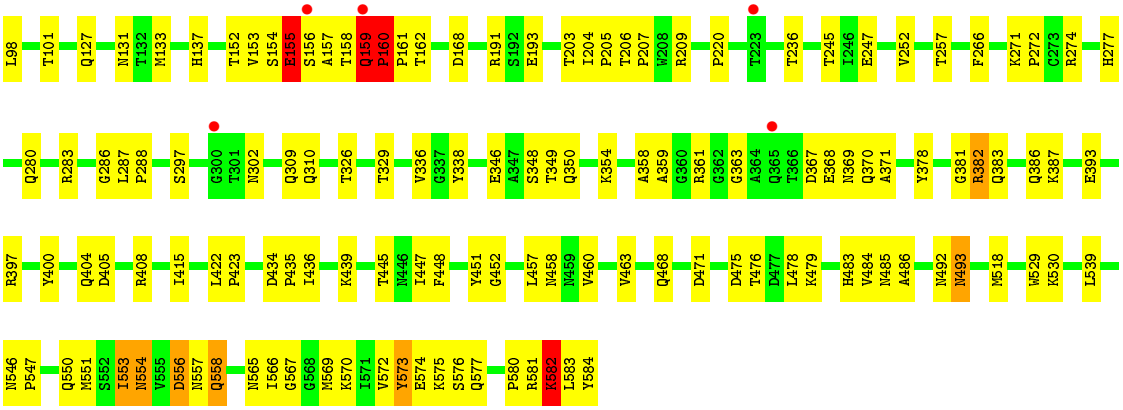


• Molecule 1: Capsid protein VP1



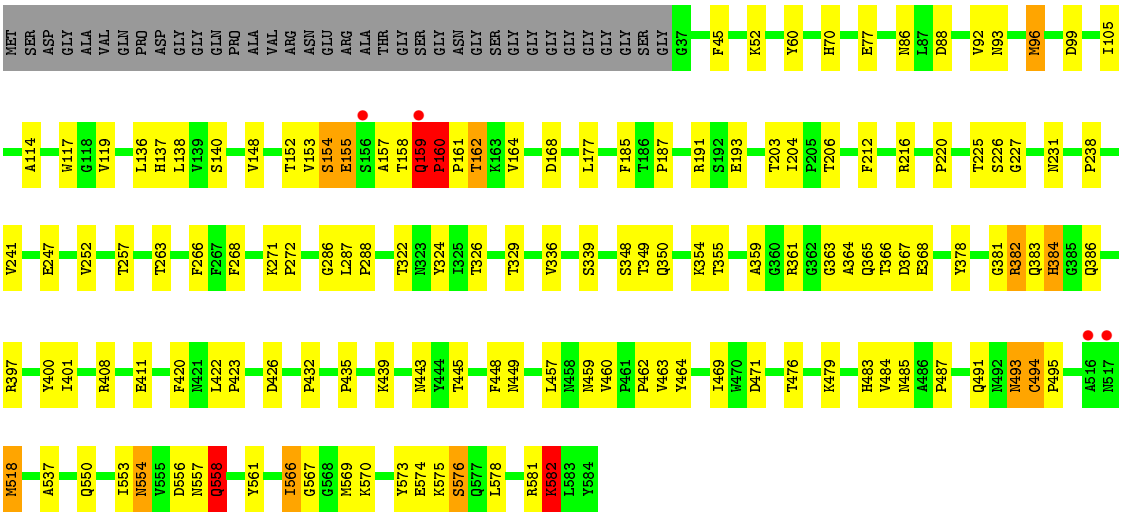
• Molecule 1: Capsid protein VP1





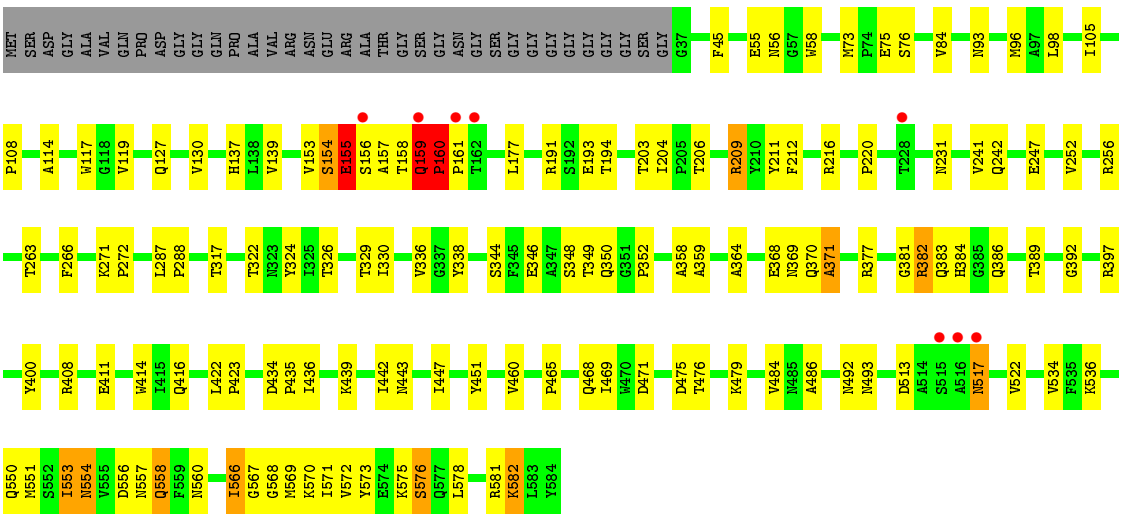
• Molecule 1: Capsid protein VP1

Chain X:



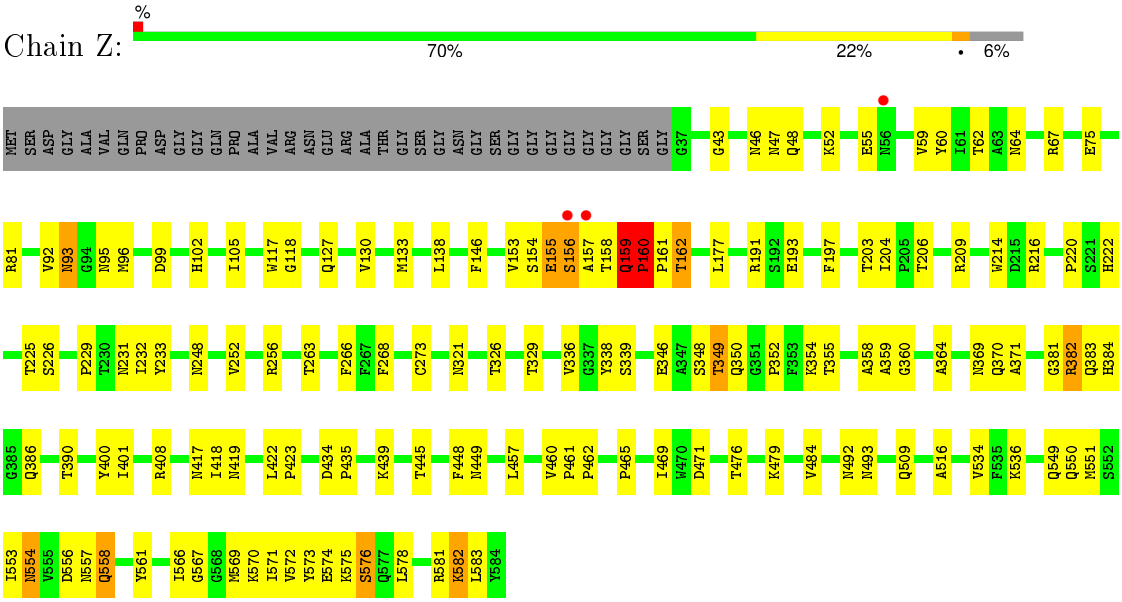
• Molecule 1: Capsid protein VP1

Chain Y:



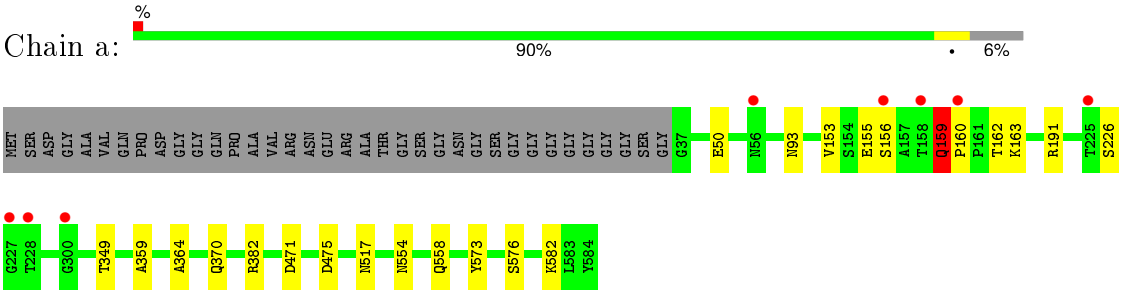
• Molecule 1: Capsid protein VP1

Chain Z:



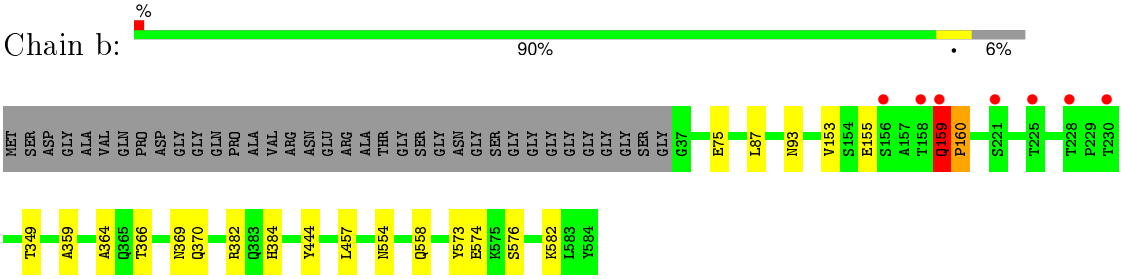
• Molecule 1: Capsid protein VP1

Chain a:



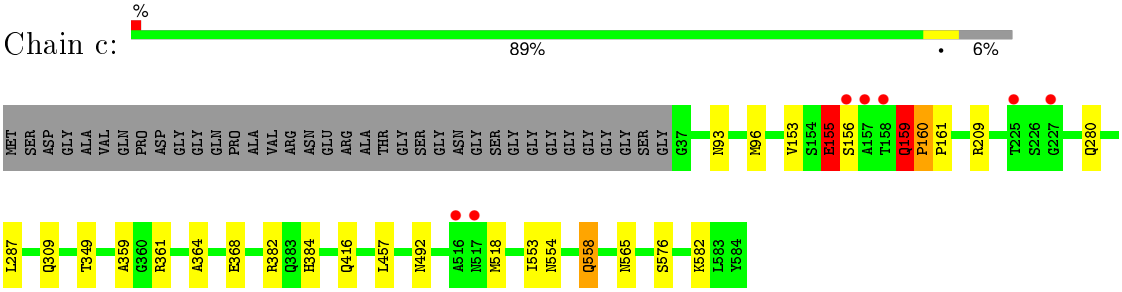
• Molecule 1: Capsid protein VP1

Chain b:



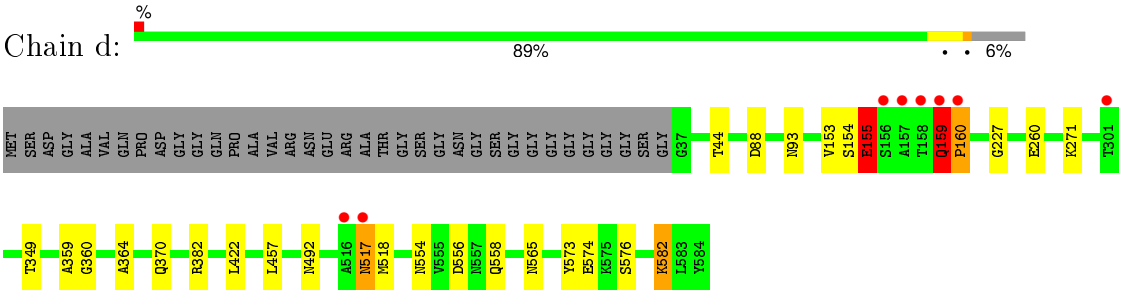
• Molecule 1: Capsid protein VP1

Chain c:



• Molecule 1: Capsid protein VP1

Chain d:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	453.10Å 453.10Å 319.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 3.50 49.99 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.99-3.50) 96.4 (49.99-3.50)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.65 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.180 , 0.221 0.175 , 0.216	Depositor DCC
R_{free} test set	19783 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	2 of 410636 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	130590	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.66	0/4483	0.70	2/6134 (0.0%)
1	B	0.63	0/4483	0.73	5/6134 (0.1%)
1	C	0.59	0/4483	0.73	4/6134 (0.1%)
1	D	0.58	0/4483	0.73	5/6134 (0.1%)
1	E	0.62	0/4483	0.73	4/6134 (0.1%)
1	F	0.63	1/4483 (0.0%)	0.84	9/6134 (0.1%)
1	G	0.59	0/4483	0.74	6/6134 (0.1%)
1	H	0.57	0/4483	0.72	3/6134 (0.0%)
1	I	0.64	0/4483	0.71	1/6134 (0.0%)
1	J	0.61	0/4483	0.71	5/6134 (0.1%)
1	K	0.67	0/4483	0.74	2/6134 (0.0%)
1	L	0.61	0/4483	0.73	3/6134 (0.0%)
1	M	0.66	0/4483	0.74	5/6134 (0.1%)
1	N	0.66	0/4483	0.72	6/6134 (0.1%)
1	O	0.58	0/4483	0.71	3/6134 (0.0%)
1	P	0.61	0/4483	0.73	4/6134 (0.1%)
1	Q	0.61	0/4483	0.72	5/6134 (0.1%)
1	R	0.63	0/4483	0.73	3/6134 (0.0%)
1	S	0.63	1/4483 (0.0%)	0.76	9/6134 (0.1%)
1	T	0.65	0/4483	0.72	4/6134 (0.1%)
1	U	0.60	0/4483	0.73	4/6134 (0.1%)
1	V	0.60	0/4483	0.70	1/6134 (0.0%)
1	W	0.55	0/4483	0.72	3/6134 (0.0%)
1	X	0.61	1/4483 (0.0%)	0.76	7/6134 (0.1%)
1	Y	0.56	0/4483	0.73	5/6134 (0.1%)
1	Z	0.60	2/4483 (0.0%)	0.74	4/6134 (0.1%)
1	a	0.55	0/4483	0.75	2/6134 (0.0%)
1	b	0.57	0/4483	0.73	3/6134 (0.0%)
1	c	0.58	0/4483	0.73	4/6134 (0.1%)
1	d	0.60	0/4483	0.76	7/6134 (0.1%)
All	All	0.61	5/134490 (0.0%)	0.73	128/184020 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	L	0	2
1	M	0	3
1	N	0	1
1	Q	0	1
1	R	0	2
1	S	0	2
1	U	0	1
1	W	0	1
1	X	0	1
1	Y	0	2
1	Z	0	1
1	a	0	1
1	b	0	1
1	c	0	2
1	d	0	3
All	All	0	34

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	222	HIS	CG-CD2	-8.08	1.22	1.35
1	F	426	ASP	CB-CG	-7.62	1.35	1.51
1	S	438	GLY	C-O	-5.81	1.14	1.23
1	X	426	ASP	CB-CG	-5.05	1.41	1.51
1	Z	273	CYS	CB-SG	-5.00	1.73	1.81

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	426	ASP	CB-CG-OD2	-27.25	93.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	159	GLN	C-N-CD	-18.61	79.65	120.60
1	X	159	GLN	C-N-CD	-16.06	85.27	120.60
1	F	426	ASP	CB-CG-OD1	15.33	132.10	118.30
1	C	159	GLN	C-N-CD	-13.92	89.97	120.60
1	D	159	GLN	C-N-CD	-13.15	91.68	120.60
1	G	159	GLN	C-N-CD	-12.82	92.40	120.60
1	W	159	GLN	C-N-CD	-12.75	92.56	120.60
1	B	159	GLN	C-N-CD	-12.73	92.59	120.60
1	Q	159	GLN	C-N-CD	-12.71	92.63	120.60
1	K	159	GLN	C-N-CD	-12.62	92.84	120.60
1	Z	159	GLN	C-N-CD	-12.36	93.41	120.60
1	R	159	GLN	C-N-CD	-12.28	93.58	120.60
1	c	159	GLN	C-N-CD	-11.80	94.65	120.60
1	b	159	GLN	C-N-CD	-11.37	95.58	120.60
1	H	159	GLN	C-N-CD	-11.17	96.03	120.60
1	M	159	GLN	C-N-CD	-10.84	96.76	120.60
1	E	160	PRO	C-N-CD	-10.82	96.78	120.60
1	S	426	ASP	CB-CG-OD1	-10.47	108.87	118.30
1	Y	159	GLN	C-N-CD	-10.42	97.67	120.60
1	d	159	GLN	C-N-CD	-9.78	99.08	120.60
1	L	159	GLN	C-N-CD	-9.60	99.47	120.60
1	A	159	GLN	C-N-CD	-8.54	101.81	120.60
1	N	159	GLN	C-N-CD	-8.37	102.19	120.60
1	J	159	GLN	C-N-CD	-8.11	102.75	120.60
1	U	159	GLN	C-N-CD	-8.06	102.86	120.60
1	M	155	GLU	N-CA-C	-8.05	89.27	111.00
1	E	159	GLN	C-N-CD	-7.99	103.03	120.60
1	X	159	GLN	C-N-CA	7.91	155.21	122.00
1	S	159	GLN	C-N-CD	-7.88	103.26	120.60
1	O	159	GLN	C-N-CD	-7.64	103.80	120.60
1	a	159	GLN	C-N-CA	7.59	153.89	122.00
1	F	159	GLN	C-N-CD	-7.56	103.96	120.60
1	T	159	GLN	C-N-CD	-7.45	104.21	120.60
1	d	227	GLY	N-CA-C	-7.14	95.25	113.10
1	T	160	PRO	C-N-CD	-7.10	104.98	120.60
1	S	160	PRO	C-N-CD	-7.10	104.99	120.60
1	b	160	PRO	C-N-CD	-7.00	105.19	120.60
1	d	155	GLU	N-CA-C	-6.99	92.13	111.00
1	B	159	GLN	C-N-CA	6.91	151.03	122.00
1	M	160	PRO	C-N-CD	-6.90	105.42	120.60
1	J	227	GLY	N-CA-C	-6.88	95.89	113.10
1	S	155	GLU	N-CA-C	-6.71	92.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	U	160	PRO	N-CA-C	6.67	129.44	112.10
1	P	158	THR	N-CA-C	-6.57	93.26	111.00
1	N	158	THR	N-CA-C	-6.53	93.36	111.00
1	F	160	PRO	N-CA-C	6.47	128.94	112.10
1	L	227	GLY	N-CA-C	-6.46	96.94	113.10
1	d	160	PRO	C-N-CD	-6.43	106.44	120.60
1	S	227	GLY	N-CA-C	-6.42	97.06	113.10
1	d	422	LEU	CA-CB-CG	6.42	130.05	115.30
1	S	426	ASP	CB-CG-OD2	6.38	124.04	118.30
1	Z	160	PRO	C-N-CD	-6.29	106.75	120.60
1	P	159	GLN	C-N-CD	-6.28	106.79	120.60
1	Y	160	PRO	C-N-CD	-6.26	106.83	120.60
1	P	160	PRO	C-N-CD	-6.20	106.95	120.60
1	Z	159	GLN	N-CA-C	6.19	127.70	111.00
1	I	155	GLU	N-CA-C	-6.18	94.32	111.00
1	L	160	PRO	C-N-CD	-6.13	107.12	120.60
1	Q	160	PRO	C-N-CD	-6.11	107.17	120.60
1	X	160	PRO	C-N-CD	-5.96	107.48	120.60
1	A	160	PRO	C-N-CD	-5.86	107.71	120.60
1	E	160	PRO	C-N-CA	5.83	146.51	122.00
1	C	160	PRO	C-N-CD	-5.79	107.85	120.60
1	S	160	PRO	N-CA-C	5.79	127.15	112.10
1	D	160	PRO	C-N-CD	-5.74	107.97	120.60
1	O	160	PRO	C-N-CD	-5.72	108.01	120.60
1	J	160	PRO	C-N-CD	-5.72	108.02	120.60
1	X	227	GLY	N-CA-C	-5.71	98.83	113.10
1	B	159	GLN	CA-CB-CG	5.70	125.95	113.40
1	X	426	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	G	209	ARG	CA-CB-CG	-5.68	100.90	113.40
1	F	426	ASP	OD1-CG-OD2	5.67	134.08	123.30
1	H	160	PRO	C-N-CD	-5.65	108.18	120.60
1	V	227	GLY	N-CA-C	-5.62	99.04	113.10
1	X	160	PRO	N-CA-C	5.60	126.67	112.10
1	T	160	PRO	N-CA-C	5.58	126.61	112.10
1	J	160	PRO	N-CA-C	5.56	126.55	112.10
1	N	160	PRO	N-CA-C	5.53	126.47	112.10
1	N	227	GLY	N-CA-C	-5.46	99.46	113.10
1	G	159	GLN	C-N-CA	5.45	144.91	122.00
1	W	160	PRO	C-N-CD	-5.44	108.63	120.60
1	c	160	PRO	C-N-CD	-5.44	108.63	120.60
1	W	155	GLU	N-CA-C	-5.44	96.31	111.00
1	Z	360	GLY	N-CA-C	-5.42	99.55	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	159	GLN	C-N-CA	5.42	144.76	122.00
1	S	160	PRO	C-N-CA	5.42	144.75	122.00
1	R	155	GLU	CA-CB-CG	5.39	125.25	113.40
1	Y	155	GLU	N-CA-C	-5.37	96.51	111.00
1	U	160	PRO	C-N-CD	-5.37	108.79	120.60
1	F	439	LYS	CG-CD-CE	-5.36	95.81	111.90
1	G	160	PRO	CA-N-CD	-5.35	104.01	111.50
1	R	160	PRO	C-N-CD	-5.34	108.84	120.60
1	D	155	GLU	N-CA-C	-5.34	96.59	111.00
1	Q	155	GLU	N-CA-C	-5.33	96.61	111.00
1	B	160	PRO	N-CA-C	5.33	125.96	112.10
1	b	160	PRO	C-N-CA	5.32	144.34	122.00
1	P	160	PRO	N-CA-C	5.31	125.91	112.10
1	M	553	ILE	C-N-CA	5.30	134.96	121.70
1	D	159	GLN	C-N-CA	5.29	144.23	122.00
1	c	155	GLU	N-CA-C	-5.29	96.72	111.00
1	Q	159	GLN	C-N-CA	5.28	144.19	122.00
1	D	154	SER	C-N-CA	5.28	134.90	121.70
1	O	160	PRO	N-CA-C	5.27	125.81	112.10
1	C	159	GLN	C-N-CA	5.27	144.15	122.00
1	F	439	LYS	CD-CE-NZ	5.25	123.77	111.70
1	Q	154	SER	C-N-CA	5.24	134.80	121.70
1	N	160	PRO	C-N-CD	-5.22	109.11	120.60
1	C	154	SER	C-N-CA	5.19	134.68	121.70
1	Y	154	SER	C-N-CA	5.19	134.66	121.70
1	N	553	ILE	C-N-CA	5.15	134.58	121.70
1	X	154	SER	C-N-CA	5.15	134.58	121.70
1	G	106	VAL	CB-CA-C	-5.09	101.72	111.40
1	K	553	ILE	C-N-CA	5.08	134.41	121.70
1	d	574	GLU	N-CA-C	5.08	124.71	111.00
1	E	553	ILE	C-N-CA	5.08	134.39	121.70
1	M	160	PRO	C-N-CA	5.07	143.29	122.00
1	d	154	SER	C-N-CA	5.07	134.36	121.70
1	T	160	PRO	C-N-CA	5.06	143.25	122.00
1	Y	553	ILE	C-N-CA	5.06	134.35	121.70
1	F	574	GLU	N-CA-C	5.05	124.63	111.00
1	U	159	GLN	C-N-CA	5.05	143.19	122.00
1	S	553	ILE	C-N-CA	5.02	134.26	121.70
1	c	553	ILE	C-N-CA	5.02	134.25	121.70
1	B	574	GLU	N-CA-C	5.02	124.54	111.00
1	G	160	PRO	C-N-CD	-5.01	109.57	120.60
1	H	553	ILE	C-N-CA	5.01	134.23	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	154	SER	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	GLN	Peptide
1	C	159	GLN	Peptide
1	C	226	SER	Peptide
1	D	159	GLN	Peptide
1	D	226	SER	Peptide
1	E	368	GLU	Peptide
1	F	226	SER	Peptide
1	G	159	GLN	Peptide
1	H	159	GLN	Peptide
1	I	226	SER	Peptide
1	L	159	GLN	Peptide
1	L	226	SER	Peptide
1	M	155	GLU	Peptide
1	M	156	SER	Peptide
1	M	159	GLN	Peptide
1	N	226	SER	Peptide
1	Q	159	GLN	Peptide
1	R	159	GLN	Peptide
1	R	226	SER	Peptide
1	S	159	GLN	Peptide
1	S	226	SER	Peptide
1	U	226	SER	Peptide
1	W	159	GLN	Peptide
1	X	226	SER	Peptide
1	Y	159	GLN	Peptide
1	Y	517	ASN	Peptide
1	Z	159	GLN	Peptide
1	a	159	GLN	Peptide
1	b	159	GLN	Peptide
1	c	155	GLU	Peptide
1	c	159	GLN	Peptide
1	d	155	GLU	Peptide
1	d	159	GLN	Peptide
1	d	360	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4352	0	4143	207	0
1	B	4352	0	4143	216	0
1	C	4352	0	4143	176	2
1	D	4352	0	4143	190	4
1	E	4352	0	4143	128	0
1	F	4352	0	4143	131	0
1	G	4352	0	4143	122	3
1	H	4352	0	4143	125	0
1	I	4352	0	4143	131	0
1	J	4352	0	4143	83	2
1	K	4352	0	4143	122	0
1	L	4352	0	4143	130	0
1	M	4352	0	4143	118	0
1	N	4352	0	4143	102	2
1	O	4352	0	4143	98	5
1	P	4352	0	4143	104	0
1	Q	4352	0	4143	81	5
1	R	4352	0	4143	120	0
1	S	4352	0	4143	92	2
1	T	4352	0	4143	110	0
1	U	4352	0	4143	106	3
1	V	4352	0	4143	128	0
1	W	4352	0	4143	124	0
1	X	4352	0	4145	93	4
1	Y	4352	0	4143	111	2
1	Z	4352	0	4143	87	2
1	a	4352	0	4143	0	3
1	b	4352	0	4143	0	0
1	c	4352	0	4143	0	1
1	d	4352	0	4143	0	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	G	1	0	0	0	0
2	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1	0	0	0	0
2	J	2	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
2	Y	2	0	0	0	0
2	Z	1	0	0	0	0
2	c	1	0	0	0	0
2	d	2	0	0	0	0
All	All	130590	0	124292	2724	20

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 11.

All (2724) 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:L:553:ILE:HA	1:L:554:ASN:HB2	1.35	1.08
1:B:553:ILE:HA	1:B:554:ASN:HB2	1.42	1.07
1:V:154:SER:HA	1:V:155:GLU:HB2	1.36	1.06
1:R:154:SER:HA	1:R:155:GLU:HG3	1.33	1.06
1:Z:553:ILE:HA	1:Z:554:ASN:HB2	1.37	1.05
1:I:553:ILE:HA	1:I:554:ASN:HB2	1.36	1.04
1:Y:553:ILE:HA	1:Y:554:ASN:HB2	1.41	1.03
1:J:553:ILE:HA	1:J:554:ASN:HB2	1.40	1.03
1:O:553:ILE:HA	1:O:554:ASN:HB2	1.40	1.01
1:D:553:ILE:HA	1:D:554:ASN:HB2	1.45	1.01
1:A:553:ILE:HA	1:A:554:ASN:HB2	1.41	1.01
1:G:553:ILE:HA	1:G:554:ASN:HB2	1.39	0.99
1:C:553:ILE:HA	1:C:554:ASN:HB2	1.42	0.99
1:Q:553:ILE:HA	1:Q:554:ASN:HB2	1.41	0.98
1:P:382:ARG:H	1:P:386:GLN:HB3	1.27	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:288:PRO:O	1:T:209:ARG:NH1	1.96	0.98
1:W:154:SER:HA	1:W:155:GLU:HB2	1.43	0.98
1:N:382:ARG:H	1:N:386:GLN:HB3	1.27	0.98
1:O:193:GLU:HB3	1:O:206:THR:HG21	1.44	0.98
1:W:553:ILE:HA	1:W:554:ASN:HB2	1.43	0.98
1:U:553:ILE:HA	1:U:554:ASN:HB2	1.46	0.98
1:X:553:ILE:HA	1:X:554:ASN:HB2	1.41	0.98
1:T:553:ILE:HA	1:T:554:ASN:HB2	1.46	0.97
1:S:553:ILE:HA	1:S:554:ASN:HB2	1.44	0.97
1:B:368:GLU:HG3	1:B:369:ASN:H	3.29	0.96
1:R:553:ILE:HA	1:R:554:ASN:HB2	1.43	0.96
1:P:553:ILE:HA	1:P:554:ASN:HB2	1.45	0.95
1:G:154:SER:HA	1:G:155:GLU:HB2	1.47	0.95
1:H:154:SER:HA	1:H:155:GLU:HB2	1.44	0.95
1:M:553:ILE:HA	1:M:554:ASN:HB2	1.49	0.95
1:A:382:ARG:H	1:A:386:GLN:HB3	1.31	0.94
1:U:154:SER:HA	1:U:155:GLU:HB2	1.45	0.94
1:E:553:ILE:HA	1:E:554:ASN:HB2	1.47	0.94
1:O:382:ARG:H	1:O:386:GLN:HB2	1.31	0.93
1:Q:193:GLU:HB3	1:Q:206:THR:HG21	1.50	0.93
1:I:382:ARG:H	1:I:386:GLN:HB3	1.33	0.93
1:H:553:ILE:HA	1:H:554:ASN:HB2	1.45	0.93
1:D:382:ARG:H	1:D:386:GLN:HB3	1.53	0.93
1:K:154:SER:HA	1:K:155:GLU:HB2	1.48	0.93
1:U:193:GLU:HB3	1:U:206:THR:HG21	1.50	0.92
1:Z:96:MET:HG2	1:Z:220:PRO:HA	1.50	0.92
1:K:553:ILE:HA	1:K:554:ASN:HB2	1.48	0.92
1:Y:193:GLU:HB3	1:Y:206:THR:HG21	1.51	0.91
1:N:287:LEU:O	1:S:191:ARG:NH1	2.04	0.90
1:X:382:ARG:H	1:X:386:GLN:HB3	1.33	0.90
1:F:553:ILE:HA	1:F:554:ASN:HB2	1.52	0.90
1:K:382:ARG:H	1:K:386:GLN:HB3	1.36	0.89
1:F:154:SER:HA	1:F:155:GLU:HB2	1.51	0.89
1:Z:154:SER:HA	1:Z:155:GLU:HB2	1.54	0.89
1:B:191:ARG:NH1	1:M:287:LEU:O	2.04	0.89
1:T:271:LYS:HG2	1:T:272:PRO:HD2	1.54	0.89
1:C:382:ARG:H	1:C:386:GLN:HB3	1.38	0.89
1:D:193:GLU:HB3	1:D:206:THR:HG21	1.60	0.89
1:B:365:GLN:O	1:B:367:ASP:N	2.69	0.88
1:M:209:ARG:NH1	1:R:288:PRO:O	2.05	0.88
1:E:209:ARG:NH1	1:I:288:PRO:O	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:193:GLU:HB3	1:P:206:THR:HG21	1.56	0.88
1:C:554:ASN:HD22	1:C:557:ASN:HD22	3.14	0.88
1:V:382:ARG:H	1:V:386:GLN:HB3	1.36	0.88
1:N:553:ILE:HA	1:N:554:ASN:HB2	1.55	0.87
1:W:193:GLU:HB3	1:W:206:THR:HG21	1.56	0.87
1:Y:193:GLU:OE1	1:Y:209:ARG:NH2	2.08	0.87
1:X:159:GLN:HG2	1:X:160:PRO:HD2	1.57	0.87
1:U:382:ARG:H	1:U:386:GLN:HB3	1.39	0.86
1:A:193:GLU:HB3	1:A:206:THR:HG21	1.67	0.85
1:C:193:GLU:HB3	1:C:206:THR:HG21	1.63	0.85
1:H:193:GLU:HB3	1:H:206:THR:HG21	1.59	0.85
1:D:154:SER:HA	1:D:155:GLU:HB2	1.62	0.85
1:E:159:GLN:HG3	1:E:160:PRO:HD2	1.58	0.84
1:A:582:LYS:NZ	1:K:244:TYR:OH	2.08	0.84
1:C:369:ASN:O	1:C:371:ALA:N	2.10	0.84
1:Y:271:LYS:HG3	1:Y:272:PRO:HD2	1.58	0.84
1:A:154:SER:HA	1:A:155:GLU:HB3	2.32	0.84
1:V:156:SER:HA	1:V:162:THR:O	1.77	0.84
1:M:193:GLU:HB3	1:M:206:THR:HG21	1.59	0.84
1:X:554:ASN:HD22	1:X:557:ASN:HD22	1.26	0.84
1:R:193:GLU:HB3	1:R:206:THR:HG21	1.57	0.84
1:V:553:ILE:HA	1:V:554:ASN:HB2	1.60	0.83
1:I:554:ASN:HB3	1:I:557:ASN:HB3	1.60	0.83
1:D:271:LYS:HG2	1:D:272:PRO:HD2	4.81	0.83
1:B:209:ARG:NH1	1:W:288:PRO:O	130.94	0.83
1:B:287:LEU:O	1:H:191:ARG:NH1	125.72	0.83
1:B:369:ASN:O	1:B:371:ALA:N	2.27	0.83
1:J:154:SER:HA	1:J:155:GLU:HB2	1.60	0.83
1:B:581:ARG:NH1	1:H:475:ASP:O	116.82	0.83
1:J:193:GLU:HB3	1:J:206:THR:HG21	1.58	0.83
1:D:191:ARG:NH1	1:L:287:LEU:O	116.77	0.83
1:G:193:GLU:HB3	1:G:206:THR:HG21	1.59	0.83
1:T:159:GLN:HG2	1:T:160:PRO:HD2	1.60	0.82
1:L:382:ARG:H	1:L:386:GLN:HB3	1.43	0.82
1:C:561:TYR:OH	1:C:574:GLU:OE2	1.97	0.82
1:S:193:GLU:HB3	1:S:206:THR:HG21	1.61	0.81
1:I:425:THR:HG22	1:I:427:ASP:H	1.45	0.81
1:V:193:GLU:HB3	1:V:206:THR:HG21	1.61	0.81
1:A:287:LEU:O	1:Y:191:ARG:NH1	152.46	0.81
1:B:401:ILE:O	1:B:575:LYS:NZ	2.37	0.81
1:M:561:TYR:OH	1:M:574:GLU:OE2	1.99	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:GLN:OE1	1:C:370:GLN:N	2.14	0.81
1:K:287:LEU:O	1:T:191:ARG:NH1	2.14	0.80
1:C:154:SER:HA	1:C:155:GLU:HB2	2.16	0.80
1:E:287:LEU:O	1:V:191:ARG:NH1	2.14	0.80
1:F:369:ASN:O	1:F:371:ALA:N	2.14	0.80
1:Y:382:ARG:H	1:Y:386:GLN:HB3	1.46	0.80
1:Q:96:MET:HG2	1:Q:220:PRO:HA	1.62	0.80
1:C:191:ARG:NH1	1:P:287:LEU:O	2.14	0.80
1:B:287:LEU:O	1:R:191:ARG:NH1	2.14	0.80
1:S:554:ASN:HB3	1:S:557:ASN:HB3	1.64	0.80
1:G:561:TYR:OH	1:G:574:GLU:OE2	2.00	0.80
1:C:348:SER:O	1:C:350:GLN:N	2.14	0.80
1:W:297:SER:O	1:W:302:ASN:ND2	2.13	0.80
1:G:554:ASN:HD22	1:G:557:ASN:HD22	1.29	0.79
1:T:554:ASN:HB3	1:T:557:ASN:HB3	1.62	0.79
1:Z:382:ARG:H	1:Z:386:GLN:HB3	1.48	0.79
1:G:382:ARG:H	1:G:386:GLN:HB3	1.47	0.79
1:B:45:PHE:HB3	1:D:252:VAL:HB	30.05	0.79
1:L:336:VAL:O	1:L:408:ARG:NH2	2.15	0.79
1:D:287:LEU:O	1:F:191:ARG:NH1	111.35	0.79
1:J:382:ARG:H	1:J:386:GLN:HB3	1.48	0.79
1:O:401:ILE:O	1:O:575:LYS:NZ	2.15	0.79
1:Q:382:ARG:H	1:Q:386:GLN:HB3	1.46	0.79
1:F:382:ARG:H	1:F:386:GLN:HB3	1.46	0.79
1:M:191:ARG:NH1	1:R:287:LEU:O	2.16	0.79
1:T:382:ARG:H	1:T:386:GLN:HB3	1.46	0.79
1:H:382:ARG:H	1:H:386:GLN:HB3	1.46	0.79
1:R:554:ASN:HB3	1:R:557:ASN:HB3	1.65	0.78
1:B:191:ARG:NH1	1:W:287:LEU:O	131.70	0.78
1:E:193:GLU:HB3	1:E:206:THR:HG21	1.64	0.78
1:S:382:ARG:H	1:S:386:GLN:HB3	1.49	0.78
1:A:96:MET:HG2	1:A:220:PRO:HA	1.65	0.78
1:I:191:ARG:NH1	1:V:287:LEU:O	2.17	0.78
1:N:158:THR:O	1:N:159:GLN:HB3	1.82	0.78
1:J:96:MET:HG2	1:J:220:PRO:HA	1.65	0.78
1:K:193:GLU:HB3	1:K:206:THR:HG21	1.63	0.78
1:F:401:ILE:O	1:F:575:LYS:NZ	2.16	0.78
1:H:348:SER:O	1:H:350:GLN:N	2.17	0.78
1:I:348:SER:O	1:I:350:GLN:N	2.17	0.78
1:Y:554:ASN:HD22	1:Y:557:ASN:HD22	1.29	0.77
1:N:550:GLN:OE1	1:T:131:ASN:ND2	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:PRO:O	1:D:209:ARG:NH1	5.04	0.77
1:L:193:GLU:HB3	1:L:206:THR:HG21	1.66	0.77
1:H:96:MET:HG2	1:H:220:PRO:HA	1.65	0.77
1:D:550:GLN:OE1	1:G:131:ASN:ND2	62.53	0.77
1:G:554:ASN:HB3	1:G:557:ASN:HB3	1.67	0.77
1:O:348:SER:O	1:O:350:GLN:N	2.17	0.77
1:A:287:LEU:O	1:K:191:ARG:NH1	2.18	0.77
1:V:96:MET:HG2	1:V:220:PRO:HA	1.65	0.77
1:U:96:MET:HG2	1:U:220:PRO:HA	1.67	0.77
1:X:348:SER:O	1:X:350:GLN:N	2.18	0.76
1:B:348:SER:O	1:B:350:GLN:N	2.18	0.76
1:J:554:ASN:HB3	1:J:557:ASN:HB3	1.66	0.76
1:E:191:ARG:NH1	1:I:287:LEU:O	2.18	0.76
1:M:382:ARG:H	1:M:386:GLN:HB3	1.50	0.76
1:H:554:ASN:HB3	1:H:557:ASN:HB3	1.67	0.76
1:S:401:ILE:O	1:S:575:LYS:NZ	2.17	0.76
1:J:191:ARG:NH1	1:U:287:LEU:O	2.19	0.76
1:N:348:SER:O	1:N:350:GLN:N	2.19	0.76
1:H:287:LEU:O	1:W:191:ARG:NH1	2.18	0.76
1:Q:361:ARG:NH2	1:Q:364:ALA:O	2.18	0.76
1:C:554:ASN:HB3	1:C:557:ASN:HB3	1.70	0.76
1:B:154:SER:HA	1:B:155:GLU:HB3	3.26	0.76
1:Z:554:ASN:HB3	1:Z:557:ASN:HB3	1.68	0.76
1:M:96:MET:HG2	1:M:220:PRO:HA	1.67	0.76
1:N:236:THR:HB	1:Q:558:GLN:HE22	1.50	0.75
1:A:191:ARG:NH1	1:T:287:LEU:O	2.19	0.75
1:N:131:ASN:ND2	1:T:550:GLN:OE1	2.17	0.75
1:Z:381:GLY:O	1:Z:383:GLN:N	2.20	0.75
1:P:369:ASN:O	1:P:371:ALA:N	2.18	0.75
1:Z:369:ASN:O	1:Z:371:ALA:N	2.19	0.75
1:C:361:ARG:NH1	1:C:363:GLY:O	2.20	0.75
1:L:348:SER:O	1:L:350:GLN:N	2.20	0.75
1:E:382:ARG:H	1:E:386:GLN:HB3	1.52	0.75
1:O:554:ASN:HD22	1:O:557:ASN:HD22	1.34	0.75
1:C:207:PRO:O	1:C:209:ARG:NH1	2.19	0.75
1:O:271:LYS:HG2	1:O:272:PRO:HD2	1.68	0.75
1:N:569:MET:HG2	1:N:570:LYS:H	1.51	0.75
1:B:96:MET:HG2	1:B:220:PRO:HA	1.67	0.75
1:I:193:GLU:OE1	1:I:209:ARG:NH2	2.20	0.75
1:U:443:ASN:OD1	1:U:446:ASN:ND2	2.20	0.75
1:Z:46:ASN:ND2	1:Z:64:ASN:HD22	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:401:ILE:O	1:I:575:LYS:NZ	2.20	0.74
1:Y:554:ASN:HB3	1:Y:557:ASN:HB3	1.70	0.74
1:H:584:TYR:OH	1:W:471:ASP:OD1	2.04	0.74
1:M:348:SER:O	1:M:350:GLN:N	2.21	0.74
1:B:554:ASN:HB3	1:B:557:ASN:HB3	1.68	0.74
1:E:96:MET:HG2	1:E:220:PRO:HA	1.68	0.74
1:W:382:ARG:H	1:W:386:GLN:HB3	1.52	0.74
1:X:193:GLU:HB3	1:X:206:THR:HG21	1.69	0.74
1:B:382:ARG:H	1:B:386:GLN:HB3	1.52	0.74
1:P:348:SER:O	1:P:350:GLN:N	2.20	0.74
1:T:193:GLU:HB3	1:T:206:THR:HG21	1.69	0.74
1:F:193:GLU:HB3	1:F:206:THR:HG21	1.69	0.73
1:K:554:ASN:HB3	1:K:557:ASN:HB3	1.70	0.73
1:C:191:ARG:NH1	1:G:287:LEU:O	123.46	0.73
1:B:56:ASN:OD1	1:B:58:TRP:HD1	4.62	0.73
1:B:193:GLU:HB3	1:B:206:THR:HG21	1.83	0.73
1:N:193:GLU:HB3	1:N:206:THR:HG21	1.70	0.73
1:A:348:SER:O	1:A:350:GLN:N	2.25	0.73
1:D:361:ARG:NH2	1:D:405:ASP:HB3	2.02	0.73
1:X:336:VAL:O	1:X:408:ARG:NH2	2.21	0.73
1:B:415:ILE:HD12	1:R:447:ILE:HG22	1.70	0.73
1:I:193:GLU:HB3	1:I:206:THR:HG21	1.70	0.73
1:B:581:ARG:NH1	1:R:475:ASP:O	2.22	0.73
1:R:348:SER:O	1:R:350:GLN:N	2.21	0.73
1:S:348:SER:O	1:S:350:GLN:N	2.22	0.73
1:G:348:SER:O	1:G:350:GLN:N	2.21	0.73
1:S:336:VAL:O	1:S:408:ARG:NH2	2.21	0.73
1:D:348:SER:O	1:D:350:GLN:N	2.21	0.73
1:A:554:ASN:HB3	1:A:557:ASN:HB3	1.70	0.73
1:U:382:ARG:NH2	1:U:392:GLY:O	2.22	0.73
1:I:558:GLN:HE22	1:K:236:THR:HB	1.53	0.72
1:Z:321:ASN:ND2	1:Z:418:ILE:O	2.21	0.72
1:G:137:HIS:CD2	1:G:272:PRO:HB3	2.24	0.72
1:I:475:ASP:O	1:V:581:ARG:NH1	2.23	0.72
1:O:154:SER:HA	1:O:155:GLU:HG2	1.70	0.72
1:O:382:ARG:N	1:O:386:GLN:HB2	2.05	0.72
1:I:209:ARG:NH1	1:V:288:PRO:O	2.22	0.72
1:M:471:ASP:OD1	1:R:584:TYR:OH	2.07	0.72
1:H:581:ARG:NH1	1:W:475:ASP:O	2.23	0.72
1:D:159:GLN:HB2	1:D:160:PRO:HD2	4.33	0.72
1:K:59:VAL:HG21	1:K:133:MET:HE2	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:348:SER:O	1:J:350:GLN:N	2.23	0.71
1:U:154:SER:CA	1:U:155:GLU:HB2	2.20	0.71
1:H:369:ASN:O	1:H:371:ALA:N	2.23	0.71
1:D:336:VAL:O	1:D:408:ARG:NH2	2.60	0.71
1:F:96:MET:HG2	1:F:220:PRO:HA	1.71	0.71
1:B:368:GLU:HG3	1:B:369:ASN:N	3.03	0.71
1:A:153:VAL:HG12	1:A:163:LYS:HE2	3.92	0.71
1:Y:381:GLY:O	1:Y:383:GLN:N	2.24	0.71
1:X:554:ASN:HB3	1:X:557:ASN:HB3	1.72	0.71
1:B:193:GLU:OE1	1:B:209:ARG:NH2	2.58	0.71
1:P:159:GLN:HE22	1:R:161:PRO:HB3	1.55	0.71
1:B:475:ASP:O	1:M:581:ARG:NH1	2.23	0.71
1:A:159:GLN:C	1:A:161:PRO:HA	2.11	0.71
1:W:368:GLU:HG2	1:W:369:ASN:N	2.04	0.71
1:D:387:LYS:HD2	1:D:570:LYS:HE2	1.73	0.71
1:N:377:ARG:HH21	1:N:397:ARG:HD2	1.55	0.71
1:J:553:ILE:CA	1:J:554:ASN:HB2	2.21	0.71
1:Z:193:GLU:HB3	1:Z:206:THR:HG21	1.71	0.71
1:Z:348:SER:O	1:Z:350:GLN:N	2.23	0.71
1:Y:369:ASN:O	1:Y:371:ALA:N	2.22	0.71
1:E:434:ASP:OD2	1:V:439:LYS:NZ	2.23	0.71
1:N:581:ARG:NH1	1:S:475:ASP:O	2.24	0.71
1:N:415:ILE:HD12	1:S:447:ILE:HG22	1.72	0.71
1:K:131:ASN:ND2	1:R:550:GLN:OE1	2.24	0.71
1:H:297:SER:O	1:V:565:ASN:ND2	2.24	0.71
1:L:260:GLU:HG3	1:L:261:PHE:N	2.05	0.71
1:E:280:GLN:NE2	1:E:583:LEU:H	1.89	0.71
1:R:154:SER:CA	1:R:155:GLU:HG3	2.19	0.70
1:F:554:ASN:HB3	1:F:557:ASN:HB3	1.73	0.70
1:W:554:ASN:HB3	1:W:557:ASN:HB3	1.72	0.70
1:K:565:ASN:HD21	1:R:302:ASN:HB2	1.55	0.70
1:O:460:VAL:HG11	1:O:484:VAL:HA	1.72	0.70
1:T:96:MET:HG2	1:T:220:PRO:HA	1.73	0.70
1:Q:381:GLY:O	1:Q:383:GLN:N	2.24	0.70
1:L:554:ASN:HB3	1:L:557:ASN:HB3	1.73	0.70
1:M:193:GLU:OE1	1:M:209:ARG:NH2	2.24	0.70
1:V:381:GLY:O	1:V:383:GLN:N	2.23	0.70
1:V:369:ASN:O	1:V:371:ALA:N	2.21	0.70
1:X:381:GLY:O	1:X:383:GLN:N	2.24	0.70
1:A:45:PHE:HB3	1:B:252:VAL:HB	136.26	0.70
1:L:381:GLY:O	1:L:383:GLN:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:348:SER:O	1:T:350:GLN:N	2.25	0.70
1:D:554:ASN:ND2	1:D:556:ASP:OD1	6.84	0.70
1:D:558:GLN:HE22	1:G:236:THR:HB	1.57	0.70
1:E:550:GLN:OE1	1:U:131:ASN:ND2	2.20	0.70
1:Q:154:SER:HA	1:Q:155:GLU:HB2	1.73	0.70
1:Y:137:HIS:CE1	1:Y:272:PRO:HB3	2.26	0.70
1:U:326:THR:H	1:U:329:THR:HB	1.57	0.70
1:K:348:SER:O	1:K:350:GLN:N	2.24	0.70
1:F:569:MET:HG2	1:F:570:LYS:H	1.56	0.70
1:D:425:THR:HG22	1:D:427:ASP:H	1.56	0.70
1:K:96:MET:HG2	1:K:220:PRO:HA	1.72	0.70
1:S:154:SER:HA	1:S:155:GLU:HB2	1.73	0.70
1:C:492:ASN:OD1	1:C:493:ASN:N	2.24	0.70
1:A:558:GLN:HE22	1:E:236:THR:HB	1.56	0.70
1:L:154:SER:HA	1:L:155:GLU:HB2	1.73	0.70
1:Z:401:ILE:O	1:Z:575:LYS:NZ	2.25	0.70
1:I:346:GLU:OE1	1:V:408:ARG:NH1	2.25	0.70
1:U:348:SER:O	1:U:350:GLN:N	2.25	0.70
1:A:550:GLN:OE1	1:W:131:ASN:ND2	118.70	0.70
1:R:154:SER:HA	1:R:155:GLU:CG	2.19	0.70
1:A:154:SER:HA	1:A:155:GLU:HB2	1.72	0.70
1:R:96:MET:HG2	1:R:220:PRO:HA	1.74	0.70
1:V:348:SER:O	1:V:350:GLN:N	2.24	0.70
1:D:269:ASP:OD1	1:D:492:ASN:ND2	2.24	0.70
1:Z:46:ASN:HD22	1:Z:64:ASN:HD22	1.39	0.70
1:N:336:VAL:O	1:N:408:ARG:NH2	2.24	0.70
1:I:381:GLY:O	1:I:383:GLN:N	2.24	0.69
1:N:381:GLY:O	1:N:383:GLN:N	2.24	0.69
1:Q:159:GLN:C	1:Q:161:PRO:HA	2.13	0.69
1:D:381:GLY:O	1:D:383:GLN:N	2.25	0.69
1:C:96:MET:HG2	1:C:220:PRO:HA	1.73	0.69
1:W:348:SER:O	1:W:350:GLN:N	2.25	0.69
1:K:287:LEU:HG	1:T:209:ARG:HH12	1.56	0.69
1:B:415:ILE:HD12	1:H:447:ILE:HG22	143.25	0.69
1:O:96:MET:HG2	1:O:220:PRO:HA	1.73	0.69
1:H:408:ARG:NH1	1:W:346:GLU:OE1	2.25	0.69
1:H:381:GLY:O	1:H:383:GLN:N	2.25	0.69
1:Y:159:GLN:C	1:Y:161:PRO:HA	2.12	0.69
1:Q:348:SER:O	1:Q:350:GLN:N	2.26	0.69
1:F:287:LEU:O	1:L:191:ARG:NH1	2.26	0.69
1:Y:566:ILE:HG22	1:Y:567:GLY:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:GLN:C	1:C:161:PRO:HA	2.18	0.69
1:G:105:ILE:C	1:G:209:ARG:HD3	2.12	0.69
1:A:475:ASP:O	1:T:581:ARG:NH1	2.25	0.69
1:K:565:ASN:ND2	1:R:302:ASN:HB2	2.08	0.69
1:E:348:SER:O	1:E:350:GLN:N	2.25	0.69
1:B:77:GLU:HB2	1:B:518:MET:HE1	1.72	0.69
1:S:425:THR:HG22	1:S:427:ASP:H	1.57	0.69
1:Z:160:PRO:N	1:Z:161:PRO:HA	2.08	0.69
1:B:338:TYR:HE1	1:B:358:ALA:HB3	1.57	0.69
1:G:361:ARG:NH2	1:G:364:ALA:O	2.21	0.68
1:M:381:GLY:O	1:M:383:GLN:N	2.25	0.68
1:H:550:GLN:OE1	1:V:131:ASN:ND2	2.26	0.68
1:W:159:GLN:C	1:W:161:PRO:HA	2.12	0.68
1:D:554:ASN:HB3	1:D:557:ASN:HB3	1.73	0.68
1:A:550:GLN:OE1	1:I:131:ASN:ND2	2.23	0.68
1:U:45:PHE:HB3	1:V:252:VAL:HB	1.75	0.68
1:Y:96:MET:HG2	1:Y:220:PRO:HA	1.74	0.68
1:F:336:VAL:O	1:F:408:ARG:NH2	2.27	0.68
1:J:45:PHE:HB3	1:Q:252:VAL:HB	1.75	0.68
1:G:369:ASN:O	1:G:371:ALA:N	2.27	0.68
1:M:382:ARG:NH2	1:M:392:GLY:O	2.26	0.68
1:B:408:ARG:NH1	1:R:346:GLU:OE1	2.26	0.68
1:L:96:MET:HG2	1:L:220:PRO:HA	1.75	0.68
1:D:159:GLN:HG2	1:D:160:PRO:CD	2.23	0.68
1:B:158:THR:O	1:B:159:GLN:HB3	1.94	0.68
1:O:45:PHE:HB3	1:P:252:VAL:HB	1.76	0.68
1:W:381:GLY:O	1:W:383:GLN:N	2.27	0.68
1:S:137:HIS:CE1	1:S:272:PRO:HB3	2.28	0.68
1:B:137:HIS:CE1	1:B:272:PRO:HB3	2.41	0.68
1:L:159:GLN:C	1:L:161:PRO:HA	2.14	0.68
1:K:336:VAL:O	1:K:408:ARG:NH2	2.27	0.68
1:A:387:LYS:NZ	1:I:298:GLU:OE1	2.26	0.68
1:T:401:ILE:O	1:T:575:LYS:NZ	2.26	0.68
1:Q:566:ILE:HG22	1:Q:567:GLY:H	1.58	0.68
1:Z:203:THR:OG1	1:Z:204:ILE:N	2.26	0.67
1:N:252:VAL:HB	1:Q:45:PHE:HB3	1.75	0.67
1:X:361:ARG:NH1	1:X:363:GLY:O	2.26	0.67
1:C:377:ARG:HH21	1:C:397:ARG:HD2	2.03	0.67
1:M:447:ILE:HG22	1:R:415:ILE:HD12	1.75	0.67
1:C:381:GLY:O	1:C:383:GLN:N	2.27	0.67
1:I:553:ILE:CA	1:I:554:ASN:HB2	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:558:GLN:HE22	1:I:236:THR:HB	1.59	0.67
1:L:369:ASN:O	1:L:371:ALA:N	2.27	0.67
1:F:381:GLY:O	1:F:383:GLN:N	2.27	0.67
1:M:569:MET:HG2	1:M:570:LYS:H	1.60	0.67
1:P:336:VAL:O	1:P:408:ARG:NH2	2.27	0.67
1:J:381:GLY:O	1:J:383:GLN:N	2.28	0.67
1:L:569:MET:HG2	1:L:570:LYS:H	1.58	0.67
1:W:368:GLU:HG2	1:W:369:ASN:H	1.60	0.67
1:C:435:PRO:HB3	1:C:439:LYS:O	1.95	0.67
1:U:381:GLY:O	1:U:383:GLN:N	2.27	0.67
1:F:408:ARG:NH1	1:L:346:GLU:OE1	2.28	0.67
1:L:553:ILE:CA	1:L:554:ASN:HB2	2.21	0.67
1:E:554:ASN:HB3	1:E:557:ASN:HB3	1.75	0.67
1:K:369:ASN:O	1:K:371:ALA:N	2.28	0.67
1:N:550:GLN:HA	1:N:578:LEU:HD23	1.77	0.66
1:B:550:GLN:OE1	1:L:131:ASN:ND2	118.96	0.66
1:G:569:MET:HG2	1:G:570:LYS:H	1.60	0.66
1:T:336:VAL:O	1:T:408:ARG:NH2	2.27	0.66
1:Z:553:ILE:CA	1:Z:554:ASN:HB2	2.19	0.66
1:P:382:ARG:N	1:P:386:GLN:HB3	2.04	0.66
1:G:336:VAL:O	1:G:408:ARG:NH2	2.29	0.66
1:O:554:ASN:HB3	1:O:557:ASN:HB3	1.76	0.66
1:F:554:ASN:HD22	1:F:557:ASN:HD22	1.43	0.66
1:T:154:SER:HA	1:T:155:GLU:HB3	1.77	0.66
1:M:554:ASN:HB3	1:M:557:ASN:HB3	1.78	0.66
1:Q:159:GLN:CD	1:Q:160:PRO:HD3	2.16	0.66
1:F:415:ILE:HD12	1:L:447:ILE:HG22	1.78	0.66
1:B:581:ARG:O	1:B:582:LYS:HB2	1.98	0.66
1:D:460:VAL:HG11	1:D:484:VAL:HA	1.81	0.66
1:D:203:THR:OG1	1:D:204:ILE:N	2.33	0.66
1:L:550:GLN:HA	1:L:578:LEU:HD23	1.78	0.66
1:R:381:GLY:O	1:R:383:GLN:N	2.29	0.66
1:O:159:GLN:C	1:O:161:PRO:HA	2.16	0.66
1:F:131:ASN:ND2	1:M:550:GLN:OE1	2.28	0.66
1:Y:348:SER:O	1:Y:350:GLN:N	2.27	0.66
1:D:475:ASP:O	1:L:581:ARG:NH1	121.72	0.66
1:P:554:ASN:HD22	1:P:557:ASN:HD22	1.44	0.66
1:N:326:THR:H	1:N:329:THR:HB	1.61	0.66
1:A:556:ASP:O	1:A:558:GLN:N	2.33	0.66
1:A:381:GLY:O	1:A:383:GLN:N	2.29	0.66
1:F:348:SER:O	1:F:350:GLN:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:336:VAL:O	1:R:408:ARG:NH2	2.28	0.66
1:K:154:SER:HA	1:K:155:GLU:CB	2.24	0.65
1:G:77:GLU:HB2	1:G:518:MET:HE1	1.76	0.65
1:B:381:GLY:O	1:B:383:GLN:N	2.28	0.65
1:G:159:GLN:C	1:G:161:PRO:HA	2.17	0.65
1:G:381:GLY:O	1:G:383:GLN:N	2.30	0.65
1:A:471:ASP:OD1	1:T:584:TYR:OH	2.12	0.65
1:G:369:ASN:HB3	1:G:372:ALA:HB3	1.78	0.65
1:D:554:ASN:HD22	1:D:557:ASN:HD22	1.44	0.65
1:A:566:ILE:HG22	1:A:567:GLY:H	1.61	0.65
1:B:558:GLN:HE22	1:C:236:THR:HB	1.61	0.65
1:P:554:ASN:HB3	1:P:557:ASN:HB3	1.77	0.65
1:A:369:ASN:O	1:A:371:ALA:N	2.30	0.65
1:B:447:ILE:HG22	1:W:415:ILE:HD12	144.76	0.65
1:E:193:GLU:OE1	1:E:209:ARG:NH2	2.30	0.65
1:F:581:ARG:NH1	1:L:475:ASP:O	2.30	0.65
1:B:565:ASN:ND2	1:L:297:SER:O	144.12	0.65
1:C:280:GLN:HG3	1:C:583:LEU:HB2	3.06	0.65
1:F:361:ARG:NH1	1:F:363:GLY:O	2.29	0.65
1:I:216:ARG:NH1	1:I:231:ASN:OD1	2.27	0.65
1:P:96:MET:HG2	1:P:220:PRO:HA	1.78	0.65
1:G:383:GLN:HB3	1:G:384:HIS:HD2	1.62	0.65
1:G:460:VAL:HG11	1:G:484:VAL:HA	1.79	0.65
1:Y:581:ARG:O	1:Y:582:LYS:HB2	1.95	0.65
1:A:336:VAL:O	1:A:408:ARG:NH2	2.30	0.65
1:R:369:ASN:O	1:R:371:ALA:N	2.30	0.65
1:I:425:THR:HG22	1:I:427:ASP:N	2.12	0.64
1:N:581:ARG:O	1:N:582:LYS:HB2	1.96	0.64
1:I:566:ILE:HG22	1:I:567:GLY:H	1.61	0.64
1:B:569:MET:HG2	1:B:570:LYS:H	1.62	0.64
1:E:565:ASN:N	1:E:565:ASN:OD1	2.30	0.64
1:U:377:ARG:NH2	1:U:397:ARG:HD2	2.11	0.64
1:E:435:PRO:HB3	1:E:439:LYS:O	1.97	0.64
1:K:581:ARG:NH1	1:T:475:ASP:O	2.30	0.64
1:H:561:TYR:OH	1:H:574:GLU:OE2	2.14	0.64
1:V:558:GLN:HE22	1:W:236:THR:HB	1.61	0.64
1:C:370:GLN:H	1:C:370:GLN:CD	1.99	0.64
1:P:70:HIS:ND1	1:R:510:TYR:HB3	2.11	0.64
1:D:326:THR:H	1:D:329:THR:HB	1.63	0.64
1:Q:363:GLY:N	1:Q:368:GLU:OE1	2.18	0.64
1:B:566:ILE:HG22	1:B:567:GLY:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:566:ILE:HG22	1:K:567:GLY:H	1.61	0.64
1:C:451:TYR:CD2	1:P:452:GLY:HA2	2.32	0.64
1:K:155:GLU:HA	1:K:163:LYS:HZ3	1.61	0.64
1:C:369:ASN:C	1:C:371:ALA:H	2.00	0.64
1:S:381:GLY:O	1:S:383:GLN:N	2.30	0.64
1:Q:365:GLN:HG2	1:Q:366:THR:HG23	1.80	0.64
1:P:381:GLY:O	1:P:383:GLN:N	2.30	0.64
1:W:131:ASN:HB3	1:W:550:GLN:NE2	2.13	0.64
1:B:550:GLN:OE1	1:P:131:ASN:ND2	2.22	0.64
1:A:415:ILE:HD12	1:K:447:ILE:HG22	1.79	0.64
1:U:581:ARG:O	1:U:582:LYS:HB2	1.96	0.64
1:N:216:ARG:NH1	1:N:231:ASN:OD1	2.30	0.64
1:W:203:THR:OG1	1:W:204:ILE:N	2.30	0.64
1:R:382:ARG:H	1:R:386:GLN:HB3	1.63	0.64
1:O:338:TYR:HE1	1:O:358:ALA:HB3	1.63	0.64
1:T:460:VAL:HG11	1:T:484:VAL:HA	1.79	0.64
1:B:203:THR:OG1	1:B:204:ILE:N	2.47	0.64
1:U:317:THR:HG21	1:U:329:THR:HG22	1.78	0.64
1:Q:159:GLN:NE2	1:Q:160:PRO:HD3	2.13	0.64
1:Z:460:VAL:HG11	1:Z:484:VAL:HA	1.80	0.64
1:E:381:GLY:O	1:E:383:GLN:N	2.31	0.64
1:Q:460:VAL:HG11	1:Q:484:VAL:HA	1.80	0.64
1:B:471:ASP:OD1	1:W:584:TYR:OH	121.46	0.64
1:M:155:GLU:H	1:M:156:SER:HB3	1.63	0.64
1:O:381:GLY:O	1:O:383:GLN:N	2.31	0.63
1:E:131:ASN:O	1:E:550:GLN:NE2	2.31	0.63
1:B:447:ILE:HG22	1:M:415:ILE:HD12	1.78	0.63
1:Q:569:MET:HG2	1:Q:570:LYS:H	1.63	0.63
1:X:569:MET:HG2	1:X:570:LYS:H	1.63	0.63
1:C:157:ALA:HA	1:C:158:THR:OG1	2.12	0.63
1:C:556:ASP:O	1:C:558:GLN:N	2.30	0.63
1:Y:553:ILE:CA	1:Y:554:ASN:HB2	2.25	0.63
1:A:153:VAL:CG1	1:A:163:LYS:HE2	3.64	0.63
1:W:369:ASN:O	1:W:371:ALA:N	2.31	0.63
1:K:159:GLN:C	1:K:161:PRO:HA	2.19	0.63
1:J:362:GLY:N	1:J:368:GLU:OE2	2.28	0.63
1:Q:336:VAL:O	1:Q:408:ARG:NH2	2.31	0.63
1:P:566:ILE:HG22	1:P:567:GLY:H	1.62	0.63
1:I:79:TYR:OH	1:I:247:GLU:OE1	2.15	0.63
1:C:447:ILE:HG22	1:P:415:ILE:HD12	1.80	0.63
1:N:460:VAL:HG11	1:N:484:VAL:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:566:ILE:HG22	1:V:567:GLY:H	1.63	0.63
1:E:471:ASP:OD1	1:I:584:TYR:OH	2.16	0.63
1:C:317:THR:HG22	1:C:330:ILE:HA	2.11	0.63
1:E:382:ARG:NH1	1:J:513:ASP:O	2.31	0.63
1:F:435:PRO:HB3	1:F:439:LYS:O	1.99	0.63
1:A:581:ARG:NH1	1:Y:475:ASP:O	141.14	0.63
1:B:476:THR:O	1:B:479:LYS:HE2	1.99	0.63
1:W:96:MET:HG2	1:W:220:PRO:HA	1.79	0.63
1:O:553:ILE:CA	1:O:554:ASN:HB2	2.24	0.63
1:B:556:ASP:O	1:B:558:GLN:N	2.28	0.63
1:K:216:ARG:NH1	1:K:231:ASN:OD1	2.28	0.63
1:I:361:ARG:NH1	1:I:363:GLY:O	2.32	0.63
1:J:447:ILE:HG22	1:U:415:ILE:HD12	1.80	0.63
1:C:475:ASP:O	1:G:581:ARG:NH1	108.75	0.63
1:X:561:TYR:OH	1:X:574:GLU:OE2	2.15	0.63
1:F:236:THR:HB	1:G:558:GLN:HE22	1.63	0.62
1:E:280:GLN:HE21	1:E:583:LEU:H	1.47	0.62
1:X:411:GLU:OE1	1:X:411:GLU:N	2.31	0.62
1:H:159:GLN:C	1:H:161:PRO:HA	2.18	0.62
1:J:369:ASN:O	1:J:371:ALA:N	2.30	0.62
1:H:415:ILE:HD12	1:W:447:ILE:HG22	1.81	0.62
1:B:252:VAL:HB	1:F:45:PHE:HB3	1.81	0.62
1:A:569:MET:HG2	1:A:570:LYS:H	1.64	0.62
1:M:401:ILE:O	1:M:575:LYS:NZ	2.32	0.62
1:T:366:THR:O	1:T:366:THR:OG1	2.14	0.62
1:S:569:MET:HG2	1:S:570:LYS:H	1.63	0.62
1:T:569:MET:HG2	1:T:570:LYS:H	1.63	0.62
1:F:460:VAL:HG11	1:F:484:VAL:HA	1.82	0.62
1:L:383:GLN:HB3	1:L:384:HIS:HD2	1.64	0.62
1:B:460:VAL:HG11	1:B:484:VAL:HA	1.80	0.62
1:T:381:GLY:O	1:T:383:GLN:N	2.33	0.62
1:U:257:THR:HG22	1:V:256:ARG:HH12	1.64	0.62
1:R:508:ASN:C	1:R:508:ASN:HD22	2.03	0.62
1:I:45:PHE:HB3	1:K:252:VAL:HB	1.82	0.62
1:W:336:VAL:O	1:W:408:ARG:NH2	2.32	0.62
1:S:556:ASP:O	1:S:558:GLN:N	2.29	0.62
1:B:553:ILE:CA	1:B:554:ASN:HB2	2.24	0.62
1:A:553:ILE:CA	1:A:554:ASN:HB2	2.24	0.62
1:I:338:TYR:HE1	1:I:358:ALA:HB3	1.65	0.62
1:D:127:GLN:HG3	1:D:551:MET:HE2	1.82	0.62
1:H:434:ASP:OD2	1:W:439:LYS:NZ	2.23	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLN:HG2	1:A:366:THR:HG23	1.81	0.62
1:V:554:ASN:HB3	1:V:557:ASN:HB3	1.81	0.62
1:B:131:ASN:ND2	1:P:550:GLN:OE1	2.26	0.62
1:K:476:THR:O	1:K:479:LYS:HE2	2.00	0.62
1:F:550:GLN:OE1	1:M:131:ASN:ND2	2.28	0.62
1:R:556:ASP:O	1:R:558:GLN:N	2.29	0.62
1:V:336:VAL:O	1:V:408:ARG:NH2	2.33	0.62
1:C:566:ILE:HG22	1:C:567:GLY:H	1.66	0.62
1:L:157:ALA:HA	1:L:158:THR:CG2	2.29	0.62
1:O:47:ASN:OD1	1:O:67:ARG:NH1	2.29	0.62
1:R:157:ALA:HA	1:R:158:THR:OG1	1.99	0.61
1:E:154:SER:HA	1:E:155:GLU:CB	2.29	0.61
1:X:553:ILE:CA	1:X:554:ASN:HB2	2.23	0.61
1:T:382:ARG:NH2	1:T:392:GLY:O	2.33	0.61
1:G:104:GLU:HG2	1:G:209:ARG:CD	2.30	0.61
1:K:581:ARG:O	1:K:582:LYS:HB2	2.00	0.61
1:O:203:THR:OG1	1:O:204:ILE:N	2.32	0.61
1:K:381:GLY:O	1:K:383:GLN:N	2.33	0.61
1:V:556:ASP:OD1	1:V:557:ASN:N	2.32	0.61
1:C:425:THR:HG22	1:C:427:ASP:H	1.82	0.61
1:G:566:ILE:HG22	1:G:567:GLY:H	1.66	0.61
1:H:269:ASP:HB3	1:H:492:ASN:HD22	1.65	0.61
1:O:359:ALA:HB1	1:O:407:GLY:HA2	1.82	0.61
1:W:207:PRO:O	1:W:209:ARG:NH1	2.34	0.61
1:M:369:ASN:O	1:M:371:ALA:N	2.33	0.61
1:G:401:ILE:O	1:G:575:LYS:NZ	2.33	0.61
1:Y:326:THR:H	1:Y:329:THR:HB	1.65	0.61
1:P:558:GLN:HE22	1:R:236:THR:HB	1.65	0.61
1:N:297:SER:O	1:N:302:ASN:ND2	2.28	0.61
1:A:565:ASN:ND2	1:I:302:ASN:O	2.33	0.61
1:Y:336:VAL:O	1:Y:408:ARG:NH2	2.33	0.61
1:N:554:ASN:HB3	1:N:557:ASN:HB3	1.82	0.61
1:B:56:ASN:HB2	1:B:58:TRP:HD1	1.66	0.61
1:J:159:GLN:C	1:J:161:PRO:HA	2.20	0.61
1:Z:566:ILE:HG22	1:Z:567:GLY:H	1.64	0.61
1:O:77:GLU:HB2	1:O:518:MET:HE1	1.83	0.61
1:N:435:PRO:HB3	1:N:439:LYS:O	2.00	0.61
1:Y:569:MET:HG2	1:Y:570:LYS:H	1.65	0.61
1:C:541:ALA:O	1:C:543:HIS:NE2	2.69	0.61
1:S:159:GLN:HG3	1:S:160:PRO:HD2	1.83	0.61
1:D:479:LYS:HD2	1:D:491:GLN:HE22	4.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:369:ASN:HB3	1:I:372:ALA:HB3	1.83	0.61
1:R:361:ARG:NH1	1:R:363:GLY:O	2.34	0.61
1:G:556:ASP:O	1:G:558:GLN:N	2.32	0.61
1:C:269:ASP:HB3	1:C:492:ASN:ND2	2.82	0.61
1:S:207:PRO:O	1:S:209:ARG:NH1	2.33	0.61
1:O:322:THR:HG1	1:O:324:TYR:HD2	1.49	0.61
1:Q:361:ARG:NH1	1:Q:363:GLY:O	2.34	0.60
1:E:408:ARG:NH1	1:V:346:GLU:OE1	2.33	0.60
1:P:432:PRO:O	1:P:443:ASN:ND2	2.26	0.60
1:G:338:TYR:HE1	1:G:358:ALA:HB3	1.65	0.60
1:X:566:ILE:HG22	1:X:567:GLY:H	1.66	0.60
1:G:550:GLN:HA	1:G:578:LEU:HD23	1.83	0.60
1:E:415:ILE:HD12	1:V:447:ILE:HG22	1.82	0.60
1:N:556:ASP:O	1:N:558:GLN:N	2.31	0.60
1:X:93:ASN:ND2	1:X:225:THR:O	2.34	0.60
1:D:457:LEU:O	1:F:476:THR:HB	99.68	0.60
1:J:203:THR:OG1	1:J:204:ILE:N	2.34	0.60
1:I:425:THR:HB	1:I:428:ASN:HB2	1.81	0.60
1:Q:216:ARG:NH1	1:Q:231:ASN:OD1	2.29	0.60
1:E:326:THR:H	1:E:329:THR:HB	1.64	0.60
1:E:338:TYR:HE1	1:E:358:ALA:HB3	1.67	0.60
1:T:77:GLU:HB2	1:T:518:MET:HE1	1.82	0.60
1:E:475:ASP:O	1:I:581:ARG:NH1	2.35	0.60
1:M:361:ARG:NH1	1:M:363:GLY:O	2.34	0.60
1:G:382:ARG:NH2	1:G:392:GLY:O	2.34	0.60
1:Y:56:ASN:OD1	1:Y:58:TRP:HD1	1.85	0.60
1:D:566:ILE:HG22	1:D:567:GLY:H	1.66	0.60
1:U:369:ASN:O	1:U:371:ALA:N	2.33	0.60
1:D:517:ASN:C	1:D:517:ASN:HD22	4.77	0.60
1:N:584:TYR:OH	1:S:471:ASP:OD1	2.18	0.60
1:E:159:GLN:C	1:E:161:PRO:HA	2.22	0.60
1:P:159:GLN:NE2	1:R:159:GLN:H	1.98	0.60
1:I:52:LYS:HE3	1:I:60:TYR:CD2	2.36	0.60
1:L:546:ASN:ND2	1:L:547:PRO:O	2.34	0.60
1:G:432:PRO:O	1:G:443:ASN:ND2	2.34	0.60
1:X:550:GLN:HA	1:X:578:LEU:HD23	1.84	0.60
1:S:553:ILE:CA	1:S:554:ASN:HB2	2.27	0.60
1:C:45:PHE:HB3	1:D:252:VAL:HB	1.84	0.60
1:N:377:ARG:NH2	1:N:397:ARG:HD2	2.17	0.60
1:B:451:TYR:CD2	1:W:452:GLY:HA2	126.93	0.60
1:P:435:PRO:HB3	1:P:439:LYS:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:566:ILE:HG22	1:O:567:GLY:H	1.67	0.60
1:U:317:THR:HG22	1:U:330:ILE:HA	1.82	0.60
1:X:137:HIS:CE1	1:X:272:PRO:HB3	2.36	0.60
1:C:476:THR:O	1:C:479:LYS:HE2	2.02	0.60
1:A:584:TYR:OH	1:Y:471:ASP:OD1	147.22	0.60
1:W:277:HIS:ND1	1:W:577:GLN:O	2.30	0.60
1:R:569:MET:HG2	1:R:570:LYS:H	1.67	0.60
1:R:550:GLN:HA	1:R:578:LEU:HD23	1.83	0.59
1:Y:56:ASN:CG	1:Y:58:TRP:HD1	2.06	0.59
1:R:216:ARG:NH1	1:R:231:ASN:OD1	2.32	0.59
1:E:569:MET:HG2	1:E:570:LYS:H	1.66	0.59
1:U:558:GLN:HE22	1:V:236:THR:HB	1.66	0.59
1:P:158:THR:O	1:P:159:GLN:HB2	2.02	0.59
1:Y:556:ASP:O	1:Y:558:GLN:N	2.30	0.59
1:A:382:ARG:N	1:A:386:GLN:HB3	2.09	0.59
1:A:565:ASN:OD1	1:I:295:PRO:HB2	2.02	0.59
1:J:346:GLU:OE1	1:U:408:ARG:NH1	2.36	0.59
1:F:566:ILE:HG22	1:F:567:GLY:H	1.67	0.59
1:K:155:GLU:HG2	1:K:163:LYS:HZ1	1.67	0.59
1:T:157:ALA:HA	1:T:158:THR:OG1	2.03	0.59
1:I:422:LEU:HA	1:I:423:PRO:C	2.22	0.59
1:A:127:GLN:HG3	1:A:551:MET:HE2	1.99	0.59
1:O:252:VAL:HB	1:S:45:PHE:HB3	1.84	0.59
1:F:252:VAL:HB	1:G:45:PHE:HB3	1.83	0.59
1:V:553:ILE:HA	1:V:554:ASN:CB	2.32	0.59
1:D:361:ARG:NH1	1:D:363:GLY:O	4.41	0.59
1:M:155:GLU:H	1:M:156:SER:CB	2.16	0.59
1:E:584:TYR:OH	1:V:471:ASP:OD1	2.14	0.59
1:N:137:HIS:CE1	1:N:272:PRO:HB3	2.38	0.59
1:B:377:ARG:HH21	1:B:397:ARG:HD2	1.98	0.59
1:H:236:THR:HB	1:L:558:GLN:HE22	1.68	0.59
1:G:131:ASN:O	1:G:550:GLN:NE2	2.36	0.59
1:U:377:ARG:HH21	1:U:397:ARG:HD2	1.68	0.59
1:P:443:ASN:OD1	1:P:446:ASN:ND2	2.35	0.59
1:Y:560:ASN:HB3	1:Y:572:VAL:HG21	1.84	0.59
1:P:476:THR:O	1:P:479:LYS:HE2	2.03	0.59
1:C:581:ARG:O	1:C:582:LYS:HB2	2.01	0.59
1:A:297:SER:O	1:A:302:ASN:ND2	2.36	0.59
1:A:510:TYR:HB3	1:N:70:HIS:ND1	2.18	0.59
1:F:339:SER:O	1:F:449:ASN:HA	2.02	0.59
1:C:216:ARG:NH1	1:C:231:ASN:OD1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LYS:NZ	1:T:434:ASP:OD2	2.25	0.59
1:A:236:THR:HB	1:Z:558:GLN:HE22	210.50	0.59
1:F:581:ARG:O	1:F:582:LYS:HB2	2.02	0.59
1:M:159:GLN:C	1:M:161:PRO:HA	2.23	0.59
1:I:336:VAL:O	1:I:408:ARG:NH2	2.35	0.59
1:K:584:TYR:OH	1:T:471:ASP:OD1	2.21	0.59
1:K:492:ASN:ND2	1:K:493:ASN:OD1	2.36	0.59
1:F:556:ASP:O	1:F:558:GLN:N	2.33	0.59
1:P:77:GLU:HB2	1:P:518:MET:HE1	1.84	0.59
1:K:415:ILE:HD12	1:T:447:ILE:HG22	1.85	0.59
1:A:447:ILE:HG22	1:T:415:ILE:HD12	1.84	0.59
1:X:238:PRO:HA	1:X:241:VAL:HG23	1.85	0.59
1:A:154:SER:HA	1:A:155:GLU:CB	2.36	0.58
1:B:154:SER:HA	1:B:155:GLU:CB	2.37	0.58
1:G:79:TYR:OH	1:G:247:GLU:OE1	2.19	0.58
1:B:159:GLN:CD	1:B:160:PRO:HD2	2.22	0.58
1:M:383:GLN:HB3	1:M:384:HIS:HD2	1.68	0.58
1:U:257:THR:HG22	1:V:256:ARG:NH1	2.18	0.58
1:R:77:GLU:HB2	1:R:518:MET:HE1	1.85	0.58
1:B:417:ASN:ND2	1:R:441:GLY:O	2.31	0.58
1:Y:137:HIS:HD2	1:Y:536:LYS:HE3	1.68	0.58
1:S:252:VAL:HB	1:T:45:PHE:HB3	1.85	0.58
1:H:569:MET:HG2	1:H:570:LYS:H	1.68	0.58
1:Y:400:TYR:CE2	1:Y:575:LYS:HA	2.38	0.58
1:D:96:MET:HG2	1:D:220:PRO:HA	3.74	0.58
1:P:556:ASP:O	1:P:558:GLN:N	2.28	0.58
1:D:569:MET:HG2	1:D:570:LYS:H	1.77	0.58
1:A:415:ILE:HD12	1:Y:447:ILE:HG22	196.85	0.58
1:U:336:VAL:O	1:U:408:ARG:NH2	2.35	0.58
1:B:411:GLU:OE1	1:B:411:GLU:N	2.57	0.58
1:L:566:ILE:HG22	1:L:567:GLY:H	1.67	0.58
1:O:154:SER:HA	1:O:155:GLU:CG	2.33	0.58
1:G:194:THR:H	1:G:384:HIS:HE1	1.52	0.58
1:L:203:THR:OG1	1:L:204:ILE:N	2.36	0.58
1:G:297:SER:OG	1:G:302:ASN:ND2	2.37	0.58
1:F:333:PRO:HG2	1:L:474:PHE:HZ	1.69	0.58
1:M:336:VAL:O	1:M:408:ARG:NH2	2.36	0.58
1:D:435:PRO:HB3	1:D:439:LYS:O	2.22	0.58
1:E:333:PRO:HG2	1:V:474:PHE:HZ	1.68	0.58
1:V:52:LYS:HE3	1:V:60:TYR:CD2	2.39	0.58
1:F:216:ARG:NH1	1:F:231:ASN:OD1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:236:THR:HB	1:M:558:GLN:NE2	2.19	0.58
1:C:363:GLY:HA3	1:C:367:ASP:O	2.04	0.58
1:C:155:GLU:HG3	1:C:156:SER:N	2.19	0.58
1:Y:422:LEU:HA	1:Y:423:PRO:C	2.24	0.58
1:J:476:THR:O	1:J:479:LYS:HE2	2.03	0.58
1:S:276:THR:HG22	1:S:579:ALA:HB3	1.84	0.58
1:C:271:LYS:HG2	1:C:272:PRO:HD2	4.46	0.58
1:E:457:LEU:HD23	1:V:478:LEU:HD12	1.86	0.58
1:Q:131:ASN:O	1:Q:550:GLN:NE2	2.37	0.58
1:C:409:TYR:CE2	1:C:411:GLU:HB2	2.38	0.58
1:S:199:PRO:HD2	1:S:200:TRP:CZ3	2.38	0.58
1:N:203:THR:OG1	1:N:204:ILE:N	2.37	0.58
1:T:159:GLN:CG	1:T:160:PRO:HD2	2.31	0.57
1:K:274:ARG:NH1	1:T:475:ASP:OD1	2.36	0.57
1:G:216:ARG:NH1	1:G:231:ASN:OD1	2.33	0.57
1:P:460:VAL:HG11	1:P:484:VAL:HA	1.85	0.57
1:M:317:THR:HG22	1:M:330:ILE:HA	1.85	0.57
1:D:550:GLN:HA	1:D:578:LEU:HD23	1.85	0.57
1:G:104:GLU:HG2	1:G:209:ARG:HD2	1.85	0.57
1:I:471:ASP:OD1	1:V:584:TYR:OH	2.19	0.57
1:W:569:MET:HG2	1:W:570:LYS:H	1.69	0.57
1:A:216:ARG:NH1	1:A:231:ASN:OD1	2.37	0.57
1:B:368:GLU:CG	1:B:369:ASN:H	3.69	0.57
1:D:159:GLN:C	1:D:161:PRO:HA	2.24	0.57
1:A:326:THR:H	1:A:329:THR:HB	1.84	0.57
1:F:248:ASN:HD22	1:G:122:ASN:HD22	1.52	0.57
1:U:476:THR:O	1:U:479:LYS:HE2	2.04	0.57
1:U:159:GLN:CB	1:U:160:PRO:HD2	2.35	0.57
1:H:158:THR:HG22	1:H:159:GLN:HG3	1.85	0.57
1:C:411:GLU:N	1:C:411:GLU:OE1	2.34	0.57
1:G:96:MET:HG2	1:G:220:PRO:HA	1.85	0.57
1:R:553:ILE:CA	1:R:554:ASN:HB2	2.27	0.57
1:V:159:GLN:C	1:V:161:PRO:HA	2.24	0.57
1:A:476:THR:O	1:A:479:LYS:HE2	2.17	0.57
1:H:287:LEU:HD12	1:H:288:PRO:HD2	1.86	0.57
1:A:473:GLU:HG2	1:A:491:GLN:HG3	1.86	0.57
1:I:59:VAL:HG21	1:I:133:MET:HE2	1.87	0.57
1:C:460:VAL:HG11	1:C:484:VAL:HA	2.09	0.57
1:A:422:LEU:HA	1:A:423:PRO:C	2.24	0.57
1:V:127:GLN:HG3	1:V:551:MET:HE2	1.86	0.57
1:N:338:TYR:HE1	1:N:358:ALA:HB3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:159:GLN:CG	1:X:160:PRO:HD2	2.31	0.57
1:I:435:PRO:HB3	1:I:439:LYS:O	2.05	0.57
1:N:476:THR:O	1:N:479:LYS:HE2	2.05	0.57
1:V:368:GLU:HG3	1:V:370:GLN:HE21	1.69	0.57
1:E:566:ILE:HG22	1:E:567:GLY:H	1.70	0.57
1:N:431:LEU:HD22	1:S:220:PRO:HB2	1.87	0.57
1:D:556:ASP:O	1:D:558:GLN:N	2.36	0.57
1:D:382:ARG:HD2	1:G:513:ASP:O	2.05	0.57
1:E:431:LEU:HD22	1:V:220:PRO:HB2	1.86	0.57
1:E:154:SER:HA	1:E:155:GLU:HB3	1.87	0.57
1:F:333:PRO:HG2	1:L:474:PHE:CZ	2.40	0.57
1:C:569:MET:HG2	1:C:570:LYS:H	1.76	0.57
1:L:58:TRP:CE3	1:L:536:LYS:HE2	2.40	0.57
1:P:137:HIS:CE1	1:P:272:PRO:HB3	2.39	0.57
1:C:77:GLU:HB2	1:C:518:MET:HE1	1.90	0.57
1:C:553:ILE:CA	1:C:554:ASN:HB2	2.27	0.57
1:A:581:ARG:NH1	1:K:475:ASP:O	2.38	0.57
1:K:159:GLN:HB3	1:K:160:PRO:HD2	1.87	0.57
1:K:157:ALA:HA	1:K:158:THR:CG2	2.35	0.57
1:O:336:VAL:O	1:O:408:ARG:NH2	2.38	0.57
1:F:452:GLY:HA2	1:L:451:TYR:CD2	2.40	0.57
1:K:157:ALA:HA	1:K:158:THR:HG22	1.85	0.57
1:D:361:ARG:O	1:D:407:GLY:N	2.34	0.56
1:M:109:TRP:CD1	1:M:246:ILE:HG13	2.38	0.56
1:Q:476:THR:O	1:Q:479:LYS:HE2	2.05	0.56
1:T:553:ILE:CA	1:T:554:ASN:HB2	2.28	0.56
1:W:157:ALA:HA	1:W:158:THR:OG1	2.05	0.56
1:D:580:PRO:HB2	1:F:242:GLN:NE2	82.79	0.56
1:F:338:TYR:HE1	1:F:358:ALA:HB3	1.69	0.56
1:L:326:THR:H	1:L:329:THR:HB	1.70	0.56
1:C:556:ASP:O	1:C:557:ASN:HB3	2.12	0.56
1:C:558:GLN:HE22	1:D:236:THR:HB	1.70	0.56
1:D:553:ILE:CA	1:D:554:ASN:HB2	2.31	0.56
1:U:513:ASP:O	1:X:382:ARG:NH1	2.38	0.56
1:P:362:GLY:N	1:P:368:GLU:OE2	2.31	0.56
1:V:581:ARG:O	1:V:582:LYS:HB2	2.04	0.56
1:D:362:GLY:O	1:F:349:THR:N	107.15	0.56
1:G:297:SER:O	1:G:302:ASN:ND2	2.35	0.56
1:P:154:SER:HA	1:P:155:GLU:CB	2.35	0.56
1:J:338:TYR:HE1	1:J:358:ALA:HB3	1.70	0.56
1:Y:247:GLU:OE1	1:Y:247:GLU:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:HIS:NE2	1:G:426:ASP:OD2	155.26	0.56
1:E:77:GLU:HB2	1:E:518:MET:HE1	1.87	0.56
1:U:435:PRO:HB3	1:U:439:LYS:O	2.05	0.56
1:U:556:ASP:O	1:U:558:GLN:N	2.33	0.56
1:H:558:GLN:NE2	1:I:236:THR:HB	2.21	0.56
1:A:435:PRO:HB3	1:A:439:LYS:O	2.13	0.56
1:V:45:PHE:HB3	1:W:252:VAL:HB	1.86	0.56
1:I:127:GLN:HG3	1:I:551:MET:HE2	1.85	0.56
1:E:447:ILE:HG22	1:I:415:ILE:HD12	1.87	0.56
1:E:572:VAL:O	1:E:574:GLU:HG3	2.05	0.56
1:O:556:ASP:O	1:O:558:GLN:N	2.31	0.56
1:C:154:SER:HA	1:C:155:GLU:CB	2.36	0.56
1:C:154:SER:HA	1:C:155:GLU:HB3	1.88	0.56
1:F:383:GLN:HB3	1:F:384:HIS:CD2	2.40	0.56
1:E:383:GLN:HB3	1:E:384:HIS:HD2	1.70	0.56
1:Y:203:THR:OG1	1:Y:204:ILE:N	2.35	0.56
1:X:401:ILE:O	1:X:575:LYS:NZ	2.36	0.56
1:I:569:MET:HG2	1:I:570:LYS:H	1.70	0.56
1:Q:557:ASN:HD21	1:Q:561:TYR:HE2	1.52	0.56
1:W:566:ILE:HG22	1:W:567:GLY:H	1.70	0.56
1:K:569:MET:HG2	1:K:570:LYS:H	1.69	0.56
1:A:131:ASN:ND2	1:I:550:GLN:OE1	2.29	0.56
1:B:565:ASN:HB3	1:L:298:GLU:HA	141.69	0.56
1:E:449:ASN:O	1:V:449:ASN:ND2	2.38	0.56
1:H:203:THR:OG1	1:H:204:ILE:N	2.35	0.56
1:T:247:GLU:OE1	1:T:247:GLU:N	2.37	0.56
1:B:150:LEU:HD22	1:B:171:ALA:HB1	1.88	0.56
1:X:252:VAL:HB	1:Y:45:PHE:HB3	1.87	0.56
1:X:203:THR:OG1	1:X:204:ILE:N	2.36	0.56
1:S:566:ILE:HG22	1:S:567:GLY:H	1.70	0.56
1:I:382:ARG:N	1:I:386:GLN:HB3	2.14	0.56
1:L:383:GLN:HB3	1:L:384:HIS:CD2	2.41	0.56
1:K:214:TRP:O	1:K:350:GLN:HG2	2.06	0.56
1:D:422:LEU:HA	1:D:423:PRO:C	2.26	0.56
1:Q:422:LEU:HA	1:Q:423:PRO:C	2.25	0.56
1:E:203:THR:OG1	1:E:204:ILE:N	2.39	0.56
1:R:572:VAL:HG12	1:R:573:TYR:O	2.05	0.56
1:O:382:ARG:NH1	1:P:513:ASP:O	2.38	0.56
1:B:346:GLU:OE1	1:M:408:ARG:NH1	2.39	0.56
1:E:422:LEU:HA	1:E:423:PRO:C	2.26	0.56
1:B:435:PRO:HB3	1:B:439:LYS:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:GLN:HG2	1:A:558:GLN:O	2.05	0.56
1:A:387:LYS:HZ3	1:A:389:THR:HG1	1.54	0.56
1:L:338:TYR:HE1	1:L:358:ALA:HB3	1.71	0.56
1:J:556:ASP:O	1:J:558:GLN:N	2.30	0.56
1:D:492:ASN:OD1	1:D:493:ASN:N	2.32	0.56
1:C:377:ARG:NH2	1:C:397:ARG:HD2	2.54	0.56
1:P:550:GLN:HA	1:P:578:LEU:HD23	1.88	0.56
1:T:566:ILE:HG22	1:T:567:GLY:H	1.70	0.56
1:D:447:ILE:HG22	1:L:415:ILE:HD12	138.71	0.56
1:Q:553:ILE:CA	1:Q:554:ASN:HB2	2.25	0.55
1:O:361:ARG:HG2	1:O:401:ILE:HG22	1.87	0.55
1:G:203:THR:OG1	1:G:204:ILE:N	2.38	0.55
1:H:452:GLY:HA2	1:W:451:TYR:CD2	2.40	0.55
1:D:581:ARG:NH1	1:F:475:ASP:O	91.61	0.55
1:F:553:ILE:CA	1:F:554:ASN:HB2	2.33	0.55
1:G:553:ILE:CA	1:G:554:ASN:HB2	2.24	0.55
1:H:553:ILE:CA	1:H:554:ASN:HB2	2.29	0.55
1:K:556:ASP:O	1:K:557:ASN:HB3	2.06	0.55
1:C:269:ASP:CG	1:C:492:ASN:HD22	2.10	0.55
1:G:383:GLN:HB3	1:G:384:HIS:CD2	2.40	0.55
1:E:333:PRO:HG2	1:V:474:PHE:CZ	2.42	0.55
1:A:401:ILE:O	1:A:575:LYS:NZ	2.39	0.55
1:K:338:TYR:HE1	1:K:358:ALA:HB3	1.72	0.55
1:A:239:ASP:HB3	1:T:549:GLN:HE21	1.70	0.55
1:V:414:TRP:HE1	1:V:416:GLN:HE21	1.53	0.55
1:W:556:ASP:O	1:W:558:GLN:N	2.31	0.55
1:C:99:ASP:CG	1:C:216:ARG:HH21	2.30	0.55
1:D:581:ARG:O	1:D:582:LYS:HB2	2.05	0.55
1:D:338:TYR:HE1	1:D:358:ALA:HB3	1.77	0.55
1:W:159:GLN:OE1	1:W:160:PRO:HD3	2.06	0.55
1:N:127:GLN:HG3	1:N:551:MET:HE2	1.88	0.55
1:A:298:GLU:HA	1:W:565:ASN:HD22	137.36	0.55
1:L:152:THR:HG23	1:L:168:ASP:HB2	1.89	0.55
1:C:422:LEU:HA	1:C:423:PRO:C	2.29	0.55
1:O:154:SER:HA	1:O:155:GLU:CB	2.36	0.55
1:B:159:GLN:C	1:B:161:PRO:HA	2.32	0.55
1:B:447:ILE:HG22	1:W:415:ILE:CD1	144.62	0.55
1:H:114:ALA:HB1	1:H:119:VAL:HG11	1.88	0.55
1:J:137:HIS:CE1	1:J:272:PRO:HB3	2.41	0.55
1:J:326:THR:H	1:J:329:THR:HB	1.71	0.55
1:E:159:GLN:CG	1:E:160:PRO:HD2	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:ALA:HA	1:E:158:THR:HB	1.88	0.55
1:N:266:PHE:HZ	1:N:493:ASN:O	1.90	0.55
1:L:271:LYS:HD2	1:L:271:LYS:H	1.71	0.55
1:J:460:VAL:HG11	1:J:484:VAL:HA	1.89	0.55
1:Y:177:LEU:HD22	1:Y:263:THR:HG22	1.89	0.55
1:U:422:LEU:HA	1:U:423:PRO:C	2.27	0.55
1:O:193:GLU:OE1	1:O:209:ARG:NH2	2.40	0.55
1:T:556:ASP:O	1:T:558:GLN:N	2.36	0.55
1:B:382:ARG:HD2	1:D:513:ASP:O	39.69	0.55
1:J:550:GLN:HA	1:J:578:LEU:HD23	1.87	0.55
1:X:460:VAL:HG11	1:X:484:VAL:HA	1.89	0.55
1:N:236:THR:HB	1:Q:558:GLN:NE2	2.21	0.55
1:P:382:ARG:NH2	1:P:392:GLY:O	2.39	0.55
1:A:584:TYR:OH	1:K:471:ASP:OD1	2.21	0.55
1:I:447:ILE:HG22	1:V:415:ILE:HD12	1.88	0.55
1:F:159:GLN:CG	1:F:160:PRO:HD2	2.37	0.55
1:I:476:THR:O	1:I:479:LYS:HE2	2.06	0.55
1:U:401:ILE:O	1:U:575:LYS:NZ	2.38	0.55
1:P:203:THR:OG1	1:P:204:ILE:N	2.38	0.55
1:X:459:ASN:HD21	1:X:487:PRO:HA	1.70	0.55
1:R:556:ASP:O	1:R:557:ASN:HB3	2.07	0.55
1:B:447:ILE:HG22	1:M:415:ILE:CD1	2.37	0.55
1:H:460:VAL:HG11	1:H:484:VAL:HA	1.87	0.55
1:M:475:ASP:O	1:R:581:ARG:NH1	2.40	0.55
1:C:59:VAL:HG21	1:C:133:MET:HE2	1.89	0.55
1:Z:383:GLN:HB3	1:Z:384:HIS:CD2	2.42	0.55
1:V:550:GLN:HA	1:V:578:LEU:HD23	1.88	0.55
1:D:447:ILE:HG22	1:L:415:ILE:CD1	138.63	0.55
1:D:297:SER:O	1:D:302:ASN:ND2	2.34	0.55
1:T:369:ASN:HB3	1:T:372:ALA:HB3	1.88	0.55
1:Z:155:GLU:HG2	1:Z:156:SER:H	1.72	0.54
1:C:317:THR:HG21	1:C:329:THR:HG22	2.14	0.54
1:H:45:PHE:HB3	1:I:252:VAL:HB	1.88	0.54
1:R:137:HIS:CE1	1:R:272:PRO:HB3	2.43	0.54
1:E:476:THR:O	1:E:479:LYS:HE2	2.07	0.54
1:K:52:LYS:HB3	1:K:60:TYR:HB3	1.89	0.54
1:C:432:PRO:O	1:C:443:ASN:ND2	2.36	0.54
1:X:52:LYS:HE3	1:X:60:TYR:CD2	2.42	0.54
1:U:238:PRO:HA	1:U:241:VAL:HG23	1.90	0.54
1:W:191:ARG:O	1:W:193:GLU:HG3	2.07	0.54
1:R:127:GLN:HG3	1:R:551:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:THR:HG23	1:D:168:ASP:HB2	2.02	0.54
1:U:256:ARG:NH1	1:X:257:THR:HG22	2.22	0.54
1:P:45:PHE:HB3	1:R:252:VAL:HB	1.88	0.54
1:Z:581:ARG:O	1:Z:582:LYS:HB2	2.07	0.54
1:C:88:ASP:OD1	1:C:89:LYS:N	2.40	0.54
1:W:558:GLN:O	1:W:558:GLN:HG2	2.07	0.54
1:D:137:HIS:CE1	1:D:272:PRO:HB3	2.58	0.54
1:D:517:ASN:ND2	1:D:517:ASN:O	4.60	0.54
1:F:158:THR:O	1:F:159:GLN:HB3	2.08	0.54
1:M:572:VAL:HG12	1:M:573:TYR:O	2.08	0.54
1:K:323:ASN:HB3	1:T:397:ARG:NH1	2.22	0.54
1:C:114:ALA:HB1	1:C:119:VAL:HG11	2.21	0.54
1:T:422:LEU:HA	1:T:423:PRO:C	2.26	0.54
1:A:432:PRO:O	1:A:443:ASN:ND2	2.49	0.54
1:S:460:VAL:HG11	1:S:484:VAL:HA	1.89	0.54
1:K:556:ASP:O	1:K:558:GLN:N	2.32	0.54
1:A:581:ARG:O	1:A:582:LYS:HB2	2.08	0.54
1:Y:368:GLU:HG3	1:Y:369:ASN:N	2.23	0.54
1:T:155:GLU:HG3	1:T:156:SER:OG	2.07	0.54
1:R:422:LEU:HA	1:R:423:PRO:C	2.28	0.54
1:Y:75:GLU:OE2	1:Y:108:PRO:HA	2.08	0.54
1:R:326:THR:H	1:R:329:THR:HB	1.72	0.54
1:H:252:VAL:HB	1:L:45:PHE:HB3	1.89	0.54
1:B:518:MET:HG3	1:B:520:ARG:HG3	4.00	0.54
1:Z:476:THR:O	1:Z:479:LYS:HE2	2.07	0.54
1:Z:558:GLN:O	1:Z:558:GLN:HG2	2.06	0.54
1:K:155:GLU:HG2	1:K:163:LYS:NZ	2.21	0.54
1:D:473:GLU:HG2	1:D:491:GLN:HE22	5.46	0.54
1:A:377:ARG:HH21	1:A:397:ARG:HD2	1.81	0.54
1:L:476:THR:O	1:L:479:LYS:HE2	2.07	0.54
1:H:556:ASP:O	1:H:558:GLN:N	2.37	0.54
1:B:154:SER:HA	1:B:155:GLU:HB2	1.88	0.54
1:Y:159:GLN:HB3	1:Y:160:PRO:HD2	1.89	0.54
1:Z:127:GLN:HG3	1:Z:551:MET:HE2	1.88	0.54
1:R:79:TYR:OH	1:R:247:GLU:OE1	2.23	0.54
1:O:127:GLN:HG3	1:O:551:MET:HE2	1.89	0.54
1:G:422:LEU:HA	1:G:423:PRO:C	2.28	0.54
1:A:460:VAL:HG11	1:A:484:VAL:HA	2.04	0.54
1:A:554:ASN:HD22	1:A:557:ASN:HD22	3.56	0.54
1:W:382:ARG:NH1	1:Y:513:ASP:O	2.41	0.54
1:C:346:GLU:OE1	1:G:408:ARG:NH1	130.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:TYR:CE2	1:B:411:GLU:HB2	2.82	0.54
1:O:369:ASN:HB3	1:O:372:ALA:HB3	1.90	0.54
1:Q:269:ASP:HB3	1:Q:492:ASN:ND2	2.23	0.54
1:M:417:ASN:OD1	1:M:419:ASN:ND2	2.39	0.54
1:X:432:PRO:O	1:X:443:ASN:ND2	2.32	0.54
1:A:150:LEU:HD22	1:A:171:ALA:HB1	2.15	0.54
1:X:554:ASN:O	1:X:558:GLN:HB2	2.07	0.54
1:K:153:VAL:HG12	1:K:163:LYS:NZ	2.23	0.54
1:U:193:GLU:OE1	1:U:209:ARG:NH2	2.41	0.54
1:B:274:ARG:NH1	1:H:475:ASP:OD1	112.34	0.54
1:C:447:ILE:HG22	1:G:415:ILE:HD12	143.83	0.54
1:M:362:GLY:N	1:M:368:GLU:OE2	2.32	0.54
1:X:154:SER:HA	1:X:155:GLU:HB2	1.89	0.54
1:G:107:THR:OG1	1:G:208:TRP:O	2.24	0.54
1:D:411:GLU:OE1	1:D:411:GLU:N	2.35	0.54
1:J:510:TYR:HE1	1:J:518:MET:HG3	1.72	0.54
1:B:513:ASP:O	1:F:382:ARG:HD2	2.08	0.54
1:J:209:ARG:NE	1:U:288:PRO:O	2.37	0.54
1:M:216:ARG:NH1	1:M:231:ASN:OD1	2.36	0.54
1:P:569:MET:HG2	1:P:570:LYS:H	1.72	0.54
1:E:369:ASN:O	1:E:371:ALA:N	2.41	0.54
1:C:109:TRP:CD1	1:C:246:ILE:HG13	2.43	0.54
1:L:236:THR:HB	1:M:558:GLN:HE22	1.73	0.53
1:C:191:ARG:O	1:C:193:GLU:HG3	2.07	0.53
1:Z:417:ASN:ND2	1:Z:419:ASN:HD22	2.05	0.53
1:D:408:ARG:NH1	1:F:346:GLU:OE1	120.00	0.53
1:V:383:GLN:HB3	1:V:384:HIS:HD2	1.73	0.53
1:U:214:TRP:O	1:U:350:GLN:HG2	2.08	0.53
1:A:194:THR:H	1:A:384:HIS:HE1	1.77	0.53
1:X:435:PRO:HB3	1:X:439:LYS:O	2.09	0.53
1:B:157:ALA:HA	1:B:158:THR:OG1	2.08	0.53
1:U:256:ARG:HH12	1:X:257:THR:HG22	1.73	0.53
1:J:422:LEU:HA	1:J:423:PRO:C	2.27	0.53
1:D:77:GLU:H	1:D:518:MET:HE1	3.19	0.53
1:C:478:LEU:HD13	1:P:481:ARG:HB3	1.91	0.53
1:A:132:THR:HG22	1:I:132:THR:HG22	1.90	0.53
1:T:339:SER:O	1:T:449:ASN:HA	2.08	0.53
1:P:326:THR:H	1:P:329:THR:HB	1.73	0.53
1:N:382:ARG:NH2	1:N:392:GLY:O	2.41	0.53
1:D:361:ARG:HG3	1:D:405:ASP:HA	1.90	0.53
1:I:581:ARG:O	1:I:582:LYS:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:154:SER:HA	1:P:155:GLU:HB3	1.90	0.53
1:B:257:THR:HG22	1:C:256:ARG:NH1	2.23	0.53
1:B:452:GLY:HA2	1:R:451:TYR:CD2	2.43	0.53
1:R:203:THR:OG1	1:R:204:ILE:N	2.40	0.53
1:F:266:PHE:HZ	1:F:493:ASN:O	1.91	0.53
1:N:573:TYR:C	1:N:574:GLU:HG2	2.27	0.53
1:S:435:PRO:HB3	1:S:439:LYS:O	2.09	0.53
1:V:326:THR:H	1:V:329:THR:HB	1.73	0.53
1:W:556:ASP:O	1:W:557:ASN:HB3	2.08	0.53
1:Y:194:THR:H	1:Y:384:HIS:HE1	1.55	0.53
1:D:566:ILE:HG12	1:G:298:GLU:HG2	80.02	0.53
1:A:493:ASN:N	1:A:493:ASN:OD1	2.40	0.53
1:I:411:GLU:OE1	1:I:411:GLU:N	2.40	0.53
1:V:569:MET:HG2	1:V:570:LYS:H	1.74	0.53
1:M:338:TYR:HE1	1:M:358:ALA:HB3	1.73	0.53
1:U:569:MET:HG2	1:U:570:LYS:H	1.74	0.53
1:J:216:ARG:NH1	1:J:231:ASN:OD1	2.38	0.53
1:D:415:ILE:HD12	1:F:447:ILE:HG22	140.17	0.53
1:W:553:ILE:CA	1:W:554:ASN:HB2	2.28	0.53
1:F:400:TYR:CE2	1:F:575:LYS:HA	2.44	0.53
1:T:154:SER:HA	1:T:155:GLU:CB	2.39	0.53
1:A:383:GLN:HB3	1:A:384:HIS:HD2	1.89	0.53
1:P:422:LEU:HA	1:P:423:PRO:C	2.28	0.53
1:J:336:VAL:O	1:J:408:ARG:NH2	2.41	0.53
1:D:368:GLU:HG3	1:D:369:ASN:N	2.68	0.53
1:U:553:ILE:CA	1:U:554:ASN:HB2	2.30	0.53
1:X:400:TYR:CE2	1:X:575:LYS:HA	2.43	0.53
1:M:203:THR:OG1	1:M:204:ILE:N	2.42	0.53
1:K:422:LEU:HA	1:K:423:PRO:C	2.29	0.53
1:X:161:PRO:HD2	1:X:162:THR:H	1.74	0.53
1:D:451:TYR:CD2	1:L:452:GLY:HA2	123.02	0.53
1:X:581:ARG:O	1:X:582:LYS:HB3	2.08	0.53
1:R:558:GLN:HE22	1:T:236:THR:HB	1.74	0.53
1:P:553:ILE:CA	1:P:554:ASN:HB2	2.29	0.53
1:B:565:ASN:HD21	1:L:302:ASN:HB3	142.81	0.53
1:O:476:THR:O	1:O:479:LYS:HE2	2.09	0.53
1:S:203:THR:OG1	1:S:204:ILE:N	2.39	0.53
1:A:382:ARG:NH2	1:A:392:GLY:O	2.36	0.53
1:L:157:ALA:HA	1:L:158:THR:HG22	1.90	0.53
1:N:566:ILE:HG22	1:N:567:GLY:H	1.72	0.53
1:L:401:ILE:O	1:L:575:LYS:NZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:546:ASN:ND2	1:W:547:PRO:O	2.35	0.53
1:E:541:ALA:HB3	1:E:543:HIS:HE1	1.74	0.53
1:V:573:TYR:O	1:V:574:GLU:HG3	2.09	0.53
1:V:266:PHE:HZ	1:V:493:ASN:O	1.91	0.53
1:J:581:ARG:O	1:J:582:LYS:HB2	2.09	0.53
1:X:422:LEU:HA	1:X:423:PRO:C	2.29	0.53
1:K:382:ARG:HD2	1:M:513:ASP:O	2.09	0.53
1:Y:400:TYR:HE2	1:Y:575:LYS:HA	1.74	0.53
1:Q:360:GLY:HA2	1:Q:373:ASP:OD2	2.09	0.53
1:F:260:GLU:HG3	1:F:261:PHE:N	2.23	0.53
1:A:148:VAL:O	1:A:257:THR:HG23	2.34	0.53
1:A:556:ASP:O	1:A:557:ASN:HB3	2.08	0.53
1:B:236:THR:HB	1:F:558:GLN:HE22	1.74	0.53
1:D:361:ARG:C	1:D:361:ARG:HH11	2.12	0.53
1:W:131:ASN:HB3	1:W:550:GLN:HE21	1.73	0.53
1:T:369:ASN:O	1:T:371:ALA:N	2.41	0.53
1:Q:138:LEU:HG	1:Q:268:PHE:CD2	2.44	0.53
1:W:338:TYR:HE1	1:W:358:ALA:HB3	1.73	0.53
1:Z:569:MET:HG2	1:Z:570:LYS:H	1.74	0.53
1:D:584:TYR:OH	1:F:471:ASP:OD1	106.56	0.53
1:T:361:ARG:NH1	1:T:363:GLY:O	2.42	0.53
1:D:323:ASN:HB3	1:F:397:ARG:NH1	137.90	0.53
1:I:558:GLN:HG2	1:I:558:GLN:O	2.08	0.52
1:K:553:ILE:CA	1:K:554:ASN:HB2	2.31	0.52
1:P:369:ASN:C	1:P:371:ALA:H	2.11	0.52
1:I:475:ASP:OD1	1:V:274:ARG:NH1	2.39	0.52
1:B:408:ARG:NH1	1:H:346:GLU:OE1	134.50	0.52
1:Y:56:ASN:OD1	1:Y:58:TRP:CD1	2.61	0.52
1:V:432:PRO:O	1:V:443:ASN:ND2	2.36	0.52
1:S:515:SER:OG	1:T:390:THR:O	2.27	0.52
1:A:548:ILE:H	1:W:127:GLN:HE22	122.00	0.52
1:O:422:LEU:HA	1:O:423:PRO:C	2.30	0.52
1:A:452:GLY:HA2	1:Y:451:TYR:CD2	176.87	0.52
1:S:476:THR:O	1:S:479:LYS:HE2	2.09	0.52
1:D:558:GLN:NE2	1:G:236:THR:HB	2.24	0.52
1:R:131:ASN:HB3	1:R:550:GLN:NE2	2.24	0.52
1:H:157:ALA:HA	1:H:158:THR:OG1	2.08	0.52
1:D:476:THR:O	1:D:479:LYS:HE2	2.13	0.52
1:V:109:TRP:CD1	1:V:246:ILE:HG13	2.44	0.52
1:D:478:LEU:HD12	1:L:457:LEU:HB3	126.90	0.52
1:V:203:THR:OG1	1:V:204:ILE:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:266:PHE:HZ	1:Z:493:ASN:O	1.92	0.52
1:U:161:PRO:HD2	1:U:162:THR:H	1.74	0.52
1:B:558:GLN:O	1:B:558:GLN:HG2	2.09	0.52
1:F:556:ASP:O	1:F:557:ASN:HB3	2.08	0.52
1:A:287:LEU:HD12	1:A:288:PRO:HD2	1.91	0.52
1:P:581:ARG:O	1:P:582:LYS:HB2	2.10	0.52
1:M:154:SER:O	1:M:154:SER:OG	2.26	0.52
1:Y:414:TRP:HE1	1:Y:416:GLN:HE21	1.56	0.52
1:D:154:SER:O	1:D:154:SER:OG	4.12	0.52
1:D:157:ALA:HA	1:D:158:THR:HG22	1.90	0.52
1:W:435:PRO:HB3	1:W:439:LYS:O	2.09	0.52
1:W:422:LEU:HA	1:W:423:PRO:C	2.30	0.52
1:X:99:ASP:CG	1:X:216:ARG:HH21	2.13	0.52
1:P:127:GLN:HG3	1:P:551:MET:HE2	1.90	0.52
1:A:157:ALA:HA	1:A:158:THR:OG1	2.09	0.52
1:X:185:PHE:CD2	1:X:187:PRO:HD3	2.45	0.52
1:Z:338:TYR:HE1	1:Z:358:ALA:HB3	1.75	0.52
1:Q:203:THR:OG1	1:Q:204:ILE:N	2.43	0.52
1:F:584:TYR:OH	1:L:471:ASP:OD1	2.18	0.52
1:C:368:GLU:HG2	1:C:369:ASN:N	2.24	0.52
1:U:443:ASN:H	1:U:446:ASN:HD22	1.57	0.52
1:Y:75:GLU:HG2	1:Y:76:SER:H	1.73	0.52
1:K:339:SER:O	1:K:449:ASN:HA	2.09	0.52
1:Z:339:SER:O	1:Z:449:ASN:HA	2.10	0.52
1:T:338:TYR:HE1	1:T:358:ALA:HB3	1.74	0.52
1:W:581:ARG:O	1:W:582:LYS:HB2	2.09	0.52
1:I:556:ASP:O	1:I:557:ASN:HB3	2.09	0.52
1:T:581:ARG:O	1:T:582:LYS:HB2	2.10	0.52
1:D:369:ASN:O	1:D:371:ALA:N	2.42	0.52
1:H:326:THR:H	1:H:329:THR:HB	1.73	0.52
1:B:132:THR:HG22	1:P:132:THR:HG22	1.91	0.52
1:O:130:VAL:HG13	1:O:576:SER:O	2.09	0.52
1:D:283:ARG:HH12	1:F:352:PRO:HD2	118.23	0.52
1:P:365:GLN:HG2	1:P:366:THR:HG23	1.91	0.52
1:C:338:TYR:HE1	1:C:358:ALA:HB3	1.74	0.52
1:D:193:GLU:OE1	1:D:209:ARG:NH2	2.42	0.52
1:U:382:ARG:N	1:U:386:GLN:HB3	2.16	0.52
1:R:191:ARG:O	1:R:193:GLU:HG3	2.10	0.52
1:J:382:ARG:HD2	1:Q:513:ASP:O	2.09	0.52
1:J:475:ASP:O	1:U:581:ARG:NH1	2.43	0.52
1:D:479:LYS:HD2	1:D:491:GLN:NE2	3.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:98:LEU:HD13	1:R:310:GLN:OE1	2.09	0.52
1:M:157:ALA:HA	1:M:158:THR:OG1	2.09	0.52
1:U:216:ARG:NH1	1:U:231:ASN:OD1	2.39	0.52
1:N:323:ASN:HB3	1:S:397:ARG:NH1	2.25	0.52
1:R:105:ILE:HG12	1:R:212:PHE:HB2	1.91	0.52
1:C:336:VAL:O	1:C:408:ARG:NH2	2.47	0.52
1:L:558:GLN:O	1:L:558:GLN:HG2	2.10	0.52
1:W:154:SER:CA	1:W:155:GLU:HB2	2.30	0.52
1:D:130:VAL:HG11	1:D:578:LEU:HD13	1.91	0.52
1:C:326:THR:H	1:C:329:THR:HB	1.73	0.52
1:V:476:THR:O	1:V:479:LYS:HE2	2.09	0.52
1:N:473:GLU:HG2	1:N:491:GLN:HE22	1.74	0.52
1:K:365:GLN:HB2	1:T:215:ASP:OD2	2.10	0.52
1:T:432:PRO:O	1:T:443:ASN:ND2	2.37	0.52
1:B:365:GLN:HG2	1:B:366:THR:HG23	2.62	0.52
1:P:383:GLN:HB3	1:P:384:HIS:CD2	2.44	0.52
1:L:114:ALA:HB1	1:L:119:VAL:HG11	1.91	0.52
1:O:411:GLU:OE1	1:O:411:GLU:N	2.43	0.52
1:J:573:TYR:O	1:J:574:GLU:HG3	2.09	0.52
1:N:69:VAL:CG1	1:N:205:PRO:HD3	2.40	0.52
1:U:382:ARG:HD2	1:V:513:ASP:O	2.09	0.52
1:R:159:GLN:C	1:R:161:PRO:HA	2.31	0.52
1:A:346:GLU:OE1	1:T:408:ARG:NH1	2.43	0.52
1:I:573:TYR:C	1:I:574:GLU:HG2	2.30	0.52
1:V:114:ALA:HB1	1:V:119:VAL:HG11	1.91	0.52
1:W:476:THR:O	1:W:479:LYS:HE2	2.10	0.52
1:P:382:ARG:NE	1:P:390:THR:O	2.32	0.51
1:B:478:LEU:HD12	1:W:457:LEU:HB3	120.85	0.51
1:C:476:THR:HB	1:G:457:LEU:O	112.68	0.51
1:I:451:TYR:CD2	1:V:452:GLY:HA2	2.45	0.51
1:C:127:GLN:HG3	1:C:551:MET:HE2	2.07	0.51
1:A:546:ASN:ND2	1:A:547:PRO:O	2.38	0.51
1:U:554:ASN:HB3	1:U:557:ASN:HB3	1.90	0.51
1:E:553:ILE:CA	1:E:554:ASN:HB2	2.30	0.51
1:V:287:LEU:HD12	1:V:288:PRO:HD2	1.92	0.51
1:H:550:GLN:HA	1:H:578:LEU:HD23	1.91	0.51
1:G:383:GLN:CB	1:G:384:HIS:HD2	2.24	0.51
1:X:96:MET:HE2	1:X:96:MET:H	1.74	0.51
1:A:138:LEU:HG	1:A:268:PHE:CD2	2.62	0.51
1:U:266:PHE:HZ	1:U:493:ASN:O	1.93	0.51
1:C:400:TYR:CE2	1:C:575:LYS:HA	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ASN:OD1	1:B:58:TRP:CD1	5.44	0.51
1:D:279:TRP:HA	1:D:405:ASP:HB2	1.91	0.51
1:B:377:ARG:NH2	1:B:397:ARG:HD2	2.43	0.51
1:C:550:GLN:HA	1:C:578:LEU:HD23	1.91	0.51
1:W:378:TYR:O	1:W:397:ARG:HA	2.10	0.51
1:E:75:GLU:OE1	1:I:294:LEU:HD12	2.11	0.51
1:D:417:ASN:OD1	1:D:419:ASN:ND2	2.50	0.51
1:A:191:ARG:O	1:A:193:GLU:HG3	2.27	0.51
1:A:452:GLY:HA2	1:K:451:TYR:CD2	2.45	0.51
1:L:422:LEU:HA	1:L:423:PRO:C	2.31	0.51
1:N:339:SER:O	1:N:449:ASN:HA	2.10	0.51
1:L:127:GLN:HG3	1:L:551:MET:HE2	1.92	0.51
1:B:573:TYR:O	1:B:574:GLU:HG3	2.10	0.51
1:P:99:ASP:CG	1:P:216:ARG:HH21	2.13	0.51
1:L:556:ASP:O	1:L:558:GLN:N	2.31	0.51
1:Q:554:ASN:O	1:Q:558:GLN:HB2	2.10	0.51
1:R:297:SER:O	1:R:302:ASN:ND2	2.40	0.51
1:L:154:SER:HA	1:L:155:GLU:CB	2.41	0.51
1:C:159:GLN:HA	1:C:159:GLN:OE1	2.09	0.51
1:X:96:MET:HG2	1:X:220:PRO:HA	1.93	0.51
1:M:460:VAL:HG11	1:M:484:VAL:HA	1.92	0.51
1:K:457:LEU:O	1:T:476:THR:HB	2.11	0.51
1:S:339:SER:O	1:S:449:ASN:HA	2.11	0.51
1:H:401:ILE:O	1:H:575:LYS:NZ	2.43	0.51
1:D:565:ASN:OD1	1:D:565:ASN:N	4.03	0.51
1:B:422:LEU:HA	1:B:423:PRO:C	2.37	0.51
1:H:154:SER:CA	1:H:155:GLU:HB2	2.31	0.51
1:Y:137:HIS:CD2	1:Y:536:LYS:HE3	2.44	0.51
1:Z:400:TYR:CE2	1:Z:575:LYS:HA	2.45	0.51
1:G:106:VAL:HG22	1:G:209:ARG:CZ	2.40	0.51
1:B:338:TYR:CE1	1:B:358:ALA:HB3	2.43	0.51
1:F:422:LEU:HA	1:F:423:PRO:C	2.31	0.51
1:C:75:GLU:HG2	1:C:76:SER:N	4.92	0.51
1:T:203:THR:OG1	1:T:204:ILE:N	2.43	0.51
1:M:137:HIS:CE1	1:M:272:PRO:HB3	2.46	0.51
1:N:382:ARG:N	1:N:386:GLN:HB3	2.10	0.51
1:A:155:GLU:HA	1:A:163:LYS:HG2	2.59	0.51
1:N:415:ILE:CD1	1:S:447:ILE:HG22	2.39	0.51
1:B:383:GLN:HB3	1:B:384:HIS:HD2	1.76	0.51
1:B:476:THR:HB	1:M:457:LEU:O	2.10	0.51
1:Y:105:ILE:HG12	1:Y:212:PHE:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:216:ARG:NH1	1:Y:231:ASN:OD1	2.35	0.51
1:Q:556:ASP:O	1:Q:558:GLN:N	2.38	0.51
1:V:558:GLN:NE2	1:W:236:THR:HB	2.25	0.51
1:B:431:LEU:HD22	1:H:220:PRO:HB2	147.50	0.51
1:E:540:ARG:HH21	1:E:550:GLN:NE2	2.09	0.51
1:Z:561:TYR:OH	1:Z:574:GLU:OE2	2.29	0.51
1:P:52:LYS:HE3	1:P:60:TYR:CD2	2.46	0.51
1:Q:572:VAL:HG12	1:Q:573:TYR:O	2.11	0.51
1:A:317:THR:HG22	1:A:330:ILE:HA	1.92	0.51
1:S:361:ARG:NH1	1:S:363:GLY:O	2.44	0.51
1:I:556:ASP:O	1:I:558:GLN:N	2.36	0.51
1:G:554:ASN:HD22	1:G:557:ASN:ND2	2.03	0.51
1:C:451:TYR:CD1	1:G:453:PRO:HD3	126.60	0.51
1:H:566:ILE:HG22	1:H:567:GLY:H	1.76	0.51
1:A:77:GLU:HB2	1:A:518:MET:HE1	3.84	0.51
1:R:566:ILE:HG22	1:R:567:GLY:H	1.76	0.51
1:D:558:GLN:O	1:D:558:GLN:HG2	2.10	0.51
1:E:556:ASP:O	1:E:558:GLN:N	2.38	0.51
1:E:382:ARG:N	1:E:386:GLN:HB3	2.25	0.51
1:R:297:SER:OG	1:R:302:ASN:ND2	2.44	0.51
1:V:194:THR:H	1:V:384:HIS:HE1	1.59	0.51
1:U:131:ASN:O	1:U:550:GLN:NE2	2.44	0.51
1:O:159:GLN:CB	1:O:160:PRO:HD2	2.40	0.51
1:O:62:THR:HG23	1:O:534:VAL:HG22	1.93	0.51
1:A:561:TYR:OH	1:A:574:GLU:OE2	2.83	0.51
1:A:247:GLU:OE1	1:A:247:GLU:N	2.53	0.51
1:D:45:PHE:HB3	1:G:252:VAL:HB	1.93	0.50
1:O:137:HIS:CE1	1:O:272:PRO:HB3	2.47	0.50
1:A:391:THR:HG22	1:B:515:SER:OG	169.53	0.50
1:O:569:MET:HG2	1:O:570:LYS:H	1.75	0.50
1:R:435:PRO:HB3	1:R:439:LYS:O	2.11	0.50
1:A:322:THR:HG21	1:A:420:PHE:CD2	2.87	0.50
1:P:558:GLN:NE2	1:R:236:THR:HB	2.27	0.50
1:F:154:SER:CA	1:F:155:GLU:HB2	2.34	0.50
1:C:269:ASP:OD1	1:C:492:ASN:ND2	2.44	0.50
1:H:131:ASN:HB3	1:H:550:GLN:NE2	2.26	0.50
1:E:137:HIS:CE1	1:E:272:PRO:HB3	2.46	0.50
1:J:566:ILE:HG22	1:J:567:GLY:H	1.76	0.50
1:P:556:ASP:O	1:P:557:ASN:HB3	2.11	0.50
1:B:211:TYR:CG	1:W:288:PRO:HG3	129.15	0.50
1:S:159:GLN:C	1:S:161:PRO:HA	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:247:GLU:N	1:U:247:GLU:OE1	2.41	0.50
1:W:137:HIS:CE1	1:W:272:PRO:HB3	2.46	0.50
1:H:572:VAL:HG12	1:H:573:TYR:O	2.11	0.50
1:L:472:LYS:HA	1:L:494:CYS:SG	2.52	0.50
1:K:153:VAL:HG12	1:K:163:LYS:HZ1	1.76	0.50
1:I:247:GLU:N	1:I:247:GLU:OE1	2.44	0.50
1:D:369:ASN:C	1:D:371:ALA:H	2.24	0.50
1:U:114:ALA:HB2	1:U:195:LEU:HD12	1.91	0.50
1:O:287:LEU:HD12	1:O:288:PRO:HD2	1.93	0.50
1:C:277:HIS:ND1	1:C:577:GLN:O	2.42	0.50
1:C:242:GLN:NE2	1:G:580:PRO:HB2	108.53	0.50
1:E:45:PHE:HB3	1:J:252:VAL:HB	1.94	0.50
1:C:295:PRO:HB3	1:C:302:ASN:OD1	2.12	0.50
1:H:377:ARG:HH21	1:H:397:ARG:HD2	1.77	0.50
1:K:203:THR:OG1	1:K:204:ILE:N	2.43	0.50
1:W:286:GLY:O	1:W:288:PRO:HD3	2.11	0.50
1:A:550:GLN:HA	1:A:578:LEU:HD23	1.92	0.50
1:X:154:SER:CA	1:X:155:GLU:HB2	2.42	0.50
1:M:566:ILE:HG22	1:M:567:GLY:H	1.77	0.50
1:Y:154:SER:HA	1:Y:155:GLU:CB	2.41	0.50
1:H:130:VAL:HG13	1:H:576:SER:O	2.11	0.50
1:T:216:ARG:NH1	1:T:231:ASN:OD1	2.36	0.50
1:X:556:ASP:O	1:X:558:GLN:N	2.35	0.50
1:K:558:GLN:OE1	1:M:236:THR:OG1	2.23	0.50
1:B:257:THR:HG22	1:D:256:ARG:NH1	14.10	0.50
1:A:157:ALA:HA	1:A:158:THR:HG22	4.67	0.50
1:D:331:MET:HE3	1:F:485:ASN:HB3	119.38	0.50
1:B:138:LEU:HG	1:B:268:PHE:CD2	2.47	0.50
1:F:362:GLY:N	1:F:368:GLU:OE2	2.41	0.50
1:U:157:ALA:HA	1:U:158:THR:HG22	1.94	0.50
1:M:581:ARG:O	1:M:582:LYS:HB2	2.11	0.50
1:S:388:THR:OG1	1:S:569:MET:N	2.44	0.50
1:Y:468:GLN:HB3	1:Y:486:ALA:HB2	1.94	0.50
1:M:75:GLU:HG2	1:M:76:SER:N	2.27	0.50
1:X:152:THR:HG23	1:X:168:ASP:HB2	1.92	0.50
1:E:132:THR:HG22	1:U:132:THR:HG22	1.93	0.50
1:Z:554:ASN:HB3	1:Z:556:ASP:O	2.12	0.50
1:R:382:ARG:NH2	1:R:392:GLY:O	2.35	0.50
1:O:573:TYR:O	1:O:574:GLU:HG2	2.12	0.50
1:U:154:SER:HA	1:U:155:GLU:CB	2.31	0.49
1:C:352:PRO:HD2	1:P:283:ARG:HH12	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLU:HA	1:I:565:ASN:HD21	1.77	0.49
1:A:157:ALA:HA	1:A:158:THR:CG2	4.02	0.49
1:A:322:THR:HG21	1:A:420:PHE:HD2	2.14	0.49
1:D:404:GLN:OE1	1:D:458:ASN:HB2	2.12	0.49
1:Z:216:ARG:NH1	1:Z:231:ASN:OD1	2.43	0.49
1:F:236:THR:HB	1:G:558:GLN:NE2	2.27	0.49
1:L:194:THR:H	1:L:384:HIS:HE1	1.60	0.49
1:A:383:GLN:CB	1:A:384:HIS:HD2	2.69	0.49
1:C:475:ASP:O	1:P:581:ARG:NH1	2.46	0.49
1:N:338:TYR:CE1	1:N:358:ALA:HB3	2.47	0.49
1:N:492:ASN:CG	1:N:493:ASN:H	2.16	0.49
1:A:453:PRO:HD3	1:Y:451:TYR:CD1	177.14	0.49
1:M:77:GLU:HB2	1:M:518:MET:HE1	1.92	0.49
1:T:150:LEU:HD22	1:T:171:ALA:HB1	1.92	0.49
1:S:493:ASN:OD1	1:S:493:ASN:N	2.42	0.49
1:D:101:THR:O	1:L:283:ARG:NH2	134.09	0.49
1:X:77:GLU:HB2	1:X:518:MET:HE1	1.93	0.49
1:B:211:TYR:CD2	1:W:288:PRO:HG3	129.68	0.49
1:O:153:VAL:HG13	1:O:163:LYS:NZ	2.27	0.49
1:B:157:ALA:HA	1:B:158:THR:HG22	4.68	0.49
1:F:383:GLN:C	1:F:384:HIS:HD2	2.15	0.49
1:A:257:THR:HG22	1:E:256:ARG:NH1	2.27	0.49
1:W:257:THR:HG22	1:Y:256:ARG:NH1	2.27	0.49
1:X:476:THR:O	1:X:479:LYS:HE2	2.12	0.49
1:X:462:PRO:HD2	1:X:576:SER:OG	2.13	0.49
1:A:554:ASN:O	1:A:558:GLN:HB2	2.20	0.49
1:B:369:ASN:C	1:B:371:ALA:H	2.15	0.49
1:I:244:TYR:OH	1:V:582:LYS:HE2	2.12	0.49
1:S:154:SER:O	1:S:154:SER:OG	2.28	0.49
1:C:492:ASN:HD22	1:C:492:ASN:H	3.25	0.49
1:P:383:GLN:HB3	1:P:384:HIS:HD2	1.76	0.49
1:R:508:ASN:ND2	1:R:508:ASN:C	2.65	0.49
1:K:266:PHE:HZ	1:K:493:ASN:O	1.96	0.49
1:C:260:GLU:HG3	1:C:261:PHE:N	2.27	0.49
1:V:42:THR:HB	1:V:260:GLU:HB3	1.94	0.49
1:K:452:GLY:HA2	1:T:451:TYR:CD2	2.47	0.49
1:L:556:ASP:O	1:L:557:ASN:HB3	2.10	0.49
1:Z:382:ARG:NE	1:Z:390:THR:O	2.40	0.49
1:Z:191:ARG:O	1:Z:193:GLU:HG3	2.12	0.49
1:D:383:GLN:HB3	1:D:384:HIS:HD2	1.77	0.49
1:P:432:PRO:C	1:P:443:ASN:HD22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:THR:HG22	1:G:583:LEU:HD11	115.62	0.49
1:Y:157:ALA:HA	1:Y:158:THR:HB	1.94	0.49
1:G:127:GLN:HG3	1:G:551:MET:HE2	1.94	0.49
1:A:252:VAL:HB	1:N:45:PHE:HB3	1.93	0.49
1:I:310:GLN:HG2	1:I:313:ARG:NH1	2.28	0.49
1:Q:148:VAL:O	1:Q:257:THR:HG23	2.13	0.49
1:O:435:PRO:HB3	1:O:439:LYS:O	2.13	0.49
1:U:556:ASP:O	1:U:557:ASN:HB3	2.11	0.49
1:P:558:GLN:O	1:P:558:GLN:HG2	2.11	0.49
1:C:513:ASP:O	1:D:382:ARG:NH1	68.45	0.49
1:B:400:TYR:CE2	1:B:575:LYS:HA	2.61	0.49
1:B:298:GLU:HG2	1:L:566:ILE:HG12	139.03	0.49
1:P:324:TYR:CE2	1:P:422:LEU:HD21	2.47	0.49
1:V:422:LEU:HA	1:V:423:PRO:C	2.32	0.49
1:K:331:MET:HG2	1:T:190:MET:HE1	1.95	0.49
1:U:460:VAL:HG11	1:U:484:VAL:HA	1.94	0.49
1:H:79:TYR:OH	1:H:247:GLU:OE1	2.27	0.49
1:E:105:ILE:HG12	1:E:212:PHE:HB2	1.94	0.49
1:D:400:TYR:CE2	1:D:575:LYS:HA	2.51	0.49
1:S:557:ASN:O	1:S:559:PHE:N	2.46	0.49
1:M:213:GLN:O	1:M:236:THR:HG22	2.13	0.49
1:D:383:GLN:C	1:D:384:HIS:HD2	2.16	0.49
1:G:322:THR:HB	1:G:324:TYR:H	1.78	0.49
1:F:247:GLU:OE1	1:F:247:GLU:N	2.36	0.49
1:S:326:THR:H	1:S:329:THR:HB	1.78	0.49
1:H:338:TYR:HE1	1:H:358:ALA:HB3	1.77	0.49
1:A:159:GLN:HB3	1:A:160:PRO:HD2	1.95	0.49
1:F:349:THR:HG22	1:F:350:GLN:HG3	1.95	0.49
1:M:155:GLU:O	1:M:156:SER:OG	2.29	0.49
1:X:464:TYR:O	1:X:573:TYR:HA	2.13	0.49
1:F:248:ASN:ND2	1:G:122:ASN:HD22	2.11	0.49
1:M:232:ILE:HG12	1:M:233:TYR:N	2.28	0.49
1:W:460:VAL:HG11	1:W:484:VAL:HA	1.95	0.49
1:A:283:ARG:HH12	1:Y:352:PRO:HD2	169.91	0.49
1:X:556:ASP:O	1:X:557:ASN:HB3	2.12	0.49
1:B:45:PHE:HB3	1:C:252:VAL:HB	1.93	0.49
1:C:45:PHE:HB3	1:Z:252:VAL:HB	110.09	0.49
1:O:361:ARG:O	1:O:405:ASP:HA	2.13	0.49
1:A:431:LEU:HD22	1:K:220:PRO:HB2	1.93	0.49
1:E:383:GLN:C	1:E:384:HIS:HD2	2.17	0.49
1:I:362:GLY:N	1:I:368:GLU:OE2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:378:TYR:CE1	1:W:463:VAL:HG11	2.47	0.49
1:A:50:GLU:HG2	1:A:62:THR:HB	4.83	0.49
1:D:339:SER:O	1:D:449:ASN:HA	2.22	0.49
1:J:478:LEU:HD13	1:U:481:ARG:HB3	1.95	0.49
1:D:286:GLY:O	1:D:288:PRO:HD3	2.19	0.49
1:B:59:VAL:HG21	1:B:133:MET:HE2	1.95	0.49
1:B:556:ASP:O	1:B:557:ASN:HB3	2.12	0.49
1:B:382:ARG:NH2	1:B:392:GLY:O	2.54	0.49
1:Q:382:ARG:NE	1:Q:390:THR:O	2.42	0.49
1:P:159:GLN:C	1:P:161:PRO:HA	2.33	0.49
1:A:383:GLN:HB3	1:A:384:HIS:CD2	2.49	0.49
1:C:451:TYR:CD2	1:G:452:GLY:HA2	126.81	0.49
1:J:475:ASP:CG	1:U:274:ARG:HH12	2.15	0.49
1:J:369:ASN:C	1:J:371:ALA:H	2.15	0.49
1:M:369:ASN:C	1:M:371:ALA:H	2.15	0.49
1:H:110:SER:HB3	1:H:205:PRO:HB2	1.95	0.49
1:L:247:GLU:N	1:L:247:GLU:OE1	2.44	0.49
1:C:572:VAL:HG12	1:C:573:TYR:O	2.13	0.49
1:D:471:ASP:OD1	1:L:584:TYR:OH	106.62	0.49
1:S:485:ASN:OD1	1:S:485:ASN:N	2.42	0.49
1:T:159:GLN:C	1:T:161:PRO:HA	2.34	0.48
1:I:191:ARG:O	1:I:193:GLU:HG3	2.12	0.48
1:H:581:ARG:O	1:H:582:LYS:HB2	2.11	0.48
1:E:439:LYS:NZ	1:I:434:ASP:OD2	2.45	0.48
1:X:155:GLU:H	1:X:164:VAL:HG22	1.76	0.48
1:F:51:PHE:CD2	1:F:61:ILE:HG12	2.47	0.48
1:I:266:PHE:HZ	1:I:493:ASN:O	1.96	0.48
1:C:339:SER:HB2	1:C:450:THR:OG1	2.19	0.48
1:H:476:THR:O	1:H:479:LYS:HE2	2.13	0.48
1:B:247:GLU:OE1	1:B:247:GLU:N	2.40	0.48
1:C:473:GLU:OE1	1:C:483:HIS:NE2	2.37	0.48
1:A:137:HIS:CE1	1:A:272:PRO:HB3	2.48	0.48
1:Q:435:PRO:HB3	1:Q:439:LYS:O	2.13	0.48
1:B:481:ARG:HB3	1:H:478:LEU:HD13	116.66	0.48
1:B:558:GLN:NE2	1:C:236:THR:HB	2.28	0.48
1:D:382:ARG:N	1:D:386:GLN:HB3	2.33	0.48
1:N:556:ASP:O	1:N:557:ASN:HB3	2.13	0.48
1:Y:382:ARG:NH2	1:Y:392:GLY:O	2.45	0.48
1:N:513:ASP:O	1:Q:382:ARG:HD2	2.13	0.48
1:U:432:PRO:O	1:U:443:ASN:ND2	2.42	0.48
1:I:338:TYR:CE1	1:I:358:ALA:HB3	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:148:VAL:O	1:X:257:THR:HG23	2.12	0.48
1:V:73:MET:CE	1:V:522:VAL:HA	2.44	0.48
1:L:148:VAL:O	1:L:257:THR:HG23	2.13	0.48
1:Q:198:TYR:HB2	1:Q:201:LYS:HB3	1.95	0.48
1:A:256:ARG:NH1	1:N:257:THR:HG22	2.28	0.48
1:I:238:PRO:HA	1:I:241:VAL:HG23	1.95	0.48
1:F:561:TYR:OH	1:F:574:GLU:OE2	2.22	0.48
1:T:193:GLU:OE1	1:T:209:ARG:NH2	2.46	0.48
1:H:159:GLN:HB3	1:H:160:PRO:HD2	1.95	0.48
1:B:424:VAL:HG12	1:H:94:GLY:HA2	148.84	0.48
1:A:572:VAL:HG12	1:A:573:TYR:O	2.30	0.48
1:J:157:ALA:HA	1:J:158:THR:HB	1.96	0.48
1:B:318:GLN:HG2	1:R:374:GLY:O	2.14	0.48
1:Q:377:ARG:NH2	1:Q:397:ARG:HD2	2.28	0.48
1:V:376:PRO:HD2	1:V:400:TYR:O	2.13	0.48
1:N:445:THR:HA	1:N:448:PHE:HB2	1.95	0.48
1:C:557:ASN:O	1:C:559:PHE:N	2.47	0.48
1:R:247:GLU:N	1:R:247:GLU:OE1	2.44	0.48
1:O:199:PRO:HD2	1:O:200:TRP:CZ3	2.48	0.48
1:U:565:ASN:N	1:U:565:ASN:OD1	2.46	0.48
1:R:417:ASN:OD1	1:R:419:ASN:ND2	2.43	0.48
1:Y:435:PRO:HB3	1:Y:439:LYS:O	2.13	0.48
1:K:460:VAL:HG11	1:K:484:VAL:HA	1.95	0.48
1:L:102:HIS:HA	1:L:214:TRP:CE2	2.48	0.48
1:C:252:VAL:HB	1:D:45:PHE:HB3	45.84	0.48
1:P:383:GLN:C	1:P:384:HIS:HD2	2.17	0.48
1:M:326:THR:H	1:M:329:THR:HB	1.79	0.48
1:E:476:THR:HB	1:I:457:LEU:O	2.13	0.48
1:Y:75:GLU:HG2	1:Y:76:SER:N	2.29	0.48
1:W:127:GLN:HG3	1:W:551:MET:HE2	1.95	0.48
1:V:338:TYR:HE1	1:V:358:ALA:HB3	1.77	0.48
1:E:148:VAL:O	1:E:257:THR:HG23	2.13	0.48
1:O:365:GLN:HG2	1:O:366:THR:HG23	1.94	0.48
1:K:551:MET:HB3	1:K:551:MET:HE3	1.75	0.48
1:P:401:ILE:O	1:P:575:LYS:NZ	2.46	0.48
1:U:566:ILE:HG22	1:U:567:GLY:H	1.78	0.48
1:A:338:TYR:HE1	1:A:358:ALA:HB3	1.78	0.48
1:L:554:ASN:O	1:L:558:GLN:HB2	2.14	0.48
1:M:554:ASN:O	1:M:558:GLN:HB2	2.13	0.48
1:K:382:ARG:N	1:K:386:GLN:HB3	2.17	0.48
1:Q:382:ARG:N	1:Q:386:GLN:HB3	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:431:LEU:HD22	1:L:220:PRO:HB2	1.96	0.48
1:P:438:GLY:O	1:P:439:LYS:HD3	2.13	0.48
1:T:369:ASN:C	1:T:371:ALA:H	2.17	0.48
1:N:256:ARG:NH1	1:Q:257:THR:HG22	2.29	0.48
1:F:558:GLN:O	1:F:558:GLN:HG2	2.13	0.48
1:Q:558:GLN:HG2	1:Q:558:GLN:O	2.11	0.48
1:G:369:ASN:C	1:G:371:ALA:H	2.17	0.48
1:O:159:GLN:HB3	1:O:160:PRO:HD2	1.96	0.48
1:C:447:ILE:HG22	1:G:415:ILE:CD1	143.63	0.48
1:K:415:ILE:CD1	1:T:447:ILE:HG22	2.43	0.48
1:C:256:ARG:HH12	1:D:257:THR:HG22	20.25	0.48
1:E:216:ARG:NH1	1:E:231:ASN:OD1	2.41	0.48
1:A:70:HIS:O	1:A:204:ILE:HG22	2.56	0.48
1:L:411:GLU:N	1:L:411:GLU:OE1	2.41	0.48
1:S:216:ARG:NH1	1:S:231:ASN:OD1	2.37	0.48
1:L:518:MET:HG3	1:L:520:ARG:CG	2.44	0.48
1:I:485:ASN:HB3	1:V:331:MET:HE3	1.95	0.48
1:J:569:MET:HG2	1:J:570:LYS:H	1.79	0.48
1:I:404:GLN:NE2	1:I:461:PRO:HD3	2.29	0.48
1:B:386:GLN:HG3	1:B:396:GLU:HB2	1.97	0.48
1:E:159:GLN:O	1:E:161:PRO:HA	2.13	0.48
1:L:513:ASP:O	1:M:382:ARG:HD2	2.14	0.48
1:B:131:ASN:HB3	1:B:550:GLN:NE2	2.56	0.48
1:B:257:THR:HG22	1:C:256:ARG:HH12	1.78	0.48
1:Y:114:ALA:HB1	1:Y:119:VAL:HG11	1.96	0.48
1:O:404:GLN:OE1	1:O:458:ASN:HB2	2.13	0.48
1:A:411:GLU:OE1	1:A:411:GLU:N	2.44	0.48
1:D:47:ASN:OD1	1:D:67:ARG:NH1	2.54	0.48
1:R:445:THR:HA	1:R:448:PHE:HB2	1.95	0.48
1:O:99:ASP:CG	1:O:216:ARG:HH21	2.16	0.48
1:D:557:ASN:O	1:D:559:PHE:N	2.65	0.48
1:Z:349:THR:HG22	1:Z:350:GLN:HG3	1.96	0.48
1:Q:77:GLU:HB2	1:Q:518:MET:HE1	1.96	0.48
1:R:411:GLU:OE1	1:R:411:GLU:N	2.43	0.48
1:Q:369:ASN:O	1:Q:371:ALA:N	2.47	0.48
1:L:176:ALA:HB2	1:L:252:VAL:HG22	1.95	0.48
1:A:66:SER:HA	1:A:529:TRP:O	2.33	0.48
1:W:572:VAL:HG12	1:W:573:TYR:O	2.14	0.48
1:Y:377:ARG:NH2	1:Y:397:ARG:HD2	2.28	0.48
1:A:159:GLN:O	1:A:161:PRO:HA	2.13	0.48
1:E:439:LYS:NZ	1:I:426:ASP:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:383:GLN:HB3	1:M:384:HIS:CD2	2.49	0.48
1:A:310:GLN:OE1	1:Y:98:LEU:HD13	179.84	0.48
1:S:266:PHE:HZ	1:S:493:ASN:O	1.96	0.48
1:F:322:THR:HG21	1:F:420:PHE:HD2	1.79	0.48
1:F:77:GLU:HB2	1:F:518:MET:HE1	1.94	0.48
1:R:257:THR:HG22	1:T:256:ARG:HH12	1.79	0.48
1:Q:287:LEU:HD12	1:Q:288:PRO:HD2	1.96	0.48
1:D:452:GLY:HA2	1:F:451:TYR:CD2	126.52	0.48
1:P:554:ASN:O	1:P:558:GLN:HB2	2.14	0.47
1:E:556:ASP:O	1:E:557:ASN:HB3	2.13	0.47
1:O:386:GLN:HG2	1:O:396:GLU:CB	2.44	0.47
1:N:569:MET:HG2	1:N:570:LYS:N	2.23	0.47
1:A:102:HIS:HB2	1:A:214:TRP:CH2	2.49	0.47
1:D:298:GLU:HG2	1:G:566:ILE:HG12	90.52	0.47
1:I:447:ILE:HG22	1:V:415:ILE:CD1	2.44	0.47
1:V:324:TYR:CE2	1:V:422:LEU:HD21	2.49	0.47
1:H:368:GLU:HG3	1:H:373:ASP:OD2	2.14	0.47
1:R:400:TYR:CE2	1:R:575:LYS:HA	2.48	0.47
1:E:445:THR:HA	1:E:448:PHE:HB2	1.96	0.47
1:W:51:PHE:CD2	1:W:61:ILE:HG12	2.49	0.47
1:K:573:TYR:C	1:K:574:GLU:HG2	2.34	0.47
1:X:117:TRP:HA	1:X:469:ILE:HD11	1.95	0.47
1:C:558:GLN:NE2	1:D:236:THR:HB	2.29	0.47
1:M:556:ASP:O	1:M:558:GLN:N	2.39	0.47
1:H:382:ARG:NH2	1:H:392:GLY:O	2.47	0.47
1:V:383:GLN:HB3	1:V:384:HIS:CD2	2.48	0.47
1:F:214:TRP:O	1:F:350:GLN:HG2	2.13	0.47
1:O:338:TYR:CE1	1:O:358:ALA:HB3	2.45	0.47
1:X:573:TYR:O	1:X:574:GLU:HG3	2.14	0.47
1:V:339:SER:O	1:V:449:ASN:HA	2.14	0.47
1:T:468:GLN:HB3	1:T:486:ALA:HB2	1.96	0.47
1:H:283:ARG:NH2	1:W:101:THR:O	2.47	0.47
1:Z:336:VAL:O	1:Z:408:ARG:NH2	2.47	0.47
1:Z:130:VAL:HG13	1:Z:576:SER:O	2.14	0.47
1:B:295:PRO:HB2	1:P:565:ASN:OD1	2.13	0.47
1:A:448:PHE:HZ	1:Y:344:SER:HG	187.43	0.47
1:A:242:GLN:NE2	1:T:580:PRO:HB2	2.29	0.47
1:A:430:LEU:HD22	1:Y:442:ILE:HG21	205.64	0.47
1:S:411:GLU:N	1:S:411:GLU:OE1	2.45	0.47
1:Y:193:GLU:CD	1:Y:209:ARG:HH22	2.10	0.47
1:D:159:GLN:HG2	1:D:160:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:383:GLN:CB	1:L:384:HIS:HD2	2.25	0.47
1:C:269:ASP:HB3	1:C:492:ASN:HD21	3.04	0.47
1:K:162:THR:HG21	1:M:155:GLU:OE2	2.13	0.47
1:D:156:SER:OG	1:D:156:SER:O	2.98	0.47
1:K:286:GLY:O	1:K:288:PRO:HD3	2.14	0.47
1:E:554:ASN:HD22	1:E:557:ASN:HD22	1.62	0.47
1:Z:417:ASN:OD1	1:Z:418:ILE:N	2.46	0.47
1:D:159:GLN:CB	1:D:160:PRO:HD2	3.39	0.47
1:V:383:GLN:CB	1:V:384:HIS:HD2	2.26	0.47
1:C:447:ILE:HG22	1:P:415:ILE:CD1	2.44	0.47
1:B:123:PRO:HB2	1:L:547:PRO:HD3	122.47	0.47
1:C:476:THR:HB	1:P:457:LEU:O	2.14	0.47
1:A:377:ARG:NH2	1:A:397:ARG:HD2	2.34	0.47
1:X:154:SER:HA	1:X:155:GLU:CB	2.44	0.47
1:N:457:LEU:O	1:S:476:THR:HB	2.13	0.47
1:X:216:ARG:NH1	1:X:231:ASN:OD1	2.42	0.47
1:X:157:ALA:HA	1:X:158:THR:OG1	2.14	0.47
1:W:266:PHE:HZ	1:W:493:ASN:O	1.97	0.47
1:Y:411:GLU:OE1	1:Y:411:GLU:N	2.46	0.47
1:I:234:HIS:ND1	1:V:365:GLN:OE1	2.47	0.47
1:H:556:ASP:O	1:H:557:ASN:HB3	2.13	0.47
1:J:154:SER:HA	1:J:155:GLU:CB	2.39	0.47
1:B:565:ASN:ND2	1:L:302:ASN:HB3	142.08	0.47
1:E:383:GLN:HB3	1:E:384:HIS:CD2	2.48	0.47
1:A:365:GLN:HB2	1:A:366:THR:HA	6.18	0.47
1:U:338:TYR:HE1	1:U:358:ALA:HB3	1.79	0.47
1:C:354:LYS:HG2	1:C:355:THR:N	2.30	0.47
1:T:105:ILE:HG12	1:T:212:PHE:HB2	1.96	0.47
1:D:102:HIS:HB2	1:D:214:TRP:CH2	2.58	0.47
1:R:460:VAL:HG11	1:R:484:VAL:HA	1.97	0.47
1:X:558:GLN:HG2	1:X:558:GLN:O	2.12	0.47
1:A:288:PRO:O	1:Y:209:ARG:HD2	146.91	0.47
1:Z:417:ASN:OD1	1:Z:418:ILE:HG22	2.13	0.47
1:Y:383:GLN:C	1:Y:384:HIS:HD2	2.18	0.47
1:D:383:GLN:HB3	1:D:384:HIS:CD2	2.49	0.47
1:V:131:ASN:O	1:V:550:GLN:NE2	2.47	0.47
1:D:434:ASP:HA	1:D:435:PRO:HD3	1.72	0.47
1:E:369:ASN:C	1:E:371:ALA:H	2.18	0.47
1:W:445:THR:HA	1:W:448:PHE:HB2	1.96	0.47
1:B:48:GLN:O	1:B:64:ASN:HB2	2.15	0.47
1:Z:326:THR:H	1:Z:329:THR:HB	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:133:MET:HE2	1:S:539:LEU:HD21	1.97	0.47
1:J:558:GLN:O	1:J:558:GLN:HG2	2.14	0.47
1:D:556:ASP:O	1:D:557:ASN:HB3	2.15	0.47
1:S:558:GLN:O	1:S:558:GLN:HG2	2.15	0.47
1:R:554:ASN:HD22	1:R:557:ASN:HD22	1.62	0.47
1:G:154:SER:HA	1:G:155:GLU:CB	2.33	0.47
1:C:382:ARG:NH2	1:C:392:GLY:O	2.47	0.47
1:U:191:ARG:O	1:U:193:GLU:HG3	2.15	0.47
1:T:137:HIS:CE1	1:T:272:PRO:HB3	2.49	0.47
1:Z:46:ASN:OD1	1:Z:48:GLN:HB2	2.15	0.47
1:W:382:ARG:HD2	1:Y:513:ASP:O	2.14	0.47
1:A:349:THR:HG22	1:A:350:GLN:HG3	1.96	0.47
1:G:104:GLU:HG2	1:G:209:ARG:NE	2.30	0.47
1:A:387:LYS:NZ	1:A:389:THR:OG1	2.40	0.47
1:B:383:GLN:HB3	1:B:384:HIS:CD2	2.50	0.47
1:T:434:ASP:HA	1:T:435:PRO:HD3	1.66	0.47
1:A:256:ARG:HH12	1:N:257:THR:HG22	1.80	0.47
1:N:369:ASN:O	1:N:371:ALA:N	2.48	0.47
1:I:185:PHE:CD2	1:I:187:PRO:HD3	2.50	0.47
1:K:411:GLU:OE1	1:K:411:GLU:N	2.46	0.47
1:N:92:VAL:O	1:N:93:ASN:HB2	2.15	0.47
1:E:581:ARG:O	1:E:582:LYS:HB2	2.14	0.47
1:A:185:PHE:CD2	1:A:187:PRO:HD3	2.49	0.47
1:U:252:VAL:HB	1:X:45:PHE:HB3	1.95	0.47
1:I:462:PRO:HD2	1:I:576:SER:OG	2.15	0.47
1:S:238:PRO:HA	1:S:241:VAL:HG23	1.96	0.47
1:B:136:LEU:HD12	1:B:537:ALA:HB2	2.19	0.47
1:U:115:ASN:ND2	1:U:470:TRP:O	2.38	0.47
1:N:546:ASN:ND2	1:N:547:PRO:O	2.39	0.47
1:R:114:ALA:HB1	1:R:119:VAL:HG11	1.96	0.47
1:G:154:SER:CA	1:G:155:GLU:HB2	2.33	0.47
1:T:550:GLN:HA	1:T:578:LEU:HD23	1.97	0.47
1:D:415:ILE:CD1	1:F:447:ILE:HG22	139.72	0.47
1:R:257:THR:HG22	1:T:256:ARG:NH1	2.30	0.47
1:Q:92:VAL:O	1:Q:93:ASN:HB2	2.14	0.47
1:L:92:VAL:O	1:L:93:ASN:HB2	2.14	0.47
1:F:411:GLU:OE1	1:F:411:GLU:N	2.41	0.47
1:T:436:ILE:HD13	1:T:436:ILE:HA	1.74	0.47
1:C:203:THR:OG1	1:C:204:ILE:N	2.47	0.47
1:O:297:SER:C	1:O:302:ASN:HD22	2.16	0.47
1:A:339:SER:O	1:A:449:ASN:HA	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:369:ASN:C	1:F:371:ALA:H	2.13	0.47
1:D:361:ARG:NH1	1:D:361:ARG:O	2.48	0.47
1:E:550:GLN:HA	1:E:578:LEU:HD23	1.96	0.47
1:G:105:ILE:HG12	1:G:212:PHE:HB2	1.96	0.47
1:M:194:THR:H	1:M:384:HIS:HE1	1.63	0.47
1:I:369:ASN:O	1:I:371:ALA:N	2.48	0.47
1:D:220:PRO:HB2	1:L:431:LEU:HD22	146.30	0.47
1:V:376:PRO:HG2	1:V:400:TYR:HB3	1.97	0.47
1:N:75:GLU:HG2	1:N:76:SER:N	2.29	0.47
1:W:152:THR:HG23	1:W:168:ASP:HB2	1.97	0.47
1:A:248:ASN:ND2	1:N:122:ASN:HD22	2.12	0.47
1:Z:177:LEU:HD22	1:Z:263:THR:HG22	1.97	0.47
1:R:107:THR:HG21	1:R:208:TRP:CE3	2.49	0.47
1:A:581:ARG:HB3	1:A:582:LYS:H	1.52	0.47
1:D:361:ARG:NH2	1:D:405:ASP:CB	2.76	0.47
1:A:457:LEU:O	1:Y:476:THR:HB	151.33	0.47
1:J:352:PRO:HD2	1:U:283:ARG:HH12	1.80	0.47
1:E:457:LEU:O	1:V:476:THR:HB	2.15	0.47
1:F:248:ASN:HD22	1:G:122:ASN:ND2	2.13	0.47
1:F:203:THR:OG1	1:F:204:ILE:N	2.48	0.47
1:P:339:SER:O	1:P:449:ASN:HA	2.15	0.47
1:P:573:TYR:O	1:P:574:GLU:HG3	2.15	0.47
1:U:137:HIS:CE1	1:U:272:PRO:HB3	2.50	0.47
1:P:492:ASN:OD1	1:P:493:ASN:N	2.48	0.47
1:O:381:GLY:HA2	1:O:386:GLN:HG3	1.97	0.46
1:K:558:GLN:HE21	1:K:558:GLN:HB3	1.52	0.46
1:N:157:ALA:HA	1:N:158:THR:OG1	2.15	0.46
1:B:566:ILE:HG12	1:L:298:GLU:HG2	139.02	0.46
1:H:266:PHE:HZ	1:H:493:ASN:O	1.97	0.46
1:Y:55:GLU:O	1:Y:56:ASN:CG	2.53	0.46
1:N:490:CYS:HB3	1:N:492:ASN:OD1	2.14	0.46
1:X:432:PRO:C	1:X:443:ASN:HD22	2.14	0.46
1:G:411:GLU:N	1:G:411:GLU:OE1	2.46	0.46
1:M:92:VAL:O	1:M:93:ASN:HB2	2.15	0.46
1:I:69:VAL:CG1	1:I:205:PRO:HD3	2.45	0.46
1:Y:139:VAL:HB	1:Y:534:VAL:O	2.15	0.46
1:L:47:ASN:OD1	1:L:67:ARG:NH1	2.42	0.46
1:B:339:SER:O	1:B:449:ASN:HA	2.18	0.46
1:J:554:ASN:CB	1:J:557:ASN:HB3	2.42	0.46
1:K:554:ASN:O	1:K:558:GLN:HB2	2.15	0.46
1:N:131:ASN:HB3	1:N:550:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:369:ASN:C	1:Z:371:ALA:H	2.16	0.46
1:C:98:LEU:HA	1:G:326:THR:HG21	140.66	0.46
1:B:572:VAL:HG12	1:B:573:TYR:O	2.20	0.46
1:A:123:PRO:HB2	1:I:547:PRO:HD3	1.96	0.46
1:Q:177:LEU:HD22	1:Q:263:THR:HG22	1.97	0.46
1:C:257:THR:HG22	1:Z:256:ARG:NH1	104.63	0.46
1:J:401:ILE:O	1:J:575:LYS:NZ	2.49	0.46
1:A:102:HIS:HA	1:A:214:TRP:CE2	2.51	0.46
1:R:159:GLN:HB3	1:R:160:PRO:HD2	1.96	0.46
1:A:159:GLN:HG3	1:A:160:PRO:HD3	3.82	0.46
1:B:560:ASN:HB3	1:B:572:VAL:HG21	2.09	0.46
1:Q:157:ALA:HA	1:Q:158:THR:OG1	2.14	0.46
1:Y:127:GLN:HG3	1:Y:551:MET:HE2	1.97	0.46
1:J:471:ASP:OD1	1:U:584:TYR:OH	2.28	0.46
1:K:435:PRO:HB3	1:K:439:LYS:O	2.14	0.46
1:G:556:ASP:O	1:G:557:ASN:HB3	2.14	0.46
1:L:286:GLY:O	1:L:288:PRO:HD3	2.15	0.46
1:I:101:THR:O	1:V:283:ARG:NH2	2.48	0.46
1:J:476:THR:HB	1:U:457:LEU:O	2.16	0.46
1:C:222:HIS:O	1:C:225:THR:HG22	2.15	0.46
1:A:239:ASP:HB3	1:T:549:GLN:NE2	2.30	0.46
1:O:369:ASN:C	1:O:371:ALA:H	2.18	0.46
1:X:161:PRO:O	1:X:162:THR:HG22	2.14	0.46
1:N:331:MET:HE3	1:S:485:ASN:HB3	1.98	0.46
1:R:183:MET:HE1	1:R:246:ILE:HD13	1.97	0.46
1:K:152:THR:HG23	1:K:168:ASP:HB2	1.98	0.46
1:Q:137:HIS:CD2	1:Q:272:PRO:HB3	2.50	0.46
1:U:133:MET:HG3	1:U:539:LEU:HD23	1.97	0.46
1:D:73:MET:CE	1:D:522:VAL:HA	2.46	0.46
1:A:369:ASN:C	1:A:371:ALA:H	2.17	0.46
1:S:159:GLN:HG3	1:S:160:PRO:CD	2.46	0.46
1:G:324:TYR:CE2	1:G:422:LEU:HD21	2.50	0.46
1:M:137:HIS:NE2	1:M:272:PRO:HB3	2.31	0.46
1:G:389:THR:HG23	1:G:568:GLY:O	2.14	0.46
1:O:378:TYR:CE1	1:O:463:VAL:HG11	2.51	0.46
1:X:247:GLU:OE1	1:X:247:GLU:N	2.42	0.46
1:T:411:GLU:OE1	1:T:411:GLU:N	2.45	0.46
1:K:462:PRO:HD2	1:K:576:SER:OG	2.15	0.46
1:Z:556:ASP:O	1:Z:557:ASN:HB3	2.15	0.46
1:P:159:GLN:NE2	1:R:161:PRO:HB3	2.25	0.46
1:M:126:TRP:NE1	1:M:130:VAL:HG21	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:550:GLN:HA	1:F:578:LEU:HD23	1.97	0.46
1:N:137:HIS:NE2	1:N:272:PRO:HB3	2.30	0.46
1:B:98:LEU:HD13	1:W:310:GLN:OE1	149.47	0.46
1:U:159:GLN:HG3	1:U:160:PRO:HD2	1.98	0.46
1:E:581:ARG:HB3	1:E:582:LYS:H	1.56	0.46
1:M:476:THR:O	1:M:479:LYS:HE2	2.15	0.46
1:F:75:GLU:HG2	1:F:76:SER:N	2.31	0.46
1:B:113:ASP:O	1:B:195:LEU:HG	2.15	0.46
1:F:547:PRO:HD3	1:M:123:PRO:HB2	1.98	0.46
1:G:271:LYS:HE2	1:G:271:LYS:HB2	1.78	0.46
1:S:422:LEU:HA	1:S:423:PRO:C	2.36	0.46
1:J:109:TRP:CD1	1:J:246:ILE:HG13	2.51	0.46
1:U:138:LEU:HG	1:U:268:PHE:CD2	2.51	0.46
1:Z:554:ASN:CB	1:Z:557:ASN:HB3	2.43	0.46
1:I:558:GLN:NE2	1:K:236:THR:HB	2.26	0.46
1:W:554:ASN:HD22	1:W:557:ASN:HD22	1.64	0.46
1:K:163:LYS:HG2	1:K:163:LYS:HZ2	1.46	0.46
1:A:214:TRP:O	1:A:350:GLN:HG2	2.15	0.46
1:V:435:PRO:HB3	1:V:439:LYS:O	2.15	0.46
1:Z:160:PRO:HG2	1:Z:162:THR:HG23	1.98	0.46
1:H:159:GLN:O	1:H:161:PRO:HA	2.15	0.46
1:Q:550:GLN:HA	1:Q:578:LEU:HD23	1.98	0.46
1:Q:557:ASN:O	1:Q:559:PHE:N	2.48	0.46
1:E:202:PRO:HD2	1:J:518:MET:HE1	1.97	0.46
1:X:161:PRO:CD	1:X:162:THR:H	2.28	0.46
1:L:518:MET:HG3	1:L:520:ARG:HG3	1.97	0.46
1:I:159:GLN:C	1:I:161:PRO:HA	2.36	0.46
1:S:550:GLN:HA	1:S:578:LEU:HD23	1.98	0.46
1:Z:550:GLN:HA	1:Z:578:LEU:HD23	1.98	0.46
1:W:436:ILE:HA	1:W:436:ILE:HD13	1.77	0.46
1:B:163:LYS:HB3	1:B:163:LYS:HE2	1.57	0.46
1:A:580:PRO:HB2	1:Y:242:GLN:NE2	132.25	0.46
1:P:126:TRP:NE1	1:P:130:VAL:HG21	2.31	0.46
1:L:51:PHE:CD2	1:L:61:ILE:HG12	2.51	0.46
1:F:465:PRO:HG3	1:F:571:ILE:HG22	1.96	0.46
1:A:554:ASN:HB2	1:A:557:ASN:HD22	1.80	0.46
1:G:191:ARG:O	1:G:193:GLU:HG3	2.15	0.46
1:I:186:THR:HB	1:V:287:LEU:HD13	1.97	0.46
1:Z:383:GLN:C	1:Z:384:HIS:HD2	2.19	0.46
1:L:369:ASN:C	1:L:371:ALA:H	2.19	0.46
1:A:568:GLY:HA3	1:A:569:MET:HB2	2.06	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:VAL:O	1:B:574:GLU:HG2	4.58	0.46
1:U:361:ARG:NH1	1:U:363:GLY:O	2.49	0.46
1:B:75:GLU:HG3	1:B:76:SER:H	4.41	0.46
1:D:464:TYR:O	1:D:573:TYR:HA	2.16	0.46
1:E:478:LEU:HD13	1:I:481:ARG:HB3	1.97	0.46
1:W:485:ASN:N	1:W:485:ASN:OD1	2.46	0.46
1:F:398:PHE:CE2	1:F:573:TYR:HB2	2.51	0.46
1:C:216:ARG:NH2	1:C:218:LEU:HD22	2.48	0.46
1:A:548:ILE:H	1:W:127:GLN:NE2	121.25	0.46
1:Y:154:SER:HA	1:Y:155:GLU:HB3	1.98	0.46
1:A:203:THR:OG1	1:A:204:ILE:N	2.51	0.46
1:G:309:GLN:HG2	1:G:311:ASP:OD1	2.16	0.46
1:E:247:GLU:OE1	1:E:247:GLU:N	2.47	0.46
1:N:401:ILE:O	1:N:575:LYS:NZ	2.49	0.46
1:H:481:ARG:NH2	1:W:478:LEU:HB3	2.30	0.46
1:Y:460:VAL:HG11	1:Y:484:VAL:HA	1.97	0.46
1:C:322:THR:HG21	1:C:420:PHE:HD2	1.81	0.46
1:A:382:ARG:HD2	1:E:513:ASP:O	2.16	0.46
1:A:287:LEU:HD11	1:Y:209:ARG:HG3	141.72	0.46
1:A:288:PRO:HG3	1:Y:211:TYR:CG	146.48	0.46
1:A:581:ARG:HD3	1:Y:475:ASP:OD2	134.67	0.46
1:B:158:THR:O	1:B:159:GLN:O	2.92	0.46
1:F:415:ILE:CD1	1:L:447:ILE:HG22	2.44	0.46
1:E:475:ASP:OD2	1:I:581:ARG:HD3	2.16	0.46
1:A:476:THR:HB	1:T:457:LEU:O	2.15	0.46
1:A:453:PRO:HD3	1:Y:451:TYR:CE1	175.87	0.46
1:S:339:SER:H	1:S:450:THR:HG1	1.63	0.46
1:Y:212:PHE:CZ	1:Y:241:VAL:HG13	2.51	0.46
1:V:338:TYR:CE1	1:V:358:ALA:HB3	2.51	0.46
1:I:148:VAL:O	1:I:257:THR:HG23	2.16	0.46
1:D:43:GLY:HA3	1:D:146:PHE:CD2	2.51	0.46
1:M:102:HIS:HB2	1:M:214:TRP:CH2	2.51	0.46
1:R:139:VAL:HB	1:R:534:VAL:O	2.16	0.46
1:B:584:TYR:OH	1:H:471:ASP:OD1	116.10	0.46
1:A:92:VAL:O	1:A:93:ASN:HB2	2.16	0.46
1:T:114:ALA:HB1	1:T:119:VAL:HG11	1.98	0.46
1:M:112:VAL:HG13	1:M:195:LEU:HD21	1.97	0.46
1:B:492:ASN:CG	1:B:493:ASN:N	2.69	0.46
1:B:558:GLN:HE22	1:D:236:THR:HB	61.54	0.45
1:E:191:ARG:O	1:E:193:GLU:HG3	2.15	0.45
1:D:155:GLU:HA	1:D:163:LYS:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:363:GLY:HA3	1:X:367:ASP:O	2.16	0.45
1:B:352:PRO:HD2	1:W:283:ARG:HH12	141.42	0.45
1:H:318:GLN:HB3	1:W:354:LYS:HE2	1.99	0.45
1:Z:435:PRO:HB3	1:Z:439:LYS:O	2.16	0.45
1:L:460:VAL:HG11	1:L:484:VAL:HA	1.98	0.45
1:E:558:GLN:NE2	1:J:236:THR:O	2.38	0.45
1:A:163:LYS:HB3	1:A:163:LYS:HE3	2.87	0.45
1:I:475:ASP:CG	1:V:274:ARG:HH12	2.19	0.45
1:E:326:THR:HG21	1:V:98:LEU:HA	1.98	0.45
1:D:257:THR:HG22	1:G:256:ARG:NH1	2.31	0.45
1:G:551:MET:HB3	1:G:551:MET:HE3	1.87	0.45
1:I:492:ASN:CG	1:I:493:ASN:N	2.69	0.45
1:F:322:THR:HG21	1:F:420:PHE:CD2	2.51	0.45
1:I:161:PRO:O	1:I:162:THR:OG1	2.30	0.45
1:L:199:PRO:HD2	1:L:200:TRP:CZ3	2.51	0.45
1:B:43:GLY:HA3	1:B:146:PHE:CD2	2.62	0.45
1:I:154:SER:O	1:I:154:SER:OG	2.28	0.45
1:M:422:LEU:HA	1:M:423:PRO:C	2.35	0.45
1:O:376:PRO:HD2	1:O:400:TYR:O	2.16	0.45
1:F:256:ARG:NH1	1:G:257:THR:HG22	2.32	0.45
1:W:280:GLN:NE2	1:W:583:LEU:H	2.13	0.45
1:D:554:ASN:O	1:D:558:GLN:HB2	2.16	0.45
1:B:415:ILE:CD1	1:R:447:ILE:HG22	2.42	0.45
1:O:153:VAL:HG13	1:O:163:LYS:HZ3	1.82	0.45
1:D:157:ALA:HA	1:D:158:THR:OG1	4.29	0.45
1:X:324:TYR:CE2	1:X:422:LEU:HD21	2.51	0.45
1:Y:154:SER:OG	1:Y:154:SER:O	2.26	0.45
1:S:581:ARG:O	1:S:582:LYS:HB2	2.15	0.45
1:U:75:GLU:HG2	1:U:76:SER:N	2.31	0.45
1:Q:266:PHE:HZ	1:Q:493:ASN:O	1.99	0.45
1:Y:382:ARG:N	1:Y:386:GLN:HB3	2.22	0.45
1:A:299:GLY:H	1:W:565:ASN:ND2	138.57	0.45
1:P:109:TRP:CD1	1:P:246:ILE:HG13	2.52	0.45
1:Y:73:MET:CE	1:Y:522:VAL:HA	2.47	0.45
1:F:317:THR:HG22	1:F:330:ILE:HA	1.99	0.45
1:Z:225:THR:HG22	1:Z:226:SER:O	2.17	0.45
1:D:462:PRO:HD2	1:D:576:SER:OG	2.28	0.45
1:J:278:THR:HB	1:J:583:LEU:HD13	1.97	0.45
1:U:473:GLU:OE1	1:U:483:HIS:NE2	2.46	0.45
1:C:43:GLY:HA3	1:C:146:PHE:CD2	2.51	0.45
1:F:554:ASN:O	1:F:558:GLN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ASP:O	1:N:382:ARG:HD2	2.16	0.45
1:T:558:GLN:O	1:T:558:GLN:HG2	2.17	0.45
1:D:191:ARG:O	1:D:193:GLU:HG3	2.17	0.45
1:B:336:VAL:O	1:B:408:ARG:NH2	2.53	0.45
1:K:369:ASN:C	1:K:371:ALA:H	2.18	0.45
1:B:378:TYR:CE1	1:B:463:VAL:HG11	2.52	0.45
1:A:447:ILE:HG22	1:T:415:ILE:CD1	2.45	0.45
1:B:434:ASP:HA	1:B:435:PRO:HD3	1.76	0.45
1:R:581:ARG:O	1:R:582:LYS:HB2	2.15	0.45
1:Z:99:ASP:CG	1:Z:216:ARG:HH21	2.20	0.45
1:W:326:THR:H	1:W:329:THR:HB	1.81	0.45
1:A:52:LYS:HB3	1:A:60:TYR:HB3	1.97	0.45
1:J:266:PHE:HZ	1:J:493:ASN:O	2.00	0.45
1:F:517:ASN:OD1	1:F:517:ASN:N	2.49	0.45
1:O:485:ASN:OD1	1:O:485:ASN:N	2.42	0.45
1:X:384:HIS:N	1:X:384:HIS:ND1	2.65	0.45
1:M:485:ASN:OD1	1:M:485:ASN:N	2.44	0.45
1:K:278:THR:HB	1:K:583:LEU:HD13	1.98	0.45
1:G:150:LEU:HD22	1:G:171:ALA:HB1	1.98	0.45
1:U:558:GLN:NE2	1:V:236:THR:HB	2.31	0.45
1:X:365:GLN:C	1:X:367:ASP:H	2.20	0.45
1:U:194:THR:H	1:U:384:HIS:HE1	1.65	0.45
1:M:155:GLU:C	1:M:156:SER:HG	2.20	0.45
1:E:408:ARG:HD3	1:E:408:ARG:HA	1.77	0.45
1:D:77:GLU:HB2	1:D:518:MET:HE1	1.98	0.45
1:R:70:HIS:O	1:R:204:ILE:HG22	2.16	0.45
1:D:573:TYR:O	1:D:574:GLU:HG3	2.16	0.45
1:X:493:ASN:N	1:X:493:ASN:OD1	2.49	0.45
1:W:247:GLU:N	1:W:247:GLU:OE1	2.45	0.45
1:K:362:GLY:O	1:T:349:THR:N	2.50	0.45
1:O:581:ARG:O	1:O:582:LYS:HB2	2.16	0.45
1:E:127:GLN:HG3	1:E:551:MET:HE2	1.97	0.45
1:N:333:PRO:HG2	1:S:474:PHE:HZ	1.82	0.45
1:M:339:SER:O	1:M:449:ASN:HA	2.16	0.45
1:E:426:ASP:HB2	1:V:222:HIS:ND1	2.31	0.45
1:P:148:VAL:O	1:P:257:THR:HG23	2.16	0.45
1:C:554:ASN:O	1:C:558:GLN:HB2	2.21	0.45
1:J:556:ASP:O	1:J:557:ASN:HB3	2.17	0.45
1:V:558:GLN:HG2	1:V:558:GLN:O	2.17	0.45
1:J:186:THR:HB	1:U:287:LEU:HB2	1.99	0.45
1:M:156:SER:OG	1:M:164:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:TYR:CE1	1:D:358:ALA:HB3	2.52	0.45
1:D:331:MET:HG2	1:F:190:MET:HE1	118.37	0.45
1:I:190:MET:HE1	1:V:331:MET:HG2	1.99	0.45
1:S:409:TYR:CE2	1:S:411:GLU:HB2	2.51	0.45
1:C:58:TRP:CZ3	1:C:538:LYS:HB2	2.90	0.45
1:S:157:ALA:HA	1:S:158:THR:OG1	2.16	0.45
1:H:92:VAL:O	1:H:93:ASN:HB2	2.17	0.45
1:I:137:HIS:CE1	1:I:272:PRO:HB3	2.51	0.45
1:L:377:ARG:HH21	1:L:397:ARG:HD2	1.81	0.45
1:F:127:GLN:HG3	1:F:551:MET:HB2	1.99	0.45
1:Z:59:VAL:O	1:Z:536:LYS:HA	2.17	0.45
1:O:386:GLN:HG2	1:O:396:GLU:HB3	1.99	0.45
1:K:558:GLN:O	1:K:558:GLN:HG2	2.15	0.45
1:Q:362:GLY:H	1:Q:368:GLU:CD	2.20	0.45
1:B:434:ASP:OD2	1:H:439:LYS:NZ	154.16	0.45
1:O:139:VAL:HB	1:O:534:VAL:O	2.16	0.45
1:M:105:ILE:HG12	1:M:212:PHE:HB2	1.98	0.45
1:T:572:VAL:HG12	1:T:573:TYR:O	2.17	0.45
1:E:411:GLU:N	1:E:411:GLU:OE1	2.44	0.45
1:X:445:THR:HA	1:X:448:PHE:HB2	1.98	0.45
1:V:200:TRP:CZ3	1:W:245:THR:HG21	2.52	0.45
1:N:424:VAL:HG12	1:S:94:GLY:HA2	1.98	0.45
1:Q:554:ASN:HB3	1:Q:556:ASP:O	2.17	0.45
1:W:369:ASN:C	1:W:371:ALA:H	2.19	0.45
1:E:434:ASP:HA	1:E:435:PRO:HD3	1.63	0.45
1:G:104:GLU:HG2	1:G:209:ARG:CZ	2.47	0.45
1:T:581:ARG:HB3	1:T:582:LYS:H	1.57	0.45
1:A:383:GLN:C	1:A:384:HIS:HD2	2.20	0.45
1:D:362:GLY:O	1:D:409:TYR:HB2	2.17	0.45
1:E:476:THR:HG22	1:I:583:LEU:HD11	1.99	0.45
1:C:98:LEU:HA	1:P:326:THR:HG21	1.99	0.45
1:Y:414:TRP:HE1	1:Y:416:GLN:NE2	2.15	0.45
1:F:137:HIS:CE1	1:F:272:PRO:HB3	2.51	0.45
1:G:367:ASP:OD1	1:G:367:ASP:N	2.49	0.45
1:S:92:VAL:O	1:S:93:ASN:HB2	2.16	0.45
1:O:48:GLN:NE2	1:P:249:SER:O	2.50	0.45
1:D:59:VAL:HG21	1:D:133:MET:HE2	2.37	0.45
1:V:117:TRP:CE2	1:V:469:ILE:HG12	2.52	0.45
1:Z:346:GLU:O	1:Z:352:PRO:HA	2.17	0.45
1:A:451:TYR:CD2	1:T:452:GLY:HA2	2.51	0.45
1:T:556:ASP:O	1:T:557:ASN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:556:ASP:O	1:S:557:ASN:HB3	2.17	0.45
1:O:382:ARG:HD2	1:P:513:ASP:O	2.17	0.45
1:K:154:SER:CA	1:K:155:GLU:HB2	2.31	0.45
1:H:382:ARG:HD2	1:I:513:ASP:O	2.16	0.45
1:E:382:ARG:HD2	1:J:513:ASP:O	2.17	0.45
1:E:447:ILE:HG22	1:I:415:ILE:CD1	2.46	0.45
1:M:338:TYR:CE1	1:M:358:ALA:HB3	2.51	0.45
1:O:216:ARG:NH1	1:O:231:ASN:OD1	2.42	0.45
1:V:411:GLU:OE1	1:V:411:GLU:N	2.49	0.45
1:Y:322:THR:HB	1:Y:324:TYR:H	1.81	0.45
1:I:92:VAL:O	1:I:93:ASN:HB2	2.17	0.45
1:O:157:ALA:HA	1:O:158:THR:OG1	2.17	0.45
1:M:556:ASP:O	1:M:557:ASN:HB3	2.16	0.44
1:P:191:ARG:O	1:P:193:GLU:HG3	2.18	0.44
1:D:153:VAL:HG12	1:D:155:GLU:HG3	1.99	0.44
1:P:368:GLU:HG3	1:P:369:ASN:N	2.33	0.44
1:C:220:PRO:HB2	1:G:431:LEU:HD22	144.68	0.44
1:H:281:THR:OG1	1:W:350:GLN:OE1	2.18	0.44
1:J:475:ASP:OD1	1:U:274:ARG:NH1	2.37	0.44
1:U:415:ILE:HG13	1:U:444:TYR:CZ	2.52	0.44
1:A:388:THR:OG1	1:A:569:MET:N	2.71	0.44
1:M:434:ASP:HA	1:M:435:PRO:HD3	1.76	0.44
1:F:583:LEU:HD11	1:L:476:THR:HG22	1.99	0.44
1:Q:551:MET:HE1	1:Q:574:GLU:HB3	1.98	0.44
1:B:457:LEU:O	1:R:476:THR:HB	2.17	0.44
1:O:297:SER:OG	1:O:302:ASN:ND2	2.49	0.44
1:Q:338:TYR:HE1	1:Q:358:ALA:HB3	1.82	0.44
1:W:45:PHE:HB3	1:Y:252:VAL:HB	1.99	0.44
1:N:238:PRO:HA	1:N:241:VAL:HG23	1.98	0.44
1:Y:338:TYR:HE1	1:Y:358:ALA:HB3	1.81	0.44
1:S:114:ALA:HB2	1:S:195:LEU:HD12	1.99	0.44
1:G:378:TYR:CE1	1:G:463:VAL:HG11	2.52	0.44
1:A:557:ASN:O	1:A:559:PHE:N	2.50	0.44
1:X:382:ARG:N	1:X:386:GLN:HB3	2.16	0.44
1:B:207:PRO:O	1:B:209:ARG:NH1	2.49	0.44
1:B:581:ARG:HD3	1:H:475:ASP:OD2	114.13	0.44
1:G:382:ARG:N	1:G:386:GLN:HB3	2.26	0.44
1:P:214:TRP:O	1:P:350:GLN:HG2	2.17	0.44
1:O:163:LYS:HB3	1:O:163:LYS:HZ2	1.81	0.44
1:G:105:ILE:O	1:G:209:ARG:HD3	2.16	0.44
1:V:415:ILE:HD11	1:V:444:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:581:ARG:HB3	1:J:582:LYS:H	1.51	0.44
1:H:326:THR:HG21	1:W:98:LEU:HA	2.00	0.44
1:C:338:TYR:CE1	1:C:358:ALA:HB3	2.52	0.44
1:X:518:MET:HB2	1:X:518:MET:HE2	1.81	0.44
1:O:434:ASP:HA	1:O:435:PRO:HD3	1.73	0.44
1:F:136:LEU:HD12	1:F:537:ALA:HB2	1.99	0.44
1:J:461:PRO:HA	1:J:462:PRO:HD3	1.89	0.44
1:E:451:TYR:CD2	1:I:452:GLY:HA2	2.51	0.44
1:E:452:GLY:HA2	1:V:451:TYR:CD2	2.53	0.44
1:B:216:ARG:NH1	1:B:231:ASN:OD1	2.39	0.44
1:A:468:GLN:HB3	1:A:485:ASN:O	2.27	0.44
1:W:133:MET:CG	1:W:539:LEU:HD23	2.47	0.44
1:A:286:GLY:O	1:A:288:PRO:HD3	2.19	0.44
1:L:287:LEU:HD12	1:L:288:PRO:HD2	1.99	0.44
1:W:382:ARG:N	1:W:386:GLN:HB3	2.27	0.44
1:K:540:ARG:HH21	1:K:550:GLN:NE2	2.15	0.44
1:R:131:ASN:HB3	1:R:550:GLN:HE21	1.81	0.44
1:E:280:GLN:NE2	1:E:583:LEU:N	2.62	0.44
1:A:549:GLN:O	1:A:550:GLN:HG3	2.43	0.44
1:M:346:GLU:OE1	1:R:408:ARG:NH1	2.51	0.44
1:W:434:ASP:HA	1:W:435:PRO:HD3	1.74	0.44
1:I:369:ASN:C	1:I:371:ALA:H	2.20	0.44
1:X:92:VAL:O	1:X:93:ASN:HB2	2.18	0.44
1:I:476:THR:HB	1:V:457:LEU:O	2.17	0.44
1:S:377:ARG:HH21	1:S:397:ARG:HD2	1.82	0.44
1:C:339:SER:O	1:C:449:ASN:HA	2.17	0.44
1:M:297:SER:O	1:M:302:ASN:ND2	2.42	0.44
1:Y:465:PRO:HG3	1:Y:571:ILE:HG22	1.99	0.44
1:B:288:PRO:O	1:H:209:ARG:NE	123.70	0.44
1:D:436:ILE:HA	1:D:436:ILE:HD13	1.96	0.44
1:W:468:GLN:HB3	1:W:486:ALA:HB2	2.00	0.44
1:X:286:GLY:O	1:X:288:PRO:HD3	2.18	0.44
1:I:96:MET:HG2	1:I:220:PRO:HA	1.99	0.44
1:G:177:LEU:HD22	1:G:263:THR:HG22	1.98	0.44
1:D:403:HIS:CD2	1:D:549:GLN:HE22	2.35	0.44
1:Y:554:ASN:O	1:Y:558:GLN:HB2	2.18	0.44
1:K:287:LEU:HG	1:T:209:ARG:NH1	2.26	0.44
1:C:193:GLU:OE1	1:C:209:ARG:NH2	2.48	0.44
1:V:369:ASN:C	1:V:371:ALA:H	2.15	0.44
1:V:408:ARG:HD3	1:V:408:ARG:HA	1.85	0.44
1:U:383:GLN:HB3	1:U:384:HIS:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:383:GLN:C	1:U:384:HIS:HD2	2.21	0.44
1:C:137:HIS:NE2	1:C:272:PRO:HB3	2.60	0.44
1:L:58:TRP:CE2	1:L:538:LYS:HE2	2.53	0.44
1:Z:434:ASP:HA	1:Z:435:PRO:HD3	1.72	0.44
1:M:302:ASN:N	1:M:302:ASN:OD1	2.47	0.44
1:H:151:LYS:NZ	1:I:168:ASP:OD2	2.44	0.44
1:X:339:SER:O	1:X:449:ASN:HA	2.17	0.44
1:V:460:VAL:HG11	1:V:484:VAL:HA	1.98	0.44
1:S:136:LEU:HD12	1:S:537:ALA:HB2	1.99	0.44
1:B:183:MET:HE1	1:B:246:ILE:HD13	1.99	0.44
1:K:298:GLU:OE2	1:R:389:THR:HG21	2.17	0.44
1:W:518:MET:HB2	1:W:518:MET:HE2	1.70	0.44
1:T:133:MET:HE2	1:T:539:LEU:HD21	1.99	0.44
1:I:157:ALA:HA	1:I:158:THR:HG22	1.98	0.44
1:R:554:ASN:O	1:R:558:GLN:HB2	2.17	0.44
1:E:558:GLN:O	1:E:558:GLN:HG2	2.16	0.44
1:H:554:ASN:O	1:H:558:GLN:HB2	2.18	0.44
1:B:154:SER:HA	1:B:155:GLU:CG	2.48	0.44
1:B:415:ILE:CD1	1:H:447:ILE:HG22	143.41	0.44
1:K:540:ARG:HH21	1:K:550:GLN:HE22	1.65	0.44
1:B:257:THR:HG21	1:D:170:THR:HG22	11.31	0.44
1:O:569:MET:HB2	1:O:569:MET:HE2	1.81	0.44
1:K:434:ASP:HA	1:K:435:PRO:HD3	1.75	0.44
1:S:66:SER:HA	1:S:529:TRP:O	2.18	0.44
1:O:456:ALA:O	1:O:457:LEU:HD12	2.18	0.44
1:R:92:VAL:O	1:R:93:ASN:HB2	2.18	0.44
1:I:387:LYS:HE3	1:I:389:THR:OG1	2.18	0.44
1:J:357:ILE:HB	1:J:373:ASP:O	2.18	0.44
1:L:256:ARG:NH1	1:M:257:THR:HG22	2.32	0.44
1:C:404:GLN:NE2	1:C:461:PRO:HD3	2.51	0.44
1:M:451:TYR:CD2	1:R:452:GLY:HA2	2.52	0.44
1:J:92:VAL:HB	1:J:95:ASN:HB2	2.00	0.44
1:F:481:ARG:NH2	1:L:478:LEU:HB3	2.33	0.44
1:B:557:ASN:O	1:B:559:PHE:N	2.51	0.44
1:H:219:ILE:HG23	1:H:220:PRO:HD2	2.00	0.44
1:K:581:ARG:HB3	1:K:582:LYS:H	1.60	0.44
1:D:581:ARG:HB3	1:D:582:LYS:H	1.55	0.44
1:F:457:LEU:O	1:L:476:THR:HB	2.17	0.44
1:V:568:GLY:HA3	1:V:569:MET:HB2	1.98	0.44
1:I:96:MET:HE3	1:I:96:MET:HB2	1.90	0.44
1:D:346:GLU:OE2	1:D:355:THR:OG1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:THR:HG22	1:E:530:LYS:NZ	2.31	0.44
1:S:338:TYR:HE1	1:S:358:ALA:HB3	1.82	0.44
1:J:483:HIS:HB3	1:J:485:ASN:OD1	2.17	0.44
1:H:43:GLY:HA3	1:H:146:PHE:CD2	2.53	0.44
1:Z:157:ALA:HA	1:Z:158:THR:OG1	2.18	0.44
1:C:92:VAL:O	1:C:93:ASN:HB2	2.20	0.44
1:B:242:GLN:NE2	1:W:580:PRO:HB2	123.30	0.44
1:K:257:THR:HG22	1:M:256:ARG:NH1	2.33	0.44
1:T:382:ARG:N	1:T:386:GLN:HB3	2.22	0.44
1:B:154:SER:CA	1:B:155:GLU:HB3	4.05	0.44
1:B:137:HIS:NE2	1:B:272:PRO:HB3	2.33	0.44
1:U:383:GLN:HB3	1:U:384:HIS:CD2	2.53	0.44
1:B:568:GLY:HA3	1:B:569:MET:HB2	2.00	0.44
1:H:492:ASN:OD1	1:H:493:ASN:N	2.35	0.44
1:O:46:ASN:OD1	1:O:48:GLN:HB2	2.17	0.44
1:P:338:TYR:HE1	1:P:358:ALA:HB3	1.81	0.44
1:H:404:GLN:NE2	1:H:461:PRO:HD3	2.33	0.44
1:L:99:ASP:CG	1:L:216:ARG:HH21	2.21	0.44
1:H:59:VAL:HG21	1:H:133:MET:HE2	2.00	0.44
1:O:105:ILE:HG12	1:O:212:PHE:HB2	2.00	0.44
1:C:459:ASN:HD21	1:C:487:PRO:HA	2.04	0.44
1:R:260:GLU:HG3	1:R:261:PHE:N	2.32	0.44
1:Z:422:LEU:HA	1:Z:423:PRO:C	2.37	0.44
1:V:137:HIS:CD2	1:V:272:PRO:HB3	2.52	0.44
1:C:47:ASN:OD1	1:C:67:ARG:NH1	2.45	0.44
1:G:357:ILE:HB	1:G:374:GLY:HA3	2.00	0.44
1:G:368:GLU:OE1	1:G:401:ILE:HD13	2.17	0.44
1:Y:434:ASP:HA	1:Y:435:PRO:HD3	1.70	0.44
1:P:583:LEU:HD12	1:P:583:LEU:HA	1.81	0.44
1:C:150:LEU:HD22	1:C:171:ALA:HB1	1.98	0.44
1:Z:556:ASP:O	1:Z:558:GLN:N	2.46	0.44
1:G:558:GLN:O	1:G:558:GLN:HG2	2.16	0.44
1:T:191:ARG:O	1:T:193:GLU:HG3	2.17	0.44
1:H:408:ARG:HD3	1:H:408:ARG:HA	1.87	0.44
1:V:346:GLU:O	1:V:352:PRO:HA	2.18	0.44
1:U:492:ASN:HB2	1:U:493:ASN:H	1.49	0.44
1:E:137:HIS:NE2	1:E:272:PRO:HB3	2.33	0.44
1:N:93:ASN:ND2	1:N:225:THR:O	2.50	0.44
1:D:549:GLN:NE2	1:F:239:ASP:OD1	81.14	0.44
1:A:478:LEU:HD13	1:T:481:ARG:HB3	2.00	0.44
1:Q:445:THR:HA	1:Q:448:PHE:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:PHE:HB2	1:C:472:LYS:HE2	2.51	0.44
1:T:322:THR:HB	1:T:324:TYR:H	1.82	0.44
1:E:378:TYR:O	1:E:397:ARG:HA	2.17	0.44
1:V:556:ASP:O	1:V:558:GLN:N	2.43	0.43
1:Z:46:ASN:ND2	1:Z:64:ASN:ND2	2.60	0.43
1:M:435:PRO:HB3	1:M:439:LYS:O	2.18	0.43
1:B:132:THR:HG22	1:L:132:THR:HG22	112.90	0.43
1:C:401:ILE:O	1:C:575:LYS:NZ	2.55	0.43
1:C:549:GLN:O	1:C:550:GLN:HG3	2.27	0.43
1:T:75:GLU:HG2	1:T:76:SER:N	2.33	0.43
1:B:436:ILE:HD13	1:B:436:ILE:HA	1.80	0.43
1:A:55:GLU:HG3	1:A:55:GLU:H	1.50	0.43
1:Q:432:PRO:O	1:Q:443:ASN:ND2	2.45	0.43
1:G:414:TRP:HE1	1:G:416:GLN:HG3	1.82	0.43
1:K:185:PHE:CD2	1:K:187:PRO:HD3	2.53	0.43
1:V:66:SER:O	1:V:67:ARG:NH1	2.47	0.43
1:K:199:PRO:HD2	1:K:200:TRP:CZ3	2.52	0.43
1:B:72:ASN:ND2	1:C:508:ASN:O	2.48	0.43
1:Z:138:LEU:HG	1:Z:268:PHE:CD2	2.52	0.43
1:T:346:GLU:O	1:T:352:PRO:HA	2.18	0.43
1:R:554:ASN:ND2	1:R:557:ASN:HD22	2.16	0.43
1:Z:382:ARG:N	1:Z:386:GLN:HB3	2.23	0.43
1:D:158:THR:O	1:D:159:GLN:O	2.35	0.43
1:Q:154:SER:HA	1:Q:155:GLU:CB	2.46	0.43
1:M:383:GLN:C	1:M:384:HIS:HD2	2.21	0.43
1:F:383:GLN:HB3	1:F:384:HIS:HD2	1.82	0.43
1:M:98:LEU:HA	1:R:326:THR:HG21	1.99	0.43
1:D:369:ASN:HB3	1:D:372:ALA:HB3	4.78	0.43
1:H:376:PRO:HG2	1:H:400:TYR:HB3	1.99	0.43
1:D:278:THR:CG2	1:D:458:ASN:HD21	2.68	0.43
1:H:338:TYR:CE1	1:H:358:ALA:HB3	2.53	0.43
1:C:177:LEU:HD22	1:C:263:THR:HG22	2.21	0.43
1:N:560:ASN:HB3	1:N:572:VAL:HG21	2.00	0.43
1:F:87:LEU:HA	1:F:90:THR:OG1	2.18	0.43
1:C:464:TYR:HA	1:C:465:PRO:HA	1.87	0.43
1:P:546:ASN:ND2	1:P:547:PRO:O	2.48	0.43
1:T:442:ILE:HG23	1:T:446:ASN:HD22	1.83	0.43
1:S:236:THR:HB	1:T:558:GLN:OE1	2.18	0.43
1:H:554:ASN:HD22	1:H:557:ASN:HB2	1.83	0.43
1:N:395:PRO:HG2	1:N:397:ARG:NH1	2.33	0.43
1:G:159:GLN:CD	1:G:160:PRO:HD2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:434:ASP:HA	1:H:435:PRO:HD3	1.70	0.43
1:Y:317:THR:HG22	1:Y:330:ILE:HA	1.99	0.43
1:V:159:GLN:HA	1:V:160:PRO:HA	1.78	0.43
1:B:168:ASP:CG	1:B:171:ALA:HB2	2.60	0.43
1:T:377:ARG:HH21	1:T:397:ARG:HD2	1.84	0.43
1:D:564:SER:OG	1:D:565:ASN:N	2.96	0.43
1:B:324:TYR:CE2	1:B:422:LEU:HD21	2.75	0.43
1:P:400:TYR:CE2	1:P:575:LYS:HA	2.53	0.43
1:N:424:VAL:HG21	1:N:429:VAL:HB	2.01	0.43
1:R:322:THR:HG21	1:R:420:PHE:CD2	2.54	0.43
1:W:92:VAL:O	1:W:93:ASN:HB2	2.18	0.43
1:B:333:PRO:HG2	1:H:474:PHE:CZ	120.96	0.43
1:Y:443:ASN:OD1	1:Y:443:ASN:N	2.50	0.43
1:W:393:GLU:O	1:W:393:GLU:HG2	2.17	0.43
1:G:92:VAL:O	1:G:93:ASN:HB2	2.19	0.43
1:E:365:GLN:HG2	1:E:366:THR:HG23	1.99	0.43
1:A:304:GLY:O	1:Y:84:VAL:HG22	154.05	0.43
1:V:130:VAL:HG13	1:V:576:SER:O	2.18	0.43
1:X:569:MET:HB2	1:X:569:MET:HE2	1.84	0.43
1:A:583:LEU:HD11	1:Y:476:THR:HG22	148.35	0.43
1:J:131:ASN:O	1:J:550:GLN:NE2	2.51	0.43
1:A:572:VAL:O	1:A:574:GLU:HG2	4.40	0.43
1:Z:461:PRO:HA	1:Z:462:PRO:HD3	1.80	0.43
1:Z:52:LYS:HE3	1:Z:60:TYR:CD2	2.53	0.43
1:E:274:ARG:HH12	1:V:475:ASP:CG	2.20	0.43
1:M:334:ALA:HB1	1:M:454:LEU:O	2.18	0.43
1:G:434:ASP:HA	1:G:435:PRO:HD3	1.76	0.43
1:S:354:LYS:HG2	1:S:355:THR:N	2.33	0.43
1:N:138:LEU:HG	1:N:268:PHE:CD2	2.54	0.43
1:F:109:TRP:CD1	1:F:246:ILE:HG13	2.53	0.43
1:B:236:THR:HB	1:F:558:GLN:NE2	2.33	0.43
1:B:191:ARG:O	1:B:193:GLU:HG3	2.19	0.43
1:L:346:GLU:O	1:L:352:PRO:HA	2.19	0.43
1:C:346:GLU:O	1:C:352:PRO:HA	2.28	0.43
1:P:408:ARG:HA	1:P:408:ARG:HD3	1.86	0.43
1:L:569:MET:HG2	1:L:570:LYS:N	2.30	0.43
1:B:439:LYS:NZ	1:M:434:ASP:OD2	2.37	0.43
1:F:583:LEU:HD12	1:F:583:LEU:HA	1.77	0.43
1:D:148:VAL:O	1:D:257:THR:HG23	2.27	0.43
1:C:256:ARG:NH1	1:D:257:THR:HG22	19.91	0.43
1:S:434:ASP:HA	1:S:435:PRO:HD3	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:TYR:C	1:A:574:GLU:HG2	3.78	0.43
1:I:354:LYS:HG2	1:I:355:THR:N	2.33	0.43
1:O:377:ARG:NH2	1:O:397:ARG:HD2	2.33	0.43
1:S:247:GLU:OE1	1:S:247:GLU:N	2.44	0.43
1:B:127:GLN:HE22	1:L:548:ILE:H	123.09	0.43
1:L:417:ASN:OD1	1:L:419:ASN:ND2	2.46	0.43
1:A:133:MET:CG	1:A:539:LEU:HD23	2.69	0.43
1:E:51:PHE:CD2	1:E:61:ILE:HG12	2.53	0.43
1:B:554:ASN:O	1:B:558:GLN:HB2	2.18	0.43
1:B:212:PHE:HE1	1:B:236:THR:HG21	1.83	0.43
1:N:558:GLN:HG2	1:N:558:GLN:O	2.17	0.43
1:B:581:ARG:HB3	1:B:582:LYS:H	1.58	0.43
1:V:369:ASN:HB3	1:V:372:ALA:HB3	2.00	0.43
1:D:493:ASN:OD1	1:D:493:ASN:N	2.51	0.43
1:R:369:ASN:C	1:R:371:ALA:H	2.20	0.43
1:X:271:LYS:NZ	1:X:459:ASN:ND2	2.66	0.43
1:M:475:ASP:CG	1:R:274:ARG:HH12	2.21	0.43
1:N:434:ASP:OD2	1:S:439:LYS:NZ	2.36	0.43
1:D:369:ASN:HD21	1:D:372:ALA:HB2	1.82	0.43
1:N:369:ASN:C	1:N:371:ALA:H	2.20	0.43
1:O:177:LEU:HD22	1:O:263:THR:HG22	2.00	0.43
1:A:363:GLY:HA2	1:A:409:TYR:HB2	2.44	0.43
1:C:105:ILE:HG12	1:C:212:PHE:HB2	2.12	0.43
1:D:118:GLY:HA3	1:D:197:PHE:CD2	2.86	0.43
1:G:210:TYR:OH	1:G:244:TYR:N	2.47	0.43
1:F:363:GLY:HA3	1:F:367:ASP:O	2.19	0.43
1:I:361:ARG:HB2	1:I:368:GLU:CD	2.39	0.43
1:P:153:VAL:HG21	1:R:508:ASN:OD1	2.18	0.43
1:Y:389:THR:HG23	1:Y:568:GLY:O	2.18	0.43
1:E:569:MET:HB2	1:E:569:MET:HE2	1.79	0.43
1:K:492:ASN:HB3	1:K:493:ASN:H	1.51	0.43
1:A:464:TYR:O	1:A:573:TYR:HA	2.18	0.43
1:A:248:ASN:HD22	1:N:122:ASN:HD22	1.66	0.43
1:D:464:TYR:HA	1:D:465:PRO:HA	1.96	0.43
1:N:333:PRO:HG2	1:S:474:PHE:CZ	2.54	0.43
1:O:294:LEU:HA	1:O:295:PRO:HD3	1.87	0.43
1:E:232:ILE:HG12	1:E:233:TYR:N	2.34	0.43
1:A:393:GLU:HG3	1:A:393:GLU:O	2.92	0.43
1:H:216:ARG:NH1	1:H:231:ASN:OD1	2.35	0.43
1:C:102:HIS:HB2	1:C:214:TRP:CH2	2.61	0.43
1:D:66:SER:HA	1:D:529:TRP:O	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:153:VAL:HG12	1:N:154:SER:N	2.34	0.43
1:Y:554:ASN:CB	1:Y:557:ASN:HB3	2.46	0.43
1:Y:556:ASP:O	1:Y:557:ASN:HB3	2.18	0.43
1:D:287:LEU:HB2	1:F:186:THR:HB	105.02	0.43
1:O:163:LYS:NZ	1:O:165:TYR:CE1	2.87	0.43
1:J:346:GLU:O	1:J:352:PRO:HA	2.19	0.43
1:A:434:ASP:HA	1:A:435:PRO:HD3	1.69	0.43
1:H:548:ILE:H	1:V:127:GLN:HE22	1.66	0.43
1:D:98:LEU:HA	1:L:326:THR:HG21	130.00	0.43
1:E:573:TYR:O	1:E:574:GLU:HG2	2.19	0.43
1:J:339:SER:OG	1:J:408:ARG:HG3	2.18	0.43
1:H:464:TYR:O	1:H:573:TYR:HA	2.19	0.43
1:W:257:THR:HG22	1:Y:256:ARG:HH12	1.84	0.43
1:D:288:PRO:O	1:F:209:ARG:NE	107.18	0.43
1:K:92:VAL:O	1:K:93:ASN:HB2	2.19	0.43
1:B:393:GLU:O	1:B:393:GLU:HG3	2.19	0.43
1:M:436:ILE:HA	1:M:436:ILE:HD13	1.79	0.43
1:A:515:SER:OG	1:N:390:THR:O	2.37	0.43
1:C:52:LYS:HB3	1:C:60:TYR:HB3	2.56	0.43
1:M:140:SER:O	1:M:533:LEU:HD12	2.19	0.43
1:H:422:LEU:HA	1:H:423:PRO:C	2.39	0.43
1:B:331:MET:HE3	1:R:485:ASN:HB3	2.00	0.43
1:D:123:PRO:HB2	1:G:547:PRO:HD3	68.29	0.43
1:O:361:ARG:HD2	1:O:402:ALA:O	2.19	0.43
1:P:131:ASN:O	1:P:550:GLN:NE2	2.51	0.43
1:M:130:VAL:HG12	1:M:578:LEU:HD22	2.00	0.43
1:G:194:THR:N	1:G:384:HIS:HE1	2.15	0.43
1:R:382:ARG:NE	1:R:390:THR:O	2.45	0.43
1:B:378:TYR:O	1:B:397:ARG:HA	2.19	0.43
1:K:568:GLY:HA3	1:K:569:MET:HB2	2.01	0.43
1:H:318:GLN:CB	1:W:354:LYS:HE2	2.48	0.43
1:A:59:VAL:HG21	1:A:133:MET:HE2	2.05	0.43
1:X:105:ILE:HG12	1:X:212:PHE:HB2	2.01	0.43
1:D:109:TRP:CD1	1:D:246:ILE:HG13	2.53	0.43
1:S:62:THR:HG23	1:S:534:VAL:HG22	2.01	0.43
1:Q:367:ASP:N	1:Q:367:ASP:OD1	2.52	0.43
1:C:247:GLU:N	1:C:247:GLU:OE1	2.47	0.43
1:D:177:LEU:HD22	1:D:263:THR:HG22	2.01	0.43
1:M:432:PRO:O	1:M:443:ASN:ND2	2.37	0.43
1:S:185:PHE:CD2	1:S:187:PRO:HD3	2.54	0.43
1:C:417:ASN:OD1	1:C:419:ASN:ND2	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:256:ARG:NH1	1:S:257:THR:HG22	2.33	0.43
1:O:257:THR:HG22	1:P:256:ARG:NH1	2.34	0.43
1:C:153:VAL:HG12	1:C:154:SER:N	2.33	0.43
1:A:348:SER:OG	1:A:349:THR:N	2.52	0.43
1:D:408:ARG:HA	1:D:408:ARG:HD3	1.86	0.43
1:R:346:GLU:O	1:R:352:PRO:HA	2.18	0.43
1:E:572:VAL:HG12	1:E:573:TYR:O	2.19	0.43
1:J:130:VAL:HG11	1:J:578:LEU:HD13	1.99	0.43
1:B:423:PRO:HA	1:H:94:GLY:O	149.39	0.43
1:F:465:PRO:HG3	1:F:571:ILE:CG2	2.49	0.43
1:A:198:TYR:HA	1:A:199:PRO:HD3	1.90	0.43
1:X:136:LEU:HD12	1:X:537:ALA:HB2	2.00	0.43
1:B:326:THR:H	1:B:329:THR:HB	1.99	0.43
1:N:422:LEU:HA	1:N:423:PRO:C	2.39	0.43
1:C:286:GLY:O	1:C:288:PRO:HD3	2.19	0.43
1:U:558:GLN:HG2	1:U:558:GLN:O	2.19	0.42
1:C:369:ASN:C	1:C:371:ALA:N	2.65	0.42
1:B:55:GLU:O	1:B:56:ASN:OD1	4.24	0.42
1:O:153:VAL:HG12	1:O:154:SER:N	2.33	0.42
1:Y:383:GLN:HB3	1:Y:384:HIS:CD2	2.54	0.42
1:B:176:ALA:HB2	1:B:252:VAL:HG22	1.99	0.42
1:I:352:PRO:HD2	1:V:283:ARG:HH12	1.84	0.42
1:M:383:GLN:CB	1:M:384:HIS:HD2	2.32	0.42
1:K:569:MET:HB2	1:K:569:MET:HE2	1.84	0.42
1:C:413:ASP:O	1:C:432:PRO:HD3	2.27	0.42
1:W:77:GLU:HB2	1:W:518:MET:HE1	2.01	0.42
1:F:59:VAL:HG21	1:F:133:MET:HE2	2.01	0.42
1:S:414:TRP:HE1	1:S:416:GLN:HE21	1.67	0.42
1:B:485:ASN:HB3	1:M:331:MET:HE3	2.01	0.42
1:I:376:PRO:HG2	1:I:400:TYR:HB3	2.00	0.42
1:S:369:ASN:O	1:S:371:ALA:N	2.52	0.42
1:L:389:THR:HG23	1:L:568:GLY:O	2.19	0.42
1:H:51:PHE:CD2	1:H:61:ILE:HG12	2.55	0.42
1:A:558:GLN:HE22	1:B:236:THR:HB	134.98	0.42
1:H:558:GLN:HG2	1:H:558:GLN:O	2.18	0.42
1:G:386:GLN:OE1	1:G:396:GLU:N	2.52	0.42
1:H:581:ARG:HB3	1:H:582:LYS:H	1.60	0.42
1:L:58:TRP:CZ2	1:L:538:LYS:HE2	2.55	0.42
1:B:323:ASN:HB3	1:H:397:ARG:NH1	132.09	0.42
1:O:581:ARG:HB3	1:O:582:LYS:H	1.55	0.42
1:K:445:THR:HA	1:K:448:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ASN:OD1	1:C:87:LEU:HD12	4.74	0.42
1:Q:130:VAL:HG13	1:Q:576:SER:O	2.20	0.42
1:J:190:MET:HE1	1:U:331:MET:HG2	2.00	0.42
1:Y:117:TRP:CE2	1:Y:469:ILE:HG12	2.54	0.42
1:D:318:GLN:HB2	1:F:354:LYS:HE2	130.70	0.42
1:M:550:GLN:HA	1:M:578:LEU:HD23	2.01	0.42
1:G:161:PRO:O	1:G:162:THR:OG1	2.29	0.42
1:E:336:VAL:O	1:E:408:ARG:NH2	2.53	0.42
1:C:137:HIS:CE1	1:C:272:PRO:HB3	2.54	0.42
1:W:569:MET:HE2	1:W:569:MET:HB2	1.88	0.42
1:A:257:THR:HG22	1:B:256:ARG:HH12	153.01	0.42
1:X:96:MET:H	1:X:96:MET:HG3	1.52	0.42
1:A:137:HIS:CD2	1:A:272:PRO:HB3	3.11	0.42
1:B:183:MET:HE1	1:B:246:ILE:CD1	2.49	0.42
1:F:309:GLN:O	1:F:313:ARG:HG3	2.20	0.42
1:L:317:THR:HG22	1:L:330:ILE:HA	2.01	0.42
1:B:114:ALA:HB1	1:B:119:VAL:HG11	2.02	0.42
1:F:318:GLN:CB	1:L:354:LYS:HE2	2.50	0.42
1:X:378:TYR:O	1:X:397:ARG:HA	2.18	0.42
1:C:238:PRO:HA	1:C:241:VAL:HG23	2.09	0.42
1:P:417:ASN:OD1	1:P:418:ILE:N	2.53	0.42
1:D:414:TRP:HE1	1:D:416:GLN:HE21	1.94	0.42
1:A:236:THR:HB	1:Z:558:GLN:NE2	210.14	0.42
1:C:186:THR:HB	1:P:287:LEU:HD13	2.02	0.42
1:L:383:GLN:C	1:L:384:HIS:HD2	2.23	0.42
1:I:550:GLN:HA	1:I:578:LEU:HD23	2.02	0.42
1:G:247:GLU:OE1	1:G:247:GLU:N	2.48	0.42
1:F:283:ARG:HH12	1:L:352:PRO:HD2	1.83	0.42
1:B:550:GLN:HA	1:B:578:LEU:HD23	2.01	0.42
1:A:326:THR:HG21	1:Y:98:LEU:HA	177.10	0.42
1:R:70:HIS:CD2	1:T:510:TYR:HB3	2.54	0.42
1:U:568:GLY:HA3	1:U:569:MET:HB2	2.02	0.42
1:H:310:GLN:OE1	1:W:98:LEU:HD13	2.19	0.42
1:H:367:ASP:O	1:H:368:GLU:HB3	2.20	0.42
1:S:93:ASN:ND2	1:S:225:THR:O	2.50	0.42
1:S:389:THR:HG23	1:S:568:GLY:O	2.19	0.42
1:E:432:PRO:CA	1:E:443:ASN:HD22	2.33	0.42
1:D:583:LEU:HD12	1:D:583:LEU:HA	1.85	0.42
1:D:114:ALA:HB1	1:D:119:VAL:HG11	2.01	0.42
1:K:55:GLU:HG3	1:R:55:GLU:HG2	2.01	0.42
1:B:234:HIS:HB3	1:M:365:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:ASN:ND2	1:F:100:ASP:HB2	2.34	0.42
1:K:191:ARG:O	1:K:193:GLU:HG3	2.20	0.42
1:P:212:PHE:O	1:P:214:TRP:HE3	2.02	0.42
1:K:131:ASN:O	1:K:550:GLN:NE2	2.52	0.42
1:C:159:GLN:O	1:C:161:PRO:HA	2.30	0.42
1:T:155:GLU:HG3	1:T:156:SER:CB	2.50	0.42
1:O:159:GLN:O	1:O:161:PRO:HA	2.19	0.42
1:B:476:THR:HB	1:W:457:LEU:O	120.11	0.42
1:E:283:ARG:HH12	1:V:352:PRO:HD2	1.84	0.42
1:D:456:ALA:O	1:D:457:LEU:HD12	2.32	0.42
1:D:96:MET:SD	1:D:220:PRO:HA	2.59	0.42
1:C:86:ASN:HB2	1:C:88:ASP:OD1	2.19	0.42
1:H:256:ARG:HH12	1:L:257:THR:HG22	1.84	0.42
1:P:266:PHE:HZ	1:P:493:ASN:O	2.03	0.42
1:C:322:THR:HG21	1:C:420:PHE:CD2	2.55	0.42
1:M:148:VAL:O	1:M:257:THR:HG23	2.19	0.42
1:K:257:THR:HG22	1:M:256:ARG:HH12	1.84	0.42
1:K:225:THR:HG22	1:K:226:SER:O	2.20	0.42
1:K:132:THR:HG22	1:R:132:THR:HG22	2.01	0.42
1:Z:465:PRO:HG3	1:Z:571:ILE:CG2	2.50	0.42
1:G:485:ASN:N	1:G:485:ASN:OD1	2.49	0.42
1:F:365:GLN:HG2	1:F:366:THR:HG23	2.02	0.42
1:N:152:THR:HG23	1:N:168:ASP:HB2	2.01	0.42
1:D:136:LEU:HD12	1:D:537:ALA:HB2	2.02	0.42
1:D:131:ASN:O	1:D:550:GLN:NE2	2.73	0.42
1:C:346:GLU:OE1	1:P:408:ARG:NH1	2.53	0.42
1:M:156:SER:CB	1:M:164:VAL:HG22	2.50	0.42
1:C:475:ASP:OD2	1:P:581:ARG:HD3	2.18	0.42
1:M:368:GLU:HG2	1:M:369:ASN:H	1.84	0.42
1:N:492:ASN:N	1:N:492:ASN:OD1	2.52	0.42
1:A:266:PHE:HZ	1:A:493:ASN:O	2.03	0.42
1:U:157:ALA:HA	1:U:158:THR:CG2	2.50	0.42
1:B:547:PRO:HD3	1:P:123:PRO:HB2	2.01	0.42
1:G:572:VAL:HG12	1:G:573:TYR:O	2.20	0.42
1:T:86:ASN:ND2	1:T:100:ASP:HB2	2.34	0.42
1:Z:572:VAL:HG12	1:Z:573:TYR:O	2.18	0.42
1:U:436:ILE:HD13	1:U:436:ILE:HA	1.71	0.42
1:F:424:VAL:HG12	1:L:94:GLY:HA2	2.01	0.42
1:A:238:PRO:HA	1:A:241:VAL:HG23	2.17	0.42
1:Z:118:GLY:HA3	1:Z:197:PHE:CD2	2.55	0.42
1:A:331:MET:HE3	1:K:485:ASN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:109:TRP:CD1	1:K:246:ILE:HG13	2.54	0.42
1:W:66:SER:HA	1:W:529:TRP:O	2.20	0.42
1:U:339:SER:O	1:U:449:ASN:HA	2.19	0.42
1:V:382:ARG:N	1:V:386:GLN:HB3	2.18	0.42
1:N:553:ILE:CA	1:N:554:ASN:HB2	2.38	0.42
1:L:382:ARG:NH2	1:L:392:GLY:O	2.49	0.42
1:I:434:ASP:HA	1:I:435:PRO:HD3	1.71	0.42
1:D:475:ASP:CG	1:L:274:ARG:HH12	116.49	0.42
1:A:583:LEU:HD11	1:K:476:THR:HG22	2.00	0.42
1:C:443:ASN:OD1	1:C:443:ASN:N	2.60	0.42
1:Z:43:GLY:HA3	1:Z:146:PHE:CD2	2.55	0.42
1:D:546:ASN:ND2	1:D:547:PRO:O	2.42	0.42
1:O:461:PRO:HA	1:O:462:PRO:HD3	1.82	0.42
1:S:432:PRO:O	1:S:443:ASN:ND2	2.43	0.42
1:F:298:GLU:OE1	1:M:387:LYS:NZ	2.44	0.42
1:X:483:HIS:HB3	1:X:485:ASN:OD1	2.20	0.42
1:T:209:ARG:HG3	1:T:209:ARG:HH11	1.83	0.42
1:H:557:ASN:O	1:H:559:PHE:N	2.53	0.42
1:B:274:ARG:HH12	1:H:475:ASP:CG	111.92	0.42
1:D:361:ARG:NE	1:D:405:ASP:OD1	2.53	0.42
1:D:492:ASN:CG	1:D:493:ASN:N	2.89	0.42
1:X:322:THR:HB	1:X:324:TYR:H	1.84	0.42
1:K:464:TYR:O	1:K:573:TYR:HA	2.20	0.42
1:A:133:MET:HG3	1:A:539:LEU:HD23	2.27	0.42
1:R:280:GLN:NE2	1:R:583:LEU:H	2.17	0.42
1:Q:59:VAL:HG21	1:Q:133:MET:HE2	2.02	0.42
1:E:88:ASP:OD1	1:E:89:LYS:HB2	2.20	0.42
1:B:403:HIS:CE1	1:B:549:GLN:HE22	3.22	0.42
1:T:461:PRO:HA	1:T:462:PRO:HD3	1.93	0.42
1:D:510:TYR:CE2	1:D:512:PRO:HD3	2.55	0.42
1:H:199:PRO:HD2	1:H:200:TRP:CZ3	2.55	0.42
1:H:271:LYS:HB2	1:H:271:LYS:HE3	1.84	0.42
1:C:122:ASN:HD22	1:Z:248:ASN:HD22	118.42	0.42
1:J:127:GLN:HA	1:J:551:MET:HE3	2.02	0.42
1:L:572:VAL:HG12	1:L:573:TYR:O	2.20	0.42
1:Q:159:GLN:O	1:Q:161:PRO:HA	2.19	0.42
1:S:383:GLN:C	1:S:384:HIS:HD2	2.23	0.42
1:Q:568:GLY:HA3	1:Q:569:MET:HB2	2.02	0.42
1:J:369:ASN:OD1	1:J:372:ALA:HB3	2.19	0.42
1:H:415:ILE:CD1	1:W:447:ILE:HG22	2.49	0.42
1:D:369:ASN:C	1:D:371:ALA:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:TYR:HA	1:A:465:PRO:HA	1.95	0.42
1:S:140:SER:HA	1:S:266:PHE:O	2.20	0.42
1:C:461:PRO:HA	1:C:462:PRO:HD3	1.91	0.42
1:U:510:TYR:HB3	1:X:70:HIS:CD2	2.55	0.42
1:G:294:LEU:HA	1:G:295:PRO:HD3	1.89	0.42
1:E:138:LEU:HG	1:E:268:PHE:CD2	2.54	0.42
1:A:212:PHE:HZ	1:N:562:VAL:HG11	1.85	0.42
1:X:326:THR:H	1:X:329:THR:HB	1.85	0.42
1:R:436:ILE:HD13	1:R:436:ILE:HA	1.75	0.42
1:W:361:ARG:HD3	1:W:405:ASP:OD1	2.20	0.42
1:B:142:GLU:HB3	1:B:265:THR:HA	2.09	0.42
1:D:92:VAL:O	1:D:93:ASN:HB2	2.20	0.42
1:U:553:ILE:HG21	1:U:553:ILE:HD13	1.83	0.42
1:L:386:GLN:HE21	1:L:390:THR:HG21	1.85	0.42
1:R:159:GLN:CB	1:R:160:PRO:HD2	2.50	0.42
1:B:475:ASP:OD1	1:W:274:ARG:NH1	115.55	0.42
1:A:408:ARG:NH1	1:Y:346:GLU:OE1	175.03	0.42
1:E:317:THR:HG21	1:E:329:THR:HG22	2.01	0.42
1:G:583:LEU:HD12	1:G:583:LEU:HA	1.75	0.42
1:C:389:THR:HG23	1:C:568:GLY:O	2.39	0.42
1:X:322:THR:HG21	1:X:420:PHE:CD2	2.54	0.42
1:U:133:MET:HE2	1:U:539:LEU:HD21	2.02	0.42
1:Q:443:ASN:N	1:Q:443:ASN:OD1	2.51	0.42
1:E:511:ASP:OD2	1:E:514:ALA:HB2	2.20	0.42
1:N:393:GLU:H	1:N:393:GLU:CD	2.23	0.42
1:W:363:GLY:HA3	1:W:367:ASP:O	2.20	0.42
1:V:59:VAL:HG21	1:V:133:MET:HE2	2.02	0.42
1:D:377:ARG:HH21	1:D:397:ARG:HD2	1.84	0.42
1:X:114:ALA:HB1	1:X:119:VAL:HG11	2.01	0.42
1:B:103:ALA:HB3	1:B:212:PHE:O	2.54	0.41
1:B:582:LYS:NZ	1:H:182:THR:O	110.50	0.41
1:Y:408:ARG:HD3	1:Y:408:ARG:HA	1.76	0.41
1:Q:369:ASN:C	1:Q:371:ALA:H	2.23	0.41
1:Q:462:PRO:HD2	1:Q:576:SER:OG	2.20	0.41
1:Z:75:GLU:H	1:Z:75:GLU:CD	2.23	0.41
1:N:96:MET:HG2	1:N:96:MET:H	1.50	0.41
1:V:247:GLU:OE1	1:V:247:GLU:N	2.47	0.41
1:L:435:PRO:HB3	1:L:439:LYS:O	2.20	0.41
1:C:390:THR:O	1:D:515:SER:OG	2.38	0.41
1:H:322:THR:HB	1:H:324:TYR:H	1.85	0.41
1:K:432:PRO:O	1:K:443:ASN:ND2	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:69:VAL:CG1	1:W:205:PRO:HD3	2.50	0.41
1:F:288:PRO:HG3	1:L:211:TYR:CG	2.55	0.41
1:Y:550:GLN:HA	1:Y:578:LEU:HD23	2.02	0.41
1:M:553:ILE:CA	1:M:554:ASN:HB2	2.35	0.41
1:A:382:ARG:HD2	1:B:513:ASP:O	162.55	0.41
1:R:158:THR:HG22	1:R:159:GLN:HG3	2.02	0.41
1:M:447:ILE:HG22	1:R:415:ILE:CD1	2.45	0.41
1:F:383:GLN:C	1:F:384:HIS:CD2	2.93	0.41
1:C:101:THR:O	1:P:283:ARG:NH2	2.53	0.41
1:C:541:ALA:O	1:C:543:HIS:CE1	2.98	0.41
1:O:130:VAL:HG11	1:O:578:LEU:HD13	2.01	0.41
1:H:256:ARG:NH1	1:L:257:THR:HG22	2.34	0.41
1:Z:408:ARG:HA	1:Z:408:ARG:HD3	1.76	0.41
1:E:92:VAL:O	1:E:93:ASN:HB2	2.20	0.41
1:U:198:TYR:HA	1:U:199:PRO:HD3	1.89	0.41
1:E:436:ILE:HD13	1:E:436:ILE:HA	1.79	0.41
1:V:393:GLU:HG2	1:V:393:GLU:O	2.19	0.41
1:I:203:THR:OG1	1:I:204:ILE:N	2.51	0.41
1:I:460:VAL:HG11	1:I:484:VAL:HA	2.01	0.41
1:L:339:SER:O	1:L:449:ASN:HA	2.19	0.41
1:F:461:PRO:HA	1:F:462:PRO:HD3	1.90	0.41
1:B:66:SER:HA	1:B:529:TRP:O	2.25	0.41
1:A:554:ASN:CB	1:A:557:ASN:HD22	2.33	0.41
1:T:271:LYS:CG	1:T:272:PRO:HD2	2.37	0.41
1:O:361:ARG:HG3	1:O:402:ALA:O	2.20	0.41
1:I:346:GLU:O	1:I:352:PRO:HA	2.21	0.41
1:G:369:ASN:O	1:G:372:ALA:N	2.51	0.41
1:A:366:THR:OG1	1:A:366:THR:O	2.82	0.41
1:M:317:THR:HG21	1:M:329:THR:HG22	2.01	0.41
1:A:378:TYR:O	1:A:397:ARG:HA	2.20	0.41
1:J:339:SER:O	1:J:449:ASN:HA	2.20	0.41
1:Q:573:TYR:O	1:Q:574:GLU:HG3	2.20	0.41
1:A:79:TYR:OH	1:A:247:GLU:OE1	2.36	0.41
1:N:278:THR:HB	1:N:583:LEU:HD13	2.03	0.41
1:Z:117:TRP:CE2	1:Z:469:ILE:HG12	2.55	0.41
1:O:560:ASN:HB3	1:O:572:VAL:HG21	2.03	0.41
1:P:198:TYR:HA	1:P:199:PRO:HD3	1.91	0.41
1:U:66:SER:HA	1:U:529:TRP:O	2.20	0.41
1:O:114:ALA:HB1	1:O:119:VAL:HG11	2.01	0.41
1:E:362:GLY:O	1:V:349:THR:N	2.52	0.41
1:X:138:LEU:HG	1:X:268:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:294:LEU:HA	1:Q:295:PRO:HD3	1.91	0.41
1:S:340:ALA:HB3	1:S:357:ILE:HD12	2.03	0.41
1:E:59:VAL:HG21	1:E:133:MET:HE2	2.02	0.41
1:L:468:GLN:HB3	1:L:485:ASN:O	2.20	0.41
1:B:432:PRO:O	1:B:443:ASN:ND2	2.46	0.41
1:P:92:VAL:O	1:P:93:ASN:HB2	2.19	0.41
1:O:346:GLU:OE2	1:O:355:THR:OG1	2.24	0.41
1:A:553:ILE:HG22	1:A:557:ASN:ND2	2.35	0.41
1:I:382:ARG:NE	1:I:390:THR:O	2.42	0.41
1:R:287:LEU:HD12	1:R:288:PRO:HD2	2.02	0.41
1:H:274:ARG:HH12	1:W:475:ASP:CG	2.23	0.41
1:F:569:MET:HB2	1:F:569:MET:HE2	1.80	0.41
1:C:266:PHE:HZ	1:C:493:ASN:O	2.08	0.41
1:U:378:TYR:O	1:U:397:ARG:HA	2.20	0.41
1:K:161:PRO:O	1:K:162:THR:OG1	2.36	0.41
1:H:159:GLN:CB	1:H:160:PRO:HD2	2.50	0.41
1:O:408:ARG:HA	1:O:408:ARG:HD3	1.86	0.41
1:A:299:GLY:N	1:W:565:ASN:ND2	138.88	0.41
1:J:94:GLY:O	1:U:423:PRO:HA	2.20	0.41
1:A:257:THR:HG22	1:B:256:ARG:NH1	152.83	0.41
1:V:109:TRP:CG	1:V:246:ILE:HG13	2.55	0.41
1:V:400:TYR:CE2	1:V:575:LYS:HA	2.55	0.41
1:B:266:PHE:HZ	1:B:493:ASN:O	2.05	0.41
1:F:481:ARG:HB3	1:L:478:LEU:HD13	2.03	0.41
1:F:298:GLU:HA	1:M:565:ASN:OD1	2.21	0.41
1:A:43:GLY:HA3	1:A:146:PHE:CD2	2.66	0.41
1:S:109:TRP:CD1	1:S:246:ILE:HG13	2.55	0.41
1:C:445:THR:HA	1:C:448:PHE:HB2	2.02	0.41
1:E:243:PHE:CD2	1:I:545:TRP:HB3	2.55	0.41
1:W:271:LYS:HE3	1:W:271:LYS:HB2	1.76	0.41
1:C:471:ASP:OD1	1:G:584:TYR:OH	114.96	0.41
1:L:414:TRP:HE1	1:L:416:GLN:HG3	1.84	0.41
1:H:232:ILE:HG12	1:H:233:TYR:N	2.36	0.41
1:D:117:TRP:CE2	1:D:469:ILE:HG12	2.55	0.41
1:Z:445:THR:HA	1:Z:448:PHE:HB2	2.01	0.41
1:W:87:LEU:HA	1:W:90:THR:OG1	2.19	0.41
1:R:408:ARG:HA	1:R:408:ARG:HD3	1.89	0.41
1:H:269:ASP:HB3	1:H:492:ASN:ND2	2.33	0.41
1:J:159:GLN:CB	1:J:160:PRO:HD2	2.50	0.41
1:I:324:TYR:CE2	1:I:422:LEU:HD21	2.56	0.41
1:C:581:ARG:HB3	1:C:582:LYS:H	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:572:VAL:O	1:I:574:GLU:HG2	2.20	0.41
1:D:288:PRO:HG3	1:F:211:TYR:CG	104.44	0.41
1:N:400:TYR:CE2	1:N:575:LYS:HA	2.55	0.41
1:E:377:ARG:NH2	1:E:397:ARG:HD2	2.35	0.41
1:R:266:PHE:HZ	1:R:493:ASN:O	2.02	0.41
1:I:200:TRP:CZ3	1:K:245:THR:HG21	2.56	0.41
1:C:384:HIS:ND1	1:C:384:HIS:N	3.70	0.41
1:N:132:THR:HG22	1:T:132:THR:HG22	2.02	0.41
1:F:389:THR:HG23	1:F:568:GLY:O	2.20	0.41
1:K:73:MET:CE	1:K:522:VAL:HA	2.50	0.41
1:I:554:ASN:O	1:I:558:GLN:HB2	2.21	0.41
1:I:286:GLY:O	1:I:288:PRO:HD3	2.21	0.41
1:A:153:VAL:HG12	1:A:163:LYS:CE	3.94	0.41
1:V:156:SER:O	1:V:157:ALA:HB3	2.21	0.41
1:F:575:LYS:O	1:F:576:SER:HB3	2.21	0.41
1:B:475:ASP:OD2	1:M:581:ARG:HD3	2.21	0.41
1:A:131:ASN:ND2	1:W:550:GLN:OE1	123.68	0.41
1:M:569:MET:HG2	1:M:570:LYS:N	2.32	0.41
1:K:90:THR:OG1	1:K:231:ASN:ND2	2.49	0.41
1:X:271:LYS:HD3	1:X:487:PRO:O	2.20	0.41
1:I:94:GLY:O	1:V:423:PRO:HA	2.20	0.41
1:K:572:VAL:HG12	1:K:573:TYR:O	2.19	0.41
1:B:492:ASN:OD1	1:B:493:ASN:N	2.89	0.41
1:E:404:GLN:NE2	1:E:461:PRO:HD3	2.36	0.41
1:M:94:GLY:HA2	1:R:424:VAL:HG12	2.03	0.41
1:T:48:GLN:O	1:T:64:ASN:HB2	2.20	0.41
1:Z:102:HIS:HB2	1:Z:214:TRP:CH2	2.55	0.41
1:L:226:SER:OG	1:L:227:GLY:N	2.53	0.41
1:R:339:SER:O	1:R:449:ASN:HA	2.20	0.41
1:Z:93:ASN:HD21	1:Z:229:PRO:HD3	1.85	0.41
1:B:430:LEU:HD22	1:R:442:ILE:HG21	2.01	0.41
1:E:48:GLN:O	1:E:64:ASN:HB2	2.20	0.41
1:H:148:VAL:O	1:H:257:THR:HG23	2.20	0.41
1:J:114:ALA:HB1	1:J:119:VAL:HG11	2.03	0.41
1:B:382:ARG:NH1	1:C:513:ASP:O	2.53	0.41
1:C:492:ASN:CG	1:C:493:ASN:H	2.24	0.41
1:G:518:MET:HE2	1:G:518:MET:HB2	1.76	0.41
1:B:388:THR:OG1	1:B:569:MET:N	2.53	0.41
1:Y:317:THR:HG21	1:Y:329:THR:HG22	2.02	0.41
1:B:346:GLU:O	1:B:352:PRO:HA	2.20	0.41
1:D:420:PHE:CE2	1:D:422:LEU:HD22	3.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:435:PRO:HA	1:S:442:ILE:O	2.20	0.41
1:Q:70:HIS:O	1:Q:204:ILE:HG22	2.19	0.41
1:T:99:ASP:CG	1:T:216:ARG:HH21	2.23	0.41
1:H:363:GLY:HA3	1:H:368:GLU:HA	2.02	0.41
1:A:445:THR:HA	1:A:448:PHE:HB2	2.03	0.41
1:T:398:PHE:CE2	1:T:573:TYR:HB2	2.56	0.41
1:H:151:LYS:HE3	1:I:505:ASN:OD1	2.20	0.41
1:X:494:CYS:SG	1:X:495:PRO:HD2	2.60	0.41
1:U:127:GLN:HG3	1:U:551:MET:HE2	2.02	0.41
1:M:442:ILE:HG23	1:M:446:ASN:HD22	1.86	0.41
1:F:326:THR:H	1:F:329:THR:HB	1.84	0.41
1:B:458:ASN:HA	1:R:477:ASP:HB2	2.03	0.41
1:L:212:PHE:HE1	1:L:236:THR:HG21	1.86	0.41
1:Q:191:ARG:O	1:Q:193:GLU:HG3	2.20	0.41
1:C:382:ARG:N	1:C:386:GLN:HB3	2.19	0.41
1:H:287:LEU:HD12	1:H:288:PRO:CD	2.51	0.41
1:L:408:ARG:HA	1:L:408:ARG:HD3	1.77	0.41
1:U:443:ASN:H	1:U:446:ASN:ND2	2.17	0.41
1:D:568:GLY:HA3	1:D:569:MET:HB2	2.04	0.41
1:C:434:ASP:HA	1:C:435:PRO:HD3	1.80	0.41
1:B:194:THR:H	1:B:384:HIS:HE1	1.69	0.41
1:N:464:TYR:O	1:N:573:TYR:HA	2.21	0.41
1:H:583:LEU:HD11	1:W:476:THR:HG22	2.03	0.41
1:G:387:LYS:HG2	1:G:389:THR:OG1	2.20	0.41
1:W:404:GLN:OE1	1:W:458:ASN:HB2	2.21	0.41
1:X:86:ASN:HB2	1:X:88:ASP:OD1	2.21	0.41
1:K:238:PRO:HA	1:K:241:VAL:HG23	2.03	0.41
1:D:485:ASN:OD1	1:D:485:ASN:N	2.52	0.41
1:A:362:GLY:HA3	1:A:407:GLY:C	2.54	0.41
1:P:46:ASN:OD1	1:P:48:GLN:HB2	2.21	0.41
1:V:102:HIS:HB2	1:V:214:TRP:CH2	2.55	0.41
1:Q:357:ILE:HB	1:Q:374:GLY:HA3	2.03	0.41
1:Y:266:PHE:HZ	1:Y:493:ASN:O	2.04	0.41
1:Q:105:ILE:HG12	1:Q:212:PHE:HB2	2.01	0.41
1:Z:354:LYS:HG2	1:Z:355:THR:N	2.36	0.41
1:O:554:ASN:O	1:O:558:GLN:HB2	2.21	0.41
1:C:382:ARG:HD2	1:D:513:ASP:O	2.21	0.41
1:B:211:TYR:CD1	1:W:288:PRO:HG3	130.05	0.41
1:A:154:SER:CA	1:A:155:GLU:HB2	2.45	0.41
1:P:105:ILE:HG12	1:P:212:PHE:HB2	2.01	0.41
1:I:475:ASP:OD2	1:V:581:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:274:ARG:HH12	1:S:475:ASP:CG	2.21	0.41
1:K:102:HIS:HB2	1:K:214:TRP:CH2	2.56	0.41
1:A:431:LEU:C	1:A:433:THR:H	2.38	0.41
1:L:154:SER:CA	1:L:155:GLU:HB2	2.48	0.41
1:G:79:TYR:HA	1:G:106:VAL:O	2.21	0.41
1:B:408:ARG:HD3	1:B:408:ARG:HA	1.90	0.41
1:L:159:GLN:O	1:L:161:PRO:HA	2.21	0.41
1:A:415:ILE:CD1	1:Y:447:ILE:HG22	195.93	0.41
1:Y:568:GLY:HA3	1:Y:569:MET:HB2	2.03	0.41
1:P:443:ASN:N	1:P:443:ASN:OD1	2.52	0.41
1:I:581:ARG:HB3	1:I:582:LYS:H	1.56	0.41
1:H:569:MET:HE2	1:H:569:MET:HB2	1.79	0.41
1:C:568:GLY:HA3	1:C:569:MET:HB2	2.03	0.41
1:T:403:HIS:CD2	1:T:549:GLN:HE22	2.38	0.41
1:I:278:THR:HB	1:I:583:LEU:HD13	2.03	0.41
1:G:326:THR:H	1:G:329:THR:HB	1.86	0.41
1:U:569:MET:HE2	1:U:569:MET:HB2	1.80	0.41
1:C:130:VAL:HG12	1:C:578:LEU:HD22	2.02	0.41
1:N:256:ARG:HH12	1:Q:257:THR:HG22	1.86	0.41
1:I:94:GLY:HA2	1:V:424:VAL:HG12	2.02	0.41
1:B:457:LEU:O	1:H:476:THR:HB	117.58	0.41
1:E:257:THR:HG22	1:J:256:ARG:NH1	2.36	0.41
1:C:148:VAL:O	1:C:257:THR:HG23	2.19	0.41
1:S:369:ASN:C	1:S:371:ALA:H	2.25	0.41
1:X:378:TYR:CE1	1:X:463:VAL:HG11	2.55	0.41
1:J:434:ASP:HA	1:J:435:PRO:HD3	1.76	0.41
1:E:266:PHE:HZ	1:E:493:ASN:O	2.03	0.41
1:J:66:SER:HA	1:J:529:TRP:O	2.21	0.41
1:O:138:LEU:HG	1:O:268:PHE:CD2	2.56	0.41
1:O:92:VAL:HB	1:O:95:ASN:HB2	2.03	0.41
1:H:442:ILE:HG23	1:H:446:ASN:HD22	1.85	0.41
1:N:545:TRP:HB3	1:S:243:PHE:CD2	2.55	0.41
1:Z:62:THR:HG23	1:Z:534:VAL:HG22	2.02	0.41
1:G:73:MET:CE	1:G:522:VAL:HA	2.51	0.41
1:Y:436:ILE:HD13	1:Y:436:ILE:HA	1.72	0.41
1:K:138:LEU:HG	1:K:268:PHE:CD2	2.56	0.41
1:R:142:GLU:HB3	1:R:265:THR:HA	2.03	0.41
1:S:256:ARG:NH1	1:T:257:THR:HG22	2.36	0.41
1:G:438:GLY:O	1:G:439:LYS:HD3	2.20	0.41
1:R:558:GLN:HG2	1:R:558:GLN:O	2.21	0.41
1:V:557:ASN:OD1	1:V:561:TYR:CE2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ASN:HB2	1:B:58:TRP:CD1	2.51	0.41
1:D:383:GLN:C	1:D:384:HIS:CD2	2.96	0.41
1:M:155:GLU:O	1:M:163:LYS:HA	2.21	0.41
1:D:473:GLU:HG2	1:D:491:GLN:NE2	4.72	0.41
1:M:159:GLN:O	1:M:161:PRO:HA	2.21	0.41
1:P:155:GLU:HA	1:P:163:LYS:HG3	2.02	0.41
1:B:424:VAL:HG12	1:R:94:GLY:HA2	2.02	0.41
1:V:137:HIS:NE2	1:V:272:PRO:HB3	2.35	0.41
1:A:198:TYR:HB2	1:A:201:LYS:HB3	2.23	0.41
1:Z:47:ASN:OD1	1:Z:67:ARG:NH1	2.53	0.41
1:S:301:THR:HG22	1:S:301:THR:O	2.21	0.41
1:K:354:LYS:HG2	1:K:355:THR:N	2.36	0.41
1:J:177:LEU:HD22	1:J:263:THR:HG22	2.03	0.41
1:Z:232:ILE:HG12	1:Z:233:TYR:N	2.36	0.41
1:B:130:VAL:HG13	1:B:576:SER:O	2.27	0.41
1:N:414:TRP:HE1	1:N:416:GLN:HE21	1.69	0.41
1:E:286:GLY:O	1:E:288:PRO:HD3	2.21	0.41
1:R:377:ARG:HH21	1:R:397:ARG:HD2	1.86	0.41
1:B:558:GLN:NE2	1:D:236:THR:HB	61.82	0.40
1:O:554:ASN:HB3	1:O:556:ASP:O	2.21	0.40
1:B:105:ILE:HG12	1:B:212:PHE:HB2	2.03	0.40
1:N:557:ASN:O	1:N:559:PHE:N	2.54	0.40
1:B:431:LEU:HD22	1:R:220:PRO:HB2	2.04	0.40
1:Y:383:GLN:HB3	1:Y:384:HIS:HD2	1.85	0.40
1:Q:153:VAL:HG12	1:Q:155:GLU:HG3	2.04	0.40
1:B:131:ASN:ND2	1:B:550:GLN:HB3	2.58	0.40
1:B:98:LEU:HA	1:M:326:THR:HG21	2.03	0.40
1:F:338:TYR:CE1	1:F:358:ALA:HB3	2.53	0.40
1:C:130:VAL:HG13	1:C:576:SER:O	2.33	0.40
1:H:400:TYR:OH	1:H:575:LYS:HA	2.21	0.40
1:B:583:LEU:HD11	1:H:476:THR:HG22	121.45	0.40
1:Z:81:ARG:HA	1:Z:105:ILE:HD13	2.03	0.40
1:Z:583:LEU:HD12	1:Z:583:LEU:HA	1.89	0.40
1:M:509:GLN:H	1:M:509:GLN:HG2	1.73	0.40
1:N:443:ASN:N	1:N:443:ASN:OD1	2.53	0.40
1:X:177:LEU:HD22	1:X:263:THR:HG22	2.04	0.40
1:O:556:ASP:O	1:O:557:ASN:HB3	2.22	0.40
1:K:408:ARG:HA	1:K:408:ARG:HD3	1.76	0.40
1:T:400:TYR:CE2	1:T:575:LYS:HA	2.56	0.40
1:J:159:GLN:O	1:J:161:PRO:HA	2.21	0.40
1:I:369:ASN:C	1:I:371:ALA:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:271:LYS:HD2	1:L:271:LYS:N	2.35	0.40
1:J:408:ARG:HA	1:J:408:ARG:HD3	1.84	0.40
1:W:127:GLN:HG3	1:W:551:MET:HB2	2.01	0.40
1:D:478:LEU:HB3	1:L:481:ARG:NH2	118.63	0.40
1:Y:155:GLU:HG2	1:Y:156:SER:N	2.36	0.40
1:Z:59:VAL:HG21	1:Z:133:MET:HE2	2.03	0.40
1:B:485:ASN:OD1	1:B:485:ASN:N	2.48	0.40
1:D:280:GLN:NE2	1:D:583:LEU:H	2.19	0.40
1:Y:130:VAL:HG13	1:Y:576:SER:O	2.21	0.40
1:U:375:ASP:HA	1:U:376:PRO:HD3	1.75	0.40
1:J:442:ILE:HG21	1:U:430:LEU:HD22	2.02	0.40
1:X:354:LYS:HG2	1:X:355:THR:N	2.35	0.40
1:Z:92:VAL:HB	1:Z:95:ASN:HB2	2.02	0.40
1:T:175:VAL:HG22	1:T:500:VAL:HG12	2.03	0.40
1:W:44:THR:O	1:W:530:LYS:HD3	2.22	0.40
1:C:73:MET:CE	1:C:522:VAL:HA	2.55	0.40
1:A:142:GLU:HB3	1:A:265:THR:HA	2.20	0.40
1:F:118:GLY:HA3	1:F:197:PHE:CD2	2.56	0.40
1:V:92:VAL:O	1:V:93:ASN:HB2	2.22	0.40
1:U:557:ASN:OD1	1:U:561:TYR:CE2	2.74	0.40
1:E:549:GLN:O	1:E:550:GLN:HG3	2.22	0.40
1:F:408:ARG:HD3	1:F:408:ARG:HA	1.78	0.40
1:D:551:MET:HB3	1:D:551:MET:HE3	1.96	0.40
1:Y:476:THR:O	1:Y:479:LYS:HE2	2.22	0.40
1:A:302:ASN:N	1:A:302:ASN:OD1	2.54	0.40
1:E:369:ASN:HB3	1:E:372:ALA:HB3	2.02	0.40
1:W:551:MET:HE3	1:W:551:MET:HB3	1.97	0.40
1:C:408:ARG:HD3	1:C:408:ARG:HA	1.72	0.40
1:H:583:LEU:HA	1:H:583:LEU:HD12	1.80	0.40
1:O:216:ARG:NH2	1:O:218:LEU:HD22	2.37	0.40
1:Q:518:MET:HB2	1:Q:518:MET:HE2	1.78	0.40
1:Q:92:VAL:HB	1:Q:95:ASN:HB2	2.04	0.40
1:W:483:HIS:HB3	1:W:485:ASN:OD1	2.20	0.40
1:E:426:ASP:HB2	1:V:222:HIS:CE1	2.57	0.40
1:B:333:PRO:HG2	1:H:474:PHE:HZ	121.26	0.40
1:Q:225:THR:HG22	1:Q:226:SER:O	2.21	0.40
1:N:286:GLY:O	1:N:288:PRO:HD3	2.21	0.40
1:V:168:ASP:CG	1:V:171:ALA:HB2	2.42	0.40
1:F:105:ILE:HG12	1:F:212:PHE:HB2	2.03	0.40
1:G:404:GLN:OE1	1:G:458:ASN:HB2	2.21	0.40
1:D:277:HIS:NE2	1:F:240:ASP:OD1	87.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:HIS:ND1	1:T:426:ASP:HB2	2.35	0.40
1:N:102:HIS:HB2	1:N:214:TRP:CH2	2.57	0.40
1:X:140:SER:HA	1:X:266:PHE:O	2.21	0.40
1:D:294:LEU:HA	1:D:295:PRO:HD3	1.86	0.40
1:L:461:PRO:HA	1:L:462:PRO:HD3	1.86	0.40
1:F:232:ILE:HG12	1:F:233:TYR:N	2.36	0.40
1:Z:383:GLN:C	1:Z:384:HIS:CD2	2.94	0.40
1:W:368:GLU:CG	1:W:369:ASN:N	2.81	0.40
1:C:492:ASN:CG	1:C:493:ASN:N	2.74	0.40
1:L:368:GLU:HG2	1:L:369:ASN:H	1.86	0.40
1:U:378:TYR:HB2	1:U:398:PHE:CE2	2.56	0.40
1:B:397:ARG:NH1	1:M:323:ASN:HB3	2.36	0.40
1:I:133:MET:CG	1:I:539:LEU:HD23	2.52	0.40
1:L:127:GLN:HG3	1:L:551:MET:HB2	2.03	0.40
1:E:98:LEU:HD13	1:I:310:GLN:OE1	2.21	0.40
1:S:133:MET:HE2	1:S:539:LEU:CD2	2.52	0.40
1:W:361:ARG:N	1:W:404:GLN:O	2.52	0.40
1:E:346:GLU:OE1	1:I:339:SER:OG	2.32	0.40
1:U:365:GLN:O	1:U:366:THR:HG22	2.22	0.40
1:V:177:LEU:HD22	1:V:263:THR:CG2	2.51	0.40
1:R:271:LYS:HB2	1:R:271:LYS:HE3	1.78	0.40
1:L:432:PRO:O	1:L:443:ASN:ND2	2.46	0.40
1:D:138:LEU:HG	1:D:268:PHE:CD2	2.56	0.40
1:K:123:PRO:HB2	1:R:547:PRO:HD3	2.03	0.40
1:K:105:ILE:HG12	1:K:212:PHE:HB2	2.03	0.40
1:G:47:ASN:OD1	1:G:67:ARG:NH1	2.52	0.40
1:J:382:ARG:NE	1:J:390:THR:O	2.43	0.40
1:J:382:ARG:NH2	1:J:392:GLY:O	2.44	0.40
1:G:569:MET:HG2	1:G:570:LYS:N	2.32	0.40
1:B:138:LEU:HA	1:B:138:LEU:HD12	1.93	0.40
1:B:133:MET:CG	1:B:539:LEU:HD23	2.51	0.40
1:B:286:GLY:O	1:B:288:PRO:HD3	2.21	0.40
1:K:198:TYR:HA	1:K:199:PRO:HD3	1.92	0.40
1:R:377:ARG:NH2	1:R:397:ARG:HD2	2.36	0.40
1:A:47:ASN:OD1	1:A:67:ARG:NH1	2.72	0.40
1:K:401:ILE:O	1:K:575:LYS:NZ	2.54	0.40
1:S:560:ASN:HB3	1:S:572:VAL:HG21	2.02	0.40
1:D:342:TYR:HA	1:D:343:TYR:HA	1.94	0.40
1:A:183:MET:HE3	1:A:208:TRP:CH2	2.75	0.40
1:O:197:PHE:CD1	1:O:197:PHE:N	2.90	0.40
1:J:506:LEU:HA	1:J:506:LEU:HD23	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:47:ASN:OD1	1:V:65:SER:HA	2.22	0.40
1:I:248:ASN:HD21	1:V:545:TRP:HE3	1.69	0.40
1:W:400:TYR:CE2	1:W:575:LYS:HA	2.56	0.40

All (20) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:209:ARG:NH1	1:Y:288:PRO:O[8_555]	2.04	0.16
1:N:182:THR:O	1:X:582:LYS:NZ[8_555]	2.06	0.14
1:S:584:TYR:OH	1:X:471:ASP:OD1[8_555]	2.07	0.13
1:O:191:ARG:NH1	1:Y:287:LEU:O[8_555]	2.10	0.10
1:C:287:LEU:O	1:Z:191:ARG:NH1[8_555]	2.10	0.10
1:J:287:LEU:O	1:Q:191:ARG:NH1[8_555]	2.12	0.08
1:D:281:THR:OG1	1:G:350:GLN:OE1[8_555]	2.12	0.08
1:D:191:ARG:NH1	1:c:287:LEU:O[8_555]	2.13	0.07
1:S:287:LEU:O	1:X:191:ARG:NH1[8_555]	2.14	0.06
1:O:584:TYR:OH	1:a:471:ASP:OD1[8_555]	2.14	0.06
1:Q:287:LEU:O	1:U:191:ARG:NH1[8_555]	2.15	0.05
1:J:584:TYR:OH	1:Q:471:ASP:OD1[8_555]	2.15	0.05
1:D:584:TYR:OH	1:G:471:ASP:OD1[8_555]	2.15	0.05
1:O:581:ARG:NH1	1:a:475:ASP:O[8_555]	2.15	0.05
1:Q:288:PRO:O	1:U:209:ARG:NH1[8_555]	2.16	0.04
1:D:287:LEU:O	1:G:191:ARG:NH1[8_555]	2.16	0.04
1:O:287:LEU:O	1:a:191:ARG:NH1[8_555]	2.17	0.03
1:N:191:ARG:NH1	1:X:287:LEU:O[8_555]	2.18	0.02
1:C:584:TYR:OH	1:Z:471:ASP:OD1[8_555]	2.18	0.02
1:Q:584:TYR:OH	1:U:471:ASP:OD1[8_555]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	546/584 (94%)	500 (92%)	31 (6%)	15 (3%)	6	44
1	B	546/584 (94%)	496 (91%)	32 (6%)	18 (3%)	5	39
1	C	546/584 (94%)	493 (90%)	39 (7%)	14 (3%)	7	45
1	D	546/584 (94%)	497 (91%)	32 (6%)	17 (3%)	5	41
1	E	546/584 (94%)	497 (91%)	33 (6%)	16 (3%)	6	42
1	F	546/584 (94%)	496 (91%)	33 (6%)	17 (3%)	5	41
1	G	546/584 (94%)	497 (91%)	32 (6%)	17 (3%)	5	41
1	H	546/584 (94%)	491 (90%)	38 (7%)	17 (3%)	5	41
1	I	546/584 (94%)	499 (91%)	34 (6%)	13 (2%)	7	47
1	J	546/584 (94%)	498 (91%)	33 (6%)	15 (3%)	6	44
1	K	546/584 (94%)	499 (91%)	31 (6%)	16 (3%)	6	42
1	L	546/584 (94%)	494 (90%)	35 (6%)	17 (3%)	5	41
1	M	546/584 (94%)	491 (90%)	40 (7%)	15 (3%)	6	44
1	N	546/584 (94%)	497 (91%)	34 (6%)	15 (3%)	6	44
1	O	546/584 (94%)	492 (90%)	35 (6%)	19 (4%)	4	38
1	P	546/584 (94%)	497 (91%)	32 (6%)	17 (3%)	5	41
1	Q	546/584 (94%)	496 (91%)	34 (6%)	16 (3%)	6	42
1	R	546/584 (94%)	490 (90%)	39 (7%)	17 (3%)	5	41
1	S	546/584 (94%)	500 (92%)	32 (6%)	14 (3%)	7	45
1	T	546/584 (94%)	501 (92%)	30 (6%)	15 (3%)	6	44
1	U	546/584 (94%)	496 (91%)	32 (6%)	18 (3%)	5	39
1	V	546/584 (94%)	492 (90%)	37 (7%)	17 (3%)	5	41
1	W	546/584 (94%)	491 (90%)	40 (7%)	15 (3%)	6	44
1	X	546/584 (94%)	495 (91%)	34 (6%)	17 (3%)	5	41
1	Y	546/584 (94%)	498 (91%)	30 (6%)	18 (3%)	5	39
1	Z	546/584 (94%)	497 (91%)	31 (6%)	18 (3%)	5	39
1	a	546/584 (94%)	497 (91%)	33 (6%)	16 (3%)	6	42
1	b	546/584 (94%)	489 (90%)	41 (8%)	16 (3%)	6	42
1	c	546/584 (94%)	499 (91%)	31 (6%)	16 (3%)	6	42
1	d	546/584 (94%)	498 (91%)	32 (6%)	16 (3%)	6	42
All	All	16380/17520 (94%)	14873 (91%)	1020 (6%)	487 (3%)	5	42

All (487) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	VAL
1	A	155	GLU
1	A	159	GLN
1	A	160	PRO
1	A	349	THR
1	A	370	GLN
1	A	382	ARG
1	A	517	ASN
1	A	582	LYS
1	E	153	VAL
1	E	155	GLU
1	E	160	PRO
1	E	349	THR
1	E	382	ARG
1	E	492	ASN
1	E	517	ASN
1	E	582	LYS
1	J	153	VAL
1	J	155	GLU
1	J	156	SER
1	J	160	PRO
1	J	349	THR
1	J	370	GLN
1	J	382	ARG
1	J	582	LYS
1	N	153	VAL
1	N	156	SER
1	N	160	PRO
1	N	349	THR
1	N	382	ARG
1	N	492	ASN
1	N	582	LYS
1	Q	153	VAL
1	Q	155	GLU
1	Q	160	PRO
1	Q	349	THR
1	Q	382	ARG
1	Q	558	GLN
1	Q	582	LYS
1	B	153	VAL
1	B	155	GLU
1	B	160	PRO
1	B	349	THR

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Mol	Chain	Res	Type
1	B	366	THR
1	B	370	GLN
1	B	382	ARG
1	B	492	ASN
1	B	558	GLN
1	B	582	LYS
1	C	153	VAL
1	C	155	GLU
1	C	159	GLN
1	C	160	PRO
1	C	349	THR
1	C	359	ALA
1	C	370	GLN
1	C	382	ARG
1	C	558	GLN
1	C	582	LYS
1	D	153	VAL
1	D	155	GLU
1	D	159	GLN
1	D	160	PRO
1	D	349	THR
1	D	382	ARG
1	D	582	LYS
1	F	153	VAL
1	F	155	GLU
1	F	156	SER
1	F	160	PRO
1	F	349	THR
1	F	359	ALA
1	F	370	GLN
1	F	382	ARG
1	F	492	ASN
1	F	558	GLN
1	F	576	SER
1	F	582	LYS
1	G	153	VAL
1	G	155	GLU
1	G	156	SER
1	G	160	PRO
1	G	349	THR
1	G	359	ALA
1	G	366	THR

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Mol	Chain	Res	Type
1	G	370	GLN
1	G	382	ARG
1	G	492	ASN
1	G	582	LYS
1	H	153	VAL
1	H	155	GLU
1	H	156	SER
1	H	159	GLN
1	H	160	PRO
1	H	349	THR
1	H	370	GLN
1	H	382	ARG
1	H	558	GLN
1	H	582	LYS
1	I	153	VAL
1	I	157	ALA
1	I	159	GLN
1	I	349	THR
1	I	382	ARG
1	I	492	ASN
1	I	582	LYS
1	K	155	GLU
1	K	160	PRO
1	K	349	THR
1	K	370	GLN
1	K	382	ARG
1	K	492	ASN
1	K	582	LYS
1	L	153	VAL
1	L	155	GLU
1	L	160	PRO
1	L	349	THR
1	L	370	GLN
1	L	382	ARG
1	L	582	LYS
1	M	153	VAL
1	M	156	SER
1	M	159	GLN
1	M	160	PRO
1	M	349	THR
1	M	370	GLN
1	M	382	ARG

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Mol	Chain	Res	Type
1	M	558	GLN
1	M	582	LYS
1	O	153	VAL
1	O	155	GLU
1	O	160	PRO
1	O	349	THR
1	O	359	ALA
1	O	382	ARG
1	O	492	ASN
1	O	582	LYS
1	P	153	VAL
1	P	155	GLU
1	P	160	PRO
1	P	349	THR
1	P	370	GLN
1	P	382	ARG
1	P	492	ASN
1	P	582	LYS
1	R	153	VAL
1	R	159	GLN
1	R	160	PRO
1	R	349	THR
1	R	359	ALA
1	R	370	GLN
1	R	382	ARG
1	R	517	ASN
1	R	582	LYS
1	S	153	VAL
1	S	156	SER
1	S	160	PRO
1	S	349	THR
1	S	364	ALA
1	S	382	ARG
1	S	558	GLN
1	S	582	LYS
1	T	153	VAL
1	T	155	GLU
1	T	160	PRO
1	T	349	THR
1	T	359	ALA
1	T	382	ARG
1	T	582	LYS

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Mol	Chain	Res	Type
1	U	153	VAL
1	U	155	GLU
1	U	160	PRO
1	U	349	THR
1	U	359	ALA
1	U	370	GLN
1	U	382	ARG
1	U	492	ASN
1	U	518	MET
1	U	558	GLN
1	U	582	LYS
1	V	153	VAL
1	V	155	GLU
1	V	156	SER
1	V	349	THR
1	V	370	GLN
1	V	382	ARG
1	V	582	LYS
1	W	153	VAL
1	W	155	GLU
1	W	156	SER
1	W	160	PRO
1	W	349	THR
1	W	359	ALA
1	W	370	GLN
1	W	382	ARG
1	W	582	LYS
1	X	153	VAL
1	X	155	GLU
1	X	160	PRO
1	X	349	THR
1	X	382	ARG
1	X	493	ASN
1	X	582	LYS
1	Y	153	VAL
1	Y	155	GLU
1	Y	160	PRO
1	Y	349	THR
1	Y	359	ALA
1	Y	382	ARG
1	Y	492	ASN
1	Y	517	ASN

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Mol	Chain	Res	Type
1	Y	582	LYS
1	Z	153	VAL
1	Z	155	GLU
1	Z	160	PRO
1	Z	349	THR
1	Z	359	ALA
1	Z	370	GLN
1	Z	382	ARG
1	Z	492	ASN
1	Z	558	GLN
1	Z	582	LYS
1	a	153	VAL
1	a	155	GLU
1	a	160	PRO
1	a	162	THR
1	a	349	THR
1	a	359	ALA
1	a	382	ARG
1	a	517	ASN
1	a	582	LYS
1	b	153	VAL
1	b	155	GLU
1	b	159	GLN
1	b	160	PRO
1	b	349	THR
1	b	366	THR
1	b	370	GLN
1	b	382	ARG
1	b	558	GLN
1	b	582	LYS
1	c	153	VAL
1	c	155	GLU
1	c	160	PRO
1	c	349	THR
1	c	382	ARG
1	c	492	ASN
1	c	582	LYS
1	d	153	VAL
1	d	155	GLU
1	d	159	GLN
1	d	160	PRO
1	d	349	THR

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Mol	Chain	Res	Type
1	d	382	ARG
1	d	492	ASN
1	d	517	ASN
1	d	558	GLN
1	d	582	LYS
1	A	359	ALA
1	A	558	GLN
1	A	576	SER
1	E	558	GLN
1	J	558	GLN
1	J	576	SER
1	N	154	SER
1	N	359	ALA
1	N	364	ALA
1	N	558	GLN
1	N	576	SER
1	Q	359	ALA
1	Q	492	ASN
1	B	359	ALA
1	B	576	SER
1	C	576	SER
1	D	156	SER
1	D	359	ALA
1	D	370	GLN
1	D	558	GLN
1	D	576	SER
1	G	558	GLN
1	G	576	SER
1	H	359	ALA
1	I	155	GLU
1	I	364	ALA
1	I	558	GLN
1	K	153	VAL
1	K	154	SER
1	K	359	ALA
1	K	366	THR
1	K	558	GLN
1	K	576	SER
1	L	359	ALA
1	L	366	THR
1	L	493	ASN
1	L	554	ASN

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Mol	Chain	Res	Type
1	L	558	GLN
1	L	576	SER
1	M	155	GLU
1	M	359	ALA
1	M	576	SER
1	O	156	SER
1	O	159	GLN
1	O	558	GLN
1	O	576	SER
1	P	359	ALA
1	P	558	GLN
1	P	576	SER
1	R	155	GLU
1	R	558	GLN
1	R	576	SER
1	S	155	GLU
1	S	359	ALA
1	S	576	SER
1	T	558	GLN
1	T	576	SER
1	U	576	SER
1	V	359	ALA
1	V	558	GLN
1	V	576	SER
1	W	162	THR
1	W	558	GLN
1	X	359	ALA
1	X	364	ALA
1	X	491	GLN
1	X	558	GLN
1	X	576	SER
1	Y	159	GLN
1	Y	370	GLN
1	Y	558	GLN
1	Y	576	SER
1	Z	364	ALA
1	Z	576	SER
1	a	558	GLN
1	a	576	SER
1	b	359	ALA
1	c	159	GLN
1	c	359	ALA

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Mol	Chain	Res	Type
1	c	364	ALA
1	c	558	GLN
1	c	576	SER
1	d	576	SER
1	A	364	ALA
1	E	359	ALA
1	E	370	GLN
1	E	554	ASN
1	E	576	SER
1	J	359	ALA
1	J	554	ASN
1	N	517	ASN
1	Q	162	THR
1	Q	227	GLY
1	Q	370	GLN
1	Q	554	ASN
1	Q	576	SER
1	B	554	ASN
1	D	364	ALA
1	F	162	THR
1	F	364	ALA
1	G	159	GLN
1	G	554	ASN
1	H	554	ASN
1	H	576	SER
1	I	554	ASN
1	I	576	SER
1	O	154	SER
1	O	554	ASN
1	P	364	ALA
1	R	156	SER
1	S	554	ASN
1	T	370	GLN
1	U	162	THR
1	U	364	ALA
1	V	159	GLN
1	V	554	ASN
1	W	576	SER
1	X	159	GLN
1	X	366	THR
1	X	554	ASN
1	Y	554	ASN

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Mol	Chain	Res	Type
1	Z	93	ASN
1	Z	156	SER
1	Z	516	ALA
1	Z	554	ASN
1	a	370	GLN
1	b	554	ASN
1	b	576	SER
1	c	156	SER
1	d	359	ALA
1	d	554	ASN
1	A	93	ASN
1	E	159	GLN
1	J	93	ASN
1	J	159	GLN
1	N	159	GLN
1	N	554	ASN
1	B	93	ASN
1	B	159	GLN
1	C	554	ASN
1	D	554	ASN
1	F	93	ASN
1	F	159	GLN
1	H	364	ALA
1	H	516	ALA
1	K	159	GLN
1	K	554	ASN
1	L	364	ALA
1	L	518	MET
1	M	154	SER
1	M	554	ASN
1	O	93	ASN
1	O	364	ALA
1	O	370	GLN
1	O	493	ASN
1	P	93	ASN
1	P	159	GLN
1	P	516	ALA
1	P	554	ASN
1	R	154	SER
1	R	554	ASN
1	T	159	GLN
1	T	554	ASN

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Mol	Chain	Res	Type
1	U	159	GLN
1	V	93	ASN
1	V	157	ALA
1	V	161	PRO
1	V	364	ALA
1	V	366	THR
1	W	492	ASN
1	W	493	ASN
1	W	554	ASN
1	Y	93	ASN
1	a	93	ASN
1	a	364	ALA
1	a	554	ASN
1	b	364	ALA
1	c	554	ASN
1	d	370	GLN
1	A	554	ASN
1	E	93	ASN
1	E	364	ALA
1	J	364	ALA
1	B	154	SER
1	B	162	THR
1	D	93	ASN
1	D	365	GLN
1	D	492	ASN
1	F	554	ASN
1	G	93	ASN
1	G	364	ALA
1	H	93	ASN
1	K	93	ASN
1	L	159	GLN
1	M	162	THR
1	R	162	THR
1	U	93	ASN
1	U	554	ASN
1	X	162	THR
1	Y	364	ALA
1	Y	371	ALA
1	Z	159	GLN
1	b	369	ASN
1	d	93	ASN
1	Q	364	ALA

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Mol	Chain	Res	Type
1	B	364	ALA
1	C	93	ASN
1	C	154	SER
1	H	154	SER
1	I	93	ASN
1	L	93	ASN
1	R	93	ASN
1	S	93	ASN
1	S	159	GLN
1	T	93	ASN
1	T	154	SER
1	T	364	ALA
1	Z	162	THR
1	b	93	ASN
1	c	93	ASN
1	d	364	ALA
1	a	159	GLN
1	Q	159	GLN
1	P	566	ILE
1	X	566	ILE
1	O	566	ILE
1	U	566	ILE
1	Y	566	ILE
1	c	161	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	476/495 (96%)	468 (98%)	8 (2%)	68 89
1	B	476/495 (96%)	472 (99%)	4 (1%)	86 95
1	C	476/495 (96%)	467 (98%)	9 (2%)	65 87
1	D	476/495 (96%)	470 (99%)	6 (1%)	76 91
1	E	476/495 (96%)	471 (99%)	5 (1%)	80 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	476/495 (96%)	470 (99%)	6 (1%)	76 91
1	G	476/495 (96%)	468 (98%)	8 (2%)	68 89
1	H	476/495 (96%)	468 (98%)	8 (2%)	68 89
1	I	476/495 (96%)	463 (97%)	13 (3%)	52 83
1	J	476/495 (96%)	471 (99%)	5 (1%)	80 92
1	K	476/495 (96%)	467 (98%)	9 (2%)	65 87
1	L	476/495 (96%)	467 (98%)	9 (2%)	65 87
1	M	476/495 (96%)	470 (99%)	6 (1%)	76 91
1	N	476/495 (96%)	470 (99%)	6 (1%)	76 91
1	O	476/495 (96%)	473 (99%)	3 (1%)	90 97
1	P	476/495 (96%)	472 (99%)	4 (1%)	86 95
1	Q	476/495 (96%)	470 (99%)	6 (1%)	76 91
1	R	476/495 (96%)	468 (98%)	8 (2%)	68 89
1	S	476/495 (96%)	465 (98%)	11 (2%)	58 85
1	T	476/495 (96%)	468 (98%)	8 (2%)	68 89
1	U	476/495 (96%)	468 (98%)	8 (2%)	68 89
1	V	476/495 (96%)	471 (99%)	5 (1%)	80 92
1	W	476/495 (96%)	468 (98%)	8 (2%)	68 89
1	X	476/495 (96%)	468 (98%)	8 (2%)	68 89
1	Y	476/495 (96%)	474 (100%)	2 (0%)	93 98
1	Z	476/495 (96%)	471 (99%)	5 (1%)	80 92
1	a	476/495 (96%)	471 (99%)	5 (1%)	80 92
1	b	476/495 (96%)	468 (98%)	8 (2%)	68 89
1	c	476/495 (96%)	463 (97%)	13 (3%)	52 83
1	d	476/495 (96%)	465 (98%)	11 (2%)	58 85
All	All	14280/14850 (96%)	14065 (98%)	215 (2%)	72 90

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	55	GLU
1	A	159	GLN

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Mol	Chain	Res	Type
1	A	209	ARG
1	A	368	GLU
1	A	457	LEU
1	A	517	ASN
1	A	549	GLN
1	E	47	ASN
1	E	52	LYS
1	E	368	GLU
1	E	565	ASN
1	E	573	TYR
1	J	44	THR
1	J	209	ARG
1	J	457	LEU
1	J	551	MET
1	J	573	TYR
1	N	96	MET
1	N	162	THR
1	N	368	GLU
1	N	393	GLU
1	N	558	GLN
1	N	574	GLU
1	Q	369	ASN
1	Q	373	ASP
1	Q	384	HIS
1	Q	492	ASN
1	Q	557	ASN
1	Q	573	TYR
1	B	88	ASP
1	B	494	CYS
1	B	554	ASN
1	B	573	TYR
1	C	75	GLU
1	C	225	THR
1	C	367	ASP
1	C	457	LEU
1	C	493	ASN
1	C	513	ASP
1	C	555	VAL
1	C	573	TYR
1	C	574	GLU
1	D	96	MET
1	D	209	ARG

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Mol	Chain	Res	Type
1	D	226	SER
1	D	271	LYS
1	D	361	ARG
1	D	518	MET
1	F	209	ARG
1	F	260	GLU
1	F	491	GLN
1	F	517	ASN
1	F	549	GLN
1	F	573	TYR
1	G	55	GLU
1	G	75	GLU
1	G	209	ARG
1	G	368	GLU
1	G	425	THR
1	G	492	ASN
1	G	573	TYR
1	G	574	GLU
1	H	367	ASP
1	H	387	LYS
1	H	457	LEU
1	H	536	LYS
1	H	549	GLN
1	H	565	ASN
1	H	573	TYR
1	H	574	GLU
1	I	88	ASP
1	I	96	MET
1	I	155	GLU
1	I	156	SER
1	I	163	LYS
1	I	209	ARG
1	I	226	SER
1	I	296	GLN
1	I	369	ASN
1	I	457	LEU
1	I	518	MET
1	I	554	ASN
1	I	574	GLU
1	K	47	ASN
1	K	55	GLU
1	K	155	GLU

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Mol	Chain	Res	Type
1	K	163	LYS
1	K	457	LEU
1	K	549	GLN
1	K	553	ILE
1	K	558	GLN
1	K	574	GLU
1	L	159	GLN
1	L	162	THR
1	L	260	GLU
1	L	302	ASN
1	L	490	CYS
1	L	492	ASN
1	L	519	SER
1	L	573	TYR
1	L	582	LYS
1	M	155	GLU
1	M	302	ASN
1	M	368	GLU
1	M	543	HIS
1	M	553	ILE
1	M	573	TYR
1	O	163	LYS
1	O	457	LEU
1	O	573	TYR
1	P	361	ARG
1	P	519	SER
1	P	536	LYS
1	P	573	TYR
1	R	75	GLU
1	R	156	SER
1	R	209	ARG
1	R	457	LEU
1	R	508	ASN
1	R	509	GLN
1	R	519	SER
1	R	573	TYR
1	S	44	THR
1	S	96	MET
1	S	154	SER
1	S	296	GLN
1	S	302	ASN
1	S	427	ASP

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Mol	Chain	Res	Type
1	S	457	LEU
1	S	549	GLN
1	S	554	ASN
1	S	558	GLN
1	S	573	TYR
1	T	88	ASP
1	T	384	HIS
1	T	457	LEU
1	T	492	ASN
1	T	509	GLN
1	T	536	LYS
1	T	565	ASN
1	T	573	TYR
1	U	159	GLN
1	U	370	GLN
1	U	457	LEU
1	U	492	ASN
1	U	543	HIS
1	U	553	ILE
1	U	565	ASN
1	U	573	TYR
1	V	159	GLN
1	V	365	GLN
1	V	493	ASN
1	V	494	CYS
1	V	573	TYR
1	W	159	GLN
1	W	309	GLN
1	W	387	LYS
1	W	553	ILE
1	W	556	ASP
1	W	573	TYR
1	W	574	GLU
1	W	582	LYS
1	X	96	MET
1	X	368	GLU
1	X	384	HIS
1	X	457	LEU
1	X	494	CYS
1	X	518	MET
1	X	558	GLN
1	X	582	LYS

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Mol	Chain	Res	Type
1	Y	209	ARG
1	Y	573	TYR
1	Z	55	GLU
1	Z	209	ARG
1	Z	457	LEU
1	Z	509	GLN
1	Z	549	GLN
1	a	50	GLU
1	a	156	SER
1	a	163	LYS
1	a	226	SER
1	a	573	TYR
1	b	75	GLU
1	b	87	LEU
1	b	159	GLN
1	b	384	HIS
1	b	444	TYR
1	b	457	LEU
1	b	573	TYR
1	b	574	GLU
1	c	96	MET
1	c	155	GLU
1	c	209	ARG
1	c	280	GLN
1	c	309	GLN
1	c	361	ARG
1	c	368	GLU
1	c	384	HIS
1	c	416	GLN
1	c	457	LEU
1	c	518	MET
1	c	558	GLN
1	c	565	ASN
1	d	44	THR
1	d	88	ASP
1	d	260	GLU
1	d	271	LYS
1	d	457	LEU
1	d	517	ASN
1	d	518	MET
1	d	556	ASP
1	d	565	ASN

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Mol	Chain	Res	Type
1	d	573	TYR
1	d	582	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	HIS
1	A	248	ASN
1	A	384	HIS
1	A	557	ASN
1	A	558	GLN
1	E	280	GLN
1	E	369	ASN
1	E	384	HIS
1	E	517	ASN
1	E	557	ASN
1	J	137	HIS
1	J	549	GLN
1	J	554	ASN
1	N	302	ASN
1	N	446	ASN
1	N	491	GLN
1	Q	280	GLN
1	Q	492	ASN
1	Q	558	GLN
1	B	56	ASN
1	B	137	HIS
1	B	384	HIS
1	C	386	GLN
1	C	549	GLN
1	C	558	GLN
1	D	280	GLN
1	D	384	HIS
1	D	557	ASN
1	D	558	GLN
1	F	137	HIS
1	F	248	ASN
1	F	384	HIS
1	F	554	ASN
1	G	302	ASN
1	G	384	HIS
1	G	446	ASN

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Mol	Chain	Res	Type
1	G	492	ASN
1	G	554	ASN
1	G	558	GLN
1	H	446	ASN
1	H	549	GLN
1	H	554	ASN
1	H	558	GLN
1	I	558	GLN
1	K	492	ASN
1	L	159	GLN
1	L	384	HIS
1	L	558	GLN
1	M	384	HIS
1	O	302	ASN
1	O	549	GLN
1	O	557	ASN
1	P	159	GLN
1	P	384	HIS
1	P	419	ASN
1	P	446	ASN
1	P	554	ASN
1	P	558	GLN
1	R	70	HIS
1	R	137	HIS
1	R	280	GLN
1	R	302	ASN
1	R	554	ASN
1	S	137	HIS
1	T	280	GLN
1	T	302	ASN
1	T	446	ASN
1	T	549	GLN
1	U	248	ASN
1	U	369	ASN
1	U	384	HIS
1	U	446	ASN
1	U	558	GLN
1	V	280	GLN
1	V	370	GLN
1	V	384	HIS
1	V	416	GLN
1	V	558	GLN

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Mol	Chain	Res	Type
1	W	280	GLN
1	W	554	ASN
1	W	558	GLN
1	W	565	ASN
1	X	137	HIS
1	X	459	ASN
1	X	557	ASN
1	Y	137	HIS
1	Y	384	HIS
1	Y	557	ASN
1	Z	46	ASN
1	Z	419	ASN
1	Z	446	ASN
1	Z	558	GLN
1	a	302	ASN
1	a	384	HIS
1	a	554	ASN
1	b	137	HIS
1	b	248	ASN
1	b	280	GLN
1	c	492	ASN
1	c	554	ASN
1	d	384	HIS
1	d	491	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 30 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	548/584 (93%)	-0.64	3 (0%)	91	88	3, 17, 60, 119	0
1	B	548/584 (93%)	-0.63	2 (0%)	93	90	4, 19, 64, 124	0
1	C	548/584 (93%)	-0.61	4 (0%)	89	82	3, 20, 64, 121	0
1	D	548/584 (93%)	-0.58	6 (1%)	82	73	5, 20, 63, 131	0
1	E	548/584 (93%)	-0.65	4 (0%)	89	82	4, 18, 62, 120	0
1	F	548/584 (93%)	-0.66	3 (0%)	91	88	3, 18, 61, 118	0
1	G	548/584 (93%)	-0.58	8 (1%)	76	67	4, 20, 62, 126	0
1	H	548/584 (93%)	-0.57	3 (0%)	91	88	4, 19, 62, 118	0
1	I	548/584 (93%)	-0.66	4 (0%)	89	82	5, 19, 62, 127	0
1	J	548/584 (93%)	-0.64	5 (0%)	85	78	3, 19, 61, 122	0
1	K	548/584 (93%)	-0.62	8 (1%)	76	67	3, 17, 61, 122	0
1	L	548/584 (93%)	-0.64	3 (0%)	91	88	4, 19, 60, 125	0
1	M	548/584 (93%)	-0.61	6 (1%)	82	73	3, 18, 62, 121	0
1	N	548/584 (93%)	-0.64	6 (1%)	82	73	5, 19, 62, 126	0
1	O	548/584 (93%)	-0.53	5 (0%)	85	78	3, 20, 64, 123	0
1	P	548/584 (93%)	-0.62	4 (0%)	89	82	3, 18, 61, 119	0
1	Q	548/584 (93%)	-0.59	8 (1%)	76	67	4, 19, 61, 130	0
1	R	548/584 (93%)	-0.63	6 (1%)	82	73	4, 18, 62, 121	0
1	S	548/584 (93%)	-0.64	4 (0%)	89	82	5, 19, 61, 131	0
1	T	548/584 (93%)	-0.61	9 (1%)	74	65	4, 18, 64, 120	0
1	U	548/584 (93%)	-0.58	8 (1%)	76	67	3, 18, 65, 118	0
1	V	548/584 (93%)	-0.59	6 (1%)	82	73	4, 19, 62, 126	0
1	W	548/584 (93%)	-0.56	5 (0%)	85	78	4, 21, 66, 121	0
1	X	548/584 (93%)	-0.64	4 (0%)	89	82	4, 19, 60, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	Y	548/584 (93%)	-0.55	8 (1%) 76 67	4, 19, 64, 123	0
1	Z	548/584 (93%)	-0.59	3 (0%) 91 88	3, 20, 64, 116	0
1	a	548/584 (93%)	-0.55	8 (1%) 76 67	4, 21, 67, 123	0
1	b	548/584 (93%)	-0.56	7 (1%) 79 70	3, 20, 66, 124	0
1	c	548/584 (93%)	-0.54	7 (1%) 79 70	4, 22, 61, 130	0
1	d	548/584 (93%)	-0.62	8 (1%) 76 67	4, 19, 64, 125	0
All	All	16440/17520 (93%)	-0.61	165 (1%) 84 76	3, 19, 64, 131	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	156	SER	4.3
1	T	156	SER	4.0
1	Q	515	SER	3.8
1	X	156	SER	3.7
1	K	156	SER	3.7
1	P	156	SER	3.7
1	V	157	ALA	3.4
1	N	156	SER	3.3
1	G	156	SER	3.3
1	D	159	GLN	3.2
1	a	156	SER	3.2
1	b	156	SER	3.1
1	J	156	SER	3.1
1	D	158	THR	3.1
1	B	156	SER	3.1
1	F	156	SER	3.1
1	M	156	SER	3.1
1	V	156	SER	3.1
1	c	156	SER	3.1
1	D	156	SER	3.1
1	Y	517	ASN	3.1
1	T	517	ASN	3.0
1	Q	156	SER	3.0
1	U	156	SER	3.0
1	W	156	SER	3.0
1	L	159	GLN	3.0
1	S	300	GLY	3.0
1	P	158	THR	3.0
1	Q	517	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	Q	516	ALA	2.9
1	U	515	SER	2.9
1	b	159	GLN	2.8
1	N	516	ALA	2.8
1	d	158	THR	2.8
1	Q	226	SER	2.8
1	Y	156	SER	2.8
1	C	158	THR	2.8
1	d	159	GLN	2.8
1	Y	159	GLN	2.7
1	T	226	SER	2.7
1	O	517	ASN	2.7
1	C	157	ALA	2.7
1	R	156	SER	2.7
1	N	301	THR	2.7
1	Z	156	SER	2.7
1	S	301	THR	2.7
1	V	228	THR	2.7
1	U	159	GLN	2.6
1	T	225	THR	2.6
1	b	228	THR	2.6
1	P	157	ALA	2.6
1	T	228	THR	2.6
1	M	155	GLU	2.6
1	a	228	THR	2.6
1	d	156	SER	2.6
1	M	226	SER	2.5
1	C	156	SER	2.5
1	b	158	THR	2.5
1	K	228	THR	2.5
1	U	160	PRO	2.5
1	E	156	SER	2.5
1	V	158	THR	2.5
1	K	516	ALA	2.5
1	X	516	ALA	2.5
1	Q	225	THR	2.4
1	K	515	SER	2.4
1	R	515	SER	2.4
1	c	158	THR	2.4
1	b	225	THR	2.4
1	G	159	GLN	2.4
1	R	516	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	516	ALA	2.4
1	D	162	THR	2.4
1	N	158	THR	2.4
1	S	159	GLN	2.4
1	W	365	GLN	2.4
1	G	228	THR	2.4
1	O	227	GLY	2.3
1	Z	157	ALA	2.3
1	A	517	ASN	2.3
1	W	159	GLN	2.3
1	c	157	ALA	2.3
1	T	227	GLY	2.3
1	V	159	GLN	2.3
1	A	162	THR	2.3
1	I	160	PRO	2.3
1	d	517	ASN	2.3
1	U	227	GLY	2.3
1	a	300	GLY	2.3
1	a	225	THR	2.3
1	G	517	ASN	2.3
1	K	301	THR	2.3
1	U	225	THR	2.3
1	Q	159	GLN	2.3
1	R	160	PRO	2.2
1	G	162	THR	2.2
1	A	159	GLN	2.2
1	c	517	ASN	2.2
1	T	224	GLY	2.2
1	F	160	PRO	2.2
1	I	227	GLY	2.2
1	Y	515	SER	2.2
1	K	161	PRO	2.2
1	R	159	GLN	2.2
1	Z	56	ASN	2.2
1	N	159	GLN	2.2
1	W	223	THR	2.2
1	H	156	SER	2.2
1	M	517	ASN	2.2
1	X	159	GLN	2.2
1	b	230	THR	2.2
1	Y	161	PRO	2.2
1	Q	223	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	227	GLY	2.2
1	O	516	ALA	2.2
1	d	516	ALA	2.2
1	Y	228	THR	2.1
1	H	224	GLY	2.1
1	E	159	GLN	2.1
1	J	301	THR	2.1
1	B	159	GLN	2.1
1	Y	516	ALA	2.1
1	J	159	GLN	2.1
1	E	160	PRO	2.1
1	b	221	SER	2.1
1	a	158	THR	2.1
1	D	157	ALA	2.1
1	G	157	ALA	2.1
1	K	162	THR	2.1
1	M	159	GLN	2.1
1	a	227	GLY	2.1
1	N	300	GLY	2.1
1	H	301	THR	2.1
1	I	161	PRO	2.1
1	U	224	GLY	2.1
1	U	157	ALA	2.1
1	V	516	ALA	2.1
1	X	517	ASN	2.1
1	K	227	GLY	2.1
1	G	229	PRO	2.1
1	J	365	GLN	2.1
1	a	160	PRO	2.1
1	F	159	GLN	2.1
1	R	365	GLN	2.1
1	d	301	THR	2.0
1	c	516	ALA	2.0
1	C	159	GLN	2.0
1	T	162	THR	2.0
1	W	300	GLY	2.0
1	c	225	THR	2.0
1	c	227	GLY	2.0
1	G	516	ALA	2.0
1	I	156	SER	2.0
1	E	56	ASN	2.0
1	d	160	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	517	ASN	2.0
1	J	162	THR	2.0
1	d	157	ALA	2.0
1	L	301	THR	2.0
1	O	157	ALA	2.0
1	P	159	GLN	2.0
1	a	56	ASN	2.0
1	T	161	PRO	2.0
1	S	156	SER	2.0
1	Y	162	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	K	800	1/1	0.93	0.36	4.05	39,39,39,39	0
2	MG	T	800	1/1	0.90	0.31	3.54	43,43,43,43	0
2	MG	Q	800	1/1	0.93	0.33	3.40	41,41,41,41	0
2	MG	Y	601	1/1	0.94	0.29	2.60	47,47,47,47	0
2	MG	O	800	1/1	0.90	0.17	1.84	41,41,41,41	0
2	MG	M	800	1/1	0.89	0.27	1.75	41,41,41,41	0
2	MG	Y	602	1/1	0.93	0.25	1.40	52,52,52,52	0
2	MG	I	800	1/1	0.97	0.24	1.28	43,43,43,43	0
2	MG	B	800	1/1	0.96	0.24	1.09	41,41,41,41	0
2	MG	D	800	1/1	0.94	0.26	1.04	43,43,43,43	0
2	MG	H	601	1/1	0.92	0.20	0.87	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	P	800	1/1	0.95	0.19	0.85	39,39,39,39	0
2	MG	J	601	1/1	0.96	0.19	0.62	40,40,40,40	0
2	MG	A	800	1/1	0.95	0.19	0.45	32,32,32,32	0
2	MG	G	800	1/1	0.93	0.18	0.42	44,44,44,44	0
2	MG	d	602	1/1	0.90	0.18	0.26	56,56,56,56	0
2	MG	W	800	1/1	0.92	0.18	0.13	47,47,47,47	0
2	MG	H	602	1/1	0.96	0.18	0.08	54,54,54,54	0
2	MG	E	601	1/1	0.90	0.16	0.07	40,40,40,40	0
2	MG	C	800	1/1	0.94	0.16	0.04	41,41,41,41	0
2	MG	J	602	1/1	0.95	0.16	-0.23	38,38,38,38	0
2	MG	L	800	1/1	0.93	0.14	-0.34	41,41,41,41	0
2	MG	N	800	1/1	0.88	0.16	-0.65	39,39,39,39	0
2	MG	Z	800	1/1	0.97	0.12	-0.74	47,47,47,47	0
2	MG	R	800	1/1	0.91	0.14	-0.77	37,37,37,37	0
2	MG	E	602	1/1	0.97	0.10	-1.42	38,38,38,38	0
2	MG	S	800	1/1	0.96	0.09	-1.71	39,39,39,39	0
2	MG	d	601	1/1	0.96	0.09	-1.71	37,37,37,37	0
2	MG	X	800	1/1	0.97	0.10	-2.16	43,43,43,43	0
2	MG	c	800	1/1	0.96	0.16	-	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.