



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:47 PM UTC

PDB ID : 4QYK / pdb_00004qyk
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

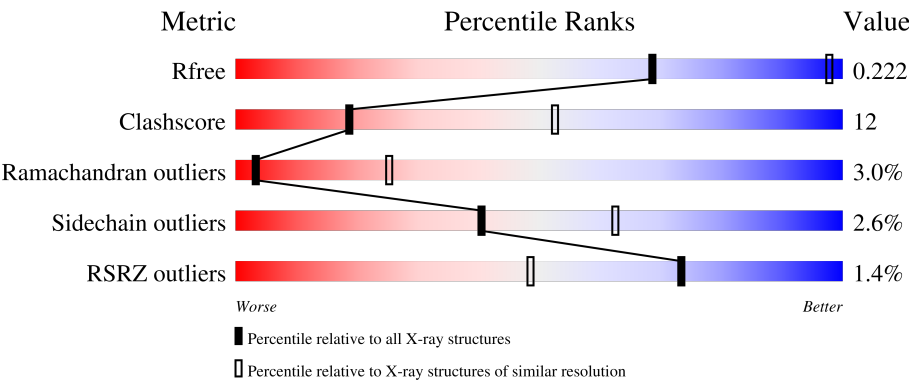
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	584	% 69%22%6%
1	B	584	% 68%23%6%
1	C	584	2% 66%24%6%
1	D	584	% 68%21%6%
1	E	584	% 67%23%6%

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Mol	Chain	Length	Quality of chain
1	F	584	
1	G	584	
1	H	584	
1	I	584	
1	J	584	
1	K	584	
1	L	584	
1	M	584	
1	N	584	
1	O	584	
1	P	584	
1	Q	584	
1	R	584	
1	S	584	
1	T	584	
1	U	584	
1	V	584	
1	W	584	
1	X	584	
1	Y	584	
1	Z	584	
1	a	584	
1	b	584	
1	c	584	
1	d	584	

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	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	E	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	J	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	N	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	Q	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			
1	F	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	G	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	H	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	I	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	K	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	L	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	M	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			
1	O	548	Total	C	N	O	S	0	0	0
			4352	2767	740	830	15			

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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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	E	2	Total Mg 2 2	0	0
2	J	2	Total Mg 2 2	0	0
2	N	1	Total Mg 1 1	0	0
2	Q	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	D	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	2	Total Mg 2 2	0	0
2	I	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0
2	L	1	Total Mg 1 1	0	0

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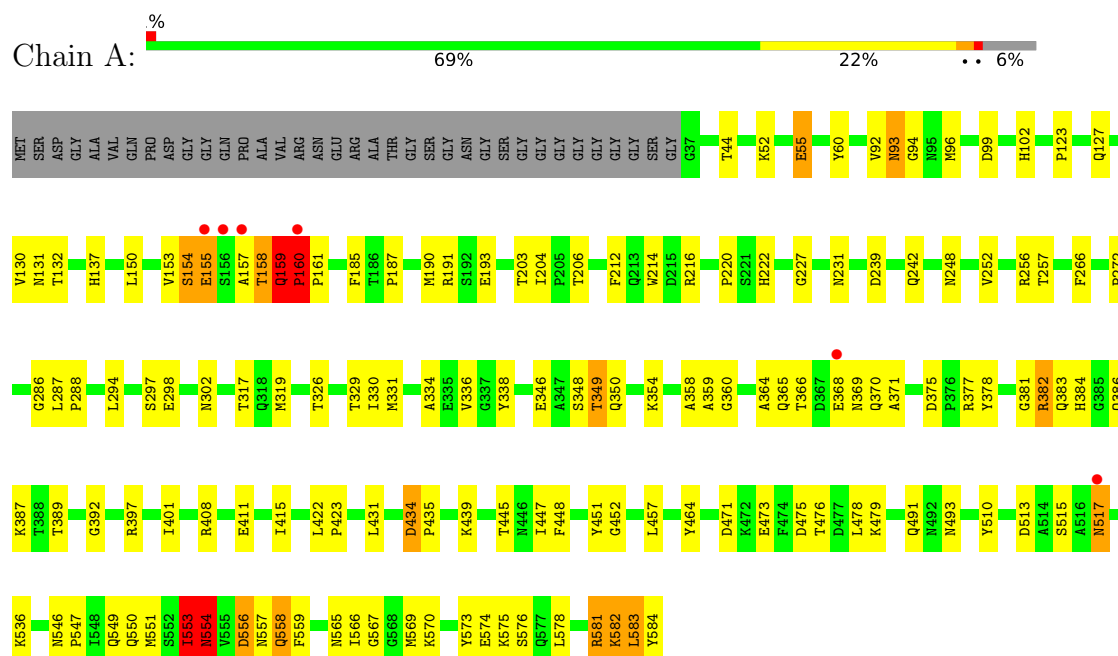
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	M	1	Total 1	Mg 1	0	0
2	O	1	Total 1	Mg 1	0	0
2	P	1	Total 1	Mg 1	0	0
2	R	1	Total 1	Mg 1	0	0
2	S	1	Total 1	Mg 1	0	0
2	T	1	Total 1	Mg 1	0	0
2	W	1	Total 1	Mg 1	0	0
2	X	1	Total 1	Mg 1	0	0
2	Y	2	Total 2	Mg 2	0	0
2	Z	1	Total 1	Mg 1	0	0
2	c	1	Total 1	Mg 1	0	0
2	d	2	Total 2	Mg 2	0	0

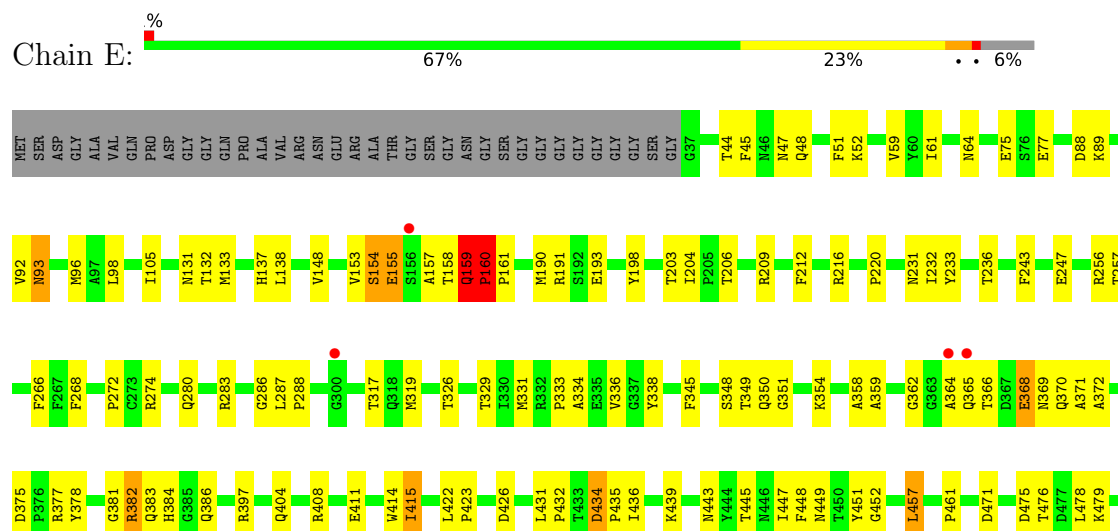
3 Residue-property plots [i](#)

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

• Molecule 1: Capsid protein VP1

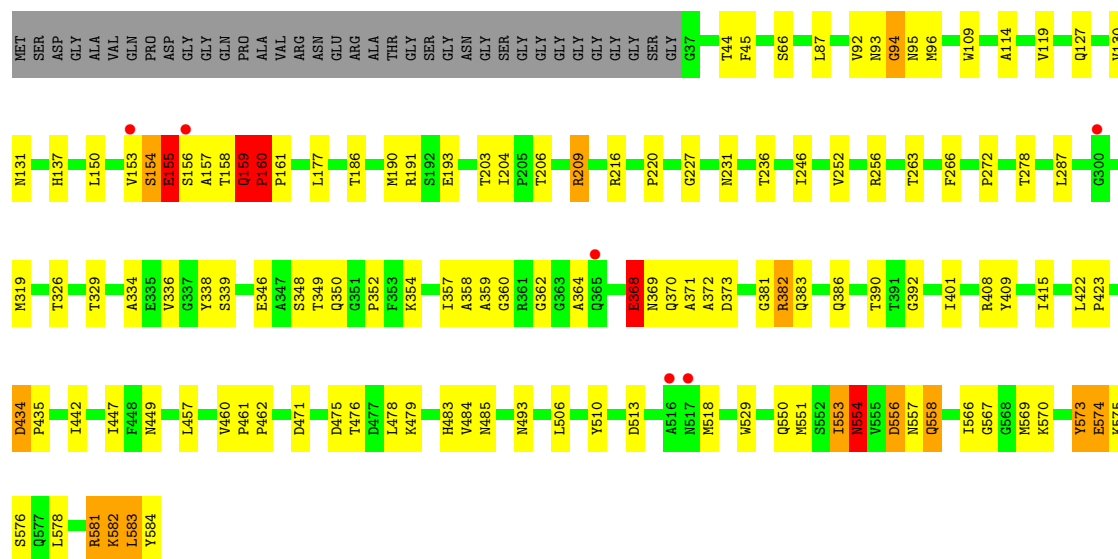


• Molecule 1: Capsid protein VP1

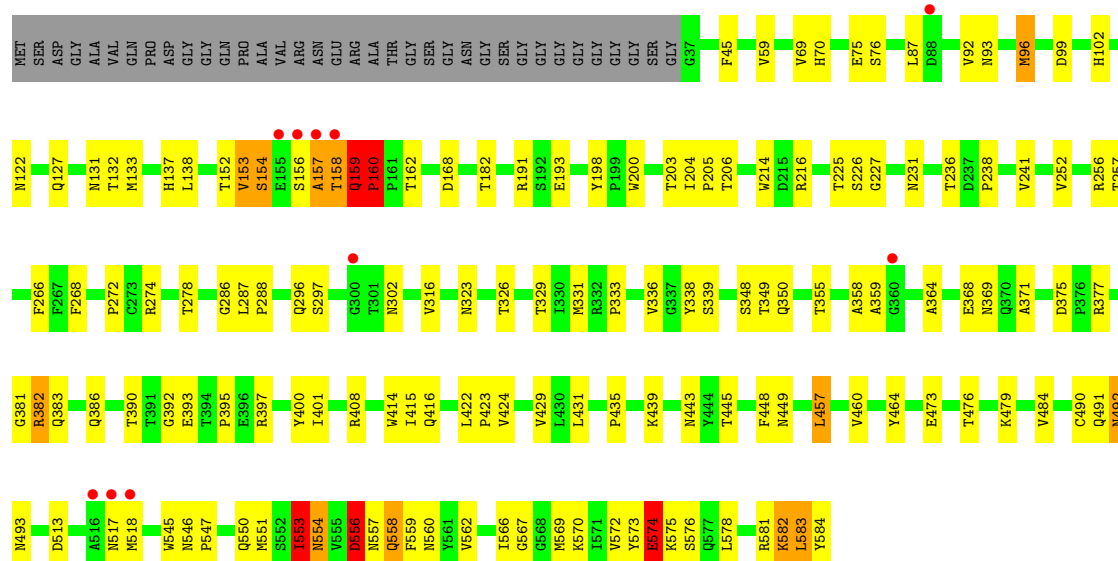




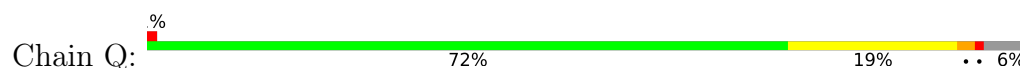
• Molecule 1: Capsid protein VP1

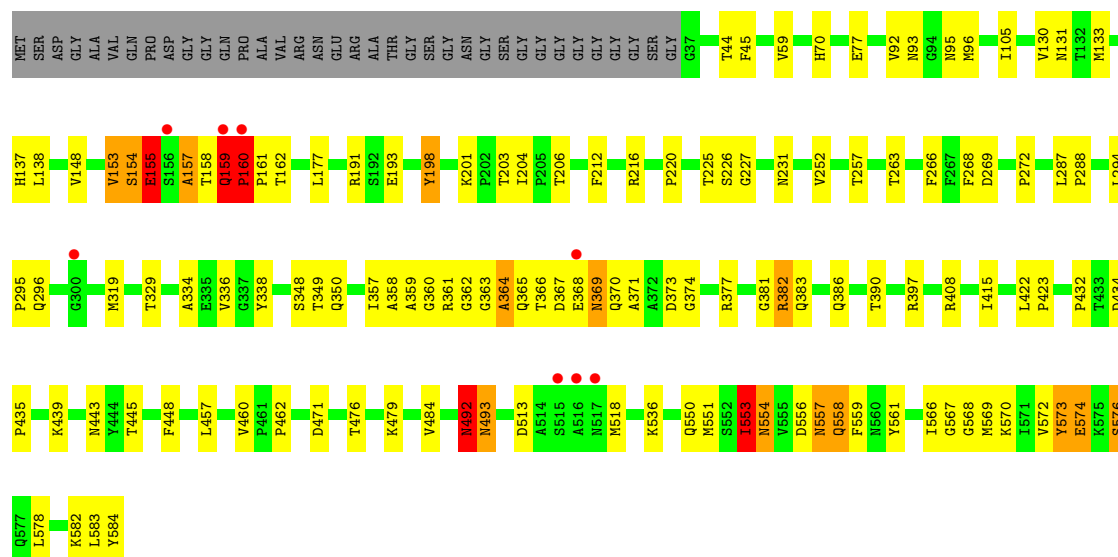


• Molecule 1: Capsid protein VP1

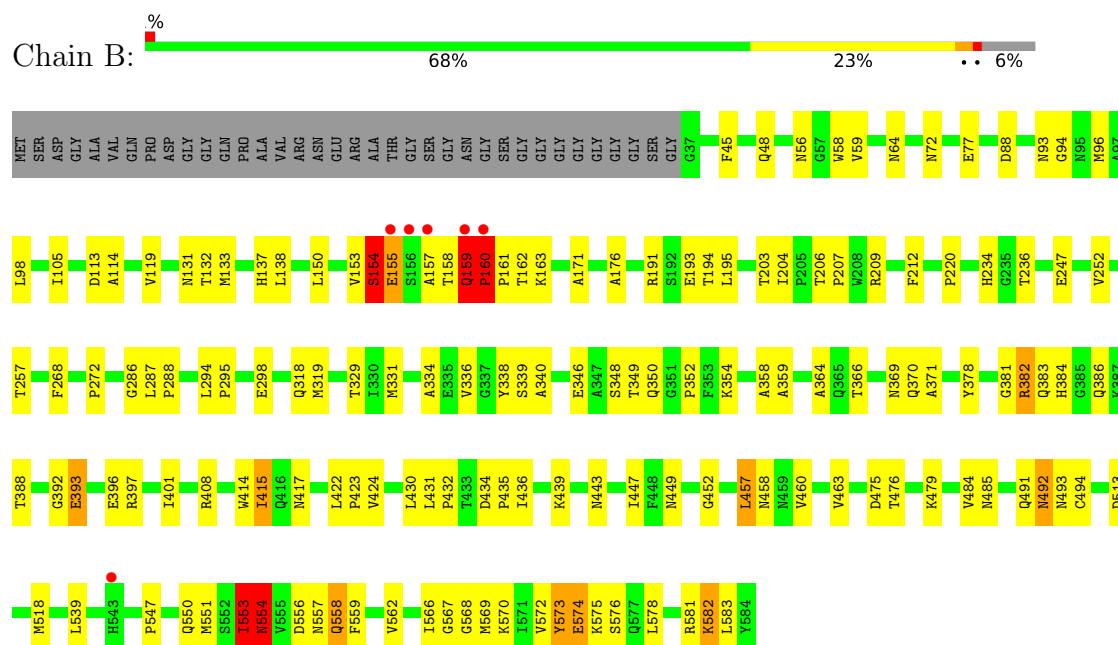


• Molecule 1: Capsid protein VP1

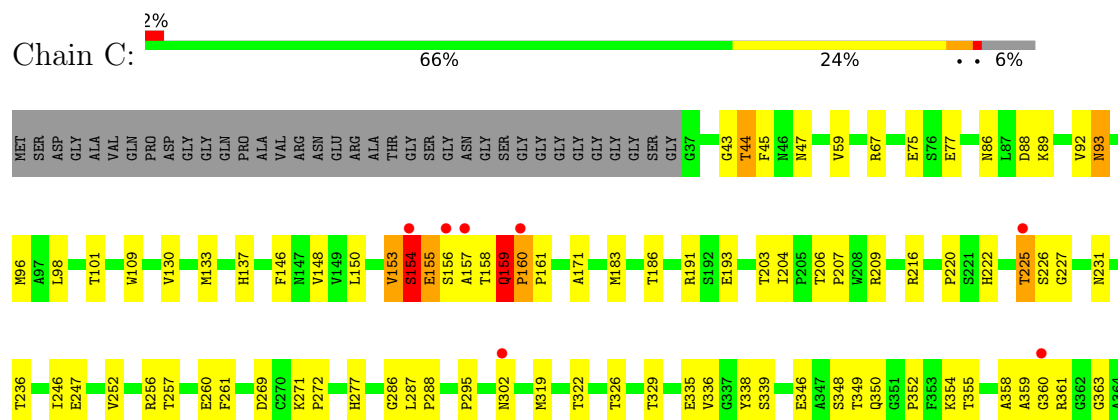




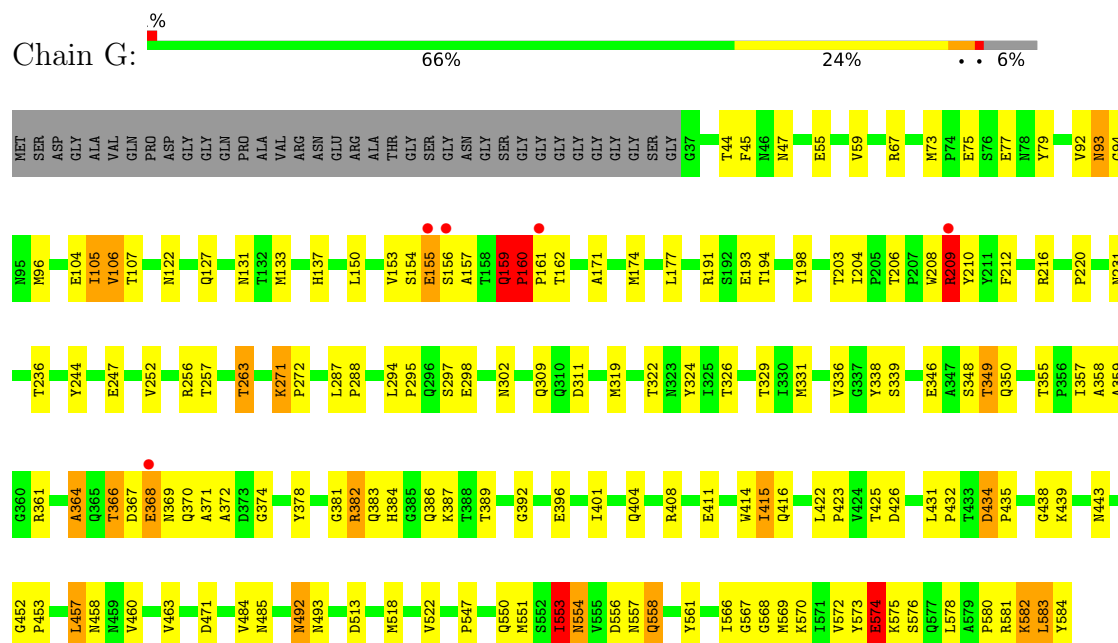
• Molecule 1: Capsid protein VP1



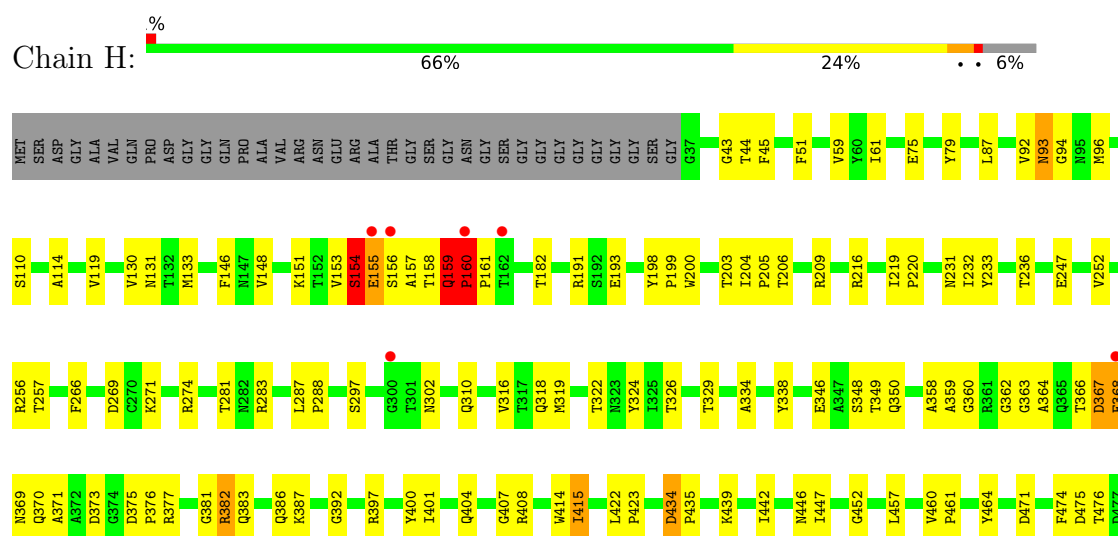
• Molecule 1: Capsid protein VP1



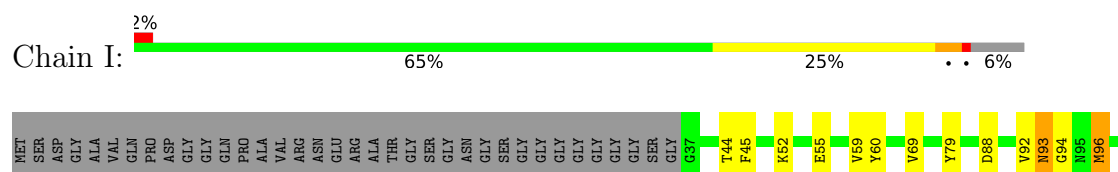
- Molecule 1: Capsid protein VP1

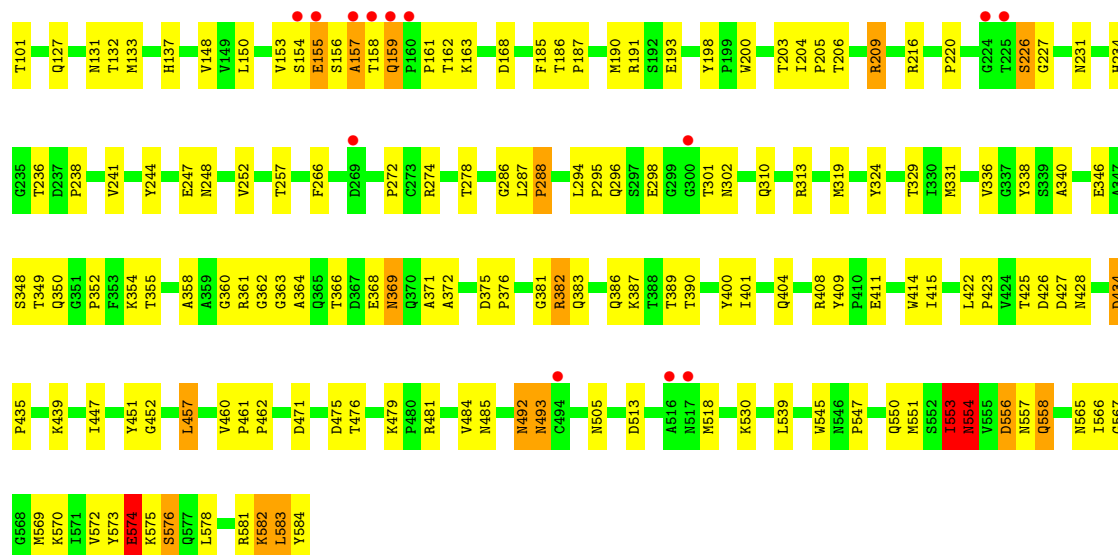


- Molecule 1: Capsid protein VP1

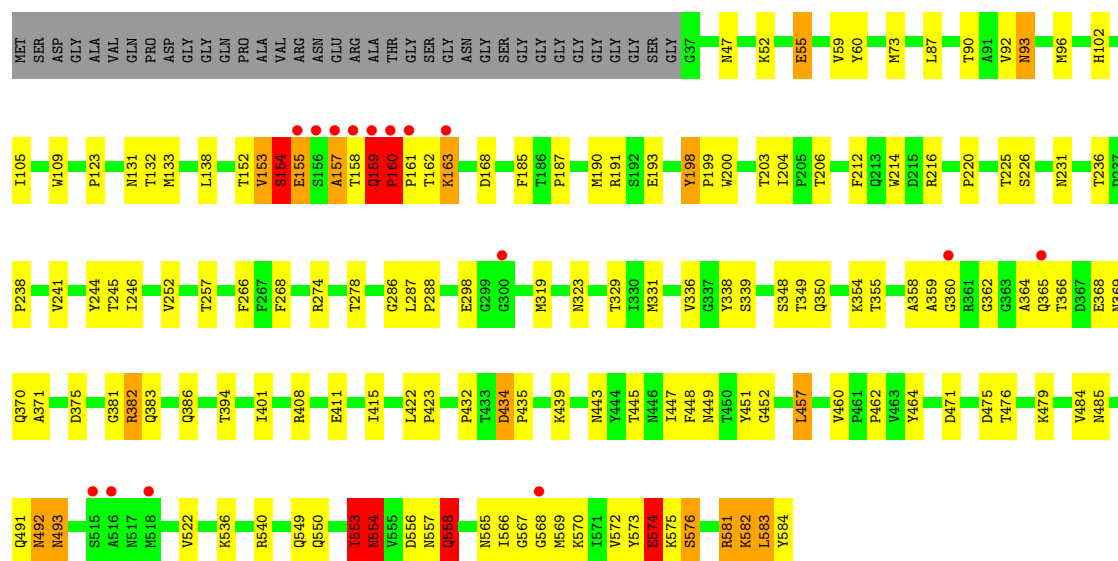


- Molecule 1: Capsid protein VP1

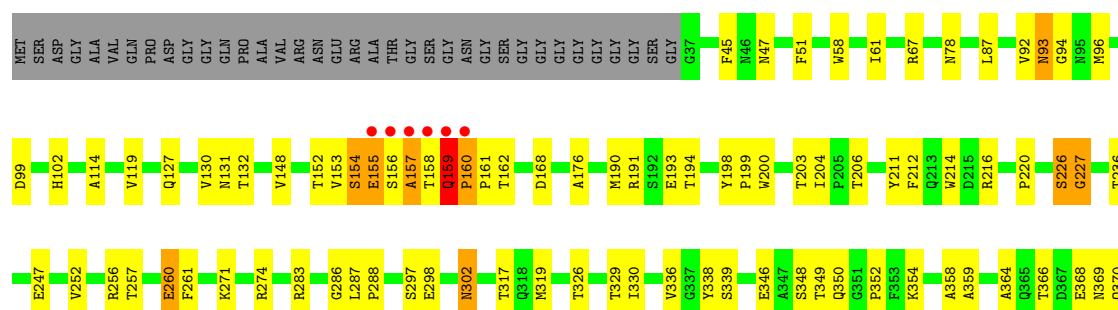


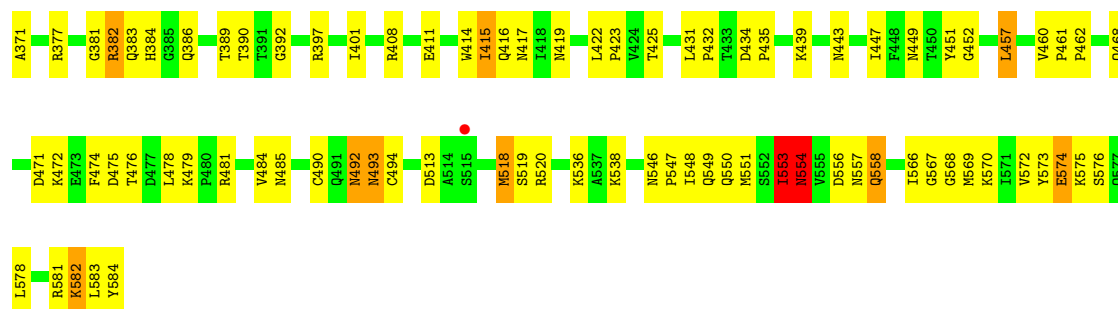


• Molecule 1: Capsid protein VP1

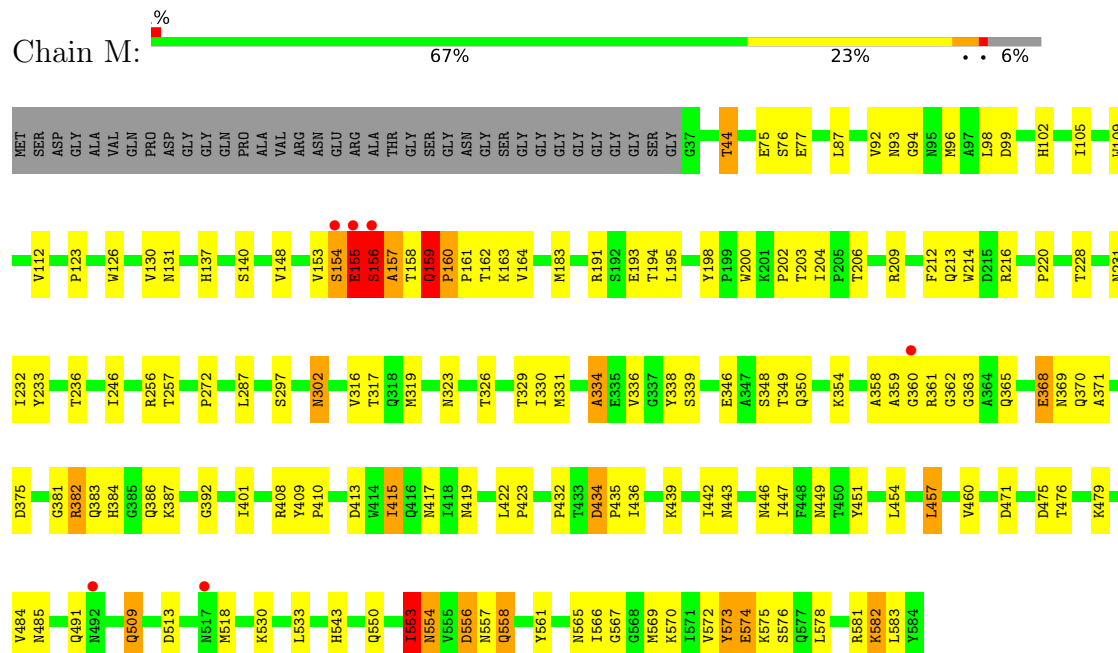


• Molecule 1: Capsid protein VP1

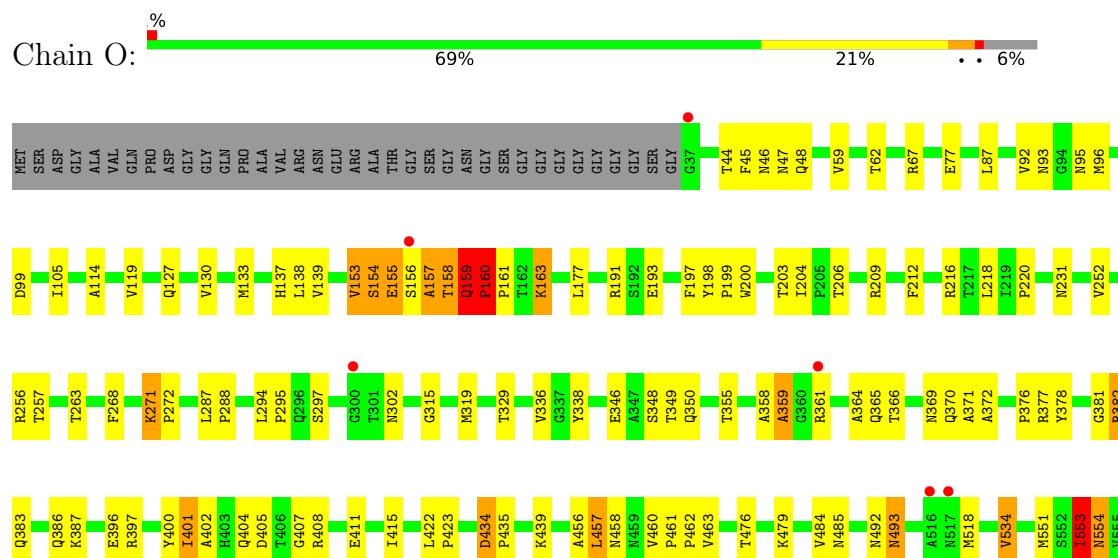




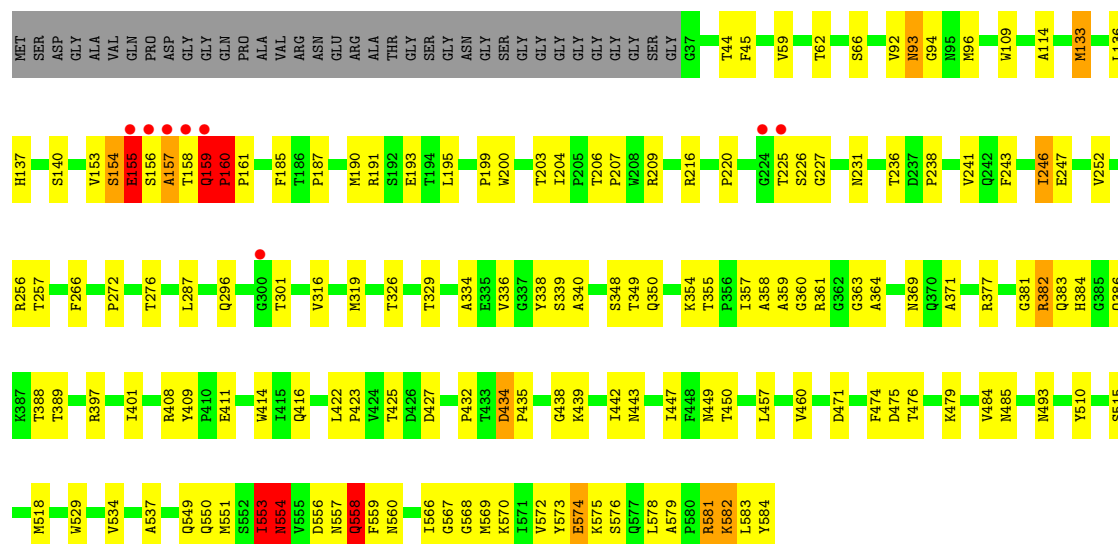
- Molecule 1: Capsid protein VP1



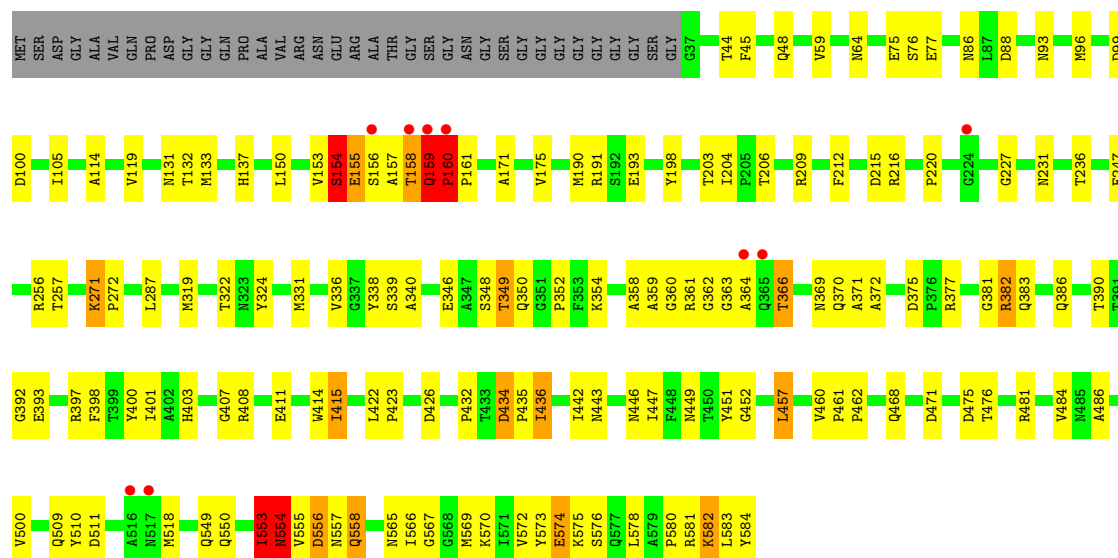
- Molecule 1: Capsid protein VP1



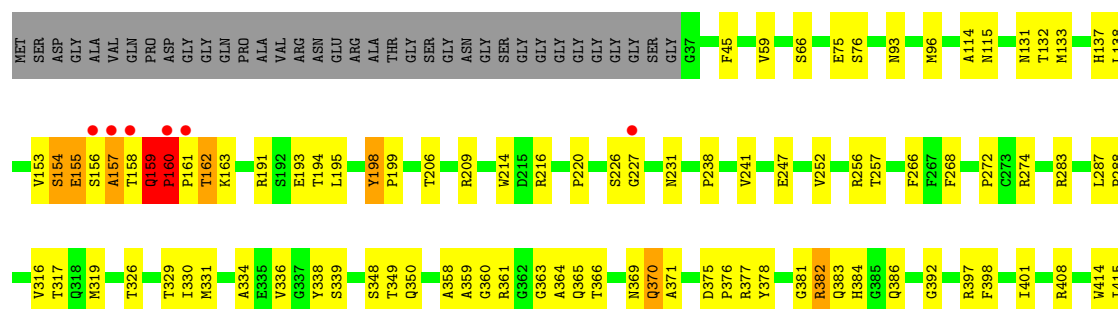


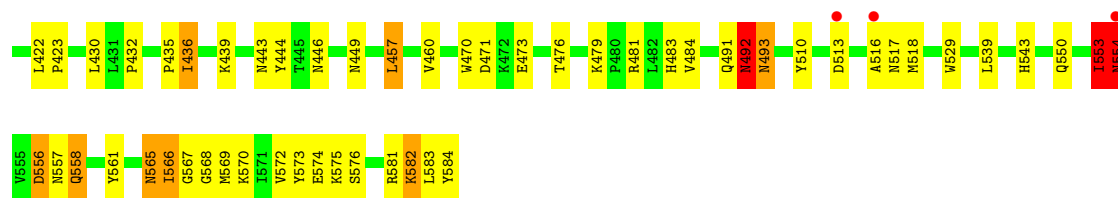


• Molecule 1: Capsid protein VP1

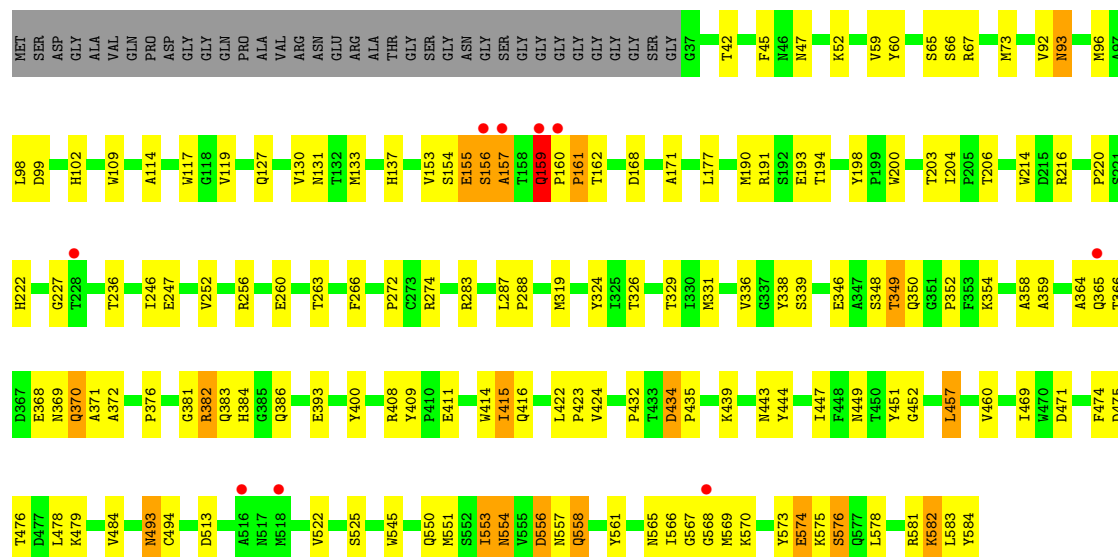


• Molecule 1: Capsid protein VP1

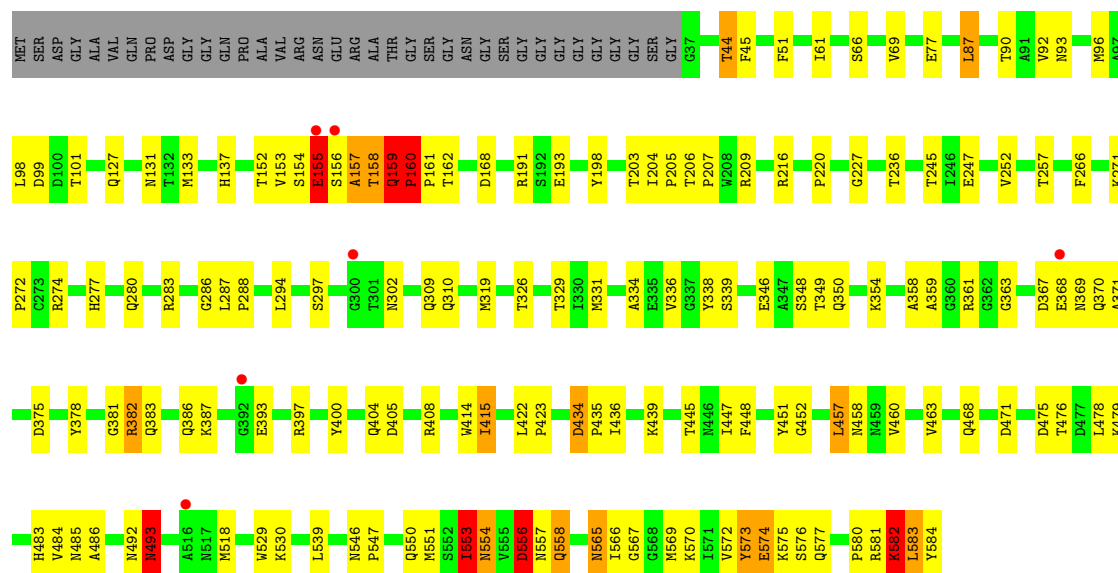




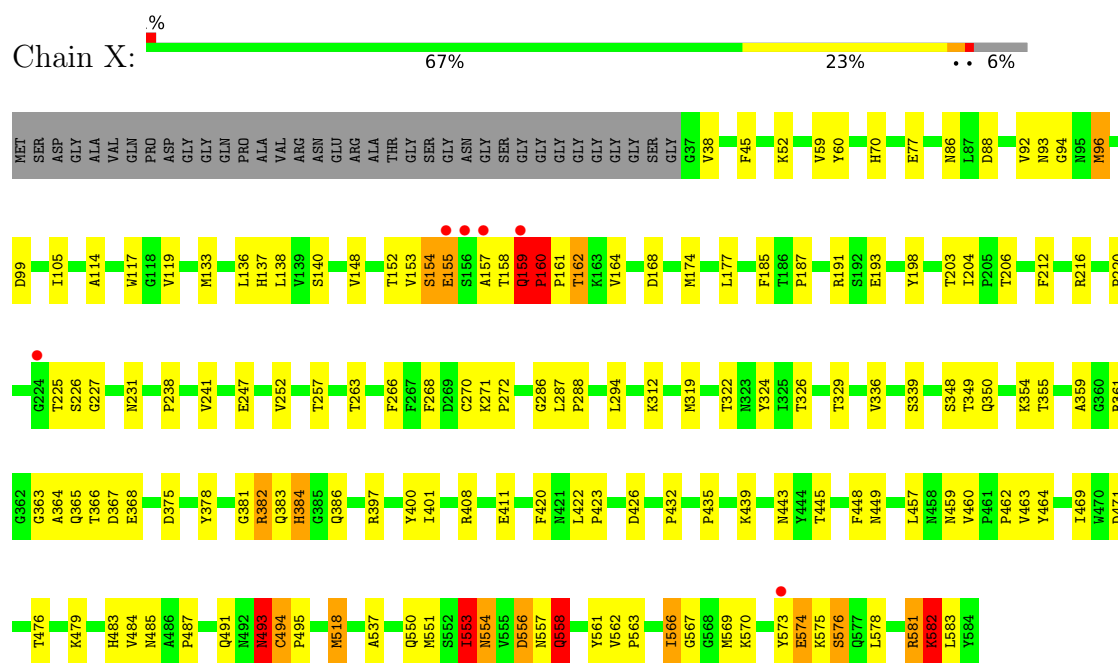
• Molecule 1: Capsid protein VP1



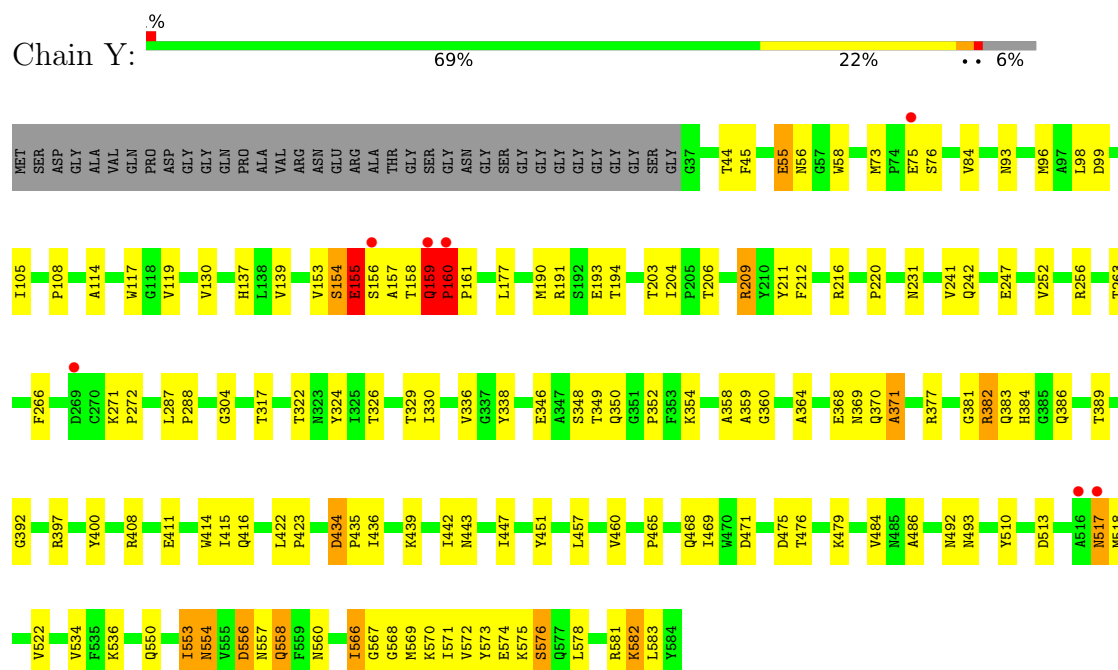
• Molecule 1: Capsid protein VP1



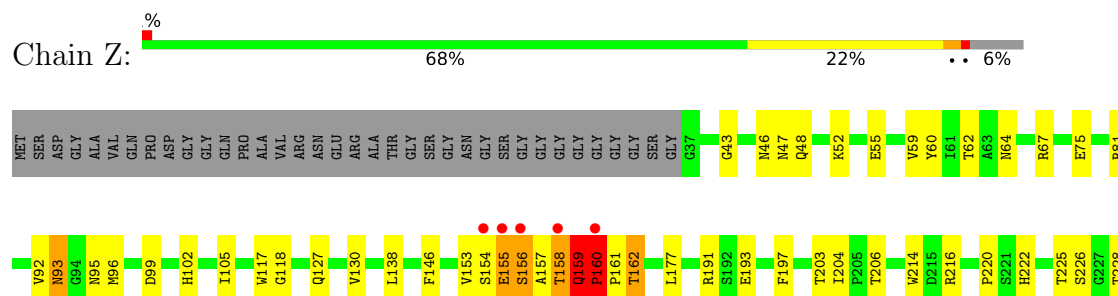
• Molecule 1: Capsid protein VP1

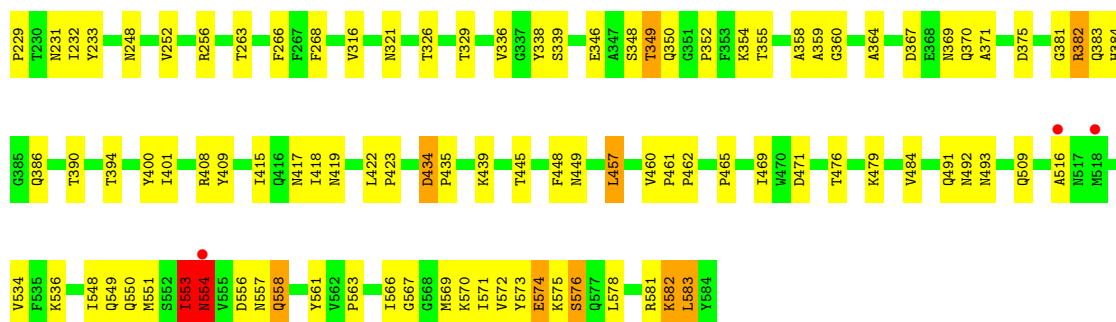


• Molecule 1: Capsid protein VP1

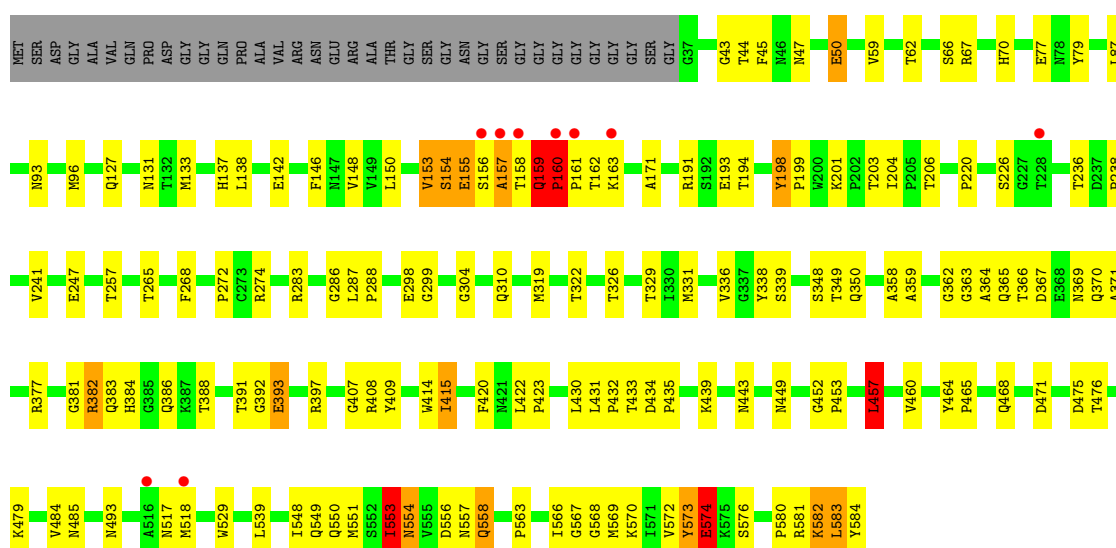


• Molecule 1: Capsid protein VP1

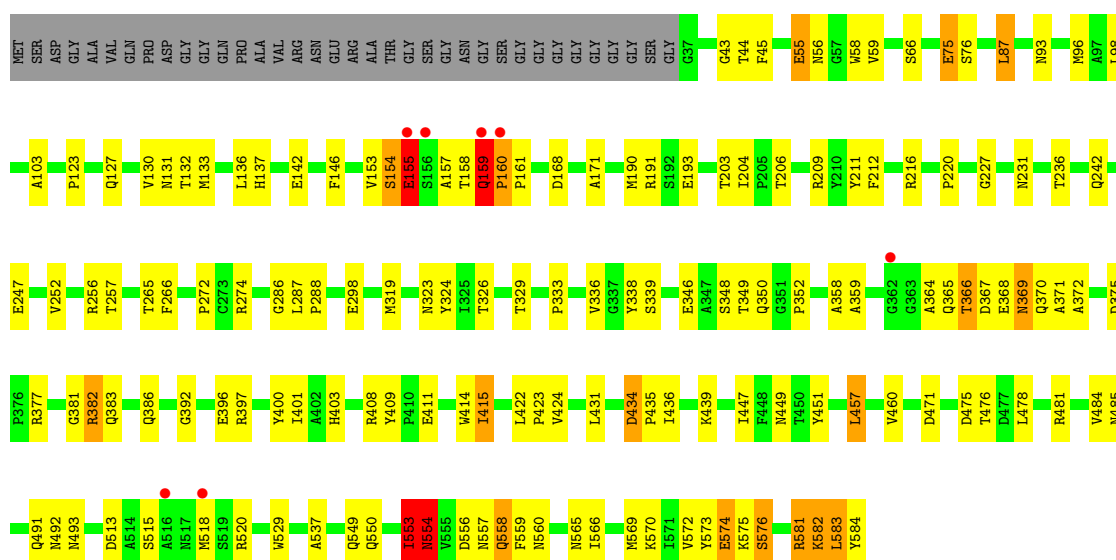




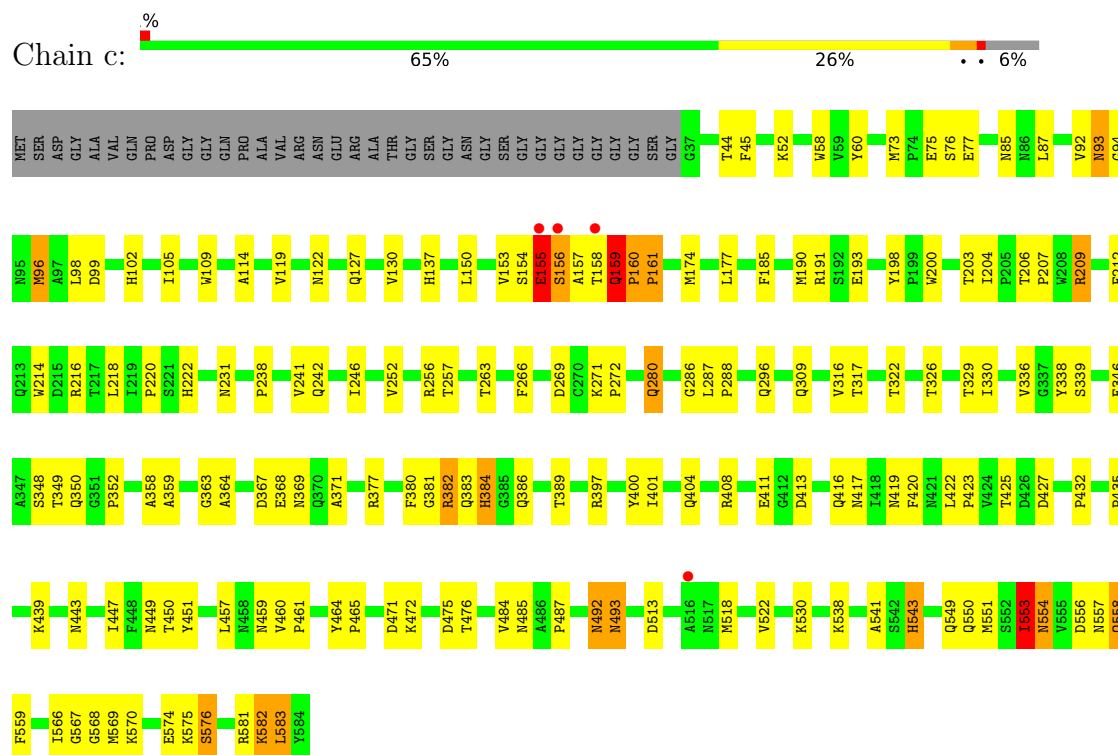
• Molecule 1: Capsid protein VP1



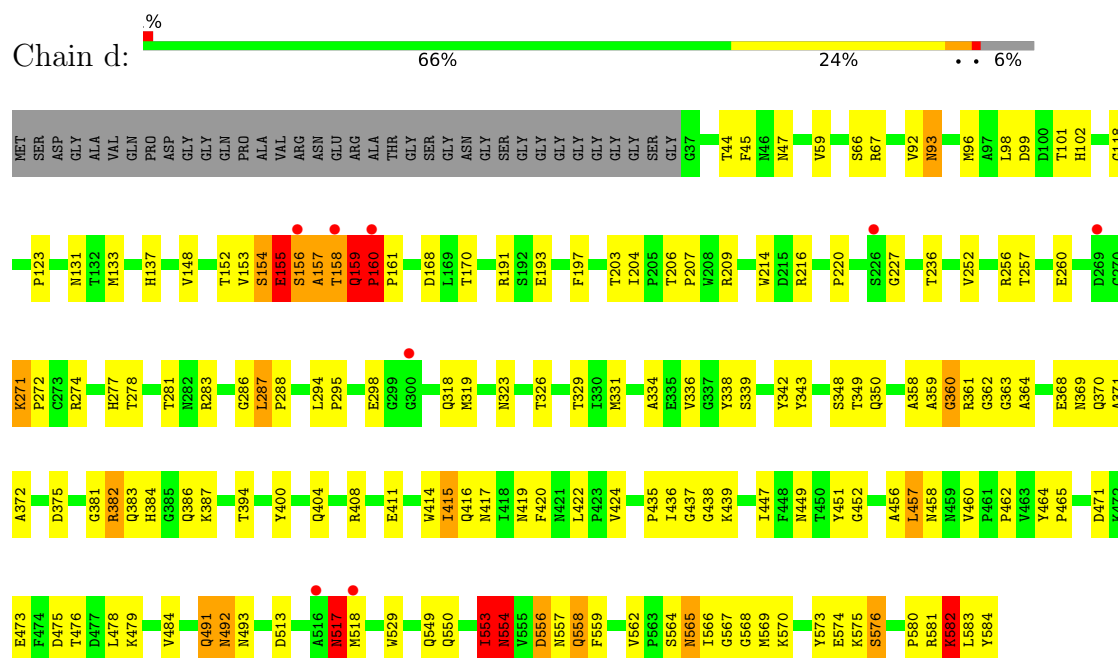
• Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.180 , 0.221 0.183 , 0.222	Depositor DCC
R_{free} test set	20538 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	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 6.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.86	1/4483 (0.0%)	1.06	24/6134 (0.4%)
1	B	0.83	2/4483 (0.0%)	1.18	16/6134 (0.3%)
1	C	0.78	0/4483	1.15	24/6134 (0.4%)
1	D	0.77	0/4483	1.12	23/6134 (0.4%)
1	E	0.82	1/4483 (0.0%)	1.11	24/6134 (0.4%)
1	F	0.83	1/4483 (0.0%)	1.17	26/6134 (0.4%)
1	G	0.78	1/4483 (0.0%)	1.15	28/6134 (0.5%)
1	H	0.76	1/4483 (0.0%)	1.10	24/6134 (0.4%)
1	I	0.84	0/4483	1.05	22/6134 (0.4%)
1	J	0.81	2/4483 (0.0%)	1.11	25/6134 (0.4%)
1	K	0.87	0/4483	1.14	28/6134 (0.5%)
1	L	0.81	0/4483	1.10	21/6134 (0.3%)
1	M	0.87	1/4483 (0.0%)	1.12	32/6134 (0.5%)
1	N	0.86	0/4483	1.11	22/6134 (0.4%)
1	O	0.76	0/4483	1.08	21/6134 (0.3%)
1	P	0.79	0/4483	1.10	25/6134 (0.4%)
1	Q	0.80	1/4483 (0.0%)	1.12	20/6134 (0.3%)
1	R	0.85	2/4483 (0.0%)	1.10	21/6134 (0.3%)
1	S	0.84	3/4483 (0.1%)	1.12	21/6134 (0.3%)
1	T	0.87	0/4483	1.10	26/6134 (0.4%)
1	U	0.78	1/4483 (0.0%)	1.14	24/6134 (0.4%)
1	V	0.78	0/4483	1.02	12/6134 (0.2%)
1	W	0.74	1/4483 (0.0%)	1.12	24/6134 (0.4%)
1	X	0.81	0/4483	1.23	25/6134 (0.4%)
1	Y	0.75	0/4483	1.11	20/6134 (0.3%)
1	Z	0.82	4/4483 (0.1%)	1.13	25/6134 (0.4%)
1	a	0.72	1/4483 (0.0%)	1.20	16/6134 (0.3%)
1	b	0.74	0/4483	1.10	21/6134 (0.3%)
1	c	0.77	0/4483	1.12	16/6134 (0.3%)
1	d	0.79	2/4483 (0.0%)	1.12	30/6134 (0.5%)
All	All	0.80	25/134490 (0.0%)	1.12	686/184020 (0.4%)

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 (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	222	HIS	CG-CD2	-12.58	1.22	1.35
1	Z	222	HIS	CD2-NE2	12.06	1.51	1.37
1	R	334	ALA	CA-CB	-8.04	1.47	1.54
1	Z	222	HIS	CG-ND1	7.96	1.47	1.38
1	W	334	ALA	CA-CB	-7.91	1.47	1.54
1	d	334	ALA	CA-CB	-7.66	1.47	1.54
1	H	334	ALA	CA-CB	-7.34	1.48	1.54
1	Z	222	HIS	ND1-CE1	-6.97	1.25	1.32
1	Q	334	ALA	CA-CB	-6.75	1.48	1.54
1	S	438	GLY	C-O	-6.52	1.14	1.24
1	F	426	ASP	CB-CG	-6.52	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	334	ALA	CA-CB	-6.06	1.49	1.54
1	J	581	ARG	CA-C	-5.88	1.49	1.52
1	U	334	ALA	CA-CB	-5.79	1.49	1.54
1	S	334	ALA	CA-CB	-5.74	1.47	1.54
1	B	334	ALA	CA-CB	-5.67	1.47	1.54
1	a	160	PRO	CA-C	5.54	1.57	1.52
1	M	334	ALA	CA-CB	-5.43	1.47	1.54
1	E	334	ALA	CA-CB	-5.38	1.47	1.54
1	R	288	PRO	CA-C	-5.28	1.49	1.51
1	A	334	ALA	CA-CB	-5.26	1.47	1.54
1	B	340	ALA	CA-CB	-5.17	1.47	1.54
1	S	246	ILE	CA-CB	-5.07	1.48	1.54
1	d	160	PRO	CA-C	5.06	1.56	1.52
1	G	209	ARG	CA-CB	-5.01	1.45	1.53

All (686) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	159	GLN	CA-C-N	33.81	155.21	120.38
1	X	159	GLN	C-N-CA	33.81	155.21	120.38
1	a	159	GLN	CA-C-N	32.53	153.89	120.38
1	a	159	GLN	C-N-CA	32.53	153.89	120.38
1	B	159	GLN	CA-C-N	29.76	151.03	120.38
1	B	159	GLN	C-N-CA	29.76	151.03	120.38
1	G	159	GLN	CA-C-N	23.81	144.91	120.38
1	G	159	GLN	C-N-CA	23.81	144.91	120.38
1	F	159	GLN	CA-C-N	23.67	144.76	120.38
1	F	159	GLN	C-N-CA	23.67	144.76	120.38
1	D	159	GLN	CA-C-N	23.16	144.23	120.38
1	D	159	GLN	C-N-CA	23.16	144.23	120.38
1	Q	159	GLN	CA-C-N	23.11	144.19	120.38
1	Q	159	GLN	C-N-CA	23.11	144.19	120.38
1	C	159	GLN	CA-C-N	23.07	144.15	120.38
1	C	159	GLN	C-N-CA	23.07	144.15	120.38
1	U	159	GLN	CA-C-N	22.15	143.19	120.38
1	U	159	GLN	C-N-CA	22.15	143.19	120.38
1	K	159	GLN	CA-C-N	21.23	142.25	120.38
1	K	159	GLN	C-N-CA	21.23	142.25	120.38
1	W	159	GLN	CA-C-N	20.91	141.92	120.38
1	W	159	GLN	C-N-CA	20.91	141.92	120.38
1	R	159	GLN	CA-C-N	20.86	141.86	120.38
1	R	159	GLN	C-N-CA	20.86	141.86	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	159	GLN	CA-C-N	20.08	141.06	120.38
1	c	159	GLN	C-N-CA	20.08	141.06	120.38
1	N	159	GLN	CA-C-N	19.38	140.34	120.38
1	N	159	GLN	C-N-CA	19.38	140.34	120.38
1	S	159	GLN	CA-C-N	19.24	140.20	120.38
1	S	159	GLN	C-N-CA	19.24	140.20	120.38
1	J	159	GLN	CA-C-N	18.52	139.45	120.38
1	J	159	GLN	C-N-CA	18.52	139.45	120.38
1	H	159	GLN	CA-C-N	18.05	138.97	120.38
1	H	159	GLN	C-N-CA	18.05	138.97	120.38
1	Z	159	GLN	CA-C-N	17.45	138.36	120.38
1	Z	159	GLN	C-N-CA	17.45	138.36	120.38
1	L	159	GLN	CA-C-N	17.41	138.31	120.38
1	L	159	GLN	C-N-CA	17.41	138.31	120.38
1	d	159	GLN	CA-C-N	16.92	137.81	120.38
1	d	159	GLN	C-N-CA	16.92	137.81	120.38
1	T	159	GLN	CA-C-N	16.86	137.75	120.38
1	T	159	GLN	C-N-CA	16.86	137.75	120.38
1	Y	159	GLN	CA-C-N	16.80	137.68	120.38
1	Y	159	GLN	C-N-CA	16.80	137.68	120.38
1	b	159	GLN	CA-C-N	16.69	137.57	120.38
1	b	159	GLN	C-N-CA	16.69	137.57	120.38
1	P	159	GLN	CA-C-N	16.30	137.17	120.38
1	P	159	GLN	C-N-CA	16.30	137.17	120.38
1	O	159	GLN	CA-C-N	15.41	136.26	120.38
1	O	159	GLN	C-N-CA	15.41	136.26	120.38
1	U	160	PRO	N-CA-C	15.36	129.44	110.70
1	E	159	GLN	CA-C-N	15.19	136.02	120.38
1	E	159	GLN	C-N-CA	15.19	136.02	120.38
1	M	159	GLN	CA-C-N	14.97	135.80	120.38
1	M	159	GLN	C-N-CA	14.97	135.80	120.38
1	F	160	PRO	N-CA-C	14.95	128.94	110.70
1	S	160	PRO	N-CA-C	13.49	127.15	110.70
1	X	160	PRO	N-CA-C	13.09	126.67	110.70
1	T	160	PRO	N-CA-C	13.04	126.61	110.70
1	J	160	PRO	N-CA-C	12.99	126.55	110.70
1	N	160	PRO	N-CA-C	12.93	126.47	110.70
1	A	159	GLN	CA-C-N	12.85	133.61	120.38
1	A	159	GLN	C-N-CA	12.85	133.61	120.38
1	B	160	PRO	N-CA-C	12.51	125.96	110.70
1	P	160	PRO	N-CA-C	12.46	125.91	110.70
1	O	160	PRO	N-CA-C	12.39	125.81	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	574	GLU	N-CA-C	11.98	124.54	110.41
1	Q	160	PRO	N-CA-C	11.40	124.60	110.70
1	c	160	PRO	N-CA-C	11.32	124.52	110.70
1	K	160	PRO	N-CA-C	11.25	124.43	110.70
1	a	159	GLN	C-N-CD	-11.06	79.65	125.00
1	a	160	PRO	N-CA-C	10.84	123.92	110.70
1	E	160	PRO	C-N-CD	-10.82	96.78	120.60
1	F	426	ASP	CB-CG-OD2	-10.71	93.78	118.40
1	R	160	PRO	N-CA-C	10.67	123.72	110.70
1	d	160	PRO	N-CA-C	10.59	123.62	110.70
1	E	160	PRO	N-CA-C	10.46	123.46	110.70
1	G	160	PRO	N-CA-C	10.35	123.33	110.70
1	D	160	PRO	N-CA-C	10.28	123.24	110.70
1	O	574	GLU	N-CA-C	10.05	122.27	110.41
1	J	227	GLY	N-CA-C	-9.96	95.89	112.83
1	Z	222	HIS	ND1-CE1-NE2	9.95	118.35	108.40
1	L	160	PRO	N-CA-C	9.86	122.73	110.70
1	Y	574	GLU	N-CA-C	9.84	122.02	110.41
1	J	574	GLU	N-CA-C	9.79	121.96	110.41
1	X	159	GLN	C-N-CD	-9.69	85.27	125.00
1	d	227	GLY	N-CA-C	-9.68	95.25	112.77
1	H	160	PRO	N-CA-C	9.65	122.47	110.70
1	c	198	TYR	CA-C-N	9.55	129.79	119.28
1	c	198	TYR	C-N-CA	9.55	129.79	119.28
1	D	574	GLU	N-CA-C	9.46	121.58	110.41
1	A	160	PRO	N-CA-C	9.41	122.18	110.70
1	a	574	GLU	N-CA-C	9.29	121.37	110.41
1	S	227	GLY	N-CA-C	-9.27	97.06	112.83
1	c	574	GLU	N-CA-C	9.26	121.34	110.41
1	W	198	TYR	CA-C-N	9.03	129.21	119.28
1	W	198	TYR	C-N-CA	9.03	129.21	119.28
1	L	227	GLY	N-CA-C	-8.75	96.94	112.77
1	Y	160	PRO	N-CA-C	8.66	121.27	110.70
1	E	434	ASP	CA-C-N	8.61	128.54	119.85
1	E	434	ASP	C-N-CA	8.61	128.54	119.85
1	C	159	GLN	C-N-CD	-8.54	89.97	125.00
1	Z	375	ASP	CA-C-N	8.47	128.23	119.76
1	Z	375	ASP	C-N-CA	8.47	128.23	119.76
1	W	160	PRO	N-CA-C	8.46	121.02	110.70
1	M	160	PRO	N-CA-C	8.33	120.86	110.70
1	Z	222	HIS	CE1-NE2-CD2	-8.32	100.68	109.00
1	b	160	PRO	N-CA-C	8.30	120.82	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	574	GLU	N-CA-C	8.29	120.20	110.41
1	X	227	GLY	N-CA-C	-8.24	98.83	112.83
1	E	160	PRO	CA-C-N	8.13	146.51	127.00
1	E	160	PRO	C-N-CA	8.13	146.51	127.00
1	D	159	GLN	C-N-CD	-8.13	91.68	125.00
1	M	360	GLY	CA-C-O	-8.13	115.54	121.88
1	I	434	ASP	CA-C-N	8.12	128.06	119.85
1	I	434	ASP	C-N-CA	8.12	128.06	119.85
1	Z	159	GLN	N-CA-C	8.10	127.70	109.81
1	G	159	GLN	C-N-CD	-7.95	92.40	125.00
1	U	516	ALA	CA-C-N	-7.93	112.06	123.00
1	U	516	ALA	C-N-CA	-7.93	112.06	123.00
1	X	574	GLU	N-CA-C	7.93	119.76	110.41
1	W	159	GLN	C-N-CD	-7.91	92.56	125.00
1	B	159	GLN	C-N-CD	-7.91	92.59	125.00
1	Q	159	GLN	C-N-CD	-7.89	92.63	125.00
1	N	227	GLY	N-CA-C	-7.86	99.46	112.83
1	K	159	GLN	C-N-CD	-7.84	92.84	125.00
1	Z	491	GLN	N-CA-C	-7.80	102.41	112.23
1	A	574	GLU	N-CA-C	7.79	119.60	110.41
1	M	155	GLU	N-CA-C	-7.76	89.27	111.00
1	Z	159	GLN	C-N-CD	-7.71	93.41	125.00
1	R	159	GLN	C-N-CD	-7.67	93.58	125.00
1	Z	367	ASP	N-CA-C	-7.64	98.17	110.32
1	Y	55	GLU	N-CA-C	-7.59	100.30	110.55
1	V	227	GLY	N-CA-C	-7.58	99.04	112.77
1	V	574	GLU	N-CA-C	7.56	119.33	110.41
1	Q	574	GLU	N-CA-C	7.51	119.28	110.41
1	M	360	GLY	N-CA-C	-7.51	102.12	112.18
1	K	574	GLU	N-CA-C	7.48	119.23	110.41
1	c	159	GLN	C-N-CD	-7.40	94.65	125.00
1	S	160	PRO	CA-C-N	7.40	144.75	127.00
1	S	160	PRO	C-N-CA	7.40	144.75	127.00
1	M	553	ILE	CA-C-N	7.37	134.96	121.70
1	M	553	ILE	C-N-CA	7.37	134.96	121.70
1	D	154	SER	CA-C-N	7.33	134.90	121.70
1	D	154	SER	C-N-CA	7.33	134.90	121.70
1	T	574	GLU	N-CA-C	7.30	119.02	110.41
1	N	375	ASP	CA-C-N	7.30	127.22	119.85
1	N	375	ASP	C-N-CA	7.30	127.22	119.85
1	Q	154	SER	CA-C-N	7.28	134.80	121.70
1	Q	154	SER	C-N-CA	7.28	134.80	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	360	GLY	CA-C-O	-7.27	117.21	122.23
1	A	434	ASP	CA-C-N	7.23	127.16	119.85
1	A	434	ASP	C-N-CA	7.23	127.16	119.85
1	S	360	GLY	CA-C-O	-7.22	117.52	122.22
1	b	160	PRO	CA-C-N	7.22	144.34	127.00
1	b	160	PRO	C-N-CA	7.22	144.34	127.00
1	C	154	SER	CA-C-N	7.21	134.68	121.70
1	C	154	SER	C-N-CA	7.21	134.68	121.70
1	Y	154	SER	CA-C-N	7.20	134.66	121.70
1	Y	154	SER	C-N-CA	7.20	134.66	121.70
1	N	574	GLU	N-CA-C	7.18	118.89	110.41
1	b	159	GLN	C-N-CD	-7.18	95.58	125.00
1	G	106	VAL	CB-CA-C	-7.17	101.72	111.33
1	N	553	ILE	CA-C-N	7.16	134.58	121.70
1	N	553	ILE	C-N-CA	7.16	134.58	121.70
1	X	154	SER	CA-C-N	7.15	134.58	121.70
1	X	154	SER	C-N-CA	7.15	134.58	121.70
1	C	160	PRO	N-CA-C	7.14	119.42	110.70
1	M	157	ALA	N-CA-C	7.14	119.91	107.49
1	G	198	TYR	CA-C-N	7.13	126.62	118.85
1	G	198	TYR	C-N-CA	7.13	126.62	118.85
1	P	375	ASP	CA-C-N	7.11	127.68	120.14
1	P	375	ASP	C-N-CA	7.11	127.68	120.14
1	T	160	PRO	C-N-CD	-7.10	104.98	120.60
1	T	434	ASP	CA-C-N	7.10	127.02	119.85
1	T	434	ASP	C-N-CA	7.10	127.02	119.85
1	S	160	PRO	C-N-CD	-7.10	104.99	120.60
1	R	288	PRO	O-C-N	7.08	124.57	121.31
1	b	375	ASP	CA-C-N	7.07	126.99	119.85
1	b	375	ASP	C-N-CA	7.07	126.99	119.85
1	H	159	GLN	C-N-CD	-7.07	96.03	125.00
1	K	553	ILE	CA-C-N	7.06	134.41	121.70
1	K	553	ILE	C-N-CA	7.06	134.41	121.70
1	E	553	ILE	CA-C-N	7.05	134.39	121.70
1	E	553	ILE	C-N-CA	7.05	134.39	121.70
1	d	491	GLN	N-CA-C	-7.04	104.16	112.89
1	A	227	GLY	N-CA-C	-7.04	100.87	112.83
1	d	154	SER	CA-C-N	7.04	134.36	121.70
1	d	154	SER	C-N-CA	7.04	134.36	121.70
1	E	198	TYR	CA-C-N	7.03	126.85	119.05
1	E	198	TYR	C-N-CA	7.03	126.85	119.05
1	Y	553	ILE	CA-C-N	7.03	134.35	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	553	ILE	C-N-CA	7.03	134.35	121.70
1	R	227	GLY	N-CA-C	-7.02	100.90	112.83
1	b	160	PRO	C-N-CD	-7.00	105.19	120.60
1	F	227	GLY	N-CA-C	-7.00	100.93	112.83
1	S	553	ILE	CA-C-N	6.98	134.26	121.70
1	S	553	ILE	C-N-CA	6.98	134.26	121.70
1	c	553	ILE	CA-C-N	6.97	134.25	121.70
1	c	553	ILE	C-N-CA	6.97	134.25	121.70
1	Z	434	ASP	CA-C-N	6.97	126.89	119.85
1	Z	434	ASP	C-N-CA	6.97	126.89	119.85
1	H	553	ILE	CA-C-N	6.96	134.23	121.70
1	H	553	ILE	C-N-CA	6.96	134.23	121.70
1	J	154	SER	CA-C-N	6.95	134.22	121.70
1	J	154	SER	C-N-CA	6.95	134.22	121.70
1	R	553	ILE	CA-C-N	6.94	134.19	121.70
1	R	553	ILE	C-N-CA	6.94	134.19	121.70
1	F	394	THR	CA-C-N	6.92	127.09	120.31
1	F	394	THR	C-N-CA	6.92	127.09	120.31
1	M	160	PRO	C-N-CD	-6.90	105.42	120.60
1	C	553	ILE	CA-C-N	6.90	134.12	121.70
1	C	553	ILE	C-N-CA	6.90	134.12	121.70
1	M	159	GLN	C-N-CD	-6.89	96.76	125.00
1	a	553	ILE	CA-C-N	6.88	134.09	121.70
1	a	553	ILE	C-N-CA	6.88	134.09	121.70
1	I	553	ILE	CA-C-N	6.88	134.08	121.70
1	I	553	ILE	C-N-CA	6.88	134.08	121.70
1	X	553	ILE	CA-C-N	6.87	134.06	121.70
1	X	553	ILE	C-N-CA	6.87	134.06	121.70
1	F	375	ASP	CA-C-N	6.85	126.77	119.85
1	F	375	ASP	C-N-CA	6.85	126.77	119.85
1	L	553	ILE	CA-C-N	6.85	134.03	121.70
1	L	553	ILE	C-N-CA	6.85	134.03	121.70
1	T	553	ILE	CA-C-N	6.85	134.03	121.70
1	T	553	ILE	C-N-CA	6.85	134.03	121.70
1	X	270	CYS	N-CA-C	6.83	118.17	108.74
1	d	553	ILE	CA-C-N	6.83	134.00	121.70
1	d	553	ILE	C-N-CA	6.83	134.00	121.70
1	Z	553	ILE	CA-C-N	6.82	133.97	121.70
1	Z	553	ILE	C-N-CA	6.82	133.97	121.70
1	J	553	ILE	CA-C-N	6.82	133.97	121.70
1	J	553	ILE	C-N-CA	6.82	133.97	121.70
1	G	553	ILE	CA-C-N	6.82	133.97	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	553	ILE	C-N-CA	6.82	133.97	121.70
1	V	553	ILE	CA-C-N	6.80	133.95	121.70
1	V	553	ILE	C-N-CA	6.80	133.95	121.70
1	M	160	PRO	CA-C-N	6.79	143.29	127.00
1	M	160	PRO	C-N-CA	6.79	143.29	127.00
1	F	553	ILE	CA-C-N	6.78	133.91	121.70
1	F	553	ILE	C-N-CA	6.78	133.91	121.70
1	d	375	ASP	CA-C-N	6.77	127.30	119.99
1	d	375	ASP	C-N-CA	6.77	127.30	119.99
1	T	160	PRO	CA-C-N	6.77	143.25	127.00
1	T	160	PRO	C-N-CA	6.77	143.25	127.00
1	U	553	ILE	CA-C-N	6.77	133.88	121.70
1	U	553	ILE	C-N-CA	6.77	133.88	121.70
1	B	553	ILE	CA-C-N	6.76	133.88	121.70
1	B	553	ILE	C-N-CA	6.76	133.88	121.70
1	T	556	ASP	N-CA-C	-6.76	101.80	110.19
1	L	154	SER	CA-C-N	6.76	133.87	121.70
1	L	154	SER	C-N-CA	6.76	133.87	121.70
1	O	553	ILE	CA-C-N	6.76	133.86	121.70
1	O	553	ILE	C-N-CA	6.76	133.86	121.70
1	J	87	LEU	N-CA-C	-6.75	103.94	111.71
1	b	553	ILE	CA-C-N	6.75	133.85	121.70
1	b	553	ILE	C-N-CA	6.75	133.85	121.70
1	d	155	GLU	N-CA-C	-6.74	92.13	111.00
1	E	574	GLU	N-CA-C	6.74	120.28	109.83
1	F	439	LYS	CG-CD-CE	-6.74	95.81	111.30
1	T	154	SER	CA-C-N	6.73	133.81	121.70
1	T	154	SER	C-N-CA	6.73	133.81	121.70
1	Q	553	ILE	CA-C-N	6.72	133.80	121.70
1	Q	553	ILE	C-N-CA	6.72	133.80	121.70
1	D	553	ILE	CA-C-N	6.72	133.80	121.70
1	D	553	ILE	C-N-CA	6.72	133.80	121.70
1	E	493	ASN	N-CA-C	-6.71	98.33	108.46
1	N	198	TYR	CA-C-N	6.71	126.66	119.28
1	N	198	TYR	C-N-CA	6.71	126.66	119.28
1	P	553	ILE	CA-C-N	6.70	133.76	121.70
1	P	553	ILE	C-N-CA	6.70	133.76	121.70
1	T	227	GLY	N-CA-C	-6.69	100.66	112.77
1	Y	159	GLN	C-N-CD	-6.67	97.67	125.00
1	C	227	GLY	N-CA-C	-6.64	101.55	112.83
1	E	154	SER	CA-C-N	6.63	133.64	121.70
1	E	154	SER	C-N-CA	6.63	133.64	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	375	ASP	CA-C-N	6.63	126.39	119.76
1	E	375	ASP	C-N-CA	6.63	126.39	119.76
1	b	87	LEU	N-CA-C	-6.62	104.47	112.54
1	F	548	ILE	N-CA-C	6.60	116.59	108.53
1	G	209	ARG	CA-CB-CG	-6.60	100.90	114.10
1	A	160	PRO	CA-C-N	6.58	142.80	127.00
1	A	160	PRO	C-N-CA	6.58	142.80	127.00
1	P	160	PRO	CA-C-N	6.58	142.79	127.00
1	P	160	PRO	C-N-CA	6.58	142.79	127.00
1	H	360	GLY	CA-C-O	-6.57	116.75	121.88
1	B	154	SER	CA-C-N	6.57	133.52	121.70
1	B	154	SER	C-N-CA	6.57	133.52	121.70
1	K	364	ALA	CA-C-N	-6.54	114.34	122.84
1	K	364	ALA	C-N-CA	-6.54	114.34	122.84
1	U	360	GLY	CA-C-O	-6.54	116.15	121.77
1	N	87	LEU	N-CA-C	-6.53	104.20	111.71
1	d	574	GLU	N-CA-C	6.53	124.71	110.80
1	G	209	ARG	N-CA-C	6.51	118.42	108.52
1	W	553	ILE	CA-C-N	6.51	133.42	121.70
1	W	553	ILE	C-N-CA	6.51	133.42	121.70
1	A	553	ILE	CA-C-N	6.50	133.41	121.70
1	A	553	ILE	C-N-CA	6.50	133.41	121.70
1	F	574	GLU	N-CA-C	6.49	124.63	110.80
1	S	155	GLU	N-CA-C	-6.47	92.87	111.00
1	L	198	TYR	CA-C-N	6.47	126.23	119.05
1	L	198	TYR	C-N-CA	6.47	126.23	119.05
1	J	360	GLY	CA-C-O	-6.45	116.85	121.88
1	C	375	ASP	CA-C-N	6.44	126.97	120.14
1	C	375	ASP	C-N-CA	6.44	126.97	120.14
1	d	160	PRO	C-N-CD	-6.43	106.44	120.60
1	I	375	ASP	CA-C-N	6.41	126.32	119.85
1	I	375	ASP	C-N-CA	6.41	126.32	119.85
1	D	227	GLY	N-CA-C	-6.40	101.95	112.83
1	C	360	GLY	CA-C-O	-6.39	116.90	121.88
1	V	198	TYR	CA-C-N	6.39	126.14	119.05
1	V	198	TYR	C-N-CA	6.39	126.14	119.05
1	Y	160	PRO	CA-C-N	6.38	142.31	127.00
1	Y	160	PRO	C-N-CA	6.38	142.31	127.00
1	d	160	PRO	CA-C-N	6.38	142.31	127.00
1	d	160	PRO	C-N-CA	6.38	142.31	127.00
1	P	154	SER	CA-C-N	6.36	133.16	121.70
1	P	154	SER	C-N-CA	6.36	133.16	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	87	LEU	N-CA-C	-6.34	104.42	111.71
1	P	158	THR	N-CA-C	-6.34	93.26	111.00
1	X	562	VAL	N-CA-C	-6.33	104.00	109.19
1	d	159	GLN	C-N-CD	-6.32	99.08	125.00
1	N	157	ALA	CA-C-N	6.31	133.06	121.70
1	N	157	ALA	C-N-CA	6.31	133.06	121.70
1	L	160	PRO	CA-C-N	6.31	142.14	127.00
1	L	160	PRO	C-N-CA	6.31	142.14	127.00
1	b	491	GLN	N-CA-C	-6.31	105.07	112.89
1	N	158	THR	N-CA-C	-6.30	93.36	111.00
1	J	434	ASP	CA-C-N	6.29	126.21	119.85
1	J	434	ASP	C-N-CA	6.29	126.21	119.85
1	Z	160	PRO	C-N-CD	-6.29	106.75	120.60
1	b	154	SER	CA-C-N	6.29	133.03	121.70
1	b	154	SER	C-N-CA	6.29	133.03	121.70
1	P	574	GLU	N-CA-C	6.29	124.19	110.80
1	Y	160	PRO	C-N-CD	-6.26	106.83	120.60
1	B	294	LEU	CA-C-N	6.25	126.22	119.78
1	B	294	LEU	C-N-CA	6.25	126.22	119.78
1	W	160	PRO	CA-C-N	6.24	141.97	127.00
1	W	160	PRO	C-N-CA	6.24	141.97	127.00
1	Z	394	THR	CA-C-N	6.23	126.42	120.31
1	Z	394	THR	C-N-CA	6.23	126.42	120.31
1	L	159	GLN	C-N-CD	-6.23	99.47	125.00
1	X	198	TYR	CA-C-N	6.22	125.96	119.05
1	X	198	TYR	C-N-CA	6.22	125.96	119.05
1	U	574	GLU	N-CA-C	6.21	124.04	110.80
1	P	160	PRO	C-N-CD	-6.20	106.95	120.60
1	K	198	TYR	CA-C-N	6.19	126.09	119.28
1	K	198	TYR	C-N-CA	6.19	126.09	119.28
1	Q	198	TYR	CA-C-N	6.18	125.91	119.05
1	Q	198	TYR	C-N-CA	6.18	125.91	119.05
1	b	227	GLY	N-CA-C	-6.18	101.58	112.77
1	H	198	TYR	CA-C-N	6.17	125.90	119.05
1	H	198	TYR	C-N-CA	6.17	125.90	119.05
1	Q	160	PRO	CA-C-N	6.16	141.78	127.00
1	Q	160	PRO	C-N-CA	6.16	141.78	127.00
1	R	360	GLY	CA-C-O	-6.15	117.08	121.88
1	L	574	GLU	N-CA-C	6.14	123.89	110.80
1	F	154	SER	CA-C-N	6.14	132.75	121.70
1	F	154	SER	C-N-CA	6.14	132.75	121.70
1	C	574	GLU	N-CA-C	6.14	123.87	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	574	GLU	N-CA-C	6.14	123.87	110.80
1	L	160	PRO	C-N-CD	-6.13	107.12	120.60
1	A	360	GLY	CA-C-O	-6.12	116.50	121.77
1	X	160	PRO	CA-C-N	6.12	141.69	127.00
1	X	160	PRO	C-N-CA	6.12	141.69	127.00
1	Q	160	PRO	C-N-CD	-6.11	107.17	120.60
1	K	394	THR	CA-C-N	6.10	126.29	120.31
1	K	394	THR	C-N-CA	6.10	126.29	120.31
1	I	409	TYR	CA-C-N	6.10	125.78	119.56
1	I	409	TYR	C-N-CA	6.10	125.78	119.56
1	A	154	SER	CA-C-N	6.09	132.67	121.70
1	A	154	SER	C-N-CA	6.09	132.67	121.70
1	M	574	GLU	N-CA-C	6.08	123.76	110.80
1	W	157	ALA	N-CA-C	6.06	117.51	107.20
1	a	574	GLU	CB-CA-C	-6.06	101.31	111.24
1	J	409	TYR	CA-C-N	6.05	125.73	119.56
1	J	409	TYR	C-N-CA	6.05	125.73	119.56
1	J	360	GLY	N-CA-C	-6.05	104.08	112.18
1	K	493	ASN	N-CA-C	-6.04	99.33	108.46
1	D	434	ASP	CA-C-N	6.04	125.95	119.85
1	D	434	ASP	C-N-CA	6.04	125.95	119.85
1	E	491	GLN	N-CA-C	-6.04	105.74	113.23
1	C	271	LYS	N-CA-C	-6.03	103.19	110.13
1	Q	434	ASP	CA-C-N	6.03	125.94	119.85
1	Q	434	ASP	C-N-CA	6.03	125.94	119.85
1	G	434	ASP	CA-C-N	6.02	125.93	119.85
1	G	434	ASP	C-N-CA	6.02	125.93	119.85
1	U	154	SER	CA-C-N	5.99	132.48	121.70
1	U	154	SER	C-N-CA	5.99	132.48	121.70
1	S	574	GLU	N-CA-C	5.99	123.55	110.80
1	M	409	TYR	CA-C-N	5.97	125.65	119.56
1	M	409	TYR	C-N-CA	5.97	125.65	119.56
1	K	375	ASP	CA-C-N	5.97	126.46	120.14
1	K	375	ASP	C-N-CA	5.97	126.46	120.14
1	X	160	PRO	C-N-CD	-5.96	107.48	120.60
1	F	426	ASP	CB-CG-OD1	5.96	132.10	118.40
1	I	155	GLU	N-CA-C	-5.96	94.32	111.00
1	U	160	PRO	CA-C-N	5.93	141.24	127.00
1	U	160	PRO	C-N-CA	5.93	141.24	127.00
1	B	159	GLN	CA-CB-CG	5.92	125.95	114.10
1	X	581	ARG	O-C-N	5.92	125.21	120.83
1	a	198	TYR	CA-C-N	5.92	125.62	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	198	TYR	C-N-CA	5.92	125.62	119.05
1	T	340	ALA	CA-C-N	5.91	125.86	119.78
1	T	340	ALA	C-N-CA	5.91	125.86	119.78
1	W	227	GLY	N-CA-C	-5.90	102.80	112.83
1	P	493	ASN	N-CA-C	-5.90	99.56	108.46
1	A	581	ARG	O-C-N	5.89	125.19	120.83
1	H	574	GLU	N-CA-C	5.89	123.34	110.80
1	M	375	ASP	CA-C-N	5.87	126.36	120.14
1	M	375	ASP	C-N-CA	5.87	126.36	120.14
1	A	160	PRO	C-N-CD	-5.86	107.71	120.60
1	X	375	ASP	CA-C-N	5.86	125.77	119.85
1	X	375	ASP	C-N-CA	5.86	125.77	119.85
1	M	154	SER	CA-C-N	5.86	132.24	121.70
1	M	154	SER	C-N-CA	5.86	132.24	121.70
1	c	493	ASN	N-CA-C	-5.85	98.74	108.75
1	D	355	THR	CA-C-N	5.85	126.34	120.14
1	D	355	THR	C-N-CA	5.85	126.34	120.14
1	C	508	ASN	CA-C-N	-5.83	114.55	122.77
1	C	508	ASN	C-N-CA	-5.83	114.55	122.77
1	M	556	ASP	N-CA-C	-5.83	102.96	110.19
1	P	434	ASP	CA-C-N	5.83	125.74	119.85
1	P	434	ASP	C-N-CA	5.83	125.74	119.85
1	R	517	ASN	N-CA-C	5.82	123.21	110.80
1	A	375	ASP	CA-C-N	5.82	125.73	119.85
1	A	375	ASP	C-N-CA	5.82	125.73	119.85
1	L	434	ASP	CA-C-N	5.82	125.73	119.85
1	L	434	ASP	C-N-CA	5.82	125.73	119.85
1	a	154	SER	CA-C-N	5.81	132.16	121.70
1	a	154	SER	C-N-CA	5.81	132.16	121.70
1	W	493	ASN	N-CA-C	-5.80	98.44	110.80
1	K	154	SER	CA-C-N	5.80	132.14	121.70
1	K	154	SER	C-N-CA	5.80	132.14	121.70
1	C	160	PRO	C-N-CD	-5.79	107.85	120.60
1	A	94	GLY	N-CA-C	-5.79	107.33	115.32
1	D	160	PRO	CA-C-N	5.78	140.88	127.00
1	D	160	PRO	C-N-CA	5.78	140.88	127.00
1	L	157	ALA	N-CA-C	5.78	117.03	107.20
1	G	574	GLU	N-CA-C	5.78	123.11	110.80
1	a	367	ASP	N-CA-C	5.76	117.45	109.15
1	I	340	ALA	CA-C-N	5.76	125.71	119.78
1	I	340	ALA	C-N-CA	5.76	125.71	119.78
1	d	360	GLY	CA-C-O	-5.76	116.09	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	491	GLN	N-CA-C	-5.76	105.75	112.89
1	d	424	VAL	N-CA-C	5.75	117.03	109.21
1	D	160	PRO	C-N-CD	-5.74	107.97	120.60
1	O	157	ALA	CA-C-N	5.74	132.04	121.70
1	O	157	ALA	C-N-CA	5.74	132.04	121.70
1	J	368	GLU	N-CA-C	-5.73	100.36	109.07
1	O	160	PRO	C-N-CD	-5.72	108.01	120.60
1	S	133	MET	N-CA-C	5.72	118.54	109.50
1	S	157	ALA	CA-C-N	5.72	132.00	121.70
1	S	157	ALA	C-N-CA	5.72	132.00	121.70
1	J	160	PRO	C-N-CD	-5.72	108.02	120.60
1	O	493	ASN	N-CA-C	-5.72	98.62	110.80
1	U	517	ASN	N-CA-C	5.71	118.26	109.07
1	G	160	PRO	CA-N-CD	-5.71	104.01	112.00
1	H	579	ALA	CA-C-N	5.69	125.66	120.03
1	H	579	ALA	C-N-CA	5.69	125.66	120.03
1	I	366	THR	N-CA-C	5.67	119.38	111.90
1	C	581	ARG	O-C-N	5.66	125.02	120.83
1	U	198	TYR	CA-C-N	5.66	125.51	119.28
1	U	198	TYR	C-N-CA	5.66	125.51	119.28
1	M	491	GLN	N-CA-C	-5.66	106.38	113.28
1	A	159	GLN	C-N-CD	-5.66	101.81	125.00
1	C	160	PRO	CA-C-N	5.65	140.55	127.00
1	C	160	PRO	C-N-CA	5.65	140.55	127.00
1	H	160	PRO	C-N-CD	-5.65	108.18	120.60
1	F	87	LEU	N-CA-C	-5.63	105.67	112.54
1	M	156	SER	N-CA-C	5.63	122.79	110.80
1	H	434	ASP	CA-C-N	5.62	125.52	119.85
1	H	434	ASP	C-N-CA	5.62	125.52	119.85
1	H	154	SER	CA-C-N	5.61	131.80	121.70
1	H	154	SER	C-N-CA	5.61	131.80	121.70
1	X	426	ASP	N-CA-C	5.61	118.93	111.75
1	Y	360	GLY	CA-C-O	-5.61	117.50	121.88
1	M	228	THR	CA-C-N	5.61	125.54	119.76
1	M	228	THR	C-N-CA	5.61	125.54	119.76
1	d	437	GLY	N-CA-C	-5.61	106.25	114.61
1	H	160	PRO	CA-C-N	5.59	140.43	127.00
1	H	160	PRO	C-N-CA	5.59	140.43	127.00
1	X	38	VAL	N-CA-C	5.59	115.72	110.30
1	R	556	ASP	N-CA-C	-5.59	103.26	110.19
1	R	155	GLU	CA-CB-CG	5.58	125.25	114.10
1	N	159	GLN	C-N-CD	-5.57	102.19	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	574	GLU	N-CA-C	5.56	122.64	110.80
1	U	493	ASN	N-CA-C	-5.55	100.08	108.46
1	W	556	ASP	N-CA-C	-5.55	103.31	110.19
1	O	160	PRO	CA-C-N	5.54	140.30	127.00
1	O	160	PRO	C-N-CA	5.54	140.30	127.00
1	I	227	GLY	N-CA-C	-5.54	102.75	112.77
1	b	581	ARG	O-C-N	5.53	124.92	120.83
1	I	556	ASP	N-CA-C	-5.52	103.34	110.19
1	K	157	ALA	CA-C-N	5.52	131.63	121.70
1	K	157	ALA	C-N-CA	5.52	131.63	121.70
1	I	198	TYR	CA-C-N	5.51	125.17	119.05
1	I	198	TYR	C-N-CA	5.51	125.17	119.05
1	V	409	TYR	CA-C-N	5.51	125.18	119.56
1	V	409	TYR	C-N-CA	5.51	125.18	119.56
1	K	87	LEU	N-CA-C	-5.50	105.83	112.54
1	U	157	ALA	N-CA-C	5.49	116.54	107.20
1	N	160	PRO	CA-C-N	5.49	140.16	127.00
1	N	160	PRO	C-N-CA	5.49	140.16	127.00
1	S	434	ASP	CA-C-N	5.49	125.39	119.85
1	S	434	ASP	C-N-CA	5.49	125.39	119.85
1	Y	434	ASP	CA-C-N	5.48	125.38	119.85
1	Y	434	ASP	C-N-CA	5.48	125.38	119.85
1	M	434	ASP	CA-C-N	5.47	125.37	119.85
1	M	434	ASP	C-N-CA	5.47	125.37	119.85
1	I	360	GLY	N-CA-C	-5.46	102.91	111.00
1	K	491	GLN	N-CA-C	-5.46	105.35	112.23
1	b	434	ASP	CA-C-N	5.45	125.36	119.85
1	b	434	ASP	C-N-CA	5.45	125.36	119.85
1	W	160	PRO	C-N-CD	-5.44	108.63	120.60
1	Y	556	ASP	N-CA-C	-5.44	103.44	110.19
1	D	556	ASP	N-CA-C	-5.44	103.44	110.19
1	O	198	TYR	CA-C-N	5.44	125.09	119.05
1	O	198	TYR	C-N-CA	5.44	125.09	119.05
1	c	160	PRO	C-N-CD	-5.44	108.63	120.60
1	G	106	VAL	N-CA-C	5.44	116.02	108.84
1	a	157	ALA	N-CA-C	5.44	116.44	107.20
1	J	159	GLN	C-N-CD	-5.43	102.75	125.00
1	R	375	ASP	CA-C-N	5.42	125.33	119.85
1	R	375	ASP	C-N-CA	5.42	125.33	119.85
1	K	434	ASP	CA-C-N	5.42	125.32	119.85
1	K	434	ASP	C-N-CA	5.42	125.32	119.85
1	Q	493	ASN	N-CA-C	-5.41	100.29	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	394	THR	CA-C-N	5.41	125.87	120.14
1	C	394	THR	C-N-CA	5.41	125.87	120.14
1	U	159	GLN	C-N-CD	-5.40	102.86	125.00
1	S	581	ARG	O-C-N	5.40	124.82	120.83
1	G	366	THR	N-CA-C	5.39	122.29	110.80
1	P	392	GLY	N-CA-C	-5.37	104.98	112.18
1	I	360	GLY	CA-C-O	-5.37	115.68	122.39
1	U	160	PRO	C-N-CD	-5.37	108.79	120.60
1	V	434	ASP	CA-C-N	5.36	125.27	119.85
1	V	434	ASP	C-N-CA	5.36	125.27	119.85
1	R	160	PRO	CA-C-N	5.36	139.87	127.00
1	R	160	PRO	C-N-CA	5.36	139.87	127.00
1	Z	548	ILE	N-CA-C	5.36	115.07	108.53
1	E	159	GLN	C-N-CD	-5.36	103.03	125.00
1	B	562	VAL	N-CA-C	-5.35	104.80	109.19
1	A	130	VAL	N-CA-C	5.35	116.12	110.72
1	J	368	GLU	CA-C-N	-5.34	114.56	123.33
1	J	368	GLU	C-N-CA	-5.34	114.56	123.33
1	R	160	PRO	C-N-CD	-5.34	108.84	120.60
1	c	156	SER	N-CA-C	5.34	122.18	110.80
1	J	556	ASP	N-CA-C	-5.33	103.59	110.19
1	X	294	LEU	CA-C-N	5.33	125.62	119.92
1	X	294	LEU	C-N-CA	5.33	125.62	119.92
1	A	556	ASP	N-CA-C	-5.32	103.59	110.19
1	F	493	ASN	N-CA-C	-5.31	100.44	108.46
1	d	287	LEU	CA-C-N	5.31	123.48	119.66
1	d	287	LEU	C-N-CA	5.31	123.48	119.66
1	E	556	ASP	N-CA-C	-5.31	103.61	110.19
1	W	87	LEU	N-CA-C	-5.31	105.66	111.82
1	c	160	PRO	CA-C-N	5.31	139.74	127.00
1	c	160	PRO	C-N-CA	5.31	139.74	127.00
1	J	160	PRO	CA-C-N	5.30	139.73	127.00
1	J	160	PRO	C-N-CA	5.30	139.73	127.00
1	G	94	GLY	N-CA-C	-5.30	108.00	115.32
1	S	154	SER	CA-C-N	5.30	131.25	121.70
1	S	154	SER	C-N-CA	5.30	131.25	121.70
1	d	394	THR	CA-C-N	5.30	125.51	120.31
1	d	394	THR	C-N-CA	5.30	125.51	120.31
1	P	157	ALA	CA-C-N	5.30	131.24	121.70
1	P	157	ALA	C-N-CA	5.30	131.24	121.70
1	S	159	GLN	C-N-CD	-5.30	103.26	125.00
1	F	133	MET	N-CA-C	5.30	117.87	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	409	TYR	CA-C-N	5.29	124.96	119.56
1	Z	409	TYR	C-N-CA	5.29	124.96	119.56
1	J	94	GLY	N-CA-C	-5.29	108.02	115.32
1	U	572	VAL	N-CA-C	5.29	116.20	108.53
1	P	360	GLY	CA-C-O	-5.29	117.22	121.77
1	K	160	PRO	CA-C-N	5.29	139.69	127.00
1	K	160	PRO	C-N-CA	5.29	139.69	127.00
1	T	375	ASP	CA-C-N	5.29	125.05	119.76
1	T	375	ASP	C-N-CA	5.29	125.05	119.76
1	F	360	GLY	CA-C-O	-5.28	117.23	121.77
1	N	556	ASP	N-CA-C	-5.28	103.64	110.19
1	d	156	SER	N-CA-C	5.28	118.68	111.39
1	U	556	ASP	N-CA-C	-5.27	103.65	110.19
1	T	511	ASP	CA-C-N	5.26	124.77	119.19
1	T	511	ASP	C-N-CA	5.26	124.77	119.19
1	d	157	ALA	CA-C-N	5.26	131.17	121.70
1	d	157	ALA	C-N-CA	5.26	131.17	121.70
1	G	157	ALA	CA-C-N	5.26	131.17	121.70
1	G	157	ALA	C-N-CA	5.26	131.17	121.70
1	K	360	GLY	CA-C-O	-5.26	117.25	121.77
1	L	87	LEU	N-CA-C	-5.25	105.67	111.71
1	H	366	THR	N-CA-C	5.25	118.82	111.90
1	W	155	GLU	N-CA-C	-5.24	96.31	111.00
1	B	160	PRO	CA-N-CD	-5.24	104.67	112.00
1	D	581	ARG	O-C-N	5.24	124.71	120.83
1	d	281	THR	N-CA-C	-5.23	102.72	110.46
1	M	87	LEU	N-CA-C	-5.23	105.76	111.82
1	N	160	PRO	C-N-CD	-5.22	109.11	120.60
1	C	160	PRO	CA-N-CD	-5.22	104.69	112.00
1	G	105	ILE	N-CA-C	5.22	115.09	107.37
1	G	160	PRO	CA-C-N	5.21	139.51	127.00
1	G	160	PRO	C-N-CA	5.21	139.51	127.00
1	N	355	THR	CA-C-N	5.21	125.66	120.14
1	N	355	THR	C-N-CA	5.21	125.66	120.14
1	I	288	PRO	O-C-N	5.21	123.60	121.15
1	B	94	GLY	N-CA-C	-5.20	108.15	115.32
1	H	87	LEU	N-CA-C	-5.19	105.80	111.82
1	R	434	ASP	CA-C-N	5.19	125.10	119.85
1	R	434	ASP	C-N-CA	5.19	125.10	119.85
1	G	493	ASN	N-CA-C	-5.19	100.14	108.55
1	M	198	TYR	CA-C-N	5.19	124.99	119.28
1	M	198	TYR	C-N-CA	5.19	124.99	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	556	ASP	N-CA-C	-5.18	103.77	110.19
1	W	434	ASP	CA-C-N	5.18	125.08	119.85
1	W	434	ASP	C-N-CA	5.18	125.08	119.85
1	Y	155	GLU	N-CA-C	-5.18	96.51	111.00
1	V	525	SER	N-CA-C	5.17	117.25	109.23
1	I	493	ASN	N-CA-C	-5.17	99.91	108.75
1	O	159	GLN	C-N-CD	-5.17	103.80	125.00
1	E	160	PRO	CA-N-CD	-5.17	104.77	112.00
1	Y	160	PRO	CA-N-CD	-5.16	104.77	112.00
1	A	294	LEU	CA-C-N	5.16	125.44	119.92
1	A	294	LEU	C-N-CA	5.16	125.44	119.92
1	T	366	THR	N-CA-C	5.16	118.87	112.47
1	d	160	PRO	CA-N-CD	-5.16	104.78	112.00
1	F	316	VAL	N-CA-C	5.15	115.54	108.12
1	I	301	THR	N-CA-C	-5.15	105.68	112.94
1	U	491	GLN	N-CA-C	-5.15	105.74	112.23
1	C	335	GLU	N-CA-C	5.15	117.46	108.76
1	R	87	LEU	N-CA-C	-5.15	105.85	111.82
1	D	155	GLU	N-CA-C	-5.15	96.59	111.00
1	Z	457	LEU	N-CA-C	5.14	116.89	109.07
1	Q	155	GLU	N-CA-C	-5.14	96.61	111.00
1	a	87	LEU	N-CA-C	-5.14	105.86	111.82
1	W	375	ASP	CA-C-N	5.14	125.54	119.99
1	W	375	ASP	C-N-CA	5.14	125.54	119.99
1	W	294	LEU	CA-C-N	5.14	125.07	119.78
1	W	294	LEU	C-N-CA	5.14	125.07	119.78
1	G	349	THR	N-CA-C	5.13	121.74	110.80
1	F	159	GLN	C-N-CD	-5.13	103.96	125.00
1	Z	360	GLY	N-CA-C	-5.13	99.55	111.04
1	K	581	ARG	O-C-N	5.13	124.63	120.83
1	a	457	LEU	N-CA-C	5.12	116.98	109.24
1	d	562	VAL	N-CA-C	-5.12	103.23	109.01
1	F	491	GLN	N-CA-C	-5.11	105.40	111.69
1	c	155	GLU	N-CA-C	-5.10	96.72	111.00
1	L	78	ASN	N-CA-C	5.10	117.91	109.85
1	Y	304	GLY	N-CA-C	-5.09	104.92	113.02
1	E	351	GLY	CA-C-N	5.09	126.21	120.66
1	E	351	GLY	C-N-CA	5.09	126.21	120.66
1	D	94	GLY	N-CA-C	-5.09	108.29	115.32
1	H	548	ILE	N-CA-C	5.09	114.74	108.53
1	H	375	ASP	CA-C-N	5.09	125.53	120.14
1	H	375	ASP	C-N-CA	5.09	125.53	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	315	GLY	N-CA-C	5.08	117.60	110.38
1	G	263	THR	N-CA-C	-5.08	103.22	110.59
1	O	534	VAL	N-CA-C	5.08	115.28	108.17
1	O	387	LYS	N-CA-C	-5.07	102.41	109.96
1	T	159	GLN	C-N-CD	-5.07	104.21	125.00
1	Q	157	ALA	CA-C-N	5.07	130.82	121.70
1	Q	157	ALA	C-N-CA	5.07	130.82	121.70
1	b	55	GLU	N-CA-C	-5.07	103.71	110.55
1	O	434	ASP	CA-C-N	5.07	124.97	119.85
1	O	434	ASP	C-N-CA	5.07	124.97	119.85
1	Z	360	GLY	CA-C-N	5.07	130.82	121.70
1	Z	360	GLY	C-N-CA	5.07	130.82	121.70
1	P	394	THR	CA-C-N	5.06	125.27	120.31
1	P	394	THR	C-N-CA	5.06	125.27	120.31
1	P	198	TYR	CA-C-N	5.06	124.67	119.05
1	P	198	TYR	C-N-CA	5.06	124.67	119.05
1	L	130	VAL	N-CA-C	5.06	115.83	110.72
1	U	227	GLY	N-CA-C	-5.06	104.23	112.83
1	D	294	LEU	CA-C-N	5.04	125.31	119.92
1	D	294	LEU	C-N-CA	5.04	125.31	119.92
1	X	556	ASP	N-CA-C	-5.03	103.95	110.19
1	M	360	GLY	CA-C-N	5.03	130.75	121.70
1	M	360	GLY	C-N-CA	5.03	130.75	121.70
1	c	380	PHE	N-CA-C	5.03	115.94	108.60
1	Z	574	GLU	N-CA-C	5.02	121.50	110.80
1	b	372	ALA	N-CA-C	-5.02	107.11	113.18
1	G	160	PRO	C-N-CD	-5.01	109.57	120.60
1	T	198	TYR	CA-C-N	5.01	124.61	119.05
1	T	198	TYR	C-N-CA	5.01	124.61	119.05
1	F	160	PRO	CA-C-N	5.01	139.02	127.00
1	F	160	PRO	C-N-CA	5.01	139.02	127.00
1	G	288	PRO	O-C-N	5.00	123.50	121.15

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

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Mol	Chain	Res	Type	Group
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 ⓘ

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	123	0
1	B	4352	0	4143	129	0
1	C	4352	0	4143	119	2
1	D	4352	0	4143	101	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4352	0	4143	136	0
1	F	4352	0	4143	146	0
1	G	4352	0	4143	129	3
1	H	4352	0	4143	134	0
1	I	4352	0	4143	141	0
1	J	4352	0	4143	86	2
1	K	4352	0	4143	127	0
1	L	4352	0	4143	142	0
1	M	4352	0	4143	132	0
1	N	4352	0	4143	109	2
1	O	4352	0	4143	100	5
1	P	4352	0	4143	111	0
1	Q	4352	0	4143	82	5
1	R	4352	0	4143	129	0
1	S	4352	0	4143	95	2
1	T	4352	0	4143	119	0
1	U	4352	0	4143	109	3
1	V	4352	0	4143	138	0
1	W	4352	0	4143	134	0
1	X	4352	0	4145	98	4
1	Y	4352	0	4143	119	2
1	Z	4352	0	4143	88	2
1	a	4352	0	4143	130	3
1	b	4352	0	4143	139	0
1	c	4352	0	4143	116	1
1	d	4352	0	4143	133	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3031	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 12.

All (3031) 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	1.37	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:J:553:ILE:HA	1:J:554:ASN:HB2	1.40	1.03
1:Y:553:ILE:HA	1:Y:554:ASN:HB2	1.41	1.03
1:A:553:ILE:HA	1:A:554:ASN:HB2	1.41	1.01
1:O:553:ILE:HA	1:O:554:ASN:HB2	1.40	1.01
1:d:553:ILE:HA	1:d:554:ASN:HB2	1.38	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	1.43	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
1:D:553:ILE:HA	1:D:554:ASN:HB2	1.45	0.98
1:N:382:ARG:H	1:N:386:GLN:HB3	1.27	0.98
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:B:553:ILE:HA	1:B:554:ASN:HB2	1.42	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:C:553:ILE:HA	1:C:554:ASN:HB2	1.42	0.98
1:U:553:ILE:HA	1:U:554:ASN:HB2	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.29	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:a:553:ILE:HA	1:a:554:ASN:HB2	1.47	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:K:154:SER:HA	1:K:155:GLU:HB2	1.48	0.93
1:d:382:ARG:H	1:d:386:GLN:HB3	1.33	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:a:382:ARG:H	1:a:386:GLN:HB3	1.36	0.90
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	1.54	0.89
1:E:209:ARG:NH1	1:I:288:PRO:O	2.06	0.88
1:M:209:ARG:NH1	1:R:288:PRO:O	2.05	0.88
1:b:365:GLN:O	1:b:367:ASP:N	2.06	0.88
1:P:193:GLU:HB3	1:P:206:THR:HG21	1.56	0.88
1:V:382:ARG:H	1:V:386:GLN:HB3	1.36	0.88
1:c:554:ASN:HD22	1:c:557:ASN:HD22	1.16	0.88
1:N:553:ILE:HA	1:N:554:ASN:HB2	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:193:GLU:HB3	1:W:206:THR:HG21	1.56	0.87
1:X:159:GLN:HG2	1:X:160:PRO:HD2	1.57	0.87
1:Y:193:GLU:OE1	1:Y:209:ARG:NH2	2.08	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	1.58	0.85
1:c:193:GLU:HB3	1:c:206:THR:HG21	1.58	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	1.57	0.85
1:A:582:LYS:NZ	1:K:244:TYR:OH	2.08	0.84
1:E:159:GLN:HG3	1:E:160:PRO:HD2	1.58	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	1.58	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:R:193:GLU:HB3	1:R:206:THR:HG21	1.57	0.84
1:X:554:ASN:HD22	1:X:557:ASN:HD22	1.26	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	1.59	0.83
1:D:193:GLU:HB3	1:D:206:THR:HG21	1.60	0.83
1:H:191:ARG:NH1	1:b:287:LEU:O	2.11	0.83
1:W:288:PRO:O	1:b:209:ARG:NH1	2.12	0.83
1:J:154:SER:HA	1:J:155:GLU:HB2	1.60	0.83
1:H:475:ASP:O	1:b:581:ARG:NH1	2.12	0.83
1:b:369:ASN:O	1:b:371:ALA:N	2.11	0.83
1:J:193:GLU:HB3	1:J:206:THR:HG21	1.58	0.83
1:L:287:LEU:O	1:d:191:ARG:NH1	2.11	0.83
1:G:193:GLU:HB3	1:G:206:THR:HG21	1.59	0.83
1:L:382:ARG:H	1:L:386:GLN:HB3	1.43	0.82
1:T:159:GLN:HG2	1:T:160:PRO:HD2	1.60	0.82
1:D:154:SER:HA	1:D:155:GLU:HB2	1.62	0.82
1:C:561:TYR:OH	1:C:574:GLU:OE2	1.97	0.82
1:I:425:THR:HG22	1:I:427:ASP:H	1.45	0.81
1:S:193:GLU:HB3	1:S:206:THR:HG21	1.61	0.81
1:V:193:GLU:HB3	1:V:206:THR:HG21	1.61	0.81
1:Y:191:ARG:NH1	1:a:287:LEU:O	2.14	0.81
1:b:401:ILE:O	1:b:575:LYS:NZ	2.13	0.81
1:C:370:GLN:N	1:C:370:GLN:OE1	2.14	0.81
1:M:561:TYR:OH	1:M:574:GLU:OE2	1.99	0.81
1:K:287:LEU:O	1:T:191:ARG:NH1	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:154:SER:HA	1:c:155:GLU:HB2	1.63	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:Q:96:MET:HG2	1:Q:220:PRO:HA	1.62	0.80
1:C:193:GLU:HB3	1:C:206:THR:HG21	1.63	0.80
1:Y:382:ARG:H	1:Y:386:GLN:HB3	1.46	0.80
1:B:287:LEU:O	1:R:191:ARG:NH1	2.14	0.80
1:C:191:ARG:NH1	1:P:287:LEU:O	2.14	0.80
1:G:331:MET:HB3	1:c:190:MET:HE1	1.64	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	1.63	0.79
1:L:336:VAL:O	1:L:408:ARG:NH2	2.15	0.79
1:J:382:ARG:H	1:J:386:GLN:HB3	1.48	0.79
1:F:191:ARG:NH1	1:d:287:LEU:O	2.16	0.79
1:Q:382:ARG:H	1:Q:386:GLN:HB3	1.46	0.79
1:O:401:ILE:O	1:O:575:LYS:NZ	2.15	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:W:287:LEU:O	1:b:191:ARG:NH1	2.16	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:J:96:MET:HG2	1:J:220:PRO:HA	1.65	0.78
1:N:158:THR:O	1:N:159:GLN:HB3	1.82	0.78
1:I:191:ARG:NH1	1:V:287:LEU:O	2.17	0.78
1:a:96:MET:HG2	1:a:220:PRO:HA	1.65	0.78
1:F:401:ILE:O	1:F:575:LYS:NZ	2.16	0.78
1:K:193:GLU:HB3	1:K:206:THR:HG21	1.63	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: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:Y:554:ASN:HD22	1:Y:557:ASN:HD22	1.29	0.77
1:G:131:ASN:ND2	1:d:550:GLN:OE1	2.16	0.77
1:H:96:MET:HG2	1:H:220:PRO:HA	1.65	0.77
1:L:193:GLU:HB3	1:L:206:THR:HG21	1.66	0.77
1:d:207:PRO:O	1:d:209:ARG:NH1	2.17	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:S:401:ILE:O	1:S:575:LYS:NZ	2.17	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:A:193:GLU:HB3	1:A:206:THR:HG21	1.67	0.76
1:B:348:SER:O	1:B:350:GLN:N	2.18	0.76
1:X:348:SER:O	1:X:350:GLN:N	2.18	0.76
1:E:191:ARG:NH1	1:I:287:LEU:O	2.18	0.76
1:J:554:ASN:HB3	1:J:557:ASN:HB3	1.66	0.76
1:A:159:GLN:C	1:A:161:PRO:HA	2.11	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: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:Q:361:ARG:NH2	1:Q:364:ALA:O	2.18	0.76
1:H:287:LEU:O	1:W:191:ARG:NH1	2.18	0.76
1:c:554:ASN:HB3	1:c:557:ASN:HB3	1.66	0.76
1:b:154:SER:HA	1:b:155:GLU:HB3	1.67	0.76
1:M:96:MET:HG2	1:M:220:PRO:HA	1.67	0.76
1:Z:554:ASN:HB3	1:Z:557:ASN:HB3	1.68	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:P:369:ASN:O	1:P:371:ALA:N	2.18	0.75
1:Z:381:GLY:O	1:Z:383:GLN:N	2.20	0.75
1:c:348:SER:O	1:c:350:GLN:N	2.20	0.75
1:Z:369:ASN:O	1:Z:371:ALA:N	2.19	0.75
1:E:382:ARG:H	1:E:386:GLN:HB3	1.52	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:554:ASN:HD22	1:O:557:ASN:HD22	1.34	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:I:401:ILE:O	1:I:575:LYS:NZ	2.20	0.74
1:Z:46:ASN:ND2	1:Z:64:ASN:HD22	1.84	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:Y:554:ASN:HB3	1:Y:557:ASN:HB3	1.70	0.74
1:E:96:MET:HG2	1:E:220:PRO:HA	1.68	0.74
1:Q:159:GLN:C	1:Q:161:PRO:HA	2.13	0.74
1:B:554:ASN:HB3	1:B:557:ASN:HB3	1.68	0.74
1:b:348:SER:O	1:b:350:GLN:N	2.19	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:P:348:SER:O	1:P:350:GLN:N	2.20	0.74
1:b:382:ARG:H	1:b:386:GLN:HB3	1.52	0.74
1:T:193:GLU:HB3	1:T:206:THR:HG21	1.69	0.74
1:Y:159:GLN:C	1:Y:161:PRO:HA	2.12	0.74
1:B:382:ARG:H	1:B:386:GLN:HB3	1.52	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:159:GLN:C	1:c:161:PRO:HA	2.14	0.73
1:G:287:LEU:O	1:c:191:ARG:NH1	2.22	0.73
1:b:56:ASN:OD1	1:b:58:TRP:HD1	1.70	0.73
1:N:193:GLU:HB3	1:N:206:THR:HG21	1.70	0.73
1:C:554:ASN:HB3	1:C:557:ASN:HB3	1.70	0.73
1:G:105:ILE:C	1:G:209:ARG:HD3	2.12	0.73
1:b:193:GLU:HB3	1:b:206:THR:HG21	1.69	0.73
1:D:361:ARG:NH2	1:D:405:ASP:HB3	2.02	0.73
1:a:348:SER:O	1:a:350:GLN:N	2.20	0.73
1:B:415:ILE:HD12	1:R:447:ILE:HG22	1.70	0.73
1:W:159:GLN:C	1:W:161:PRO:HA	2.12	0.73
1:X:336:VAL:O	1:X:408:ARG:NH2	2.21	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:D:348:SER:O	1:D:350:GLN:N	2.21	0.73
1:G:348:SER:O	1:G:350:GLN:N	2.21	0.73
1:R:348:SER:O	1:R:350:GLN:N	2.21	0.73
1:S:336:VAL:O	1:S:408:ARG:NH2	2.21	0.73
1:S:348:SER:O	1:S:350:GLN:N	2.22	0.73
1:A:554:ASN:HB3	1:A:557:ASN:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:159:GLN:C	1:L:161:PRO:HA	2.14	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:D:382:ARG:H	1:D:386:GLN:HB3	1.53	0.72
1:H:581:ARG:NH1	1:W:475:ASP:O	2.23	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:O:382:ARG:N	1:O:386:GLN:HB2	2.05	0.72
1:d:159:GLN:HB2	1:d:160:PRO:HD2	1.71	0.72
1:J:348:SER:O	1:J:350:GLN:N	2.23	0.71
1:F:96:MET:HG2	1:F:220:PRO:HA	1.71	0.71
1:H:369:ASN:O	1:H:371:ALA:N	2.23	0.71
1:U:154:SER:CA	1:U:155:GLU:HB2	2.20	0.71
1:d:336:VAL:O	1:d:408:ARG:NH2	2.23	0.71
1:d:348:SER:O	1:d:350:GLN:N	2.22	0.71
1:Y:381:GLY:O	1:Y:383:GLN:N	2.24	0.71
1:a:153:VAL:HG12	1:a:163:LYS:HE2	1.71	0.71
1:b:368:GLU:HG3	1:b:369:ASN:N	2.05	0.71
1:B:475:ASP:O	1:M:581:ARG:NH1	2.23	0.71
1:P:159:GLN:HE22	1:R:161:PRO:HB3	1.55	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	2.24	0.71
1:D:387:LYS:HD2	1:D:570:LYS:HE2	1.73	0.71
1:W:368:GLU:HG2	1:W:369:ASN:N	2.04	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:Y:369:ASN:O	1:Y:371:ALA:N	2.22	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:N:415:ILE:HD12	1:S:447:ILE:HG22	1.72	0.71
1:N:581:ARG:NH1	1:S:475:ASP:O	2.24	0.71
1:K:131:ASN:ND2	1:R:550:GLN:OE1	2.24	0.71
1:E:280:GLN:NE2	1:E:583:LEU:H	1.89	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:O:159:GLN:C	1:O:161:PRO:HA	2.16	0.71
1:c:207:PRO:O	1:c:209:ARG:NH1	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:381:GLY:O	1:Q:383:GLN:N	2.24	0.70
1:F:554:ASN:HB3	1:F:557:ASN:HB3	1.73	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:R:154:SER:CA	1:R:155:GLU:HG3	2.19	0.70
1:T:96:MET:HG2	1:T:220:PRO:HA	1.73	0.70
1:W:554:ASN:HB3	1:W:557:ASN:HB3	1.72	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:b:554:ASN:HB3	1:b:557:ASN:HB3	1.72	0.70
1:L:381:GLY:O	1:L:383:GLN:N	2.24	0.70
1:T:348:SER:O	1:T:350:GLN:N	2.25	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	1.72	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:D:558:GLN:HE22	1:G:236:THR:HB	1.57	0.70
1:d:554:ASN:ND2	1:d:556:ASP:OD1	2.23	0.70
1:F:569:MET:HG2	1:F:570:LYS:H	1.56	0.70
1:K:348:SER:O	1:K:350:GLN:N	2.24	0.70
1:U:326:THR:H	1:U:329:THR:HB	1.57	0.70
1:Y:137:HIS:CE1	1:Y:272:PRO:HB3	2.26	0.70
1:C:492:ASN:OD1	1:C:493:ASN:N	2.24	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: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: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:W:131:ASN:ND2	1:a:550:GLN:OE1	2.22	0.70
1:Z:401:ILE:O	1:Z:575:LYS:NZ	2.25	0.70
1:A:154:SER:HA	1:A:155:GLU:HB2	1.72	0.70
1:Q:159:GLN:CD	1:Q:160:PRO:HD3	2.16	0.70
1:D:269:ASP:OD1	1:D:492:ASN:ND2	2.24	0.70
1:R:96:MET:HG2	1:R:220:PRO:HA	1.74	0.70
1:R:154:SER:HA	1:R:155:GLU:CG	2.19	0.70
1:V:348:SER:O	1:V:350:GLN:N	2.24	0.70
1:N:336:VAL:O	1:N:408:ARG:NH2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:46:ASN:HD22	1:Z:64:ASN:HD22	1.39	0.70
1:A:348:SER:O	1:A:350:GLN:N	2.25	0.69
1:G:159:GLN:C	1:G:161:PRO:HA	2.17	0.69
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:C:96:MET:HG2	1:C:220:PRO:HA	1.73	0.69
1:D:381:GLY:O	1:D:383:GLN:N	2.25	0.69
1:W:348:SER:O	1:W:350:GLN:N	2.25	0.69
1:H:447:ILE:HG22	1:b:415:ILE:HD12	1.75	0.69
1:K:287:LEU:HG	1:T:209:ARG:HH12	1.56	0.69
1:O:96:MET:HG2	1:O:220:PRO:HA	1.73	0.69
1:C:370:GLN:CD	1:C:370:GLN:H	1.99	0.69
1:H:381:GLY:O	1:H:383:GLN:N	2.25	0.69
1:H:408:ARG:NH1	1:W:346:GLU:OE1	2.25	0.69
1:A:475:ASP:O	1:T:581:ARG:NH1	2.25	0.69
1:Q:348:SER:O	1:Q:350:GLN:N	2.26	0.69
1:C:159:GLN:C	1:C:161:PRO:HA	2.18	0.69
1:C:369:ASN:C	1:C:371:ALA:H	2.00	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
1:E:348:SER:O	1:E:350:GLN:N	2.25	0.69
1:K:565:ASN:ND2	1:R:302:ASN:HB2	2.08	0.69
1:B:338:TYR:HE1	1:B:358:ALA:HB3	1.57	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: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:b:96:MET:HG2	1:b:220:PRO:HA	1.76	0.68
1:A:550:GLN:OE1	1:I:131:ASN:ND2	2.23	0.68
1:D:554:ASN:HB3	1:D:557:ASN:HB3	1.73	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:J:45:PHE:HB3	1:Q:252:VAL:HB	1.75	0.68
1:F:336:VAL:O	1:F:408:ARG:NH2	2.27	0.68
1:G:369:ASN:O	1:G:371:ALA:N	2.27	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:M:382:ARG:NH2	1:M:392:GLY:O	2.26	0.68
1:B:158:THR:O	1:B:159:GLN:HB3	1.94	0.68
1:D:159:GLN:HG2	1:D:160:PRO:CD	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:159:GLN:C	1:H:161:PRO:HA	2.18	0.68
1:K:159:GLN:C	1:K:161:PRO:HA	2.19	0.68
1:c:382:ARG:H	1:c:386:GLN:HB3	1.57	0.68
1:O:45:PHE:HB3	1:P:252:VAL:HB	1.76	0.68
1:S:137:HIS:CE1	1:S:272:PRO:HB3	2.28	0.68
1:W:381:GLY:O	1:W:383:GLN:N	2.27	0.68
1:b:137:HIS:CE1	1:b:272:PRO:HB3	2.29	0.68
1:A:387:LYS:NZ	1:I:298:GLU:OE1	2.26	0.68
1:Q:566:ILE:HG22	1:Q:567:GLY:H	1.58	0.68
1:K:336:VAL:O	1:K:408:ARG:NH2	2.27	0.68
1:T:401:ILE:O	1:T:575:LYS:NZ	2.26	0.68
1:N:252:VAL:HB	1:Q:45:PHE:HB3	1.75	0.67
1:K:59:VAL:HG21	1:K:133:MET:HE2	1.76	0.67
1:M:447:ILE:HG22	1:R:415:ILE:HD12	1.75	0.67
1:X:361:ARG:NH1	1:X:363:GLY:O	2.26	0.67
1:Z:203:THR:OG1	1:Z:204:ILE:N	2.26	0.67
1:c:377:ARG:HH21	1:c:397:ARG:HD2	1.59	0.67
1:C:381:GLY:O	1:C:383:GLN:N	2.27	0.67
1:F:381:GLY:O	1:F:383:GLN:N	2.27	0.67
1:H:558:GLN:HE22	1:I:236:THR:HB	1.59	0.67
1:I:553:ILE:CA	1:I:554:ASN:HB2	2.20	0.67
1:L:369:ASN:O	1:L:371:ALA:N	2.27	0.67
1:B:369:ASN:O	1:B:371:ALA: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:b:59:VAL:HG21	1:b:133:MET:HE2	1.76	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:C:435:PRO:HB3	1:C:439:LYS:O	1.95	0.67
1:W:368:GLU:HG2	1:W:369:ASN:H	1.60	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:R:508:ASN:C	1:R:508:ASN:HD22	2.03	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:L:553:ILE:CA	1:L:554:ASN:HB2	2.21	0.67
1:N:550:GLN:HA	1:N:578:LEU:HD23	1.77	0.66
1:G:569:MET:HG2	1:G:570:LYS:H	1.60	0.66
1:L:131:ASN:ND2	1:b:550:GLN:OE1	2.27	0.66
1:T:336:VAL:O	1:T:408:ARG:NH2	2.27	0.66
1:G:336:VAL:O	1:G:408:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:382:ARG:N	1:P:386:GLN:HB3	2.04	0.66
1:Z:553:ILE:CA	1:Z:554:ASN:HB2	2.19	0.66
1:F:554:ASN:HD22	1:F:557:ASN:HD22	1.43	0.66
1:O:554:ASN:HB3	1:O:557:ASN:HB3	1.76	0.66
1:T:154:SER:HA	1:T:155:GLU:HB3	1.77	0.66
1:F:415:ILE:HD12	1:L:447:ILE:HG22	1.78	0.66
1:M:554:ASN:HB3	1:M:557:ASN:HB3	1.78	0.66
1:B:77:GLU:HB2	1:B:518:MET:HE1	1.77	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:b:581:ARG:O	1:b:582:LYS:HB2	1.96	0.66
1:d:203:THR:OG1	1:d:204:ILE:N	2.26	0.66
1:d:460:VAL:HG11	1:d:484:VAL:HA	1.77	0.66
1:F:131:ASN:ND2	1:M:550:GLN:OE1	2.28	0.66
1:L:581:ARG:NH1	1:d:475:ASP:O	2.29	0.66
1:Y:348:SER:O	1:Y:350:GLN:N	2.27	0.66
1:J:159:GLN:C	1:J:161:PRO:HA	2.20	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: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
1:R:336:VAL:O	1:R:408:ARG:NH2	2.28	0.66
1:a:554:ASN:HB3	1:a:557:ASN:HB3	1.76	0.66
1:a:556:ASP:O	1:a:558:GLN:N	2.25	0.66
1:K:154:SER:HA	1:K:155:GLU:CB	2.24	0.65
1:B:381:GLY:O	1:B:383:GLN:N	2.28	0.65
1:A:471:ASP:OD1	1:T:584:TYR:OH	2.12	0.65
1:G:381:GLY:O	1:G:383:GLN:N	2.30	0.65
1:G:369:ASN:HB3	1:G:372:ALA:HB3	1.78	0.65
1:A:566:ILE:HG22	1:A:567:GLY:H	1.61	0.65
1:D:554:ASN:HD22	1:D:557:ASN:HD22	1.44	0.65
1:a:159:GLN:C	1:a:161:PRO:HA	2.22	0.65
1:A:369:ASN:O	1:A:371:ALA:N	2.30	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:W:415:ILE:HD12	1:b:447:ILE:HG22	1.77	0.65
1:b:381:GLY:O	1:b:383:GLN:N	2.30	0.65
1:E:193:GLU:OE1	1:E:209:ARG:NH2	2.30	0.65
1:F:319:MET:HE2	1:L:354:LYS:HD2	1.78	0.65
1:F:361:ARG:NH1	1:F:363:GLY:O	2.29	0.65
1:F:581:ARG:NH1	1:L:475:ASP:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:216:ARG:NH1	1:I:231:ASN:OD1	2.27	0.65
1:L:297:SER:O	1:b:565:ASN:ND2	2.29	0.65
1:P:96:MET:HG2	1:P:220:PRO:HA	1.78	0.65
1:c:280:GLN:HG3	1:c:583:LEU:HB2	1.79	0.65
1:d:517:ASN:HD22	1:d:517:ASN:C	2.05	0.65
1:A:336:VAL:O	1:A:408:ARG:NH2	2.30	0.65
1:E:159:GLN:C	1:E:161:PRO:HA	2.22	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:R:369:ASN:O	1:R:371:ALA:N	2.30	0.65
1:Y:581:ARG:O	1:Y:582:LYS:HB2	1.95	0.65
1:E:565:ASN:N	1:E:565:ASN:OD1	2.30	0.64
1:N:581:ARG:O	1:N:582:LYS:HB2	1.96	0.64
1:B:569:MET:HG2	1:B:570:LYS:H	1.62	0.64
1:G:77:GLU:HB2	1:G:518:MET:HE1	1.78	0.64
1:I:425:THR:HG22	1:I:427:ASP:N	2.12	0.64
1:I:566:ILE:HG22	1:I:567:GLY:H	1.61	0.64
1:U:377:ARG:NH2	1:U:397:ARG:HD2	2.11	0.64
1:c:381:GLY:O	1:c:383:GLN:N	2.29	0.64
1:E:435:PRO:HB3	1:E:439:LYS:O	1.97	0.64
1:H:561:TYR:OH	1:H:574:GLU:OE2	2.14	0.64
1:K:581:ARG:NH1	1:T:475:ASP:O	2.30	0.64
1:D:326:THR:H	1:D:329:THR:HB	1.63	0.64
1:P:70:HIS:ND1	1:R:510:TYR:HB3	2.11	0.64
1:V:558:GLN:HE22	1:W:236:THR:HB	1.61	0.64
1:Y:56:ASN:CG	1:Y:58:TRP:HD1	2.06	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
1:C:451:TYR:CD2	1:P:452:GLY:HA2	2.32	0.64
1:K:566:ILE:HG22	1:K:567:GLY:H	1.61	0.64
1:K:155:GLU:HA	1:K:163:LYS:HZ3	1.61	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:A:415:ILE:HD12	1:K:447:ILE:HG22	1.79	0.64
1:N:216:ARG:NH1	1:N:231:ASN:OD1	2.30	0.64
1:B:550:GLN:OE1	1:P:131:ASN:ND2	2.22	0.64
1:I:422:LEU:HA	1:I:423:PRO:C	2.22	0.64
1:R:382:ARG:H	1:R:386:GLN:HB3	1.63	0.64
1:U:581:ARG:O	1:U:582:LYS:HB2	1.96	0.64
1:W:131:ASN:HB3	1:W:550:GLN:NE2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:203:THR:OG1	1:W:204:ILE:N	2.30	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:E:381:GLY:O	1:E:383:GLN:N	2.31	0.64
1:Q:159:GLN:NE2	1:Q:160:PRO:HD3	2.13	0.64
1:Q:460:VAL:HG11	1:Q:484:VAL:HA	1.80	0.64
1:U:317:THR:HG21	1:U:329:THR:HG22	1.78	0.64
1:W:584:TYR:OH	1:b:471:ASP:OD1	2.15	0.64
1:Z:460:VAL:HG11	1:Z:484:VAL:HA	1.80	0.64
1:M:155:GLU:H	1:M:156:SER:HB3	1.63	0.64
1:E:131:ASN:O	1:E:550:GLN:NE2	2.31	0.63
1:Q:569:MET:HG2	1:Q:570:LYS:H	1.63	0.63
1:B:447:ILE:HG22	1:M:415:ILE:HD12	1.78	0.63
1:M:159:GLN:C	1:M:161:PRO:HA	2.23	0.63
1:O:381:GLY:O	1:O:383:GLN:N	2.31	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	1.97	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:B:159:GLN:CD	1:B:160:PRO:HD2	2.22	0.63
1:B:581:ARG:O	1:B:582:LYS:HB2	1.98	0.63
1:I:79:TYR:OH	1:I:247:GLU:OE1	2.15	0.63
1:P:566:ILE:HG22	1:P:567:GLY:H	1.62	0.63
1:W:369:ASN:O	1:W:371:ALA:N	2.31	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	2.27	0.63
1:c:556:ASP:O	1:c:558:GLN:N	2.27	0.63
1:E:471:ASP:OD1	1:I:584:TYR:OH	2.16	0.63
1:N:460:VAL:HG11	1:N:484:VAL:HA	1.81	0.63
1:C:447:ILE:HG22	1:P:415:ILE:HD12	1.80	0.63
1:V:566:ILE:HG22	1:V:567:GLY:H	1.63	0.63
1:c:317:THR:HG22	1:c:330:ILE:HA	1.80	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: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:Y:475:ASP:O	1:a:581:ARG:NH1	2.32	0.63
1:O:553:ILE:CA	1:O:554:ASN:HB2	2.24	0.63
1:Y:422:LEU:HA	1:Y:423:PRO:C	2.24	0.63
1:J:447:ILE:HG22	1:U:415:ILE:HD12	1.80	0.63
1:B:556:ASP:O	1:B:558:GLN:N	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:581:ARG:NH1	1:c:475:ASP:O	2.32	0.63
1:I:361:ARG:NH1	1:I:363:GLY:O	2.32	0.63
1:K:216:ARG:NH1	1:K:231:ASN:OD1	2.28	0.63
1:X:561:TYR:OH	1:X:574:GLU:OE2	2.15	0.63
1:E:280:GLN:HE21	1:E:583:LEU:H	1.47	0.62
1:F:236:THR:HB	1:G:558:GLN:HE22	1.63	0.62
1:X:411:GLU:OE1	1:X:411:GLU:N	2.31	0.62
1:a:336:VAL:O	1:a:408:ARG:NH2	2.32	0.62
1:d:381:GLY:O	1:d:383:GLN:N	2.32	0.62
1:J:369:ASN:O	1:J:371:ALA:N	2.30	0.62
1:F:59:VAL:HG21	1:F:133:MET:HE2	1.81	0.62
1:H:415:ILE:HD12	1:W:447:ILE:HG22	1.81	0.62
1:A:569:MET:HG2	1:A:570:LYS:H	1.64	0.62
1:B:252:VAL:HB	1:F:45:PHE:HB3	1.81	0.62
1:D:460:VAL:HG11	1:D:484:VAL:HA	1.81	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:b:203:THR:OG1	1:b:204:ILE:N	2.30	0.62
1:c:435:PRO:HB3	1:c:439:LYS:O	1.98	0.62
1:F:460:VAL:HG11	1:F:484:VAL:HA	1.82	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:B:460:VAL:HG11	1:B:484:VAL:HA	1.80	0.62
1:L:383:GLN:HB3	1:L:384:HIS:HD2	1.64	0.62
1:T:381:GLY:O	1:T:383:GLN:N	2.33	0.62
1:D:159:GLN:C	1:D:161:PRO:HA	2.24	0.62
1:I:45:PHE:HB3	1:K:252:VAL:HB	1.82	0.62
1:U:257:THR:HG22	1:V:256:ARG:HH12	1.64	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:A:365:GLN:HG2	1:A:366:THR:HG23	1.81	0.62
1:A:553:ILE:CA	1:A:554:ASN:HB2	2.24	0.62
1:B:553:ILE:CA	1:B:554:ASN:HB2	2.24	0.62
1:H:434:ASP:OD2	1:W:439:LYS:NZ	2.23	0.62
1:I:338:TYR:HE1	1:I:358:ALA:HB3	1.65	0.62
1:V:159:GLN:C	1:V:161:PRO:HA	2.24	0.62
1:B:131:ASN:ND2	1:P:550:GLN:OE1	2.26	0.62
1:F:550:GLN:OE1	1:M:131:ASN:ND2	2.28	0.62
1:K:476:THR:O	1:K:479:LYS:HE2	2.00	0.62
1:V:554:ASN:HB3	1:V:557:ASN:HB3	1.81	0.62
1:A:422:LEU:HA	1:A:423:PRO:C	2.24	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:MET:HE2	1:d:414:TRP:CE2	2.34	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: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:b:569:MET:HG2	1:b:570:LYS:H	1.65	0.62
1:c:566:ILE:HG22	1:c:567:GLY:H	1.64	0.62
1:E:154:SER:HA	1:E:155:GLU:CB	2.29	0.61
1:R:157:ALA:HA	1:R:158:THR:OG1	1.99	0.61
1:G:104:GLU:HG2	1:G:209:ARG:CD	2.30	0.61
1:K:381:GLY:O	1:K:383:GLN:N	2.33	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:T:382:ARG:NH2	1:T:392:GLY:O	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	1.66	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:M:369:ASN:O	1:M:371:ALA:N	2.33	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: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:A:565:ASN:ND2	1:I:302:ASN:O	2.33	0.61
1:N:297:SER:O	1:N:302:ASN:ND2	2.28	0.61
1:P:558:GLN:HE22	1:R:236:THR:HB	1.65	0.61
1:Y:336:VAL:O	1:Y:408:ARG:NH2	2.33	0.61
1:N:435:PRO:HB3	1:N:439:LYS:O	2.00	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:D:203:THR:OG1	1:D:204:ILE:N	2.33	0.61
1:Y:354:LYS:HD2	1:a:319:MET:HE2	1.83	0.61
1:Y:569:MET:HG2	1:Y:570:LYS:H	1.65	0.61
1:Z:566:ILE:HG22	1:Z:567:GLY:H	1.64	0.61
1:S:159:GLN:HG3	1:S:160:PRO:HD2	1.83	0.61
1:c:541:ALA:O	1:c:543:HIS:NE2	2.34	0.61
1:d:479:LYS:HD2	1:d:491:GLN:HE22	1.65	0.61
1:E:434:ASP:OD2	1:V:439:LYS:NZ	2.23	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:207:PRO:O	1:S:209:ARG:NH1	2.33	0.61
1:c:269:ASP:HB3	1:c:492:ASN:ND2	2.16	0.61
1:E:408:ARG:NH1	1:V:346:GLU:OE1	2.33	0.60
1:Q:361:ARG:NH1	1:Q:363:GLY:O	2.34	0.60
1:P:432:PRO:O	1:P:443:ASN:ND2	2.26	0.60
1:E:422:LEU:HA	1:E:423:PRO:C	2.26	0.60
1:Q:422:LEU:HA	1:Q:423:PRO:C	2.25	0.60
1:D:422:LEU:HA	1:D:423:PRO:C	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:E:415:ILE:HD12	1:V:447:ILE:HG22	1.82	0.60
1:C:566:ILE:HG22	1:C:567:GLY:H	1.66	0.60
1:G:550:GLN:HA	1:G:578:LEU:HD23	1.83	0.60
1:d:159:GLN:C	1:d:161:PRO:HA	2.25	0.60
1:J:203:THR:OG1	1:J:204:ILE:N	2.34	0.60
1:N:556:ASP:O	1:N:558:GLN:N	2.31	0.60
1:F:476:THR:HB	1:d:457:LEU:O	2.01	0.60
1:X:93:ASN:ND2	1:X:225:THR:O	2.34	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:E:475:ASP:O	1:I:581:ARG:NH1	2.35	0.60
1:Q:216:ARG:NH1	1:Q:231:ASN:OD1	2.29	0.60
1:D:59:VAL:HG21	1:D:133:MET:HE2	1.82	0.60
1:I:425:THR:HB	1:I:428:ASN:HB2	1.81	0.60
1:M:361:ARG:NH1	1:M:363:GLY:O	2.34	0.60
1:C:269:ASP:CG	1:C:492:ASN:HD22	2.10	0.60
1:G:382:ARG:NH2	1:G:392:GLY:O	2.34	0.60
1:c:99:ASP:CG	1:c:216:ARG:HH21	2.10	0.60
1:N:584:TYR:OH	1:S:471:ASP:OD1	2.18	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:Y:56:ASN:OD1	1:Y:58:TRP:HD1	1.85	0.60
1:G:432:PRO:O	1:G:443:ASN:ND2	2.34	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:P:159:GLN:NE2	1:R:159:GLN:H	1.98	0.60
1:X:550:GLN:HA	1:X:578:LEU:HD23	1.84	0.60
1:c:422:LEU:HA	1:c:423:PRO:C	2.27	0.60
1:N:377:ARG:NH2	1:N:397:ARG:HD2	2.17	0.60
1:B:193:GLU:HB3	1:B:206:THR:HG21	1.83	0.60
1:C:45:PHE:HB3	1:D:252:VAL:HB	1.84	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:P:435:PRO:HB3	1:P:439:LYS:O	2.01	0.60
1:S:553:ILE:CA	1:S:554:ASN:HB2	2.27	0.60
1:W:452:GLY:HA2	1:b:451:TYR:CD2	2.37	0.60
1:b:159:GLN:C	1:b:161:PRO:HA	2.27	0.60
1:C:476:THR:O	1:C:479:LYS:HE2	2.02	0.60
1:R:569:MET:HG2	1:R:570:LYS:H	1.67	0.60
1:U:317:THR:HG22	1:U:330:ILE:HA	1.82	0.60
1:W:277:HIS:ND1	1:W:577:GLN:O	2.30	0.60
1:X:137:HIS:CE1	1:X:272:PRO:HB3	2.36	0.60
1:Y:471:ASP:OD1	1:a:584:TYR:OH	2.16	0.60
1:E:569:MET:HG2	1:E:570:LYS:H	1.66	0.59
1:R:216:ARG:NH1	1:R:231:ASN:OD1	2.32	0.59
1:R:550:GLN:HA	1:R:578:LEU:HD23	1.83	0.59
1:C:556:ASP:O	1:C:558:GLN:N	2.30	0.59
1:H:319:MET:HE2	1:W:354:LYS:HD2	1.84	0.59
1:P:158:THR:O	1:P:159:GLN:HB2	2.02	0.59
1:U:422:LEU:HA	1:U:423:PRO:C	2.27	0.59
1:U:558:GLN:HE22	1:V:236:THR:HB	1.66	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:S:59:VAL:HG21	1:S:133:MET:HE2	1.85	0.59
1:Y:556:ASP:O	1:Y:558:GLN:N	2.30	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:D:127:GLN:HG3	1:D:551:MET:HE2	1.85	0.59
1:F:252:VAL:HB	1:G:45:PHE:HB3	1.83	0.59
1:K:155:GLU:HG2	1:K:163:LYS:HZ1	1.67	0.59
1:O:252:VAL:HB	1:S:45:PHE:HB3	1.84	0.59
1:T:157:ALA:HA	1:T:158:THR:OG1	2.03	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:M:155:GLU:H	1:M:156:SER:CB	2.16	0.59
1:V:553:ILE:HA	1:V:554:ASN:CB	2.32	0.59
1:a:127:GLN:HG3	1:a:551:MET:HE2	1.84	0.59
1:b:377:ARG:HH21	1:b:397:ARG:HD2	1.68	0.59
1:d:361:ARG:NH1	1:d:363:GLY:O	2.34	0.59
1:A:297:SER:O	1:A:302:ASN:ND2	2.36	0.59
1:C:581:ARG:O	1:C:582:LYS:HB2	2.01	0.59
1:G:131:ASN:O	1:G:550:GLN:NE2	2.36	0.59
1:H:236:THR:HB	1:L:558:GLN:HE22	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:443:ASN:OD1	1:P:446:ASN:ND2	2.35	0.59
1:P:476:THR:O	1:P:479:LYS:HE2	2.03	0.59
1:U:377:ARG:HH21	1:U:397:ARG:HD2	1.68	0.59
1:Y:560:ASN:HB3	1:Y:572:VAL:HG21	1.84	0.59
1:A:439:LYS:NZ	1:T:434:ASP:OD2	2.25	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:T:422:LEU:HA	1:T:423:PRO:C	2.26	0.59
1:c:216:ARG:NH1	1:c:231:ASN:OD1	2.33	0.59
1:F:581:ARG:O	1:F:582:LYS:HB2	2.02	0.59
1:I:336:VAL:O	1:I:408:ARG:NH2	2.35	0.59
1:K:492:ASN:ND2	1:K:493:ASN:OD1	2.36	0.59
1:Z:558:GLN:HE22	1:a:236:THR:HB	1.67	0.59
1:A:447:ILE:HG22	1:T:415:ILE:HD12	1.84	0.59
1:F:556:ASP:O	1:F:558:GLN:N	2.33	0.59
1:K:415:ILE:HD12	1:T:447:ILE:HG22	1.85	0.59
1:X:238:PRO:HA	1:X:241:VAL:HG23	1.85	0.59
1:G:79:TYR:OH	1:G:247:GLU:OE1	2.19	0.58
1:a:154:SER:HA	1:a:155:GLU:CB	2.30	0.58
1:b:154:SER:HA	1:b:155:GLU:CB	2.31	0.58
1:E:331:MET:HB3	1:V:190:MET:HE1	1.85	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:B:417:ASN:ND2	1:R:441:GLY:O	2.31	0.58
1:U:59:VAL:HG21	1:U:133:MET:HE2	1.84	0.58
1:H:569:MET:HG2	1:H:570:LYS:H	1.68	0.58
1:O:77:GLU:HB2	1:O:518:MET:HE1	1.86	0.58
1:S:252:VAL:HB	1:T:45:PHE:HB3	1.85	0.58
1:Y:137:HIS:HD2	1:Y:536:LYS:HE3	1.68	0.58
1:Y:400:TYR:CE2	1:Y:575:LYS:HA	2.38	0.58
1:a:381:GLY:O	1:a:383:GLN:N	2.36	0.58
1:d:96:MET:HG2	1:d:220:PRO:HA	1.84	0.58
1:L:566:ILE:HG22	1:L:567:GLY:H	1.67	0.58
1:P:556:ASP:O	1:P:558:GLN:N	2.28	0.58
1:U:336:VAL:O	1:U:408:ARG:NH2	2.35	0.58
1:Y:447:ILE:HG22	1:a:415:ILE:HD12	1.85	0.58
1:b:411:GLU:OE1	1:b:411:GLU:N	2.34	0.58
1:d:569:MET:HG2	1:d:570:LYS:H	1.67	0.58
1:J:422:LEU:HA	1:J:423:PRO:C	2.27	0.58
1:F:333:PRO:HG2	1:L:474:PHE:HZ	1.69	0.58
1:G:194:THR:H	1:G:384:HIS:HE1	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:SER:OG	1:G:302:ASN:ND2	2.37	0.58
1:L:203:THR:OG1	1:L:204:ILE:N	2.36	0.58
1:O:154:SER:HA	1:O:155:GLU:CG	2.33	0.58
1:d:59:VAL:HG21	1:d:133:MET:HE2	1.84	0.58
1:E:333:PRO:HG2	1:V:474:PHE:HZ	1.68	0.58
1:F:216:ARG:NH1	1:F:231:ASN:OD1	2.34	0.58
1:M:336:VAL:O	1:M:408:ARG:NH2	2.36	0.58
1:R:422:LEU:HA	1:R:423:PRO:C	2.28	0.58
1:V:52:LYS:HE3	1:V:60:TYR:CD2	2.39	0.58
1:d:435:PRO:HB3	1:d:439:LYS:O	2.03	0.58
1:B:401:ILE:O	1:B:575:LYS:NZ	2.37	0.58
1:C:363:GLY:HA3	1:C:367:ASP:O	2.04	0.58
1:L:236:THR:HB	1:M:558:GLN:NE2	2.19	0.58
1:a:59:VAL:HG21	1:a:133:MET:HE2	1.84	0.58
1:J:476:THR:O	1:J:479:LYS:HE2	2.03	0.58
1:N:573:TYR:C	1:N:574:GLU:HG2	2.27	0.58
1:C:155:GLU:HG3	1:C:156:SER:N	2.19	0.58
1:P:422:LEU:HA	1:P:423:PRO:C	2.28	0.58
1:T:77:GLU:HB2	1:T:518:MET:HE1	1.84	0.58
1:X:401:ILE:O	1:X:575:LYS:NZ	2.36	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:S:276:THR:HG22	1:S:579:ALA:HB3	1.84	0.58
1:c:271:LYS:HG2	1:c:272:PRO:HD2	1.84	0.58
1:G:216:ARG:NH1	1:G:231:ASN:OD1	2.33	0.57
1:K:274:ARG:NH1	1:T:475:ASP:OD1	2.36	0.57
1:M:317:THR:HG22	1:M:330:ILE:HA	1.85	0.57
1:O:319:MET:HE3	1:O:329:THR:HG23	1.84	0.57
1:P:460:VAL:HG11	1:P:484:VAL:HA	1.85	0.57
1:T:159:GLN:CG	1:T:160:PRO:HD2	2.31	0.57
1:A:216:ARG:NH1	1:A:231:ASN:OD1	2.37	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:X:422:LEU:HA	1:X:423:PRO:C	2.29	0.57
1:F:248:ASN:HD22	1:G:122:ASN:HD22	1.52	0.57
1:U:159:GLN:CB	1:U:160:PRO:HD2	2.35	0.57
1:U:476:THR:O	1:U:479:LYS:HE2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:326:THR:H	1:a:329:THR:HB	1.68	0.57
1:b:368:GLU:CG	1:b:369:ASN:H	2.10	0.57
1:d:566:ILE:HG22	1:d:567:GLY:H	1.69	0.57
1:C:411:GLU:N	1:C:411:GLU:OE1	2.34	0.57
1:D:361:ARG:HH11	1:D:361:ARG:C	2.12	0.57
1:G:96:MET:HG2	1:G:220:PRO:HA	1.85	0.57
1:G:422:LEU:HA	1:G:423:PRO:C	2.28	0.57
1:H:158:THR:HG22	1:H:159:GLN:HG3	1.85	0.57
1:P:369:ASN:C	1:P:371:ALA:H	2.11	0.57
1:a:476:THR:O	1:a:479:LYS:HE2	2.04	0.57
1:A:473:GLU:HG2	1:A:491:GLN:HG3	1.86	0.57
1:E:414:TRP:CE2	1:V:96:MET:HE2	2.40	0.57
1:N:338:TYR:HE1	1:N:358:ALA:HB3	1.69	0.57
1:H:287:LEU:HD12	1:H:288:PRO:HD2	1.86	0.57
1:c:460:VAL:HG11	1:c:484:VAL:HA	1.86	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:N:476:THR:O	1:N:479:LYS:HE2	2.05	0.57
1:I:435:PRO:HB3	1:I:439:LYS:O	2.05	0.57
1:K:422:LEU:HA	1:K:423:PRO:C	2.29	0.57
1:V:368:GLU:HG3	1:V:370:GLN:HE21	1.69	0.57
1:X:159:GLN:CG	1:X:160:PRO:HD2	2.31	0.57
1:E:154:SER:HA	1:E:155:GLU:HB3	1.87	0.57
1:E:431:LEU:HD22	1:V:220:PRO:HB2	1.86	0.57
1:B:59:VAL:HG21	1:B:133:MET:HE2	1.86	0.57
1:C:59:VAL:HG21	1:C:133:MET:HE2	1.87	0.57
1:D:382:ARG:HD2	1:G:513:ASP:O	2.05	0.57
1:F:333:PRO:HG2	1:L:474:PHE:CZ	2.40	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:W:422:LEU:HA	1:W:423:PRO:C	2.30	0.57
1:X:99:ASP:CG	1:X:216:ARG:HH21	2.13	0.57
1:X:553:ILE:CA	1:X:554:ASN:HB2	2.23	0.57
1:c:569:MET:HG2	1:c:570:LYS:H	1.68	0.57
1:d:556:ASP:O	1:d:558:GLN:N	2.33	0.57
1:A:581:ARG:NH1	1:K:475:ASP:O	2.38	0.57
1:E:319:MET:HE2	1:V:354:LYS:HD2	1.87	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:CG2	2.35	0.57
1:K:159:GLN:HB3	1:K:160:PRO:HD2	1.87	0.57
1:O:336:VAL:O	1:O:408:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:432:PRO:C	1:P:443:ASN:HD22	2.13	0.57
1:b:338:TYR:HE1	1:b:358:ALA:HB3	1.69	0.57
1:K:157:ALA:HA	1:K:158:THR:HG22	1.85	0.57
1:Q:476:THR:O	1:Q:479:LYS:HE2	2.05	0.56
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:C:422:LEU:HA	1:C:423:PRO:C	2.29	0.56
1:F:242:GLN:NE2	1:d:580:PRO:HB2	2.19	0.56
1:F:338:TYR:HE1	1:F:358:ALA:HB3	1.69	0.56
1:F:369:ASN:C	1:F:371:ALA:H	2.13	0.56
1:L:326:THR:H	1:L:329:THR:HB	1.70	0.56
1:P:77:GLU:HB2	1:P:518:MET:HE1	1.87	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:J:338:TYR:HE1	1:J:358:ALA:HB3	1.70	0.56
1:B:319:MET:HE2	1:R:354:LYS:HD2	1.86	0.56
1:C:558:GLN:HE22	1:D:236:THR:HB	1.70	0.56
1:F:349:THR:N	1:d:362:GLY:O	2.36	0.56
1:G:297:SER:O	1:G:302:ASN:ND2	2.35	0.56
1:G:426:ASP:OD2	1:c:222:HIS:NE2	2.39	0.56
1:O:422:LEU:HA	1:O:423:PRO:C	2.30	0.56
1:P:154:SER:HA	1:P:155:GLU:CB	2.35	0.56
1:P:362:GLY:N	1:P:368:GLU:OE2	2.31	0.56
1:R:159:GLN:C	1:R:161:PRO:HA	2.31	0.56
1:U:435:PRO:HB3	1:U:439:LYS:O	2.05	0.56
1:U:513:ASP:O	1:X:382:ARG:NH1	2.38	0.56
1:V:581:ARG:O	1:V:582:LYS:HB2	2.04	0.56
1:Y:247:GLU:OE1	1:Y:247:GLU:N	2.38	0.56
1:c:556:ASP:O	1:c:557:ASN:HB3	2.05	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:H:558:GLN:NE2	1:I:236:THR:HB	2.21	0.56
1:I:573:TYR:C	1:I:574:GLU:HG2	2.30	0.56
1:U:556:ASP:O	1:U:558:GLN:N	2.33	0.56
1:V:45:PHE:HB3	1:W:252:VAL:HB	1.86	0.56
1:a:435:PRO:HB3	1:a:439:LYS:O	2.05	0.56
1:E:383:GLN:HB3	1:E:384:HIS:HD2	1.70	0.56
1:Q:557:ASN:HD21	1:Q:561:TYR:HE2	1.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:569:MET:HG2	1:I:570:LYS:H	1.70	0.56
1:K:569:MET:HG2	1:K:570:LYS:H	1.69	0.56
1:O:556:ASP:O	1:O:558:GLN:N	2.31	0.56
1:W:566:ILE:HG22	1:W:567:GLY:H	1.70	0.56
1:Y:203:THR:OG1	1:Y:204:ILE:N	2.35	0.56
1:A:131:ASN:ND2	1:I:550:GLN:OE1	2.29	0.56
1:E:449:ASN:O	1:V:449:ASN:ND2	2.38	0.56
1:B:150:LEU:HD22	1:B:171:ALA:HB1	1.88	0.56
1:F:354:LYS:HD2	1:d:319:MET:HE2	1.86	0.56
1:H:203:THR:OG1	1:H:204:ILE:N	2.35	0.56
1:L:298:GLU:HA	1:b:565:ASN:HB3	1.86	0.56
1:L:422:LEU:HA	1:L:423:PRO:C	2.31	0.56
1:S:566:ILE:HG22	1:S:567:GLY:H	1.70	0.56
1:T:247:GLU:OE1	1:T:247:GLU:N	2.37	0.56
1:X:203:THR:OG1	1:X:204:ILE:N	2.36	0.56
1:X:252:VAL:HB	1:Y:45:PHE:HB3	1.87	0.56
1:E:203:THR:OG1	1:E:204:ILE:N	2.39	0.56
1:I:382:ARG:N	1:I:386:GLN:HB3	2.14	0.56
1:K:214:TRP:O	1:K:350:GLN:HG2	2.06	0.56
1:L:383:GLN:HB3	1:L:384:HIS:CD2	2.41	0.56
1:P:99:ASP:CG	1:P:216:ARG:HH21	2.13	0.56
1:R:572:VAL:HG12	1:R:573:TYR:O	2.05	0.56
1:A:319:MET:HE2	1:K:354:LYS:HD2	1.87	0.56
1:N:59:VAL:HG21	1:N:133:MET:HE2	1.87	0.56
1:Q:319:MET:HE3	1:Q:329:THR:HG23	1.87	0.56
1:B:346:GLU:OE1	1:M:408:ARG:NH1	2.39	0.56
1:B:435:PRO:HB3	1:B:439:LYS:O	2.06	0.56
1:I:127:GLN:HG3	1:I:551:MET:HE2	1.88	0.56
1:O:382:ARG:NH1	1:P:513:ASP:O	2.38	0.56
1:b:422:LEU:HA	1:b:423:PRO:C	2.31	0.56
1:A:558:GLN:HG2	1:A:558:GLN:O	2.05	0.56
1:F:422:LEU:HA	1:F:423:PRO:C	2.31	0.56
1:L:338:TYR:HE1	1:L:358:ALA:HB3	1.71	0.56
1:X:432:PRO:C	1:X:443:ASN:HD22	2.14	0.56
1:A:154:SER:HA	1:A:155:GLU:CB	2.36	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:L:415:ILE:HD12	1:d:447:ILE:HG22	1.88	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:c:377:ARG:NH2	1:c:397:ARG:HD2	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:475:ASP:O	1:d:581:ARG:NH1	2.39	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:L:319:MET:HE3	1:L:329:THR:HG23	1.87	0.55
1:O:361:ARG:HG2	1:O:401:ILE:HG22	1.87	0.55
1:a:566:ILE:HG22	1:a:567:GLY:H	1.71	0.55
1:d:326:THR:H	1:d:329:THR:HB	1.70	0.55
1:A:239:ASP:HB3	1:T:549:GLN:HE21	1.70	0.55
1:A:401:ILE:O	1:A:575:LYS:NZ	2.39	0.55
1:E:333:PRO:HG2	1:V:474:PHE:CZ	2.42	0.55
1:F:553:ILE:CA	1:F:554:ASN:HB2	2.33	0.55
1:G:383:GLN:HB3	1:G:384:HIS:CD2	2.40	0.55
1:H:553:ILE:CA	1:H:554:ASN:HB2	2.29	0.55
1:K:338:TYR:HE1	1:K:358:ALA:HB3	1.72	0.55
1:K:556:ASP:O	1:K:557:ASN:HB3	2.06	0.55
1:V:414:TRP:HE1	1:V:416:GLN:HE21	1.53	0.55
1:D:581:ARG:O	1:D:582:LYS:HB2	2.05	0.55
1:V:319:MET:HE3	1:V:329:THR:HG23	1.87	0.55
1:W:556:ASP:O	1:W:558:GLN:N	2.31	0.55
1:c:553:ILE:CA	1:c:554:ASN:HB2	2.28	0.55
1:d:338:TYR:HE1	1:d:358:ALA:HB3	1.71	0.55
1:B:137:HIS:CE1	1:B:272:PRO:HB3	2.41	0.55
1:B:354:LYS:HD2	1:M:319:MET:HE2	1.88	0.55
1:L:152:THR:HG23	1:L:168:ASP:HB2	1.89	0.55
1:W:159:GLN:OE1	1:W:160:PRO:HD3	2.06	0.55
1:W:565:ASN:HD22	1:a:298:GLU:HA	1.71	0.55
1:a:422:LEU:HA	1:a:423:PRO:C	2.31	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:B:154:SER:HA	1:B:155:GLU:CB	2.37	0.55
1:H:114:ALA:HB1	1:H:119:VAL:HG11	1.88	0.55
1:I:59:VAL:HG21	1:I:133:MET:HE2	1.88	0.55
1:O:154:SER:HA	1:O:155:GLU:CB	2.36	0.55
1:W:415:ILE:CD1	1:b:447:ILE:HG22	2.37	0.55
1:E:157:ALA:HA	1:E:158:THR:HB	1.88	0.55
1:E:159:GLN:CG	1:E:160:PRO:HD2	2.33	0.55
1:J:460:VAL:HG11	1:J:484:VAL:HA	1.89	0.55
1:N:266:PHE:HZ	1:N:493:ASN:O	1.90	0.55
1:L:271:LYS:H	1:L:271:LYS:HD2	1.71	0.55
1:S:159:GLN:C	1:S:161:PRO:HA	2.32	0.55
1:Y:177:LEU:HD22	1:Y:263:THR:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:553:ILE:CA	1:a:554:ASN:HB2	2.30	0.55
1:J:550:GLN:HA	1:J:578:LEU:HD23	1.87	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:X:460:VAL:HG11	1:X:484:VAL:HA	1.89	0.55
1:a:569:MET:HG2	1:a:570:LYS:H	1.71	0.55
1:b:382:ARG:HD2	1:d:513:ASP:O	2.06	0.55
1:A:584:TYR:OH	1:K:471:ASP:OD1	2.21	0.55
1:N:236:THR:HB	1:Q:558:GLN:NE2	2.21	0.55
1:F:159:GLN:CG	1:F:160:PRO:HD2	2.37	0.55
1:I:447:ILE:HG22	1:V:415:ILE:HD12	1.88	0.55
1:I:476:THR:O	1:I:479:LYS:HE2	2.06	0.55
1:P:203:THR:OG1	1:P:204:ILE:N	2.38	0.55
1:P:382:ARG:NH2	1:P:392:GLY:O	2.39	0.55
1:U:401:ILE:O	1:U:575:LYS:NZ	2.38	0.55
1:X:459:ASN:HD21	1:X:487:PRO:HA	1.70	0.55
1:J:127:GLN:HA	1:J:551:MET:HE3	1.87	0.55
1:N:203:THR:OG1	1:N:204:ILE:N	2.37	0.55
1:B:439:LYS:NZ	1:M:434:ASP:OD2	2.37	0.55
1:B:447:ILE:HG22	1:M:415:ILE:CD1	2.37	0.55
1:C:553:ILE:CA	1:C:554:ASN:HB2	2.27	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:R:556:ASP:O	1:R:557:ASN:HB3	2.07	0.55
1:d:369:ASN:C	1:d:371:ALA:H	2.13	0.55
1:D:297:SER:O	1:D:302:ASN:ND2	2.34	0.55
1:L:415:ILE:CD1	1:d:447:ILE:HG22	2.37	0.55
1:T:369:ASN:HB3	1:T:372:ALA:HB3	1.88	0.55
1:V:550:GLN:HA	1:V:578:LEU:HD23	1.88	0.55
1:Z:383:GLN:HB3	1:Z:384:HIS:CD2	2.42	0.55
1:E:476:THR:O	1:E:479:LYS:HE2	2.07	0.54
1:C:432:PRO:O	1:C:443:ASN:ND2	2.36	0.54
1:H:45:PHE:HB3	1:I:252:VAL:HB	1.88	0.54
1:K:52:LYS:HB3	1:K:60:TYR:HB3	1.89	0.54
1:K:331:MET:HB3	1:T:190:MET:HE1	1.89	0.54
1:R:137:HIS:CE1	1:R:272:PRO:HB3	2.43	0.54
1:U:238:PRO:HA	1:U:241:VAL:HG23	1.90	0.54
1:X:52:LYS:HE3	1:X:60:TYR:CD2	2.42	0.54
1:Z:155:GLU:HG2	1:Z:156:SER:H	1.72	0.54
1:c:317:THR:HG21	1:c:329:THR:HG22	1.89	0.54
1:C:88:ASP:OD1	1:C:89:LYS:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:153:VAL:HG13	1:O:163:LYS:HZ3	1.73	0.54
1:P:45:PHE:HB3	1:R:252:VAL:HB	1.88	0.54
1:U:256:ARG:NH1	1:X:257:THR:HG22	2.22	0.54
1:W:191:ARG:O	1:W:193:GLU:HG3	2.07	0.54
1:Z:581:ARG:O	1:Z:582:LYS:HB2	2.07	0.54
1:d:152:THR:HG23	1:d:168:ASP:HB2	1.89	0.54
1:B:159:GLN:C	1:B:161:PRO:HA	2.32	0.54
1:F:158:THR:O	1:F:159:GLN:HB3	2.08	0.54
1:K:323:ASN:HB3	1:T:397:ARG:NH1	2.22	0.54
1:M:572:VAL:HG12	1:M:573:TYR:O	2.08	0.54
1:S:460:VAL:HG11	1:S:484:VAL:HA	1.89	0.54
1:W:558:GLN:O	1:W:558:GLN:HG2	2.07	0.54
1:a:432:PRO:O	1:a:443:ASN:ND2	2.37	0.54
1:c:114:ALA:HB1	1:c:119:VAL:HG11	1.89	0.54
1:d:137:HIS:CE1	1:d:272:PRO:HB3	2.42	0.54
1:d:517:ASN:O	1:d:517:ASN:ND2	2.23	0.54
1:A:581:ARG:O	1:A:582:LYS:HB2	2.08	0.54
1:C:216:ARG:NH1	1:C:231:ASN:OD1	2.34	0.54
1:H:252:VAL:HB	1:L:45:PHE:HB3	1.89	0.54
1:K:556:ASP:O	1:K:558:GLN:N	2.32	0.54
1:R:326:THR:H	1:R:329:THR:HB	1.72	0.54
1:T:155:GLU:HG3	1:T:156:SER:OG	2.07	0.54
1:Y:75:GLU:OE2	1:Y:108:PRO:HA	2.08	0.54
1:Y:368:GLU:HG3	1:Y:369:ASN:N	2.23	0.54
1:B:331:MET:HB3	1:R:190:MET:HE1	1.89	0.54
1:F:383:GLN:C	1:F:384:HIS:HD2	2.15	0.54
1:M:439:LYS:NZ	1:R:434:ASP:OD2	2.31	0.54
1:Z:476:THR:O	1:Z:479:LYS:HE2	2.07	0.54
1:b:518:MET:HG3	1:b:520:ARG:HG3	1.88	0.54
1:J:369:ASN:C	1:J:371:ALA:H	2.15	0.54
1:B:369:ASN:C	1:B:371:ALA:H	2.15	0.54
1:K:155:GLU:HG2	1:K:163:LYS:NZ	2.21	0.54
1:L:476:THR:O	1:L:479:LYS:HE2	2.07	0.54
1:R:508:ASN:C	1:R:508:ASN:ND2	2.65	0.54
1:Z:558:GLN:O	1:Z:558:GLN:HG2	2.06	0.54
1:a:377:ARG:HH21	1:a:397:ARG:HD2	1.73	0.54
1:d:473:GLU:HG2	1:d:491:GLN:HE22	1.73	0.54
1:B:154:SER:HA	1:B:155:GLU:HB2	1.88	0.54
1:H:556:ASP:O	1:H:558:GLN:N	2.37	0.54
1:R:79:TYR:OH	1:R:247:GLU:OE1	2.23	0.54
1:Y:159:GLN:HB3	1:Y:160:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:460:VAL:HG11	1:a:484:VAL:HA	1.90	0.54
1:Q:269:ASP:HB3	1:Q:492:ASN:ND2	2.23	0.54
1:G:408:ARG:NH1	1:c:346:GLU:OE1	2.40	0.54
1:M:417:ASN:OD1	1:M:419:ASN:ND2	2.39	0.54
1:O:369:ASN:HB3	1:O:372:ALA:HB3	1.90	0.54
1:W:382:ARG:NH1	1:Y:513:ASP:O	2.41	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	1.90	0.54
1:a:554:ASN:HD22	1:a:557:ASN:HD22	1.56	0.54
1:b:409:TYR:CE2	1:b:411:GLU:HB2	2.43	0.54
1:J:510:TYR:HE1	1:J:518:MET:HG3	1.72	0.54
1:D:411:GLU:OE1	1:D:411:GLU:N	2.35	0.54
1:G:107:THR:OG1	1:G:208:TRP:O	2.24	0.54
1:G:415:ILE:HD12	1:c:447:ILE:HG22	1.90	0.54
1:H:475:ASP:OD1	1:b:274:ARG:NH1	2.39	0.54
1:K:153:VAL:HG12	1:K:163:LYS:NZ	2.23	0.54
1:M:362:GLY:N	1:M:368:GLU:OE2	2.32	0.54
1:U:193:GLU:OE1	1:U:209:ARG:NH2	2.41	0.54
1:V:422:LEU:HA	1:V:423:PRO:C	2.32	0.54
1:X:154:SER:HA	1:X:155:GLU:HB2	1.89	0.54
1:X:554:ASN:O	1:X:558:GLN:HB2	2.07	0.54
1:c:77:GLU:HB2	1:c:518:MET:HE1	1.89	0.54
1:E:369:ASN:O	1:E:371:ALA:N	2.41	0.54
1:J:209:ARG:NE	1:U:288:PRO:O	2.37	0.54
1:B:513:ASP:O	1:F:382:ARG:HD2	2.08	0.54
1:C:109:TRP:CD1	1:C:246:ILE:HG13	2.43	0.54
1:G:59:VAL:HG21	1:G:133:MET:HE2	1.89	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:A:387:LYS:NZ	1:A:389:THR:OG1	2.40	0.53
1:E:383:GLN:C	1:E:384:HIS:HD2	2.17	0.53
1:C:191:ARG:O	1:C:193:GLU:HG3	2.07	0.53
1:F:346:GLU:OE1	1:d:408:ARG:NH1	2.41	0.53
1:L:236:THR:HB	1:M:558:GLN:HE22	1.73	0.53
1:U:214:TRP:O	1:U:350:GLN:HG2	2.08	0.53
1:V:383:GLN:HB3	1:V:384:HIS:HD2	1.73	0.53
1:X:435:PRO:HB3	1:X:439:LYS:O	2.09	0.53
1:Z:417:ASN:ND2	1:Z:419:ASN:HD22	2.05	0.53
1:a:194:THR:H	1:a:384:HIS:HE1	1.54	0.53
1:A:132:THR:HG22	1:I:132:THR:HG22	1.90	0.53
1:J:475:ASP:CG	1:U:274:ARG:HH12	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ALA:HA	1:B:158:THR:OG1	2.08	0.53
1:C:478:LEU:HD13	1:P:481:ARG:HB3	1.91	0.53
1:M:369:ASN:C	1:M:371:ALA:H	2.15	0.53
1:P:159:GLN:C	1:P:161:PRO:HA	2.33	0.53
1:P:326:THR:H	1:P:329:THR:HB	1.73	0.53
1:T:339:SER:O	1:T:449:ASN:HA	2.08	0.53
1:U:256:ARG:HH12	1:X:257:THR:HG22	1.73	0.53
1:X:59:VAL:HG21	1:X:133:MET:HE2	1.90	0.53
1:N:382:ARG:NH2	1:N:392:GLY:O	2.41	0.53
1:Q:59:VAL:HG21	1:Q:133:MET:HE2	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:D:361:ARG:HG3	1:D:405:ASP:HA	1.90	0.53
1:F:266:PHE:HZ	1:F:493:ASN:O	1.91	0.53
1:I:581:ARG:O	1:I:582:LYS:HB2	2.08	0.53
1:P:154:SER:HA	1:P:155:GLU:HB3	1.90	0.53
1:S:435:PRO:HB3	1:S:439:LYS:O	2.09	0.53
1:T:159:GLN:C	1:T:161:PRO:HA	2.34	0.53
1:V:326:THR:H	1:V:329:THR:HB	1.73	0.53
1:A:493:ASN:N	1:A:493:ASN:OD1	2.40	0.53
1:J:216:ARG:NH1	1:J:231:ASN:OD1	2.38	0.53
1:F:447:ILE:HG22	1:d:415:ILE:HD12	1.89	0.53
1:G:298:GLU:HG2	1:d:566:ILE:HG12	1.90	0.53
1:I:411:GLU:OE1	1:I:411:GLU:N	2.40	0.53
1:K:584:TYR:OH	1:T:471:ASP:OD1	2.21	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:V:569:MET:HG2	1:V:570:LYS:H	1.74	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:A:556:ASP:O	1:A:558:GLN:N	2.33	0.53
1:J:336:VAL:O	1:J:408:ARG:NH2	2.41	0.53
1:N:127:GLN:HG3	1:N:551:MET:HE2	1.90	0.53
1:F:174:MET:HE2	1:F:252:VAL:HG11	1.91	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	1.72	0.53
1:d:368:GLU:HG3	1:d:369:ASN:N	2.22	0.53
1:Q:553:ILE:CA	1:Q:554:ASN:HB2	2.25	0.53
1:D:383:GLN:C	1:D:384:HIS:HD2	2.16	0.53
1:L:452:GLY:HA2	1:d:451:TYR:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:203:THR:OG1	1:M:204:ILE:N	2.42	0.53
1:X:161:PRO:HD2	1:X:162:THR:H	1.74	0.53
1:X:400:TYR:CE2	1:X:575:LYS:HA	2.43	0.53
1:X:581:ARG:O	1:X:582:LYS:HB3	2.08	0.53
1:L:302:ASN:HB3	1:b:565:ASN:HD21	1.73	0.53
1:O:476:THR:O	1:O:479:LYS:HE2	2.09	0.53
1:R:558:GLN:HE22	1:T:236:THR:HB	1.74	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:E:541:ALA:HB3	1:E:543:HIS:HE1	1.74	0.53
1:J:581:ARG:O	1:J:582:LYS:HB2	2.09	0.53
1:N:566:ILE:HG22	1:N:567:GLY:H	1.72	0.53
1:L:157:ALA:HA	1:L:158:THR:HG22	1.90	0.53
1:L:401:ILE:O	1:L:575:LYS:NZ	2.42	0.53
1:P:383:GLN:C	1:P:384:HIS:HD2	2.17	0.53
1:T:369:ASN:C	1:T:371:ALA:H	2.17	0.53
1:V:266:PHE:HZ	1:V:493:ASN:O	1.91	0.53
1:V:573:TYR:O	1:V:574:GLU:HG3	2.09	0.53
1:W:546:ASN:ND2	1:W:547:PRO:O	2.35	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:G:369:ASN:C	1:G:371:ALA:H	2.17	0.53
1:G:553:ILE:CA	1:G:554:ASN:HB2	2.24	0.53
1:K:382:ARG:HD2	1:M:513:ASP:O	2.09	0.53
1:O:99:ASP:CG	1:O:216:ARG:HH21	2.16	0.53
1:R:77:GLU:HB2	1:R:518:MET:HE1	1.91	0.53
1:Y:400:TYR:HE2	1:Y:575:LYS:HA	1.74	0.53
1:a:148:VAL:O	1:a:257:THR:HG23	2.09	0.53
1:d:383:GLN:C	1:d:384:HIS:HD2	2.17	0.53
1:A:556:ASP:O	1:A:557:ASN:HB3	2.08	0.53
1:Q:138:LEU:HG	1:Q:268:PHE:CD2	2.44	0.53
1:B:236:THR:HB	1:F:558:GLN:HE22	1.74	0.53
1:F:397:ARG:NH1	1:d:323:ASN:HB3	2.23	0.53
1:F:471:ASP:OD1	1:d:584:TYR:OH	2.21	0.53
1:K:319:MET:HE2	1:T:354:LYS:HD2	1.90	0.53
1:T:361:ARG:NH1	1:T:363:GLY:O	2.42	0.53
1:T:369:ASN:O	1:T:371:ALA:N	2.41	0.53
1:W:131:ASN:HB3	1:W:550:GLN:HE21	1.73	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:H:346:GLU:OE1	1:b:408:ARG:NH1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:475:ASP:OD1	1:V:274:ARG:NH1	2.39	0.52
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:S:476:THR:O	1:S:479:LYS:HE2	2.09	0.52
1:S:515:SER:OG	1:T:390:THR:O	2.27	0.52
1:V:432:PRO:O	1:V:443:ASN:ND2	2.36	0.52
1:W:127:GLN:HE22	1:a:548:ILE:H	1.56	0.52
1:Y:56:ASN:OD1	1:Y:58:TRP:CD1	2.61	0.52
1:Y:451:TYR:CD2	1:a:452:GLY:HA2	2.44	0.52
1:b:319:MET:HE3	1:b:329:THR:HG23	1.91	0.52
1:D:558:GLN:NE2	1:G:236:THR:HB	2.24	0.52
1:H:157:ALA:HA	1:H:158:THR:OG1	2.08	0.52
1:L:457:LEU:HB3	1:d:478:LEU:HD12	1.90	0.52
1:R:131:ASN:HB3	1:R:550:GLN:NE2	2.24	0.52
1:U:161:PRO:HD2	1:U:162:THR:H	1.74	0.52
1:V:109:TRP:CD1	1:V:246:ILE:HG13	2.44	0.52
1:V:203:THR:OG1	1:V:204:ILE:N	2.42	0.52
1:Z:266:PHE:HZ	1:Z:493:ASN:O	1.92	0.52
1:d:476:THR:O	1:d:479:LYS:HE2	2.09	0.52
1:A:287:LEU:HD12	1:A:288:PRO:HD2	1.91	0.52
1:J:319:MET:HE3	1:J:329:THR:HG23	1.89	0.52
1:B:558:GLN:O	1:B:558:GLN:HG2	2.09	0.52
1:D:96:MET:HE2	1:D:221:SER:O	2.09	0.52
1:F:556:ASP:O	1:F:557:ASN:HB3	2.08	0.52
1:P:581:ARG:O	1:P:582:LYS:HB2	2.10	0.52
1:Y:414:TRP:HE1	1:Y:416:GLN:HE21	1.56	0.52
1:b:553:ILE:CA	1:b:554:ASN:HB2	2.23	0.52
1:A:157:ALA:HA	1:A:158:THR:OG1	2.09	0.52
1:N:492:ASN:CG	1:N:493:ASN:H	2.16	0.52
1:Q:203:THR:OG1	1:Q:204:ILE:N	2.43	0.52
1:D:157:ALA:HA	1:D:158:THR:HG22	1.90	0.52
1:F:584:TYR:OH	1:L:471:ASP:OD1	2.18	0.52
1:W:435:PRO:HB3	1:W:439:LYS:O	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:c:581:ARG:O	1:c:582:LYS:HB2	2.08	0.52
1:d:154:SER:O	1:d:154:SER:OG	2.24	0.52
1:C:368:GLU:HG2	1:C:369:ASN:N	2.24	0.52
1:K:339:SER:O	1:K:449:ASN:HA	2.09	0.52
1:T:338:TYR:HE1	1:T:358:ALA:HB3	1.74	0.52
1:U:443:ASN:H	1:U:446:ASN:HD22	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:581:ARG:O	1:W:582:LYS:HB2	2.09	0.52
1:Y:75:GLU:HG2	1:Y:76:SER:H	1.73	0.52
1:Y:193:GLU:CD	1:Y:209:ARG:HH22	2.10	0.52
1:Z:339:SER:O	1:Z:449:ASN:HA	2.10	0.52
1:B:132:THR:HG22	1:P:132:THR:HG22	1.91	0.52
1:C:338:TYR:HE1	1:C:358:ALA:HB3	1.74	0.52
1:D:369:ASN:O	1:D:371:ALA:N	2.42	0.52
1:F:331:MET:HB3	1:L:190:MET:HE1	1.92	0.52
1:F:352:PRO:HD2	1:d:283:ARG:HH12	1.73	0.52
1:H:326:THR:H	1:H:329:THR:HB	1.73	0.52
1:I:556:ASP:O	1:I:557:ASN:HB3	2.09	0.52
1:K:573:TYR:C	1:K:574:GLU:HG2	2.34	0.52
1:O:130:VAL:HG13	1:O:576:SER:O	2.09	0.52
1:P:365:GLN:HG2	1:P:366:THR:HG23	1.91	0.52
1:T:581:ARG:O	1:T:582:LYS:HB2	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:N:323:ASN:HB3	1:S:397:ARG:NH1	2.25	0.52
1:D:193:GLU:OE1	1:D:209:ARG:NH2	2.42	0.52
1:H:96:MET:HE2	1:b:414:TRP:CE2	2.44	0.52
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:R:105:ILE:HG12	1:R:212:PHE:HB2	1.91	0.52
1:R:191:ARG:O	1:R:193:GLU:HG3	2.10	0.52
1:U:216:ARG:NH1	1:U:231:ASN:OD1	2.39	0.52
1:U:382:ARG:N	1:U:386:GLN:HB3	2.16	0.52
1:V:127:GLN:HG3	1:V:551:MET:HE2	1.91	0.52
1:c:336:VAL:O	1:c:408:ARG:NH2	2.43	0.52
1:c:363:GLY:HA3	1:c:367:ASP:O	2.10	0.52
1:d:411:GLU:OE1	1:d:411:GLU:N	2.39	0.52
1:d:479:LYS:HD2	1:d:491:GLN:NE2	2.24	0.52
1:N:473:GLU:HG2	1:N:491:GLN:HE22	1.74	0.52
1:C:326:THR:H	1:C:329:THR:HB	1.73	0.52
1:D:130:VAL:HG11	1:D:578:LEU:HD13	1.91	0.52
1:K:365:GLN:HB2	1:T:215:ASP:OD2	2.10	0.52
1:L:558:GLN:HG2	1:L:558:GLN:O	2.10	0.52
1:T:432:PRO:O	1:T:443:ASN:ND2	2.37	0.52
1:V:476:THR:O	1:V:479:LYS:HE2	2.09	0.52
1:Y:383:GLN:C	1:Y:384:HIS:HD2	2.18	0.52
1:A:96:MET:HE2	1:T:414:TRP:CE2	2.45	0.52
1:E:369:ASN:C	1:E:371:ALA:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:P:383:GLN:HB3	1:P:384:HIS:CD2	2.44	0.52
1:R:127:GLN:HG3	1:R:551:MET:HE2	1.91	0.52
1:R:203:THR:OG1	1:R:204:ILE:N	2.40	0.52
1:T:59:VAL:HG21	1:T:133:MET:HE2	1.91	0.52
1:b:365:GLN:HG2	1:b:366:THR:HG23	1.92	0.52
1:A:346:GLU:OE1	1:T:408:ARG:NH1	2.43	0.52
1:U:382:ARG:HD2	1:V:513:ASP:O	2.09	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:A:546:ASN:ND2	1:A:547:PRO:O	2.38	0.51
1:G:457:LEU:O	1:c:476:THR:HB	2.11	0.51
1:I:451:TYR:CD2	1:V:452:GLY:HA2	2.45	0.51
1:O:297:SER:C	1:O:302:ASN:HD22	2.16	0.51
1:O:369:ASN:C	1:O:371:ALA:H	2.18	0.51
1:P:382:ARG:NE	1:P:390:THR:O	2.32	0.51
1:W:457:LEU:HB3	1:b:478:LEU:HD12	1.93	0.51
1:c:369:ASN:C	1:c:371:ALA:H	2.17	0.51
1:E:77:GLU:HB2	1:E:518:MET:HE1	1.92	0.51
1:G:383:GLN:CB	1:G:384:HIS:HD2	2.24	0.51
1:H:550:GLN:HA	1:H:578:LEU:HD23	1.91	0.51
1:U:266:PHE:HZ	1:U:493:ASN:O	1.93	0.51
1:U:554:ASN:HB3	1:U:557:ASN:HB3	1.90	0.51
1:V:287:LEU:HD12	1:V:288:PRO:HD2	1.92	0.51
1:a:138:LEU:HG	1:a:268:PHE:CD2	2.45	0.51
1:c:400:TYR:CE2	1:c:575:LYS:HA	2.44	0.51
1:E:75:GLU:OE1	1:I:294:LEU:HD12	2.11	0.51
1:C:550:GLN:HA	1:C:578:LEU:HD23	1.91	0.51
1:D:279:TRP:HA	1:D:405:ASP:HB2	1.91	0.51
1:W:378:TYR:O	1:W:397:ARG:HA	2.10	0.51
1:Y:55:GLU:O	1:Y:56:ASN:CG	2.53	0.51
1:b:56:ASN:OD1	1:b:58:TRP:CD1	2.59	0.51
1:b:377:ARG:NH2	1:b:397:ARG:HD2	2.24	0.51
1:d:417:ASN:OD1	1:d:419:ASN:ND2	2.33	0.51
1:A:452:GLY:HA2	1:K:451:TYR:CD2	2.45	0.51
1:N:339:SER:O	1:N:449:ASN:HA	2.10	0.51
1:B:573:TYR:O	1:B:574:GLU:HG3	2.10	0.51
1:R:553:ILE:CA	1:R:554:ASN:HB2	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:191:ARG:O	1:a:193:GLU:HG3	2.10	0.51
1:Q:554:ASN:O	1:Q:558:GLN:HB2	2.10	0.51
1:C:159:GLN:HA	1:C:159:GLN:OE1	2.09	0.51
1:H:401:ILE:O	1:H:575:LYS:NZ	2.43	0.51
1:K:457:LEU:O	1:T:476:THR:HB	2.11	0.51
1:K:558:GLN:OE1	1:M:236:THR:OG1	2.23	0.51
1:L:154:SER:HA	1:L:155:GLU:CB	2.41	0.51
1:L:556:ASP:O	1:L:558:GLN:N	2.31	0.51
1:M:460:VAL:HG11	1:M:484:VAL:HA	1.92	0.51
1:R:297:SER:O	1:R:302:ASN:ND2	2.40	0.51
1:S:339:SER:O	1:S:449:ASN:HA	2.11	0.51
1:X:96:MET:HG2	1:X:220:PRO:HA	1.93	0.51
1:Z:369:ASN:C	1:Z:371:ALA:H	2.16	0.51
1:d:565:ASN:OD1	1:d:565:ASN:N	2.44	0.51
1:B:338:TYR:CE1	1:B:358:ALA:HB3	2.43	0.51
1:C:77:GLU:HB2	1:C:518:MET:HE1	1.92	0.51
1:G:106:VAL:HG22	1:G:209:ARG:CZ	2.40	0.51
1:H:154:SER:CA	1:H:155:GLU:HB2	2.31	0.51
1:M:137:HIS:CE1	1:M:272:PRO:HB3	2.46	0.51
1:T:203:THR:OG1	1:T:204:ILE:N	2.43	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:c:75:GLU:HG2	1:c:76:SER:N	2.25	0.51
1:N:382:ARG:N	1:N:386:GLN:HB3	2.10	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:414:TRP:CE2	1:R:96:MET:HE2	2.45	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
1:Y:216:ARG:NH1	1:Y:231:ASN:OD1	2.35	0.51
1:a:155:GLU:HA	1:a:163:LYS:HG2	1.93	0.51
1:b:369:ASN:C	1:b:371:ALA:H	2.14	0.51
1:A:317:THR:HG22	1:A:330:ILE:HA	1.92	0.51
1:A:369:ASN:C	1:A:371:ALA:H	2.17	0.51
1:E:540:ARG:HH21	1:E:550:GLN:NE2	2.09	0.51
1:Q:556:ASP:O	1:Q:558:GLN:N	2.38	0.51
1:Q:572:VAL:HG12	1:Q:573:TYR:O	2.11	0.51
1:H:220:PRO:HB2	1:b:431:LEU:HD22	1.93	0.51
1:I:190:MET:HE1	1:V:331:MET:HB3	1.92	0.51
1:P:52:LYS:HE3	1:P:60:TYR:CD2	2.46	0.51
1:S:361:ARG:NH1	1:S:363:GLY:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:558:GLN:NE2	1:W:236:THR:HB	2.25	0.51
1:Z:561:TYR:OH	1:Z:574:GLU:OE2	2.29	0.51
1:C:569:MET:HG2	1:C:570:LYS:H	1.76	0.51
1:G:453:PRO:HD3	1:c:451:TYR:CD1	2.46	0.51
1:G:554:ASN:HD22	1:G:557:ASN:ND2	2.03	0.51
1:H:566:ILE:HG22	1:H:567:GLY:H	1.76	0.51
1:I:556:ASP:O	1:I:558:GLN:N	2.36	0.51
1:R:566:ILE:HG22	1:R:567:GLY:H	1.76	0.51
1:S:422:LEU:HA	1:S:423:PRO:C	2.36	0.51
1:Z:127:GLN:HG3	1:Z:551:MET:HE2	1.93	0.51
1:E:382:ARG:N	1:E:386:GLN:HB3	2.25	0.51
1:E:556:ASP:O	1:E:558:GLN:N	2.38	0.51
1:D:558:GLN:O	1:D:558:GLN:HG2	2.10	0.51
1:I:159:GLN:C	1:I:161:PRO:HA	2.36	0.51
1:O:62:THR:HG23	1:O:534:VAL:HG22	1.93	0.51
1:O:159:GLN:CB	1:O:160:PRO:HD2	2.40	0.51
1:R:297:SER:OG	1:R:302:ASN:ND2	2.44	0.51
1:U:131:ASN:O	1:U:550:GLN:NE2	2.44	0.51
1:V:194:THR:H	1:V:384:HIS:HE1	1.59	0.51
1:a:247:GLU:OE1	1:a:247:GLU:N	2.42	0.51
1:D:45:PHE:HB3	1:G:252:VAL:HB	1.93	0.50
1:L:369:ASN:C	1:L:371:ALA:H	2.19	0.50
1:O:137:HIS:CE1	1:O:272:PRO:HB3	2.47	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:W:319:MET:HE3	1:W:329:THR:HG23	1.94	0.50
1:Z:383:GLN:C	1:Z:384:HIS:HD2	2.19	0.50
1:a:322:THR:HG21	1:a:420:PHE:CD2	2.45	0.50
1:a:391:THR:HG22	1:b:515:SER:OG	2.11	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:C:269:ASP:OD1	1:C:492:ASN:ND2	2.44	0.50
1:F:154:SER:CA	1:F:155:GLU:HB2	2.34	0.50
1:H:131:ASN:HB3	1:H:550:GLN:NE2	2.26	0.50
1:M:96:MET:HE2	1:R:414:TRP:CE2	2.47	0.50
1:P:558:GLN:NE2	1:R:236:THR:HB	2.27	0.50
1:d:554:ASN:HB3	1:d:557:ASN:HB3	1.93	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:P:556:ASP:O	1:P:557:ASN:HB3	2.11	0.50
1:U:247:GLU:OE1	1:U:247:GLU:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:137:HIS:CE1	1:W:272:PRO:HB3	2.46	0.50
1:W:288:PRO:HG3	1:b:211:TYR:CG	2.47	0.50
1:W:414:TRP:CE2	1:b:96:MET:HE2	2.46	0.50
1:C:277:HIS:ND1	1:C:577:GLN:O	2.42	0.50
1:D:563:PRO:HB3	1:D:569:MET:HE2	1.93	0.50
1:G:580:PRO:HB2	1:c:242:GLN:NE2	2.27	0.50
1:I:247:GLU:OE1	1:I:247:GLU:N	2.44	0.50
1:K:153:VAL:HG12	1:K:163:LYS:HZ1	1.76	0.50
1:M:155:GLU:O	1:M:156:SER:OG	2.29	0.50
1:O:287:LEU:HD12	1:O:288:PRO:HD2	1.93	0.50
1:U:114:ALA:HB2	1:U:195:LEU:HD12	1.91	0.50
1:U:553:ILE:CA	1:U:554:ASN:HB2	2.30	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:I:475:ASP:CG	1:V:274:ARG:HH12	2.19	0.50
1:K:203:THR:OG1	1:K:204:ILE:N	2.43	0.50
1:M:422:LEU:HA	1:M:423:PRO:C	2.35	0.50
1:b:556:ASP:O	1:b:558:GLN:N	2.41	0.50
1:A:550:GLN:HA	1:A:578:LEU:HD23	1.92	0.50
1:C:319:MET:HE3	1:C:329:THR:HG23	1.92	0.50
1:H:130:VAL:HG13	1:H:576:SER:O	2.11	0.50
1:M:566:ILE:HG22	1:M:567:GLY:H	1.77	0.50
1:T:216:ARG:NH1	1:T:231:ASN:OD1	2.36	0.50
1:W:286:GLY:O	1:W:288:PRO:HD3	2.11	0.50
1:X:154:SER:CA	1:X:155:GLU:HB2	2.42	0.50
1:Y:154:SER:HA	1:Y:155:GLU:CB	2.41	0.50
1:c:127:GLN:HG3	1:c:551:MET:HE2	1.94	0.50
1:J:354:LYS:HD2	1:U:319:MET:HE2	1.92	0.50
1:B:138:LEU:HG	1:B:268:PHE:CD2	2.47	0.50
1:C:556:ASP:O	1:C:557:ASN:HB3	2.12	0.50
1:F:362:GLY:N	1:F:368:GLU:OE2	2.41	0.50
1:P:127:GLN:HG3	1:P:551:MET:HE2	1.94	0.50
1:P:183:MET:HE1	1:P:246:ILE:HD13	1.93	0.50
1:U:157:ALA:HA	1:U:158:THR:HG22	1.94	0.50
1:X:556:ASP:O	1:X:558:GLN:N	2.35	0.50
1:a:157:ALA:HA	1:a:158:THR:HG22	1.94	0.50
1:b:257:THR:HG22	1:d:256:ARG:NH1	2.26	0.50
1:E:132:THR:HG22	1:U:132:THR:HG22	1.93	0.50
1:E:354:LYS:HD2	1:I:319:MET:HE2	1.94	0.50
1:K:369:ASN:C	1:K:371:ALA:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:75:GLU:HG2	1:M:76:SER:N	2.27	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:X:152:THR:HG23	1:X:168:ASP:HB2	1.92	0.50
1:Y:468:GLN:HB3	1:Y:486:ALA:HB2	1.94	0.50
1:Z:99:ASP:CG	1:Z:216:ARG:HH21	2.20	0.50
1:D:338:TYR:HE1	1:D:358:ALA:HB3	1.77	0.50
1:O:573:TYR:O	1:O:574:GLU:HG2	2.12	0.50
1:R:382:ARG:NH2	1:R:392:GLY:O	2.35	0.50
1:X:365:GLN:C	1:X:367:ASP:H	2.20	0.50
1:Z:554:ASN:HB3	1:Z:556:ASP:O	2.12	0.50
1:A:298:GLU:HA	1:I:565:ASN:HD21	1.77	0.49
1:N:331:MET:HE3	1:S:485:ASN:HB3	1.94	0.49
1:B:422:LEU:HA	1:B:423:PRO:C	2.37	0.49
1:C:352:PRO:HD2	1:P:283:ARG:HH12	1.76	0.49
1:U:154:SER:HA	1:U:155:GLU:CB	2.31	0.49
1:Z:216:ARG:NH1	1:Z:231:ASN:OD1	2.43	0.49
1:a:157:ALA:HA	1:a:158:THR:CG2	2.42	0.49
1:a:322:THR:HG21	1:a:420:PHE:HD2	1.77	0.49
1:d:404:GLN:OE1	1:d:458:ASN:HB2	2.12	0.49
1:N:338:TYR:CE1	1:N:358:ALA:HB3	2.47	0.49
1:Q:362:GLY:H	1:Q:368:GLU:CD	2.20	0.49
1:C:475:ASP:O	1:P:581:ARG:NH1	2.46	0.49
1:F:236:THR:HB	1:G:558:GLN:NE2	2.27	0.49
1:G:174:MET:HE2	1:G:252:VAL:HG11	1.94	0.49
1:I:492:ASN:CG	1:I:493:ASN:N	2.69	0.49
1:L:194:THR:H	1:L:384:HIS:HE1	1.60	0.49
1:L:283:ARG:NH2	1:d:101:THR:O	2.45	0.49
1:S:493:ASN:OD1	1:S:493:ASN:N	2.42	0.49
1:T:150:LEU:HD22	1:T:171:ALA:HB1	1.92	0.49
1:Y:451:TYR:CD1	1:a:453:PRO:HD3	2.47	0.49
1:a:383:GLN:CB	1:a:384:HIS:HD2	2.24	0.49
1:A:257:THR:HG22	1:E:256:ARG:NH1	2.27	0.49
1:C:183:MET:HE1	1:C:246:ILE:HD13	1.93	0.49
1:W:257:THR:HG22	1:Y:256:ARG:NH1	2.27	0.49
1:W:288:PRO:HG3	1:b:211:TYR:CD2	2.48	0.49
1:W:369:ASN:C	1:W:371:ALA:H	2.19	0.49
1:X:462:PRO:HD2	1:X:576:SER:OG	2.13	0.49
1:X:476:THR:O	1:X:479:LYS:HE2	2.12	0.49
1:b:157:ALA:HA	1:b:158:THR:HG22	1.94	0.49
1:A:435:PRO:HB3	1:A:439:LYS:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:GLU:HG3	1:C:261:PHE:N	2.27	0.49
1:I:244:TYR:OH	1:V:582:LYS:HE2	2.12	0.49
1:K:266:PHE:HZ	1:K:493:ASN:O	1.96	0.49
1:K:452:GLY:HA2	1:T:451:TYR:CD2	2.47	0.49
1:P:383:GLN:HB3	1:P:384:HIS:HD2	1.76	0.49
1:S:154:SER:O	1:S:154:SER:OG	2.28	0.49
1:V:42:THR:HB	1:V:260:GLU:HB3	1.94	0.49
1:X:94:GLY:C	1:X:96:MET:HE2	2.37	0.49
1:a:554:ASN:O	1:a:558:GLN:HB2	2.13	0.49
1:c:492:ASN:H	1:c:492:ASN:HD22	1.61	0.49
1:A:252:VAL:HB	1:N:45:PHE:HB3	1.93	0.49
1:Q:148:VAL:O	1:Q:257:THR:HG23	2.13	0.49
1:D:383:GLN:HB3	1:D:384:HIS:HD2	1.77	0.49
1:D:404:GLN:OE1	1:D:458:ASN:HB2	2.12	0.49
1:G:583:LEU:HD11	1:c:476:THR:HG22	1.95	0.49
1:I:310:GLN:HG2	1:I:313:ARG:NH1	2.28	0.49
1:L:556:ASP:O	1:L:557:ASN:HB3	2.10	0.49
1:O:435:PRO:HB3	1:O:439:LYS:O	2.13	0.49
1:Y:157:ALA:HA	1:Y:158:THR:HB	1.94	0.49
1:Z:191:ARG:O	1:Z:193:GLU:HG3	2.12	0.49
1:Z:382:ARG:NE	1:Z:390:THR:O	2.40	0.49
1:E:105:ILE:HG12	1:E:212:PHE:HB2	1.94	0.49
1:H:79:TYR:OH	1:H:247:GLU:OE1	2.27	0.49
1:L:566:ILE:HG12	1:b:298:GLU:HG2	1.94	0.49
1:P:324:TYR:CE2	1:P:422:LEU:HD21	2.47	0.49
1:P:558:GLN:O	1:P:558:GLN:HG2	2.11	0.49
1:U:460:VAL:HG11	1:U:484:VAL:HA	1.94	0.49
1:U:556:ASP:O	1:U:557:ASN:HB3	2.11	0.49
1:b:400:TYR:CE2	1:b:575:LYS:HA	2.48	0.49
1:c:369:ASN:O	1:c:371:ALA:N	2.45	0.49
1:c:513:ASP:O	1:d:382:ARG:NH1	2.46	0.49
1:d:400:TYR:CE2	1:d:575:LYS:HA	2.48	0.49
1:F:247:GLU:OE1	1:F:247:GLU:N	2.36	0.49
1:G:322:THR:HB	1:G:324:TYR:H	1.78	0.49
1:H:338:TYR:HE1	1:H:358:ALA:HB3	1.77	0.49
1:M:213:GLN:O	1:M:236:THR:HG22	2.13	0.49
1:S:326:THR:H	1:S:329:THR:HB	1.78	0.49
1:S:557:ASN:O	1:S:559:PHE:N	2.46	0.49
1:A:159:GLN:HB3	1:A:160:PRO:HD2	1.95	0.49
1:B:485:ASN:HB3	1:M:331:MET:HE3	1.94	0.49
1:F:248:ASN:ND2	1:G:122:ASN:HD22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:THR:HG22	1:F:350:GLN:HG3	1.95	0.49
1:I:369:ASN:C	1:I:371:ALA:H	2.20	0.49
1:M:232:ILE:HG12	1:M:233:TYR:N	2.28	0.49
1:V:369:ASN:C	1:V:371:ALA:H	2.15	0.49
1:W:460:VAL:HG11	1:W:484:VAL:HA	1.95	0.49
1:X:464:TYR:O	1:X:573:TYR:HA	2.13	0.49
1:Y:352:PRO:HD2	1:a:283:ARG:HH12	1.78	0.49
1:A:431:LEU:HD22	1:K:220:PRO:HB2	1.93	0.49
1:J:478:LEU:HD13	1:U:481:ARG:HB3	1.95	0.49
1:B:45:PHE:HB3	1:C:252:VAL:HB	1.93	0.49
1:C:157:ALA:HA	1:C:158:THR:OG1	2.12	0.49
1:D:476:THR:O	1:D:479:LYS:HE2	2.13	0.49
1:I:362:GLY:N	1:I:368:GLU:OE2	2.42	0.49
1:O:361:ARG:O	1:O:405:ASP:HA	2.13	0.49
1:W:378:TYR:CE1	1:W:463:VAL:HG11	2.47	0.49
1:X:556:ASP:O	1:X:557:ASN:HB3	2.12	0.49
1:Z:252:VAL:HB	1:c:45:PHE:HB3	1.94	0.49
1:a:50:GLU:HG2	1:a:62:THR:HB	1.94	0.49
1:d:286:GLY:O	1:d:288:PRO:HD3	2.13	0.49
1:d:339:SER:O	1:d:449:ASN:HA	2.13	0.49
1:Q:382:ARG:NE	1:Q:390:THR:O	2.42	0.49
1:C:572:VAL:HG12	1:C:573:TYR:O	2.13	0.49
1:D:569:MET:HG2	1:D:570:LYS:H	1.77	0.49
1:G:452:GLY:HA2	1:c:451:TYR:CD2	2.47	0.49
1:H:110:SER:HB3	1:H:205:PRO:HB2	1.95	0.49
1:H:414:TRP:CE2	1:W:96:MET:HE2	2.47	0.49
1:L:127:GLN:HG3	1:L:551:MET:HE2	1.94	0.49
1:L:247:GLU:OE1	1:L:247:GLU:N	2.44	0.49
1:L:584:TYR:OH	1:d:471:ASP:OD1	2.23	0.49
1:S:485:ASN:OD1	1:S:485:ASN:N	2.42	0.49
1:a:383:GLN:HB3	1:a:384:HIS:CD2	2.47	0.49
1:b:382:ARG:NH2	1:b:392:GLY:O	2.45	0.49
1:A:137:HIS:CE1	1:A:272:PRO:HB3	2.48	0.48
1:A:383:GLN:C	1:A:384:HIS:HD2	2.20	0.48
1:Q:435:PRO:HB3	1:Q:439:LYS:O	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:F:51:PHE:CD2	1:F:61:ILE:HG12	2.47	0.48
1:H:476:THR:O	1:H:479:LYS:HE2	2.13	0.48
1:H:478:LEU:HD13	1:b:481:ARG:HB3	1.94	0.48
1:H:581:ARG:O	1:H:582:LYS:HB2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:191:ARG:O	1:I:193:GLU:HG3	2.12	0.48
1:I:266:PHE:HZ	1:I:493:ASN:O	1.96	0.48
1:L:99:ASP:CG	1:L:216:ARG:HH21	2.21	0.48
1:O:127:GLN:HG3	1:O:551:MET:HE2	1.94	0.48
1:O:163:LYS:HZ2	1:O:163:LYS:HB3	1.77	0.48
1:X:155:GLU:H	1:X:164:VAL:HG22	1.76	0.48
1:Y:510:TYR:HE1	1:Y:518:MET:HE2	1.78	0.48
1:Z:422:LEU:HA	1:Z:423:PRO:C	2.37	0.48
1:c:339:SER:HB2	1:c:450:THR:OG1	2.14	0.48
1:A:256:ARG:NH1	1:N:257:THR:HG22	2.28	0.48
1:N:513:ASP:O	1:Q:382:ARG:HD2	2.13	0.48
1:N:556:ASP:O	1:N:557:ASN:HB3	2.13	0.48
1:Q:198:TYR:HB2	1:Q:201:LYS:HB3	1.95	0.48
1:B:558:GLN:NE2	1:C:236:THR:HB	2.28	0.48
1:F:561:TYR:OH	1:F:574:GLU:OE2	2.22	0.48
1:I:238:PRO:HA	1:I:241:VAL:HG23	1.95	0.48
1:I:338:TYR:CE1	1:I:358:ALA:HB3	2.46	0.48
1:L:148:VAL:O	1:L:257:THR:HG23	2.13	0.48
1:U:432:PRO:O	1:U:443:ASN:ND2	2.42	0.48
1:V:73:MET:CE	1:V:522:VAL:HA	2.44	0.48
1:X:148:VAL:O	1:X:257:THR:HG23	2.12	0.48
1:Y:382:ARG:NH2	1:Y:392:GLY:O	2.45	0.48
1:d:382:ARG:N	1:d:386:GLN:HB3	2.15	0.48
1:J:157:ALA:HA	1:J:158:THR:HB	1.96	0.48
1:N:445:THR:HA	1:N:448:PHE:HB2	1.95	0.48
1:Q:377:ARG:NH2	1:Q:397:ARG:HD2	2.28	0.48
1:B:318:GLN:HG2	1:R:374:GLY:O	2.14	0.48
1:B:492:ASN:CG	1:B:493:ASN:N	2.69	0.48
1:H:94:GLY:HA2	1:b:424:VAL:HG12	1.95	0.48
1:H:159:GLN:HB3	1:H:160:PRO:HD2	1.95	0.48
1:R:369:ASN:C	1:R:371:ALA:H	2.20	0.48
1:T:193:GLU:OE1	1:T:209:ARG:NH2	2.46	0.48
1:V:376:PRO:HD2	1:V:400:TYR:O	2.13	0.48
1:a:556:ASP:O	1:a:557:ASN:HB3	2.12	0.48
1:a:572:VAL:HG12	1:a:573:TYR:O	2.13	0.48
1:E:439:LYS:NZ	1:I:434:ASP:OD2	2.45	0.48
1:C:557:ASN:O	1:C:559:PHE:N	2.47	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:O:199:PRO:HD2	1:O:200:TRP:CZ3	2.48	0.48
1:R:247:GLU:OE1	1:R:247:GLU:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:338:TYR:HE1	1:A:358:ALA:HB3	1.78	0.48
1:E:148:VAL:O	1:E:257:THR:HG23	2.13	0.48
1:E:476:THR:HB	1:I:457:LEU:O	2.13	0.48
1:M:326:THR:H	1:M:329:THR:HB	1.79	0.48
1:M:383:GLN:C	1:M:384:HIS:HD2	2.21	0.48
1:O:365:GLN:HG2	1:O:366:THR:HG23	1.94	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:V:59:VAL:HG21	1:V:133:MET:HE2	1.95	0.48
1:V:338:TYR:HE1	1:V:358:ALA:HB3	1.77	0.48
1:Y:75:GLU:HG2	1:Y:76:SER:N	2.29	0.48
1:a:369:ASN:O	1:a:371:ALA:N	2.47	0.48
1:c:252:VAL:HB	1:d:45:PHE:HB3	1.95	0.48
1:d:553:ILE:CA	1:d:554:ASN:HB2	2.23	0.48
1:J:96:MET:HE2	1:U:414:TRP:CE2	2.49	0.48
1:N:256:ARG:NH1	1:Q:257:THR:HG22	2.29	0.48
1:Q:382:ARG:N	1:Q:386:GLN:HB3	2.24	0.48
1:F:431:LEU:HD22	1:L:220:PRO:HB2	1.96	0.48
1:G:127:GLN:HG3	1:G:551:MET:HE2	1.96	0.48
1:K:382:ARG:N	1:K:386:GLN:HB3	2.17	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:O:153:VAL:HG13	1:O:163:LYS:NZ	2.27	0.48
1:P:438:GLY:O	1:P:439:LYS:HD3	2.13	0.48
1:U:565:ASN:N	1:U:565:ASN:OD1	2.46	0.48
1:E:216:ARG:NH1	1:E:231:ASN:OD1	2.41	0.48
1:E:274:ARG:HH12	1:V:475:ASP:CG	2.20	0.48
1:J:569:MET:HG2	1:J:570:LYS:H	1.79	0.48
1:Q:558:GLN:HG2	1:Q:558:GLN:O	2.11	0.48
1:B:556:ASP:O	1:B:557:ASN:HB3	2.12	0.48
1:F:558:GLN:HG2	1:F:558:GLN:O	2.13	0.48
1:G:415:ILE:CD1	1:c:447:ILE:HG22	2.43	0.48
1:I:404:GLN:NE2	1:I:461:PRO:HD3	2.29	0.48
1:K:415:ILE:CD1	1:T:447:ILE:HG22	2.43	0.48
1:L:411:GLU:OE1	1:L:411:GLU:N	2.41	0.48
1:L:518:MET:HG3	1:L:520:ARG:CG	2.44	0.48
1:O:159:GLN:HB3	1:O:160:PRO:HD2	1.96	0.48
1:S:216:ARG:NH1	1:S:231:ASN:OD1	2.37	0.48
1:a:70:HIS:O	1:a:204:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:432:PRO:C	1:a:443:ASN:HD22	2.21	0.48
1:c:256:ARG:HH12	1:d:257:THR:HG22	1.78	0.48
1:A:411:GLU:OE1	1:A:411:GLU:N	2.44	0.48
1:B:257:THR:HG22	1:C:256:ARG:HH12	1.78	0.48
1:L:513:ASP:O	1:M:382:ARG:HD2	2.14	0.48
1:L:551:MET:HE3	1:L:551:MET:HB3	1.74	0.48
1:O:404:GLN:OE1	1:O:458:ASN:HB2	2.13	0.48
1:R:445:THR:HA	1:R:448:PHE:HB2	1.95	0.48
1:Y:114:ALA:HB1	1:Y:119:VAL:HG11	1.96	0.48
1:a:573:TYR:C	1:a:574:GLU:HG2	2.39	0.48
1:b:131:ASN:HB3	1:b:550:GLN:NE2	2.29	0.48
1:b:386:GLN:HG3	1:b:396:GLU:HB2	1.96	0.48
1:d:47:ASN:OD1	1:d:67:ARG:NH1	2.39	0.48
1:N:369:ASN:C	1:N:371:ALA:H	2.20	0.48
1:Q:369:ASN:O	1:Q:371:ALA:N	2.47	0.48
1:H:151:LYS:NZ	1:I:168:ASP:OD2	2.44	0.48
1:L:176:ALA:HB2	1:L:252:VAL:HG22	1.95	0.48
1:R:411:GLU:OE1	1:R:411:GLU:N	2.43	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:Z:349:THR:HG22	1:Z:350:GLN:HG3	1.96	0.48
1:a:66:SER:HA	1:a:529:TRP:O	2.14	0.48
1:b:435:PRO:HB3	1:b:439:LYS:O	2.14	0.48
1:d:557:ASN:O	1:d:559:PHE:N	2.47	0.48
1:A:159:GLN:O	1:A:161:PRO:HA	2.13	0.48
1:Q:287:LEU:HD12	1:Q:288:PRO:HD2	1.96	0.48
1:B:331:MET:HE3	1:R:485:ASN:HB3	1.96	0.48
1:F:322:THR:HG21	1:F:420:PHE:HD2	1.79	0.48
1:F:451:TYR:CD2	1:d:452:GLY:HA2	2.49	0.48
1:I:361:ARG:HB2	1:I:368:GLU:CD	2.39	0.48
1:M:383:GLN:HB3	1:M:384:HIS:CD2	2.49	0.48
1:M:475:ASP:CG	1:R:274:ARG:HH12	2.21	0.48
1:R:257:THR:HG22	1:T:256:ARG:HH12	1.79	0.48
1:S:266:PHE:HZ	1:S:493:ASN:O	1.96	0.48
1:Y:98:LEU:HD13	1:a:310:GLN:OE1	2.14	0.48
1:d:369:ASN:O	1:d:371:ALA:N	2.46	0.48
1:A:102:HIS:HB2	1:A:214:TRP:CH2	2.49	0.47
1:E:445:THR:HA	1:E:448:PHE:HB2	1.96	0.47
1:N:569:MET:HG2	1:N:570:LYS:N	2.23	0.47
1:G:566:ILE:HG12	1:d:298:GLU:HG2	1.96	0.47
1:H:368:GLU:HG3	1:H:373:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:422:LEU:HA	1:H:423:PRO:C	2.39	0.47
1:I:447:ILE:HG22	1:V:415:ILE:CD1	2.44	0.47
1:O:386:GLN:HG2	1:O:396:GLU:CB	2.44	0.47
1:P:554:ASN:O	1:P:558:GLN:HB2	2.14	0.47
1:R:400:TYR:CE2	1:R:575:LYS:HA	2.48	0.47
1:V:324:TYR:CE2	1:V:422:LEU:HD21	2.49	0.47
1:W:51:PHE:CD2	1:W:61:ILE:HG12	2.49	0.47
1:X:117:TRP:HA	1:X:469:ILE:HD11	1.95	0.47
1:b:168:ASP:CG	1:b:171:ALA:HB2	2.39	0.47
1:c:551:MET:HE3	1:c:551:MET:HB3	1.76	0.47
1:A:242:GLN:NE2	1:T:580:PRO:HB2	2.29	0.47
1:B:295:PRO:HB2	1:P:565:ASN:OD1	2.13	0.47
1:C:558:GLN:NE2	1:D:236:THR:HB	2.29	0.47
1:F:214:TRP:O	1:F:350:GLN:HG2	2.13	0.47
1:H:283:ARG:NH2	1:W:101:THR:O	2.47	0.47
1:H:382:ARG:NH2	1:H:392:GLY:O	2.47	0.47
1:M:556:ASP:O	1:M:558:GLN:N	2.39	0.47
1:O:338:TYR:CE1	1:O:358:ALA:HB3	2.45	0.47
1:S:411:GLU:OE1	1:S:411:GLU:N	2.45	0.47
1:T:468:GLN:HB3	1:T:486:ALA:HB2	1.96	0.47
1:U:383:GLN:C	1:U:384:HIS:HD2	2.21	0.47
1:V:339:SER:O	1:V:449:ASN:HA	2.14	0.47
1:V:383:GLN:HB3	1:V:384:HIS:CD2	2.48	0.47
1:X:573:TYR:O	1:X:574:GLU:HG3	2.14	0.47
1:Y:442:ILE:HG21	1:a:430:LEU:HD22	1.96	0.47
1:Z:130:VAL:HG13	1:Z:576:SER:O	2.14	0.47
1:Z:336:VAL:O	1:Z:408:ARG:NH2	2.47	0.47
1:E:159:GLN:O	1:E:161:PRO:HA	2.13	0.47
1:D:159:GLN:HG2	1:D:160:PRO:HD3	1.96	0.47
1:H:563:PRO:HB3	1:H:569:MET:HE2	1.97	0.47
1:K:162:THR:HG21	1:M:155:GLU:OE2	2.13	0.47
1:L:383:GLN:CB	1:L:384:HIS:HD2	2.25	0.47
1:a:79:TYR:OH	1:a:247:GLU:OE1	2.28	0.47
1:c:269:ASP:HB3	1:c:492:ASN:HD21	1.78	0.47
1:d:156:SER:O	1:d:156:SER:OG	2.20	0.47
1:A:383:GLN:HB3	1:A:384:HIS:CD2	2.49	0.47
1:E:554:ASN:HD22	1:E:557:ASN:HD22	1.62	0.47
1:N:457:LEU:O	1:S:476:THR:HB	2.13	0.47
1:C:447:ILE:HG22	1:P:415:ILE:CD1	2.44	0.47
1:C:476:THR:HB	1:P:457:LEU:O	2.14	0.47
1:F:434:ASP:OD2	1:L:439:LYS:NZ	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:234:HIS:ND1	1:V:365:GLN:OE1	2.47	0.47
1:K:286:GLY:O	1:K:288:PRO:HD3	2.14	0.47
1:L:547:PRO:HD3	1:b:123:PRO:HB2	1.96	0.47
1:V:383:GLN:CB	1:V:384:HIS:HD2	2.26	0.47
1:W:266:PHE:HZ	1:W:493:ASN:O	1.97	0.47
1:X:154:SER:HA	1:X:155:GLU:CB	2.44	0.47
1:X:157:ALA:HA	1:X:158:THR:OG1	2.14	0.47
1:X:216:ARG:NH1	1:X:231:ASN:OD1	2.42	0.47
1:Y:411:GLU:OE1	1:Y:411:GLU:N	2.46	0.47
1:Z:417:ASN:OD1	1:Z:418:ILE:N	2.46	0.47
1:a:377:ARG:NH2	1:a:397:ARG:HD2	2.29	0.47
1:c:109:TRP:CD1	1:c:246:ILE:HG13	2.50	0.47
1:d:159:GLN:CB	1:d:160:PRO:HD2	2.43	0.47
1:E:383:GLN:HB3	1:E:384:HIS:CD2	2.48	0.47
1:E:556:ASP:O	1:E:557:ASN:HB3	2.13	0.47
1:J:154:SER:HA	1:J:155:GLU:CB	2.39	0.47
1:N:422:LEU:HA	1:N:423:PRO:C	2.39	0.47
1:C:354:LYS:HG2	1:C:355:THR:N	2.30	0.47
1:F:319:MET:HE3	1:F:329:THR:HG23	1.95	0.47
1:G:159:GLN:CD	1:G:160:PRO:HD2	2.39	0.47
1:H:556:ASP:O	1:H:557:ASN:HB3	2.13	0.47
1:L:302:ASN:HB3	1:b:565:ASN:ND2	2.29	0.47
1:R:460:VAL:HG11	1:R:484:VAL:HA	1.97	0.47
1:T:105:ILE:HG12	1:T:212:PHE:HB2	1.96	0.47
1:U:338:TYR:HE1	1:U:358:ALA:HB3	1.79	0.47
1:a:365:GLN:HB2	1:a:366:THR:HA	1.97	0.47
1:d:102:HIS:HB2	1:d:214:TRP:CH2	2.50	0.47
1:B:48:GLN:O	1:B:64:ASN:HB2	2.15	0.47
1:D:383:GLN:HB3	1:D:384:HIS:CD2	2.49	0.47
1:D:434:ASP:HA	1:D:435:PRO:HD3	1.72	0.47
1:V:131:ASN:O	1:V:550:GLN:NE2	2.47	0.47
1:W:445:THR:HA	1:W:448:PHE:HB2	1.96	0.47
1:X:558:GLN:O	1:X:558:GLN:HG2	2.12	0.47
1:Y:209:ARG:HD2	1:a:288:PRO:O	2.14	0.47
1:Z:326:THR:H	1:Z:329:THR:HB	1.80	0.47
1:Z:417:ASN:OD1	1:Z:418:ILE:HG22	2.13	0.47
1:A:185:PHE:CD2	1:A:187:PRO:HD3	2.49	0.47
1:A:256:ARG:HH12	1:N:257:THR:HG22	1.80	0.47
1:A:349:THR:HG22	1:A:350:GLN:HG3	1.96	0.47
1:E:581:ARG:O	1:E:582:LYS:HB2	2.14	0.47
1:J:558:GLN:O	1:J:558:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:92:VAL:O	1:N:93:ASN:HB2	2.15	0.47
1:N:369:ASN:O	1:N:371:ALA:N	2.48	0.47
1:N:546:ASN:ND2	1:N:547:PRO:O	2.39	0.47
1:B:383:GLN:HB3	1:B:384:HIS:CD2	2.50	0.47
1:C:382:ARG:NH2	1:C:392:GLY:O	2.47	0.47
1:F:77:GLU:HB2	1:F:518:MET:HE1	1.95	0.47
1:G:104:GLU:HG2	1:G:209:ARG:NE	2.30	0.47
1:G:154:SER:HA	1:G:155:GLU:CB	2.33	0.47
1:I:185:PHE:CD2	1:I:187:PRO:HD3	2.50	0.47
1:I:462:PRO:HD2	1:I:576:SER:OG	2.15	0.47
1:K:411:GLU:OE1	1:K:411:GLU:N	2.46	0.47
1:R:114:ALA:HB1	1:R:119:VAL:HG11	1.96	0.47
1:R:554:ASN:HD22	1:R:557:ASN:HD22	1.62	0.47
1:S:238:PRO:HA	1:S:241:VAL:HG23	1.96	0.47
1:S:558:GLN:HG2	1:S:558:GLN:O	2.15	0.47
1:T:137:HIS:CE1	1:T:272:PRO:HB3	2.49	0.47
1:T:434:ASP:HA	1:T:435:PRO:HD3	1.66	0.47
1:U:115:ASN:ND2	1:U:470:TRP:O	2.38	0.47
1:U:191:ARG:O	1:U:193:GLU:HG3	2.15	0.47
1:U:252:VAL:HB	1:X:45:PHE:HB3	1.95	0.47
1:W:382:ARG:HD2	1:Y:513:ASP:O	2.14	0.47
1:Z:46:ASN:OD1	1:Z:48:GLN:HB2	2.15	0.47
1:a:77:GLU:HB2	1:a:518:MET:HE1	1.96	0.47
1:b:136:LEU:HD12	1:b:537:ALA:HB2	1.97	0.47
1:b:556:ASP:O	1:b:557:ASN:HB3	2.14	0.47
1:c:44:THR:O	1:c:530:LYS:NZ	2.39	0.47
1:c:338:TYR:HE1	1:c:358:ALA:HB3	1.80	0.47
1:d:556:ASP:O	1:d:557:ASN:HB3	2.15	0.47
1:Q:92:VAL:O	1:Q:93:ASN:HB2	2.14	0.47
1:C:369:ASN:C	1:C:371:ALA:N	2.65	0.47
1:F:411:GLU:OE1	1:F:411:GLU:N	2.41	0.47
1:F:447:ILE:HG22	1:d:415:ILE:CD1	2.45	0.47
1:H:59:VAL:HG21	1:H:133:MET:HE2	1.97	0.47
1:L:92:VAL:O	1:L:93:ASN:HB2	2.14	0.47
1:L:383:GLN:C	1:L:384:HIS:HD2	2.23	0.47
1:M:354:LYS:HD2	1:R:319:MET:HE2	1.96	0.47
1:R:257:THR:HG22	1:T:256:ARG:NH1	2.30	0.47
1:T:436:ILE:HD13	1:T:436:ILE:HA	1.74	0.47
1:T:550:GLN:HA	1:T:578:LEU:HD23	1.97	0.47
1:a:339:SER:O	1:a:449:ASN:HA	2.13	0.47
1:A:248:ASN:ND2	1:N:122:ASN:HD22	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:550:GLN:HA	1:E:578:LEU:HD23	1.96	0.47
1:N:75:GLU:HG2	1:N:76:SER:N	2.29	0.47
1:D:361:ARG:O	1:D:361:ARG:NH1	2.48	0.47
1:D:556:ASP:O	1:D:558:GLN:N	2.36	0.47
1:G:105:ILE:HG12	1:G:212:PHE:HB2	1.96	0.47
1:I:369:ASN:O	1:I:371:ALA:N	2.48	0.47
1:L:274:ARG:HH12	1:d:475:ASP:CG	2.22	0.47
1:L:431:LEU:HD22	1:d:220:PRO:HB2	1.97	0.47
1:M:194:THR:H	1:M:384:HIS:HE1	1.63	0.47
1:R:107:THR:HG21	1:R:208:TRP:CE3	2.49	0.47
1:V:376:PRO:HG2	1:V:400:TYR:HB3	1.97	0.47
1:W:152:THR:HG23	1:W:168:ASP:HB2	1.97	0.47
1:W:339:SER:OG	1:b:346:GLU:OE1	2.26	0.47
1:Y:414:TRP:NE1	1:Y:416:GLN:HE21	2.13	0.47
1:Z:177:LEU:HD22	1:Z:263:THR:HG22	1.97	0.47
1:E:457:LEU:O	1:V:476:THR:HB	2.15	0.47
1:J:352:PRO:HD2	1:U:283:ARG:HH12	1.80	0.47
1:D:361:ARG:NH2	1:D:405:ASP:CB	2.76	0.47
1:F:203:THR:OG1	1:F:204:ILE:N	2.48	0.47
1:F:248:ASN:HD22	1:G:122:ASN:ND2	2.13	0.47
1:H:475:ASP:CG	1:b:274:ARG:HH12	2.22	0.47
1:P:339:SER:O	1:P:449:ASN:HA	2.15	0.47
1:P:492:ASN:OD1	1:P:493:ASN:N	2.48	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:W:77:GLU:HB2	1:W:518:MET:HE1	1.97	0.47
1:Y:476:THR:HB	1:a:457:LEU:O	2.14	0.47
1:a:581:ARG:HB3	1:a:582:LYS:H	1.51	0.47
1:N:157:ALA:HA	1:N:158:THR:OG1	2.15	0.46
1:N:490:CYS:HB3	1:N:492:ASN:OD1	2.14	0.46
1:C:336:VAL:O	1:C:408:ARG:NH2	2.47	0.46
1:G:411:GLU:OE1	1:G:411:GLU:N	2.46	0.46
1:H:266:PHE:HZ	1:H:493:ASN:O	1.97	0.46
1:I:69:VAL:CG1	1:I:205:PRO:HD3	2.45	0.46
1:K:558:GLN:HE21	1:K:558:GLN:HB3	1.52	0.46
1:L:47:ASN:OD1	1:L:67:ARG:NH1	2.42	0.46
1:L:298:GLU:HG2	1:b:566:ILE:HG12	1.97	0.46
1:M:92:VAL:O	1:M:93:ASN:HB2	2.15	0.46
1:O:381:GLY:HA2	1:O:386:GLN:HG3	1.97	0.46
1:Y:139:VAL:HB	1:Y:534:VAL:O	2.15	0.46
1:b:339:SER:O	1:b:449:ASN:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:203:THR:OG1	1:c:204:ILE:N	2.48	0.46
1:d:369:ASN:C	1:d:371:ALA:N	2.73	0.46
1:d:492:ASN:CG	1:d:493:ASN:N	2.72	0.46
1:A:123:PRO:HB2	1:I:547:PRO:HD3	1.96	0.46
1:J:401:ILE:O	1:J:575:LYS:NZ	2.49	0.46
1:J:554:ASN:CB	1:J:557:ASN:HB3	2.42	0.46
1:N:131:ASN:HB3	1:N:550:GLN:NE2	2.30	0.46
1:N:393:GLU:H	1:N:393:GLU:CD	2.23	0.46
1:Q:177:LEU:HD22	1:Q:263:THR:HG22	1.97	0.46
1:F:183:MET:HE1	1:F:246:ILE:HD13	1.96	0.46
1:F:383:GLN:C	1:F:384:HIS:CD2	2.93	0.46
1:G:326:THR:HG21	1:c:98:LEU:HA	1.97	0.46
1:K:554:ASN:O	1:K:558:GLN:HB2	2.15	0.46
1:S:319:MET:HE3	1:S:329:THR:HG23	1.96	0.46
1:S:383:GLN:C	1:S:384:HIS:HD2	2.23	0.46
1:Z:256:ARG:NH1	1:c:257:THR:HG22	2.31	0.46
1:b:572:VAL:HG12	1:b:573:TYR:O	2.15	0.46
1:A:102:HIS:HA	1:A:214:TRP:CE2	2.51	0.46
1:J:471:ASP:OD1	1:U:584:TYR:OH	2.28	0.46
1:Q:157:ALA:HA	1:Q:158:THR:OG1	2.14	0.46
1:K:435:PRO:HB3	1:K:439:LYS:O	2.14	0.46
1:L:518:MET:HE1	1:M:202:PRO:HG2	1.97	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	1.98	0.46
1:b:560:ASN:HB3	1:b:572:VAL:HG21	1.97	0.46
1:A:239:ASP:HB3	1:T:549:GLN:NE2	2.30	0.46
1:J:476:THR:HB	1:U:457:LEU:O	2.16	0.46
1:Q:137:HIS:CD2	1:Q:272:PRO:HB3	2.50	0.46
1:Q:369:ASN:C	1:Q:371:ALA:H	2.23	0.46
1:C:222:HIS:O	1:C:225:THR:HG22	2.15	0.46
1:D:73:MET:CE	1:D:522:VAL:HA	2.46	0.46
1:D:400:TYR:CE2	1:D:575:LYS:HA	2.51	0.46
1:D:556:ASP:O	1:D:557:ASN:HB3	2.15	0.46
1:G:556:ASP:O	1:G:557:ASN:HB3	2.14	0.46
1:I:101:THR:O	1:V:283:ARG:NH2	2.48	0.46
1:K:152:THR:HG23	1:K:168:ASP:HB2	1.98	0.46
1:L:286:GLY:O	1:L:288:PRO:HD3	2.15	0.46
1:U:133:MET:HG3	1:U:539:LEU:HD23	1.97	0.46
1:X:161:PRO:O	1:X:162:THR:HG22	2.14	0.46
1:a:558:GLN:HG2	1:a:558:GLN:O	2.15	0.46
1:N:274:ARG:HH12	1:S:475:ASP:CG	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:319:MET:HE3	1:G:329:THR:HG23	1.97	0.46
1:G:324:TYR:CE2	1:G:422:LEU:HD21	2.50	0.46
1:G:389:THR:HG23	1:G:568:GLY:O	2.14	0.46
1:H:274:ARG:HH12	1:W:475:ASP:CG	2.23	0.46
1:K:462:PRO:HD2	1:K:576:SER:OG	2.15	0.46
1:M:137:HIS:NE2	1:M:272:PRO:HB3	2.31	0.46
1:O:378:TYR:CE1	1:O:463:VAL:HG11	2.51	0.46
1:S:159:GLN:HG3	1:S:160:PRO:CD	2.46	0.46
1:T:411:GLU:OE1	1:T:411:GLU:N	2.45	0.46
1:X:247:GLU:OE1	1:X:247:GLU:N	2.42	0.46
1:A:354:LYS:HD2	1:T:319:MET:HE2	1.98	0.46
1:E:581:ARG:HB3	1:E:582:LYS:H	1.56	0.46
1:J:109:TRP:CD1	1:J:246:ILE:HG13	2.51	0.46
1:N:137:HIS:NE2	1:N:272:PRO:HB3	2.30	0.46
1:B:113:ASP:O	1:B:195:LEU:HG	2.15	0.46
1:B:203:THR:OG1	1:B:204:ILE:N	2.47	0.46
1:F:75:GLU:HG2	1:F:76:SER:N	2.31	0.46
1:F:547:PRO:HD3	1:M:123:PRO:HB2	1.98	0.46
1:F:550:GLN:HA	1:F:578:LEU:HD23	1.97	0.46
1:G:271:LYS:HB2	1:G:271:LYS:HE2	1.78	0.46
1:M:126:TRP:NE1	1:M:130:VAL:HG21	2.30	0.46
1:M:476:THR:O	1:M:479:LYS:HE2	2.15	0.46
1:P:159:GLN:NE2	1:R:161:PRO:HB3	2.25	0.46
1:U:138:LEU:HG	1:U:268:PHE:CD2	2.51	0.46
1:U:159:GLN:HG3	1:U:160:PRO:HD2	1.98	0.46
1:W:310:GLN:OE1	1:b:98:LEU:HD13	2.16	0.46
1:Z:556:ASP:O	1:Z:557:ASN:HB3	2.15	0.46
1:A:214:TRP:O	1:A:350:GLN:HG2	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:B:163:LYS:HE2	1:B:163:LYS:HB3	1.57	0.46
1:C:96:MET:HE2	1:P:414:TRP:CE2	2.51	0.46
1:F:465:PRO:HG3	1:F:571:ILE:HG22	1.96	0.46
1:F:485:ASN:HB3	1:d:331:MET:HE3	1.97	0.46
1:H:159:GLN:O	1:H:161:PRO:HA	2.15	0.46
1:I:558:GLN:NE2	1:K:236:THR:HB	2.26	0.46
1:K:163:LYS:HZ2	1:K:163:LYS:HG2	1.46	0.46
1:L:51:PHE:CD2	1:L:61:ILE:HG12	2.51	0.46
1:L:518:MET:HG3	1:L:520:ARG:HG3	1.97	0.46
1:M:319:MET:HE3	1:M:329:THR:HG23	1.98	0.46
1:P:126:TRP:NE1	1:P:130:VAL:HG21	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:550:GLN:HA	1:S:578:LEU:HD23	1.98	0.46
1:V:435:PRO:HB3	1:V:439:LYS:O	2.15	0.46
1:W:436:ILE:HD13	1:W:436:ILE:HA	1.77	0.46
1:W:554:ASN:HD22	1:W:557:ASN:HD22	1.64	0.46
1:X:161:PRO:CD	1:X:162:THR:H	2.28	0.46
1:Y:96:MET:HE2	1:a:414:TRP:CE2	2.50	0.46
1:Y:242:GLN:NE2	1:a:580:PRO:HB2	2.31	0.46
1:Z:160:PRO:HG2	1:Z:162:THR:HG23	1.98	0.46
1:Z:550:GLN:HA	1:Z:578:LEU:HD23	1.98	0.46
1:Z:554:ASN:CB	1:Z:557:ASN:HB3	2.43	0.46
1:a:127:GLN:CG	1:a:551:MET:HE2	2.46	0.46
1:A:554:ASN:HB2	1:A:557:ASN:HD22	1.80	0.46
1:E:478:LEU:HD13	1:I:481:ARG:HB3	1.97	0.46
1:D:464:TYR:O	1:D:573:TYR:HA	2.16	0.46
1:F:398:PHE:CE2	1:F:573:TYR:HB2	2.51	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:I:485:ASN:HB3	1:V:331:MET:HE3	1.98	0.46
1:U:361:ARG:NH1	1:U:363:GLY:O	2.49	0.46
1:V:414:TRP:NE1	1:V:416:GLN:HE21	2.14	0.46
1:W:485:ASN:OD1	1:W:485:ASN:N	2.46	0.46
1:a:382:ARG:NH2	1:a:392:GLY:O	2.48	0.46
1:a:568:GLY:HA3	1:a:569:MET:HB2	1.97	0.46
1:b:75:GLU:HG3	1:b:76:SER:H	1.81	0.46
1:b:572:VAL:O	1:b:574:GLU:HG2	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:C:322:THR:HG21	1:C:420:PHE:HD2	1.81	0.46
1:C:492:ASN:CG	1:C:493:ASN:H	2.24	0.46
1:G:309:GLN:HG2	1:G:311:ASP:OD1	2.16	0.46
1:H:481:ARG:NH2	1:W:478:LEU:HB3	2.30	0.46
1:T:99:ASP:CG	1:T:216:ARG:HH21	2.23	0.46
1:W:127:GLN:NE2	1:a:548:ILE:H	2.14	0.46
1:Y:154:SER:HA	1:Y:155:GLU:HB3	1.98	0.46
1:Y:460:VAL:HG11	1:Y:484:VAL:HA	1.97	0.46
1:a:203:THR:OG1	1:a:204:ILE:N	2.47	0.46
1:c:216:ARG:NH2	1:c:218:LEU:HD22	2.31	0.46
1:A:92:VAL:O	1:A:93:ASN:HB2	2.16	0.46
1:A:382:ARG:HD2	1:E:513:ASP:O	2.16	0.46
1:A:476:THR:HB	1:T:457:LEU:O	2.15	0.46
1:E:475:ASP:OD2	1:I:581:ARG:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:553:ILE:CA	1:E:554:ASN:HB2	2.30	0.46
1:D:43:GLY:HA3	1:D:146:PHE:CD2	2.51	0.46
1:F:415:ILE:CD1	1:L:447:ILE:HG22	2.44	0.46
1:H:471:ASP:OD1	1:b:584:TYR:OH	2.22	0.46
1:I:148:VAL:O	1:I:257:THR:HG23	2.16	0.46
1:M:102:HIS:HB2	1:M:214:TRP:CH2	2.51	0.46
1:M:112:VAL:HG13	1:M:195:LEU:HD21	1.97	0.46
1:R:139:VAL:HB	1:R:534:VAL:O	2.16	0.46
1:S:339:SER:H	1:S:450:THR:HG1	1.63	0.46
1:T:114:ALA:HB1	1:T:119:VAL:HG11	1.98	0.46
1:V:338:TYR:CE1	1:V:358:ALA:HB3	2.51	0.46
1:X:551:MET:HB3	1:X:551:MET:HE2	1.63	0.46
1:Y:209:ARG:HG3	1:a:287:LEU:HD11	1.98	0.46
1:Y:211:TYR:CG	1:a:288:PRO:HG3	2.51	0.46
1:Y:212:PHE:CZ	1:Y:241:VAL:HG13	2.51	0.46
1:Y:451:TYR:CE1	1:a:453:PRO:HD3	2.50	0.46
1:Y:475:ASP:OD2	1:a:581:ARG:HD3	2.16	0.46
1:b:158:THR:O	1:b:159:GLN:O	2.34	0.46
1:c:326:THR:H	1:c:329:THR:HB	1.81	0.46
1:A:190:MET:HE1	1:T:331:MET:HB3	1.98	0.45
1:E:191:ARG:O	1:E:193:GLU:HG3	2.15	0.45
1:N:551:MET:HE3	1:N:551:MET:HB3	1.78	0.45
1:D:155:GLU:HA	1:D:163:LYS:HG3	1.97	0.45
1:H:318:GLN:HB3	1:W:354:LYS:HE2	1.99	0.45
1:L:460:VAL:HG11	1:L:484:VAL:HA	1.98	0.45
1:W:283:ARG:HH12	1:b:352:PRO:HD2	1.80	0.45
1:W:331:MET:HE3	1:b:485:ASN:HB3	1.98	0.45
1:X:363:GLY:HA3	1:X:367:ASP:O	2.16	0.45
1:Z:435:PRO:HB3	1:Z:439:LYS:O	2.16	0.45
1:a:431:LEU:C	1:a:433:THR:H	2.24	0.45
1:b:558:GLN:HE22	1:d:236:THR:HB	1.80	0.45
1:E:326:THR:HG21	1:V:98:LEU:HA	1.98	0.45
1:E:558:GLN:NE2	1:J:236:THR:O	2.38	0.45
1:B:518:MET:HE2	1:B:518:MET:HB2	1.69	0.45
1:C:203:THR:OG1	1:C:204:ILE:N	2.47	0.45
1:D:257:THR:HG22	1:G:256:ARG:NH1	2.31	0.45
1:F:256:ARG:NH1	1:G:257:THR:HG22	2.32	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:O:376:PRO:HD2	1:O:400:TYR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:369:ASN:C	1:S:371:ALA:H	2.25	0.45
1:W:280:GLN:NE2	1:W:583:LEU:H	2.13	0.45
1:Z:75:GLU:CD	1:Z:75:GLU:H	2.23	0.45
1:a:163:LYS:HB3	1:a:163:LYS:HE3	1.43	0.45
1:a:362:GLY:HA3	1:a:407:GLY:C	2.40	0.45
1:a:563:PRO:HB3	1:a:569:MET:HE2	1.98	0.45
1:b:43:GLY:HA3	1:b:146:PHE:CD2	2.51	0.45
1:d:383:GLN:C	1:d:384:HIS:CD2	2.94	0.45
1:Q:266:PHE:HZ	1:Q:493:ASN:O	1.99	0.45
1:B:415:ILE:CD1	1:R:447:ILE:HG22	2.42	0.45
1:D:554:ASN:O	1:D:558:GLN:HB2	2.16	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:X:324:TYR:CE2	1:X:422:LEU:HD21	2.51	0.45
1:Y:154:SER:O	1:Y:154:SER:OG	2.26	0.45
1:d:157:ALA:HA	1:d:158:THR:OG1	2.16	0.45
1:J:278:THR:HB	1:J:583:LEU:HD13	1.97	0.45
1:C:43:GLY:HA3	1:C:146:PHE:CD2	2.51	0.45
1:F:317:THR:HG22	1:F:330:ILE:HA	1.99	0.45
1:I:369:ASN:C	1:I:371:ALA:N	2.74	0.45
1:P:109:TRP:CD1	1:P:246:ILE:HG13	2.52	0.45
1:U:473:GLU:OE1	1:U:483:HIS:NE2	2.46	0.45
1:W:565:ASN:ND2	1:a:299:GLY:H	2.14	0.45
1:Y:73:MET:CE	1:Y:522:VAL:HA	2.47	0.45
1:Y:382:ARG:N	1:Y:386:GLN:HB3	2.22	0.45
1:Z:225:THR:HG22	1:Z:226:SER:O	2.17	0.45
1:d:383:GLN:HB3	1:d:384:HIS:CD2	2.51	0.45
1:d:462:PRO:HD2	1:d:576:SER:OG	2.16	0.45
1:A:52:LYS:HB3	1:A:60:TYR:HB3	1.97	0.45
1:A:447:ILE:HG22	1:T:415:ILE:CD1	2.45	0.45
1:A:513:ASP:O	1:N:382:ARG:HD2	2.16	0.45
1:J:266:PHE:HZ	1:J:493:ASN:O	2.00	0.45
1:B:378:TYR:CE1	1:B:463:VAL:HG11	2.52	0.45
1:B:434:ASP:HA	1:B:435:PRO:HD3	1.76	0.45
1:D:191:ARG:O	1:D:193:GLU:HG3	2.17	0.45
1:F:517:ASN:OD1	1:F:517:ASN:N	2.49	0.45
1:F:554:ASN:O	1:F:558:GLN:HB2	2.17	0.45
1:G:150:LEU:HD22	1:G:171:ALA:HB1	1.98	0.45
1:I:154:SER:O	1:I:154:SER:OG	2.28	0.45
1:K:278:THR:HB	1:K:583:LEU:HD13	1.98	0.45
1:M:485:ASN:OD1	1:M:485:ASN:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:485:ASN:OD1	1:O:485:ASN:N	2.42	0.45
1:R:581:ARG:O	1:R:582:LYS:HB2	2.15	0.45
1:T:558:GLN:O	1:T:558:GLN:HG2	2.17	0.45
1:W:326:THR:H	1:W:329:THR:HB	1.81	0.45
1:X:384:HIS:ND1	1:X:384:HIS:N	2.65	0.45
1:a:338:TYR:HE1	1:a:358:ALA:HB3	1.82	0.45
1:b:336:VAL:O	1:b:408:ARG:NH2	2.49	0.45
1:d:191:ARG:O	1:d:193:GLU:HG3	2.16	0.45
1:E:408:ARG:HD3	1:E:408:ARG:HA	1.77	0.45
1:E:426:ASP:HB2	1:V:222:HIS:ND1	2.31	0.45
1:N:333:PRO:HG2	1:S:474:PHE:HZ	1.82	0.45
1:D:573:TYR:O	1:D:574:GLU:HG3	2.16	0.45
1:K:362:GLY:O	1:T:349:THR:N	2.50	0.45
1:M:339:SER:O	1:M:449:ASN:HA	2.16	0.45
1:O:581:ARG:O	1:O:582:LYS:HB2	2.16	0.45
1:P:148:VAL:O	1:P:257:THR:HG23	2.16	0.45
1:R:70:HIS:O	1:R:204:ILE:HG22	2.16	0.45
1:R:183:MET:HE1	1:R:246:ILE:HD13	1.98	0.45
1:U:194:THR:H	1:U:384:HIS:HE1	1.65	0.45
1:U:558:GLN:NE2	1:V:236:THR:HB	2.31	0.45
1:V:168:ASP:CG	1:V:171:ALA:HB2	2.42	0.45
1:W:247:GLU:OE1	1:W:247:GLU:N	2.45	0.45
1:Z:383:GLN:C	1:Z:384:HIS:CD2	2.94	0.45
1:J:186:THR:HB	1:U:287:LEU:HB2	1.99	0.45
1:J:556:ASP:O	1:J:557:ASN:HB3	2.17	0.45
1:B:386:GLN:HG3	1:B:396:GLU:HB2	1.97	0.45
1:C:492:ASN:CG	1:C:493:ASN:N	2.74	0.45
1:D:338:TYR:CE1	1:D:358:ALA:HB3	2.52	0.45
1:F:127:GLN:HG3	1:F:551:MET:HB2	1.99	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:M:156:SER:OG	1:M:164:VAL:HG22	2.16	0.45
1:S:157:ALA:HA	1:S:158:THR:OG1	2.16	0.45
1:S:409:TYR:CE2	1:S:411:GLU:HB2	2.51	0.45
1:U:369:ASN:C	1:U:371:ALA:H	2.24	0.45
1:V:558:GLN:O	1:V:558:GLN:HG2	2.17	0.45
1:Z:59:VAL:O	1:Z:536:LYS:HA	2.17	0.45
1:b:247:GLU:OE1	1:b:247:GLU:N	2.47	0.45
1:c:58:TRP:CZ3	1:c:538:LYS:HB2	2.51	0.45
1:c:554:ASN:O	1:c:558:GLN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:MET:HE2	1:I:414:TRP:CE2	2.51	0.45
1:E:411:GLU:OE1	1:E:411:GLU:N	2.44	0.45
1:N:424:VAL:HG12	1:S:94:GLY:HA2	1.98	0.45
1:G:518:MET:HE2	1:G:518:MET:HB2	1.71	0.45
1:H:439:LYS:NZ	1:b:434:ASP:OD2	2.31	0.45
1:I:319:MET:HE3	1:I:329:THR:HG23	1.98	0.45
1:K:558:GLN:O	1:K:558:GLN:HG2	2.15	0.45
1:M:105:ILE:HG12	1:M:212:PHE:HB2	1.98	0.45
1:O:139:VAL:HB	1:O:534:VAL:O	2.16	0.45
1:O:386:GLN:HG2	1:O:396:GLU:HB3	1.99	0.45
1:T:572:VAL:HG12	1:T:573:TYR:O	2.17	0.45
1:V:200:TRP:CZ3	1:W:245:THR:HG21	2.52	0.45
1:X:445:THR:HA	1:X:448:PHE:HB2	1.98	0.45
1:X:493:ASN:OD1	1:X:493:ASN:N	2.49	0.45
1:X:518:MET:HE2	1:X:518:MET:HB2	1.74	0.45
1:A:451:TYR:CD2	1:T:452:GLY:HA2	2.51	0.45
1:E:434:ASP:HA	1:E:435:PRO:HD3	1.63	0.45
1:E:476:THR:HG22	1:I:583:LEU:HD11	1.99	0.45
1:Q:554:ASN:HB3	1:Q:556:ASP:O	2.17	0.45
1:C:98:LEU:HA	1:P:326:THR:HG21	1.99	0.45
1:C:432:PRO:C	1:C:443:ASN:HD22	2.24	0.45
1:D:362:GLY:O	1:D:409:TYR:HB2	2.17	0.45
1:D:369:ASN:C	1:D:371:ALA:H	2.24	0.45
1:F:137:HIS:CE1	1:F:272:PRO:HB3	2.51	0.45
1:G:104:GLU:HG2	1:G:209:ARG:CZ	2.47	0.45
1:G:367:ASP:N	1:G:367:ASP:OD1	2.49	0.45
1:O:48:GLN:NE2	1:P:249:SER:O	2.50	0.45
1:S:92:VAL:O	1:S:93:ASN:HB2	2.16	0.45
1:T:581:ARG:HB3	1:T:582:LYS:H	1.57	0.45
1:V:117:TRP:CE2	1:V:469:ILE:HG12	2.52	0.45
1:Y:414:TRP:HE1	1:Y:416:GLN:NE2	2.15	0.45
1:Z:346:GLU:O	1:Z:352:PRO:HA	2.17	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:B:383:GLN:C	1:B:384:HIS:HD2	2.25	0.45
1:G:432:PRO:C	1:G:443:ASN:HD22	2.20	0.45
1:H:382:ARG:HD2	1:I:513:ASP:O	2.16	0.45
1:I:92:VAL:O	1:I:93:ASN:HB2	2.17	0.45
1:K:154:SER:CA	1:K:155:GLU:HB2	2.31	0.45
1:L:414:TRP:CE2	1:d:96:MET:HE2	2.52	0.45
1:M:338:TYR:CE1	1:M:358:ALA:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:157:ALA:HA	1:O:158:THR:OG1	2.17	0.45
1:O:216:ARG:NH1	1:O:231:ASN:OD1	2.42	0.45
1:O:382:ARG:HD2	1:P:513:ASP:O	2.17	0.45
1:S:556:ASP:O	1:S:557:ASN:HB3	2.17	0.45
1:T:556:ASP:O	1:T:557:ASN:HB3	2.16	0.45
1:V:411:GLU:OE1	1:V:411:GLU:N	2.49	0.45
1:V:551:MET:HE3	1:V:551:MET:HB3	1.80	0.45
1:Y:322:THR:HB	1:Y:324:TYR:H	1.81	0.45
1:J:475:ASP:OD1	1:U:274:ARG:NH1	2.37	0.44
1:N:238:PRO:HA	1:N:241:VAL:HG23	1.98	0.44
1:Q:338:TYR:HE1	1:Q:358:ALA:HB3	1.82	0.44
1:B:457:LEU:O	1:R:476:THR:HB	2.17	0.44
1:D:153:VAL:HG12	1:D:155:GLU:HG3	1.99	0.44
1:D:383:GLN:C	1:D:384:HIS:CD2	2.96	0.44
1:F:583:LEU:HD11	1:L:476:THR:HG22	1.99	0.44
1:G:378:TYR:CE1	1:G:463:VAL:HG11	2.52	0.44
1:G:431:LEU:HD22	1:c:220:PRO:HB2	1.98	0.44
1:H:281:THR:OG1	1:W:350:GLN:OE1	2.18	0.44
1:M:434:ASP:HA	1:M:435:PRO:HD3	1.76	0.44
1:M:556:ASP:O	1:M:557:ASN:HB3	2.16	0.44
1:O:297:SER:OG	1:O:302:ASN:ND2	2.49	0.44
1:P:191:ARG:O	1:P:193:GLU:HG3	2.18	0.44
1:P:368:GLU:HG3	1:P:369:ASN:N	2.33	0.44
1:S:114:ALA:HB2	1:S:195:LEU:HD12	1.99	0.44
1:U:415:ILE:HG13	1:U:444:TYR:CZ	2.52	0.44
1:W:45:PHE:HB3	1:Y:252:VAL:HB	1.99	0.44
1:Y:338:TYR:HE1	1:Y:358:ALA:HB3	1.81	0.44
1:a:388:THR:OG1	1:a:569:MET:N	2.49	0.44
1:A:557:ASN:O	1:A:559:PHE:N	2.50	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:J:461:PRO:HA	1:J:462:PRO:HD3	1.89	0.44
1:J:581:ARG:HB3	1:J:582:LYS:H	1.51	0.44
1:B:207:PRO:O	1:B:209:ARG:NH1	2.49	0.44
1:B:339:SER:O	1:B:449:ASN:HA	2.18	0.44
1:B:369:ASN:C	1:B:371:ALA:N	2.75	0.44
1:C:338:TYR:CE1	1:C:358:ALA:HB3	2.52	0.44
1:C:425:THR:HG22	1:C:427:ASP:H	1.82	0.44
1:F:136:LEU:HD12	1:F:537:ALA:HB2	1.99	0.44
1:G:105:ILE:O	1:G:209:ARG:HD3	2.16	0.44
1:G:382:ARG:N	1:G:386:GLN:HB3	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:319:MET:HE3	1:H:329:THR:HG23	1.98	0.44
1:H:326:THR:HG21	1:W:98:LEU:HA	2.00	0.44
1:H:475:ASP:OD2	1:b:581:ARG:HD3	2.18	0.44
1:O:434:ASP:HA	1:O:435:PRO:HD3	1.73	0.44
1:P:214:TRP:O	1:P:350:GLN:HG2	2.17	0.44
1:V:415:ILE:HD11	1:V:444:TYR:CE2	2.52	0.44
1:W:133:MET:CG	1:W:539:LEU:HD23	2.47	0.44
1:W:551:MET:HE3	1:W:551:MET:HB3	1.75	0.44
1:X:382:ARG:N	1:X:386:GLN:HB3	2.16	0.44
1:a:468:GLN:HB3	1:a:485:ASN:O	2.17	0.44
1:b:216:ARG:NH1	1:b:231:ASN:OD1	2.49	0.44
1:E:280:GLN:NE2	1:E:583:LEU:N	2.62	0.44
1:D:403:HIS:CD2	1:D:549:GLN:HE22	2.35	0.44
1:G:177:LEU:HD22	1:G:263:THR:HG22	1.98	0.44
1:H:209:ARG:NE	1:b:288:PRO:O	2.37	0.44
1:I:96:MET:HG2	1:I:220:PRO:HA	1.99	0.44
1:I:476:THR:HB	1:V:457:LEU:O	2.17	0.44
1:K:540:ARG:HH21	1:K:550:GLN:NE2	2.15	0.44
1:L:287:LEU:HD12	1:L:288:PRO:HD2	1.99	0.44
1:M:297:SER:O	1:M:302:ASN:ND2	2.42	0.44
1:M:346:GLU:OE1	1:R:408:ARG:NH1	2.51	0.44
1:R:131:ASN:HB3	1:R:550:GLN:HE21	1.81	0.44
1:S:377:ARG:HH21	1:S:397:ARG:HD2	1.82	0.44
1:W:382:ARG:N	1:W:386:GLN:HB3	2.27	0.44
1:W:434:ASP:HA	1:W:435:PRO:HD3	1.74	0.44
1:W:468:GLN:HB3	1:W:486:ALA:HB2	2.00	0.44
1:X:92:VAL:O	1:X:93:ASN:HB2	2.18	0.44
1:X:286:GLY:O	1:X:288:PRO:HD3	2.18	0.44
1:Y:465:PRO:HG3	1:Y:571:ILE:HG22	1.99	0.44
1:a:286:GLY:O	1:a:288:PRO:HD3	2.18	0.44
1:a:549:GLN:O	1:a:550:GLN:HG3	2.17	0.44
1:c:269:ASP:HB3	1:c:492:ASN:CG	2.42	0.44
1:c:339:SER:O	1:c:449:ASN:HA	2.18	0.44
1:d:338:TYR:CE1	1:d:358:ALA:HB3	2.52	0.44
1:d:436:ILE:HD13	1:d:436:ILE:HA	1.76	0.44
1:B:193:GLU:CD	1:B:209:ARG:HH22	2.26	0.44
1:C:193:GLU:OE1	1:C:209:ARG:NH2	2.48	0.44
1:I:157:ALA:HA	1:I:158:THR:HG22	1.98	0.44
1:K:287:LEU:HG	1:T:209:ARG:NH1	2.26	0.44
1:K:298:GLU:OE2	1:R:389:THR:HG21	2.17	0.44
1:L:58:TRP:CE2	1:L:538:LYS:HE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:302:ASN:OD1	1:M:302:ASN:N	2.47	0.44
1:S:136:LEU:HD12	1:S:537:ALA:HB2	1.99	0.44
1:U:383:GLN:HB3	1:U:384:HIS:HD2	1.82	0.44
1:V:408:ARG:HA	1:V:408:ARG:HD3	1.85	0.44
1:V:460:VAL:HG11	1:V:484:VAL:HA	1.98	0.44
1:W:127:GLN:HG3	1:W:551:MET:HE2	2.00	0.44
1:X:339:SER:O	1:X:449:ASN:HA	2.17	0.44
1:Y:554:ASN:O	1:Y:558:GLN:HB2	2.18	0.44
1:Z:434:ASP:HA	1:Z:435:PRO:HD3	1.72	0.44
1:c:137:HIS:NE2	1:c:272:PRO:HB3	2.33	0.44
1:A:203:THR:OG1	1:A:204:ILE:N	2.51	0.44
1:E:558:GLN:O	1:E:558:GLN:HG2	2.16	0.44
1:J:92:VAL:HB	1:J:95:ASN:HB2	2.00	0.44
1:J:357:ILE:HB	1:J:373:ASP:O	2.18	0.44
1:B:154:SER:HA	1:B:155:GLU:CG	2.48	0.44
1:B:319:MET:HE3	1:B:329:THR:HG23	1.99	0.44
1:F:481:ARG:NH2	1:L:478:LEU:HB3	2.33	0.44
1:H:447:ILE:HG22	1:b:415:ILE:CD1	2.44	0.44
1:H:554:ASN:O	1:H:558:GLN:HB2	2.18	0.44
1:I:387:LYS:HE3	1:I:389:THR:OG1	2.18	0.44
1:K:434:ASP:HA	1:K:435:PRO:HD3	1.75	0.44
1:K:540:ARG:HH21	1:K:550:GLN:HE22	1.65	0.44
1:L:256:ARG:NH1	1:M:257:THR:HG22	2.32	0.44
1:M:451:TYR:CD2	1:R:452:GLY:HA2	2.52	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:R:554:ASN:O	1:R:558:GLN:HB2	2.17	0.44
1:S:66:SER:HA	1:S:529:TRP:O	2.18	0.44
1:b:257:THR:HG21	1:d:170:THR:HG22	1.99	0.44
1:c:404:GLN:NE2	1:c:461:PRO:HD3	2.31	0.44
1:E:44:THR:HG22	1:E:530:LYS:NZ	2.31	0.44
1:J:483:HIS:HB3	1:J:485:ASN:OD1	2.17	0.44
1:B:557:ASN:O	1:B:559:PHE:N	2.51	0.44
1:D:346:GLU:OE2	1:D:355:THR:OG1	2.29	0.44
1:F:457:LEU:O	1:L:476:THR:HB	2.17	0.44
1:H:43:GLY:HA3	1:H:146:PHE:CD2	2.53	0.44
1:H:219:ILE:HG23	1:H:220:PRO:HD2	2.00	0.44
1:K:257:THR:HG22	1:M:256:ARG:NH1	2.33	0.44
1:K:581:ARG:HB3	1:K:582:LYS:H	1.60	0.44
1:S:338:TYR:HE1	1:S:358:ALA:HB3	1.82	0.44
1:V:568:GLY:HA3	1:V:569:MET:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:580:PRO:HB2	1:b:242:GLN:NE2	2.33	0.44
1:Z:157:ALA:HA	1:Z:158:THR:OG1	2.18	0.44
1:d:581:ARG:HB3	1:d:582:LYS:H	1.62	0.44
1:B:137:HIS:NE2	1:B:272:PRO:HB3	2.33	0.44
1:B:551:MET:HE3	1:B:551:MET:HB3	1.79	0.44
1:B:568:GLY:HA3	1:B:569:MET:HB2	2.00	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:H:404:GLN:NE2	1:H:461:PRO:HD3	2.33	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:O:105:ILE:HG12	1:O:212:PHE:HB2	2.00	0.44
1:P:338:TYR:HE1	1:P:358:ALA:HB3	1.81	0.44
1:R:260:GLU:HG3	1:R:261:PHE:N	2.32	0.44
1:T:382:ARG:N	1:T:386:GLN:HB3	2.22	0.44
1:U:383:GLN:HB3	1:U:384:HIS:CD2	2.53	0.44
1:V:137:HIS:CD2	1:V:272:PRO:HB3	2.52	0.44
1:Y:190:MET:HE1	1:a:331:MET:HB3	1.99	0.44
1:b:154:SER:CA	1:b:155:GLU:HB3	2.42	0.44
1:c:459:ASN:HD21	1:c:487:PRO:HA	1.83	0.44
1:c:557:ASN:O	1:c:559:PHE:N	2.50	0.44
1:C:150:LEU:HD22	1:C:171:ALA:HB1	1.98	0.44
1:G:368:GLU:OE1	1:G:401:ILE:HD13	2.17	0.44
1:P:583:LEU:HA	1:P:583:LEU:HD12	1.81	0.44
1:X:77:GLU:HB2	1:X:518:MET:HE1	1.98	0.44
1:Y:434:ASP:HA	1:Y:435:PRO:HD3	1.70	0.44
1:A:478:LEU:HD13	1:T:481:ARG:HB3	2.00	0.44
1:E:137:HIS:NE2	1:E:272:PRO:HB3	2.33	0.44
1:E:378:TYR:O	1:E:397:ARG:HA	2.17	0.44
1:N:93:ASN:ND2	1:N:225:THR:O	2.50	0.44
1:N:331:MET:HB3	1:S:190:MET:HE1	2.00	0.44
1:Q:445:THR:HA	1:Q:448:PHE:HB2	1.98	0.44
1:F:239:ASP:OD1	1:d:549:GLN:NE2	2.44	0.44
1:G:558:GLN:O	1:G:558:GLN:HG2	2.16	0.44
1:H:408:ARG:HA	1:H:408:ARG:HD3	1.87	0.44
1:T:191:ARG:O	1:T:193:GLU:HG3	2.17	0.44
1:T:322:THR:HB	1:T:324:TYR:H	1.82	0.44
1:U:492:ASN:HB2	1:U:493:ASN:H	1.49	0.44
1:V:346:GLU:O	1:V:352:PRO:HA	2.18	0.44
1:Z:556:ASP:O	1:Z:558:GLN:N	2.46	0.44
1:c:185:PHE:HB2	1:c:472:LYS:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:H	1:A:55:GLU:HG3	1.50	0.43
1:A:476:THR:O	1:A:479:LYS:HE2	2.17	0.43
1:A:551:MET:HE3	1:A:551:MET:HB3	1.76	0.43
1:N:99:ASP:CG	1:N:216:ARG:HH21	2.25	0.43
1:N:200:TRP:HZ2	1:N:569:MET:HE1	1.82	0.43
1:Q:432:PRO:O	1:Q:443:ASN:ND2	2.45	0.43
1:B:72:ASN:ND2	1:C:508:ASN:O	2.48	0.43
1:C:339:SER:O	1:C:449:ASN:HA	2.17	0.43
1:G:414:TRP:HE1	1:G:416:GLN:HG3	1.82	0.43
1:I:96:MET:HE3	1:I:96:MET:HB2	1.83	0.43
1:K:185:PHE:CD2	1:K:187:PRO:HD3	2.53	0.43
1:K:199:PRO:HD2	1:K:200:TRP:CZ3	2.52	0.43
1:L:132:THR:HG22	1:b:132:THR:HG22	2.00	0.43
1:M:435:PRO:HB3	1:M:439:LYS:O	2.18	0.43
1:T:75:GLU:HG2	1:T:76:SER:N	2.33	0.43
1:T:346:GLU:O	1:T:352:PRO:HA	2.18	0.43
1:V:66:SER:O	1:V:67:ARG:NH1	2.47	0.43
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:Z:138:LEU:HG	1:Z:268:PHE:CD2	2.52	0.43
1:b:436:ILE:HD13	1:b:436:ILE:HA	1.74	0.43
1:c:174:MET:HE2	1:c:252:VAL:HG11	2.00	0.43
1:c:338:TYR:CE1	1:c:358:ALA:HB3	2.53	0.43
1:c:401:ILE:O	1:c:575:LYS:NZ	2.50	0.43
1:c:549:GLN:O	1:c:550:GLN:HG3	2.18	0.43
1:A:377:ARG:HH21	1:A:397:ARG:HD2	1.81	0.43
1:E:475:ASP:CG	1:I:274:ARG:HH12	2.26	0.43
1:N:560:ASN:HB3	1:N:572:VAL:HG21	2.00	0.43
1:Q:154:SER:HA	1:Q:155:GLU:CB	2.46	0.43
1:D:158:THR:O	1:D:159:GLN:O	2.35	0.43
1:F:87:LEU:HA	1:F:90:THR:OG1	2.18	0.43
1:F:383:GLN:HB3	1:F:384:HIS:HD2	1.82	0.43
1:H:338:TYR:CE1	1:H:358:ALA:HB3	2.53	0.43
1:H:376:PRO:HG2	1:H:400:TYR:HB3	1.99	0.43
1:M:77:GLU:HB2	1:M:518:MET:HE1	1.99	0.43
1:M:98:LEU:HA	1:R:326:THR:HG21	1.99	0.43
1:P:546:ASN:ND2	1:P:547:PRO:O	2.48	0.43
1:R:554:ASN:ND2	1:R:557:ASN:HD22	2.16	0.43
1:T:442:ILE:HG23	1:T:446:ASN:HD22	1.83	0.43
1:Z:382:ARG:N	1:Z:386:GLN:HB3	2.23	0.43
1:b:434:ASP:HA	1:b:435:PRO:HD3	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:177:LEU:HD22	1:c:263:THR:HG22	2.00	0.43
1:c:464:TYR:HA	1:c:465:PRO:HA	1.82	0.43
1:d:278:THR:CG2	1:d:458:ASN:HD21	2.31	0.43
1:d:369:ASN:HB3	1:d:372:ALA:HB3	2.00	0.43
1:A:383:GLN:C	1:A:384:HIS:CD2	2.97	0.43
1:E:365:GLN:HG2	1:E:366:THR:HG23	1.99	0.43
1:N:395:PRO:HG2	1:N:397:ARG:NH1	2.33	0.43
1:N:424:VAL:HG21	1:N:429:VAL:HB	2.01	0.43
1:G:92:VAL:O	1:G:93:ASN:HB2	2.19	0.43
1:H:434:ASP:HA	1:H:435:PRO:HD3	1.70	0.43
1:H:474:PHE:CZ	1:b:333:PRO:HG2	2.54	0.43
1:H:554:ASN:HD22	1:H:557:ASN:HB2	1.83	0.43
1:P:400:TYR:CE2	1:P:575:LYS:HA	2.53	0.43
1:R:322:THR:HG21	1:R:420:PHE:CD2	2.54	0.43
1:S:236:THR:HB	1:T:558:GLN:OE1	2.18	0.43
1:T:377:ARG:HH21	1:T:397:ARG:HD2	1.84	0.43
1:V:130:VAL:HG13	1:V:576:SER:O	2.18	0.43
1:V:159:GLN:HA	1:V:160:PRO:HA	1.78	0.43
1:W:92:VAL:O	1:W:93:ASN:HB2	2.18	0.43
1:W:393:GLU:O	1:W:393:GLU:HG2	2.17	0.43
1:Y:84:VAL:HG22	1:a:304:GLY:O	2.19	0.43
1:Y:317:THR:HG22	1:Y:330:ILE:HA	1.99	0.43
1:Y:443:ASN:OD1	1:Y:443:ASN:N	2.50	0.43
1:b:324:TYR:CE2	1:b:422:LEU:HD21	2.54	0.43
1:c:92:VAL:O	1:c:93:ASN:HB2	2.18	0.43
1:d:564:SER:OG	1:d:565:ASN:N	2.51	0.43
1:A:582:LYS:HB2	1:A:582:LYS:HZ3	1.83	0.43
1:J:131:ASN:O	1:J:550:GLN:NE2	2.51	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:G:434:ASP:HA	1:G:435:PRO:HD3	1.76	0.43
1:H:369:ASN:C	1:H:371:ALA:H	2.24	0.43
1:M:334:ALA:HB1	1:M:454:LEU:O	2.18	0.43
1:P:200:TRP:HZ2	1:P:569:MET:HE1	1.84	0.43
1:S:354:LYS:HG2	1:S:355:THR:N	2.33	0.43
1:T:555:VAL:C	1:T:556:ASP:O	2.60	0.43
1:Y:476:THR:HG22	1:a:583:LEU:HD11	2.00	0.43
1:Z:52:LYS:HE3	1:Z:60:TYR:CD2	2.53	0.43
1:Z:461:PRO:HA	1:Z:462:PRO:HD3	1.80	0.43
1:a:572:VAL:O	1:a:574:GLU:HG2	2.18	0.43
1:E:51:PHE:CD2	1:E:61:ILE:HG12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:O	1:B:193:GLU:HG3	2.19	0.43
1:B:236:THR:HB	1:F:558:GLN:NE2	2.33	0.43
1:F:583:LEU:HA	1:F:583:LEU:HD12	1.77	0.43
1:I:354:LYS:HG2	1:I:355:THR:N	2.33	0.43
1:L:346:GLU:O	1:L:352:PRO:HA	2.19	0.43
1:L:417:ASN:OD1	1:L:419:ASN:ND2	2.46	0.43
1:L:548:ILE:H	1:b:127:GLN:HE22	1.66	0.43
1:L:569:MET:HG2	1:L:570:LYS:N	2.30	0.43
1:O:377:ARG:NH2	1:O:397:ARG:HD2	2.33	0.43
1:P:408:ARG:HA	1:P:408:ARG:HD3	1.86	0.43
1:S:247:GLU:OE1	1:S:247:GLU:N	2.44	0.43
1:S:434:ASP:HA	1:S:435:PRO:HD3	1.73	0.43
1:a:133:MET:CG	1:a:539:LEU:HD23	2.49	0.43
1:c:256:ARG:NH1	1:d:257:THR:HG22	2.34	0.43
1:c:346:GLU:O	1:c:352:PRO:HA	2.19	0.43
1:d:148:VAL:O	1:d:257:THR:HG23	2.18	0.43
1:J:510:TYR:OH	1:J:518:MET:HE2	2.19	0.43
1:N:518:MET:HE3	1:N:518:MET:HB2	1.77	0.43
1:N:558:GLN:O	1:N:558:GLN:HG2	2.17	0.43
1:B:212:PHE:HE1	1:B:236:THR:HG21	1.83	0.43
1:B:554:ASN:O	1:B:558:GLN:HB2	2.18	0.43
1:D:155:GLU:O	1:D:156:SER:C	2.61	0.43
1:D:369:ASN:HD21	1:D:372:ALA:HB2	1.82	0.43
1:D:493:ASN:N	1:D:493:ASN:OD1	2.51	0.43
1:G:210:TYR:OH	1:G:244:TYR:N	2.47	0.43
1:H:297:SER:C	1:H:302:ASN:HD22	2.18	0.43
1:M:200:TRP:HZ2	1:M:569:MET:HE1	1.84	0.43
1:O:177:LEU:HD22	1:O:263:THR:HG22	2.00	0.43
1:V:369:ASN:HB3	1:V:372:ALA:HB3	2.00	0.43
1:X:271:LYS:NZ	1:X:459:ASN:ND2	2.66	0.43
1:a:363:GLY:HA2	1:a:409:TYR:HB2	2.00	0.43
1:b:581:ARG:HB3	1:b:582:LYS:H	1.54	0.43
1:c:105:ILE:HG12	1:c:212:PHE:HB2	2.00	0.43
1:d:118:GLY:HA3	1:d:197:PHE:CD2	2.54	0.43
1:A:248:ASN:HD22	1:N:122:ASN:HD22	1.66	0.43
1:A:464:TYR:O	1:A:573:TYR:HA	2.18	0.43
1:E:232:ILE:HG12	1:E:233:TYR:N	2.34	0.43
1:N:153:VAL:HG12	1:N:154:SER:N	2.34	0.43
1:N:333:PRO:HG2	1:S:474:PHE:CZ	2.54	0.43
1:Q:551:MET:HE1	1:Q:574:GLU:HB3	2.00	0.43
1:F:363:GLY:HA3	1:F:367:ASP:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:216:ARG:NH1	1:H:231:ASN:OD1	2.35	0.43
1:K:492:ASN:HB3	1:K:493:ASN:H	1.51	0.43
1:O:294:LEU:HA	1:O:295:PRO:HD3	1.87	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:a:393:GLU:O	1:a:393:GLU:HG3	2.18	0.43
1:c:102:HIS:HB2	1:c:214:TRP:CH2	2.53	0.43
1:d:66:SER:HA	1:d:529:TRP:O	2.19	0.43
1:d:464:TYR:HA	1:d:465:PRO:HA	1.82	0.43
1:A:515:SER:OG	1:N:390:THR:O	2.37	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:J:346:GLU:O	1:J:352:PRO:HA	2.19	0.43
1:N:297:SER:C	1:N:302:ASN:HD22	2.21	0.43
1:F:186:THR:HB	1:d:287:LEU:HB2	2.01	0.43
1:F:209:ARG:NE	1:d:288:PRO:O	2.43	0.43
1:G:547:PRO:HD3	1:d:123:PRO:HB2	2.00	0.43
1:H:464:TYR:O	1:H:573:TYR:HA	2.19	0.43
1:H:548:ILE:H	1:V:127:GLN:HE22	1.66	0.43
1:K:92:VAL:O	1:K:93:ASN:HB2	2.19	0.43
1:K:153:VAL:O	1:K:154:SER:C	2.61	0.43
1:L:326:THR:HG21	1:d:98:LEU:HA	1.99	0.43
1:M:99:ASP:CG	1:M:216:ARG:HH21	2.26	0.43
1:M:140:SER:O	1:M:533:LEU:HD12	2.19	0.43
1:M:436:ILE:HD13	1:M:436:ILE:HA	1.79	0.43
1:P:383:GLN:C	1:P:384:HIS:CD2	2.96	0.43
1:W:257:THR:HG22	1:Y:256:ARG:HH12	1.84	0.43
1:Y:99:ASP:CG	1:Y:216:ARG:HH21	2.27	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:a:434:ASP:HA	1:a:435:PRO:HD3	1.81	0.43
1:b:338:TYR:CE1	1:b:358:ALA:HB3	2.51	0.43
1:c:52:LYS:HB3	1:c:60:TYR:HB3	2.00	0.43
1:E:439:LYS:NZ	1:I:426:ASP:O	2.46	0.43
1:Q:367:ASP:N	1:Q:367:ASP:OD1	2.52	0.43
1:B:378:TYR:O	1:B:397:ARG:HA	2.19	0.43
1:C:247:GLU:OE1	1:C:247:GLU:N	2.47	0.43
1:D:109:TRP:CD1	1:D:246:ILE:HG13	2.53	0.43
1:D:177:LEU:HD22	1:D:263:THR:HG22	2.01	0.43
1:F:159:GLN:CD	1:F:160:PRO:HD2	2.44	0.43
1:G:194:THR:N	1:G:384:HIS:HE1	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:318:GLN:CB	1:W:354:LYS:HE2	2.48	0.43
1:K:568:GLY:HA3	1:K:569:MET:HB2	2.01	0.43
1:M:130:VAL:HG12	1:M:578:LEU:HD22	2.00	0.43
1:M:432:PRO:O	1:M:443:ASN:ND2	2.37	0.43
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: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:R:382:ARG:NE	1:R:390:THR:O	2.45	0.43
1:S:62:THR:HG23	1:S:534:VAL:HG22	2.01	0.43
1:S:185:PHE:CD2	1:S:187:PRO:HD3	2.54	0.43
1:X:105:ILE:HG12	1:X:212:PHE:HB2	2.01	0.43
1:c:417:ASN:OD1	1:c:419:ASN:ND2	2.45	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:C:153:VAL:HG12	1:C:154:SER:N	2.33	0.43
1:C:286:GLY:O	1:C:288:PRO:HD3	2.19	0.43
1:F:465:PRO:HG3	1:F:571:ILE:CG2	2.49	0.43
1:H:94:GLY:O	1:b:423:PRO:HA	2.18	0.43
1:K:319:MET:HE3	1:K:329:THR:HG23	1.99	0.43
1:R:346:GLU:O	1:R:352:PRO:HA	2.18	0.43
1:X:136:LEU:HD12	1:X:537:ALA:HB2	2.00	0.43
1:Z:563:PRO:HB3	1:Z:569:MET:HE2	2.01	0.43
1:a:198:TYR:HA	1:a:199:PRO:HD3	1.88	0.43
1:b:326:THR:H	1:b:329:THR:HB	1.84	0.43
1:c:411:GLU:OE1	1:c:411:GLU:N	2.51	0.43
1:c:518:MET:HB2	1:c:518:MET:HE2	1.67	0.43
1:d:408:ARG:HA	1:d:408:ARG:HD3	1.89	0.43
1:B:176:ALA:HB2	1:B:252:VAL:HG22	1.99	0.42
1:B:581:ARG:HB3	1:B:582:LYS:H	1.58	0.42
1:D:127:GLN:CG	1:D:551:MET:HE2	2.49	0.42
1:H:51:PHE:CD2	1:H:61:ILE:HG12	2.55	0.42
1:I:352:PRO:HD2	1:V:283:ARG:HH12	1.84	0.42
1:I:376:PRO:HG2	1:I:400:TYR:HB3	2.00	0.42
1:L:389:THR:HG23	1:L:568:GLY:O	2.19	0.42
1:M:383:GLN:CB	1:M:384:HIS:HD2	2.32	0.42
1:O:153:VAL:HG12	1:O:154:SER:N	2.33	0.42
1:P:77:GLU:CD	1:P:504:PRO:HG3	2.44	0.42
1:S:369:ASN:O	1:S:371:ALA:N	2.52	0.42
1:S:414:TRP:HE1	1:S:416:GLN:HE21	1.67	0.42
1:U:558:GLN:O	1:U:558:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:99:ASP:CG	1:W:216:ARG:HH21	2.25	0.42
1:Y:383:GLN:HB3	1:Y:384:HIS:CD2	2.54	0.42
1:Y:475:ASP:CG	1:a:274:ARG:HH12	2.26	0.42
1:b:55:GLU:O	1:b:56:ASN:OD1	2.36	0.42
1:c:413:ASP:O	1:c:432:PRO:HD3	2.18	0.42
1:E:59:VAL:HG21	1:E:133:MET:HE2	2.00	0.42
1:N:369:ASN:C	1:N:371:ALA:N	2.77	0.42
1:Q:130:VAL:HG13	1:Q:576:SER:O	2.20	0.42
1:F:354:LYS:HE2	1:d:318:GLN:HB2	1.99	0.42
1:G:386:GLN:OE1	1:G:396:GLU:N	2.52	0.42
1:H:397:ARG:NH1	1:b:323:ASN:HB3	2.34	0.42
1:H:558:GLN:O	1:H:558:GLN:HG2	2.18	0.42
1:H:581:ARG:HB3	1:H:582:LYS:H	1.60	0.42
1:K:445:THR:HA	1:K:448:PHE:HB2	2.01	0.42
1:L:58:TRP:CZ2	1:L:538:LYS:HE2	2.55	0.42
1:O:581:ARG:HB3	1:O:582:LYS:H	1.55	0.42
1:Y:117:TRP:CE2	1:Y:469:ILE:HG12	2.54	0.42
1:Y:383:GLN:C	1:Y:384:HIS:CD2	2.97	0.42
1:a:558:GLN:HE22	1:b:236:THR:HB	1.84	0.42
1:c:85:ASN:OD1	1:c:87:LEU:HD12	2.20	0.42
1:A:377:ARG:NH2	1:A:397:ARG:HD2	2.34	0.42
1:E:336:VAL:O	1:E:408:ARG:NH2	2.53	0.42
1:B:114:ALA:HB1	1:B:119:VAL:HG11	2.02	0.42
1:B:393:GLU:O	1:B:393:GLU:HG3	2.19	0.42
1:C:137:HIS:CE1	1:C:272:PRO:HB3	2.54	0.42
1:F:309:GLN:O	1:F:313:ARG:HG3	2.20	0.42
1:F:318:GLN:CB	1:L:354:LYS:HE2	2.50	0.42
1:F:414:TRP:CE2	1:L:96:MET:HE2	2.55	0.42
1:F:492:ASN:CG	1:F:493:ASN:N	2.75	0.42
1:G:161:PRO:O	1:G:162:THR:OG1	2.29	0.42
1:L:317:THR:HG22	1:L:330:ILE:HA	2.01	0.42
1:M:550:GLN:HA	1:M:578:LEU:HD23	2.01	0.42
1:P:417:ASN:OD1	1:P:418:ILE:N	2.53	0.42
1:R:551:MET:HE3	1:R:551:MET:HB3	1.71	0.42
1:X:96:MET:H	1:X:96:MET:HG3	1.52	0.42
1:X:378:TYR:O	1:X:397:ARG:HA	2.18	0.42
1:a:137:HIS:CD2	1:a:272:PRO:HB3	2.54	0.42
1:a:257:THR:HG22	1:b:256:ARG:HH12	1.84	0.42
1:a:493:ASN:OD1	1:a:493:ASN:N	2.51	0.42
1:c:238:PRO:HA	1:c:241:VAL:HG23	2.02	0.42
1:d:383:GLN:HB3	1:d:384:HIS:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:414:TRP:HE1	1:d:416:GLN:HE21	1.66	0.42
1:A:348:SER:OG	1:A:349:THR:N	2.52	0.42
1:A:434:ASP:HA	1:A:435:PRO:HD3	1.69	0.42
1:E:345:PHE:CZ	1:I:319:MET:HE1	2.54	0.42
1:E:432:PRO:CA	1:E:443:ASN:HD22	2.33	0.42
1:Q:557:ASN:ND2	1:Q:557:ASN:C	2.77	0.42
1:B:234:HIS:HB3	1:M:365:GLN:OE1	2.19	0.42
1:B:550:GLN:HA	1:B:578:LEU:HD23	2.01	0.42
1:C:186:THR:HB	1:P:287:LEU:HD13	2.02	0.42
1:D:114:ALA:HB1	1:D:119:VAL:HG11	2.01	0.42
1:D:583:LEU:HD12	1:D:583:LEU:HA	1.85	0.42
1:F:86:ASN:ND2	1:F:100:ASP:HB2	2.34	0.42
1:F:283:ARG:HH12	1:L:352:PRO:HD2	1.83	0.42
1:G:247:GLU:OE1	1:G:247:GLU:N	2.48	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:I:550:GLN:HA	1:I:578:LEU:HD23	2.02	0.42
1:K:55:GLU:HG3	1:R:55:GLU:HG2	2.01	0.42
1:R:70:HIS:CD2	1:T:510:TYR:HB3	2.54	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:U:568:GLY:HA3	1:U:569:MET:HB2	2.02	0.42
1:Y:98:LEU:HA	1:a:326:THR:HG21	2.01	0.42
1:Z:558:GLN:NE2	1:a:236:THR:HB	2.33	0.42
1:c:369:ASN:C	1:c:371:ALA:N	2.76	0.42
1:E:283:ARG:HH12	1:V:352:PRO:HD2	1.84	0.42
1:E:369:ASN:C	1:E:371:ALA:N	2.78	0.42
1:N:152:THR:HG23	1:N:168:ASP:HB2	2.01	0.42
1:C:86:ASN:HB2	1:C:88:ASP:OD1	2.19	0.42
1:D:96:MET:SD	1:D:220:PRO:HA	2.59	0.42
1:D:136:LEU:HD12	1:D:537:ALA:HB2	2.02	0.42
1:F:365:GLN:HG2	1:F:366:THR:HG23	2.02	0.42
1:G:485:ASN:OD1	1:G:485:ASN:N	2.49	0.42
1:H:256:ARG:HH12	1:L:257:THR:HG22	1.84	0.42
1:K:131:ASN:O	1:K:550:GLN:NE2	2.52	0.42
1:K:132:THR:HG22	1:R:132:THR:HG22	2.01	0.42
1:K:191:ARG:O	1:K:193:GLU:HG3	2.20	0.42
1:K:225:THR:HG22	1:K:226:SER:O	2.20	0.42
1:K:257:THR:HG22	1:M:256:ARG:HH12	1.84	0.42
1:M:148:VAL:O	1:M:257:THR:HG23	2.19	0.42
1:M:410:PRO:HA	1:M:413:ASP:CG	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:159:GLN:O	1:O:161:PRO:HA	2.19	0.42
1:P:212:PHE:O	1:P:214:TRP:HE3	2.02	0.42
1:P:266:PHE:HZ	1:P:493:ASN:O	2.03	0.42
1:T:155:GLU:HG3	1:T:156:SER:CB	2.50	0.42
1:U:432:PRO:C	1:U:443:ASN:HD22	2.26	0.42
1:W:457:LEU:O	1:b:476:THR:HB	2.19	0.42
1:Z:465:PRO:HG3	1:Z:571:ILE:CG2	2.50	0.42
1:c:159:GLN:O	1:c:161:PRO:HA	2.19	0.42
1:c:322:THR:HG21	1:c:420:PHE:CD2	2.54	0.42
1:d:456:ALA:O	1:d:457:LEU:HD12	2.20	0.42
1:A:266:PHE:HZ	1:A:493:ASN:O	2.03	0.42
1:N:492:ASN:OD1	1:N:492:ASN:N	2.52	0.42
1:B:547:PRO:HD3	1:P:123:PRO:HB2	2.01	0.42
1:C:92:VAL:O	1:C:93:ASN:HB2	2.20	0.42
1:C:346:GLU:OE1	1:P:408:ARG:NH1	2.53	0.42
1:C:475:ASP:OD2	1:P:581:ARG:HD3	2.18	0.42
1:F:424:VAL:HG12	1:L:94:GLY:HA2	2.01	0.42
1:G:331:MET:HE3	1:c:485:ASN:HB3	2.00	0.42
1:G:572:VAL:HG12	1:G:573:TYR:O	2.20	0.42
1:K:109:TRP:CD1	1:K:246:ILE:HG13	2.54	0.42
1:M:156:SER:CB	1:M:164:VAL:HG22	2.50	0.42
1:M:368:GLU:HG2	1:M:369:ASN:H	1.84	0.42
1:T:86:ASN:ND2	1:T:100:ASP:HB2	2.34	0.42
1:U:157:ALA:HA	1:U:158:THR:CG2	2.50	0.42
1:U:339:SER:O	1:U:449:ASN:HA	2.19	0.42
1:U:436:ILE:HD13	1:U:436:ILE:HA	1.71	0.42
1:W:66:SER:HA	1:W:529:TRP:O	2.20	0.42
1:Z:118:GLY:HA3	1:Z:197:PHE:CD2	2.55	0.42
1:Z:572:VAL:HG12	1:Z:573:TYR:O	2.18	0.42
1:a:238:PRO:HA	1:a:241:VAL:HG23	2.01	0.42
1:d:131:ASN:O	1:d:550:GLN:NE2	2.52	0.42
1:A:583:LEU:HD11	1:K:476:THR:HG22	2.00	0.42
1:C:339:SER:HB2	1:C:450:THR:OG1	2.19	0.42
1:D:546:ASN:ND2	1:D:547:PRO:O	2.42	0.42
1:F:298:GLU:OE1	1:M:387:LYS:NZ	2.44	0.42
1:F:551:MET:HE2	1:F:551:MET:HB3	1.71	0.42
1:I:434:ASP:HA	1:I:435:PRO:HD3	1.71	0.42
1:L:382:ARG:NH2	1:L:392:GLY:O	2.49	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:S:518:MET:HE3	1:S:518:MET:HB2	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:382:ARG:N	1:V:386:GLN:HB3	2.18	0.42
1:X:483:HIS:HB3	1:X:485:ASN:OD1	2.20	0.42
1:X:563:PRO:HB3	1:X:569:MET:HE2	2.01	0.42
1:Z:43:GLY:HA3	1:Z:146:PHE:CD2	2.55	0.42
1:b:554:ASN:O	1:b:558:GLN:HB2	2.20	0.42
1:c:443:ASN:OD1	1:c:443:ASN:N	2.51	0.42
1:d:436:ILE:C	1:d:438:GLY:N	2.77	0.42
1:E:88:ASP:OD1	1:E:89:LYS:HB2	2.20	0.42
1:C:269:ASP:CG	1:C:269:ASP:O	2.62	0.42
1:C:269:ASP:CG	1:C:492:ASN:ND2	2.77	0.42
1:D:319:MET:HE3	1:D:329:THR:HG23	2.02	0.42
1:D:361:ARG:NE	1:D:405:ASP:OD1	2.53	0.42
1:D:510:TYR:CE2	1:D:512:PRO:HD3	2.55	0.42
1:F:190:MET:HE1	1:d:331:MET:HG2	2.02	0.42
1:G:339:SER:OG	1:c:346:GLU:OE1	2.32	0.42
1:H:199:PRO:HD2	1:H:200:TRP:CZ3	2.55	0.42
1:H:271:LYS:HE3	1:H:271:LYS:HB2	1.84	0.42
1:H:557:ASN:O	1:H:559:PHE:N	2.53	0.42
1:K:464:TYR:O	1:K:573:TYR:HA	2.20	0.42
1:L:572:VAL:HG12	1:L:573:TYR:O	2.20	0.42
1:O:551:MET:HE3	1:O:551:MET:HB3	1.84	0.42
1:R:75:GLU:CD	1:R:75:GLU:H	2.28	0.42
1:R:280:GLN:NE2	1:R:583:LEU:H	2.17	0.42
1:T:209:ARG:HH11	1:T:209:ARG:HG3	1.83	0.42
1:T:461:PRO:HA	1:T:462:PRO:HD3	1.93	0.42
1:W:553:ILE:HG22	1:W:557:ASN:CG	2.44	0.42
1:X:322:THR:HB	1:X:324:TYR:H	1.84	0.42
1:Z:248:ASN:HD22	1:c:122:ASN:HD22	1.67	0.42
1:a:133:MET:HG3	1:a:539:LEU:HD23	2.02	0.42
1:b:403:HIS:CE1	1:b:549:GLN:HE22	2.37	0.42
1:A:212:PHE:HZ	1:N:562:VAL:HG11	1.85	0.42
1:A:326:THR:H	1:A:329:THR:HB	1.84	0.42
1:E:138:LEU:HG	1:E:268:PHE:CD2	2.54	0.42
1:J:369:ASN:OD1	1:J:372:ALA:HB3	2.19	0.42
1:Q:77:GLU:HB2	1:Q:518:MET:HE1	2.02	0.42
1:Q:159:GLN:O	1:Q:161:PRO:HA	2.19	0.42
1:Q:568:GLY:HA3	1:Q:569:MET:HB2	2.02	0.42
1:C:461:PRO:HA	1:C:462:PRO:HD3	1.91	0.42
1:D:92:VAL:O	1:D:93:ASN:HB2	2.20	0.42
1:F:190:MET:HE1	1:d:331:MET:HB3	2.02	0.42
1:G:294:LEU:HA	1:G:295:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:415:ILE:CD1	1:W:447:ILE:HG22	2.49	0.42
1:I:190:MET:HE1	1:V:331:MET:HG2	2.02	0.42
1:L:155:GLU:O	1:L:156:SER:C	2.63	0.42
1:M:183:MET:HE1	1:M:246:ILE:HD13	2.01	0.42
1:M:383:GLN:C	1:M:384:HIS:CD2	2.98	0.42
1:R:436:ILE:HA	1:R:436:ILE:HD13	1.75	0.42
1:S:140:SER:HA	1:S:266:PHE:O	2.20	0.42
1:U:510:TYR:HB3	1:X:70:HIS:CD2	2.55	0.42
1:W:159:GLN:CD	1:W:160:PRO:HD3	2.44	0.42
1:W:361:ARG:HD3	1:W:405:ASP:OD1	2.20	0.42
1:X:326:THR:H	1:X:329:THR:HB	1.85	0.42
1:a:464:TYR:HA	1:a:465:PRO:HA	1.86	0.42
1:b:142:GLU:HB3	1:b:265:THR:HA	2.01	0.42
1:A:554:ASN:O	1:A:558:GLN:HB2	2.20	0.42
1:E:190:MET:HE1	1:I:331:MET:HB3	2.01	0.42
1:E:317:THR:HG21	1:E:329:THR:HG22	2.01	0.42
1:E:511:ASP:OD2	1:E:514:ALA:HB2	2.20	0.42
1:Q:443:ASN:OD1	1:Q:443:ASN:N	2.51	0.42
1:D:377:ARG:HH21	1:D:397:ARG:HD2	1.84	0.42
1:G:583:LEU:HA	1:G:583:LEU:HD12	1.75	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:U:553:ILE:HG21	1:U:553:ILE:HD13	1.83	0.42
1:W:274:ARG:NH1	1:b:475:ASP:OD1	2.43	0.42
1:W:363:GLY:HA3	1:W:367:ASP:O	2.20	0.42
1:X:114:ALA:HB1	1:X:119:VAL:HG11	2.01	0.42
1:X:322:THR:HG21	1:X:420:PHE:CD2	2.54	0.42
1:Y:346:GLU:OE1	1:a:408:ARG:NH1	2.53	0.42
1:c:286:GLY:O	1:c:288:PRO:HD3	2.20	0.42
1:c:389:THR:HG23	1:c:568:GLY:O	2.20	0.42
1:N:96:MET:H	1:N:96:MET:HG2	1.50	0.41
1:Q:462:PRO:HD2	1:Q:576:SER:OG	2.20	0.41
1:C:390:THR:O	1:D:515:SER:OG	2.38	0.41
1:D:286:GLY:O	1:D:288:PRO:HD3	2.19	0.41
1:F:288:PRO:HG3	1:L:211:TYR:CG	2.55	0.41
1:H:182:THR:O	1:b:582:LYS:NZ	2.43	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
1:L:435:PRO:HB3	1:L:439:LYS:O	2.20	0.41
1:M:518:MET:HE2	1:M:518:MET:HB2	1.81	0.41
1:P:553:ILE:CA	1:P:554:ASN:HB2	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:247:GLU:OE1	1:V:247:GLU:N	2.47	0.41
1:V:432:PRO:C	1:V:443:ASN:HD22	2.23	0.41
1:W:69:VAL:CG1	1:W:205:PRO:HD3	2.50	0.41
1:X:319:MET:HE3	1:X:329:THR:HG23	2.02	0.41
1:Y:408:ARG:HD3	1:Y:408:ARG:HA	1.76	0.41
1:Y:550:GLN:HA	1:Y:578:LEU:HD23	2.02	0.41
1:a:551:MET:HE3	1:a:551:MET:HB3	1.76	0.41
1:b:103:ALA:HB3	1:b:212:PHE:O	2.20	0.41
1:E:92:VAL:O	1:E:93:ASN:HB2	2.20	0.41
1:E:436:ILE:HD13	1:E:436:ILE:HA	1.79	0.41
1:J:190:MET:HE1	1:U:331:MET:HG2	2.02	0.41
1:C:101:THR:O	1:P:283:ARG:NH2	2.53	0.41
1:F:274:ARG:HH12	1:L:475:ASP:CG	2.28	0.41
1:F:461:PRO:HA	1:F:462:PRO:HD3	1.90	0.41
1:G:383:GLN:C	1:G:384:HIS:HD2	2.28	0.41
1:H:256:ARG:NH1	1:L:257:THR:HG22	2.34	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:M:447:ILE:HG22	1:R:415:ILE:CD1	2.45	0.41
1:M:553:ILE:CA	1:M:554:ASN:HB2	2.35	0.41
1:O:130:VAL:HG11	1:O:578:LEU:HD13	2.01	0.41
1:R:158:THR:HG22	1:R:159:GLN:HG3	2.02	0.41
1:U:198:TYR:HA	1:U:199:PRO:HD3	1.89	0.41
1:V:393:GLU:O	1:V:393:GLU:HG2	2.19	0.41
1:Z:408:ARG:HA	1:Z:408:ARG:HD3	1.76	0.41
1:a:382:ARG:HD2	1:b:513:ASP:O	2.19	0.41
1:b:66:SER:HA	1:b:529:TRP:O	2.20	0.41
1:c:541:ALA:O	1:c:543:HIS:CE1	2.73	0.41
1:A:378:TYR:O	1:A:397:ARG:HA	2.20	0.41
1:A:554:ASN:CB	1:A:557:ASN:HD22	2.33	0.41
1:E:362:GLY:O	1:V:349:THR:N	2.52	0.41
1:E:383:GLN:C	1:E:384:HIS:CD2	2.97	0.41
1:J:339:SER:O	1:J:449:ASN:HA	2.20	0.41
1:N:278:THR:HB	1:N:583:LEU:HD13	2.03	0.41
1:Q:294:LEU:HA	1:Q:295:PRO:HD3	1.91	0.41
1:Q:573:TYR:O	1:Q:574:GLU:HG3	2.20	0.41
1:B:432:PRO:O	1:B:443:ASN:ND2	2.46	0.41
1:B:436:ILE:HD13	1:B:436:ILE:HA	1.80	0.41
1:G:369:ASN:O	1:G:372:ALA:N	2.51	0.41
1:I:346:GLU:O	1:I:352:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:492:ASN:CG	1:I:493:ASN:H	2.27	0.41
1:L:468:GLN:HB3	1:L:485:ASN:O	2.20	0.41
1:M:317:THR:HG21	1:M:329:THR:HG22	2.01	0.41
1:O:114:ALA:HB1	1:O:119:VAL:HG11	2.01	0.41
1:O:346:GLU:OE2	1:O:355:THR:OG1	2.24	0.41
1:O:361:ARG:HG3	1:O:402:ALA:O	2.20	0.41
1:O:560:ASN:HB3	1:O:572:VAL:HG21	2.03	0.41
1:P:92:VAL:O	1:P:93:ASN:HB2	2.19	0.41
1:P:198:TYR:HA	1:P:199:PRO:HD3	1.91	0.41
1:S:340:ALA:HB3	1:S:357:ILE:HD12	2.03	0.41
1:T:271:LYS:CG	1:T:272:PRO:HD2	2.37	0.41
1:U:66:SER:HA	1:U:529:TRP:O	2.20	0.41
1:X:138:LEU:HG	1:X:268:PHE:CD2	2.56	0.41
1:X:174:MET:HE2	1:X:252:VAL:HG11	2.02	0.41
1:X:471:ASP:CG	1:X:485:ASN:HD21	2.28	0.41
1:Z:117:TRP:CE2	1:Z:469:ILE:HG12	2.55	0.41
1:a:366:THR:O	1:a:366:THR:OG1	2.35	0.41
1:b:557:ASN:O	1:b:559:PHE:N	2.52	0.41
1:A:286:GLY:O	1:A:288:PRO:HD3	2.19	0.41
1:A:553:ILE:HG22	1:A:557:ASN:ND2	2.35	0.41
1:E:243:PHE:CD2	1:I:545:TRP:HB3	2.55	0.41
1:J:94:GLY:O	1:U:423:PRO:HA	2.20	0.41
1:B:336:VAL:O	1:B:408:ARG:NH2	2.53	0.41
1:C:445:THR:HA	1:C:448:PHE:HB2	2.02	0.41
1:D:77:GLU:HB2	1:D:518:MET:HE1	2.01	0.41
1:D:117:TRP:CE2	1:D:469:ILE:HG12	2.55	0.41
1:F:298:GLU:HA	1:M:565:ASN:OD1	2.21	0.41
1:F:481:ARG:HB3	1:L:478:LEU:HD13	2.03	0.41
1:G:584:TYR:OH	1:c:471:ASP:OD1	2.17	0.41
1:H:159:GLN:CB	1:H:160:PRO:HD2	2.50	0.41
1:H:232:ILE:HG12	1:H:233:TYR:N	2.36	0.41
1:I:382:ARG:NE	1:I:390:THR:O	2.42	0.41
1:I:439:LYS:NZ	1:V:434:ASP:OD2	2.48	0.41
1:L:414:TRP:HE1	1:L:416:GLN:HG3	1.84	0.41
1:M:155:GLU:CD	1:M:156:SER:H	2.28	0.41
1:O:408:ARG:HA	1:O:408:ARG:HD3	1.86	0.41
1:R:287:LEU:HD12	1:R:288:PRO:HD2	2.02	0.41
1:S:109:TRP:CD1	1:S:246:ILE:HG13	2.55	0.41
1:U:378:TYR:O	1:U:397:ARG:HA	2.20	0.41
1:V:99:ASP:CG	1:V:216:ARG:HH21	2.29	0.41
1:V:109:TRP:CG	1:V:246:ILE:HG13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:400:TYR:CE2	1:V:575:LYS:HA	2.55	0.41
1:W:87:LEU:HA	1:W:90:THR:OG1	2.19	0.41
1:W:271:LYS:HE3	1:W:271:LYS:HB2	1.76	0.41
1:W:565:ASN:ND2	1:a:299:GLY:N	2.68	0.41
1:Z:445:THR:HA	1:Z:448:PHE:HB2	2.01	0.41
1:a:43:GLY:HA3	1:a:146:PHE:CD2	2.55	0.41
1:a:257:THR:HG22	1:b:256:ARG:NH1	2.35	0.41
1:b:266:PHE:HZ	1:b:493:ASN:O	2.02	0.41
1:c:266:PHE:HZ	1:c:493:ASN:O	2.02	0.41
1:A:99:ASP:CG	1:A:216:ARG:HH21	2.28	0.41
1:E:377:ARG:NH2	1:E:397:ARG:HD2	2.35	0.41
1:J:159:GLN:CB	1:J:160:PRO:HD2	2.50	0.41
1:N:132:THR:HG22	1:T:132:THR:HG22	2.02	0.41
1:N:400:TYR:CE2	1:N:575:LYS:HA	2.55	0.41
1:B:298:GLU:CD	1:P:387:LYS:HZ3	2.27	0.41
1:C:410:PRO:HA	1:C:413:ASP:CG	2.46	0.41
1:C:581:ARG:HB3	1:C:582:LYS:H	1.58	0.41
1:F:211:TYR:CG	1:d:288:PRO:HG3	2.54	0.41
1:F:389:THR:HG23	1:F:568:GLY:O	2.20	0.41
1:H:269:ASP:HB3	1:H:492:ASN:ND2	2.33	0.41
1:I:200:TRP:CZ3	1:K:245:THR:HG21	2.56	0.41
1:I:324:TYR:CE2	1:I:422:LEU:HD21	2.56	0.41
1:I:572:VAL:O	1:I:574:GLU:HG2	2.20	0.41
1:K:73:MET:CE	1:K:522:VAL:HA	2.50	0.41
1:R:266:PHE:HZ	1:R:493:ASN:O	2.02	0.41
1:R:408:ARG:HA	1:R:408:ARG:HD3	1.89	0.41
1:W:331:MET:HB3	1:b:190:MET:HE1	2.03	0.41
1:b:460:VAL:HG11	1:b:484:VAL:HA	2.02	0.41
1:c:384:HIS:ND1	1:c:384:HIS:N	2.69	0.41
1:A:127:GLN:HG3	1:A:551:MET:HE2	2.02	0.41
1:E:48:GLN:O	1:E:64:ASN:HB2	2.20	0.41
1:E:404:GLN:NE2	1:E:461:PRO:HD3	2.36	0.41
1:J:114:ALA:HB1	1:J:119:VAL:HG11	2.03	0.41
1:B:430:LEU:HD22	1:R:442:ILE:HG21	2.01	0.41
1:B:475:ASP:OD2	1:M:581:ARG:HD3	2.21	0.41
1:F:575:LYS:O	1:F:576:SER:HB3	2.21	0.41
1:H:148:VAL:O	1:H:257:THR:HG23	2.20	0.41
1:I:94:GLY:O	1:V:423:PRO:HA	2.20	0.41
1:I:286:GLY:O	1:I:288:PRO:HD3	2.21	0.41
1:I:554:ASN:O	1:I:558:GLN:HB2	2.21	0.41
1:K:90:THR:OG1	1:K:231:ASN:ND2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:432:PRO:C	1:K:443:ASN:HD22	2.28	0.41
1:K:572:VAL:HG12	1:K:573:TYR:O	2.19	0.41
1:L:226:SER:OG	1:L:227:GLY:N	2.53	0.41
1:M:94:GLY:HA2	1:R:424:VAL:HG12	2.03	0.41
1:M:569:MET:HG2	1:M:570:LYS:N	2.32	0.41
1:P:75:GLU:H	1:P:75:GLU:CD	2.28	0.41
1:R:339:SER:O	1:R:449:ASN:HA	2.20	0.41
1:T:48:GLN:O	1:T:64:ASN:HB2	2.20	0.41
1:V:156:SER:O	1:V:157:ALA:HB3	2.21	0.41
1:W:550:GLN:OE1	1:a:131:ASN:ND2	2.49	0.41
1:X:271:LYS:HD3	1:X:487:PRO:O	2.20	0.41
1:Z:93:ASN:HD21	1:Z:229:PRO:HD3	1.85	0.41
1:Z:102:HIS:HB2	1:Z:214:TRP:CH2	2.55	0.41
1:a:153:VAL:HG12	1:a:163:LYS:CE	2.43	0.41
1:b:492:ASN:OD1	1:b:493:ASN:N	2.54	0.41
1:c:94:GLY:C	1:c:96:MET:HE2	2.45	0.41
1:A:445:THR:HA	1:A:448:PHE:HB2	2.03	0.41
1:Q:70:HIS:O	1:Q:204:ILE:HG22	2.19	0.41
1:B:346:GLU:O	1:B:352:PRO:HA	2.20	0.41
1:B:382:ARG:NH1	1:C:513:ASP:O	2.53	0.41
1:B:388:THR:OG1	1:B:569:MET:N	2.53	0.41
1:B:458:ASN:HA	1:R:477:ASP:HB2	2.03	0.41
1:F:326:THR:H	1:F:329:THR:HB	1.84	0.41
1:H:151:LYS:HE3	1:I:505:ASN:OD1	2.20	0.41
1:H:363:GLY:HA3	1:H:368:GLU:HA	2.02	0.41
1:M:442:ILE:HG23	1:M:446:ASN:HD22	1.86	0.41
1:O:563:PRO:HB3	1:O:569:MET:HE2	2.02	0.41
1:S:435:PRO:HA	1:S:442:ILE:O	2.20	0.41
1:T:398:PHE:CE2	1:T:573:TYR:HB2	2.56	0.41
1:X:494:CYS:SG	1:X:495:PRO:HD2	2.60	0.41
1:Y:317:THR:HG21	1:Y:329:THR:HG22	2.02	0.41
1:Z:369:ASN:C	1:Z:371:ALA:N	2.78	0.41
1:d:420:PHE:CE2	1:d:422:LEU:HD22	2.56	0.41
1:A:331:MET:HB3	1:K:190:MET:HE1	2.03	0.41
1:E:345:PHE:HZ	1:I:319:MET:HE1	1.86	0.41
1:E:551:MET:HB3	1:E:551:MET:HE3	1.83	0.41
1:N:464:TYR:O	1:N:573:TYR:HA	2.21	0.41
1:Q:105:ILE:HG12	1:Q:212:PHE:HB2	2.01	0.41
1:Q:191:ARG:O	1:Q:193:GLU:HG3	2.20	0.41
1:Q:357:ILE:HB	1:Q:374:GLY:HA3	2.03	0.41
1:B:194:THR:H	1:B:384:HIS:HE1	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:VAL:HG12	1:B:573:TYR:O	2.20	0.41
1:C:382:ARG:N	1:C:386:GLN:HB3	2.19	0.41
1:C:434:ASP:HA	1:C:435:PRO:HD3	1.80	0.41
1:C:518:MET:HE2	1:C:518:MET:HB2	1.78	0.41
1:D:485:ASN:OD1	1:D:485:ASN:N	2.52	0.41
1:G:387:LYS:HG2	1:G:389:THR:OG1	2.20	0.41
1:H:287:LEU:HD12	1:H:288:PRO:CD	2.51	0.41
1:H:551:MET:HE2	1:H:551:MET:HB3	1.68	0.41
1:H:583:LEU:HD11	1:W:476:THR:HG22	2.03	0.41
1:K:238:PRO:HA	1:K:241:VAL:HG23	2.03	0.41
1:L:212:PHE:HE1	1:L:236:THR:HG21	1.86	0.41
1:L:408:ARG:HD3	1:L:408:ARG:HA	1.77	0.41
1:M:369:ASN:C	1:M:371:ALA:N	2.77	0.41
1:P:46:ASN:OD1	1:P:48:GLN:HB2	2.21	0.41
1:U:443:ASN:H	1:U:446:ASN:ND2	2.17	0.41
1:V:102:HIS:HB2	1:V:214:TRP:CH2	2.55	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:Y:266:PHE:HZ	1:Y:493:ASN:O	2.04	0.41
1:Z:354:LYS:HG2	1:Z:355:THR:N	2.36	0.41
1:d:568:GLY:HA3	1:d:569:MET:HB2	2.02	0.41
1:A:154:SER:CA	1:A:155:GLU:HB2	2.45	0.41
1:E:257:THR:HG22	1:J:256:ARG:NH1	2.36	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:J:434:ASP:HA	1:J:435:PRO:HD3	1.76	0.41
1:N:256:ARG:HH12	1:Q:257:THR:HG22	1.86	0.41
1:N:545:TRP:HB3	1:S:243:PHE:CD2	2.55	0.41
1:C:130:VAL:HG12	1:C:578:LEU:HD22	2.02	0.41
1:C:148:VAL:O	1:C:257:THR:HG23	2.19	0.41
1:C:322:THR:HG21	1:C:420:PHE:CD2	2.55	0.41
1:C:382:ARG:HD2	1:D:513:ASP:O	2.21	0.41
1:C:568:GLY:HA3	1:C:569:MET:HB2	2.03	0.41
1:G:73:MET:CE	1:G:522:VAL:HA	2.51	0.41
1:G:79:TYR:HA	1:G:106:VAL:O	2.21	0.41
1:G:326:THR:H	1:G:329:THR:HB	1.86	0.41
1:G:438:GLY:O	1:G:439:LYS:HD3	2.20	0.41
1:H:442:ILE:HG23	1:H:446:ASN:HD22	1.85	0.41
1:H:476:THR:HB	1:b:457:LEU:O	2.21	0.41
1:I:94:GLY:HA2	1:V:424:VAL:HG12	2.02	0.41
1:I:278:THR:HB	1:I:583:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:475:ASP:OD2	1:V:581:ARG:HD3	2.20	0.41
1:I:581:ARG:HB3	1:I:582:LYS:H	1.56	0.41
1:K:102:HIS:HB2	1:K:214:TRP:CH2	2.56	0.41
1:K:138:LEU:HG	1:K:268:PHE:CD2	2.56	0.41
1:L:154:SER:CA	1:L:155:GLU:HB2	2.48	0.41
1:L:159:GLN:O	1:L:161:PRO:HA	2.21	0.41
1:L:383:GLN:C	1:L:384:HIS:CD2	2.98	0.41
1:O:92:VAL:HB	1:O:95:ASN:HB2	2.03	0.41
1:O:138:LEU:HG	1:O:268:PHE:CD2	2.56	0.41
1:O:554:ASN:O	1:O:558:GLN:HB2	2.21	0.41
1:P:105:ILE:HG12	1:P:212:PHE:HB2	2.01	0.41
1:P:443:ASN:OD1	1:P:443:ASN:N	2.52	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:T:348:SER:O	1:T:349:THR:C	2.63	0.41
1:T:403:HIS:CD2	1:T:549:GLN:HE22	2.38	0.41
1:T:432:PRO:C	1:T:443:ASN:HD22	2.24	0.41
1:W:288:PRO:HG3	1:b:211:TYR:CD1	2.56	0.41
1:X:378:TYR:CE1	1:X:463:VAL:HG11	2.55	0.41
1:Y:436:ILE:HD13	1:Y:436:ILE:HA	1.72	0.41
1:Y:447:ILE:HG22	1:a:415:ILE:CD1	2.51	0.41
1:Y:568:GLY:HA3	1:Y:569:MET:HB2	2.03	0.41
1:Z:62:THR:HG23	1:Z:534:VAL:HG22	2.02	0.41
1:b:408:ARG:HA	1:b:408:ARG:HD3	1.72	0.41
1:c:137:HIS:CE1	1:c:272:PRO:HB3	2.56	0.41
1:A:331:MET:HE3	1:K:485:ASN:HB3	2.03	0.41
1:E:286:GLY:O	1:E:288:PRO:HD3	2.21	0.41
1:J:177:LEU:HD22	1:J:263:THR:HG22	2.03	0.41
1:N:414:TRP:HE1	1:N:416:GLN:HE21	1.69	0.41
1:B:56:ASN:HB2	1:B:58:TRP:CD1	2.51	0.41
1:B:424:VAL:HG12	1:R:94:GLY:HA2	2.02	0.41
1:D:152:THR:HG23	1:D:168:ASP:HB2	2.02	0.41
1:F:369:ASN:C	1:F:371:ALA:N	2.77	0.41
1:H:362:GLY:HA3	1:H:407:GLY:C	2.46	0.41
1:K:354:LYS:HG2	1:K:355:THR:N	2.36	0.41
1:M:155:GLU:O	1:M:163:LYS:HA	2.21	0.41
1:M:155:GLU:C	1:M:156:SER:OG	2.63	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:R:377:ARG:HH21	1:R:397:ARG:HD2	1.86	0.41
1:R:558:GLN:O	1:R:558:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:301:THR:HG22	1:S:301:THR:O	2.21	0.41
1:T:362:GLY:HA3	1:T:407:GLY:C	2.46	0.41
1:T:369:ASN:C	1:T:371:ALA:N	2.78	0.41
1:V:137:HIS:NE2	1:V:272:PRO:HB3	2.35	0.41
1:V:557:ASN:OD1	1:V:561:TYR:CE2	2.74	0.41
1:Z:47:ASN:OD1	1:Z:67:ARG:NH1	2.53	0.41
1:a:198:TYR:HB2	1:a:201:LYS:HB3	2.03	0.41
1:b:130:VAL:HG13	1:b:576:SER:O	2.21	0.41
1:d:473:GLU:HG2	1:d:491:GLN:NE2	2.36	0.41
1:N:557:ASN:O	1:N:559:PHE:N	2.54	0.40
1:Q:153:VAL:HG12	1:Q:155:GLU:HG3	2.04	0.40
1:B:98:LEU:HA	1:M:326:THR:HG21	2.03	0.40
1:B:105:ILE:HG12	1:B:212:PHE:HB2	2.03	0.40
1:B:431:LEU:HD22	1:R:220:PRO:HB2	2.04	0.40
1:F:338:TYR:CE1	1:F:358:ALA:HB3	2.53	0.40
1:F:475:ASP:CG	1:d:274:ARG:HH12	2.29	0.40
1:H:400:TYR:OH	1:H:575:LYS:HA	2.21	0.40
1:H:476:THR:HG22	1:b:583:LEU:HD11	2.02	0.40
1:I:44:THR:O	1:I:530:LYS:NZ	2.45	0.40
1:K:553:ILE:HG22	1:K:557:ASN:CG	2.46	0.40
1:M:509:GLN:H	1:M:509:GLN:HG2	1.73	0.40
1:O:554:ASN:HB3	1:O:556:ASP:O	2.21	0.40
1:X:177:LEU:HD22	1:X:263:THR:HG22	2.04	0.40
1:Y:383:GLN:HB3	1:Y:384:HIS:HD2	1.85	0.40
1:Z:81:ARG:HA	1:Z:105:ILE:HD13	2.03	0.40
1:Z:232:ILE:HG12	1:Z:233:TYR:N	2.36	0.40
1:Z:583:LEU:HD12	1:Z:583:LEU:HA	1.89	0.40
1:b:131:ASN:ND2	1:b:550:GLN:HB3	2.35	0.40
1:b:558:GLN:NE2	1:d:236:THR:HB	2.37	0.40
1:c:130:VAL:HG13	1:c:576:SER:O	2.21	0.40
1:J:159:GLN:O	1:J:161:PRO:HA	2.21	0.40
1:J:408:ARG:HA	1:J:408:ARG:HD3	1.84	0.40
1:J:442:ILE:HG21	1:U:430:LEU:HD22	2.02	0.40
1:N:159:GLN:CD	1:N:160:PRO:HD2	2.46	0.40
1:B:382:ARG:NH2	1:B:392:GLY:O	2.54	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:D:417:ASN:OD1	1:D:419:ASN:ND2	2.50	0.40
1:D:551:MET:HE3	1:D:551:MET:HB3	1.82	0.40
1:F:118:GLY:HA3	1:F:197:PHE:CD2	2.56	0.40
1:G:346:GLU:OE2	1:G:355:THR:OG1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:408:ARG:HD3	1:K:408:ARG:HA	1.76	0.40
1:L:271:LYS:HD2	1:L:271:LYS:N	2.35	0.40
1:L:481:ARG:NH2	1:d:478:LEU:HB3	2.36	0.40
1:O:59:VAL:HG21	1:O:133:MET:HE2	2.04	0.40
1:O:569:MET:HE3	1:O:569:MET:HB2	1.81	0.40
1:T:175:VAL:HG22	1:T:500:VAL:HG12	2.03	0.40
1:T:400:TYR:CE2	1:T:575:LYS:HA	2.56	0.40
1:U:155:GLU:O	1:U:156:SER:C	2.64	0.40
1:U:375:ASP:HA	1:U:376:PRO:HD3	1.75	0.40
1:V:92:VAL:O	1:V:93:ASN:HB2	2.22	0.40
1:W:44:THR:O	1:W:530:LYS:HD3	2.22	0.40
1:W:127:GLN:HG3	1:W:551:MET:HB2	2.01	0.40
1:X:354:LYS:HG2	1:X:355:THR:N	2.35	0.40
1:Y:130:VAL:HG13	1:Y:576:SER:O	2.21	0.40
1:Y:155:GLU:HG2	1:Y:156:SER:N	2.36	0.40
1:Z:92:VAL:HB	1:Z:95:ASN:HB2	2.02	0.40
1:a:142:GLU:HB3	1:a:265:THR:HA	2.03	0.40
1:c:73:MET:CE	1:c:522:VAL:HA	2.51	0.40
1:c:200:TRP:HZ2	1:c:569:MET:HE1	1.86	0.40
1:d:92:VAL:O	1:d:93:ASN:HB2	2.20	0.40
1:A:222:HIS:ND1	1:T:426:ASP:HB2	2.35	0.40
1:E:369:ASN:HB3	1:E:372:ALA:HB3	2.02	0.40
1:E:426:ASP:HB2	1:V:222:HIS:CE1	2.57	0.40
1:E:549:GLN:O	1:E:550:GLN:HG3	2.22	0.40
1:N:102:HIS:HB2	1:N:214:TRP:CH2	2.57	0.40
1:N:286:GLY:O	1:N:288:PRO:HD3	2.21	0.40
1:N:443:ASN:OD1	1:N:443:ASN:N	2.53	0.40
1:Q:92:VAL:HB	1:Q:95:ASN:HB2	2.04	0.40
1:Q:225:THR:HG22	1:Q:226:SER:O	2.21	0.40
1:C:545:TRP:CD1	1:C:545:TRP:C	3.00	0.40
1:F:105:ILE:HG12	1:F:212:PHE:HB2	2.03	0.40
1:F:232:ILE:HG12	1:F:233:TYR:N	2.36	0.40
1:F:240:ASP:OD1	1:d:277:HIS:NE2	2.52	0.40
1:F:408:ARG:HD3	1:F:408:ARG:HA	1.78	0.40
1:G:404:GLN:OE1	1:G:458:ASN:HB2	2.21	0.40
1:H:288:PRO:C	1:W:191:ARG:HH12	2.29	0.40
1:H:474:PHE:HZ	1:b:333:PRO:HG2	1.86	0.40
1:H:583:LEU:HD12	1:H:583:LEU:HA	1.80	0.40
1:L:461:PRO:HA	1:L:462:PRO:HD3	1.86	0.40
1:M:44:THR:O	1:M:530:LYS:NZ	2.50	0.40
1:O:216:ARG:NH2	1:O:218:LEU:HD22	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:556:ASP:O	1:O:557:ASN:HB3	2.22	0.40
1:S:510:TYR:HE1	1:S:518:MET:HE2	1.86	0.40
1:S:551:MET:HE2	1:S:551:MET:HB3	1.96	0.40
1:U:557:ASN:OD1	1:U:561:TYR:CE2	2.74	0.40
1:W:297:SER:C	1:W:302:ASN:HD22	2.19	0.40
1:W:483:HIS:HB3	1:W:485:ASN:OD1	2.20	0.40
1:W:518:MET:HE2	1:W:518:MET:HB2	1.72	0.40
1:X:140:SER:HA	1:X:266:PHE:O	2.21	0.40
1:Y:75:GLU:CD	1:Y:75:GLU:H	2.29	0.40
1:Y:476:THR:O	1:Y:479:LYS:HE2	2.22	0.40
1:c:408:ARG:HA	1:c:408:ARG:HD3	1.88	0.40
1:d:99:ASP:CG	1:d:216:ARG:HH21	2.29	0.40
1:d:294:LEU:HA	1:d:295:PRO:HD3	1.92	0.40
1:A:581:ARG:HB3	1:A:582:LYS:H	1.52	0.40
1:E:98:LEU:HD13	1:I:310:GLN:OE1	2.21	0.40
1:B:397:ARG:NH1	1:M:323:ASN:HB3	2.36	0.40
1:D:138:LEU:HG	1:D:268:PHE:CD2	2.56	0.40
1:G:47:ASN:OD1	1:G:67:ARG:NH1	2.52	0.40
1:I:133:MET:CG	1:I:539:LEU:HD23	2.52	0.40
1:K:105:ILE:HG12	1:K:212:PHE:HB2	2.03	0.40
1:K:123:PRO:HB2	1:R:547:PRO:HD3	2.03	0.40
1:L:127:GLN:HG3	1:L:551:MET:HB2	2.03	0.40
1:L:368:GLU:HG2	1:L:369:ASN:H	1.86	0.40
1:L:432:PRO:O	1:L:443:ASN:ND2	2.46	0.40
1:L:492:ASN:CG	1:L:493:ASN:N	2.79	0.40
1:R:271:LYS:HE3	1:R:271:LYS:HB2	1.78	0.40
1:U:365:GLN:O	1:U:366:THR:HG22	2.22	0.40
1:U:378:TYR:HB2	1:U:398:PHE:CE2	2.56	0.40
1:V:177:LEU:HD22	1:V:263:THR:CG2	2.51	0.40
1:W:361:ARG:N	1:W:404:GLN:O	2.52	0.40
1:W:368:GLU:CG	1:W:369:ASN:N	2.81	0.40
1:W:553:ILE:CA	1:W:554:ASN:HB2	2.28	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:J:506:LEU:HA	1:J:506:LEU:HD23	1.90	0.40
1:B:133:MET:CG	1:B:539:LEU:HD23	2.51	0.40
1:B:138:LEU:HD12	1:B:138:LEU:HA	1.93	0.40
1:B:286:GLY:O	1:B:288:PRO:HD3	2.21	0.40
1:C:44:THR:O	1:C:530:LYS:NZ	2.49	0.40
1:G:569:MET:HG2	1:G:570:LYS:N	2.32	0.40
1:I:248:ASN:HD21	1:V:545:TRP:HE3	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:198:TYR:HA	1:K:199:PRO:HD3	1.92	0.40
1:K:401:ILE:O	1:K:575:LYS:NZ	2.54	0.40
1:K:557:ASN:OD1	1:K:557:ASN:C	2.65	0.40
1:O:197:PHE:N	1:O:197:PHE:CD1	2.90	0.40
1:R:377:ARG:NH2	1:R:397:ARG:HD2	2.36	0.40
1:R:518:MET:HE2	1:R:518:MET:HB2	1.85	0.40
1:S:560:ASN:HB3	1:S:572:VAL:HG21	2.02	0.40
1:V:47:ASN:OD1	1:V:65:SER:HA	2.22	0.40
1:W:400:TYR:CE2	1:W:575:LYS:HA	2.56	0.40
1:Y:439:LYS:NZ	1:a:434:ASP:OD2	2.43	0.40
1:a:47:ASN:OD1	1:a:67:ARG:NH1	2.53	0.40
1:b:286:GLY:O	1:b:288:PRO:HD3	2.21	0.40
1:c:382:ARG:N	1:c:386:GLN:HB3	2.32	0.40
1:d:342:TYR:HA	1:d:343:TYR:HA	1.93	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:C:287:LEU:O	1:Z:191:ARG:NH1[8_555]	2.10	0.10
1:O:191:ARG:NH1	1:Y:287:LEU:O[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:O:584:TYR:OH	1:a:471:ASP:OD1[8_555]	2.14	0.06
1:S:287:LEU:O	1:X:191:ARG:NH1[8_555]	2.14	0.06
1:J:584:TYR:OH	1:Q:471:ASP:OD1[8_555]	2.15	0.05
1:Q:287:LEU:O	1:U:191:ARG:NH1[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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	4	27
1	B	546/584 (94%)	496 (91%)	32 (6%)	18 (3%)	3	23
1	C	546/584 (94%)	493 (90%)	39 (7%)	14 (3%)	4	27
1	D	546/584 (94%)	497 (91%)	32 (6%)	17 (3%)	3	25
1	E	546/584 (94%)	497 (91%)	33 (6%)	16 (3%)	3	26
1	F	546/584 (94%)	496 (91%)	33 (6%)	17 (3%)	3	25
1	G	546/584 (94%)	497 (91%)	32 (6%)	17 (3%)	3	25
1	H	546/584 (94%)	491 (90%)	38 (7%)	17 (3%)	3	25
1	I	546/584 (94%)	499 (91%)	34 (6%)	13 (2%)	4	29
1	J	546/584 (94%)	498 (91%)	33 (6%)	15 (3%)	4	27
1	K	546/584 (94%)	499 (91%)	31 (6%)	16 (3%)	3	26
1	L	546/584 (94%)	494 (90%)	35 (6%)	17 (3%)	3	25
1	M	546/584 (94%)	491 (90%)	40 (7%)	15 (3%)	4	27
1	N	546/584 (94%)	497 (91%)	34 (6%)	15 (3%)	4	27
1	O	546/584 (94%)	492 (90%)	35 (6%)	19 (4%)	3	23
1	P	546/584 (94%)	497 (91%)	32 (6%)	17 (3%)	3	25
1	Q	546/584 (94%)	496 (91%)	34 (6%)	16 (3%)	3	26
1	R	546/584 (94%)	490 (90%)	39 (7%)	17 (3%)	3	25
1	S	546/584 (94%)	500 (92%)	32 (6%)	14 (3%)	4	27
1	T	546/584 (94%)	501 (92%)	30 (6%)	15 (3%)	4	27
1	U	546/584 (94%)	496 (91%)	32 (6%)	18 (3%)	3	23
1	V	546/584 (94%)	492 (90%)	37 (7%)	17 (3%)	3	25
1	W	546/584 (94%)	491 (90%)	40 (7%)	15 (3%)	4	27
1	X	546/584 (94%)	495 (91%)	34 (6%)	17 (3%)	3	25
1	Y	546/584 (94%)	498 (91%)	30 (6%)	18 (3%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	546/584 (94%)	497 (91%)	31 (6%)	18 (3%)	3	23
1	a	546/584 (94%)	497 (91%)	33 (6%)	16 (3%)	3	26
1	b	546/584 (94%)	489 (90%)	41 (8%)	16 (3%)	3	26
1	c	546/584 (94%)	499 (91%)	31 (6%)	16 (3%)	3	26
1	d	546/584 (94%)	498 (91%)	32 (6%)	16 (3%)	3	26
All	All	16380/17520 (94%)	14873 (91%)	1020 (6%)	487 (3%)	3	25

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	463 (97%)	13 (3%)	39	62
1	B	476/495 (96%)	467 (98%)	9 (2%)	50	68
1	C	476/495 (96%)	458 (96%)	18 (4%)	29	55
1	D	476/495 (96%)	462 (97%)	14 (3%)	37	60
1	E	476/495 (96%)	467 (98%)	9 (2%)	50	68
1	F	476/495 (96%)	463 (97%)	13 (3%)	39	62
1	G	476/495 (96%)	462 (97%)	14 (3%)	37	60
1	H	476/495 (96%)	460 (97%)	16 (3%)	32	57
1	I	476/495 (96%)	460 (97%)	16 (3%)	32	57
1	J	476/495 (96%)	466 (98%)	10 (2%)	47	66
1	K	476/495 (96%)	464 (98%)	12 (2%)	42	63
1	L	476/495 (96%)	460 (97%)	16 (3%)	32	57
1	M	476/495 (96%)	464 (98%)	12 (2%)	42	63
1	N	476/495 (96%)	466 (98%)	10 (2%)	47	66
1	O	476/495 (96%)	465 (98%)	11 (2%)	44	64
1	P	476/495 (96%)	469 (98%)	7 (2%)	57	71
1	Q	476/495 (96%)	465 (98%)	11 (2%)	44	64
1	R	476/495 (96%)	461 (97%)	15 (3%)	34	59
1	S	476/495 (96%)	464 (98%)	12 (2%)	42	63
1	T	476/495 (96%)	462 (97%)	14 (3%)	37	60
1	U	476/495 (96%)	463 (97%)	13 (3%)	39	62
1	V	476/495 (96%)	470 (99%)	6 (1%)	61	72
1	W	476/495 (96%)	462 (97%)	14 (3%)	37	60
1	X	476/495 (96%)	464 (98%)	12 (2%)	42	63
1	Y	476/495 (96%)	470 (99%)	6 (1%)	61	72
1	Z	476/495 (96%)	465 (98%)	11 (2%)	44	64
1	a	476/495 (96%)	465 (98%)	11 (2%)	44	64
1	b	476/495 (96%)	465 (98%)	11 (2%)	44	64
1	c	476/495 (96%)	462 (97%)	14 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	d	476/495 (96%)	460 (97%)	16 (3%)	32	57
All	All	14280/14850 (96%)	13914 (97%)	366 (3%)	40	62

All (366) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	55	GLU
1	A	150	LEU
1	A	158	THR
1	A	159	GLN
1	A	368	GLU
1	A	457	LEU
1	A	517	ASN
1	A	536	LYS
1	A	549	GLN
1	A	553	ILE
1	A	554	ASN
1	A	583	LEU
1	E	47	ASN
1	E	52	LYS
1	E	368	GLU
1	E	415	ILE
1	E	457	LEU
1	E	553	ILE
1	E	565	ASN
1	E	573	TYR
1	E	583	LEU
1	J	44	THR
1	J	150	LEU
1	J	155	GLU
1	J	209	ARG
1	J	368	GLU
1	J	415	ILE
1	J	457	LEU
1	J	554	ASN
1	J	573	TYR
1	J	583	LEU
1	N	96	MET
1	N	162	THR
1	N	296	GLN
1	N	316	VAL

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Mol	Chain	Res	Type
1	N	368	GLU
1	N	457	LEU
1	N	553	ILE
1	N	556	ASP
1	N	574	GLU
1	N	583	LEU
1	Q	44	THR
1	Q	296	GLN
1	Q	369	ASN
1	Q	415	ILE
1	Q	457	LEU
1	Q	492	ASN
1	Q	536	LYS
1	Q	553	ILE
1	Q	557	ASN
1	Q	573	TYR
1	Q	583	LEU
1	B	88	ASP
1	B	393	GLU
1	B	415	ILE
1	B	457	LEU
1	B	494	CYS
1	B	553	ILE
1	B	554	ASN
1	B	573	TYR
1	B	583	LEU
1	C	44	THR
1	C	75	GLU
1	C	159	GLN
1	C	225	THR
1	C	367	ASP
1	C	370	GLN
1	C	415	ILE
1	C	457	LEU
1	C	493	ASN
1	C	513	ASP
1	C	553	ILE
1	C	554	ASN
1	C	555	VAL
1	C	556	ASP
1	C	566	ILE
1	C	573	TYR

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Mol	Chain	Res	Type
1	C	574	GLU
1	C	583	LEU
1	D	44	THR
1	D	55	GLU
1	D	56	ASN
1	D	96	MET
1	D	155	GLU
1	D	209	ARG
1	D	226	SER
1	D	271	LYS
1	D	296	GLN
1	D	316	VAL
1	D	361	ARG
1	D	457	LEU
1	D	518	MET
1	D	553	ILE
1	F	55	GLU
1	F	260	GLU
1	F	357	ILE
1	F	368	GLU
1	F	383	GLN
1	F	415	ILE
1	F	457	LEU
1	F	517	ASN
1	F	549	GLN
1	F	553	ILE
1	F	573	TYR
1	F	574	GLU
1	F	583	LEU
1	G	44	THR
1	G	55	GLU
1	G	75	GLU
1	G	209	ARG
1	G	271	LYS
1	G	368	GLU
1	G	415	ILE
1	G	425	THR
1	G	457	LEU
1	G	492	ASN
1	G	553	ILE
1	G	574	GLU
1	G	582	LYS

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Mol	Chain	Res	Type
1	G	583	LEU
1	H	44	THR
1	H	75	GLU
1	H	316	VAL
1	H	367	ASP
1	H	368	GLU
1	H	387	LYS
1	H	415	ILE
1	H	457	LEU
1	H	536	LYS
1	H	549	GLN
1	H	553	ILE
1	H	556	ASP
1	H	565	ASN
1	H	573	TYR
1	H	574	GLU
1	H	583	LEU
1	I	55	GLU
1	I	88	ASP
1	I	96	MET
1	I	150	LEU
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	553	ILE
1	I	554	ASN
1	I	574	GLU
1	I	583	LEU
1	K	47	ASN
1	K	55	GLU
1	K	163	LYS
1	K	368	GLU
1	K	457	LEU
1	K	536	LYS
1	K	549	GLN
1	K	553	ILE
1	K	554	ASN

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Mol	Chain	Res	Type
1	K	558	GLN
1	K	574	GLU
1	K	583	LEU
1	L	159	GLN
1	L	162	THR
1	L	260	GLU
1	L	302	ASN
1	L	415	ILE
1	L	425	THR
1	L	457	LEU
1	L	490	CYS
1	L	492	ASN
1	L	519	SER
1	L	549	GLN
1	L	553	ILE
1	L	554	ASN
1	L	574	GLU
1	L	582	LYS
1	L	583	LEU
1	M	44	THR
1	M	155	GLU
1	M	302	ASN
1	M	316	VAL
1	M	368	GLU
1	M	415	ILE
1	M	457	LEU
1	M	509	GLN
1	M	543	HIS
1	M	553	ILE
1	M	573	TYR
1	M	583	LEU
1	O	44	THR
1	O	158	THR
1	O	163	LYS
1	O	271	LYS
1	O	401	ILE
1	O	415	ILE
1	O	457	LEU
1	O	553	ILE
1	O	573	TYR
1	O	574	GLU
1	O	583	LEU

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Mol	Chain	Res	Type
1	P	361	ARG
1	P	457	LEU
1	P	519	SER
1	P	536	LYS
1	P	549	GLN
1	P	553	ILE
1	P	573	TYR
1	R	44	THR
1	R	75	GLU
1	R	156	SER
1	R	209	ARG
1	R	316	VAL
1	R	415	ILE
1	R	457	LEU
1	R	508	ASN
1	R	509	GLN
1	R	519	SER
1	R	549	GLN
1	R	553	ILE
1	R	573	TYR
1	R	574	GLU
1	R	583	LEU
1	S	44	THR
1	S	96	MET
1	S	296	GLN
1	S	316	VAL
1	S	457	LEU
1	S	549	GLN
1	S	553	ILE
1	S	554	ASN
1	S	558	GLN
1	S	573	TYR
1	S	574	GLU
1	S	583	LEU
1	T	44	THR
1	T	88	ASP
1	T	158	THR
1	T	271	LYS
1	T	393	GLU
1	T	415	ILE
1	T	436	ILE
1	T	457	LEU

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Mol	Chain	Res	Type
1	T	509	GLN
1	T	553	ILE
1	T	554	ASN
1	T	565	ASN
1	T	574	GLU
1	T	583	LEU
1	U	159	GLN
1	U	163	LYS
1	U	316	VAL
1	U	370	GLN
1	U	436	ILE
1	U	457	LEU
1	U	492	ASN
1	U	543	HIS
1	U	553	ILE
1	U	554	ASN
1	U	565	ASN
1	U	573	TYR
1	U	583	LEU
1	V	159	GLN
1	V	415	ILE
1	V	457	LEU
1	V	493	ASN
1	V	494	CYS
1	V	583	LEU
1	W	44	THR
1	W	158	THR
1	W	159	GLN
1	W	309	GLN
1	W	387	LYS
1	W	415	ILE
1	W	457	LEU
1	W	553	ILE
1	W	556	ASP
1	W	565	ASN
1	W	573	TYR
1	W	574	GLU
1	W	582	LYS
1	W	583	LEU
1	X	96	MET
1	X	312	LYS
1	X	368	GLU

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Mol	Chain	Res	Type
1	X	384	HIS
1	X	457	LEU
1	X	493	ASN
1	X	494	CYS
1	X	518	MET
1	X	553	ILE
1	X	558	GLN
1	X	582	LYS
1	X	583	LEU
1	Y	44	THR
1	Y	209	ARG
1	Y	415	ILE
1	Y	457	LEU
1	Y	573	TYR
1	Y	583	LEU
1	Z	55	GLU
1	Z	158	THR
1	Z	228	THR
1	Z	316	VAL
1	Z	415	ILE
1	Z	457	LEU
1	Z	509	GLN
1	Z	549	GLN
1	Z	553	ILE
1	Z	554	ASN
1	Z	583	LEU
1	a	44	THR
1	a	50	GLU
1	a	156	SER
1	a	226	SER
1	a	393	GLU
1	a	415	ILE
1	a	457	LEU
1	a	553	ILE
1	a	573	TYR
1	a	574	GLU
1	a	583	LEU
1	b	44	THR
1	b	75	GLU
1	b	87	LEU
1	b	155	GLU
1	b	159	GLN

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Mol	Chain	Res	Type
1	b	415	ILE
1	b	457	LEU
1	b	553	ILE
1	b	554	ASN
1	b	574	GLU
1	b	583	LEU
1	c	96	MET
1	c	150	LEU
1	c	209	ARG
1	c	280	GLN
1	c	296	GLN
1	c	309	GLN
1	c	316	VAL
1	c	368	GLU
1	c	384	HIS
1	c	416	GLN
1	c	457	LEU
1	c	543	HIS
1	c	553	ILE
1	c	583	LEU
1	d	44	THR
1	d	158	THR
1	d	260	GLU
1	d	271	LYS
1	d	387	LYS
1	d	415	ILE
1	d	457	LEU
1	d	517	ASN
1	d	518	MET
1	d	553	ILE
1	d	554	ASN
1	d	556	ASP
1	d	565	ASN
1	d	573	TYR
1	d	582	LYS
1	d	583	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (204) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	72	ASN

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Mol	Chain	Res	Type
1	A	137	HIS
1	A	248	ASN
1	A	253	HIS
1	A	383	GLN
1	A	384	HIS
1	A	509	GLN
1	A	549	GLN
1	A	557	ASN
1	A	558	GLN
1	E	95	ASN
1	E	159	GLN
1	E	280	GLN
1	E	302	ASN
1	E	383	GLN
1	E	384	HIS
1	E	517	ASN
1	E	543	HIS
1	E	557	ASN
1	J	137	HIS
1	J	383	GLN
1	J	549	GLN
1	N	167	ASN
1	N	248	ASN
1	N	419	ASN
1	N	446	ASN
1	N	458	ASN
1	N	466	ASN
1	N	491	GLN
1	Q	280	GLN
1	Q	302	ASN
1	Q	403	HIS
1	Q	492	ASN
1	Q	493	ASN
1	Q	558	GLN
1	B	56	ASN
1	B	137	HIS
1	B	159	GLN
1	B	302	ASN
1	B	384	HIS
1	B	386	GLN
1	B	554	ASN
1	B	565	ASN

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Mol	Chain	Res	Type
1	C	137	HIS
1	C	321	ASN
1	C	386	GLN
1	C	549	GLN
1	D	137	HIS
1	D	253	HIS
1	D	370	GLN
1	D	384	HIS
1	D	557	ASN
1	D	558	GLN
1	F	72	ASN
1	F	137	HIS
1	F	248	ASN
1	F	302	ASN
1	F	383	GLN
1	F	384	HIS
1	F	466	ASN
1	F	554	ASN
1	F	558	GLN
1	G	253	HIS
1	G	302	ASN
1	G	365	GLN
1	G	384	HIS
1	G	446	ASN
1	G	466	ASN
1	G	554	ASN
1	H	72	ASN
1	H	242	GLN
1	H	383	GLN
1	H	446	ASN
1	H	517	ASN
1	H	543	HIS
1	H	549	GLN
1	H	554	ASN
1	I	137	HIS
1	I	248	ASN
1	I	253	HIS
1	I	383	GLN
1	I	419	ASN
1	I	558	GLN
1	K	302	ASN
1	K	492	ASN

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Mol	Chain	Res	Type
1	L	159	GLN
1	L	321	ASN
1	L	365	GLN
1	L	383	GLN
1	L	384	HIS
1	L	386	GLN
1	L	565	ASN
1	L	577	GLN
1	M	253	HIS
1	M	383	GLN
1	M	384	HIS
1	M	543	HIS
1	M	558	GLN
1	O	137	HIS
1	O	253	HIS
1	O	302	ASN
1	O	309	GLN
1	O	369	ASN
1	O	557	ASN
1	P	137	HIS
1	P	159	GLN
1	P	384	HIS
1	P	543	HIS
1	P	554	ASN
1	P	558	GLN
1	R	64	ASN
1	R	70	HIS
1	R	137	HIS
1	R	242	GLN
1	R	280	GLN
1	R	302	ASN
1	R	369	ASN
1	R	383	GLN
1	R	458	ASN
1	R	554	ASN
1	R	558	GLN
1	S	137	HIS
1	S	321	ASN
1	S	384	HIS
1	S	416	GLN
1	S	446	ASN
1	S	491	GLN

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Mol	Chain	Res	Type
1	S	554	ASN
1	T	137	HIS
1	T	253	HIS
1	T	302	ASN
1	T	446	ASN
1	T	543	HIS
1	T	549	GLN
1	U	56	ASN
1	U	137	HIS
1	U	248	ASN
1	U	302	ASN
1	U	369	ASN
1	U	383	GLN
1	U	384	HIS
1	U	446	ASN
1	U	558	GLN
1	U	577	GLN
1	V	64	ASN
1	V	280	GLN
1	V	321	ASN
1	V	383	GLN
1	V	384	HIS
1	V	416	GLN
1	V	558	GLN
1	W	280	GLN
1	W	549	GLN
1	W	554	ASN
1	W	558	GLN
1	W	565	ASN
1	X	137	HIS
1	X	280	GLN
1	X	321	ASN
1	X	383	GLN
1	X	386	GLN
1	X	459	ASN
1	X	466	ASN
1	X	557	ASN
1	Y	137	HIS
1	Y	248	ASN
1	Y	321	ASN
1	Y	383	GLN
1	Y	384	HIS

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Mol	Chain	Res	Type
1	Y	416	GLN
1	Y	458	ASN
1	Y	557	ASN
1	Z	46	ASN
1	Z	350	GLN
1	Z	383	GLN
1	Z	384	HIS
1	Z	419	ASN
1	Z	446	ASN
1	Z	550	GLN
1	Z	558	GLN
1	a	253	HIS
1	a	302	ASN
1	a	384	HIS
1	a	466	ASN
1	a	554	ASN
1	a	577	GLN
1	b	137	HIS
1	b	248	ASN
1	b	280	GLN
1	b	302	ASN
1	b	577	GLN
1	c	253	HIS
1	c	321	ASN
1	c	466	ASN
1	c	492	ASN
1	c	554	ASN
1	c	577	GLN
1	d	137	HIS
1	d	302	ASN
1	d	384	HIS
1	d	416	GLN
1	d	458	ASN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	548/584 (93%)	-0.25	6 (1%) 78 54	3, 17, 60, 119	0
1	B	548/584 (93%)	-0.22	6 (1%) 78 54	4, 19, 64, 124	0
1	C	548/584 (93%)	-0.12	10 (1%) 67 42	3, 20, 64, 121	0
1	D	548/584 (93%)	-0.15	8 (1%) 72 47	5, 20, 63, 131	0
1	E	548/584 (93%)	-0.19	7 (1%) 75 50	4, 18, 62, 120	0
1	F	548/584 (93%)	-0.20	7 (1%) 75 50	3, 18, 61, 118	0
1	G	548/584 (93%)	-0.15	5 (0%) 81 58	4, 20, 62, 126	0
1	H	548/584 (93%)	-0.17	7 (1%) 75 50	4, 19, 62, 118	0
1	I	548/584 (93%)	-0.16	13 (2%) 59 35	5, 19, 62, 127	0
1	J	548/584 (93%)	-0.23	6 (1%) 78 54	3, 19, 61, 122	0
1	K	548/584 (93%)	-0.20	15 (2%) 56 33	3, 17, 61, 122	0
1	L	548/584 (93%)	-0.12	7 (1%) 75 50	4, 19, 60, 125	0
1	M	548/584 (93%)	-0.23	6 (1%) 78 54	3, 18, 62, 121	0
1	N	548/584 (93%)	-0.19	10 (1%) 67 42	5, 19, 62, 126	0
1	O	548/584 (93%)	-0.14	6 (1%) 78 54	3, 20, 64, 123	0
1	P	548/584 (93%)	-0.18	7 (1%) 75 50	3, 18, 61, 119	0
1	Q	548/584 (93%)	-0.21	8 (1%) 72 47	4, 19, 61, 130	0
1	R	548/584 (93%)	-0.20	9 (1%) 70 45	4, 18, 62, 121	0
1	S	548/584 (93%)	-0.14	8 (1%) 72 47	5, 19, 61, 131	0
1	T	548/584 (93%)	-0.19	9 (1%) 70 45	4, 18, 64, 120	0
1	U	548/584 (93%)	-0.18	9 (1%) 70 45	3, 18, 65, 118	0
1	V	548/584 (93%)	-0.12	9 (1%) 70 45	4, 19, 62, 126	0
1	W	548/584 (93%)	-0.13	6 (1%) 78 54	4, 21, 66, 121	0
1	X	548/584 (93%)	-0.17	6 (1%) 78 54	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%)	-0.13	7 (1%) 75 50	4, 19, 64, 123	0
1	Z	548/584 (93%)	-0.07	8 (1%) 72 47	3, 20, 64, 116	0
1	a	548/584 (93%)	-0.04	9 (1%) 70 45	4, 21, 67, 123	0
1	b	548/584 (93%)	-0.17	7 (1%) 75 50	3, 20, 66, 124	0
1	c	548/584 (93%)	-0.06	4 (0%) 84 63	4, 22, 61, 130	0
1	d	548/584 (93%)	-0.11	8 (1%) 72 47	4, 19, 64, 125	0
All	All	16440/17520 (93%)	-0.16	233 (1%) 73 48	3, 19, 64, 131	0

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	368	GLU	4.8
1	a	156	SER	4.7
1	N	158	THR	4.4
1	Q	516	ALA	4.4
1	M	156	SER	4.4
1	M	155	GLU	4.4
1	K	156	SER	4.2
1	R	516	ALA	4.1
1	c	156	SER	4.0
1	T	517	ASN	4.0
1	d	516	ALA	3.9
1	T	156	SER	3.9
1	N	516	ALA	3.9
1	S	300	GLY	3.8
1	N	156	SER	3.7
1	C	156	SER	3.7
1	X	156	SER	3.6
1	H	518	MET	3.6
1	c	516	ALA	3.6
1	Q	156	SER	3.6
1	U	516	ALA	3.5
1	V	159	GLN	3.5
1	V	160	PRO	3.5
1	I	224	GLY	3.4
1	W	156	SER	3.4
1	D	156	SER	3.4
1	O	156	SER	3.4
1	K	157	ALA	3.4
1	U	157	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	Q	515	SER	3.4
1	T	516	ALA	3.3
1	V	516	ALA	3.3
1	d	156	SER	3.3
1	F	156	SER	3.2
1	K	300	GLY	3.2
1	K	155	GLU	3.2
1	I	154	SER	3.2
1	X	224	GLY	3.2
1	I	155	GLU	3.2
1	C	365	GLN	3.1
1	H	300	GLY	3.1
1	D	157	ALA	3.1
1	d	158	THR	3.1
1	V	156	SER	3.1
1	J	365	GLN	3.1
1	G	156	SER	3.0
1	I	516	ALA	3.0
1	A	156	SER	3.0
1	K	518	MET	3.0
1	U	160	PRO	3.0
1	I	225	THR	3.0
1	K	158	THR	3.0
1	b	518	MET	3.0
1	S	224	GLY	2.9
1	a	516	ALA	2.9
1	F	157	ALA	2.9
1	Z	518	MET	2.9
1	E	364	ALA	2.9
1	L	160	PRO	2.9
1	A	155	GLU	2.9
1	Q	517	ASN	2.9
1	I	517	ASN	2.9
1	I	157	ALA	2.9
1	N	300	GLY	2.8
1	E	516	ALA	2.8
1	a	157	ALA	2.8
1	G	155	GLU	2.8
1	b	156	SER	2.8
1	A	517	ASN	2.8
1	E	517	ASN	2.8
1	C	157	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	X	157	ALA	2.8
1	a	160	PRO	2.8
1	B	159	GLN	2.8
1	L	155	GLU	2.8
1	O	516	ALA	2.8
1	P	156	SER	2.8
1	L	159	GLN	2.8
1	O	517	ASN	2.8
1	H	156	SER	2.8
1	T	160	PRO	2.8
1	P	158	THR	2.8
1	T	364	ALA	2.8
1	Z	516	ALA	2.7
1	V	157	ALA	2.7
1	B	155	GLU	2.7
1	V	518	MET	2.7
1	U	161	PRO	2.6
1	T	159	GLN	2.6
1	b	160	PRO	2.6
1	J	156	SER	2.6
1	M	154	SER	2.6
1	U	156	SER	2.6
1	Y	160	PRO	2.6
1	F	224	GLY	2.6
1	d	518	MET	2.6
1	c	158	THR	2.6
1	Y	156	SER	2.6
1	Z	158	THR	2.5
1	C	302	ASN	2.5
1	H	160	PRO	2.5
1	I	158	THR	2.5
1	N	155	GLU	2.5
1	J	516	ALA	2.5
1	K	160	PRO	2.5
1	P	161	PRO	2.5
1	W	155	GLU	2.5
1	I	494	CYS	2.5
1	d	160	PRO	2.5
1	N	518	MET	2.5
1	A	160	PRO	2.5
1	N	88	ASP	2.5
1	O	300	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	R	518	MET	2.5
1	J	517	ASN	2.4
1	Q	159	GLN	2.4
1	b	516	ALA	2.4
1	G	161	PRO	2.4
1	S	156	SER	2.4
1	D	153	VAL	2.4
1	L	157	ALA	2.4
1	M	517	ASN	2.4
1	S	159	GLN	2.4
1	F	160	PRO	2.4
1	W	300	GLY	2.4
1	R	156	SER	2.4
1	I	159	GLN	2.4
1	Y	159	GLN	2.4
1	C	517	ASN	2.4
1	Q	160	PRO	2.4
1	d	300	GLY	2.4
1	B	156	SER	2.4
1	U	513	ASP	2.4
1	G	209	ARG	2.4
1	a	161	PRO	2.4
1	a	163	LYS	2.4
1	R	158	THR	2.4
1	S	155	GLU	2.4
1	R	365	GLN	2.4
1	W	516	ALA	2.4
1	b	159	GLN	2.4
1	K	568	GLY	2.4
1	P	159	GLN	2.3
1	F	360	GLY	2.3
1	S	157	ALA	2.3
1	T	365	GLN	2.3
1	B	543	HIS	2.3
1	D	516	ALA	2.3
1	E	365	GLN	2.3
1	Y	75	GLU	2.3
1	I	300	GLY	2.3
1	L	515	SER	2.3
1	P	160	PRO	2.3
1	U	227	GLY	2.3
1	S	158	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	a	228	THR	2.3
1	B	157	ALA	2.3
1	X	573	TYR	2.3
1	H	155	GLU	2.3
1	H	162	THR	2.3
1	a	518	MET	2.3
1	P	516	ALA	2.3
1	W	392	GLY	2.3
1	L	158	THR	2.3
1	C	154	SER	2.3
1	N	360	GLY	2.3
1	N	517	ASN	2.2
1	E	156	SER	2.2
1	C	225	THR	2.2
1	R	515	SER	2.2
1	X	155	GLU	2.2
1	S	225	THR	2.2
1	Y	269	ASP	2.2
1	C	516	ALA	2.2
1	Y	516	ALA	2.2
1	L	156	SER	2.2
1	d	226	SER	2.2
1	V	568	GLY	2.2
1	b	155	GLU	2.2
1	B	160	PRO	2.2
1	I	160	PRO	2.2
1	U	158	THR	2.2
1	Z	554	ASN	2.2
1	K	163	LYS	2.2
1	X	159	GLN	2.2
1	J	300	GLY	2.2
1	D	227	GLY	2.2
1	Z	160	PRO	2.2
1	K	159	GLN	2.2
1	O	361	ARG	2.2
1	Q	368	GLU	2.2
1	K	161	PRO	2.2
1	W	368	GLU	2.2
1	V	228	THR	2.2
1	Y	517	ASN	2.2
1	E	300	GLY	2.1
1	T	224	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	368	GLU	2.1
1	R	155	GLU	2.1
1	a	158	THR	2.1
1	P	517	ASN	2.1
1	d	269	ASP	2.1
1	R	568	GLY	2.1
1	K	516	ALA	2.1
1	U	554	ASN	2.1
1	Z	156	SER	2.1
1	D	159	GLN	2.1
1	K	365	GLN	2.1
1	R	159	GLN	2.1
1	K	360	GLY	2.1
1	b	362	GLY	2.1
1	Z	155	GLU	2.1
1	c	155	GLU	2.1
1	C	160	PRO	2.1
1	F	161	PRO	2.1
1	D	155	GLU	2.1
1	H	368	GLU	2.1
1	K	515	SER	2.1
1	Z	154	SER	2.1
1	F	159	GLN	2.1
1	M	492	ASN	2.1
1	V	365	GLN	2.1
1	J	153	VAL	2.1
1	C	360	GLY	2.0
1	E	515	SER	2.0
1	N	157	ALA	2.0
1	Q	300	GLY	2.0
1	M	360	GLY	2.0
1	A	157	ALA	2.0
1	D	517	ASN	2.0
1	O	37	GLY	2.0
1	T	158	THR	2.0
1	I	269	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	Y	602	1/1	0.76	0.36	52,52,52,52	0
2	MG	K	800	1/1	0.82	0.35	39,39,39,39	0
2	MG	D	800	1/1	0.86	0.17	43,43,43,43	0
2	MG	T	800	1/1	0.87	0.29	43,43,43,43	0
2	MG	M	800	1/1	0.87	0.29	41,41,41,41	0
2	MG	N	800	1/1	0.88	0.26	39,39,39,39	0
2	MG	O	800	1/1	0.89	0.18	41,41,41,41	0
2	MG	d	602	1/1	0.89	0.32	56,56,56,56	0
2	MG	G	800	1/1	0.90	0.24	44,44,44,44	0
2	MG	H	602	1/1	0.91	0.23	54,54,54,54	0
2	MG	Q	800	1/1	0.91	0.25	41,41,41,41	0
2	MG	R	800	1/1	0.91	0.21	37,37,37,37	0
2	MG	c	800	1/1	0.92	0.18	53,53,53,53	0
2	MG	C	800	1/1	0.93	0.20	41,41,41,41	0
2	MG	L	800	1/1	0.93	0.18	41,41,41,41	0
2	MG	W	800	1/1	0.93	0.19	47,47,47,47	0
2	MG	E	601	1/1	0.94	0.18	40,40,40,40	0
2	MG	H	601	1/1	0.95	0.16	36,36,36,36	0
2	MG	Y	601	1/1	0.95	0.15	47,47,47,47	0
2	MG	P	800	1/1	0.95	0.19	39,39,39,39	0
2	MG	J	602	1/1	0.95	0.22	38,38,38,38	0
2	MG	d	601	1/1	0.95	0.14	37,37,37,37	0
2	MG	I	800	1/1	0.95	0.20	43,43,43,43	0
2	MG	E	602	1/1	0.96	0.14	38,38,38,38	0
2	MG	B	800	1/1	0.96	0.17	41,41,41,41	0
2	MG	X	800	1/1	0.96	0.15	43,43,43,43	0
2	MG	S	800	1/1	0.96	0.16	39,39,39,39	0
2	MG	J	601	1/1	0.97	0.16	40,40,40,40	0
2	MG	A	800	1/1	0.97	0.11	32,32,32,32	0
2	MG	Z	800	1/1	0.99	0.14	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.