



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:58 am GMT

PDB ID : 3HQQ
Title : Crystal structure of Leishmania mexicana pyruvate kinase (LmPYK) in complex with Fructose 2,6 biphosphate
Authors : Morgan, H.P.; Walkinshaw, M.D.
Deposited on : 2009-06-08
Resolution : 5.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28972

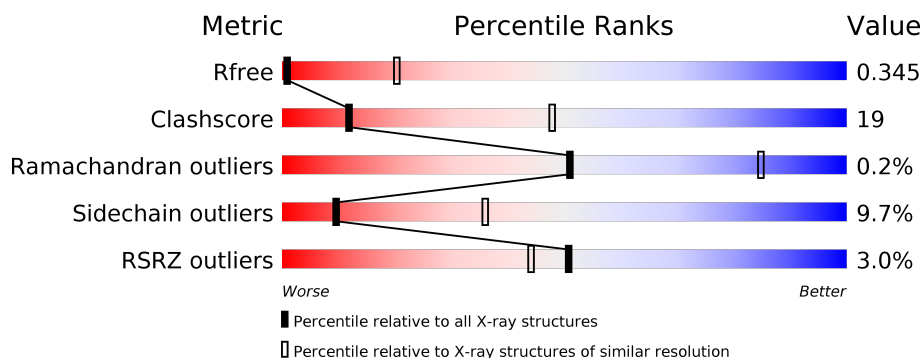
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.07 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}	100719	1005 (6.46-3.68)
Clashscore	112137	1095 (6.46-3.70)
Ramachandran outliers	110173	1028 (6.46-3.70)
Sidechain outliers	110143	1005 (6.46-3.70)
RSRZ outliers	101464	1006 (6.46-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	499	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div></div> </div> </div>
1	B	499	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div></div> </div> </div>
1	C	499	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>5%</div> </div> </div>
1	D	499	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div></div> </div> </div>
1	E	499	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div></div> </div> </div>
1	F	499	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	499	
1	H	499	
1	I	499	
1	J	499	
1	K	499	
1	L	499	
1	M	499	
1	N	499	
1	O	499	
1	P	499	
1	Q	499	
1	R	499	
1	S	499	
1	T	499	
1	U	499	
1	V	499	
1	W	499	
1	X	499	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 91656 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	B	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	C	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	D	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	E	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	F	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	G	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	H	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	I	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	J	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	K	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	L	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	M	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	N	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	O	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	P	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	R	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	S	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	T	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	U	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	V	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	W	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	X	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	SER	GLY	SEE REMARK 999	UNP Q27686
A	389	TYR	SER	SEE REMARK 999	UNP Q27686
A	404	ARG	ALA	SEE REMARK 999	UNP Q27686
A	405	SER	GLY	SEE REMARK 999	UNP Q27686
B	382	SER	GLY	SEE REMARK 999	UNP Q27686
B	389	TYR	SER	SEE REMARK 999	UNP Q27686
B	404	ARG	ALA	SEE REMARK 999	UNP Q27686
B	405	SER	GLY	SEE REMARK 999	UNP Q27686
C	382	SER	GLY	SEE REMARK 999	UNP Q27686
C	389	TYR	SER	SEE REMARK 999	UNP Q27686
C	404	ARG	ALA	SEE REMARK 999	UNP Q27686
C	405	SER	GLY	SEE REMARK 999	UNP Q27686
D	382	SER	GLY	SEE REMARK 999	UNP Q27686
D	389	TYR	SER	SEE REMARK 999	UNP Q27686
D	404	ARG	ALA	SEE REMARK 999	UNP Q27686
D	405	SER	GLY	SEE REMARK 999	UNP Q27686
E	382	SER	GLY	SEE REMARK 999	UNP Q27686
E	389	TYR	SER	SEE REMARK 999	UNP Q27686
E	404	ARG	ALA	SEE REMARK 999	UNP Q27686
E	405	SER	GLY	SEE REMARK 999	UNP Q27686
F	382	SER	GLY	SEE REMARK 999	UNP Q27686
F	389	TYR	SER	SEE REMARK 999	UNP Q27686
F	404	ARG	ALA	SEE REMARK 999	UNP Q27686

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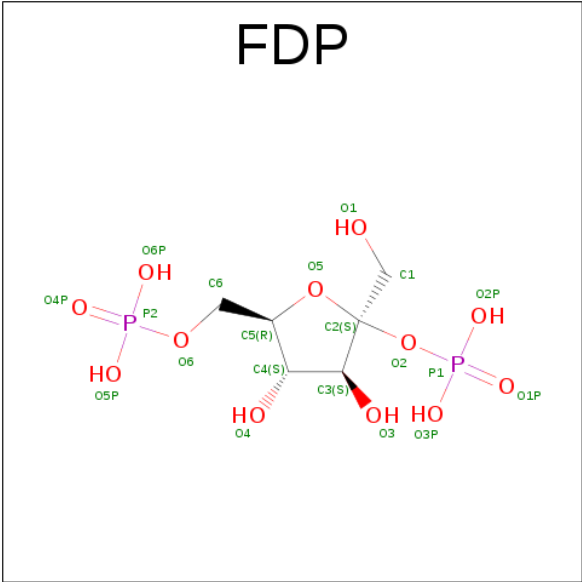
Chain	Residue	Modelled	Actual	Comment	Reference
F	405	SER	GLY	SEE REMARK 999	UNP Q27686
G	382	SER	GLY	SEE REMARK 999	UNP Q27686
G	389	TYR	SER	SEE REMARK 999	UNP Q27686
G	404	ARG	ALA	SEE REMARK 999	UNP Q27686
G	405	SER	GLY	SEE REMARK 999	UNP Q27686
H	382	SER	GLY	SEE REMARK 999	UNP Q27686
H	389	TYR	SER	SEE REMARK 999	UNP Q27686
H	404	ARG	ALA	SEE REMARK 999	UNP Q27686
H	405	SER	GLY	SEE REMARK 999	UNP Q27686
I	382	SER	GLY	SEE REMARK 999	UNP Q27686
I	389	TYR	SER	SEE REMARK 999	UNP Q27686
I	404	ARG	ALA	SEE REMARK 999	UNP Q27686
I	405	SER	GLY	SEE REMARK 999	UNP Q27686
J	382	SER	GLY	SEE REMARK 999	UNP Q27686
J	389	TYR	SER	SEE REMARK 999	UNP Q27686
J	404	ARG	ALA	SEE REMARK 999	UNP Q27686
J	405	SER	GLY	SEE REMARK 999	UNP Q27686
K	382	SER	GLY	SEE REMARK 999	UNP Q27686
K	389	TYR	SER	SEE REMARK 999	UNP Q27686
K	404	ARG	ALA	SEE REMARK 999	UNP Q27686
K	405	SER	GLY	SEE REMARK 999	UNP Q27686
L	382	SER	GLY	SEE REMARK 999	UNP Q27686
L	389	TYR	SER	SEE REMARK 999	UNP Q27686
L	404	ARG	ALA	SEE REMARK 999	UNP Q27686
L	405	SER	GLY	SEE REMARK 999	UNP Q27686
M	382	SER	GLY	SEE REMARK 999	UNP Q27686
M	389	TYR	SER	SEE REMARK 999	UNP Q27686
M	404	ARG	ALA	SEE REMARK 999	UNP Q27686
M	405	SER	GLY	SEE REMARK 999	UNP Q27686
N	382	SER	GLY	SEE REMARK 999	UNP Q27686
N	389	TYR	SER	SEE REMARK 999	UNP Q27686
N	404	ARG	ALA	SEE REMARK 999	UNP Q27686
N	405	SER	GLY	SEE REMARK 999	UNP Q27686
O	382	SER	GLY	SEE REMARK 999	UNP Q27686
O	389	TYR	SER	SEE REMARK 999	UNP Q27686
O	404	ARG	ALA	SEE REMARK 999	UNP Q27686
O	405	SER	GLY	SEE REMARK 999	UNP Q27686
P	382	SER	GLY	SEE REMARK 999	UNP Q27686
P	389	TYR	SER	SEE REMARK 999	UNP Q27686
P	404	ARG	ALA	SEE REMARK 999	UNP Q27686
P	405	SER	GLY	SEE REMARK 999	UNP Q27686
Q	382	SER	GLY	SEE REMARK 999	UNP Q27686

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	389	TYR	SER	SEE REMARK 999	UNP Q27686
Q	404	ARG	ALA	SEE REMARK 999	UNP Q27686
Q	405	SER	GLY	SEE REMARK 999	UNP Q27686
R	382	SER	GLY	SEE REMARK 999	UNP Q27686
R	389	TYR	SER	SEE REMARK 999	UNP Q27686
R	404	ARG	ALA	SEE REMARK 999	UNP Q27686
R	405	SER	GLY	SEE REMARK 999	UNP Q27686
S	382	SER	GLY	SEE REMARK 999	UNP Q27686
S	389	TYR	SER	SEE REMARK 999	UNP Q27686
S	404	ARG	ALA	SEE REMARK 999	UNP Q27686
S	405	SER	GLY	SEE REMARK 999	UNP Q27686
T	382	SER	GLY	SEE REMARK 999	UNP Q27686
T	389	TYR	SER	SEE REMARK 999	UNP Q27686
T	404	ARG	ALA	SEE REMARK 999	UNP Q27686
T	405	SER	GLY	SEE REMARK 999	UNP Q27686
U	382	SER	GLY	SEE REMARK 999	UNP Q27686
U	389	TYR	SER	SEE REMARK 999	UNP Q27686
U	404	ARG	ALA	SEE REMARK 999	UNP Q27686
U	405	SER	GLY	SEE REMARK 999	UNP Q27686
V	382	SER	GLY	SEE REMARK 999	UNP Q27686
V	389	TYR	SER	SEE REMARK 999	UNP Q27686
V	404	ARG	ALA	SEE REMARK 999	UNP Q27686
V	405	SER	GLY	SEE REMARK 999	UNP Q27686
W	382	SER	GLY	SEE REMARK 999	UNP Q27686
W	389	TYR	SER	SEE REMARK 999	UNP Q27686
W	404	ARG	ALA	SEE REMARK 999	UNP Q27686
W	405	SER	GLY	SEE REMARK 999	UNP Q27686
X	382	SER	GLY	SEE REMARK 999	UNP Q27686
X	389	TYR	SER	SEE REMARK 999	UNP Q27686
X	404	ARG	ALA	SEE REMARK 999	UNP Q27686
X	405	SER	GLY	SEE REMARK 999	UNP Q27686

- Molecule 2 is SUGAR (FRUCTOSE-2,6-DIPHOSPHATE) (three-letter code: FDP) (formula: C₆H₁₄O₁₂P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		
2	E	1	Total	C	O	P	0	0
			20	6	12	2		
2	F	1	Total	C	O	P	0	0
			20	6	12	2		
2	G	1	Total	C	O	P	0	0
			20	6	12	2		
2	H	1	Total	C	O	P	0	0
			20	6	12	2		
2	I	1	Total	C	O	P	0	0
			20	6	12	2		
2	J	1	Total	C	O	P	0	0
			20	6	12	2		
2	K	1	Total	C	O	P	0	0
			20	6	12	2		
2	L	1	Total	C	O	P	0	0
			20	6	12	2		
2	M	1	Total	C	O	P	0	0
			20	6	12	2		
2	N	1	Total	C	O	P	0	0
			20	6	12	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total	C	O	P	0	0
			20	6	12	2		
2	P	1	Total	C	O	P	0	0
			20	6	12	2		
2	Q	1	Total	C	O	P	0	0
			20	6	12	2		
2	R	1	Total	C	O	P	0	0
			20	6	12	2		
2	S	1	Total	C	O	P	0	0
			20	6	12	2		
2	T	1	Total	C	O	P	0	0
			20	6	12	2		
2	U	1	Total	C	O	P	0	0
			20	6	12	2		
2	V	1	Total	C	O	P	0	0
			20	6	12	2		
2	W	1	Total	C	O	P	0	0
			20	6	12	2		
2	X	1	Total	C	O	P	0	0
			20	6	12	2		

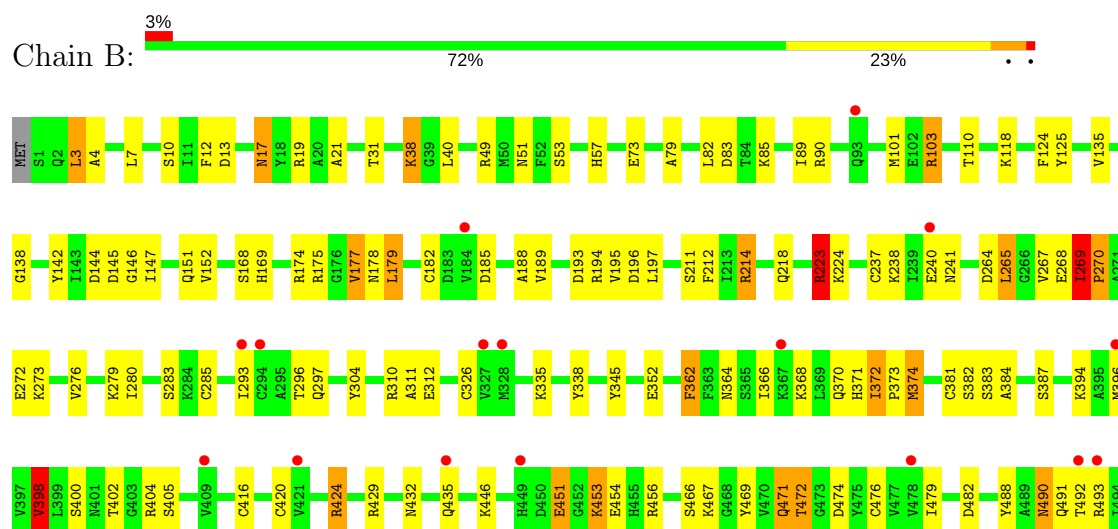
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

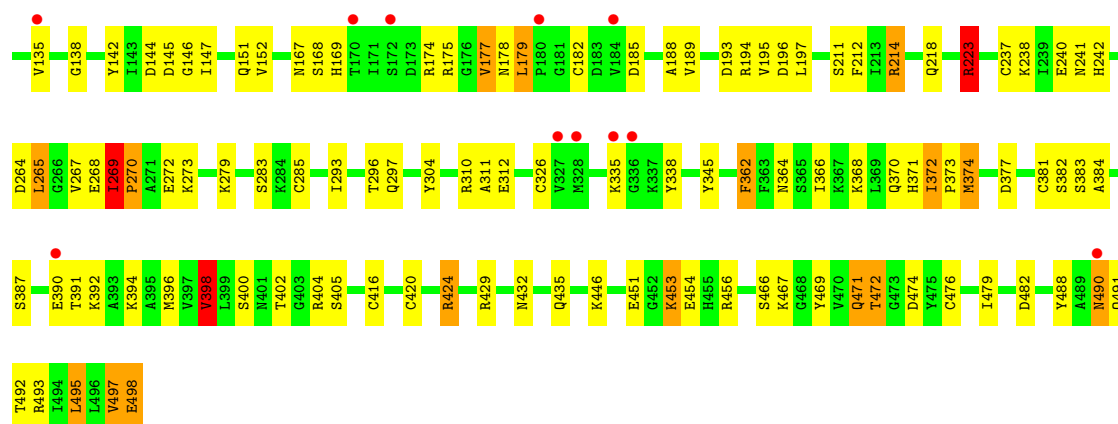
• Molecule 1: Pyruvate kinase



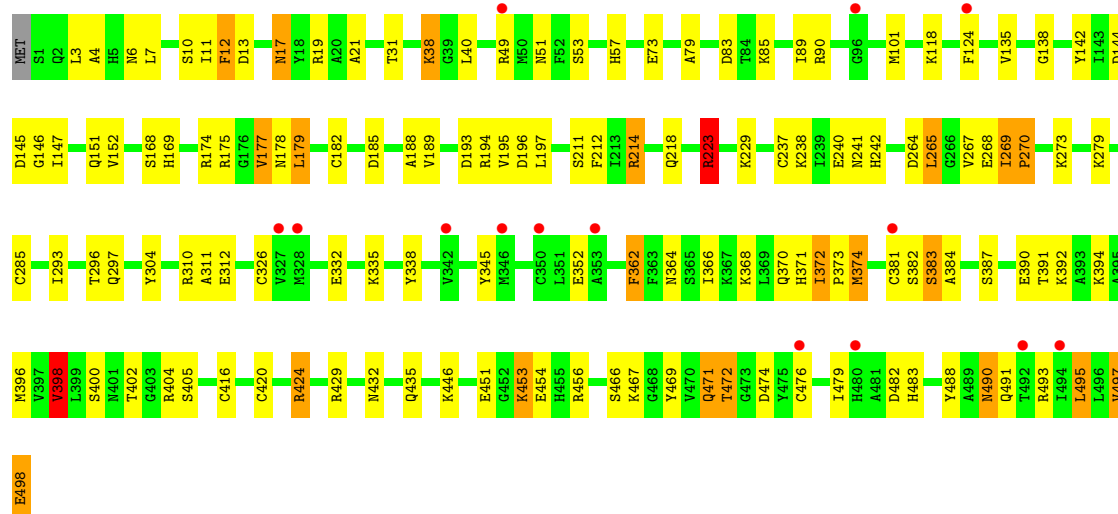
• Molecule 1: Pyruvate kinase



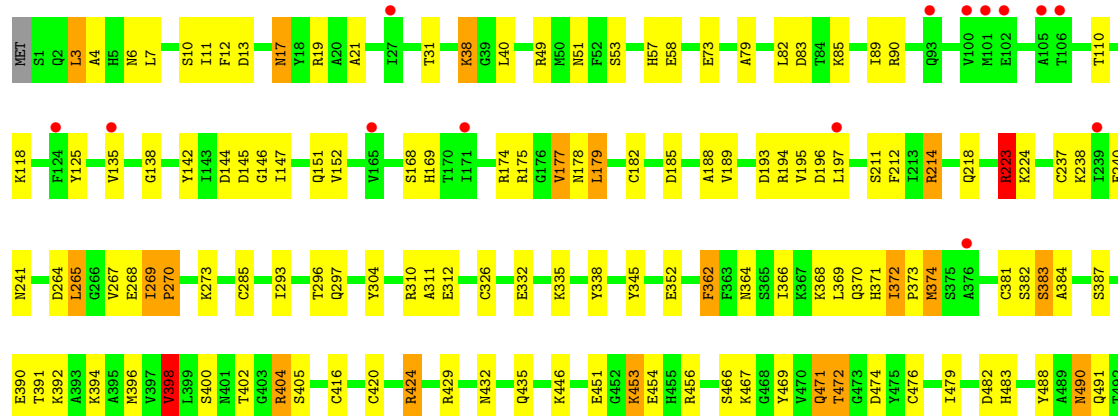
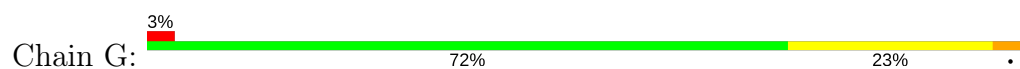


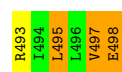


• Molecule 1: Pyruvate kinase

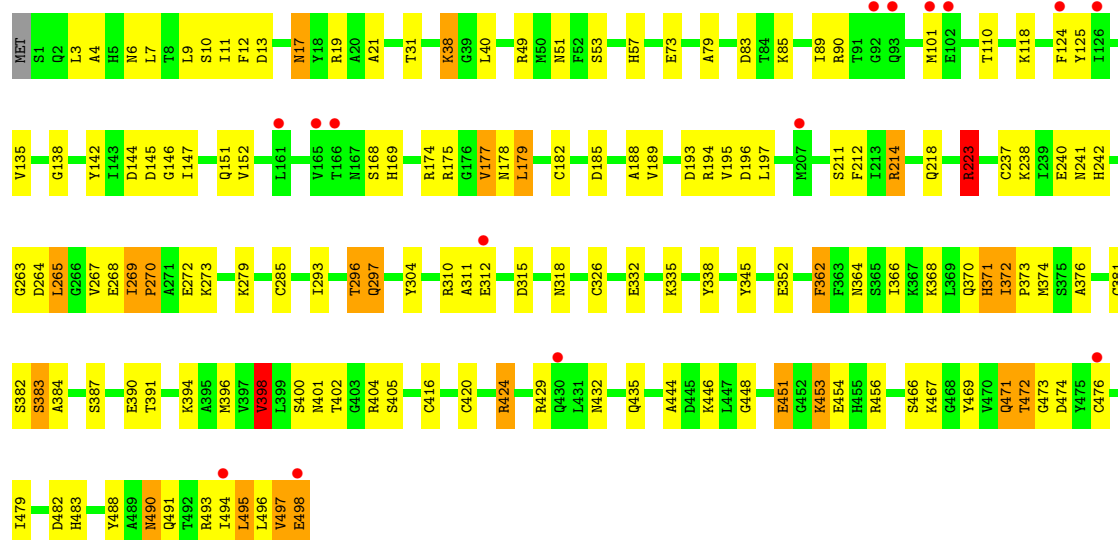


• Molecule 1: Pyruvate kinase

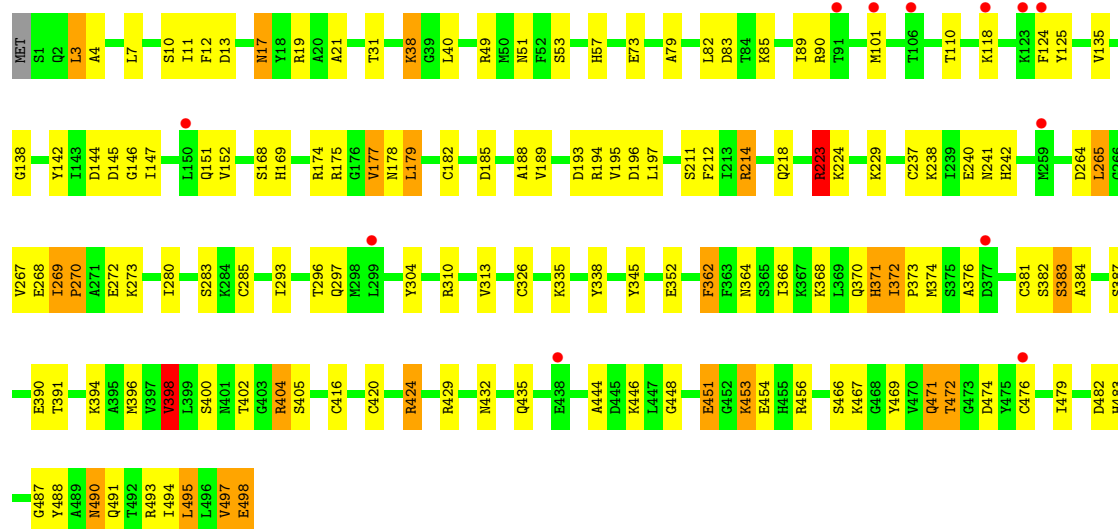




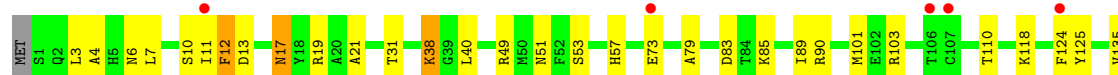
• Molecule 1: Pyruvate kinase

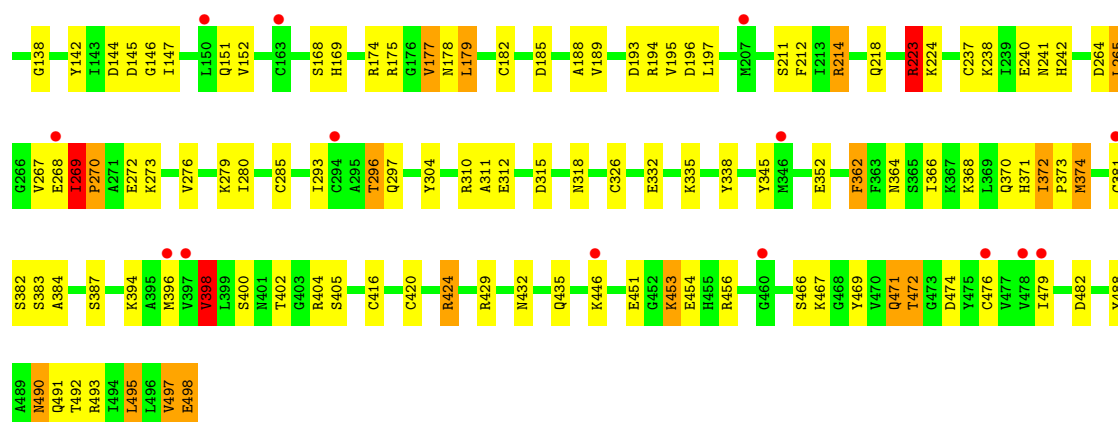


• Molecule 1: Pyruvate kinase

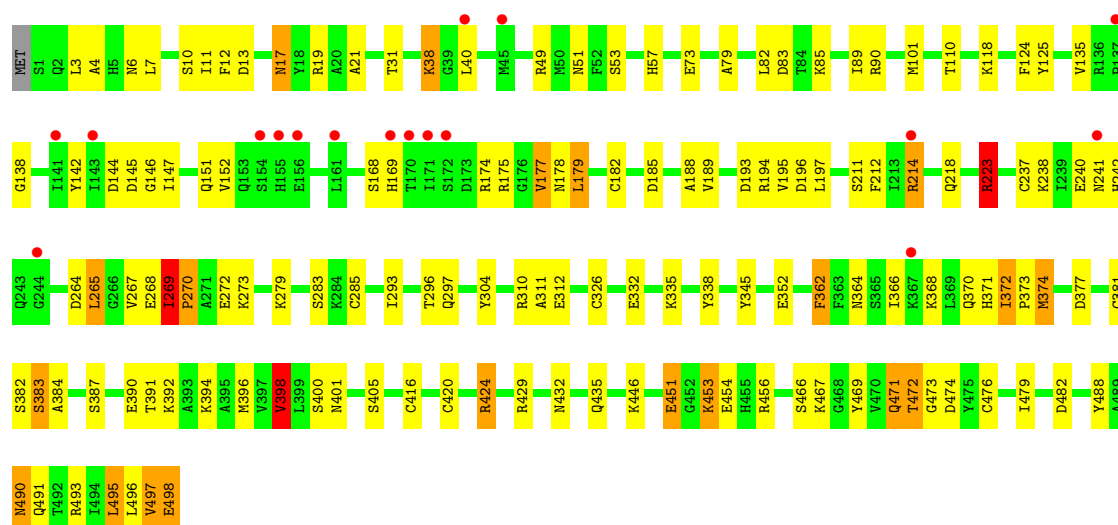


• Molecule 1: Pyruvate kinase

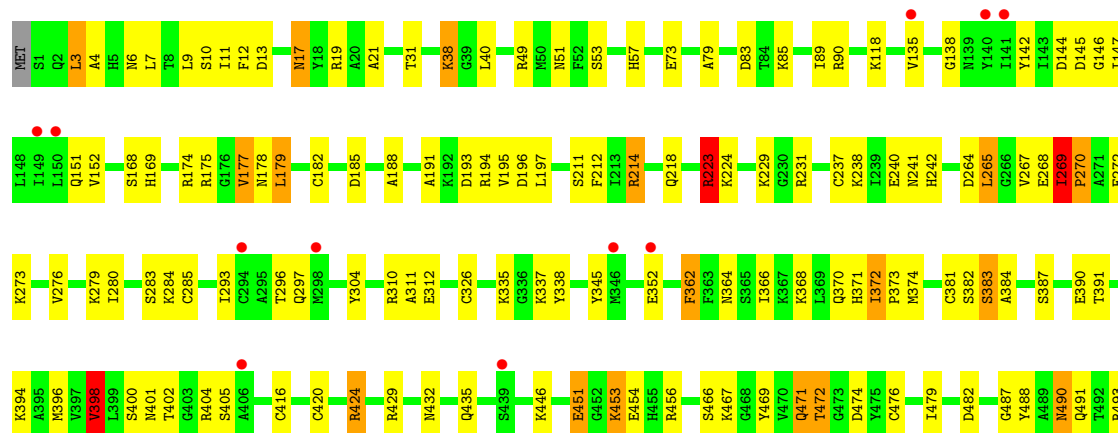


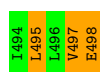


• Molecule 1: Pyruvate kinase

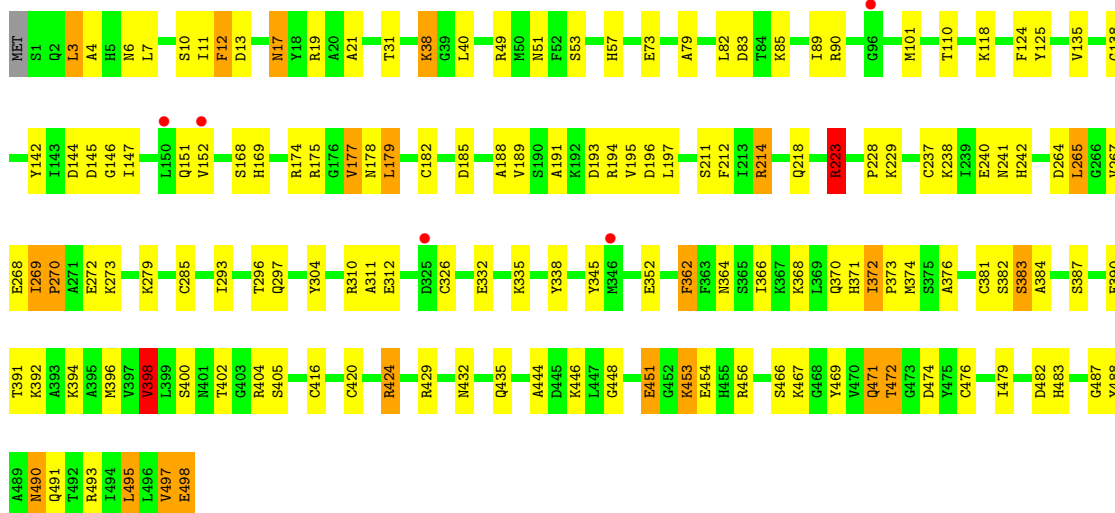


• Molecule 1: Pyruvate kinase

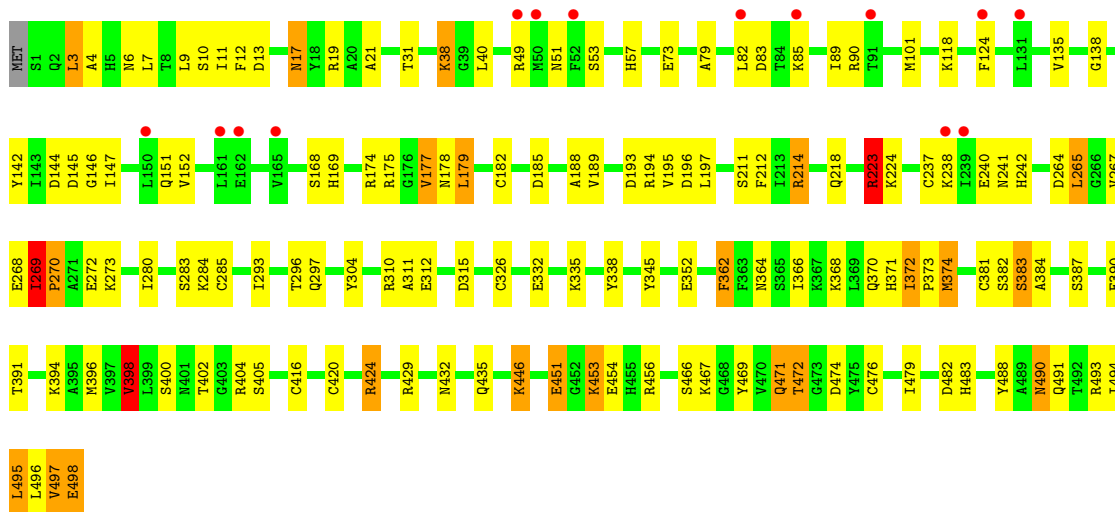




• Molecule 1: Pyruvate kinase

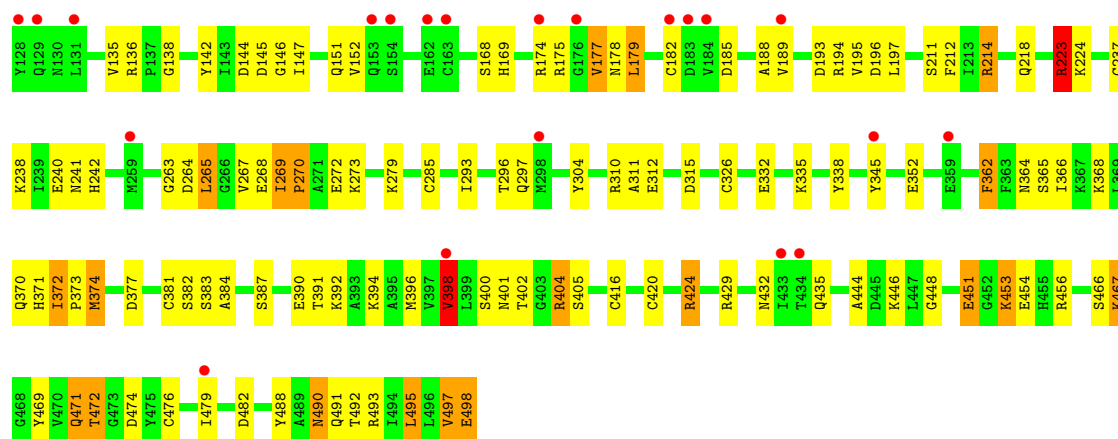


• Molecule 1: Pyruvate kinase

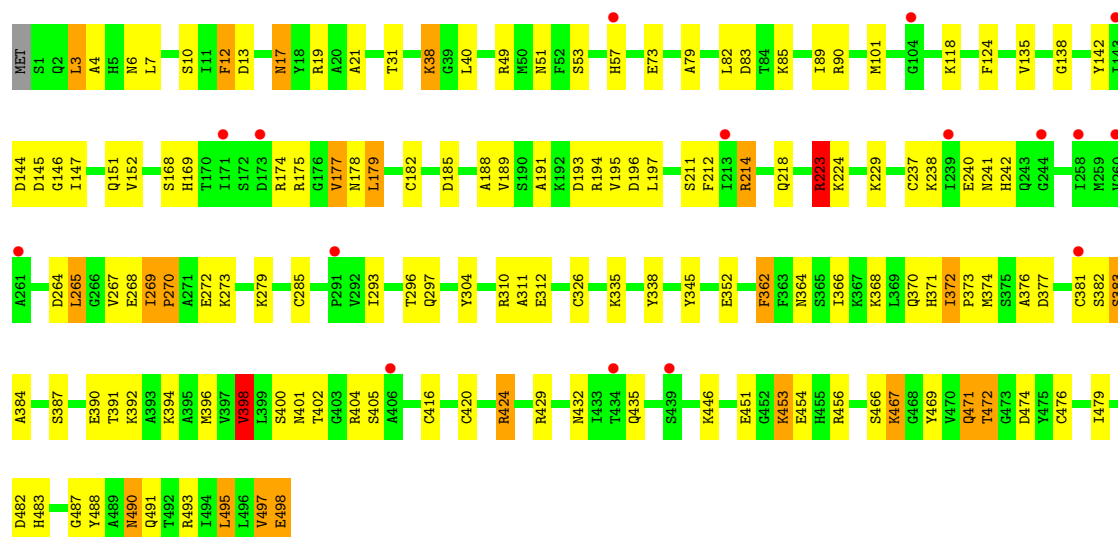


• Molecule 1: Pyruvate kinase

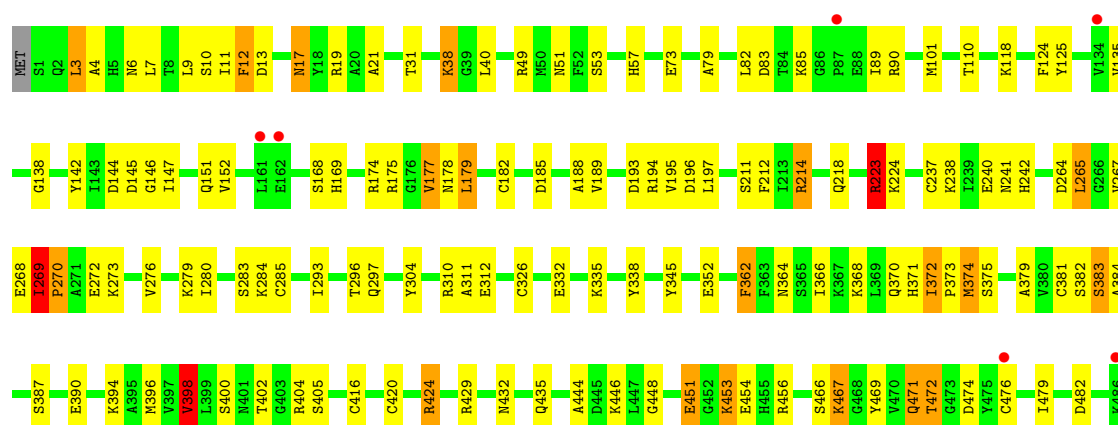


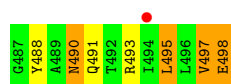


• Molecule 1: Pyruvate kinase

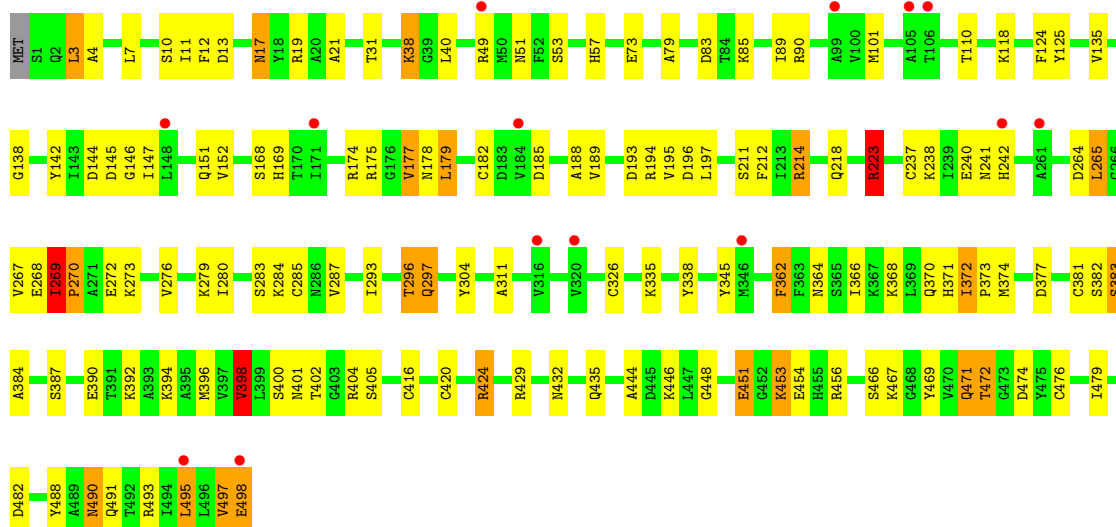
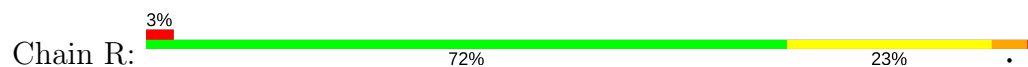


• Molecule 1: Pyruvate kinase

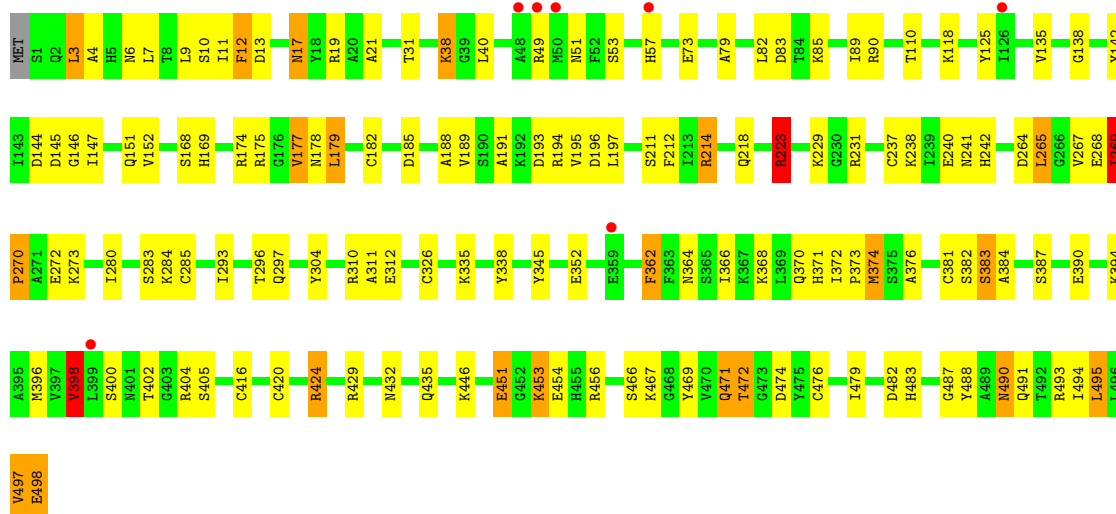




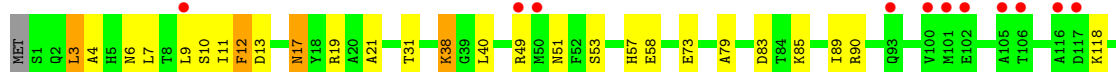
● Molecule 1: Pyruvate kinase

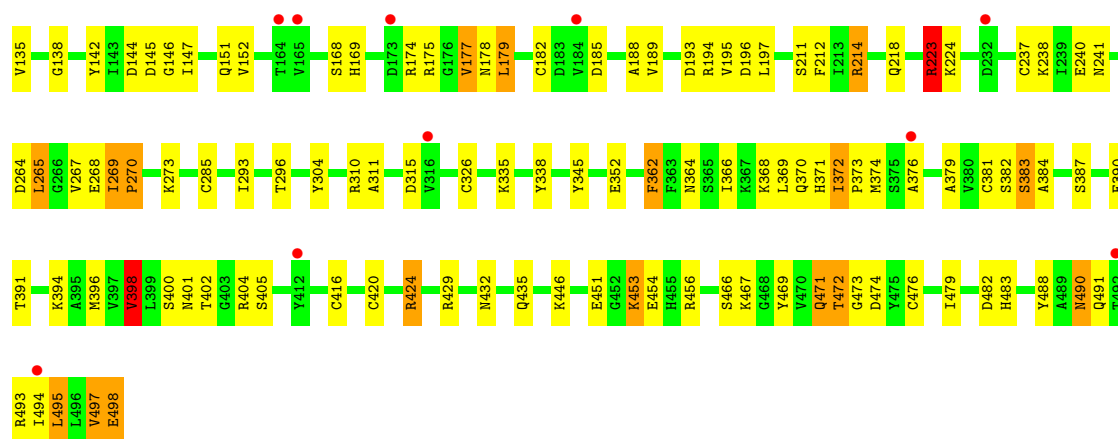


● Molecule 1: Pyruvate kinase

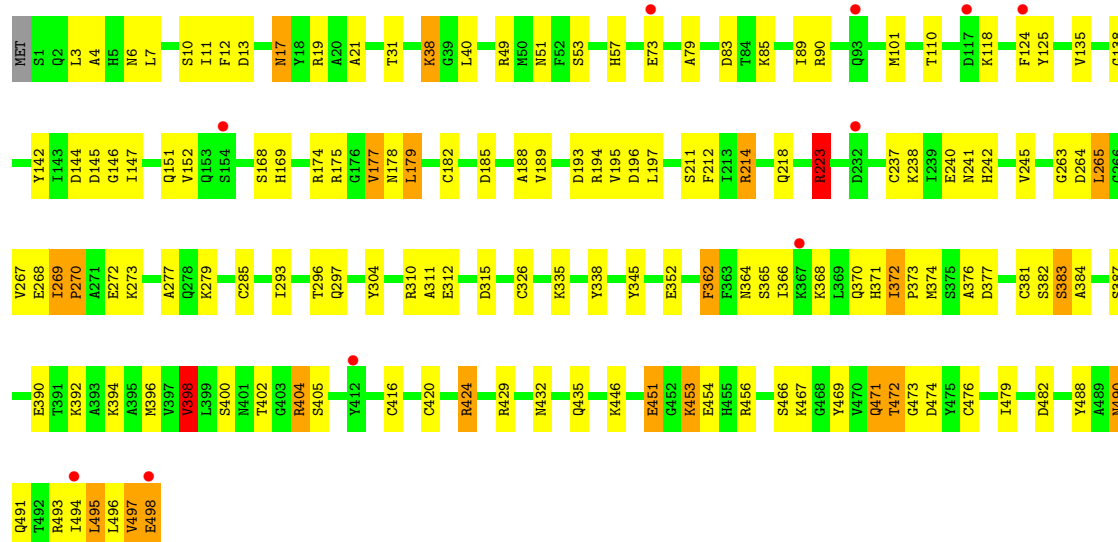


● Molecule 1: Pyruvate kinase

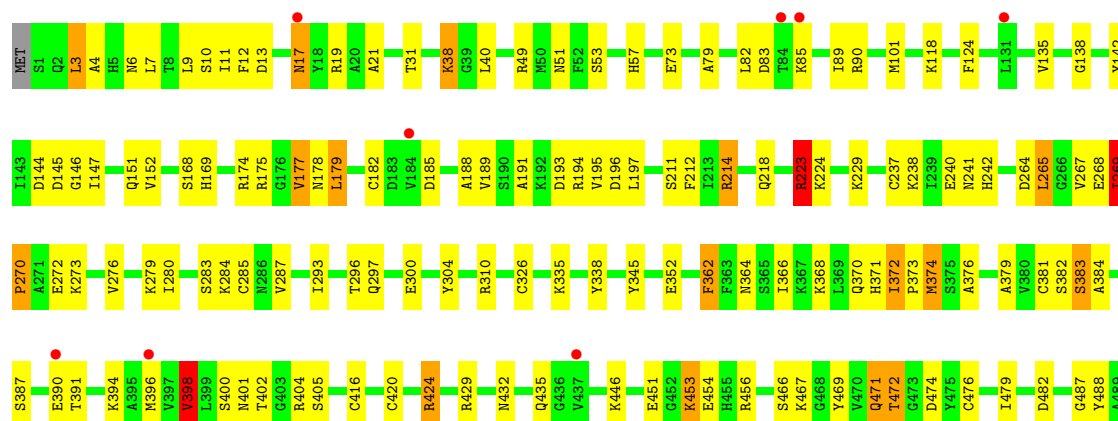




• Molecule 1: Pyruvate kinase




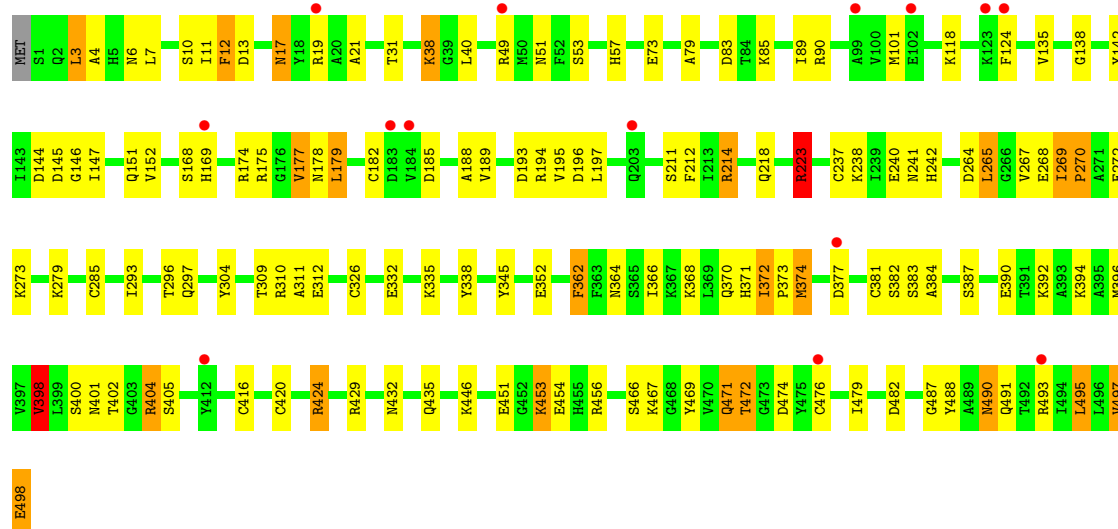
• Molecule 1: Pyruvate kinase



R490
Q491
T492
R493
L494
L495
V496
E497
E498

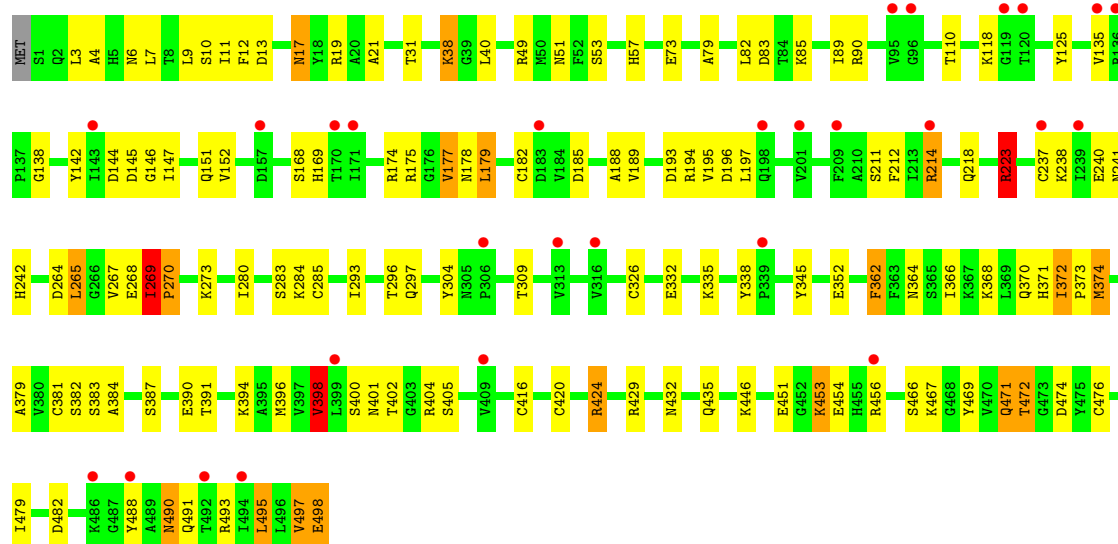
• Molecule 1: Pyruvate kinase

Chain W:  3% 72% 23%



• Molecule 1: Pyruvate kinase

Chain X:  6% 72% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	243.84Å 254.69Å 892.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.81 – 5.07 39.81 – 5.07	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.81-5.07) 86.3 (39.81-5.07)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 5.09Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.353 , 0.357 0.343 , 0.345	Depositor DCC
R_{free} test set	5652 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	131.8	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.118 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	91656	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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: FDP

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	1.44	12/3856 (0.3%)	0.85	7/5220 (0.1%)
1	B	1.44	10/3856 (0.3%)	0.85	8/5220 (0.2%)
1	C	1.44	11/3856 (0.3%)	0.85	7/5220 (0.1%)
1	D	1.44	12/3856 (0.3%)	0.85	7/5220 (0.1%)
1	E	1.44	10/3856 (0.3%)	0.85	8/5220 (0.2%)
1	F	1.44	11/3856 (0.3%)	0.85	7/5220 (0.1%)
1	G	1.44	13/3856 (0.3%)	0.85	8/5220 (0.2%)
1	H	1.44	12/3856 (0.3%)	0.85	7/5220 (0.1%)
1	I	1.44	10/3856 (0.3%)	0.85	8/5220 (0.2%)
1	J	1.44	11/3856 (0.3%)	0.85	7/5220 (0.1%)
1	K	1.44	11/3856 (0.3%)	0.85	8/5220 (0.2%)
1	L	1.44	10/3856 (0.3%)	0.85	7/5220 (0.1%)
1	M	1.44	11/3856 (0.3%)	0.85	8/5220 (0.2%)
1	N	1.44	11/3856 (0.3%)	0.85	8/5220 (0.2%)
1	O	1.44	11/3856 (0.3%)	0.85	8/5220 (0.2%)
1	P	1.44	11/3856 (0.3%)	0.85	8/5220 (0.2%)
1	Q	1.44	11/3856 (0.3%)	0.85	8/5220 (0.2%)
1	R	1.44	10/3856 (0.3%)	0.85	7/5220 (0.1%)
1	S	1.44	11/3856 (0.3%)	0.85	8/5220 (0.2%)
1	T	1.44	11/3856 (0.3%)	0.85	7/5220 (0.1%)
1	U	1.44	10/3856 (0.3%)	0.85	7/5220 (0.1%)
1	V	1.44	11/3856 (0.3%)	0.85	8/5220 (0.2%)
1	W	1.44	12/3856 (0.3%)	0.85	7/5220 (0.1%)
1	X	1.44	13/3856 (0.3%)	0.85	8/5220 (0.2%)
All	All	1.44	266/92544 (0.3%)	0.85	181/125280 (0.1%)

All (266) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	476	CYS	CB-SG	-7.67	1.69	1.82
1	R	476	CYS	CB-SG	-7.64	1.69	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	476	CYS	CB-SG	-7.64	1.69	1.82
1	D	476	CYS	CB-SG	-7.63	1.69	1.82
1	E	476	CYS	CB-SG	-7.62	1.69	1.82
1	Q	476	CYS	CB-SG	-7.61	1.69	1.82
1	W	476	CYS	CB-SG	-7.61	1.69	1.82
1	H	476	CYS	CB-SG	-7.60	1.69	1.82
1	V	476	CYS	CB-SG	-7.60	1.69	1.82
1	I	476	CYS	CB-SG	-7.60	1.69	1.82
1	U	476	CYS	CB-SG	-7.60	1.69	1.82
1	G	476	CYS	CB-SG	-7.59	1.69	1.82
1	O	476	CYS	CB-SG	-7.59	1.69	1.82
1	N	476	CYS	CB-SG	-7.59	1.69	1.82
1	T	476	CYS	CB-SG	-7.58	1.69	1.82
1	P	476	CYS	CB-SG	-7.58	1.69	1.82
1	M	476	CYS	CB-SG	-7.57	1.69	1.82
1	S	476	CYS	CB-SG	-7.57	1.69	1.82
1	K	476	CYS	CB-SG	-7.56	1.69	1.82
1	F	476	CYS	CB-SG	-7.55	1.69	1.82
1	X	476	CYS	CB-SG	-7.54	1.69	1.82
1	A	476	CYS	CB-SG	-7.53	1.69	1.82
1	C	476	CYS	CB-SG	-7.52	1.69	1.82
1	B	476	CYS	CB-SG	-7.51	1.69	1.82
1	S	416	CYS	CB-SG	-7.26	1.70	1.82
1	Q	416	CYS	CB-SG	-7.25	1.70	1.82
1	W	416	CYS	CB-SG	-7.23	1.70	1.82
1	G	416	CYS	CB-SG	-7.23	1.70	1.82
1	H	416	CYS	CB-SG	-7.23	1.70	1.82
1	N	416	CYS	CB-SG	-7.22	1.70	1.82
1	D	416	CYS	CB-SG	-7.21	1.70	1.82
1	R	416	CYS	CB-SG	-7.21	1.70	1.82
1	O	416	CYS	CB-SG	-7.20	1.70	1.82
1	U	416	CYS	CB-SG	-7.20	1.70	1.82
1	L	416	CYS	CB-SG	-7.20	1.70	1.82
1	B	416	CYS	CB-SG	-7.18	1.70	1.82
1	V	416	CYS	CB-SG	-7.18	1.70	1.82
1	C	416	CYS	CB-SG	-7.18	1.70	1.82
1	T	416	CYS	CB-SG	-7.17	1.70	1.82
1	X	416	CYS	CB-SG	-7.17	1.70	1.82
1	I	416	CYS	CB-SG	-7.16	1.70	1.82
1	P	416	CYS	CB-SG	-7.16	1.70	1.82
1	E	416	CYS	CB-SG	-7.16	1.70	1.82
1	F	416	CYS	CB-SG	-7.15	1.70	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	CYS	CB-SG	-7.14	1.70	1.82
1	J	416	CYS	CB-SG	-7.14	1.70	1.82
1	M	416	CYS	CB-SG	-7.13	1.70	1.82
1	K	416	CYS	CB-SG	-7.12	1.70	1.82
1	H	469	TYR	CD2-CE2	-5.82	1.30	1.39
1	K	469	TYR	CD2-CE2	-5.82	1.30	1.39
1	F	469	TYR	CD2-CE2	-5.79	1.30	1.39
1	P	469	TYR	CD2-CE2	-5.78	1.30	1.39
1	N	469	TYR	CD2-CE2	-5.78	1.30	1.39
1	U	469	TYR	CD2-CE2	-5.78	1.30	1.39
1	O	469	TYR	CD2-CE2	-5.77	1.30	1.39
1	X	469	TYR	CD2-CE2	-5.77	1.30	1.39
1	V	469	TYR	CD2-CE2	-5.77	1.30	1.39
1	M	469	TYR	CD2-CE2	-5.76	1.30	1.39
1	L	469	TYR	CD2-CE2	-5.76	1.30	1.39
1	R	469	TYR	CD2-CE2	-5.75	1.30	1.39
1	S	469	TYR	CD2-CE2	-5.75	1.30	1.39
1	J	469	TYR	CD2-CE2	-5.74	1.30	1.39
1	D	469	TYR	CD2-CE2	-5.74	1.30	1.39
1	A	469	TYR	CD2-CE2	-5.73	1.30	1.39
1	T	469	TYR	CD2-CE2	-5.73	1.30	1.39
1	W	469	TYR	CD2-CE2	-5.72	1.30	1.39
1	C	469	TYR	CD2-CE2	-5.71	1.30	1.39
1	E	469	TYR	CD2-CE2	-5.70	1.30	1.39
1	I	469	TYR	CD2-CE2	-5.69	1.30	1.39
1	B	469	TYR	CD2-CE2	-5.69	1.30	1.39
1	G	469	TYR	CD2-CE2	-5.69	1.30	1.39
1	Q	469	TYR	CD2-CE2	-5.69	1.30	1.39
1	Q	420	CYS	CB-SG	-5.65	1.72	1.81
1	J	420	CYS	CB-SG	-5.64	1.72	1.81
1	S	420	CYS	CB-SG	-5.64	1.72	1.81
1	E	420	CYS	CB-SG	-5.62	1.72	1.81
1	N	420	CYS	CB-SG	-5.62	1.72	1.81
1	H	420	CYS	CB-SG	-5.61	1.72	1.81
1	C	420	CYS	CB-SG	-5.60	1.72	1.81
1	L	420	CYS	CB-SG	-5.60	1.72	1.81
1	U	420	CYS	CB-SG	-5.60	1.72	1.81
1	X	420	CYS	CB-SG	-5.60	1.72	1.81
1	F	420	CYS	CB-SG	-5.59	1.72	1.81
1	B	381	CYS	CB-SG	-5.59	1.72	1.81
1	V	420	CYS	CB-SG	-5.59	1.72	1.81
1	G	420	CYS	CB-SG	-5.59	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	420	CYS	CB-SG	-5.57	1.72	1.81
1	D	420	CYS	CB-SG	-5.57	1.72	1.81
1	I	420	CYS	CB-SG	-5.57	1.72	1.81
1	K	420	CYS	CB-SG	-5.57	1.72	1.81
1	M	420	CYS	CB-SG	-5.57	1.72	1.81
1	I	381	CYS	CB-SG	-5.56	1.72	1.81
1	N	381	CYS	CB-SG	-5.56	1.72	1.81
1	D	381	CYS	CB-SG	-5.56	1.72	1.81
1	W	420	CYS	CB-SG	-5.55	1.72	1.81
1	M	381	CYS	CB-SG	-5.55	1.72	1.81
1	R	381	CYS	CB-SG	-5.55	1.72	1.81
1	R	420	CYS	CB-SG	-5.55	1.72	1.81
1	P	420	CYS	CB-SG	-5.54	1.72	1.81
1	C	381	CYS	CB-SG	-5.53	1.72	1.81
1	T	420	CYS	CB-SG	-5.53	1.72	1.81
1	F	381	CYS	CB-SG	-5.52	1.72	1.81
1	O	420	CYS	CB-SG	-5.52	1.72	1.81
1	X	381	CYS	CB-SG	-5.52	1.72	1.81
1	V	381	CYS	CB-SG	-5.52	1.72	1.81
1	B	420	CYS	CB-SG	-5.52	1.72	1.81
1	W	381	CYS	CB-SG	-5.52	1.72	1.81
1	K	381	CYS	CB-SG	-5.51	1.72	1.81
1	Q	381	CYS	CB-SG	-5.51	1.72	1.81
1	S	381	CYS	CB-SG	-5.51	1.72	1.81
1	O	381	CYS	CB-SG	-5.50	1.72	1.81
1	L	381	CYS	CB-SG	-5.49	1.72	1.81
1	E	381	CYS	CB-SG	-5.49	1.72	1.81
1	H	381	CYS	CB-SG	-5.48	1.72	1.81
1	J	381	CYS	CB-SG	-5.48	1.72	1.81
1	U	381	CYS	CB-SG	-5.48	1.72	1.81
1	A	381	CYS	CB-SG	-5.48	1.72	1.81
1	P	381	CYS	CB-SG	-5.46	1.73	1.81
1	T	381	CYS	CB-SG	-5.46	1.73	1.81
1	C	237	CYS	CB-SG	-5.46	1.73	1.81
1	G	381	CYS	CB-SG	-5.43	1.73	1.81
1	B	237	CYS	CB-SG	-5.43	1.73	1.81
1	F	237	CYS	CB-SG	-5.42	1.73	1.81
1	H	237	CYS	CB-SG	-5.42	1.73	1.81
1	Q	237	CYS	CB-SG	-5.41	1.73	1.81
1	I	237	CYS	CB-SG	-5.40	1.73	1.81
1	U	237	CYS	CB-SG	-5.40	1.73	1.81
1	N	237	CYS	CB-SG	-5.40	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	237	CYS	CB-SG	-5.39	1.73	1.81
1	J	237	CYS	CB-SG	-5.38	1.73	1.81
1	K	237	CYS	CB-SG	-5.38	1.73	1.81
1	O	469	TYR	CD1-CE1	-5.37	1.31	1.39
1	P	237	CYS	CB-SG	-5.37	1.73	1.81
1	G	237	CYS	CB-SG	-5.36	1.73	1.81
1	L	237	CYS	CB-SG	-5.35	1.73	1.81
1	D	237	CYS	CB-SG	-5.34	1.73	1.81
1	S	237	CYS	CB-SG	-5.34	1.73	1.81
1	I	469	TYR	CD1-CE1	-5.34	1.31	1.39
1	B	469	TYR	CD1-CE1	-5.34	1.31	1.39
1	X	237	CYS	CB-SG	-5.34	1.73	1.81
1	A	237	CYS	CB-SG	-5.33	1.73	1.81
1	M	469	TYR	CD1-CE1	-5.33	1.31	1.39
1	G	469	TYR	CD1-CE1	-5.33	1.31	1.39
1	W	469	TYR	CD1-CE1	-5.33	1.31	1.39
1	M	237	CYS	CB-SG	-5.32	1.73	1.81
1	T	237	CYS	CB-SG	-5.32	1.73	1.81
1	L	469	TYR	CD1-CE1	-5.32	1.31	1.39
1	R	237	CYS	CB-SG	-5.32	1.73	1.81
1	E	237	CYS	CB-SG	-5.32	1.73	1.81
1	V	237	CYS	CB-SG	-5.31	1.73	1.81
1	O	237	CYS	CB-SG	-5.31	1.73	1.81
1	N	469	TYR	CD1-CE1	-5.31	1.31	1.39
1	S	469	TYR	CD1-CE1	-5.30	1.31	1.39
1	F	469	TYR	CD1-CE1	-5.30	1.31	1.39
1	V	469	TYR	CD1-CE1	-5.30	1.31	1.39
1	J	469	TYR	CD1-CE1	-5.29	1.31	1.39
1	Q	469	TYR	CD1-CE1	-5.29	1.31	1.39
1	P	469	TYR	CD1-CE1	-5.29	1.31	1.39
1	X	469	TYR	CD1-CE1	-5.29	1.31	1.39
1	E	469	TYR	CD1-CE1	-5.29	1.31	1.39
1	K	469	TYR	CD1-CE1	-5.29	1.31	1.39
1	U	469	TYR	CD1-CE1	-5.28	1.31	1.39
1	D	469	TYR	CD1-CE1	-5.28	1.31	1.39
1	R	469	TYR	CD1-CE1	-5.27	1.31	1.39
1	H	469	TYR	CD1-CE1	-5.27	1.31	1.39
1	T	469	TYR	CD1-CE1	-5.27	1.31	1.39
1	C	469	TYR	CD1-CE1	-5.26	1.31	1.39
1	V	285	CYS	CB-SG	-5.25	1.73	1.81
1	G	285	CYS	CB-SG	-5.25	1.73	1.81
1	H	338	TYR	CD2-CE2	-5.24	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	TYR	CD1-CE1	-5.24	1.31	1.39
1	D	338	TYR	CD2-CE2	-5.24	1.31	1.39
1	J	285	CYS	CB-SG	-5.23	1.73	1.81
1	O	285	CYS	CB-SG	-5.23	1.73	1.81
1	B	338	TYR	CD2-CE2	-5.22	1.31	1.39
1	B	488	TYR	CD2-CE2	-5.22	1.31	1.39
1	F	338	TYR	CD2-CE2	-5.22	1.31	1.39
1	N	488	TYR	CD2-CE2	-5.22	1.31	1.39
1	A	488	TYR	CD2-CE2	-5.22	1.31	1.39
1	F	285	CYS	CB-SG	-5.22	1.73	1.81
1	O	488	TYR	CD2-CE2	-5.22	1.31	1.39
1	N	285	CYS	CB-SG	-5.22	1.73	1.81
1	R	285	CYS	CB-SG	-5.22	1.73	1.81
1	W	338	TYR	CD2-CE2	-5.21	1.31	1.39
1	X	285	CYS	CB-SG	-5.21	1.73	1.81
1	B	285	CYS	CB-SG	-5.20	1.73	1.81
1	C	285	CYS	CB-SG	-5.20	1.73	1.81
1	C	488	TYR	CD2-CE2	-5.20	1.31	1.39
1	F	488	TYR	CD2-CE2	-5.20	1.31	1.39
1	P	285	CYS	CB-SG	-5.20	1.73	1.81
1	E	338	TYR	CD2-CE2	-5.20	1.31	1.39
1	I	285	CYS	CB-SG	-5.20	1.73	1.81
1	T	285	CYS	CB-SG	-5.20	1.73	1.81
1	G	488	TYR	CD2-CE2	-5.19	1.31	1.39
1	S	338	TYR	CD2-CE2	-5.19	1.31	1.39
1	D	488	TYR	CD2-CE2	-5.19	1.31	1.39
1	U	338	TYR	CD2-CE2	-5.19	1.31	1.39
1	H	285	CYS	CB-SG	-5.18	1.73	1.81
1	Q	488	TYR	CD2-CE2	-5.18	1.31	1.39
1	K	338	TYR	CD2-CE2	-5.18	1.31	1.39
1	V	488	TYR	CD2-CE2	-5.18	1.31	1.39
1	W	488	TYR	CD2-CE2	-5.18	1.31	1.39
1	D	285	CYS	CB-SG	-5.18	1.73	1.81
1	U	285	CYS	CB-SG	-5.17	1.73	1.81
1	A	338	TYR	CD2-CE2	-5.17	1.31	1.39
1	I	338	TYR	CD2-CE2	-5.17	1.31	1.39
1	G	338	TYR	CD2-CE2	-5.17	1.31	1.39
1	J	488	TYR	CD2-CE2	-5.17	1.31	1.39
1	Q	285	CYS	CB-SG	-5.17	1.73	1.81
1	C	338	TYR	CD2-CE2	-5.17	1.31	1.39
1	J	338	TYR	CD2-CE2	-5.17	1.31	1.39
1	L	338	TYR	CD2-CE2	-5.17	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	285	CYS	CB-SG	-5.17	1.73	1.81
1	R	488	TYR	CD2-CE2	-5.17	1.31	1.39
1	L	488	TYR	CD2-CE2	-5.16	1.31	1.39
1	P	338	TYR	CD2-CE2	-5.16	1.31	1.39
1	E	285	CYS	CB-SG	-5.16	1.73	1.81
1	N	338	TYR	CD2-CE2	-5.16	1.31	1.39
1	S	488	TYR	CD2-CE2	-5.16	1.31	1.39
1	T	488	TYR	CD2-CE2	-5.16	1.31	1.39
1	V	338	TYR	CD2-CE2	-5.16	1.31	1.39
1	S	285	CYS	CB-SG	-5.15	1.73	1.81
1	U	488	TYR	CD2-CE2	-5.15	1.31	1.39
1	K	285	CYS	CB-SG	-5.15	1.73	1.81
1	T	338	TYR	CD2-CE2	-5.15	1.31	1.39
1	L	285	CYS	CB-SG	-5.15	1.73	1.81
1	R	338	TYR	CD2-CE2	-5.15	1.31	1.39
1	X	488	TYR	CD2-CE2	-5.14	1.31	1.39
1	A	285	CYS	CB-SG	-5.14	1.73	1.81
1	Q	338	TYR	CD2-CE2	-5.14	1.31	1.39
1	W	285	CYS	CB-SG	-5.14	1.73	1.81
1	O	338	TYR	CD2-CE2	-5.13	1.31	1.39
1	X	338	TYR	CD2-CE2	-5.13	1.31	1.39
1	E	488	TYR	CD2-CE2	-5.13	1.31	1.39
1	K	488	TYR	CD2-CE2	-5.13	1.31	1.39
1	I	488	TYR	CD2-CE2	-5.13	1.31	1.39
1	P	488	TYR	CD2-CE2	-5.11	1.31	1.39
1	O	332	GLU	CD-OE1	-5.11	1.20	1.25
1	H	488	TYR	CD2-CE2	-5.10	1.31	1.39
1	M	488	TYR	CD2-CE2	-5.10	1.31	1.39
1	M	338	TYR	CD2-CE2	-5.08	1.31	1.39
1	D	338	TYR	CD1-CE1	-5.08	1.31	1.39
1	G	332	GLU	CD-OE1	-5.07	1.20	1.25
1	W	332	GLU	CD-OE1	-5.07	1.20	1.25
1	X	332	GLU	CD-OE1	-5.05	1.20	1.25
1	N	332	GLU	CD-OE1	-5.05	1.20	1.25
1	X	488	TYR	CD1-CE1	-5.05	1.31	1.39
1	G	488	TYR	CD1-CE1	-5.05	1.31	1.39
1	G	338	TYR	CD1-CE1	-5.05	1.31	1.39
1	P	338	TYR	CD1-CE1	-5.04	1.31	1.39
1	T	338	TYR	CD1-CE1	-5.04	1.31	1.39
1	A	332	GLU	CD-OE1	-5.03	1.20	1.25
1	H	488	TYR	CD1-CE1	-5.03	1.31	1.39
1	D	332	GLU	CD-OE1	-5.03	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	332	GLU	CD-OE1	-5.03	1.20	1.25
1	K	332	GLU	CD-OE1	-5.02	1.20	1.25
1	J	332	GLU	CD-OE1	-5.02	1.20	1.25
1	F	332	GLU	CD-OE1	-5.02	1.20	1.25
1	W	338	TYR	CD1-CE1	-5.01	1.31	1.39
1	X	338	TYR	CD1-CE1	-5.01	1.31	1.39
1	S	338	TYR	CD1-CE1	-5.01	1.31	1.39
1	H	332	GLU	CD-OE1	-5.01	1.20	1.25
1	Q	332	GLU	CD-OE1	-5.01	1.20	1.25
1	A	488	TYR	CD1-CE1	-5.00	1.31	1.39
1	V	488	TYR	CD1-CE1	-5.00	1.31	1.39
1	M	332	GLU	CD-OE1	-5.00	1.20	1.25

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	270	PRO	O-C-N	7.21	134.24	122.70
1	K	270	PRO	O-C-N	7.19	134.21	122.70
1	P	270	PRO	O-C-N	7.17	134.18	122.70
1	I	270	PRO	O-C-N	7.17	134.17	122.70
1	C	270	PRO	O-C-N	7.16	134.16	122.70
1	O	270	PRO	O-C-N	7.16	134.16	122.70
1	E	270	PRO	O-C-N	7.15	134.14	122.70
1	H	270	PRO	O-C-N	7.15	134.14	122.70
1	U	270	PRO	O-C-N	7.15	134.14	122.70
1	M	270	PRO	O-C-N	7.15	134.14	122.70
1	L	270	PRO	O-C-N	7.15	134.14	122.70
1	T	270	PRO	O-C-N	7.15	134.14	122.70
1	A	270	PRO	O-C-N	7.14	134.13	122.70
1	B	270	PRO	O-C-N	7.14	134.13	122.70
1	G	270	PRO	O-C-N	7.14	134.12	122.70
1	W	270	PRO	O-C-N	7.14	134.12	122.70
1	R	270	PRO	O-C-N	7.13	134.11	122.70
1	Q	270	PRO	O-C-N	7.13	134.11	122.70
1	X	270	PRO	O-C-N	7.13	134.11	122.70
1	S	270	PRO	O-C-N	7.13	134.10	122.70
1	J	270	PRO	O-C-N	7.10	134.07	122.70
1	F	270	PRO	O-C-N	7.10	134.06	122.70
1	N	270	PRO	O-C-N	7.10	134.06	122.70
1	D	270	PRO	O-C-N	7.07	134.01	122.70
1	I	398	VAL	CB-CA-C	-7.07	97.98	111.40
1	T	398	VAL	CB-CA-C	-7.05	98.00	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	398	VAL	CB-CA-C	-7.05	98.00	111.40
1	G	398	VAL	CB-CA-C	-7.05	98.01	111.40
1	B	398	VAL	CB-CA-C	-7.04	98.02	111.40
1	V	398	VAL	CB-CA-C	-7.04	98.01	111.40
1	E	398	VAL	CB-CA-C	-7.04	98.02	111.40
1	L	398	VAL	CB-CA-C	-7.04	98.03	111.40
1	W	398	VAL	CB-CA-C	-7.03	98.04	111.40
1	J	398	VAL	CB-CA-C	-7.03	98.04	111.40
1	X	398	VAL	CB-CA-C	-7.03	98.04	111.40
1	Q	398	VAL	CB-CA-C	-7.02	98.06	111.40
1	A	398	VAL	CB-CA-C	-7.02	98.06	111.40
1	F	398	VAL	CB-CA-C	-7.02	98.06	111.40
1	H	398	VAL	CB-CA-C	-7.02	98.06	111.40
1	R	398	VAL	CB-CA-C	-7.02	98.07	111.40
1	S	398	VAL	CB-CA-C	-7.01	98.08	111.40
1	M	398	VAL	CB-CA-C	-7.01	98.08	111.40
1	O	398	VAL	CB-CA-C	-7.01	98.08	111.40
1	K	398	VAL	CB-CA-C	-7.00	98.09	111.40
1	U	398	VAL	CB-CA-C	-7.00	98.09	111.40
1	D	398	VAL	CB-CA-C	-7.00	98.09	111.40
1	N	398	VAL	CB-CA-C	-6.99	98.12	111.40
1	P	398	VAL	CB-CA-C	-6.98	98.14	111.40
1	B	223	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	H	223	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	D	223	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	223	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	R	223	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	C	223	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	X	223	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	Q	223	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	N	223	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	S	223	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	E	223	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	G	223	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	W	223	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	O	223	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	F	223	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	K	223	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	T	223	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	U	223	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	L	223	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	I	223	ARG	NE-CZ-NH1	6.44	123.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	223	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	M	223	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	V	223	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	P	223	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	V	495	LEU	CA-CB-CG	6.33	129.86	115.30
1	O	495	LEU	CA-CB-CG	6.33	129.86	115.30
1	E	495	LEU	CA-CB-CG	6.32	129.84	115.30
1	I	495	LEU	CA-CB-CG	6.32	129.84	115.30
1	L	495	LEU	CA-CB-CG	6.32	129.83	115.30
1	R	495	LEU	CA-CB-CG	6.32	129.83	115.30
1	W	495	LEU	CA-CB-CG	6.32	129.83	115.30
1	X	495	LEU	CA-CB-CG	6.31	129.82	115.30
1	P	495	LEU	CA-CB-CG	6.31	129.82	115.30
1	M	495	LEU	CA-CB-CG	6.31	129.80	115.30
1	K	495	LEU	CA-CB-CG	6.30	129.80	115.30
1	N	495	LEU	CA-CB-CG	6.30	129.80	115.30
1	T	495	LEU	CA-CB-CG	6.30	129.79	115.30
1	D	495	LEU	CA-CB-CG	6.30	129.78	115.30
1	F	495	LEU	CA-CB-CG	6.30	129.78	115.30
1	G	495	LEU	CA-CB-CG	6.29	129.77	115.30
1	B	495	LEU	CA-CB-CG	6.29	129.77	115.30
1	C	495	LEU	CA-CB-CG	6.29	129.76	115.30
1	H	495	LEU	CA-CB-CG	6.29	129.76	115.30
1	U	495	LEU	CA-CB-CG	6.29	129.76	115.30
1	S	495	LEU	CA-CB-CG	6.28	129.75	115.30
1	A	495	LEU	CA-CB-CG	6.28	129.74	115.30
1	Q	495	LEU	CA-CB-CG	6.28	129.75	115.30
1	J	495	LEU	CA-CB-CG	6.28	129.74	115.30
1	C	185	ASP	CB-CG-OD2	6.20	123.88	118.30
1	W	185	ASP	CB-CG-OD2	6.18	123.86	118.30
1	I	185	ASP	CB-CG-OD2	6.17	123.85	118.30
1	S	185	ASP	CB-CG-OD2	6.17	123.85	118.30
1	G	185	ASP	CB-CG-OD2	6.16	123.84	118.30
1	X	185	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	185	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	185	ASP	CB-CG-OD2	6.15	123.83	118.30
1	T	185	ASP	CB-CG-OD2	6.14	123.83	118.30
1	U	185	ASP	CB-CG-OD2	6.14	123.83	118.30
1	L	185	ASP	CB-CG-OD2	6.13	123.82	118.30
1	D	185	ASP	CB-CG-OD2	6.12	123.81	118.30
1	E	185	ASP	CB-CG-OD2	6.12	123.81	118.30
1	N	185	ASP	CB-CG-OD2	6.12	123.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	185	ASP	CB-CG-OD2	6.12	123.81	118.30
1	M	185	ASP	CB-CG-OD2	6.12	123.81	118.30
1	P	185	ASP	CB-CG-OD2	6.12	123.81	118.30
1	V	185	ASP	CB-CG-OD2	6.11	123.80	118.30
1	O	185	ASP	CB-CG-OD2	6.11	123.80	118.30
1	F	185	ASP	CB-CG-OD2	6.10	123.79	118.30
1	J	185	ASP	CB-CG-OD2	6.09	123.78	118.30
1	K	185	ASP	CB-CG-OD2	6.09	123.78	118.30
1	H	185	ASP	CB-CG-OD2	6.08	123.77	118.30
1	R	185	ASP	CB-CG-OD2	6.08	123.77	118.30
1	M	269	ILE	N-CA-C	-5.52	96.11	111.00
1	P	269	ILE	N-CA-C	-5.51	96.13	111.00
1	B	269	ILE	N-CA-C	-5.50	96.16	111.00
1	E	269	ILE	N-CA-C	-5.50	96.16	111.00
1	N	269	ILE	N-CA-C	-5.50	96.16	111.00
1	S	269	ILE	N-CA-C	-5.50	96.16	111.00
1	F	269	ILE	N-CA-C	-5.49	96.17	111.00
1	V	269	ILE	N-CA-C	-5.49	96.18	111.00
1	A	269	ILE	N-CA-C	-5.49	96.19	111.00
1	Q	269	ILE	N-CA-C	-5.49	96.19	111.00
1	U	269	ILE	N-CA-C	-5.49	96.19	111.00
1	R	269	ILE	N-CA-C	-5.48	96.20	111.00
1	L	269	ILE	N-CA-C	-5.48	96.21	111.00
1	H	269	ILE	N-CA-C	-5.48	96.21	111.00
1	I	269	ILE	N-CA-C	-5.47	96.22	111.00
1	O	269	ILE	N-CA-C	-5.47	96.22	111.00
1	T	269	ILE	N-CA-C	-5.47	96.22	111.00
1	K	269	ILE	N-CA-C	-5.47	96.23	111.00
1	D	269	ILE	N-CA-C	-5.47	96.24	111.00
1	C	269	ILE	N-CA-C	-5.47	96.24	111.00
1	W	269	ILE	N-CA-C	-5.47	96.24	111.00
1	X	269	ILE	N-CA-C	-5.47	96.24	111.00
1	G	269	ILE	N-CA-C	-5.46	96.25	111.00
1	M	265	LEU	CB-CG-CD2	5.46	120.29	111.00
1	J	269	ILE	N-CA-C	-5.46	96.26	111.00
1	O	265	LEU	CB-CG-CD2	5.45	120.26	111.00
1	C	265	LEU	CB-CG-CD2	5.44	120.25	111.00
1	R	265	LEU	CB-CG-CD2	5.44	120.26	111.00
1	L	265	LEU	CB-CG-CD2	5.44	120.25	111.00
1	T	265	LEU	CB-CG-CD2	5.44	120.25	111.00
1	H	265	LEU	CB-CG-CD2	5.44	120.25	111.00
1	A	265	LEU	CB-CG-CD2	5.44	120.24	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	265	LEU	CB-CG-CD2	5.43	120.24	111.00
1	B	265	LEU	CB-CG-CD2	5.43	120.23	111.00
1	W	265	LEU	CB-CG-CD2	5.43	120.23	111.00
1	S	265	LEU	CB-CG-CD2	5.42	120.22	111.00
1	J	265	LEU	CB-CG-CD2	5.41	120.20	111.00
1	F	265	LEU	CB-CG-CD2	5.41	120.19	111.00
1	E	265	LEU	CB-CG-CD2	5.40	120.18	111.00
1	G	265	LEU	CB-CG-CD2	5.40	120.18	111.00
1	D	265	LEU	CB-CG-CD2	5.40	120.17	111.00
1	Q	265	LEU	CB-CG-CD2	5.40	120.17	111.00
1	P	265	LEU	CB-CG-CD2	5.39	120.17	111.00
1	V	265	LEU	CB-CG-CD2	5.39	120.17	111.00
1	N	265	LEU	CB-CG-CD2	5.38	120.15	111.00
1	U	265	LEU	CB-CG-CD2	5.38	120.15	111.00
1	X	265	LEU	CB-CG-CD2	5.38	120.15	111.00
1	I	265	LEU	CB-CG-CD2	5.38	120.14	111.00
1	N	82	LEU	O-C-N	5.05	130.78	122.70
1	B	82	LEU	O-C-N	5.04	130.76	122.70
1	Q	82	LEU	O-C-N	5.04	130.76	122.70
1	P	82	LEU	O-C-N	5.03	130.75	122.70
1	X	82	LEU	O-C-N	5.03	130.75	122.70
1	E	82	LEU	O-C-N	5.02	130.73	122.70
1	G	82	LEU	O-C-N	5.02	130.73	122.70
1	O	82	LEU	O-C-N	5.02	130.73	122.70
1	I	82	LEU	O-C-N	5.01	130.72	122.70
1	V	82	LEU	O-C-N	5.01	130.72	122.70
1	M	82	LEU	O-C-N	5.01	130.71	122.70
1	K	82	LEU	O-C-N	5.00	130.70	122.70
1	S	82	LEU	O-C-N	5.00	130.70	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3799	0	3802	142	0
1	B	3799	0	3802	165	0
1	C	3799	0	3802	208	0
1	D	3799	0	3802	134	0
1	E	3799	0	3802	154	0
1	F	3799	0	3802	144	3
1	G	3799	0	3802	154	0
1	H	3799	0	3802	238	0
1	I	3799	0	3802	178	0
1	J	3799	0	3802	197	1
1	K	3799	0	3802	172	0
1	L	3799	0	3802	229	0
1	M	3799	0	3802	194	0
1	N	3799	0	3802	235	0
1	O	3799	0	3802	167	0
1	P	3799	0	3802	197	0
1	Q	3799	0	3802	191	0
1	R	3799	0	3802	200	0
1	S	3799	0	3802	230	0
1	T	3799	0	3802	213	1
1	U	3799	0	3802	218	0
1	V	3799	0	3802	257	0
1	W	3799	0	3802	188	3
1	X	3799	0	3802	186	0
2	A	20	0	10	4	0
2	B	20	0	10	4	0
2	C	20	0	10	4	0
2	D	20	0	10	4	0
2	E	20	0	10	4	0
2	F	20	0	10	4	0
2	G	20	0	10	4	0
2	H	20	0	10	5	0
2	I	20	0	10	4	0
2	J	20	0	10	4	0
2	K	20	0	10	5	0
2	L	20	0	10	5	0
2	M	20	0	10	4	0
2	N	20	0	10	4	0
2	O	20	0	10	5	0
2	P	20	0	10	5	0
2	Q	20	0	10	4	0
2	R	20	0	10	5	0
2	S	20	0	10	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	20	0	10	5	0
2	U	20	0	10	4	0
2	V	20	0	10	5	0
2	W	20	0	10	5	0
2	X	20	0	10	5	0
All	All	91656	0	91488	3536	4

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 19.

All (3536) 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:C:216:ALA:CB	1:N:446:LYS:HD3	1.49	1.42
1:C:250:SER:CB	1:N:446:LYS:HG2	1.49	1.41
1:U:242:HIS:HE1	1:W:12:PHE:CZ	1.42	1.38
1:H:12:PHE:CZ	1:J:242:HIS:HE1	1.41	1.37
1:P:487:GLY:HA2	1:V:229:LYS:CE	1.56	1.33
1:F:188:ALA:CB	1:F:218:GLN:HG3	1.62	1.30
1:M:188:ALA:CB	1:M:218:GLN:HG3	1.62	1.30
1:B:188:ALA:CB	1:B:218:GLN:HG3	1.62	1.30
1:J:188:ALA:CB	1:J:218:GLN:HG3	1.62	1.30
1:D:188:ALA:CB	1:D:218:GLN:HG3	1.62	1.29
1:K:12:PHE:CZ	1:M:242:HIS:HE1	1.49	1.29
1:G:188:ALA:CB	1:G:218:GLN:HG3	1.62	1.29
1:U:188:ALA:CB	1:U:218:GLN:HG3	1.62	1.29
1:O:188:ALA:CB	1:O:218:GLN:HG3	1.62	1.28
1:R:188:ALA:CB	1:R:218:GLN:HG3	1.62	1.28
1:C:250:SER:HB2	1:N:446:LYS:CG	1.61	1.28
1:K:188:ALA:CB	1:K:218:GLN:HG3	1.62	1.28
1:V:284:LYS:HG3	1:X:7:LEU:CD2	1.60	1.28
1:L:188:ALA:CB	1:L:218:GLN:HG3	1.62	1.28
1:N:188:ALA:CB	1:N:218:GLN:HG3	1.62	1.28
1:T:188:ALA:CB	1:T:218:GLN:HG3	1.62	1.28
1:E:188:ALA:CB	1:E:218:GLN:HG3	1.62	1.28
1:U:242:HIS:CE1	1:W:12:PHE:CZ	2.20	1.28
1:C:188:ALA:CB	1:C:218:GLN:HG3	1.62	1.28
1:V:188:ALA:CB	1:V:218:GLN:HG3	1.62	1.28
1:W:188:ALA:CB	1:W:218:GLN:HG3	1.62	1.28
1:S:188:ALA:CB	1:S:218:GLN:HG3	1.62	1.28
1:A:188:ALA:CB	1:A:218:GLN:HG3	1.62	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:188:ALA:CB	1:I:218:GLN:HG3	1.62	1.27
1:P:188:ALA:CB	1:P:218:GLN:HG3	1.62	1.27
1:X:188:ALA:CB	1:X:218:GLN:HG3	1.62	1.27
1:Q:188:ALA:CB	1:Q:218:GLN:HG3	1.62	1.27
1:H:188:ALA:CB	1:H:218:GLN:HG3	1.62	1.27
1:L:242:HIS:HE1	1:N:12:PHE:CE2	1.51	1.27
1:I:229:LYS:CE	1:M:487:GLY:HA2	1.64	1.26
1:R:280:ILE:HG12	1:T:6:ASN:O	1.35	1.23
1:L:242:HIS:CE1	1:N:12:PHE:CE2	2.28	1.21
1:R:284:LYS:HG3	1:T:7:LEU:CD2	1.69	1.21
1:K:12:PHE:CE2	1:M:242:HIS:CE1	2.28	1.20
1:U:372:ILE:HG13	1:V:390:GLU:HA	1.22	1.19
1:E:297:GLN:OE1	1:G:310:ARG:HG2	1.44	1.18
1:D:472:THR:HG22	1:D:498:GLU:HA	1.25	1.17
1:Q:472:THR:HG22	1:Q:498:GLU:HA	1.25	1.17
1:S:373:PRO:HB3	1:T:391:THR:HA	1.25	1.17
1:H:310:ARG:HG2	1:J:297:GLN:CG	1.75	1.17
1:C:390:GLU:HA	1:P:372:ILE:HG13	1.23	1.17
1:H:310:ARG:HG2	1:J:297:GLN:CB	1.73	1.17
1:I:487:GLY:CA	1:M:229:LYS:HG3	1.73	1.17
1:M:472:THR:HG22	1:M:498:GLU:HA	1.25	1.16
1:L:283:SER:HB3	1:N:3:LEU:CD2	1.75	1.16
1:H:12:PHE:CZ	1:J:242:HIS:CE1	2.31	1.16
1:H:371:HIS:O	1:H:374:MET:HG2	1.44	1.16
1:R:472:THR:HG22	1:R:498:GLU:HA	1.25	1.16
1:K:472:THR:HG22	1:K:498:GLU:HA	1.25	1.16
1:F:373:PRO:HA	1:G:390:GLU:O	1.40	1.15
1:I:487:GLY:HA2	1:M:229:LYS:CG	1.76	1.15
1:A:472:THR:HG22	1:A:498:GLU:HA	1.25	1.15
1:U:12:PHE:CE2	1:W:242:HIS:HE1	1.64	1.15
1:L:472:THR:HG22	1:L:498:GLU:HA	1.25	1.14
1:S:472:THR:HG22	1:S:498:GLU:HA	1.25	1.14
1:V:472:THR:HG22	1:V:498:GLU:HA	1.25	1.14
1:H:310:ARG:CG	1:J:297:GLN:HB2	1.76	1.14
1:S:372:ILE:HD11	1:T:390:GLU:HG2	1.29	1.13
1:P:487:GLY:HA2	1:V:229:LYS:CD	1.77	1.13
1:B:12:PHE:CE2	1:C:242:HIS:HE1	1.65	1.13
1:B:472:THR:HG22	1:B:498:GLU:HA	1.25	1.13
1:H:297:GLN:HB2	1:J:310:ARG:HG2	1.26	1.13
1:S:372:ILE:CG1	1:T:390:GLU:HA	1.77	1.13
1:U:242:HIS:CE1	1:W:12:PHE:CE2	2.37	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:297:GLN:OE1	1:S:310:ARG:HG2	1.43	1.13
1:U:11:ILE:HB	1:W:273:LYS:CG	1.77	1.12
1:H:312:GLU:HA	1:J:311:ALA:CB	1.78	1.12
1:K:12:PHE:CZ	1:M:242:HIS:CE1	2.36	1.12
1:U:297:GLN:HB2	1:W:310:ARG:HG2	1.32	1.12
1:W:472:THR:HG22	1:W:498:GLU:HA	1.25	1.12
1:K:12:PHE:CE2	1:M:242:HIS:HE1	1.65	1.12
1:U:472:THR:HG22	1:U:498:GLU:HA	1.25	1.12
1:B:188:ALA:CB	1:B:218:GLN:CG	2.28	1.12
1:L:188:ALA:CB	1:L:218:GLN:CG	2.28	1.12
1:T:3:LEU:HD23	1:T:3:LEU:C	1.70	1.12
1:F:188:ALA:CB	1:F:218:GLN:CG	2.28	1.11
1:O:472:THR:HG22	1:O:498:GLU:HA	1.25	1.11
1:T:188:ALA:CB	1:T:218:GLN:CG	2.28	1.11
1:S:373:PRO:HA	1:T:390:GLU:O	1.49	1.11
1:M:188:ALA:CB	1:M:218:GLN:CG	2.28	1.11
1:C:472:THR:HG22	1:C:498:GLU:HA	1.25	1.11
1:H:188:ALA:CB	1:H:218:GLN:CG	2.28	1.11
1:U:188:ALA:CB	1:U:218:GLN:CG	2.28	1.11
1:O:188:ALA:CB	1:O:218:GLN:CG	2.28	1.11
1:S:188:ALA:CB	1:S:218:GLN:CG	2.28	1.11
1:U:11:ILE:HB	1:W:273:LYS:HG2	1.13	1.11
1:F:472:THR:HG22	1:F:498:GLU:HA	1.25	1.11
1:Q:188:ALA:CB	1:Q:218:GLN:CG	2.28	1.11
1:I:188:ALA:CB	1:I:218:GLN:CG	2.28	1.11
1:C:188:ALA:CB	1:C:218:GLN:CG	2.28	1.11
1:H:242:HIS:CE1	1:J:12:PHE:CE2	2.39	1.11
1:I:229:LYS:HE3	1:M:487:GLY:HA2	1.15	1.11
1:V:242:HIS:CE1	1:X:12:PHE:CE2	2.39	1.11
1:X:472:THR:HG22	1:X:498:GLU:HA	1.25	1.11
1:O:11:ILE:HB	1:P:273:LYS:HG2	1.27	1.10
1:R:371:HIS:O	1:R:374:MET:HG2	1.48	1.10
1:V:188:ALA:CB	1:V:218:GLN:CG	2.29	1.10
1:V:280:ILE:HG12	1:X:6:ASN:O	1.51	1.10
1:X:188:ALA:CB	1:X:218:GLN:CG	2.28	1.10
1:U:11:ILE:CB	1:W:273:LYS:HG2	1.81	1.10
1:W:188:ALA:CB	1:W:218:GLN:CG	2.28	1.10
1:A:188:ALA:CB	1:A:218:GLN:CG	2.28	1.10
1:J:188:ALA:CB	1:J:218:GLN:CG	2.28	1.10
1:P:487:GLY:CA	1:V:229:LYS:HE3	1.82	1.10
1:A:392:LYS:HD2	1:J:373:PRO:HD3	1.34	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:188:ALA:CB	1:P:218:GLN:CG	2.28	1.10
1:E:188:ALA:CB	1:E:218:GLN:CG	2.28	1.10
1:G:472:THR:HG22	1:G:498:GLU:HA	1.25	1.10
1:K:188:ALA:CB	1:K:218:GLN:CG	2.28	1.10
1:E:472:THR:HG22	1:E:498:GLU:HA	1.25	1.09
1:I:188:ALA:HB2	1:I:218:GLN:CG	1.82	1.09
1:N:188:ALA:CB	1:N:218:GLN:CG	2.28	1.09
1:R:188:ALA:CB	1:R:218:GLN:CG	2.28	1.09
1:S:188:ALA:HB2	1:S:218:GLN:CG	1.82	1.09
1:D:188:ALA:CB	1:D:218:GLN:CG	2.28	1.09
1:I:472:THR:HG22	1:I:498:GLU:HA	1.25	1.09
1:O:12:PHE:CE2	1:P:242:HIS:HE1	1.69	1.09
1:P:188:ALA:HB2	1:P:218:GLN:CG	1.82	1.09
1:U:312:GLU:HA	1:W:311:ALA:HB1	1.32	1.09
1:A:188:ALA:HB2	1:A:218:GLN:CG	1.83	1.09
1:G:188:ALA:CB	1:G:218:GLN:CG	2.28	1.09
1:G:188:ALA:HB2	1:G:218:GLN:CG	1.82	1.09
1:M:188:ALA:HB2	1:M:218:GLN:CG	1.82	1.09
1:L:188:ALA:HB2	1:L:218:GLN:CG	1.83	1.09
1:Q:188:ALA:HB2	1:Q:218:GLN:CG	1.82	1.09
1:S:372:ILE:HG12	1:T:390:GLU:HA	1.30	1.09
1:C:188:ALA:HB2	1:C:218:GLN:CG	1.83	1.09
1:N:472:THR:HG22	1:N:498:GLU:HA	1.25	1.09
1:F:390:GLU:O	1:G:373:PRO:HA	1.52	1.09
1:R:272:GLU:CG	1:T:352:GLU:HG2	1.80	1.09
1:D:188:ALA:HB2	1:D:218:GLN:CG	1.83	1.08
1:K:188:ALA:HB2	1:K:218:GLN:CG	1.83	1.08
1:P:472:THR:HG22	1:P:498:GLU:HA	1.25	1.08
1:R:269:ILE:HG12	1:T:11:ILE:HD12	1.29	1.08
1:R:270:PRO:HG2	1:R:273:LYS:HE2	1.36	1.08
1:V:188:ALA:HB2	1:V:218:GLN:CG	1.83	1.08
1:X:188:ALA:HB2	1:X:218:GLN:CG	1.83	1.08
1:E:270:PRO:HG2	1:E:273:LYS:HE2	1.35	1.08
1:P:371:HIS:O	1:P:374:MET:HG2	1.51	1.08
1:V:270:PRO:HG2	1:V:273:LYS:HE2	1.35	1.08
1:L:424:ARG:HG2	1:L:424:ARG:NH1	1.55	1.08
1:B:188:ALA:HB2	1:B:218:GLN:CG	1.83	1.08
1:H:188:ALA:HB2	1:H:218:GLN:CG	1.83	1.08
1:O:188:ALA:HB2	1:O:218:GLN:CG	1.82	1.08
1:T:472:THR:HG22	1:T:498:GLU:HA	1.25	1.08
1:U:371:HIS:O	1:U:374:MET:HG2	1.54	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:ALA:HB2	1:F:218:GLN:CG	1.83	1.08
1:C:216:ALA:HB3	1:N:446:LYS:HD3	1.28	1.08
1:T:188:ALA:HB2	1:T:218:GLN:CG	1.83	1.07
1:C:424:ARG:HG2	1:C:424:ARG:NH1	1.55	1.07
1:H:472:THR:HG22	1:H:498:GLU:HA	1.25	1.07
1:B:424:ARG:HG2	1:B:424:ARG:NH1	1.56	1.07
1:N:188:ALA:HB2	1:N:218:GLN:CG	1.83	1.07
1:L:270:PRO:HG2	1:L:273:LYS:HE2	1.35	1.07
1:U:188:ALA:HB2	1:U:218:GLN:CG	1.83	1.07
1:I:424:ARG:NH1	1:I:424:ARG:HG2	1.55	1.07
1:H:242:HIS:HE1	1:J:12:PHE:CE2	1.69	1.07
1:L:297:GLN:OE1	1:N:310:ARG:HG2	1.50	1.07
1:U:11:ILE:O	1:W:273:LYS:HE3	1.54	1.07
1:E:188:ALA:HB2	1:E:218:GLN:CG	1.83	1.07
1:H:496:LEU:HG	1:M:195:VAL:CG2	1.85	1.07
1:H:242:HIS:HE1	1:J:12:PHE:CZ	1.72	1.07
1:J:472:THR:HG22	1:J:498:GLU:HA	1.25	1.06
1:T:424:ARG:HH11	1:T:424:ARG:CG	1.68	1.06
1:J:188:ALA:HB2	1:J:218:GLN:CG	1.82	1.06
1:P:229:LYS:HG3	1:V:487:GLY:CA	1.84	1.06
1:V:284:LYS:HG3	1:X:7:LEU:HD21	1.35	1.06
1:I:270:PRO:HG2	1:I:273:LYS:HE2	1.36	1.06
1:R:188:ALA:HB2	1:R:218:GLN:CG	1.83	1.06
1:J:296:THR:HG22	1:J:297:GLN:HG2	1.37	1.06
1:H:496:LEU:CD2	1:M:195:VAL:HG22	1.83	1.06
1:C:216:ALA:HB3	1:N:446:LYS:O	1.55	1.06
1:S:424:ARG:CG	1:S:424:ARG:HH11	1.68	1.06
1:W:188:ALA:HB2	1:W:218:GLN:CG	1.83	1.06
1:B:424:ARG:CG	1:B:424:ARG:HH11	1.68	1.06
1:B:297:GLN:OE1	1:C:310:ARG:HG2	1.55	1.06
1:I:424:ARG:HH11	1:I:424:ARG:CG	1.68	1.06
1:H:311:ALA:CB	1:J:312:GLU:HA	1.85	1.06
1:I:229:LYS:HE3	1:M:487:GLY:CA	1.86	1.06
1:I:229:LYS:CD	1:M:487:GLY:HA2	1.86	1.06
1:U:311:ALA:HB1	1:W:312:GLU:HA	1.32	1.06
1:C:216:ALA:CB	1:N:446:LYS:CD	2.34	1.06
1:D:424:ARG:CG	1:D:424:ARG:HH11	1.68	1.06
1:I:371:HIS:O	1:I:374:MET:HG2	1.55	1.06
1:O:12:PHE:CZ	1:P:242:HIS:HE1	1.73	1.05
1:W:424:ARG:NH1	1:W:424:ARG:HG2	1.55	1.05
1:U:372:ILE:HG13	1:V:390:GLU:CA	1.87	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:424:ARG:HH11	1:N:424:ARG:CG	1.69	1.05
1:A:424:ARG:CG	1:A:424:ARG:HH11	1.68	1.05
1:C:424:ARG:HH11	1:C:424:ARG:CG	1.68	1.05
1:F:424:ARG:NH1	1:F:424:ARG:HG2	1.55	1.05
1:R:424:ARG:NH1	1:R:424:ARG:HG2	1.55	1.05
1:P:229:LYS:HG3	1:V:487:GLY:HA2	1.36	1.05
1:H:496:LEU:CG	1:M:195:VAL:HG22	1.85	1.04
1:H:312:GLU:HA	1:J:311:ALA:HB1	1.06	1.04
1:G:424:ARG:CG	1:G:424:ARG:HH11	1.68	1.04
1:O:12:PHE:CE2	1:P:242:HIS:CE1	2.45	1.04
1:U:12:PHE:HE2	1:W:242:HIS:CE1	1.75	1.04
1:L:371:HIS:O	1:L:374:MET:HG2	1.58	1.04
1:K:424:ARG:HH11	1:K:424:ARG:CG	1.68	1.04
1:V:424:ARG:HH11	1:V:424:ARG:CG	1.68	1.04
1:M:373:PRO:HA	1:N:390:GLU:O	1.58	1.04
1:H:372:ILE:HG23	1:I:390:GLU:O	1.57	1.04
1:R:284:LYS:HG3	1:T:7:LEU:HD22	1.36	1.04
1:M:424:ARG:HH11	1:M:424:ARG:CG	1.68	1.04
1:L:424:ARG:CG	1:L:424:ARG:HH11	1.68	1.04
1:X:424:ARG:CG	1:X:424:ARG:HH11	1.68	1.03
1:V:242:HIS:HE1	1:X:12:PHE:CE2	1.74	1.03
1:O:424:ARG:HH11	1:O:424:ARG:CG	1.68	1.03
1:P:424:ARG:CG	1:P:424:ARG:HH11	1.68	1.03
1:Q:424:ARG:CG	1:Q:424:ARG:HH11	1.68	1.03
1:M:372:ILE:HG13	1:N:390:GLU:HA	1.36	1.03
1:W:424:ARG:HH11	1:W:424:ARG:CG	1.68	1.03
1:H:424:ARG:CG	1:H:424:ARG:HH11	1.68	1.03
1:J:424:ARG:CG	1:J:424:ARG:HH11	1.68	1.03
1:Q:242:HIS:CE1	1:S:12:PHE:CE2	2.47	1.03
1:S:371:HIS:O	1:S:374:MET:HG2	1.58	1.03
1:U:424:ARG:CG	1:U:424:ARG:HH11	1.68	1.02
1:F:424:ARG:HH11	1:F:424:ARG:CG	1.69	1.02
1:U:373:PRO:HA	1:V:390:GLU:O	1.59	1.02
1:V:276:VAL:HG12	1:V:280:ILE:HD11	1.36	1.02
1:R:269:ILE:HG12	1:T:11:ILE:CD1	1.89	1.02
1:S:372:ILE:HG13	1:T:390:GLU:CA	1.89	1.02
1:R:297:GLN:HG3	1:T:310:ARG:HG3	1.40	1.02
1:H:372:ILE:HG13	1:I:390:GLU:HA	1.40	1.02
1:P:487:GLY:HA2	1:V:229:LYS:HE3	1.06	1.02
1:H:310:ARG:HG2	1:J:297:GLN:HB2	1.30	1.01
1:S:372:ILE:HG13	1:T:390:GLU:O	1.59	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:373:PRO:HB3	1:X:391:THR:HA	1.39	1.01
1:K:424:ARG:HG2	1:K:424:ARG:NH1	1.55	1.01
1:O:311:ALA:HB1	1:P:312:GLU:HA	1.41	1.01
1:H:310:ARG:HG2	1:J:297:GLN:HG3	1.42	1.01
1:L:283:SER:CB	1:N:3:LEU:CD2	2.38	1.01
1:M:371:HIS:O	1:M:374:MET:HG2	1.60	1.01
1:E:242:HIS:HE1	1:G:12:PHE:CZ	1.77	1.01
1:U:12:PHE:CE2	1:W:242:HIS:CE1	2.49	1.01
1:V:284:LYS:CG	1:X:7:LEU:CD2	2.37	1.00
1:T:371:HIS:O	1:T:374:MET:HG2	1.61	1.00
1:W:372:ILE:HG13	1:X:390:GLU:HA	1.39	1.00
1:E:424:ARG:HG2	1:E:424:ARG:NH1	1.55	1.00
1:K:496:LEU:HG	1:S:195:VAL:HG22	1.40	1.00
1:R:424:ARG:HH11	1:R:424:ARG:CG	1.68	1.00
1:P:195:VAL:HG22	1:U:496:LEU:HG	1.43	1.00
1:H:311:ALA:HB1	1:J:312:GLU:CA	1.90	1.00
1:Q:283:SER:HB3	1:S:3:LEU:CD2	1.92	1.00
1:E:424:ARG:CG	1:E:424:ARG:HH11	1.68	1.00
1:R:272:GLU:HG3	1:T:352:GLU:HB2	1.42	1.00
1:D:424:ARG:NH1	1:D:424:ARG:HG2	1.55	0.99
1:H:496:LEU:HG	1:M:195:VAL:HG22	1.39	0.99
1:U:372:ILE:HG23	1:V:390:GLU:O	1.62	0.99
1:H:12:PHE:CE2	1:J:242:HIS:HE1	1.80	0.99
1:I:229:LYS:HG3	1:M:487:GLY:CA	1.91	0.99
1:K:12:PHE:HE2	1:M:242:HIS:CE1	1.75	0.99
1:P:424:ARG:HG2	1:P:424:ARG:NH1	1.55	0.99
1:M:424:ARG:NH1	1:M:424:ARG:HG2	1.55	0.99
1:J:424:ARG:HG2	1:J:424:ARG:NH1	1.55	0.98
1:I:229:LYS:HG3	1:M:487:GLY:HA3	1.42	0.98
1:O:12:PHE:HE2	1:P:242:HIS:CE1	1.81	0.98
1:V:297:GLN:HE21	1:V:300:GLU:CB	1.76	0.98
1:A:424:ARG:HG2	1:A:424:ARG:NH1	1.55	0.98
1:B:12:PHE:HE2	1:C:242:HIS:CE1	1.80	0.98
1:T:424:ARG:HG2	1:T:424:ARG:NH1	1.55	0.98
1:U:424:ARG:NH1	1:U:424:ARG:HG2	1.55	0.98
1:H:310:ARG:CB	1:J:297:GLN:HB2	1.93	0.98
1:O:312:GLU:HA	1:P:311:ALA:HB1	1.45	0.98
1:G:424:ARG:NH1	1:G:424:ARG:HG2	1.55	0.97
1:H:311:ALA:HB1	1:J:312:GLU:HA	0.98	0.97
1:K:373:PRO:HA	1:L:390:GLU:O	1.63	0.97
1:S:373:PRO:HB3	1:T:391:THR:CA	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:195:VAL:HG22	1:U:496:LEU:CD2	1.95	0.97
1:T:3:LEU:HD23	1:T:3:LEU:O	1.63	0.97
1:X:424:ARG:NH1	1:X:424:ARG:HG2	1.55	0.97
1:H:297:GLN:CB	1:J:310:ARG:HG2	1.94	0.97
1:K:242:HIS:CE1	1:M:12:PHE:CE2	2.53	0.97
1:S:424:ARG:NH1	1:S:424:ARG:HG2	1.55	0.97
1:C:473:GLY:HA3	1:V:191:ALA:HB1	1.46	0.97
1:L:283:SER:CB	1:N:3:LEU:HD23	1.95	0.96
1:H:424:ARG:NH1	1:H:424:ARG:HG2	1.55	0.96
1:A:3:LEU:CD2	1:I:283:SER:HB3	1.95	0.96
1:S:373:PRO:CB	1:T:391:THR:HA	1.95	0.96
1:H:472:THR:HG22	1:H:498:GLU:CA	1.96	0.96
1:F:472:THR:HG22	1:F:498:GLU:CA	1.96	0.96
1:H:297:GLN:HB2	1:J:310:ARG:CG	1.94	0.96
1:C:496:LEU:HG	1:V:195:VAL:HG22	1.48	0.96
1:V:424:ARG:NH1	1:V:424:ARG:HG2	1.56	0.96
1:B:472:THR:HG22	1:B:498:GLU:CA	1.96	0.96
1:L:472:THR:HG22	1:L:498:GLU:CA	1.96	0.96
1:Q:472:THR:HG22	1:Q:498:GLU:CA	1.96	0.96
1:V:297:GLN:NE2	1:V:300:GLU:CG	2.29	0.96
1:D:472:THR:HG22	1:D:498:GLU:CA	1.96	0.96
1:Q:424:ARG:HG2	1:Q:424:ARG:NH1	1.55	0.96
1:A:472:THR:HG22	1:A:498:GLU:CA	1.96	0.96
1:C:390:GLU:O	1:P:373:PRO:HA	1.66	0.95
1:R:472:THR:HG22	1:R:498:GLU:CA	1.96	0.95
1:B:373:PRO:HD3	1:O:392:LYS:HD2	1.45	0.95
1:F:372:ILE:HG13	1:G:390:GLU:HA	1.48	0.95
1:K:472:THR:HG22	1:K:498:GLU:CA	1.96	0.95
1:S:472:THR:HG22	1:S:498:GLU:CA	1.96	0.95
1:R:269:ILE:CG1	1:T:11:ILE:HD12	1.96	0.95
1:P:195:VAL:HG22	1:U:496:LEU:CG	1.95	0.95
1:U:472:THR:HG22	1:U:498:GLU:CA	1.96	0.95
1:V:472:THR:HG22	1:V:498:GLU:CA	1.96	0.95
1:C:472:THR:HG22	1:C:498:GLU:CA	1.96	0.95
1:V:297:GLN:NE2	1:V:300:GLU:CB	2.30	0.95
1:O:472:THR:HG22	1:O:498:GLU:CA	1.96	0.95
1:X:472:THR:HG22	1:X:498:GLU:CA	1.96	0.95
1:G:472:THR:HG22	1:G:498:GLU:CA	1.96	0.94
1:C:373:PRO:HA	1:P:390:GLU:O	1.66	0.94
1:P:472:THR:HG22	1:P:498:GLU:CA	1.96	0.94
1:W:472:THR:HG22	1:W:498:GLU:CA	1.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:472:THR:HG22	1:E:498:GLU:CA	1.96	0.94
1:D:12:PHE:CZ	1:F:242:HIS:HE1	1.84	0.94
1:N:472:THR:HG22	1:N:498:GLU:CA	1.96	0.94
1:I:472:THR:HG22	1:I:498:GLU:CA	1.96	0.94
1:M:472:THR:HG22	1:M:498:GLU:CA	1.96	0.94
1:T:472:THR:HG22	1:T:498:GLU:CA	1.96	0.94
1:F:188:ALA:HB1	1:F:218:GLN:CG	1.98	0.94
1:H:6:ASN:OD1	1:J:279:LYS:HE3	1.64	0.94
1:S:372:ILE:CG1	1:T:390:GLU:CA	2.44	0.94
1:D:12:PHE:CE2	1:F:242:HIS:CE1	2.55	0.94
1:U:188:ALA:HB1	1:U:218:GLN:CG	1.98	0.94
1:D:188:ALA:HB1	1:D:218:GLN:CG	1.98	0.93
1:Q:390:GLU:HA	1:R:372:ILE:HG13	1.45	0.93
1:W:372:ILE:HG13	1:X:390:GLU:CA	1.98	0.93
1:N:188:ALA:HB1	1:N:218:GLN:CG	1.98	0.93
1:E:242:HIS:CE1	1:G:12:PHE:CE2	2.56	0.93
1:N:424:ARG:HG2	1:N:424:ARG:NH1	1.55	0.93
1:P:487:GLY:HA3	1:V:229:LYS:HG3	1.51	0.93
1:R:276:VAL:HG12	1:R:280:ILE:HD11	1.50	0.93
1:U:373:PRO:HB3	1:V:391:THR:HA	1.51	0.93
1:B:12:PHE:CE2	1:C:242:HIS:CE1	2.56	0.93
1:D:392:LYS:HD2	1:E:373:PRO:HD3	1.51	0.93
1:J:472:THR:HG22	1:J:498:GLU:CA	1.96	0.93
1:R:370:GLN:HB3	1:R:374:MET:SD	2.08	0.93
1:E:242:HIS:HE1	1:G:12:PHE:CE2	1.86	0.93
1:I:487:GLY:HA2	1:M:229:LYS:HG3	0.93	0.93
1:W:188:ALA:HB1	1:W:218:GLN:CG	1.98	0.93
1:I:188:ALA:HB1	1:I:218:GLN:CG	1.98	0.93
1:O:11:ILE:HB	1:P:273:LYS:CG	1.99	0.93
1:O:6:ASN:OD1	1:P:279:LYS:HE3	1.68	0.93
1:G:188:ALA:HB1	1:G:218:GLN:CG	1.98	0.93
1:M:188:ALA:HB1	1:M:218:GLN:CG	1.98	0.93
1:L:283:SER:OG	1:N:3:LEU:HD23	1.67	0.93
1:R:272:GLU:HG3	1:T:352:GLU:CB	1.98	0.93
1:B:188:ALA:HB1	1:B:218:GLN:CG	1.98	0.93
1:H:473:GLY:HA3	1:M:191:ALA:HB1	1.51	0.93
1:K:373:PRO:HB3	1:L:391:THR:HA	1.50	0.93
1:Q:269:ILE:HG12	1:S:11:ILE:HD12	1.51	0.93
1:R:188:ALA:HB1	1:R:218:GLN:CG	1.98	0.93
1:K:188:ALA:HB1	1:K:218:GLN:CG	1.98	0.92
1:V:276:VAL:HG12	1:V:280:ILE:CD1	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ALA:HB1	1:A:218:GLN:CG	1.98	0.92
1:O:188:ALA:HB1	1:O:218:GLN:CG	1.98	0.92
1:P:188:ALA:HB1	1:P:218:GLN:CG	1.98	0.92
1:D:12:PHE:CE2	1:F:242:HIS:HE1	1.88	0.92
1:H:242:HIS:CE1	1:J:12:PHE:CZ	2.55	0.92
1:J:188:ALA:HB1	1:J:218:GLN:CG	1.98	0.92
1:R:272:GLU:CG	1:T:352:GLU:CG	2.46	0.92
1:L:280:ILE:HG12	1:N:6:ASN:O	1.69	0.92
1:L:487:GLY:CA	1:S:229:LYS:HG3	1.99	0.92
1:H:188:ALA:HB1	1:H:218:GLN:CG	1.98	0.92
1:Q:188:ALA:HB1	1:Q:218:GLN:CG	1.98	0.91
1:F:373:PRO:HB3	1:G:391:THR:HA	1.52	0.91
1:V:283:SER:CB	1:X:3:LEU:HG	2.00	0.91
1:K:188:ALA:HB2	1:K:218:GLN:HG3	0.91	0.91
1:L:188:ALA:HB2	1:L:218:GLN:HG3	0.91	0.91
1:M:188:ALA:HB2	1:M:218:GLN:HG3	0.91	0.91
1:L:242:HIS:CE1	1:N:12:PHE:HE2	1.81	0.91
1:X:188:ALA:HB2	1:X:218:GLN:HG3	0.91	0.91
1:C:188:ALA:HB1	1:C:218:GLN:CG	1.98	0.91
1:I:188:ALA:HB2	1:I:218:GLN:HG3	0.91	0.91
1:L:188:ALA:HB1	1:L:218:GLN:CG	1.98	0.91
1:U:6:ASN:OD1	1:W:279:LYS:HE3	1.69	0.91
1:D:188:ALA:HB2	1:D:218:GLN:HG3	0.91	0.91
1:A:242:HIS:CE1	1:I:12:PHE:CE2	2.59	0.91
1:K:312:GLU:HA	1:M:311:ALA:HB1	1.53	0.91
1:N:371:HIS:O	1:N:374:MET:HG2	1.71	0.91
1:O:424:ARG:HG2	1:O:424:ARG:NH1	1.55	0.91
1:S:372:ILE:CD1	1:T:390:GLU:HG2	2.00	0.91
1:M:390:GLU:O	1:N:373:PRO:HA	1.69	0.91
1:C:216:ALA:HB2	1:N:446:LYS:HD3	1.52	0.91
1:E:188:ALA:HB1	1:E:218:GLN:CG	1.98	0.91
1:O:371:HIS:O	1:O:374:MET:HG2	1.71	0.91
1:P:487:GLY:CA	1:V:229:LYS:HG3	2.00	0.91
1:S:188:ALA:HB1	1:S:218:GLN:CG	1.98	0.91
1:X:188:ALA:HB1	1:X:218:GLN:CG	1.98	0.91
1:K:242:HIS:HE1	1:M:12:PHE:CE2	1.89	0.90
1:T:188:ALA:HB1	1:T:218:GLN:CG	1.98	0.90
1:S:372:ILE:HG13	1:T:390:GLU:C	1.91	0.90
1:G:371:HIS:O	1:G:374:MET:HG2	1.71	0.90
1:A:188:ALA:HB2	1:A:218:GLN:HG3	0.91	0.90
1:A:371:HIS:O	1:A:374:MET:HG2	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:188:ALA:HB2	1:G:218:GLN:HG3	0.91	0.90
1:H:188:ALA:HB2	1:H:218:GLN:HG3	0.91	0.90
1:R:272:GLU:HG2	1:T:352:GLU:HG2	1.53	0.90
1:R:273:LYS:HD3	1:T:11:ILE:O	1.69	0.90
1:P:195:VAL:CG2	1:U:496:LEU:HG	2.01	0.90
1:I:370:GLN:HB3	1:I:374:MET:SD	2.11	0.90
1:V:297:GLN:HE21	1:V:300:GLU:HB2	1.34	0.90
1:R:296:THR:HG22	1:R:297:GLN:HG2	1.54	0.90
1:S:372:ILE:HG23	1:T:390:GLU:O	1.70	0.90
1:U:188:ALA:HB2	1:U:218:GLN:HG3	0.91	0.90
1:V:188:ALA:HB1	1:V:218:GLN:CG	1.98	0.90
1:P:487:GLY:CA	1:V:229:LYS:CD	2.50	0.90
1:I:229:LYS:CG	1:M:487:GLY:HA2	2.02	0.90
1:E:371:HIS:O	1:E:374:MET:HG2	1.71	0.90
1:K:371:HIS:O	1:K:374:MET:HG2	1.71	0.90
1:Q:188:ALA:HB2	1:Q:218:GLN:HG3	0.91	0.90
1:R:297:GLN:HG3	1:T:310:ARG:CG	2.02	0.90
1:V:188:ALA:HB2	1:V:218:GLN:HG3	0.91	0.90
1:B:371:HIS:O	1:B:374:MET:HG2	1.71	0.90
1:C:371:HIS:O	1:C:374:MET:HG2	1.71	0.90
1:H:312:GLU:CA	1:J:311:ALA:HB1	2.00	0.90
1:U:263:GLY:HA2	1:W:310:ARG:HH11	1.34	0.90
1:R:276:VAL:CG1	1:T:9:LEU:HB3	2.02	0.89
1:T:188:ALA:HB2	1:T:218:GLN:HG3	0.91	0.89
1:F:188:ALA:HB2	1:F:218:GLN:HG3	0.91	0.89
1:D:11:ILE:HB	1:F:273:LYS:HG2	1.52	0.89
1:W:373:PRO:HA	1:X:390:GLU:O	1.72	0.89
1:K:12:PHE:HZ	1:M:242:HIS:HE1	1.20	0.89
1:P:144:ASP:O	1:P:145:ASP:HB2	1.73	0.89
1:O:11:ILE:CB	1:P:273:LYS:HG2	2.03	0.89
1:S:144:ASP:O	1:S:145:ASP:HB2	1.73	0.89
1:R:284:LYS:CG	1:T:7:LEU:HD22	2.01	0.89
1:U:312:GLU:HA	1:W:311:ALA:CB	2.01	0.89
1:E:144:ASP:O	1:E:145:ASP:HB2	1.72	0.89
1:F:144:ASP:O	1:F:145:ASP:HB2	1.72	0.89
1:G:144:ASP:O	1:G:145:ASP:HB2	1.72	0.89
1:N:144:ASP:O	1:N:145:ASP:HB2	1.72	0.89
1:C:216:ALA:HB1	1:N:446:LYS:HE2	1.54	0.89
1:L:487:GLY:HA2	1:S:229:LYS:HE3	1.53	0.89
1:S:188:ALA:HB2	1:S:218:GLN:HG3	0.91	0.89
1:W:144:ASP:O	1:W:145:ASP:HB2	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ALA:HB2	1:B:218:GLN:HG3	0.91	0.89
1:V:371:HIS:O	1:V:374:MET:HG2	1.71	0.89
1:J:188:ALA:HB2	1:J:218:GLN:HG3	0.91	0.89
1:P:188:ALA:HB2	1:P:218:GLN:HG3	0.91	0.89
1:Q:144:ASP:O	1:Q:145:ASP:HB2	1.72	0.89
1:W:188:ALA:HB2	1:W:218:GLN:HG3	0.91	0.89
1:X:371:HIS:O	1:X:374:MET:HG2	1.71	0.89
1:K:144:ASP:O	1:K:145:ASP:HB2	1.72	0.89
1:L:242:HIS:HE1	1:N:12:PHE:CZ	1.90	0.89
1:O:144:ASP:O	1:O:145:ASP:HB2	1.72	0.89
1:Q:371:HIS:O	1:Q:374:MET:HG2	1.71	0.89
1:V:284:LYS:CG	1:X:7:LEU:HD22	2.01	0.89
1:D:144:ASP:O	1:D:145:ASP:HB2	1.72	0.88
1:W:371:HIS:O	1:W:374:MET:HG2	1.71	0.88
1:E:188:ALA:HB2	1:E:218:GLN:HG3	0.91	0.88
1:R:188:ALA:HB2	1:R:218:GLN:HG3	0.91	0.88
1:Q:280:ILE:HG12	1:S:6:ASN:O	1.71	0.88
1:U:272:GLU:O	1:W:352:GLU:HG2	1.72	0.88
1:J:371:HIS:O	1:J:374:MET:HG2	1.71	0.88
1:R:297:GLN:HB2	1:T:310:ARG:HB2	1.53	0.88
1:N:188:ALA:HB2	1:N:218:GLN:HG3	0.91	0.88
1:T:144:ASP:O	1:T:145:ASP:HB2	1.72	0.88
1:P:229:LYS:CG	1:V:487:GLY:HA2	2.03	0.88
1:B:144:ASP:O	1:B:145:ASP:HB2	1.72	0.88
1:H:383:SER:HB2	1:I:383:SER:HB2	1.54	0.88
1:H:11:ILE:HB	1:J:273:LYS:HG2	1.53	0.88
1:X:144:ASP:O	1:X:145:ASP:HB2	1.73	0.88
1:F:371:HIS:O	1:F:374:MET:HG2	1.71	0.88
1:F:373:PRO:CA	1:G:390:GLU:O	2.20	0.88
1:U:144:ASP:O	1:U:145:ASP:HB2	1.72	0.88
1:C:144:ASP:O	1:C:145:ASP:HB2	1.72	0.88
1:D:371:HIS:O	1:D:374:MET:HG2	1.71	0.88
1:J:144:ASP:O	1:J:145:ASP:HB2	1.72	0.88
1:C:390:GLU:CA	1:P:372:ILE:HG13	2.04	0.87
1:D:297:GLN:OE1	1:F:310:ARG:HG2	1.75	0.87
1:V:297:GLN:HE21	1:V:300:GLU:CG	1.87	0.87
1:B:272:GLU:HG3	1:C:352:GLU:HB2	1.55	0.87
1:H:144:ASP:O	1:H:145:ASP:HB2	1.72	0.87
1:L:144:ASP:O	1:L:145:ASP:HB2	1.72	0.87
1:Q:242:HIS:HE1	1:S:12:PHE:CE2	1.87	0.87
1:H:188:ALA:HB1	1:H:218:GLN:HG2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:LEU:HG	1:V:195:VAL:CG2	2.05	0.87
1:I:404:ARG:NH2	1:M:228:PRO:HG2	1.89	0.87
1:L:229:LYS:HG3	1:S:487:GLY:CA	2.05	0.87
1:V:144:ASP:O	1:V:145:ASP:HB2	1.72	0.87
1:B:312:GLU:HA	1:C:311:ALA:HB1	1.56	0.87
1:C:188:ALA:HB2	1:C:218:GLN:HG3	0.91	0.87
1:G:188:ALA:HB1	1:G:218:GLN:HG2	1.56	0.87
1:O:188:ALA:HB2	1:O:218:GLN:HG3	0.91	0.87
1:R:188:ALA:HB1	1:R:218:GLN:HG2	1.56	0.87
1:R:272:GLU:HG3	1:T:352:GLU:CG	2.05	0.87
1:T:3:LEU:CD2	1:T:3:LEU:C	2.42	0.87
1:W:372:ILE:HG23	1:X:390:GLU:O	1.75	0.87
1:L:269:ILE:HG12	1:N:11:ILE:HD12	1.57	0.87
1:M:144:ASP:O	1:M:145:ASP:HB2	1.72	0.87
1:J:188:ALA:HB1	1:J:218:GLN:HG2	1.56	0.86
1:R:144:ASP:O	1:R:145:ASP:HB2	1.72	0.86
1:F:188:ALA:HB1	1:F:218:GLN:HG2	1.56	0.86
1:I:144:ASP:O	1:I:145:ASP:HB2	1.72	0.86
1:M:188:ALA:HB1	1:M:218:GLN:HG2	1.56	0.86
1:T:188:ALA:HB1	1:T:218:GLN:HG2	1.57	0.86
1:U:390:GLU:O	1:V:373:PRO:CB	2.22	0.86
1:K:311:ALA:HB1	1:M:312:GLU:HA	1.57	0.86
1:A:144:ASP:O	1:A:145:ASP:HB2	1.72	0.86
1:S:390:GLU:OE1	1:T:379:ALA:CB	2.23	0.86
1:U:11:ILE:CA	1:W:273:LYS:HG2	2.05	0.86
1:U:188:ALA:HB1	1:U:218:GLN:HG2	1.56	0.86
1:D:188:ALA:HB1	1:D:218:GLN:HG2	1.57	0.86
1:H:310:ARG:HB2	1:J:297:GLN:HB2	1.58	0.86
1:K:188:ALA:HB1	1:K:218:GLN:HG2	1.56	0.86
1:Q:188:ALA:HB1	1:Q:218:GLN:HG2	1.56	0.86
1:U:12:PHE:CZ	1:W:242:HIS:HE1	1.93	0.86
1:L:188:ALA:HB1	1:L:218:GLN:HG2	1.56	0.86
1:O:310:ARG:HG2	1:P:297:GLN:OE1	1.75	0.86
1:P:188:ALA:HB1	1:P:218:GLN:HG2	1.56	0.86
1:R:279:LYS:HB3	1:T:6:ASN:CG	1.96	0.86
1:E:11:ILE:CG1	1:E:12:PHE:CE2	2.60	0.85
1:H:11:ILE:O	1:J:273:LYS:CD	2.24	0.85
1:N:188:ALA:HB1	1:N:218:GLN:HG2	1.56	0.85
1:H:12:PHE:CE2	1:J:242:HIS:CE1	2.59	0.85
1:H:370:GLN:HB3	1:H:374:MET:SD	2.16	0.85
1:V:424:ARG:HH11	1:V:424:ARG:HG2	0.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ALA:HB1	1:A:218:GLN:HG2	1.56	0.85
1:E:242:HIS:CE1	1:G:12:PHE:CZ	2.64	0.85
1:H:272:GLU:O	1:J:352:GLU:HG2	1.76	0.85
1:U:310:ARG:HG2	1:W:297:GLN:OE1	1.77	0.85
1:C:188:ALA:HB1	1:C:218:GLN:HG2	1.56	0.85
1:M:383:SER:HB2	1:N:383:SER:HB2	1.59	0.85
1:M:424:ARG:HH11	1:M:424:ARG:HG2	0.74	0.85
1:O:242:HIS:HE1	1:P:12:PHE:CZ	1.94	0.85
1:O:188:ALA:HB1	1:O:218:GLN:HG2	1.56	0.85
1:K:496:LEU:CG	1:S:195:VAL:HG22	2.06	0.85
1:X:188:ALA:HB1	1:X:218:GLN:HG2	1.56	0.85
1:H:352:GLU:HG2	1:J:272:GLU:O	1.77	0.85
1:I:11:ILE:CG1	1:I:12:PHE:CE2	2.60	0.85
1:I:188:ALA:HB1	1:I:218:GLN:HG2	1.56	0.85
1:I:11:ILE:HD11	1:I:12:PHE:CE2	2.12	0.85
1:L:11:ILE:CG1	1:L:12:PHE:CE2	2.59	0.85
1:U:372:ILE:CG1	1:V:390:GLU:HA	2.04	0.85
1:U:11:ILE:O	1:W:273:LYS:CE	2.25	0.85
1:B:188:ALA:HB1	1:B:218:GLN:HG2	1.56	0.84
1:E:188:ALA:HB1	1:E:218:GLN:HG2	1.56	0.84
1:R:11:ILE:CG1	1:R:12:PHE:CE2	2.59	0.84
1:Q:272:GLU:HG3	1:S:352:GLU:HB2	1.59	0.84
1:V:11:ILE:HD11	1:V:12:PHE:CE2	2.12	0.84
1:L:11:ILE:HG13	1:L:12:PHE:CD2	2.12	0.84
1:V:188:ALA:HB1	1:V:218:GLN:HG2	1.56	0.84
1:S:483:HIS:CD2	1:T:483:HIS:NE2	2.44	0.84
1:I:11:ILE:HG13	1:I:12:PHE:CD2	2.13	0.84
1:K:390:GLU:HA	1:L:372:ILE:HG13	1.60	0.84
1:O:12:PHE:CZ	1:P:242:HIS:CE1	2.64	0.84
1:S:483:HIS:NE2	1:T:483:HIS:CD2	2.44	0.84
1:R:11:ILE:HD11	1:R:12:PHE:CE2	2.12	0.84
1:S:483:HIS:NE2	1:T:483:HIS:HD2	1.75	0.84
1:L:11:ILE:HD11	1:L:12:PHE:CE2	2.12	0.84
1:L:297:GLN:HB2	1:N:310:ARG:HG3	1.59	0.84
1:S:188:ALA:HB1	1:S:218:GLN:HG2	1.57	0.84
1:V:11:ILE:CG1	1:V:12:PHE:CE2	2.60	0.84
1:E:11:ILE:HD11	1:E:12:PHE:CE2	2.12	0.84
1:R:11:ILE:HG13	1:R:12:PHE:CD2	2.12	0.84
1:E:424:ARG:HG2	1:E:424:ARG:HH11	0.74	0.84
1:K:297:GLN:OE1	1:M:310:ARG:HG2	1.77	0.84
1:W:188:ALA:HB1	1:W:218:GLN:HG2	1.56	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:310:ARG:HG2	1:W:297:GLN:HB2	1.59	0.84
1:W:373:PRO:HB3	1:X:391:THR:CA	2.07	0.84
1:R:272:GLU:CB	1:T:352:GLU:HG2	2.08	0.83
1:U:297:GLN:HB2	1:W:310:ARG:CG	2.08	0.83
1:E:11:ILE:HG13	1:E:12:PHE:CD2	2.12	0.83
1:H:10:SER:HB3	1:H:13:ASP:OD1	1.78	0.83
1:S:10:SER:HB3	1:S:13:ASP:OD1	1.79	0.83
1:I:229:LYS:CG	1:M:487:GLY:CA	2.56	0.83
1:L:11:ILE:HD11	1:L:12:PHE:HE2	1.44	0.83
1:R:10:SER:HB3	1:R:13:ASP:OD1	1.79	0.83
1:T:10:SER:HB3	1:T:13:ASP:OD1	1.78	0.83
1:V:11:ILE:HG13	1:V:12:PHE:CD2	2.12	0.83
1:B:279:LYS:HE3	1:C:6:ASN:OD1	1.78	0.83
1:L:10:SER:HB3	1:L:13:ASP:OD1	1.78	0.83
1:H:496:LEU:CD2	1:M:195:VAL:CG2	2.56	0.83
1:G:10:SER:HB3	1:G:13:ASP:OD1	1.79	0.83
1:M:10:SER:HB3	1:M:13:ASP:OD1	1.79	0.83
1:C:254:GLU:HG2	1:N:446:LYS:HE2	1.60	0.83
1:O:10:SER:HB3	1:O:13:ASP:OD1	1.78	0.83
1:R:11:ILE:HD11	1:R:12:PHE:HE2	1.43	0.83
1:V:272:GLU:CG	1:X:352:GLU:HG2	2.09	0.83
1:E:279:LYS:HE3	1:G:6:ASN:OD1	1.76	0.83
1:I:11:ILE:HD11	1:I:12:PHE:HE2	1.44	0.83
1:A:242:HIS:NE2	1:I:12:PHE:CZ	2.47	0.83
1:H:315:ASP:HB2	1:J:311:ALA:HA	1.61	0.83
1:M:390:GLU:O	1:N:373:PRO:CB	2.27	0.83
1:A:10:SER:HB3	1:A:13:ASP:OD1	1.78	0.83
1:V:10:SER:HB3	1:V:13:ASP:OD1	1.79	0.83
1:F:10:SER:HB3	1:F:13:ASP:OD1	1.79	0.83
1:N:10:SER:HB3	1:N:13:ASP:OD1	1.79	0.83
1:M:390:GLU:O	1:N:373:PRO:CA	2.26	0.83
1:U:10:SER:HB3	1:U:13:ASP:OD1	1.78	0.83
1:V:3:LEU:HD23	1:X:283:SER:HB3	1.61	0.83
1:I:10:SER:HB3	1:I:13:ASP:OD1	1.79	0.83
1:J:10:SER:HB3	1:J:13:ASP:OD1	1.79	0.83
1:K:424:ARG:HH11	1:K:424:ARG:HG2	0.74	0.83
1:L:280:ILE:CG1	1:N:6:ASN:O	2.26	0.83
1:R:280:ILE:HD11	1:T:9:LEU:HB2	1.59	0.82
1:V:7:LEU:CD2	1:X:284:LYS:HG3	2.08	0.82
1:E:10:SER:HB3	1:E:13:ASP:OD1	1.79	0.82
1:H:310:ARG:CG	1:J:297:GLN:CG	2.57	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD21	1:I:283:SER:HB3	1.61	0.82
1:K:12:PHE:HZ	1:M:242:HIS:CE1	1.91	0.82
1:I:229:LYS:CD	1:M:487:GLY:CA	2.57	0.82
1:C:10:SER:HB3	1:C:13:ASP:OD1	1.78	0.82
1:F:390:GLU:O	1:G:373:PRO:CA	2.26	0.82
1:V:284:LYS:CG	1:X:7:LEU:HD21	2.07	0.82
1:B:10:SER:HB3	1:B:13:ASP:OD1	1.79	0.82
1:F:373:PRO:CB	1:G:391:THR:HA	2.09	0.82
1:A:453:LYS:NZ	2:A:700:FDP:O1P	2.12	0.82
1:C:453:LYS:NZ	2:C:700:FDP:O1P	2.12	0.82
1:O:424:ARG:HG2	1:O:424:ARG:HH11	0.74	0.82
1:D:10:SER:HB3	1:D:13:ASP:OD1	1.79	0.82
1:H:11:ILE:CA	1:J:273:LYS:HG2	2.08	0.82
1:Q:310:ARG:HG2	1:S:297:GLN:OE1	1.80	0.82
1:C:496:LEU:CG	1:V:195:VAL:HG22	2.10	0.82
1:F:453:LYS:NZ	2:F:700:FDP:O1P	2.13	0.82
1:I:424:ARG:HH11	1:I:424:ARG:HG2	0.74	0.82
1:V:11:ILE:HD11	1:V:12:PHE:HE2	1.44	0.82
1:W:10:SER:HB3	1:W:13:ASP:OD1	1.79	0.82
1:A:424:ARG:HG2	1:A:424:ARG:HH11	0.74	0.82
1:Q:283:SER:CB	1:S:3:LEU:CD2	2.57	0.82
1:Q:283:SER:CB	1:S:3:LEU:HD23	2.09	0.82
1:X:10:SER:HB3	1:X:13:ASP:OD1	1.78	0.82
1:B:453:LYS:NZ	2:B:700:FDP:O1P	2.13	0.81
1:E:453:LYS:NZ	2:E:700:FDP:O1P	2.13	0.81
1:K:10:SER:HB3	1:K:13:ASP:OD1	1.79	0.81
1:L:11:ILE:O	1:N:273:LYS:HE3	1.79	0.81
1:P:487:GLY:HA2	1:V:229:LYS:CG	2.09	0.81
1:R:424:ARG:HH11	1:R:424:ARG:HG2	0.74	0.81
1:D:453:LYS:NZ	2:D:700:FDP:O1P	2.13	0.81
1:J:453:LYS:NZ	2:J:700:FDP:O1P	2.13	0.81
1:H:496:LEU:CG	1:M:195:VAL:CG2	2.52	0.81
1:N:453:LYS:NZ	2:N:700:FDP:O1P	2.13	0.81
1:Q:10:SER:HB3	1:Q:13:ASP:OD1	1.78	0.81
1:L:487:GLY:HA2	1:S:229:LYS:HG3	1.59	0.81
1:Q:453:LYS:NZ	2:Q:700:FDP:O1P	2.13	0.81
1:C:424:ARG:HH11	1:C:424:ARG:HG2	0.74	0.81
1:D:12:PHE:HE2	1:F:242:HIS:CE1	1.95	0.81
1:E:11:ILE:HD11	1:E:12:PHE:HE2	1.44	0.81
1:N:446:LYS:O	1:N:446:LYS:HD2	1.81	0.81
1:S:453:LYS:NZ	2:S:700:FDP:O1P	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:10:SER:HB3	1:P:13:ASP:OD1	1.79	0.81
1:F:373:PRO:HB3	1:G:391:THR:CA	2.11	0.81
1:V:280:ILE:CG1	1:X:6:ASN:O	2.29	0.81
1:L:311:ALA:HB1	1:N:312:GLU:HA	1.63	0.81
1:V:12:PHE:CE2	1:X:242:HIS:CE1	2.69	0.81
1:D:12:PHE:CZ	1:F:242:HIS:CE1	2.69	0.81
1:L:229:LYS:HE3	1:S:487:GLY:HA2	1.61	0.81
1:L:487:GLY:HA2	1:S:229:LYS:CE	2.09	0.81
1:M:370:GLN:HB3	1:M:374:MET:SD	2.20	0.81
1:K:496:LEU:HG	1:S:195:VAL:CG2	2.10	0.81
1:S:483:HIS:CD2	1:T:483:HIS:CD2	2.69	0.81
1:T:424:ARG:HG2	1:T:424:ARG:HH11	0.74	0.81
1:W:390:GLU:OE1	1:X:379:ALA:CB	2.29	0.81
1:I:453:LYS:NZ	2:I:700:FDP:O1P	2.13	0.81
1:S:424:ARG:HG2	1:S:424:ARG:HH11	0.74	0.81
1:U:390:GLU:OE1	1:V:379:ALA:CB	2.29	0.81
1:K:372:ILE:HG13	1:L:390:GLU:HA	1.61	0.81
1:H:11:ILE:HB	1:J:273:LYS:CG	2.10	0.80
1:R:453:LYS:NZ	2:R:700:FDP:O1P	2.13	0.80
1:I:270:PRO:HG2	1:I:273:LYS:CE	2.11	0.80
1:D:424:ARG:HG2	1:D:424:ARG:HH11	0.74	0.80
1:G:424:ARG:HG2	1:G:424:ARG:HH11	0.74	0.80
1:V:283:SER:OG	1:X:3:LEU:HG	1.82	0.80
1:E:270:PRO:HG2	1:E:273:LYS:CE	2.11	0.80
1:H:315:ASP:CB	1:J:311:ALA:HA	2.12	0.80
1:R:280:ILE:CG1	1:T:6:ASN:O	2.26	0.80
1:U:310:ARG:CG	1:W:297:GLN:HB2	2.11	0.80
1:V:453:LYS:NZ	2:V:700:FDP:O1P	2.15	0.80
1:W:453:LYS:NZ	2:W:700:FDP:O1P	2.15	0.80
1:B:269:ILE:HG12	1:C:11:ILE:HD12	1.64	0.80
1:H:390:GLU:O	1:I:373:PRO:HA	1.79	0.80
1:R:270:PRO:HG2	1:R:273:LYS:CE	2.11	0.80
1:V:270:PRO:HG2	1:V:273:LYS:CE	2.11	0.80
1:X:424:ARG:HH11	1:X:424:ARG:HG2	0.74	0.80
1:U:453:LYS:NZ	2:U:700:FDP:O1P	2.13	0.80
1:X:453:LYS:NZ	2:X:700:FDP:O1P	2.15	0.80
1:H:453:LYS:NZ	2:H:700:FDP:O1P	2.15	0.79
1:K:453:LYS:NZ	2:K:700:FDP:O1P	2.15	0.79
1:O:453:LYS:NZ	2:O:700:FDP:O1P	2.14	0.79
1:N:142:TYR:HB3	1:N:146:GLY:HA2	1.65	0.79
1:U:242:HIS:NE2	1:W:12:PHE:CE2	2.49	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ILE:HG13	1:O:390:GLU:HA	1.64	0.79
1:H:11:ILE:O	1:J:273:LYS:CG	2.30	0.79
1:L:142:TYR:HB3	1:L:146:GLY:HA2	1.65	0.79
1:H:496:LEU:HD23	1:M:195:VAL:HG22	1.64	0.79
1:L:487:GLY:HA2	1:S:229:LYS:CG	2.11	0.79
1:V:276:VAL:CG1	1:V:280:ILE:HD11	2.11	0.79
1:W:390:GLU:OE1	1:X:379:ALA:HB1	1.82	0.79
1:H:424:ARG:HH11	1:H:424:ARG:HG2	0.74	0.79
1:N:446:LYS:O	1:N:446:LYS:CD	2.30	0.79
1:O:312:GLU:HA	1:P:311:ALA:CB	2.13	0.79
1:P:370:GLN:HB3	1:P:374:MET:SD	2.22	0.79
1:P:453:LYS:NZ	2:P:700:FDP:O1P	2.15	0.79
1:G:142:TYR:HB3	1:G:146:GLY:HA2	1.65	0.79
1:L:312:GLU:HA	1:N:311:ALA:HB1	1.64	0.79
1:T:142:TYR:HB3	1:T:146:GLY:HA2	1.65	0.79
1:T:453:LYS:NZ	2:T:700:FDP:O1P	2.15	0.79
1:V:242:HIS:HE1	1:X:12:PHE:CZ	2.00	0.79
1:P:487:GLY:CA	1:V:229:LYS:CG	2.61	0.79
1:Q:280:ILE:HD11	1:S:9:LEU:HB2	1.65	0.79
1:K:142:TYR:HB3	1:K:146:GLY:HA2	1.65	0.79
1:Q:142:TYR:HB3	1:Q:146:GLY:HA2	1.65	0.79
1:H:11:ILE:O	1:J:273:LYS:HE3	1.83	0.79
1:L:12:PHE:CZ	1:N:242:HIS:CE1	2.70	0.79
1:M:453:LYS:NZ	2:M:700:FDP:O1P	2.15	0.79
1:R:3:LEU:HD13	1:T:369:LEU:HD12	1.65	0.79
1:W:142:TYR:HB3	1:W:146:GLY:HA2	1.65	0.79
1:B:424:ARG:HG2	1:B:424:ARG:HH11	0.74	0.79
1:L:453:LYS:NZ	2:L:700:FDP:O1P	2.15	0.79
1:R:371:HIS:O	1:R:374:MET:CG	2.30	0.79
1:V:269:ILE:HG12	1:X:11:ILE:HD12	1.64	0.79
1:A:142:TYR:HB3	1:A:146:GLY:HA2	1.65	0.78
1:B:142:TYR:HB3	1:B:146:GLY:HA2	1.65	0.78
1:H:11:ILE:CB	1:J:273:LYS:HG2	2.13	0.78
1:B:4:ALA:O	1:B:7:LEU:HB2	1.84	0.78
1:H:142:TYR:HB3	1:H:146:GLY:HA2	1.64	0.78
1:L:270:PRO:HG2	1:L:273:LYS:CE	2.11	0.78
1:C:216:ALA:HB1	1:N:446:LYS:CE	2.13	0.78
1:L:284:LYS:HG3	1:N:7:LEU:CD2	2.13	0.78
1:S:4:ALA:O	1:S:7:LEU:HB2	1.83	0.78
1:N:424:ARG:HG2	1:N:424:ARG:HH11	0.74	0.78
1:T:4:ALA:O	1:T:7:LEU:HB2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:284:LYS:HG3	1:T:7:LEU:HD21	1.59	0.78
1:W:373:PRO:CB	1:X:391:THR:HA	2.12	0.78
1:D:142:TYR:HB3	1:D:146:GLY:HA2	1.65	0.78
1:L:370:GLN:HB3	1:L:374:MET:SD	2.22	0.78
1:K:242:HIS:HE1	1:M:12:PHE:CZ	2.01	0.78
1:P:4:ALA:O	1:P:7:LEU:HB2	1.84	0.78
1:W:4:ALA:O	1:W:7:LEU:HB2	1.84	0.78
1:G:453:LYS:NZ	2:G:700:FDP:O1P	2.15	0.78
1:I:4:ALA:O	1:I:7:LEU:HB2	1.84	0.78
1:J:142:TYR:HB3	1:J:146:GLY:HA2	1.65	0.78
1:N:4:ALA:O	1:N:7:LEU:HB2	1.84	0.78
1:R:142:TYR:HB3	1:R:146:GLY:HA2	1.65	0.78
1:U:142:TYR:HB3	1:U:146:GLY:HA2	1.65	0.78
1:H:373:PRO:HA	1:I:390:GLU:O	1.84	0.78
1:K:4:ALA:O	1:K:7:LEU:HB2	1.84	0.78
1:R:284:LYS:CG	1:T:7:LEU:CD2	2.56	0.78
1:C:223:ARG:HH11	1:C:223:ARG:HG2	1.49	0.78
1:F:424:ARG:HG2	1:F:424:ARG:HH11	0.74	0.78
1:L:272:GLU:CG	1:N:352:GLU:HG2	2.13	0.78
1:P:223:ARG:HG2	1:P:223:ARG:HH11	1.49	0.78
1:Q:283:SER:HB3	1:S:3:LEU:HD23	1.65	0.78
1:D:4:ALA:O	1:D:7:LEU:HB2	1.83	0.78
1:E:4:ALA:O	1:E:7:LEU:HB2	1.84	0.78
1:H:372:ILE:HG13	1:I:390:GLU:CA	2.14	0.78
1:K:390:GLU:O	1:L:373:PRO:HA	1.83	0.78
1:V:7:LEU:CD2	1:X:284:LYS:CG	2.62	0.78
1:B:223:ARG:HH11	1:B:223:ARG:HG2	1.49	0.78
1:C:4:ALA:O	1:C:7:LEU:HB2	1.84	0.78
1:R:4:ALA:O	1:R:7:LEU:HB2	1.84	0.78
1:W:223:ARG:HG2	1:W:223:ARG:HH11	1.49	0.78
1:D:223:ARG:HG2	1:D:223:ARG:HH11	1.49	0.78
1:L:223:ARG:HG2	1:L:223:ARG:HH11	1.49	0.78
1:L:4:ALA:O	1:L:7:LEU:HB2	1.83	0.78
1:P:142:TYR:HB3	1:P:146:GLY:HA2	1.65	0.78
1:C:142:TYR:HB3	1:C:146:GLY:HA2	1.65	0.77
1:F:223:ARG:HH11	1:F:223:ARG:HG2	1.49	0.77
1:X:4:ALA:O	1:X:7:LEU:HB2	1.84	0.77
1:P:424:ARG:HG2	1:P:424:ARG:HH11	0.74	0.77
1:A:4:ALA:O	1:A:7:LEU:HB2	1.84	0.77
1:G:4:ALA:O	1:G:7:LEU:HB2	1.83	0.77
1:I:142:TYR:HB3	1:I:146:GLY:HA2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:223:ARG:HG2	1:J:223:ARG:HH11	1.49	0.77
1:L:487:GLY:HA3	1:S:229:LYS:HG3	1.64	0.77
1:X:142:TYR:HB3	1:X:146:GLY:HA2	1.64	0.77
1:J:4:ALA:O	1:J:7:LEU:HB2	1.84	0.77
1:O:4:ALA:O	1:O:7:LEU:HB2	1.84	0.77
1:Q:424:ARG:HG2	1:Q:424:ARG:HH11	0.74	0.77
1:R:279:LYS:HE3	1:T:6:ASN:OD1	1.85	0.77
1:V:276:VAL:O	1:V:280:ILE:HD12	1.85	0.77
1:A:223:ARG:HG2	1:A:223:ARG:HH11	1.49	0.77
1:H:297:GLN:CG	1:J:310:ARG:HG2	2.15	0.77
1:V:142:TYR:HB3	1:V:146:GLY:HA2	1.65	0.77
1:B:311:ALA:HB1	1:C:312:GLU:HA	1.65	0.77
1:E:142:TYR:HB3	1:E:146:GLY:HA2	1.65	0.77
1:F:4:ALA:O	1:F:7:LEU:HB2	1.83	0.77
1:Q:223:ARG:HH11	1:Q:223:ARG:HG2	1.49	0.77
1:S:223:ARG:HG2	1:S:223:ARG:HH11	1.49	0.77
1:S:370:GLN:HB3	1:S:374:MET:SD	2.25	0.77
1:W:424:ARG:HG2	1:W:424:ARG:HH11	0.74	0.77
1:D:372:ILE:HG13	1:E:390:GLU:HA	1.67	0.77
1:F:142:TYR:HB3	1:F:146:GLY:HA2	1.65	0.77
1:H:4:ALA:O	1:H:7:LEU:HB2	1.84	0.77
1:M:4:ALA:O	1:M:7:LEU:HB2	1.84	0.77
1:M:142:TYR:HB3	1:M:146:GLY:HA2	1.65	0.77
1:O:142:TYR:HB3	1:O:146:GLY:HA2	1.65	0.77
1:Q:283:SER:OG	1:S:3:LEU:HD23	1.83	0.77
1:Q:284:LYS:HG3	1:S:7:LEU:CD2	2.15	0.77
1:T:223:ARG:HH11	1:T:223:ARG:HG2	1.49	0.77
1:U:223:ARG:HG2	1:U:223:ARG:HH11	1.49	0.77
1:U:4:ALA:O	1:U:7:LEU:HB2	1.84	0.77
1:V:283:SER:HB3	1:X:3:LEU:HG	1.66	0.77
1:G:223:ARG:HG2	1:G:223:ARG:HH11	1.49	0.76
1:H:223:ARG:HG2	1:H:223:ARG:HH11	1.49	0.76
1:M:214:ARG:H	1:M:218:GLN:HE22	1.33	0.76
1:Q:4:ALA:O	1:Q:7:LEU:HB2	1.84	0.76
1:S:142:TYR:HB3	1:S:146:GLY:HA2	1.64	0.76
1:V:12:PHE:CZ	1:X:242:HIS:CE1	2.72	0.76
1:V:283:SER:HB3	1:X:3:LEU:CD2	2.15	0.76
1:Q:390:GLU:O	1:R:372:ILE:HG23	1.86	0.76
1:V:214:ARG:H	1:V:218:GLN:HE22	1.33	0.76
1:A:392:LYS:CD	1:J:373:PRO:HD3	2.13	0.76
1:K:223:ARG:HH11	1:K:223:ARG:HG2	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:269:ILE:HG12	1:N:11:ILE:CD1	2.15	0.76
1:X:223:ARG:HH11	1:X:223:ARG:HG2	1.49	0.76
1:K:214:ARG:H	1:K:218:GLN:HE22	1.34	0.76
1:N:223:ARG:HH11	1:N:223:ARG:HG2	1.49	0.76
1:B:373:PRO:HB3	1:O:391:THR:C	2.06	0.76
1:B:214:ARG:H	1:B:218:GLN:HE22	1.33	0.76
1:I:214:ARG:H	1:I:218:GLN:HE22	1.33	0.76
1:O:223:ARG:HH11	1:O:223:ARG:HG2	1.49	0.76
1:L:229:LYS:HG3	1:S:487:GLY:HA3	1.67	0.76
1:I:223:ARG:HG2	1:I:223:ARG:HH11	1.49	0.76
1:R:223:ARG:HH11	1:R:223:ARG:HG2	1.49	0.76
1:L:229:LYS:HG3	1:S:487:GLY:HA2	1.66	0.76
1:M:223:ARG:HG2	1:M:223:ARG:HH11	1.49	0.76
1:C:373:PRO:CA	1:P:390:GLU:O	2.34	0.76
1:B:12:PHE:HE2	1:C:242:HIS:HE1	0.88	0.75
1:O:11:ILE:O	1:P:273:LYS:HE3	1.85	0.75
1:U:390:GLU:O	1:V:373:PRO:HB3	1.85	0.75
1:L:283:SER:HB3	1:N:3:LEU:HD23	1.57	0.75
1:C:214:ARG:H	1:C:218:GLN:HE22	1.33	0.75
1:F:383:SER:HB2	1:G:383:SER:HB2	1.69	0.75
1:V:223:ARG:HG2	1:V:223:ARG:HH11	1.49	0.75
1:V:4:ALA:O	1:V:7:LEU:HB2	1.84	0.75
1:B:297:GLN:HB2	1:C:310:ARG:CG	2.15	0.75
1:D:373:PRO:HA	1:E:390:GLU:O	1.85	0.75
1:Q:12:PHE:HE2	1:S:242:HIS:CE1	2.05	0.75
1:H:310:ARG:CG	1:J:297:GLN:CB	2.49	0.75
1:P:214:ARG:H	1:P:218:GLN:HE22	1.33	0.75
1:S:390:GLU:OE1	1:T:379:ALA:HB1	1.86	0.75
1:A:214:ARG:H	1:A:218:GLN:HE22	1.33	0.75
1:E:214:ARG:H	1:E:218:GLN:HE22	1.33	0.75
1:O:214:ARG:H	1:O:218:GLN:HE22	1.34	0.75
1:L:214:ARG:H	1:L:218:GLN:HE22	1.33	0.74
1:K:272:GLU:HG3	1:M:352:GLU:HB2	1.68	0.74
1:R:276:VAL:CG1	1:T:9:LEU:CB	2.64	0.74
1:E:223:ARG:HG2	1:E:223:ARG:HH11	1.49	0.74
1:H:297:GLN:HG3	1:J:310:ARG:HG2	1.69	0.74
1:S:491:GLN:HG3	1:T:491:GLN:HG3	1.68	0.74
1:U:242:HIS:CE1	1:W:12:PHE:HZ	2.00	0.74
1:V:280:ILE:HD11	1:X:9:LEU:HB2	1.68	0.74
1:I:195:VAL:HG22	1:N:496:LEU:HG	1.69	0.74
1:X:214:ARG:H	1:X:218:GLN:HE22	1.33	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:GLU:HA	1:G:372:ILE:HG13	1.69	0.74
1:K:11:ILE:HB	1:M:273:LYS:HG2	1.68	0.74
1:P:229:LYS:HG3	1:V:487:GLY:HA3	1.69	0.74
1:L:191:ALA:HB1	1:T:473:GLY:HA3	1.69	0.74
1:U:214:ARG:H	1:U:218:GLN:HE22	1.33	0.74
1:Q:280:ILE:CG1	1:S:6:ASN:O	2.34	0.74
1:D:214:ARG:H	1:D:218:GLN:HE22	1.33	0.74
1:G:214:ARG:H	1:G:218:GLN:HE22	1.33	0.74
1:C:373:PRO:HB3	1:P:391:THR:HA	1.69	0.74
1:T:214:ARG:H	1:T:218:GLN:HE22	1.33	0.74
1:V:297:GLN:NE2	1:V:300:GLU:HG2	2.02	0.74
1:I:193:ASP:HA	1:I:196:ASP:HB2	1.70	0.74
1:F:391:THR:HA	1:G:373:PRO:HB3	1.70	0.74
1:J:214:ARG:H	1:J:218:GLN:HE22	1.33	0.74
1:K:193:ASP:HA	1:K:196:ASP:HB2	1.70	0.74
1:M:193:ASP:HA	1:M:196:ASP:HB2	1.70	0.74
1:Q:214:ARG:H	1:Q:218:GLN:HE22	1.33	0.74
1:Q:12:PHE:CE2	1:S:242:HIS:HE1	2.06	0.74
1:W:193:ASP:HA	1:W:196:ASP:HB2	1.70	0.74
1:O:193:ASP:HA	1:O:196:ASP:HB2	1.70	0.74
1:R:276:VAL:HG13	1:T:9:LEU:CB	2.18	0.74
1:W:392:LYS:HD2	1:X:373:PRO:HD3	1.69	0.74
1:V:9:LEU:HB2	1:X:280:ILE:HD11	1.68	0.74
1:V:297:GLN:OE1	1:X:309:THR:HB	1.88	0.74
1:L:193:ASP:HA	1:L:196:ASP:HB2	1.70	0.73
1:L:283:SER:CB	1:N:3:LEU:HD21	2.17	0.73
1:S:494:ILE:HD12	1:T:376:ALA:HB1	1.68	0.73
1:H:214:ARG:H	1:H:218:GLN:HE22	1.34	0.73
1:Q:390:GLU:O	1:R:373:PRO:HA	1.88	0.73
1:S:214:ARG:H	1:S:218:GLN:HE22	1.33	0.73
1:A:179:LEU:HB3	1:A:182:CYS:HB2	1.71	0.73
1:E:11:ILE:CG1	1:E:12:PHE:CD2	2.71	0.73
1:F:193:ASP:HA	1:F:196:ASP:HB2	1.70	0.73
1:N:179:LEU:HB3	1:N:182:CYS:HB2	1.70	0.73
1:P:193:ASP:HA	1:P:196:ASP:HB2	1.70	0.73
1:C:383:SER:HB2	1:P:383:SER:HB2	1.70	0.73
1:V:310:ARG:HG2	1:X:297:GLN:OE1	1.88	0.73
1:I:11:ILE:CG1	1:I:12:PHE:CD2	2.71	0.73
1:R:11:ILE:CG1	1:R:12:PHE:CD2	2.71	0.73
1:C:216:ALA:HB3	1:N:446:LYS:CD	2.12	0.73
1:F:214:ARG:H	1:F:218:GLN:HE22	1.33	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:179:LEU:HB3	1:J:182:CYS:HB2	1.70	0.73
1:U:193:ASP:HA	1:U:196:ASP:HB2	1.70	0.73
1:K:242:HIS:CE1	1:M:12:PHE:CZ	2.75	0.73
1:L:424:ARG:HG2	1:L:424:ARG:HH11	0.74	0.73
1:B:373:PRO:HA	1:O:390:GLU:O	1.88	0.73
1:O:242:HIS:CE1	1:P:12:PHE:CZ	2.77	0.73
1:Q:297:GLN:OE1	1:S:310:ARG:CG	2.31	0.73
1:R:214:ARG:H	1:R:218:GLN:HE22	1.33	0.73
1:S:193:ASP:HA	1:S:196:ASP:HB2	1.70	0.73
1:C:216:ALA:HB1	1:N:446:LYS:CD	2.15	0.73
1:D:179:LEU:HB3	1:D:182:CYS:HB2	1.70	0.73
1:N:214:ARG:H	1:N:218:GLN:HE22	1.33	0.73
1:Q:312:GLU:HA	1:S:311:ALA:HB1	1.70	0.73
1:V:11:ILE:CG1	1:V:12:PHE:CD2	2.71	0.73
1:W:179:LEU:HB3	1:W:182:CYS:HB2	1.70	0.73
1:C:179:LEU:HB3	1:C:182:CYS:HB2	1.70	0.73
1:D:193:ASP:HA	1:D:196:ASP:HB2	1.70	0.73
1:I:179:LEU:HB3	1:I:182:CYS:HB2	1.70	0.73
1:N:193:ASP:HA	1:N:196:ASP:HB2	1.70	0.73
1:T:179:LEU:HB3	1:T:182:CYS:HB2	1.70	0.73
1:U:179:LEU:HB3	1:U:182:CYS:HB2	1.70	0.73
1:C:496:LEU:CD2	1:V:195:VAL:HG22	2.19	0.73
1:W:214:ARG:H	1:W:218:GLN:HE22	1.33	0.73
1:O:179:LEU:HB3	1:O:182:CYS:HB2	1.71	0.73
1:T:370:GLN:HB3	1:T:374:MET:SD	2.29	0.73
1:A:193:ASP:HA	1:A:196:ASP:HB2	1.70	0.72
1:L:11:ILE:CG1	1:L:12:PHE:CD2	2.71	0.72
1:Q:193:ASP:HA	1:Q:196:ASP:HB2	1.70	0.72
1:U:424:ARG:HH11	1:U:424:ARG:HG2	0.74	0.72
1:X:179:LEU:HB3	1:X:182:CYS:HB2	1.70	0.72
1:M:390:GLU:O	1:N:373:PRO:HB3	1.87	0.72
1:Q:373:PRO:HA	1:R:390:GLU:O	1.89	0.72
1:L:229:LYS:CE	1:S:487:GLY:HA2	2.19	0.72
1:R:193:ASP:HA	1:R:196:ASP:HB2	1.70	0.72
1:U:370:GLN:HB3	1:U:374:MET:SD	2.29	0.72
1:P:191:ALA:HB1	1:U:473:GLY:HA3	1.69	0.72
1:L:487:GLY:HA2	1:S:229:LYS:CD	2.20	0.72
1:V:179:LEU:HB3	1:V:182:CYS:HB2	1.70	0.72
1:Q:179:LEU:HB3	1:Q:182:CYS:HB2	1.71	0.72
1:V:193:ASP:HA	1:V:196:ASP:HB2	1.70	0.72
1:C:193:ASP:HA	1:C:196:ASP:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:193:ASP:HA	1:J:196:ASP:HB2	1.70	0.72
1:S:179:LEU:HB3	1:S:182:CYS:HB2	1.70	0.72
1:Q:11:ILE:HB	1:S:273:LYS:HG2	1.72	0.72
1:Q:3:LEU:CD2	1:S:283:SER:HB3	2.20	0.72
1:R:276:VAL:HG13	1:T:9:LEU:HD13	1.71	0.72
1:U:373:PRO:CB	1:V:391:THR:HA	2.19	0.72
1:V:242:HIS:CE1	1:X:12:PHE:CZ	2.75	0.72
1:F:179:LEU:HB3	1:F:182:CYS:HB2	1.70	0.72
1:L:272:GLU:HG3	1:N:352:GLU:HB2	1.70	0.72
1:Q:373:PRO:HD3	1:R:392:LYS:HD2	1.72	0.72
1:U:373:PRO:HB3	1:V:391:THR:CA	2.19	0.72
1:A:390:GLU:HA	1:J:372:ILE:HG13	1.70	0.72
1:E:193:ASP:HA	1:E:196:ASP:HB2	1.70	0.72
1:F:491:GLN:HG3	1:G:491:GLN:HG3	1.72	0.72
1:J:424:ARG:HH11	1:J:424:ARG:HG2	0.74	0.72
1:L:179:LEU:HB3	1:L:182:CYS:HB2	1.70	0.72
1:P:179:LEU:HB3	1:P:182:CYS:HB2	1.70	0.72
1:U:372:ILE:HD11	1:V:390:GLU:HG2	1.71	0.72
1:H:11:ILE:O	1:J:273:LYS:HG2	1.90	0.72
1:M:179:LEU:HB3	1:M:182:CYS:HB2	1.70	0.72
1:R:276:VAL:HG13	1:T:9:LEU:HB3	1.71	0.72
1:U:315:ASP:HB2	1:W:311:ALA:HA	1.71	0.72
1:B:193:ASP:HA	1:B:196:ASP:HB2	1.70	0.72
1:A:242:HIS:CE1	1:I:12:PHE:CZ	2.77	0.72
1:V:6:ASN:O	1:X:280:ILE:HG12	1.90	0.72
1:H:193:ASP:HA	1:H:196:ASP:HB2	1.70	0.71
1:H:179:LEU:HB3	1:H:182:CYS:HB2	1.70	0.71
1:K:179:LEU:HB3	1:K:182:CYS:HB2	1.70	0.71
1:G:179:LEU:HB3	1:G:182:CYS:HB2	1.70	0.71
1:H:11:ILE:O	1:J:273:LYS:CE	2.37	0.71
1:S:376:ALA:HA	1:T:494:ILE:HD12	1.71	0.71
1:K:297:GLN:HB2	1:M:310:ARG:HG2	1.71	0.71
1:R:179:LEU:HB3	1:R:182:CYS:HB2	1.70	0.71
1:A:283:SER:HB3	1:I:3:LEU:CD2	2.21	0.71
1:Q:272:GLU:CG	1:S:352:GLU:HG2	2.21	0.71
1:I:370:GLN:CB	1:I:374:MET:SD	2.78	0.71
1:K:473:GLY:HA3	1:S:191:ALA:HB1	1.73	0.71
1:L:273:LYS:HD3	1:N:11:ILE:O	1.90	0.71
1:R:276:VAL:HG12	1:R:280:ILE:CD1	2.21	0.71
1:P:487:GLY:CA	1:V:229:LYS:CE	2.49	0.71
1:U:315:ASP:CB	1:W:311:ALA:HA	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:GLU:CG	1:N:446:LYS:HE2	2.21	0.71
1:E:179:LEU:HB3	1:E:182:CYS:HB2	1.70	0.71
1:G:193:ASP:HA	1:G:196:ASP:HB2	1.70	0.71
1:O:310:ARG:HG2	1:P:297:GLN:HB2	1.72	0.71
1:L:229:LYS:CG	1:S:487:GLY:HA2	2.20	0.71
1:X:193:ASP:HA	1:X:196:ASP:HB2	1.70	0.71
1:B:179:LEU:HB3	1:B:182:CYS:HB2	1.70	0.70
1:L:273:LYS:CG	1:N:11:ILE:HB	2.21	0.70
1:C:270:PRO:HG2	1:C:273:LYS:CD	2.21	0.70
1:B:297:GLN:HB2	1:C:310:ARG:HG2	1.73	0.70
1:V:3:LEU:CD2	1:X:283:SER:HB3	2.20	0.70
1:H:311:ALA:HB3	1:J:312:GLU:HG3	1.73	0.70
1:K:496:LEU:CD2	1:S:195:VAL:HG22	2.21	0.70
1:Q:270:PRO:HG2	1:Q:273:LYS:CD	2.22	0.70
1:Q:311:ALA:HB1	1:S:312:GLU:HA	1.74	0.70
1:L:242:HIS:CE1	1:N:12:PHE:CZ	2.71	0.70
1:R:276:VAL:O	1:R:280:ILE:HG13	1.91	0.70
1:T:193:ASP:HA	1:T:196:ASP:HB2	1.70	0.70
1:V:7:LEU:HD22	1:X:284:LYS:HG2	1.74	0.70
1:M:491:GLN:HG3	1:N:491:GLN:HG3	1.72	0.70
1:R:370:GLN:CB	1:R:374:MET:SD	2.78	0.70
1:X:456:ARG:NH2	2:X:700:FDP:O1P	2.25	0.70
1:A:270:PRO:HG2	1:A:273:LYS:CD	2.21	0.70
1:R:11:ILE:CD1	1:R:12:PHE:CE2	2.75	0.70
1:S:372:ILE:CG1	1:T:390:GLU:O	2.36	0.70
1:U:390:GLU:OE1	1:V:379:ALA:HB1	1.91	0.70
1:A:135:VAL:HG11	1:A:152:VAL:HG21	1.74	0.70
1:I:11:ILE:CD1	1:I:12:PHE:CE2	2.75	0.70
1:B:373:PRO:HD3	1:O:392:LYS:CD	2.22	0.70
1:R:280:ILE:HG23	1:T:7:LEU:HA	1.74	0.70
1:Q:38:LYS:HE3	1:Q:73:GLU:OE1	1.92	0.70
1:R:38:LYS:HE3	1:R:73:GLU:OE1	1.92	0.70
1:B:135:VAL:HG11	1:B:152:VAL:HG21	1.74	0.70
1:C:38:LYS:HE3	1:C:73:GLU:OE1	1.92	0.70
1:E:11:ILE:CD1	1:E:12:PHE:CE2	2.75	0.70
1:O:38:LYS:HE3	1:O:73:GLU:OE1	1.92	0.70
1:T:38:LYS:HE3	1:T:73:GLU:OE1	1.92	0.70
1:X:135:VAL:HG11	1:X:152:VAL:HG21	1.74	0.70
1:I:38:LYS:HE3	1:I:73:GLU:OE1	1.92	0.69
1:V:11:ILE:CD1	1:V:12:PHE:CE2	2.75	0.69
1:B:270:PRO:HG2	1:B:273:LYS:CD	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:GLU:CD	1:E:103:ARG:HD2	2.12	0.69
1:E:38:LYS:HE3	1:E:73:GLU:OE1	1.92	0.69
1:F:38:LYS:HE3	1:F:73:GLU:OE1	1.92	0.69
1:L:11:ILE:CD1	1:L:12:PHE:CE2	2.75	0.69
1:M:135:VAL:HG11	1:M:152:VAL:HG21	1.74	0.69
1:A:391:THR:C	1:J:373:PRO:HB3	2.13	0.69
1:D:310:ARG:HG2	1:F:297:GLN:OE1	1.92	0.69
1:D:38:LYS:HE3	1:D:73:GLU:OE1	1.92	0.69
1:K:270:PRO:HG2	1:K:273:LYS:CD	2.22	0.69
1:K:383:SER:HB2	1:L:383:SER:HB2	1.74	0.69
1:N:38:LYS:HE3	1:N:73:GLU:OE1	1.92	0.69
1:R:276:VAL:HG11	1:T:9:LEU:HB3	1.74	0.69
1:U:38:LYS:HE3	1:U:73:GLU:OE1	1.92	0.69
1:V:272:GLU:HG3	1:X:352:GLU:HB2	1.73	0.69
1:A:38:LYS:HE3	1:A:73:GLU:OE1	1.92	0.69
1:F:373:PRO:HD3	1:G:392:LYS:HD2	1.75	0.69
1:H:270:PRO:HG2	1:H:273:LYS:CD	2.22	0.69
1:H:456:ARG:NH2	2:H:700:FDP:O1P	2.25	0.69
1:L:38:LYS:HE3	1:L:73:GLU:OE1	1.92	0.69
1:O:297:GLN:HB2	1:P:310:ARG:HG2	1.74	0.69
1:X:38:LYS:HE3	1:X:73:GLU:OE1	1.92	0.69
1:A:3:LEU:HD23	1:I:283:SER:HB3	1.74	0.69
1:B:272:GLU:CG	1:C:352:GLU:HG2	2.23	0.69
1:D:270:PRO:HG2	1:D:273:LYS:CD	2.22	0.69
1:J:38:LYS:HE3	1:J:73:GLU:OE1	1.92	0.69
1:U:270:PRO:HG2	1:U:273:LYS:CD	2.22	0.69
1:V:135:VAL:HG11	1:V:152:VAL:HG21	1.74	0.69
1:H:12:PHE:HZ	1:J:242:HIS:CE1	2.02	0.69
1:K:272:GLU:O	1:M:352:GLU:HG2	1.92	0.69
1:M:456:ARG:NH2	2:M:700:FDP:O1P	2.25	0.69
1:V:276:VAL:HG13	1:X:9:LEU:HD13	1.75	0.69
1:U:297:GLN:CB	1:W:310:ARG:HG2	2.17	0.69
1:W:38:LYS:HE3	1:W:73:GLU:OE1	1.92	0.69
1:J:135:VAL:HG11	1:J:152:VAL:HG21	1.74	0.69
1:O:310:ARG:CG	1:P:297:GLN:HB2	2.22	0.69
1:T:135:VAL:HG11	1:T:152:VAL:HG21	1.74	0.69
1:H:38:LYS:HE3	1:H:73:GLU:OE1	1.92	0.69
1:W:372:ILE:HG13	1:X:390:GLU:O	1.93	0.69
1:G:135:VAL:HG11	1:G:152:VAL:HG21	1.74	0.69
1:O:135:VAL:HG11	1:O:152:VAL:HG21	1.74	0.69
1:O:270:PRO:HG2	1:O:273:LYS:CD	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:456:ARG:NH2	2:P:700:FDP:O1P	2.25	0.69
1:R:135:VAL:HG11	1:R:152:VAL:HG21	1.74	0.69
1:S:38:LYS:HE3	1:S:73:GLU:OE1	1.92	0.69
1:W:456:ARG:NH2	2:W:700:FDP:O1P	2.25	0.69
1:G:38:LYS:HE3	1:G:73:GLU:OE1	1.92	0.69
1:H:11:ILE:HB	1:J:273:LYS:HB3	1.74	0.69
1:H:11:ILE:HD12	1:J:269:ILE:HG12	1.74	0.69
1:H:311:ALA:HB3	1:J:312:GLU:CG	2.23	0.69
1:M:38:LYS:HE3	1:M:73:GLU:OE1	1.92	0.69
1:P:38:LYS:HE3	1:P:73:GLU:OE1	1.92	0.69
1:V:272:GLU:HG2	1:X:352:GLU:HG2	1.73	0.69
1:G:456:ARG:NH2	2:G:700:FDP:O1P	2.25	0.69
1:N:135:VAL:HG11	1:N:152:VAL:HG21	1.74	0.69
1:O:456:ARG:NH2	2:O:700:FDP:O1P	2.25	0.69
1:V:38:LYS:HE3	1:V:73:GLU:OE1	1.92	0.69
1:E:135:VAL:HG11	1:E:152:VAL:HG21	1.74	0.68
1:L:297:GLN:HB2	1:N:310:ARG:CG	2.24	0.68
1:S:372:ILE:CG2	1:T:390:GLU:O	2.42	0.68
1:K:38:LYS:HE3	1:K:73:GLU:OE1	1.92	0.68
1:S:135:VAL:HG11	1:S:152:VAL:HG21	1.74	0.68
1:B:273:LYS:HB3	1:C:11:ILE:HB	1.75	0.68
1:K:297:GLN:HB2	1:M:310:ARG:CG	2.23	0.68
1:P:135:VAL:HG11	1:P:152:VAL:HG21	1.74	0.68
1:V:297:GLN:HE21	1:V:300:GLU:CD	1.97	0.68
1:B:38:LYS:HE3	1:B:73:GLU:OE1	1.92	0.68
1:L:456:ARG:NH2	2:L:700:FDP:O1P	2.25	0.68
1:Q:135:VAL:HG11	1:Q:152:VAL:HG21	1.74	0.68
1:F:392:LYS:HD2	1:G:373:PRO:HD3	1.74	0.68
1:H:135:VAL:HG11	1:H:152:VAL:HG21	1.74	0.68
1:V:242:HIS:CE1	1:X:12:PHE:HE2	2.06	0.68
1:K:456:ARG:NH2	2:K:700:FDP:O1P	2.25	0.68
1:L:11:ILE:HG13	1:L:12:PHE:CE2	2.29	0.68
1:R:372:ILE:HD12	1:R:374:MET:HG3	1.75	0.68
1:W:135:VAL:HG11	1:W:152:VAL:HG21	1.74	0.68
1:F:135:VAL:HG11	1:F:152:VAL:HG21	1.74	0.68
1:I:135:VAL:HG11	1:I:152:VAL:HG21	1.74	0.68
1:C:390:GLU:O	1:P:372:ILE:HG23	1.92	0.68
1:Q:269:ILE:HG12	1:S:11:ILE:CD1	2.22	0.68
1:S:483:HIS:HD2	1:T:483:HIS:NE2	1.90	0.68
1:K:279:LYS:HE3	1:M:6:ASN:OD1	1.94	0.68
1:U:135:VAL:HG11	1:U:152:VAL:HG21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:371:HIS:CD2	1:U:373:PRO:O	2.47	0.68
1:V:11:ILE:HG13	1:V:12:PHE:CE2	2.29	0.68
1:L:135:VAL:HG11	1:L:152:VAL:HG21	1.74	0.68
1:R:297:GLN:CG	1:T:310:ARG:CG	2.71	0.68
1:V:456:ARG:NH2	2:V:700:FDP:O1P	2.25	0.68
1:B:297:GLN:OE1	1:C:310:ARG:CG	2.39	0.67
1:T:456:ARG:NH2	2:T:700:FDP:O1P	2.25	0.67
1:U:242:HIS:NE2	1:W:12:PHE:HE2	1.93	0.67
1:L:12:PHE:CE2	1:N:242:HIS:CE1	2.82	0.67
1:N:446:LYS:C	1:N:446:LYS:HD2	2.14	0.67
1:R:296:THR:HG22	1:R:297:GLN:CG	2.25	0.67
1:Q:12:PHE:HE2	1:S:242:HIS:HE1	1.40	0.67
1:C:135:VAL:HG11	1:C:152:VAL:HG21	1.74	0.67
1:H:370:GLN:CB	1:H:374:MET:SD	2.82	0.67
1:A:390:GLU:O	1:J:373:PRO:HA	1.94	0.67
1:C:391:THR:HA	1:P:373:PRO:HB3	1.75	0.67
1:S:383:SER:HB2	1:T:383:SER:HB2	1.76	0.67
1:D:135:VAL:HG11	1:D:152:VAL:HG21	1.74	0.67
1:A:371:HIS:CD2	1:A:373:PRO:O	2.48	0.67
1:D:390:GLU:O	1:E:373:PRO:HA	1.94	0.67
1:L:283:SER:HB3	1:N:3:LEU:HD21	1.71	0.67
1:W:371:HIS:CD2	1:W:373:PRO:O	2.48	0.67
1:X:371:HIS:CD2	1:X:373:PRO:O	2.48	0.67
1:B:371:HIS:CD2	1:B:373:PRO:O	2.48	0.67
1:C:371:HIS:CD2	1:C:373:PRO:O	2.48	0.67
1:L:273:LYS:HB3	1:N:11:ILE:HB	1.77	0.67
1:K:392:LYS:HD2	1:L:373:PRO:HD3	1.77	0.67
1:H:263:GLY:HA2	1:J:310:ARG:HH11	1.60	0.67
1:C:254:GLU:HG2	1:N:446:LYS:CE	2.24	0.67
1:R:11:ILE:HG13	1:R:12:PHE:CE2	2.29	0.67
1:V:283:SER:HB3	1:X:3:LEU:CG	2.25	0.67
1:D:373:PRO:HD3	1:E:392:LYS:HD2	1.76	0.67
1:J:371:HIS:CD2	1:J:373:PRO:O	2.48	0.67
1:K:135:VAL:HG11	1:K:152:VAL:HG21	1.74	0.67
1:L:280:ILE:HD11	1:N:9:LEU:HB2	1.76	0.67
1:N:371:HIS:CD2	1:N:373:PRO:O	2.48	0.66
1:U:311:ALA:CB	1:W:312:GLU:HA	2.19	0.66
1:L:272:GLU:CB	1:N:352:GLU:HG2	2.24	0.66
1:S:491:GLN:HG3	1:T:491:GLN:CG	2.24	0.66
1:V:371:HIS:CD2	1:V:373:PRO:O	2.48	0.66
1:H:53:SER:OG	1:H:85:LYS:HA	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:371:HIS:CD2	1:K:373:PRO:O	2.48	0.66
1:F:371:HIS:CD2	1:F:373:PRO:O	2.48	0.66
1:F:391:THR:HA	1:G:373:PRO:CB	2.25	0.66
1:H:310:ARG:CG	1:J:297:GLN:HG3	2.22	0.66
1:L:53:SER:OG	1:L:85:LYS:HA	1.96	0.66
1:S:373:PRO:HB3	1:T:391:THR:C	2.16	0.66
1:U:242:HIS:HE1	1:W:12:PHE:CE2	1.85	0.66
1:G:53:SER:OG	1:G:85:LYS:HA	1.96	0.66
1:R:53:SER:OG	1:R:85:LYS:HA	1.96	0.66
1:R:279:LYS:HB3	1:T:6:ASN:OD1	1.95	0.66
1:V:12:PHE:CZ	1:X:242:HIS:NE2	2.63	0.66
1:V:3:LEU:HD23	1:X:283:SER:CB	2.26	0.66
1:D:53:SER:OG	1:D:85:LYS:HA	1.96	0.66
1:E:371:HIS:CD2	1:E:373:PRO:O	2.48	0.66
1:F:53:SER:OG	1:F:85:LYS:HA	1.96	0.66
1:L:352:GLU:HG2	1:N:272:GLU:O	1.96	0.66
1:O:12:PHE:HZ	1:P:242:HIS:HE1	1.42	0.66
1:Q:371:HIS:CD2	1:Q:373:PRO:O	2.48	0.66
1:X:53:SER:OG	1:X:85:LYS:HA	1.96	0.66
1:D:371:HIS:CD2	1:D:373:PRO:O	2.48	0.66
1:O:371:HIS:CD2	1:O:373:PRO:O	2.48	0.66
1:C:53:SER:OG	1:C:85:LYS:HA	1.96	0.66
1:F:373:PRO:HB3	1:G:391:THR:C	2.16	0.66
1:H:352:GLU:HG2	1:J:272:GLU:C	2.16	0.66
1:L:279:LYS:HE3	1:N:6:ASN:OD1	1.96	0.66
1:S:53:SER:OG	1:S:85:LYS:HA	1.96	0.66
1:R:283:SER:HB3	1:T:3:LEU:HG	1.77	0.66
1:A:53:SER:OG	1:A:85:LYS:HA	1.96	0.66
1:C:250:SER:HB3	1:N:446:LYS:HG2	1.71	0.66
1:E:283:SER:OG	1:G:3:LEU:HD23	1.97	0.65
1:M:53:SER:OG	1:M:85:LYS:HA	1.96	0.65
1:U:11:ILE:O	1:W:273:LYS:CD	2.45	0.65
1:B:144:ASP:O	1:B:145:ASP:CB	2.45	0.65
1:E:11:ILE:HG13	1:E:12:PHE:CE2	2.29	0.65
1:E:53:SER:OG	1:E:85:LYS:HA	1.96	0.65
1:N:53:SER:OG	1:N:85:LYS:HA	1.96	0.65
1:V:269:ILE:HG12	1:X:11:ILE:CD1	2.27	0.65
1:W:53:SER:OG	1:W:85:LYS:HA	1.96	0.65
1:A:242:HIS:HE1	1:I:12:PHE:CE2	2.10	0.65
1:B:272:GLU:O	1:C:352:GLU:HG2	1.96	0.65
1:H:352:GLU:HB2	1:J:272:GLU:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:53:SER:OG	1:I:85:LYS:HA	1.96	0.65
1:T:53:SER:OG	1:T:85:LYS:HA	1.96	0.65
1:U:390:GLU:O	1:V:373:PRO:CA	2.44	0.65
1:A:3:LEU:CD2	1:I:283:SER:CB	2.74	0.65
1:V:144:ASP:O	1:V:145:ASP:CB	2.45	0.65
1:W:144:ASP:O	1:W:145:ASP:CB	2.45	0.65
1:E:312:GLU:HA	1:G:311:ALA:HB1	1.78	0.65
1:G:371:HIS:CD2	1:G:373:PRO:O	2.48	0.65
1:H:144:ASP:O	1:H:145:ASP:CB	2.45	0.65
1:J:53:SER:OG	1:J:85:LYS:HA	1.96	0.65
1:O:242:HIS:CE1	1:P:12:PHE:CE2	2.84	0.65
1:U:315:ASP:CG	1:W:311:ALA:HA	2.16	0.65
1:A:144:ASP:O	1:A:145:ASP:CB	2.45	0.65
1:O:53:SER:OG	1:O:85:LYS:HA	1.96	0.65
1:R:269:ILE:CG1	1:T:11:ILE:CD1	2.65	0.65
1:K:53:SER:OG	1:K:85:LYS:HA	1.96	0.65
1:Q:144:ASP:O	1:Q:145:ASP:CB	2.45	0.65
1:Q:373:PRO:CB	1:R:390:GLU:O	2.45	0.65
1:V:297:GLN:HE22	1:V:300:GLU:HG2	1.62	0.65
1:D:144:ASP:O	1:D:145:ASP:CB	2.45	0.65
1:O:311:ALA:CB	1:P:312:GLU:HA	2.23	0.65
1:P:53:SER:OG	1:P:85:LYS:HA	1.96	0.65
1:Q:53:SER:OG	1:Q:85:LYS:HA	1.96	0.65
1:U:372:ILE:CG2	1:V:390:GLU:O	2.43	0.65
1:B:53:SER:OG	1:B:85:LYS:HA	1.96	0.65
1:H:11:ILE:HB	1:J:273:LYS:CB	2.27	0.65
1:R:3:LEU:HD13	1:T:369:LEU:CD1	2.26	0.65
1:T:371:HIS:CD2	1:T:373:PRO:O	2.49	0.65
1:V:370:GLN:HB3	1:V:374:MET:SD	2.37	0.65
1:Q:390:GLU:CA	1:R:372:ILE:HG13	2.24	0.64
1:U:53:SER:OG	1:U:85:LYS:HA	1.96	0.64
1:V:269:ILE:CG1	1:X:11:ILE:HD12	2.27	0.64
1:T:214:ARG:N	1:T:218:GLN:HE22	1.96	0.64
1:Q:383:SER:HB2	1:R:383:SER:HB2	1.79	0.64
1:R:144:ASP:O	1:R:145:ASP:CB	2.45	0.64
1:X:370:GLN:HB3	1:X:374:MET:SD	2.37	0.64
1:F:144:ASP:O	1:F:145:ASP:CB	2.45	0.64
1:G:370:GLN:HB3	1:G:374:MET:SD	2.38	0.64
1:K:370:GLN:HB3	1:K:374:MET:SD	2.37	0.64
1:L:269:ILE:CG1	1:N:11:ILE:HD12	2.27	0.64
1:U:245:VAL:HG11	1:W:11:ILE:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLU:HG3	1:C:352:GLU:CB	2.26	0.64
1:M:214:ARG:N	1:M:218:GLN:HE22	1.96	0.64
1:L:310:ARG:HG2	1:N:297:GLN:HB2	1.78	0.64
1:Q:370:GLN:HB3	1:Q:374:MET:SD	2.38	0.64
1:X:214:ARG:N	1:X:218:GLN:HE22	1.96	0.64
1:B:370:GLN:HB3	1:B:374:MET:SD	2.38	0.64
1:C:214:ARG:N	1:C:218:GLN:HE22	1.96	0.64
1:D:370:GLN:HB3	1:D:374:MET:SD	2.38	0.64
1:N:370:GLN:HB3	1:N:374:MET:SD	2.37	0.64
1:R:273:LYS:CD	1:T:11:ILE:O	2.42	0.64
1:Q:373:PRO:CA	1:R:390:GLU:O	2.46	0.64
1:Q:272:GLU:HG3	1:S:352:GLU:CB	2.27	0.64
1:U:11:ILE:HB	1:W:273:LYS:CB	2.27	0.64
1:V:53:SER:OG	1:V:85:LYS:HA	1.96	0.64
1:W:370:GLN:HB3	1:W:374:MET:SD	2.37	0.64
1:O:370:GLN:HB3	1:O:374:MET:SD	2.37	0.64
1:S:390:GLU:OE1	1:T:379:ALA:HB2	1.98	0.64
1:U:310:ARG:NH2	1:W:297:GLN:OE1	2.30	0.64
1:E:370:GLN:HB3	1:E:374:MET:SD	2.37	0.64
1:I:371:HIS:CD2	1:I:373:PRO:O	2.50	0.64
1:E:144:ASP:O	1:E:145:ASP:CB	2.45	0.64
1:F:370:GLN:HB3	1:F:374:MET:SD	2.38	0.64
1:K:373:PRO:CA	1:L:390:GLU:O	2.42	0.64
1:K:373:PRO:CB	1:L:391:THR:HA	2.25	0.64
1:W:214:ARG:N	1:W:218:GLN:HE22	1.96	0.64
1:A:370:GLN:HB3	1:A:374:MET:SD	2.38	0.64
1:B:214:ARG:N	1:B:218:GLN:HE22	1.96	0.64
1:C:370:GLN:HB3	1:C:374:MET:SD	2.37	0.64
1:H:214:ARG:N	1:H:218:GLN:HE22	1.96	0.64
1:J:214:ARG:N	1:J:218:GLN:HE22	1.96	0.64
1:Q:6:ASN:O	1:S:280:ILE:HG12	1.98	0.64
1:U:214:ARG:N	1:U:218:GLN:HE22	1.96	0.64
1:T:144:ASP:O	1:T:145:ASP:CB	2.45	0.63
1:E:297:GLN:OE1	1:G:310:ARG:CG	2.35	0.63
1:Q:214:ARG:N	1:Q:218:GLN:HE22	1.95	0.63
1:A:214:ARG:N	1:A:218:GLN:HE22	1.96	0.63
1:O:11:ILE:CA	1:P:273:LYS:HG2	2.28	0.63
1:V:214:ARG:N	1:V:218:GLN:HE22	1.96	0.63
1:F:214:ARG:N	1:F:218:GLN:HE22	1.96	0.63
1:F:391:THR:CA	1:G:373:PRO:HB3	2.29	0.63
1:H:297:GLN:HB2	1:J:310:ARG:CB	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:THR:HG22	1:J:492:THR:HG22	1.79	0.63
1:L:311:ALA:CB	1:N:312:GLU:HA	2.28	0.63
1:G:214:ARG:N	1:G:218:GLN:HE22	1.96	0.63
1:I:371:HIS:O	1:I:374:MET:CG	2.41	0.63
1:J:370:GLN:HB3	1:J:374:MET:SD	2.37	0.63
1:M:370:GLN:CB	1:M:374:MET:SD	2.86	0.63
1:R:214:ARG:N	1:R:218:GLN:HE22	1.96	0.63
1:P:195:VAL:CG2	1:U:496:LEU:CD2	2.73	0.63
1:L:272:GLU:CG	1:N:352:GLU:CG	2.76	0.63
1:P:214:ARG:N	1:P:218:GLN:HE22	1.96	0.63
1:D:214:ARG:N	1:D:218:GLN:HE22	1.96	0.63
1:K:214:ARG:N	1:K:218:GLN:HE22	1.96	0.63
1:L:9:LEU:HB2	1:N:280:ILE:HD11	1.81	0.63
1:L:11:ILE:HD12	1:N:269:ILE:HG12	1.80	0.63
1:X:144:ASP:O	1:X:145:ASP:CB	2.45	0.63
1:H:315:ASP:CG	1:J:311:ALA:HA	2.19	0.63
1:O:144:ASP:O	1:O:145:ASP:CB	2.45	0.63
1:O:214:ARG:N	1:O:218:GLN:HE22	1.96	0.63
1:P:487:GLY:CA	1:V:229:LYS:HD2	2.27	0.63
1:V:7:LEU:HD23	1:X:284:LYS:HG3	1.80	0.63
1:B:272:GLU:C	1:C:352:GLU:HG2	2.20	0.62
1:L:214:ARG:N	1:L:218:GLN:HE22	1.96	0.62
1:S:214:ARG:N	1:S:218:GLN:HE22	1.96	0.62
1:E:11:ILE:CD1	1:E:12:PHE:HE2	2.12	0.62
1:I:11:ILE:HG13	1:I:12:PHE:CE2	2.29	0.62
1:I:214:ARG:N	1:I:218:GLN:HE22	1.96	0.62
1:K:456:ARG:NH1	2:K:700:FDP:O2P	2.28	0.62
1:M:373:PRO:HB3	1:N:391:THR:HA	1.80	0.62
1:P:144:ASP:O	1:P:145:ASP:CB	2.45	0.62
1:F:372:ILE:HD11	1:G:390:GLU:HG2	1.81	0.62
1:H:372:ILE:HD12	1:H:374:MET:HG3	1.81	0.62
1:G:144:ASP:O	1:G:145:ASP:CB	2.45	0.62
1:K:310:ARG:HG2	1:M:297:GLN:HB2	1.80	0.62
1:S:371:HIS:CD2	1:S:373:PRO:O	2.53	0.62
1:H:372:ILE:CG2	1:I:390:GLU:O	2.43	0.62
1:L:370:GLN:CB	1:L:374:MET:SD	2.87	0.62
1:H:273:LYS:HB3	1:J:11:ILE:HB	1.82	0.62
1:O:315:ASP:HB2	1:P:311:ALA:HA	1.82	0.62
1:P:371:HIS:CD2	1:P:373:PRO:O	2.53	0.62
1:P:456:ARG:NH1	2:P:700:FDP:O2P	2.28	0.62
1:L:310:ARG:HG2	1:N:297:GLN:OE1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:144:ASP:O	1:L:145:ASP:CB	2.45	0.62
1:N:214:ARG:N	1:N:218:GLN:HE22	1.96	0.62
1:Q:372:ILE:HD11	1:Q:374:MET:HE1	1.81	0.62
1:R:276:VAL:CG1	1:R:280:ILE:HD11	2.27	0.62
1:L:242:HIS:NE2	1:N:12:PHE:HE2	1.98	0.61
1:B:283:SER:OG	1:C:3:LEU:HD23	1.99	0.61
1:K:269:ILE:HG12	1:M:11:ILE:HD12	1.82	0.61
1:S:144:ASP:O	1:S:145:ASP:CB	2.45	0.61
1:L:283:SER:HB3	1:N:3:LEU:HD22	1.79	0.61
1:D:492:THR:HG22	1:E:492:THR:HG22	1.83	0.61
1:H:315:ASP:HB2	1:J:311:ALA:CA	2.30	0.61
1:C:250:SER:HB2	1:N:446:LYS:HG2	0.69	0.61
1:V:456:ARG:NH1	2:V:700:FDP:O2P	2.28	0.61
1:C:390:GLU:HA	1:P:372:ILE:CG1	2.15	0.61
1:E:214:ARG:N	1:E:218:GLN:HE22	1.96	0.61
1:C:391:THR:C	1:P:373:PRO:HB3	2.21	0.61
1:Q:270:PRO:HG2	1:Q:273:LYS:HE2	1.83	0.61
1:V:272:GLU:HG3	1:X:352:GLU:CB	2.30	0.61
1:V:7:LEU:CD2	1:X:284:LYS:HG2	2.30	0.61
1:H:352:GLU:CG	1:J:272:GLU:O	2.49	0.61
1:S:373:PRO:CA	1:T:390:GLU:O	2.37	0.61
1:S:491:GLN:HG3	1:T:491:GLN:CD	2.21	0.61
1:V:297:GLN:NE2	1:V:300:GLU:CD	2.53	0.61
1:B:270:PRO:HG2	1:B:273:LYS:HE2	1.83	0.61
1:C:250:SER:CB	1:N:446:LYS:CG	2.46	0.61
1:L:11:ILE:CD1	1:L:12:PHE:HE2	2.12	0.61
1:P:370:GLN:CB	1:P:374:MET:SD	2.88	0.61
1:U:270:PRO:HG2	1:U:273:LYS:HE2	1.83	0.61
1:U:352:GLU:HG2	1:W:272:GLU:CB	2.30	0.61
1:U:310:ARG:CZ	1:W:297:GLN:OE1	2.49	0.61
1:E:11:ILE:HB	1:G:273:LYS:HG2	1.82	0.61
1:H:279:LYS:HE3	1:J:6:ASN:OD1	2.01	0.61
1:J:144:ASP:O	1:J:145:ASP:CB	2.45	0.61
1:K:373:PRO:HB3	1:L:391:THR:CA	2.26	0.61
1:O:456:ARG:NH1	2:O:700:FDP:O2P	2.28	0.61
1:R:287:VAL:HG23	1:T:3:LEU:HD11	1.83	0.61
1:M:456:ARG:NH1	2:M:700:FDP:O2P	2.28	0.61
1:T:456:ARG:NH1	2:T:700:FDP:O2P	2.28	0.61
1:B:103:ARG:HD2	1:G:58:GLU:OE1	2.01	0.60
1:Q:456:ARG:NH2	2:Q:700:FDP:O1P	2.34	0.60
1:D:400:SER:HB2	1:D:405:SER:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:ALA:HB1	1:G:312:GLU:HA	1.82	0.60
1:H:270:PRO:HG2	1:H:273:LYS:HE2	1.83	0.60
1:N:446:LYS:O	1:N:446:LYS:HD3	2.00	0.60
1:V:7:LEU:HD22	1:X:284:LYS:CG	2.28	0.60
1:D:270:PRO:HG2	1:D:273:LYS:HE2	1.83	0.60
1:N:456:ARG:NH2	2:N:700:FDP:O1P	2.34	0.60
1:O:400:SER:HB2	1:O:405:SER:HB2	1.83	0.60
1:Q:400:SER:HB2	1:Q:405:SER:HB2	1.84	0.60
1:K:270:PRO:HG2	1:K:273:LYS:HE2	1.83	0.60
1:M:400:SER:HB2	1:M:405:SER:HB2	1.83	0.60
1:O:270:PRO:HG2	1:O:273:LYS:HE2	1.83	0.60
1:B:272:GLU:CB	1:C:352:GLU:HG2	2.30	0.60
1:C:58:GLU:OE1	1:E:103:ARG:HD2	2.02	0.60
1:E:472:THR:CG2	1:E:498:GLU:C	2.70	0.60
1:H:296:THR:HG22	1:H:297:GLN:HG2	1.83	0.60
1:N:472:THR:CG2	1:N:498:GLU:C	2.70	0.60
1:T:472:THR:CG2	1:T:498:GLU:C	2.70	0.60
1:U:390:GLU:O	1:V:373:PRO:HA	2.02	0.60
1:U:372:ILE:HG13	1:V:390:GLU:O	2.01	0.60
1:V:242:HIS:NE2	1:X:12:PHE:HE2	1.99	0.60
1:X:472:THR:CG2	1:X:498:GLU:C	2.70	0.60
1:F:490:ASN:H	1:F:490:ASN:HD22	1.50	0.60
1:E:242:HIS:CE1	1:G:12:PHE:HE2	2.17	0.60
1:H:400:SER:HB2	1:H:405:SER:HB2	1.84	0.60
1:K:400:SER:HB2	1:K:405:SER:HB2	1.84	0.60
1:L:400:SER:HB2	1:L:405:SER:HB2	1.84	0.60
1:S:490:ASN:H	1:S:490:ASN:HD22	1.50	0.60
1:T:400:SER:HB2	1:T:405:SER:HB2	1.83	0.60
1:A:242:HIS:NE2	1:I:12:PHE:HZ	1.99	0.60
1:A:270:PRO:HG2	1:A:273:LYS:HE2	1.83	0.60
1:A:472:THR:CG2	1:A:498:GLU:C	2.70	0.60
1:D:212:PHE:CE1	1:D:241:ASN:ND2	2.70	0.60
1:E:212:PHE:CE1	1:E:241:ASN:ND2	2.70	0.60
1:G:400:SER:HB2	1:G:405:SER:HB2	1.83	0.60
1:G:472:THR:CG2	1:G:498:GLU:C	2.70	0.60
1:O:490:ASN:HD22	1:O:490:ASN:H	1.50	0.60
1:W:212:PHE:CE1	1:W:241:ASN:ND2	2.70	0.60
1:W:472:THR:CG2	1:W:498:GLU:C	2.70	0.60
1:F:472:THR:CG2	1:F:498:GLU:C	2.70	0.60
1:J:472:THR:CG2	1:J:498:GLU:C	2.70	0.60
1:L:276:VAL:CG1	1:N:9:LEU:HB3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:472:THR:CG2	1:P:498:GLU:C	2.70	0.60
1:R:472:THR:CG2	1:R:498:GLU:C	2.70	0.60
1:U:144:ASP:O	1:U:145:ASP:CB	2.45	0.60
1:U:12:PHE:CZ	1:W:242:HIS:CE1	2.84	0.60
1:W:490:ASN:H	1:W:490:ASN:HD22	1.50	0.60
1:B:103:ARG:HB3	1:G:58:GLU:OE1	2.02	0.60
1:B:472:THR:CG2	1:B:498:GLU:C	2.70	0.60
1:D:456:ARG:NH2	2:D:700:FDP:O1P	2.34	0.60
1:E:11:ILE:O	1:G:273:LYS:HE3	2.01	0.60
1:H:472:THR:CG2	1:H:498:GLU:C	2.70	0.60
1:H:390:GLU:O	1:I:373:PRO:CA	2.48	0.60
1:J:490:ASN:H	1:J:490:ASN:HD22	1.50	0.60
1:N:472:THR:HG22	1:N:498:GLU:C	2.22	0.60
1:P:212:PHE:CE1	1:P:241:ASN:ND2	2.70	0.60
1:R:400:SER:HB2	1:R:405:SER:HB2	1.84	0.60
1:S:372:ILE:CG1	1:T:390:GLU:HG2	2.32	0.60
1:U:383:SER:HB2	1:V:383:SER:HB2	1.81	0.60
1:V:472:THR:CG2	1:V:498:GLU:C	2.70	0.60
1:C:270:PRO:HG2	1:C:273:LYS:HE2	1.83	0.60
1:C:456:ARG:NH2	2:C:700:FDP:O1P	2.34	0.60
1:F:456:ARG:NH2	2:F:700:FDP:O1P	2.35	0.60
1:J:456:ARG:NH2	2:J:700:FDP:O1P	2.34	0.60
1:M:490:ASN:HD22	1:M:490:ASN:H	1.50	0.60
1:O:472:THR:CG2	1:O:498:GLU:C	2.70	0.60
1:P:400:SER:HB2	1:P:405:SER:HB2	1.83	0.60
1:R:11:ILE:CD1	1:R:12:PHE:HE2	2.12	0.60
1:R:297:GLN:CG	1:T:310:ARG:HG2	2.32	0.60
1:P:195:VAL:CG2	1:U:496:LEU:CG	2.68	0.60
1:B:147:ILE:CG2	1:B:169:HIS:CD2	2.85	0.59
1:C:400:SER:HB2	1:C:405:SER:HB2	1.84	0.59
1:C:490:ASN:H	1:C:490:ASN:HD22	1.50	0.59
1:F:400:SER:HB2	1:F:405:SER:HB2	1.83	0.59
1:I:472:THR:CG2	1:I:498:GLU:C	2.70	0.59
1:L:472:THR:CG2	1:L:498:GLU:C	2.70	0.59
1:Q:3:LEU:HD23	1:S:283:SER:HB3	1.84	0.59
1:U:472:THR:CG2	1:U:498:GLU:C	2.70	0.59
1:X:456:ARG:HH22	2:X:700:FDP:P1	2.25	0.59
1:A:490:ASN:HD22	1:A:490:ASN:H	1.50	0.59
1:C:212:PHE:CE1	1:C:241:ASN:ND2	2.70	0.59
1:H:147:ILE:CG2	1:H:169:HIS:CD2	2.85	0.59
1:O:147:ILE:CG2	1:O:169:HIS:CD2	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:472:THR:HG22	1:O:498:GLU:C	2.23	0.59
1:R:276:VAL:HG13	1:T:9:LEU:CD1	2.32	0.59
1:U:311:ALA:HB1	1:W:312:GLU:CA	2.21	0.59
1:V:147:ILE:CG2	1:V:169:HIS:CD2	2.85	0.59
1:V:297:GLN:NE2	1:V:300:GLU:HB2	2.05	0.59
1:V:456:ARG:HH22	2:V:700:FDP:P1	2.25	0.59
1:V:490:ASN:H	1:V:490:ASN:HD22	1.50	0.59
1:X:400:SER:HB2	1:X:405:SER:HB2	1.83	0.59
1:X:456:ARG:NH1	2:X:700:FDP:O2P	2.28	0.59
1:B:400:SER:HB2	1:B:405:SER:HB2	1.83	0.59
1:C:144:ASP:O	1:C:145:ASP:CB	2.45	0.59
1:G:147:ILE:CG2	1:G:169:HIS:CD2	2.86	0.59
1:J:472:THR:HG22	1:J:498:GLU:C	2.23	0.59
1:M:147:ILE:CG2	1:M:169:HIS:CD2	2.86	0.59
1:M:472:THR:HG22	1:M:498:GLU:C	2.23	0.59
1:U:147:ILE:CG2	1:U:169:HIS:CD2	2.85	0.59
1:U:400:SER:HB2	1:U:405:SER:HB2	1.84	0.59
1:V:400:SER:HB2	1:V:405:SER:HB2	1.84	0.59
1:D:472:THR:HG22	1:D:498:GLU:C	2.22	0.59
1:E:400:SER:HB2	1:E:405:SER:HB2	1.84	0.59
1:F:472:THR:HG22	1:F:498:GLU:C	2.23	0.59
1:I:147:ILE:CG2	1:I:169:HIS:CD2	2.85	0.59
1:I:404:ARG:CZ	1:M:228:PRO:HG2	2.31	0.59
1:K:490:ASN:HD22	1:K:490:ASN:H	1.50	0.59
1:Q:297:GLN:HB2	1:S:310:ARG:CG	2.32	0.59
1:S:456:ARG:NH2	2:S:700:FDP:O1P	2.34	0.59
1:T:472:THR:HG22	1:T:498:GLU:C	2.23	0.59
1:V:472:THR:HG22	1:V:498:GLU:C	2.23	0.59
1:C:472:THR:CG2	1:C:498:GLU:C	2.70	0.59
1:D:472:THR:CG2	1:D:498:GLU:C	2.70	0.59
1:F:212:PHE:CE1	1:F:241:ASN:ND2	2.70	0.59
1:H:472:THR:HG22	1:H:498:GLU:C	2.23	0.59
1:L:371:HIS:CD2	1:L:373:PRO:O	2.55	0.59
1:P:490:ASN:HD22	1:P:490:ASN:H	1.50	0.59
1:S:383:SER:HB2	1:T:383:SER:CB	2.33	0.59
1:A:147:ILE:CG2	1:A:169:HIS:CD2	2.85	0.59
1:A:456:ARG:NH2	2:A:700:FDP:O1P	2.34	0.59
1:B:272:GLU:CG	1:C:352:GLU:CG	2.79	0.59
1:G:456:ARG:NH1	2:G:700:FDP:O2P	2.28	0.59
1:I:11:ILE:CD1	1:I:12:PHE:HE2	2.12	0.59
1:H:352:GLU:HG2	1:J:272:GLU:CB	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:352:GLU:HG2	1:M:272:GLU:O	2.03	0.59
1:K:472:THR:CG2	1:K:498:GLU:C	2.70	0.59
1:L:490:ASN:HD22	1:L:490:ASN:H	1.50	0.59
1:M:472:THR:CG2	1:M:498:GLU:C	2.70	0.59
1:Q:147:ILE:CG2	1:Q:169:HIS:CD2	2.85	0.59
1:Q:472:THR:CG2	1:Q:498:GLU:C	2.70	0.59
1:Q:472:THR:HG22	1:Q:498:GLU:C	2.23	0.59
1:S:147:ILE:CG2	1:S:169:HIS:CD2	2.85	0.59
1:S:370:GLN:CB	1:S:374:MET:SD	2.90	0.59
1:U:456:ARG:NH2	2:U:700:FDP:O1P	2.35	0.59
1:A:400:SER:HB2	1:A:405:SER:HB2	1.83	0.59
1:B:311:ALA:CB	1:C:312:GLU:HA	2.32	0.59
1:E:456:ARG:NH2	2:E:700:FDP:O1P	2.34	0.59
1:F:147:ILE:CG2	1:F:169:HIS:CD2	2.85	0.59
1:H:371:HIS:O	1:H:374:MET:CG	2.36	0.59
1:K:212:PHE:CE1	1:K:241:ASN:ND2	2.70	0.59
1:K:311:ALA:CB	1:M:312:GLU:HA	2.32	0.59
1:K:456:ARG:HH22	2:K:700:FDP:P1	2.26	0.59
1:L:147:ILE:CG2	1:L:169:HIS:CD2	2.86	0.59
1:L:472:THR:HG22	1:L:498:GLU:C	2.22	0.59
1:L:272:GLU:HG3	1:N:352:GLU:CG	2.33	0.59
1:O:456:ARG:HH22	2:O:700:FDP:P1	2.25	0.59
1:P:147:ILE:CG2	1:P:169:HIS:CD2	2.86	0.59
1:P:456:ARG:HH22	2:P:700:FDP:P1	2.26	0.59
1:R:147:ILE:CG2	1:R:169:HIS:CD2	2.85	0.59
1:W:147:ILE:CG2	1:W:169:HIS:CD2	2.85	0.59
1:X:472:THR:HG22	1:X:498:GLU:C	2.23	0.59
1:C:373:PRO:CB	1:P:390:GLU:O	2.51	0.59
1:H:383:SER:HB2	1:I:383:SER:CB	2.29	0.59
1:L:273:LYS:CB	1:N:11:ILE:HB	2.33	0.59
1:L:270:PRO:CG	1:L:273:LYS:HE2	2.23	0.59
1:O:242:HIS:HE1	1:P:12:PHE:CE2	2.20	0.59
1:Q:372:ILE:HD11	1:Q:374:MET:CE	2.33	0.59
1:S:400:SER:HB2	1:S:405:SER:HB2	1.84	0.59
1:T:490:ASN:H	1:T:490:ASN:HD22	1.50	0.59
1:S:491:GLN:CD	1:T:491:GLN:NE2	2.56	0.59
1:W:472:THR:HG22	1:W:498:GLU:C	2.23	0.59
1:B:372:ILE:HD11	1:B:374:MET:CE	2.33	0.59
1:B:490:ASN:H	1:B:490:ASN:HD22	1.50	0.59
1:G:456:ARG:HH22	2:G:700:FDP:P1	2.26	0.59
1:J:400:SER:HB2	1:J:405:SER:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:212:PHE:CE1	1:U:241:ASN:ND2	2.70	0.59
1:U:365:SER:HB3	1:W:3:LEU:HD12	1.84	0.59
1:W:372:ILE:HD11	1:W:374:MET:CE	2.33	0.59
1:W:400:SER:HB2	1:W:405:SER:HB2	1.84	0.59
1:I:490:ASN:H	1:I:490:ASN:HD22	1.50	0.59
1:J:372:ILE:HD11	1:J:374:MET:CE	2.33	0.59
1:K:147:ILE:CG2	1:K:169:HIS:CD2	2.86	0.59
1:K:372:ILE:HD11	1:K:374:MET:CE	2.33	0.59
1:L:229:LYS:HE3	1:S:487:GLY:CA	2.33	0.59
1:L:456:ARG:NH1	2:L:700:FDP:O2P	2.29	0.59
1:M:371:HIS:CD2	1:M:373:PRO:O	2.55	0.59
1:M:456:ARG:HH22	2:M:700:FDP:P1	2.26	0.59
1:R:272:GLU:HG2	1:T:352:GLU:CG	2.21	0.59
1:S:472:THR:CG2	1:S:498:GLU:C	2.70	0.59
1:U:352:GLU:HG2	1:W:272:GLU:HB2	1.85	0.59
1:E:272:GLU:CG	1:G:352:GLU:HG2	2.32	0.58
1:N:372:ILE:HD11	1:N:374:MET:CE	2.33	0.58
1:P:472:THR:HG22	1:P:498:GLU:C	2.23	0.58
1:R:490:ASN:HD22	1:R:490:ASN:H	1.50	0.58
1:E:270:PRO:CG	1:E:273:LYS:HE2	2.24	0.58
1:H:311:ALA:CB	1:J:312:GLU:CG	2.81	0.58
1:N:147:ILE:CG2	1:N:169:HIS:CD2	2.85	0.58
1:U:472:THR:HG22	1:U:498:GLU:C	2.23	0.58
1:V:372:ILE:HD11	1:V:374:MET:CE	2.33	0.58
1:W:372:ILE:CG1	1:X:390:GLU:HA	2.23	0.58
1:A:472:THR:HG22	1:A:498:GLU:C	2.22	0.58
1:C:472:THR:HG22	1:C:498:GLU:C	2.23	0.58
1:E:490:ASN:HD22	1:E:490:ASN:H	1.50	0.58
1:G:372:ILE:HD11	1:G:374:MET:CE	2.33	0.58
1:I:472:THR:HG22	1:I:498:GLU:C	2.23	0.58
1:J:147:ILE:CG2	1:J:169:HIS:CD2	2.85	0.58
1:N:490:ASN:H	1:N:490:ASN:HD22	1.50	0.58
1:O:212:PHE:CE1	1:O:241:ASN:ND2	2.70	0.58
1:O:372:ILE:HD11	1:O:374:MET:CE	2.33	0.58
1:R:212:PHE:CE1	1:R:241:ASN:ND2	2.70	0.58
1:L:487:GLY:CA	1:S:229:LYS:HE3	2.28	0.58
1:U:372:ILE:HD12	1:U:374:MET:CG	2.33	0.58
1:V:212:PHE:CE1	1:V:241:ASN:ND2	2.70	0.58
1:W:456:ARG:HH22	2:W:700:FDP:P1	2.26	0.58
1:A:372:ILE:HD11	1:A:374:MET:CE	2.33	0.58
1:K:57:HIS:HE1	1:K:195:VAL:HG12	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:297:GLN:HB2	1:N:310:ARG:HB2	1.84	0.58
1:L:456:ARG:HH22	2:L:700:FDP:P1	2.26	0.58
1:M:212:PHE:CE1	1:M:241:ASN:ND2	2.70	0.58
1:N:144:ASP:O	1:N:145:ASP:CB	2.45	0.58
1:Q:242:HIS:CE1	1:S:12:PHE:CZ	2.91	0.58
1:T:147:ILE:CG2	1:T:169:HIS:CD2	2.85	0.58
1:X:372:ILE:HD11	1:X:374:MET:CE	2.33	0.58
1:V:283:SER:O	1:X:3:LEU:HD21	2.03	0.58
1:D:490:ASN:HD22	1:D:490:ASN:H	1.50	0.58
1:E:147:ILE:CG2	1:E:169:HIS:CD2	2.85	0.58
1:F:372:ILE:HD11	1:F:374:MET:CE	2.33	0.58
1:H:456:ARG:NH1	2:H:700:FDP:O2P	2.29	0.58
1:I:212:PHE:CE1	1:I:241:ASN:ND2	2.70	0.58
1:M:57:HIS:HE1	1:M:195:VAL:HG12	1.69	0.58
1:N:400:SER:HB2	1:N:405:SER:HB2	1.84	0.58
1:T:212:PHE:CE1	1:T:241:ASN:ND2	2.70	0.58
1:X:57:HIS:HE1	1:X:195:VAL:HG12	1.69	0.58
1:B:283:SER:HB3	1:C:3:LEU:CD2	2.34	0.58
1:H:371:HIS:CD2	1:H:373:PRO:O	2.57	0.58
1:H:57:HIS:HE1	1:H:195:VAL:HG12	1.69	0.58
1:I:400:SER:HB2	1:I:405:SER:HB2	1.84	0.58
1:H:11:ILE:C	1:J:273:LYS:HG2	2.23	0.58
1:K:472:THR:HG22	1:K:498:GLU:C	2.23	0.58
1:O:57:HIS:HE1	1:O:195:VAL:HG12	1.69	0.58
1:Q:212:PHE:CE1	1:Q:241:ASN:ND2	2.70	0.58
1:Q:269:ILE:CG1	1:S:11:ILE:HD12	2.31	0.58
1:Q:11:ILE:HD12	1:S:269:ILE:HG12	1.85	0.58
1:U:490:ASN:HD22	1:U:490:ASN:H	1.50	0.58
1:V:57:HIS:HE1	1:V:195:VAL:HG12	1.69	0.58
1:X:147:ILE:CG2	1:X:169:HIS:CD2	2.86	0.58
1:A:212:PHE:CE1	1:A:241:ASN:ND2	2.70	0.58
1:C:147:ILE:CG2	1:C:169:HIS:CD2	2.86	0.58
1:D:11:ILE:HB	1:F:273:LYS:CG	2.31	0.58
1:A:242:HIS:CE1	1:I:12:PHE:HE2	2.18	0.58
1:C:391:THR:HA	1:P:373:PRO:CB	2.32	0.58
1:S:472:THR:HG22	1:S:498:GLU:C	2.23	0.58
1:B:212:PHE:CE1	1:B:241:ASN:ND2	2.70	0.58
1:B:472:THR:HG22	1:B:498:GLU:C	2.22	0.58
1:B:57:HIS:HE1	1:B:195:VAL:HG12	1.69	0.58
1:D:147:ILE:CG2	1:D:169:HIS:CD2	2.85	0.58
1:D:372:ILE:HD11	1:D:374:MET:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:483:HIS:CD2	1:G:483:HIS:CD2	2.92	0.58
1:H:490:ASN:H	1:H:490:ASN:HD22	1.50	0.58
1:I:456:ARG:NH2	2:I:700:FDP:O1P	2.34	0.58
1:H:11:ILE:HA	1:J:273:LYS:HG2	1.86	0.58
1:L:212:PHE:CE1	1:L:241:ASN:ND2	2.70	0.58
1:X:490:ASN:H	1:X:490:ASN:HD22	1.50	0.58
1:C:372:ILE:HD11	1:C:374:MET:CE	2.33	0.58
1:E:372:ILE:HD11	1:E:374:MET:CE	2.33	0.58
1:D:279:LYS:HE3	1:F:6:ASN:OD1	2.04	0.58
1:H:11:ILE:O	1:J:273:LYS:HD3	2.04	0.58
1:M:472:THR:HA	1:M:497:VAL:O	2.04	0.58
1:N:212:PHE:CE1	1:N:241:ASN:ND2	2.70	0.58
1:H:456:ARG:HH22	2:H:700:FDP:P1	2.26	0.58
1:L:283:SER:OG	1:N:3:LEU:CD2	2.42	0.58
1:N:472:THR:HA	1:N:497:VAL:O	2.04	0.58
1:C:391:THR:CA	1:P:373:PRO:HB3	2.33	0.58
1:T:456:ARG:HH22	2:T:700:FDP:P1	2.26	0.58
1:T:472:THR:HA	1:T:497:VAL:O	2.04	0.58
1:U:372:ILE:HG13	1:V:390:GLU:C	2.24	0.58
1:U:310:ARG:HG2	1:W:297:GLN:CB	2.30	0.58
1:F:57:HIS:HE1	1:F:195:VAL:HG12	1.69	0.57
1:G:472:THR:HA	1:G:497:VAL:O	2.04	0.57
1:H:9:LEU:HB3	1:J:276:VAL:HG13	1.85	0.57
1:R:472:THR:HA	1:R:497:VAL:O	2.04	0.57
1:U:472:THR:HA	1:U:497:VAL:O	2.04	0.57
1:U:272:GLU:HG3	1:W:352:GLU:HB2	1.86	0.57
1:E:472:THR:HG22	1:E:498:GLU:C	2.23	0.57
1:G:212:PHE:CE1	1:G:241:ASN:ND2	2.70	0.57
1:N:57:HIS:HE1	1:N:195:VAL:HG12	1.69	0.57
1:P:472:THR:HA	1:P:497:VAL:O	2.04	0.57
1:R:472:THR:HG22	1:R:498:GLU:C	2.23	0.57
1:C:472:THR:HA	1:C:497:VAL:O	2.04	0.57
1:E:272:GLU:HG3	1:G:352:GLU:HB2	1.85	0.57
1:H:491:GLN:HG3	1:I:491:GLN:HG3	1.86	0.57
1:I:472:THR:HA	1:I:497:VAL:O	2.05	0.57
1:U:57:HIS:HE1	1:U:195:VAL:HG12	1.69	0.57
1:B:456:ARG:NH2	2:B:700:FDP:O1P	2.34	0.57
1:C:57:HIS:HE1	1:C:195:VAL:HG12	1.69	0.57
1:L:472:THR:HA	1:L:497:VAL:O	2.04	0.57
1:L:272:GLU:HG3	1:N:352:GLU:CB	2.33	0.57
1:Q:490:ASN:H	1:Q:490:ASN:HD22	1.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:280:ILE:CD1	1:T:9:LEU:HB2	2.32	0.57
1:A:283:SER:HB3	1:I:3:LEU:HD23	1.86	0.57
1:A:310:ARG:HG2	1:I:297:GLN:OE1	2.04	0.57
1:C:372:ILE:HG13	1:P:390:GLU:HA	1.85	0.57
1:E:57:HIS:HE1	1:E:195:VAL:HG12	1.69	0.57
1:H:212:PHE:CE1	1:H:241:ASN:ND2	2.70	0.57
1:P:57:HIS:HE1	1:P:195:VAL:HG12	1.69	0.57
1:Q:472:THR:HA	1:Q:497:VAL:O	2.05	0.57
1:S:372:ILE:HG13	1:T:390:GLU:CB	2.33	0.57
1:T:472:THR:CG2	1:T:498:GLU:HA	2.18	0.57
1:W:372:ILE:HG13	1:X:390:GLU:C	2.24	0.57
1:G:490:ASN:H	1:G:490:ASN:HD22	1.50	0.57
1:H:496:LEU:HD21	1:M:195:VAL:CG2	2.33	0.57
1:J:57:HIS:HE1	1:J:195:VAL:HG12	1.69	0.57
1:T:57:HIS:HE1	1:T:195:VAL:HG12	1.69	0.57
1:V:242:HIS:NE2	1:X:12:PHE:CE2	2.73	0.57
1:X:472:THR:HA	1:X:497:VAL:O	2.04	0.57
1:A:472:THR:HA	1:A:497:VAL:O	2.04	0.57
1:B:472:THR:HA	1:B:497:VAL:O	2.05	0.57
1:D:57:HIS:HE1	1:D:195:VAL:HG12	1.69	0.57
1:E:472:THR:HA	1:E:497:VAL:O	2.04	0.57
1:F:472:THR:HA	1:F:497:VAL:O	2.04	0.57
1:H:242:HIS:CE1	1:J:12:PHE:HE2	2.13	0.57
1:I:57:HIS:HE1	1:I:195:VAL:HG12	1.69	0.57
1:L:57:HIS:HE1	1:L:195:VAL:HG12	1.69	0.57
1:L:6:ASN:O	1:N:280:ILE:HG12	2.04	0.57
1:B:373:PRO:HB3	1:O:391:THR:O	2.03	0.57
1:Q:11:ILE:O	1:S:273:LYS:HE3	2.05	0.57
1:Q:57:HIS:HE1	1:Q:195:VAL:HG12	1.69	0.57
1:W:472:THR:HA	1:W:497:VAL:O	2.04	0.57
1:G:57:HIS:HE1	1:G:195:VAL:HG12	1.69	0.57
1:E:283:SER:HB3	1:G:3:LEU:CD2	2.35	0.57
1:G:472:THR:HG22	1:G:498:GLU:C	2.23	0.57
1:L:280:ILE:HG13	1:N:6:ASN:O	2.03	0.57
1:C:373:PRO:CB	1:P:391:THR:HA	2.33	0.57
1:R:11:ILE:HG12	1:R:12:PHE:CE2	2.40	0.57
1:R:57:HIS:HE1	1:R:195:VAL:HG12	1.69	0.57
1:S:212:PHE:CE1	1:S:241:ASN:ND2	2.70	0.57
1:H:472:THR:HA	1:H:497:VAL:O	2.04	0.57
1:L:273:LYS:CD	1:N:11:ILE:O	2.53	0.57
1:Q:12:PHE:CE2	1:S:242:HIS:CE1	2.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:273:LYS:HB3	1:T:11:ILE:HB	1.85	0.57
1:R:456:ARG:NH2	2:R:700:FDP:O1P	2.34	0.57
1:V:472:THR:HA	1:V:497:VAL:O	2.04	0.57
1:G:372:ILE:HD11	1:G:374:MET:HE1	1.86	0.57
1:J:212:PHE:CE1	1:J:241:ASN:ND2	2.70	0.57
1:V:272:GLU:CG	1:X:352:GLU:CG	2.82	0.57
1:W:57:HIS:HE1	1:W:195:VAL:HG12	1.69	0.57
1:J:472:THR:HA	1:J:497:VAL:O	2.04	0.56
1:K:472:THR:HA	1:K:497:VAL:O	2.04	0.56
1:L:472:THR:CG2	1:L:498:GLU:HA	2.18	0.56
1:S:472:THR:HA	1:S:497:VAL:O	2.04	0.56
1:A:57:HIS:HE1	1:A:195:VAL:HG12	1.69	0.56
1:A:3:LEU:HD23	1:I:283:SER:CB	2.34	0.56
1:D:472:THR:HA	1:D:497:VAL:O	2.04	0.56
1:M:372:ILE:HG23	1:N:390:GLU:O	2.05	0.56
1:C:57:HIS:CE1	1:C:195:VAL:HG12	2.41	0.56
1:I:229:LYS:HE3	1:M:487:GLY:N	2.19	0.56
1:K:310:ARG:HG2	1:M:297:GLN:OE1	2.05	0.56
1:U:11:ILE:HA	1:W:273:LYS:HG2	1.85	0.56
1:C:498:GLU:HG2	1:V:195:VAL:HG11	1.87	0.56
1:D:373:PRO:HB3	1:E:391:THR:C	2.25	0.56
1:F:57:HIS:CE1	1:F:195:VAL:HG12	2.41	0.56
1:M:372:ILE:HD11	1:N:390:GLU:HG2	1.87	0.56
1:O:472:THR:HA	1:O:497:VAL:O	2.04	0.56
1:P:195:VAL:HG22	1:U:496:LEU:HD23	1.85	0.56
1:Q:272:GLU:HG2	1:S:352:GLU:HG2	1.85	0.56
1:S:493:ARG:NE	1:T:482:ASP:OD2	2.34	0.56
1:U:223:ARG:CG	1:U:223:ARG:HH11	2.19	0.56
1:U:315:ASP:HB2	1:W:311:ALA:CA	2.34	0.56
1:X:212:PHE:CE1	1:X:241:ASN:ND2	2.70	0.56
1:X:57:HIS:CE1	1:X:195:VAL:HG12	2.41	0.56
1:G:472:THR:CG2	1:G:498:GLU:HA	2.18	0.56
1:K:491:GLN:HG3	1:L:491:GLN:HG3	1.87	0.56
1:L:352:GLU:HB2	1:N:272:GLU:HG3	1.87	0.56
1:N:57:HIS:CE1	1:N:195:VAL:HG12	2.41	0.56
1:O:57:HIS:CE1	1:O:195:VAL:HG12	2.41	0.56
1:P:223:ARG:CG	1:P:223:ARG:HH11	2.19	0.56
1:U:57:HIS:CE1	1:U:195:VAL:HG12	2.41	0.56
1:V:57:HIS:CE1	1:V:195:VAL:HG12	2.41	0.56
1:D:312:GLU:HA	1:F:311:ALA:HB1	1.87	0.56
1:E:57:HIS:CE1	1:E:195:VAL:HG12	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:HIS:CE1	1:G:195:VAL:HG12	2.41	0.56
1:L:11:ILE:HG12	1:L:12:PHE:CE2	2.40	0.56
1:S:57:HIS:HE1	1:S:195:VAL:HG12	1.69	0.56
1:A:223:ARG:HH11	1:A:223:ARG:CG	2.19	0.56
1:H:390:GLU:HA	1:I:372:ILE:HG13	1.88	0.56
1:K:57:HIS:CE1	1:K:195:VAL:HG12	2.41	0.56
1:Q:272:GLU:CG	1:S:352:GLU:CG	2.83	0.56
1:Q:57:HIS:CE1	1:Q:195:VAL:HG12	2.41	0.56
1:S:57:HIS:CE1	1:S:195:VAL:HG12	2.41	0.56
1:B:57:HIS:CE1	1:B:195:VAL:HG12	2.41	0.56
1:E:273:LYS:CG	1:G:11:ILE:HB	2.36	0.56
1:L:297:GLN:OE1	1:N:310:ARG:CG	2.41	0.56
1:V:372:ILE:HD11	1:V:374:MET:HE1	1.87	0.56
1:C:223:ARG:CG	1:C:223:ARG:HH11	2.19	0.56
1:I:57:HIS:CE1	1:I:195:VAL:HG12	2.41	0.56
1:J:57:HIS:CE1	1:J:195:VAL:HG12	2.41	0.56
1:T:370:GLN:CB	1:T:374:MET:SD	2.94	0.56
1:T:57:HIS:CE1	1:T:195:VAL:HG12	2.41	0.56
1:C:472:THR:CG2	1:C:498:GLU:HA	2.18	0.56
1:I:270:PRO:CG	1:I:273:LYS:HE2	2.24	0.56
1:R:57:HIS:CE1	1:R:195:VAL:HG12	2.41	0.56
1:B:269:ILE:HG12	1:C:11:ILE:CD1	2.35	0.56
1:A:3:LEU:HD21	1:I:283:SER:CB	2.34	0.56
1:L:297:GLN:CB	1:N:310:ARG:HG3	2.33	0.56
1:T:223:ARG:HH11	1:T:223:ARG:CG	2.19	0.56
1:U:392:LYS:HD2	1:V:373:PRO:HD3	1.87	0.56
1:X:223:ARG:CG	1:X:223:ARG:HH11	2.19	0.56
1:D:311:ALA:HB1	1:F:312:GLU:HA	1.88	0.55
1:K:144:ASP:O	1:K:145:ASP:CB	2.45	0.55
1:W:223:ARG:CG	1:W:223:ARG:HH11	2.19	0.55
1:W:456:ARG:NH1	2:W:700:FDP:O2P	2.28	0.55
1:E:223:ARG:CG	1:E:223:ARG:HH11	2.19	0.55
1:H:472:THR:CG2	1:H:498:GLU:HA	2.18	0.55
1:M:144:ASP:O	1:M:145:ASP:CB	2.45	0.55
1:U:370:GLN:CB	1:U:374:MET:SD	2.94	0.55
1:D:57:HIS:CE1	1:D:195:VAL:HG12	2.41	0.55
1:H:57:HIS:CE1	1:H:195:VAL:HG12	2.41	0.55
1:I:223:ARG:CG	1:I:223:ARG:HH11	2.19	0.55
1:K:272:GLU:C	1:M:352:GLU:HG2	2.26	0.55
1:P:57:HIS:CE1	1:P:195:VAL:HG12	2.41	0.55
1:Q:9:LEU:HB2	1:S:280:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:57:HIS:CE1	1:W:195:VAL:HG12	2.41	0.55
1:B:297:GLN:HB2	1:C:310:ARG:HB2	1.87	0.55
1:N:446:LYS:C	1:N:446:LYS:CD	2.72	0.55
1:R:283:SER:CB	1:T:3:LEU:HG	2.36	0.55
1:D:223:ARG:CG	1:D:223:ARG:HH11	2.19	0.55
1:H:273:LYS:HG2	1:J:11:ILE:O	2.07	0.55
1:H:318:ASN:ND2	1:J:318:ASN:ND2	2.55	0.55
1:L:57:HIS:CE1	1:L:195:VAL:HG12	2.41	0.55
1:N:372:ILE:HD11	1:N:374:MET:HE1	1.89	0.55
1:P:487:GLY:HA3	1:V:229:LYS:CG	2.27	0.55
1:U:365:SER:CB	1:W:3:LEU:HD12	2.37	0.55
1:V:11:ILE:CD1	1:V:12:PHE:HE2	2.12	0.55
1:A:57:HIS:CE1	1:A:195:VAL:HG12	2.41	0.55
1:Q:272:GLU:O	1:S:352:GLU:HG2	2.07	0.55
1:S:372:ILE:HG12	1:T:390:GLU:CA	2.16	0.55
1:H:147:ILE:HG22	1:H:169:HIS:CD2	2.42	0.55
1:H:352:GLU:OE1	1:J:272:GLU:CG	2.54	0.55
1:M:57:HIS:CE1	1:M:195:VAL:HG12	2.41	0.55
1:Q:372:ILE:HD12	1:Q:374:MET:HG2	1.89	0.55
1:R:272:GLU:C	1:T:352:GLU:HG2	2.27	0.55
1:U:147:ILE:HG22	1:U:169:HIS:CD2	2.42	0.55
1:D:372:ILE:HD12	1:D:374:MET:HG2	1.89	0.55
1:D:53:SER:HA	1:D:85:LYS:HG3	1.89	0.55
1:I:147:ILE:HG22	1:I:169:HIS:CD2	2.42	0.55
1:H:372:ILE:CG1	1:I:390:GLU:HA	2.26	0.55
1:S:390:GLU:O	1:T:373:PRO:CB	2.55	0.55
1:W:147:ILE:HG22	1:W:169:HIS:CD2	2.42	0.55
1:X:147:ILE:HG22	1:X:169:HIS:CD2	2.42	0.55
1:I:11:ILE:HG12	1:I:12:PHE:CE2	2.40	0.55
1:J:193:ASP:O	1:J:197:LEU:N	2.38	0.55
1:N:147:ILE:HG22	1:N:169:HIS:CD2	2.42	0.55
1:N:223:ARG:HH11	1:N:223:ARG:CG	2.19	0.55
1:N:372:ILE:HD12	1:N:374:MET:HG2	1.89	0.55
1:P:147:ILE:HG22	1:P:169:HIS:CD2	2.42	0.55
1:Q:242:HIS:HE1	1:S:12:PHE:CZ	2.25	0.55
1:R:147:ILE:HG22	1:R:169:HIS:CD2	2.42	0.55
1:V:372:ILE:HD12	1:V:374:MET:HG2	1.89	0.55
1:W:372:ILE:CG2	1:X:390:GLU:O	2.53	0.55
1:B:53:SER:HA	1:B:85:LYS:HG3	1.89	0.54
1:C:372:ILE:HD12	1:C:374:MET:HG2	1.89	0.54
1:D:147:ILE:HG22	1:D:169:HIS:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:GLU:HA	1:E:372:ILE:HG13	1.89	0.54
1:H:352:GLU:OE1	1:J:272:GLU:HG3	2.07	0.54
1:L:147:ILE:HG22	1:L:169:HIS:CD2	2.42	0.54
1:L:53:SER:HA	1:L:85:LYS:HG3	1.89	0.54
1:W:372:ILE:HD12	1:W:374:MET:HG2	1.89	0.54
1:Q:147:ILE:HG22	1:Q:169:HIS:CD2	2.42	0.54
1:Q:223:ARG:CG	1:Q:223:ARG:HH11	2.19	0.54
1:V:147:ILE:HG22	1:V:169:HIS:CD2	2.42	0.54
1:X:49:ARG:NE	1:X:83:ASP:OD2	2.33	0.54
1:A:147:ILE:HG22	1:A:169:HIS:CD2	2.42	0.54
1:A:53:SER:HA	1:A:85:LYS:HG3	1.89	0.54
1:G:372:ILE:HD12	1:G:374:MET:HG2	1.89	0.54
1:O:147:ILE:HG22	1:O:169:HIS:CD2	2.42	0.54
1:O:372:ILE:HD12	1:O:374:MET:HG2	1.89	0.54
1:C:147:ILE:HG22	1:C:169:HIS:CD2	2.42	0.54
1:J:372:ILE:HD12	1:J:374:MET:HG2	1.89	0.54
1:J:53:SER:HA	1:J:85:LYS:HG3	1.89	0.54
1:K:372:ILE:HD12	1:K:374:MET:HG2	1.89	0.54
1:K:53:SER:HA	1:K:85:LYS:HG3	1.89	0.54
1:L:284:LYS:HG3	1:N:7:LEU:HD21	1.89	0.54
1:R:270:PRO:CG	1:R:273:LYS:HE2	2.23	0.54
1:T:147:ILE:HG22	1:T:169:HIS:CD2	2.42	0.54
1:V:272:GLU:HG3	1:X:352:GLU:CG	2.37	0.54
1:B:147:ILE:HG22	1:B:169:HIS:CD2	2.42	0.54
1:E:11:ILE:HG12	1:E:12:PHE:CE2	2.40	0.54
1:M:147:ILE:HG22	1:M:169:HIS:CD2	2.42	0.54
1:Q:11:ILE:HB	1:S:273:LYS:CG	2.37	0.54
1:R:456:ARG:NH1	2:R:700:FDP:O2P	2.34	0.54
1:V:276:VAL:O	1:V:280:ILE:CD1	2.54	0.54
1:H:9:LEU:O	1:J:280:ILE:HD11	2.07	0.54
1:K:223:ARG:CG	1:K:223:ARG:HH11	2.19	0.54
1:K:390:GLU:HG2	1:L:374:MET:HE2	1.89	0.54
1:O:223:ARG:CG	1:O:223:ARG:HH11	2.19	0.54
1:O:53:SER:HA	1:O:85:LYS:HG3	1.89	0.54
1:S:147:ILE:HG22	1:S:169:HIS:CD2	2.42	0.54
1:T:53:SER:HA	1:T:85:LYS:HG3	1.89	0.54
1:U:53:SER:HA	1:U:85:LYS:HG3	1.89	0.54
1:V:273:LYS:HD3	1:X:11:ILE:O	2.08	0.54
1:C:373:PRO:HB3	1:P:391:THR:CA	2.38	0.54
1:F:193:ASP:O	1:F:197:LEU:N	2.38	0.54
1:H:223:ARG:CG	1:H:223:ARG:HH11	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:144:ASP:O	1:I:145:ASP:CB	2.45	0.54
1:J:147:ILE:HG22	1:J:169:HIS:CD2	2.42	0.54
1:V:279:LYS:HB3	1:X:6:ASN:CG	2.28	0.54
1:E:472:THR:CG2	1:E:498:GLU:HA	2.18	0.54
1:F:147:ILE:HG22	1:F:169:HIS:CD2	2.42	0.54
1:F:223:ARG:CG	1:F:223:ARG:HH11	2.19	0.54
1:F:53:SER:HA	1:F:85:LYS:HG3	1.89	0.54
1:G:147:ILE:HG22	1:G:169:HIS:CD2	2.42	0.54
1:J:456:ARG:NH1	2:J:700:FDP:O2P	2.34	0.54
1:N:53:SER:HA	1:N:85:LYS:HG3	1.89	0.54
1:Q:53:SER:HA	1:Q:85:LYS:HG3	1.89	0.54
1:R:49:ARG:NE	1:R:83:ASP:OD2	2.33	0.54
1:S:53:SER:HA	1:S:85:LYS:HG3	1.89	0.54
1:V:270:PRO:CG	1:V:273:LYS:HE2	2.24	0.54
1:E:372:ILE:HD12	1:E:374:MET:HG2	1.89	0.54
1:H:270:PRO:HB2	1:H:273:LYS:HD2	1.90	0.54
1:P:53:SER:HA	1:P:85:LYS:HG3	1.89	0.54
1:Q:273:LYS:HB3	1:S:11:ILE:HB	1.88	0.54
1:Q:283:SER:CB	1:S:3:LEU:HD21	2.38	0.54
1:V:276:VAL:CG1	1:X:9:LEU:HB3	2.37	0.54
1:W:53:SER:HA	1:W:85:LYS:HG3	1.89	0.54
1:X:472:THR:CG2	1:X:498:GLU:HA	2.18	0.54
1:B:273:LYS:HG2	1:C:11:ILE:O	2.07	0.54
1:C:373:PRO:HB3	1:P:390:GLU:O	2.08	0.54
1:D:12:PHE:HZ	1:F:242:HIS:CE1	2.24	0.54
1:K:270:PRO:HB2	1:K:273:LYS:HD2	1.90	0.54
1:U:270:PRO:HB2	1:U:273:LYS:HD2	1.90	0.54
1:V:11:ILE:HG12	1:V:12:PHE:CE2	2.40	0.54
1:A:270:PRO:HG2	1:A:273:LYS:CE	2.38	0.53
1:C:270:PRO:HB2	1:C:273:LYS:HD2	1.90	0.53
1:E:147:ILE:HG22	1:E:169:HIS:CD2	2.42	0.53
1:E:53:SER:HA	1:E:85:LYS:HG3	1.89	0.53
1:H:11:ILE:CD1	1:J:269:ILE:HG12	2.38	0.53
1:I:195:VAL:HG22	1:N:496:LEU:CG	2.36	0.53
1:L:276:VAL:HG13	1:N:9:LEU:HB3	1.90	0.53
1:O:272:GLU:O	1:P:352:GLU:HG2	2.08	0.53
1:S:223:ARG:CG	1:S:223:ARG:HH11	2.19	0.53
1:R:273:LYS:CD	1:T:11:ILE:HB	2.39	0.53
1:U:297:GLN:OE1	1:W:310:ARG:NH2	2.41	0.53
1:K:147:ILE:HG22	1:K:169:HIS:CD2	2.42	0.53
1:B:270:PRO:HB2	1:B:273:LYS:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:GLU:O	1:G:373:PRO:CB	2.56	0.53
1:I:53:SER:HA	1:I:85:LYS:HG3	1.89	0.53
1:L:229:LYS:CD	1:S:487:GLY:HA2	2.38	0.53
1:O:12:PHE:HZ	1:P:242:HIS:CE1	2.21	0.53
1:W:373:PRO:HB3	1:X:391:THR:C	2.28	0.53
1:A:456:ARG:NH1	2:A:700:FDP:O2P	2.34	0.53
1:B:270:PRO:HG2	1:B:273:LYS:CE	2.38	0.53
1:F:372:ILE:HD12	1:F:374:MET:HG2	1.89	0.53
1:L:297:GLN:CB	1:N:310:ARG:HB2	2.38	0.53
1:R:472:THR:CG2	1:R:498:GLU:HA	2.18	0.53
1:U:494:ILE:HD12	1:V:376:ALA:HB1	1.89	0.53
1:D:270:PRO:HG2	1:D:273:LYS:CE	2.38	0.53
1:L:223:ARG:CG	1:L:223:ARG:HH11	2.19	0.53
1:N:472:THR:CG2	1:N:498:GLU:HA	2.18	0.53
1:Q:272:GLU:C	1:S:352:GLU:HG2	2.28	0.53
1:B:297:GLN:CD	1:C:310:ARG:HG2	2.26	0.53
1:F:483:HIS:NE2	1:G:483:HIS:HD2	2.07	0.53
1:G:223:ARG:CG	1:G:223:ARG:HH11	2.19	0.53
1:Q:270:PRO:HG2	1:Q:273:LYS:CE	2.38	0.53
1:X:372:ILE:HD12	1:X:374:MET:HG2	1.89	0.53
1:G:53:SER:HA	1:G:85:LYS:HG3	1.89	0.53
1:K:270:PRO:HG2	1:K:273:LYS:CE	2.38	0.53
1:L:310:ARG:CG	1:N:297:GLN:HB2	2.37	0.53
1:O:270:PRO:HB2	1:O:273:LYS:HD2	1.90	0.53
1:O:472:THR:CG2	1:O:498:GLU:HA	2.18	0.53
1:Q:270:PRO:HB2	1:Q:273:LYS:HD2	1.90	0.53
1:Q:352:GLU:HB2	1:S:272:GLU:HG3	1.89	0.53
1:R:193:ASP:O	1:R:197:LEU:N	2.38	0.53
1:R:273:LYS:CG	1:T:11:ILE:HB	2.39	0.53
1:B:372:ILE:HD12	1:B:374:MET:HG2	1.89	0.53
1:C:89:ILE:CG2	1:C:177:VAL:HG22	2.39	0.53
1:H:53:SER:HA	1:H:85:LYS:HG3	1.89	0.53
1:M:392:LYS:HD2	1:N:373:PRO:HD3	1.91	0.53
1:P:89:ILE:CG2	1:P:177:VAL:HG22	2.39	0.53
1:P:472:THR:CG2	1:P:498:GLU:HA	2.18	0.53
1:R:53:SER:HA	1:R:85:LYS:HG3	1.89	0.53
1:X:53:SER:HA	1:X:85:LYS:HG3	1.89	0.53
1:B:297:GLN:CB	1:C:310:ARG:HG2	2.38	0.53
1:D:89:ILE:CG2	1:D:177:VAL:HG22	2.39	0.53
1:K:89:ILE:CG2	1:K:177:VAL:HG22	2.39	0.53
1:L:89:ILE:CG2	1:L:177:VAL:HG22	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:89:ILE:CG2	1:N:177:VAL:HG22	2.39	0.53
1:O:311:ALA:HB1	1:P:312:GLU:CA	2.26	0.53
1:S:89:ILE:CG2	1:S:177:VAL:HG22	2.39	0.53
1:V:11:ILE:HG13	1:V:12:PHE:HD2	1.72	0.53
1:V:53:SER:HA	1:V:85:LYS:HG3	1.89	0.53
1:U:352:GLU:OE1	1:W:272:GLU:HG3	2.09	0.53
1:A:270:PRO:HB2	1:A:273:LYS:HD2	1.90	0.53
1:B:89:ILE:CG2	1:B:177:VAL:HG22	2.39	0.53
1:C:193:ASP:O	1:C:197:LEU:N	2.38	0.53
1:B:297:GLN:HB2	1:C:310:ARG:CB	2.39	0.53
1:B:3:LEU:HD13	1:C:369:LEU:HD12	1.90	0.53
1:F:89:ILE:CG2	1:F:177:VAL:HG22	2.39	0.53
1:H:296:THR:HG22	1:H:297:GLN:CG	2.39	0.53
1:J:240:GLU:HB3	1:J:264:ASP:HB2	1.91	0.53
1:M:240:GLU:HB3	1:M:264:ASP:HB2	1.91	0.53
1:R:270:PRO:O	1:R:273:LYS:HB2	2.09	0.53
1:T:89:ILE:CG2	1:T:177:VAL:HG22	2.39	0.53
1:U:89:ILE:CG2	1:U:177:VAL:HG22	2.39	0.53
1:U:270:PRO:HG2	1:U:273:LYS:CE	2.38	0.53
1:W:89:ILE:CG2	1:W:177:VAL:HG22	2.39	0.53
1:A:240:GLU:HB3	1:A:264:ASP:HB2	1.91	0.52
1:A:372:ILE:HD12	1:A:374:MET:HG2	1.89	0.52
1:E:270:PRO:O	1:E:273:LYS:HB2	2.09	0.52
1:I:270:PRO:O	1:I:273:LYS:HB2	2.09	0.52
1:M:383:SER:HB2	1:N:383:SER:CB	2.33	0.52
1:L:272:GLU:HG2	1:N:352:GLU:HG2	1.91	0.52
1:L:276:VAL:HG13	1:N:9:LEU:CB	2.39	0.52
1:C:270:PRO:HG2	1:C:273:LYS:CE	2.38	0.52
1:C:390:GLU:HG2	1:P:372:ILE:HD11	1.91	0.52
1:C:53:SER:HA	1:C:85:LYS:HG3	1.90	0.52
1:G:89:ILE:CG2	1:G:177:VAL:HG22	2.39	0.52
1:J:89:ILE:CG2	1:J:177:VAL:HG22	2.39	0.52
1:L:273:LYS:CD	1:N:11:ILE:HB	2.39	0.52
1:M:53:SER:HA	1:M:85:LYS:HG3	1.89	0.52
1:N:193:ASP:O	1:N:197:LEU:N	2.38	0.52
1:S:240:GLU:HB3	1:S:264:ASP:HB2	1.91	0.52
1:H:372:ILE:HD12	1:H:374:MET:CG	2.38	0.52
1:I:89:ILE:CG2	1:I:177:VAL:HG22	2.39	0.52
1:R:273:LYS:HG2	1:T:11:ILE:HA	1.91	0.52
1:T:193:ASP:O	1:T:197:LEU:N	2.38	0.52
1:S:372:ILE:CG1	1:T:390:GLU:CB	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:49:ARG:NE	1:U:83:ASP:OD2	2.33	0.52
1:W:240:GLU:HB3	1:W:264:ASP:HB2	1.91	0.52
1:X:89:ILE:CG2	1:X:177:VAL:HG22	2.39	0.52
1:H:352:GLU:HG2	1:J:272:GLU:HB2	1.92	0.52
1:K:273:LYS:HB3	1:M:11:ILE:HB	1.91	0.52
1:M:89:ILE:CG2	1:M:177:VAL:HG22	2.39	0.52
1:M:193:ASP:O	1:M:197:LEU:N	2.38	0.52
1:M:223:ARG:HH11	1:M:223:ARG:CG	2.19	0.52
1:V:240:GLU:HB3	1:V:264:ASP:HB2	1.91	0.52
1:V:270:PRO:O	1:V:273:LYS:HB2	2.09	0.52
1:X:193:ASP:O	1:X:197:LEU:N	2.38	0.52
1:B:240:GLU:HB3	1:B:264:ASP:HB2	1.91	0.52
1:E:240:GLU:HB3	1:E:264:ASP:HB2	1.91	0.52
1:H:270:PRO:HG2	1:H:273:LYS:CE	2.38	0.52
1:O:270:PRO:HG2	1:O:273:LYS:CE	2.38	0.52
1:O:89:ILE:CG2	1:O:177:VAL:HG22	2.39	0.52
1:R:89:ILE:CG2	1:R:177:VAL:HG22	2.39	0.52
1:V:287:VAL:HG23	1:X:3:LEU:CD2	2.40	0.52
1:D:270:PRO:HB2	1:D:273:LYS:HD2	1.90	0.52
1:D:12:PHE:HZ	1:F:242:HIS:HE1	1.51	0.52
1:H:391:THR:HA	1:I:373:PRO:HB3	1.91	0.52
1:J:223:ARG:CG	1:J:223:ARG:HH11	2.19	0.52
1:J:372:ILE:HD11	1:J:374:MET:HE1	1.92	0.52
1:M:373:PRO:CB	1:N:391:THR:HA	2.39	0.52
1:O:193:ASP:O	1:O:197:LEU:N	2.38	0.52
1:O:270:PRO:HG2	1:O:273:LYS:HD2	1.92	0.52
1:P:193:ASP:O	1:P:197:LEU:N	2.38	0.52
1:Q:471:GLN:O	1:Q:497:VAL:CG2	2.58	0.52
1:S:390:GLU:O	1:T:373:PRO:HB3	2.09	0.52
1:U:240:GLU:HB3	1:U:264:ASP:HB2	1.91	0.52
1:U:471:GLN:O	1:U:497:VAL:CG2	2.58	0.52
1:X:240:GLU:HB3	1:X:264:ASP:HB2	1.91	0.52
1:V:280:ILE:HA	1:X:6:ASN:HB3	1.90	0.52
1:A:89:ILE:CG2	1:A:177:VAL:HG22	2.39	0.52
1:B:193:ASP:O	1:B:197:LEU:N	2.38	0.52
1:H:89:ILE:CG2	1:H:177:VAL:HG22	2.39	0.52
1:H:193:ASP:O	1:H:197:LEU:N	2.38	0.52
1:H:240:GLU:HB3	1:H:264:ASP:HB2	1.91	0.52
1:N:240:GLU:HB3	1:N:264:ASP:HB2	1.91	0.52
1:Q:89:ILE:CG2	1:Q:177:VAL:HG22	2.39	0.52
1:V:89:ILE:CG2	1:V:177:VAL:HG22	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:GLN:O	1:C:497:VAL:CG2	2.58	0.52
1:M:471:GLN:O	1:M:497:VAL:CG2	2.58	0.52
1:O:310:ARG:CZ	1:P:297:GLN:OE1	2.58	0.52
1:Q:270:PRO:HG2	1:Q:273:LYS:HD2	1.92	0.52
1:U:390:GLU:OE1	1:V:379:ALA:HB2	2.10	0.52
1:X:471:GLN:O	1:X:497:VAL:CG2	2.58	0.52
1:A:270:PRO:HG2	1:A:273:LYS:HD2	1.92	0.52
1:K:270:PRO:HG2	1:K:273:LYS:HD2	1.92	0.52
1:O:471:GLN:O	1:O:497:VAL:CG2	2.58	0.52
1:Q:373:PRO:HB3	1:R:390:GLU:O	2.09	0.52
1:S:193:ASP:O	1:S:197:LEU:N	2.38	0.52
1:U:272:GLU:C	1:W:352:GLU:HG2	2.29	0.52
1:W:471:GLN:O	1:W:497:VAL:CG2	2.58	0.52
1:D:471:GLN:O	1:D:497:VAL:CG2	2.58	0.51
1:E:456:ARG:HH22	2:E:700:FDP:P1	2.33	0.51
1:G:240:GLU:HB3	1:G:264:ASP:HB2	1.91	0.51
1:L:193:ASP:O	1:L:197:LEU:N	2.38	0.51
1:N:471:GLN:O	1:N:497:VAL:CG2	2.58	0.51
1:B:223:ARG:CG	1:B:223:ARG:HH11	2.19	0.51
1:C:240:GLU:HB3	1:C:264:ASP:HB2	1.91	0.51
1:B:280:ILE:HG12	1:C:6:ASN:O	2.10	0.51
1:D:270:PRO:HG2	1:D:273:LYS:HD2	1.92	0.51
1:F:188:ALA:HA	1:F:218:GLN:OE1	2.11	0.51
1:L:188:ALA:HA	1:L:218:GLN:OE1	2.11	0.51
1:L:270:PRO:O	1:L:273:LYS:HB2	2.09	0.51
1:L:471:GLN:O	1:L:497:VAL:CG2	2.58	0.51
1:R:223:ARG:CG	1:R:223:ARG:HH11	2.19	0.51
1:R:240:GLU:HB3	1:R:264:ASP:HB2	1.91	0.51
1:R:471:GLN:O	1:R:497:VAL:CG2	2.58	0.51
1:B:297:GLN:OE1	1:C:310:ARG:CZ	2.58	0.51
1:E:89:ILE:CG2	1:E:177:VAL:HG22	2.39	0.51
1:F:471:GLN:O	1:F:497:VAL:CG2	2.58	0.51
1:G:471:GLN:O	1:G:497:VAL:CG2	2.58	0.51
1:H:270:PRO:HG2	1:H:273:LYS:HD2	1.92	0.51
1:H:471:GLN:O	1:H:497:VAL:CG2	2.58	0.51
1:P:240:GLU:HB3	1:P:264:ASP:HB2	1.92	0.51
1:S:372:ILE:HD11	1:T:390:GLU:CG	2.21	0.51
1:S:372:ILE:CB	1:T:390:GLU:O	2.58	0.51
1:T:471:GLN:O	1:T:497:VAL:CG2	2.58	0.51
1:V:471:GLN:O	1:V:497:VAL:CG2	2.58	0.51
1:W:188:ALA:HA	1:W:218:GLN:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:GLN:O	1:B:497:VAL:CG2	2.58	0.51
1:I:193:ASP:O	1:I:197:LEU:N	2.38	0.51
1:L:372:ILE:HD12	1:L:374:MET:CG	2.41	0.51
1:N:456:ARG:HH22	2:N:700:FDP:P1	2.34	0.51
1:P:471:GLN:O	1:P:497:VAL:CG2	2.58	0.51
1:Q:279:LYS:HE3	1:S:6:ASN:OD1	2.10	0.51
1:V:223:ARG:CG	1:V:223:ARG:HH11	2.19	0.51
1:V:352:GLU:OE1	1:X:273:LYS:NZ	2.43	0.51
1:A:188:ALA:HA	1:A:218:GLN:OE1	2.11	0.51
1:A:471:GLN:O	1:A:497:VAL:CG2	2.58	0.51
1:M:188:ALA:HA	1:M:218:GLN:OE1	2.11	0.51
1:N:456:ARG:NH1	2:N:700:FDP:O2P	2.34	0.51
1:C:491:GLN:HG3	1:P:491:GLN:HG3	1.93	0.51
1:Q:3:LEU:HD23	1:S:283:SER:CB	2.41	0.51
1:S:471:GLN:O	1:S:497:VAL:CG2	2.58	0.51
1:T:188:ALA:HA	1:T:218:GLN:OE1	2.11	0.51
1:V:188:ALA:HA	1:V:218:GLN:OE1	2.11	0.51
1:B:103:ARG:CB	1:G:58:GLU:OE1	2.59	0.51
1:B:270:PRO:HG2	1:B:273:LYS:HD2	1.92	0.51
1:I:188:ALA:HA	1:I:218:GLN:OE1	2.11	0.51
1:M:483:HIS:NE2	1:N:483:HIS:HD2	2.09	0.51
1:B:492:THR:HG22	1:O:492:THR:HG22	1.92	0.51
1:P:211:SER:HA	1:P:238:LYS:HD3	1.93	0.51
1:T:240:GLU:HB3	1:T:264:ASP:HB2	1.91	0.51
1:R:297:GLN:CB	1:T:310:ARG:HB2	2.34	0.51
1:V:11:ILE:O	1:X:273:LYS:HE3	2.10	0.51
1:C:456:ARG:NH1	2:C:700:FDP:O2P	2.34	0.51
1:B:276:VAL:HG13	1:C:9:LEU:HB3	1.93	0.51
1:F:240:GLU:HB3	1:F:264:ASP:HB2	1.91	0.51
1:I:471:GLN:O	1:I:497:VAL:CG2	2.58	0.51
1:Q:240:GLU:HB3	1:Q:264:ASP:HB2	1.91	0.51
1:U:372:ILE:HG23	1:V:390:GLU:C	2.29	0.51
1:W:372:ILE:CG1	1:X:390:GLU:O	2.58	0.51
1:C:211:SER:HA	1:C:238:LYS:HD3	1.93	0.51
1:D:188:ALA:HA	1:D:218:GLN:OE1	2.11	0.51
1:D:193:ASP:O	1:D:197:LEU:N	2.38	0.51
1:D:211:SER:HA	1:D:238:LYS:HD3	1.93	0.51
1:E:193:ASP:O	1:E:196:ASP:N	2.44	0.51
1:E:471:GLN:O	1:E:497:VAL:CG2	2.58	0.51
1:H:193:ASP:O	1:H:196:ASP:N	2.44	0.51
1:I:270:PRO:HD2	1:I:273:LYS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:193:ASP:O	1:J:196:ASP:N	2.44	0.51
1:J:471:GLN:O	1:J:497:VAL:CG2	2.58	0.51
1:J:49:ARG:NE	1:J:83:ASP:OD2	2.33	0.51
1:K:211:SER:HA	1:K:238:LYS:HD3	1.93	0.51
1:K:240:GLU:HB3	1:K:264:ASP:HB2	1.91	0.51
1:L:49:ARG:NE	1:L:83:ASP:OD2	2.33	0.51
1:P:372:ILE:HD12	1:P:374:MET:CG	2.40	0.51
1:S:188:ALA:HA	1:S:218:GLN:OE1	2.11	0.51
1:U:373:PRO:HB3	1:V:391:THR:C	2.32	0.51
1:V:193:ASP:O	1:V:196:ASP:N	2.44	0.51
1:V:49:ARG:NE	1:V:83:ASP:OD2	2.33	0.51
1:E:269:ILE:HG12	1:G:11:ILE:HD12	1.93	0.51
1:I:147:ILE:HG21	1:I:169:HIS:CD2	2.46	0.51
1:I:240:GLU:HB3	1:I:264:ASP:HB2	1.91	0.51
1:H:373:PRO:HB3	1:I:391:THR:HA	1.92	0.51
1:K:188:ALA:HA	1:K:218:GLN:OE1	2.11	0.51
1:M:483:HIS:CD2	1:N:483:HIS:CD2	2.98	0.51
1:Q:193:ASP:O	1:Q:196:ASP:N	2.44	0.51
1:R:456:ARG:HH22	2:R:700:FDP:P1	2.34	0.51
1:S:147:ILE:HG21	1:S:169:HIS:NE2	2.26	0.51
1:U:211:SER:HA	1:U:238:LYS:HD3	1.93	0.51
1:V:270:PRO:HD2	1:V:273:LYS:HD2	1.93	0.51
1:U:352:GLU:HG2	1:W:272:GLU:CG	2.40	0.51
1:V:284:LYS:HG2	1:X:7:LEU:HD22	1.86	0.51
1:A:193:ASP:O	1:A:196:ASP:N	2.44	0.51
1:A:193:ASP:O	1:A:197:LEU:N	2.38	0.51
1:B:270:PRO:O	1:B:273:LYS:HB2	2.11	0.51
1:B:272:GLU:HG2	1:C:352:GLU:HG2	1.93	0.51
1:C:270:PRO:O	1:C:273:LYS:HB2	2.11	0.51
1:E:456:ARG:NH1	2:E:700:FDP:O2P	2.34	0.51
1:F:483:HIS:HD2	1:G:483:HIS:NE2	2.08	0.51
1:K:270:PRO:O	1:K:273:LYS:HB2	2.11	0.51
1:L:147:ILE:HG21	1:L:169:HIS:CD2	2.46	0.51
1:M:193:ASP:O	1:M:196:ASP:N	2.44	0.51
1:O:11:ILE:O	1:P:273:LYS:CE	2.56	0.51
1:O:188:ALA:HA	1:O:218:GLN:OE1	2.11	0.51
1:O:240:GLU:HB3	1:O:264:ASP:HB2	1.91	0.51
1:Q:270:PRO:O	1:Q:273:LYS:HB2	2.11	0.51
1:Q:456:ARG:HH22	2:Q:700:FDP:P1	2.34	0.51
1:S:193:ASP:O	1:S:196:ASP:N	2.44	0.51
1:S:49:ARG:NE	1:S:83:ASP:OD2	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:193:ASP:O	1:V:197:LEU:N	2.38	0.51
1:W:211:SER:HA	1:W:238:LYS:HD3	1.93	0.51
1:X:193:ASP:O	1:X:196:ASP:N	2.44	0.51
1:X:211:SER:HA	1:X:238:LYS:HD3	1.93	0.51
1:B:188:ALA:HA	1:B:218:GLN:OE1	2.11	0.50
1:B:310:ARG:HG2	1:C:297:GLN:HB2	1.92	0.50
1:D:193:ASP:O	1:D:196:ASP:N	2.44	0.50
1:E:147:ILE:HG21	1:E:169:HIS:NE2	2.27	0.50
1:E:188:ALA:HA	1:E:218:GLN:OE1	2.11	0.50
1:E:283:SER:CB	1:G:3:LEU:CD2	2.89	0.50
1:K:193:ASP:O	1:K:196:ASP:N	2.44	0.50
1:K:471:GLN:O	1:K:497:VAL:CG2	2.58	0.50
1:O:147:ILE:HG21	1:O:169:HIS:NE2	2.26	0.50
1:O:270:PRO:O	1:O:273:LYS:HB2	2.11	0.50
1:U:193:ASP:O	1:U:196:ASP:N	2.44	0.50
1:U:188:ALA:HA	1:U:218:GLN:OE1	2.11	0.50
1:P:195:VAL:CG2	1:U:496:LEU:HD21	2.40	0.50
1:V:147:ILE:HG21	1:V:169:HIS:NE2	2.26	0.50
1:W:193:ASP:O	1:W:197:LEU:N	2.38	0.50
1:A:270:PRO:O	1:A:273:LYS:HB2	2.11	0.50
1:B:193:ASP:O	1:B:196:ASP:N	2.44	0.50
1:C:147:ILE:HG21	1:C:169:HIS:NE2	2.27	0.50
1:C:456:ARG:HH22	2:C:700:FDP:P1	2.34	0.50
1:E:270:PRO:HD2	1:E:273:LYS:HD2	1.93	0.50
1:F:147:ILE:HG21	1:F:169:HIS:NE2	2.26	0.50
1:F:193:ASP:O	1:F:196:ASP:N	2.44	0.50
1:H:49:ARG:NE	1:H:83:ASP:OD2	2.33	0.50
1:I:211:SER:HA	1:I:238:LYS:HD3	1.93	0.50
1:H:311:ALA:HA	1:J:315:ASP:HB2	1.93	0.50
1:J:456:ARG:HH22	2:J:700:FDP:P1	2.34	0.50
1:J:472:THR:CG2	1:J:498:GLU:HA	2.18	0.50
1:L:193:ASP:O	1:L:196:ASP:N	2.44	0.50
1:L:240:GLU:HB3	1:L:264:ASP:HB2	1.91	0.50
1:L:270:PRO:HD2	1:L:273:LYS:HD2	1.93	0.50
1:L:297:GLN:CB	1:N:310:ARG:CG	2.89	0.50
1:L:297:GLN:HB2	1:N:310:ARG:CB	2.41	0.50
1:M:211:SER:HA	1:M:238:LYS:HD3	1.93	0.50
1:N:147:ILE:HG21	1:N:169:HIS:NE2	2.27	0.50
1:N:193:ASP:O	1:N:196:ASP:N	2.44	0.50
1:N:211:SER:HA	1:N:238:LYS:HD3	1.93	0.50
1:O:193:ASP:O	1:O:196:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:147:ILE:HG21	1:P:169:HIS:NE2	2.27	0.50
1:P:188:ALA:HA	1:P:218:GLN:OE1	2.11	0.50
1:R:188:ALA:HA	1:R:218:GLN:OE1	2.11	0.50
1:R:193:ASP:O	1:R:196:ASP:N	2.44	0.50
1:T:147:ILE:HG21	1:T:169:HIS:NE2	2.27	0.50
1:T:193:ASP:O	1:T:196:ASP:N	2.44	0.50
1:X:147:ILE:HG21	1:X:169:HIS:CD2	2.47	0.50
1:A:147:ILE:HG21	1:A:169:HIS:NE2	2.27	0.50
1:A:211:SER:HA	1:A:238:LYS:HD3	1.93	0.50
1:A:456:ARG:HH22	2:A:700:FDP:P1	2.33	0.50
1:B:147:ILE:HG21	1:B:169:HIS:CD2	2.46	0.50
1:C:372:ILE:HD11	1:C:374:MET:HE1	1.92	0.50
1:D:270:PRO:O	1:D:273:LYS:HB2	2.11	0.50
1:F:147:ILE:HG21	1:F:169:HIS:CD2	2.46	0.50
1:E:273:LYS:HG2	1:G:11:ILE:HB	1.92	0.50
1:H:211:SER:HA	1:H:238:LYS:HD3	1.93	0.50
1:J:188:ALA:HA	1:J:218:GLN:OE1	2.11	0.50
1:P:193:ASP:O	1:P:196:ASP:N	2.44	0.50
1:R:270:PRO:HD2	1:R:273:LYS:HD2	1.93	0.50
1:S:211:SER:HA	1:S:238:LYS:HD3	1.93	0.50
1:V:211:SER:HA	1:V:238:LYS:HD3	1.93	0.50
1:D:240:GLU:HB3	1:D:264:ASP:HB2	1.91	0.50
1:D:456:ARG:HH22	2:D:700:FDP:P1	2.34	0.50
1:I:472:THR:CG2	1:I:498:GLU:HA	2.18	0.50
1:J:193:ASP:CA	1:J:196:ASP:HB2	2.41	0.50
1:N:147:ILE:HG21	1:N:169:HIS:CD2	2.46	0.50
1:N:188:ALA:HA	1:N:218:GLN:OE1	2.11	0.50
1:Q:147:ILE:HG21	1:Q:169:HIS:NE2	2.26	0.50
1:U:147:ILE:HG21	1:U:169:HIS:CD2	2.46	0.50
1:U:270:PRO:O	1:U:273:LYS:HB2	2.11	0.50
1:W:147:ILE:HG21	1:W:169:HIS:NE2	2.26	0.50
1:W:193:ASP:O	1:W:196:ASP:N	2.44	0.50
1:V:280:ILE:CD1	1:X:9:LEU:HB2	2.40	0.50
1:B:147:ILE:HG21	1:B:169:HIS:NE2	2.27	0.50
1:B:211:SER:HA	1:B:238:LYS:HD3	1.93	0.50
1:G:188:ALA:HA	1:G:218:GLN:OE1	2.11	0.50
1:H:312:GLU:CA	1:J:311:ALA:CB	2.71	0.50
1:M:147:ILE:HG21	1:M:169:HIS:CD2	2.46	0.50
1:K:352:GLU:HB2	1:M:272:GLU:HG3	1.94	0.50
1:O:352:GLU:HG2	1:P:272:GLU:O	2.11	0.50
1:R:147:ILE:HG21	1:R:169:HIS:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:193:ASP:CA	1:T:196:ASP:HB2	2.42	0.50
1:U:11:ILE:O	1:W:273:LYS:CG	2.60	0.50
1:U:297:GLN:OE1	1:W:309:THR:HA	2.12	0.50
1:W:390:GLU:OE1	1:X:379:ALA:HA	2.12	0.50
1:B:456:ARG:HH22	2:B:700:FDP:P1	2.34	0.50
1:C:188:ALA:HA	1:C:218:GLN:OE1	2.11	0.50
1:D:147:ILE:HG21	1:D:169:HIS:NE2	2.26	0.50
1:E:211:SER:HA	1:E:238:LYS:HD3	1.93	0.50
1:J:147:ILE:HG21	1:J:169:HIS:CD2	2.46	0.50
1:J:147:ILE:HG21	1:J:169:HIS:NE2	2.26	0.50
1:K:372:ILE:HD11	1:L:390:GLU:HG2	1.93	0.50
1:K:297:GLN:OE1	1:M:310:ARG:NH2	2.45	0.50
1:O:147:ILE:HG21	1:O:169:HIS:CD2	2.46	0.50
1:R:211:SER:HA	1:R:238:LYS:HD3	1.93	0.50
1:U:263:GLY:HA2	1:W:310:ARG:NH1	2.16	0.50
1:X:372:ILE:HD11	1:X:374:MET:HE2	1.93	0.50
1:B:472:THR:CG2	1:B:498:GLU:HA	2.18	0.50
1:C:193:ASP:O	1:C:196:ASP:N	2.44	0.50
1:E:193:ASP:O	1:E:197:LEU:N	2.38	0.50
1:H:188:ALA:HA	1:H:218:GLN:OE1	2.11	0.50
1:H:270:PRO:O	1:H:273:LYS:HB2	2.11	0.50
1:I:11:ILE:HG13	1:I:12:PHE:HD2	1.72	0.50
1:L:7:LEU:CD2	1:N:284:LYS:HG3	2.42	0.50
1:T:211:SER:HA	1:T:238:LYS:HD3	1.93	0.50
1:R:311:ALA:HB1	1:T:315:ASP:HB2	1.94	0.50
1:V:11:ILE:HG12	1:V:12:PHE:CD2	2.47	0.50
1:A:49:ARG:NE	1:A:83:ASP:OD2	2.33	0.50
1:G:147:ILE:HG21	1:G:169:HIS:NE2	2.27	0.50
1:G:211:SER:HA	1:G:238:LYS:HD3	1.93	0.50
1:L:211:SER:HA	1:L:238:LYS:HD3	1.93	0.50
1:P:372:ILE:HD12	1:P:374:MET:HG3	1.92	0.50
1:Q:211:SER:HA	1:Q:238:LYS:HD3	1.93	0.50
1:Q:491:GLN:HG3	1:R:491:GLN:HG3	1.93	0.50
1:S:51:ASN:HA	1:S:83:ASP:HB3	1.94	0.50
1:V:284:LYS:CE	1:X:7:LEU:HD22	2.41	0.50
1:X:188:ALA:HA	1:X:218:GLN:OE1	2.11	0.50
1:B:51:ASN:HA	1:B:83:ASP:HB3	1.94	0.50
1:C:51:ASN:HA	1:C:83:ASP:HB3	1.94	0.50
1:D:49:ARG:NE	1:D:83:ASP:OD2	2.33	0.50
1:I:193:ASP:O	1:I:196:ASP:N	2.44	0.50
1:J:211:SER:HA	1:J:238:LYS:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:147:ILE:HG21	1:K:169:HIS:NE2	2.27	0.50
1:Q:272:GLU:CB	1:S:352:GLU:HG2	2.42	0.50
1:S:456:ARG:HH22	2:S:700:FDP:P1	2.34	0.50
1:V:147:ILE:HG21	1:V:169:HIS:CD2	2.46	0.50
1:W:472:THR:CG2	1:W:498:GLU:HA	2.18	0.50
1:X:147:ILE:HG21	1:X:169:HIS:NE2	2.27	0.50
1:F:211:SER:HA	1:F:238:LYS:HD3	1.93	0.49
1:I:12:PHE:N	1:I:12:PHE:CD2	2.79	0.49
1:K:147:ILE:HG21	1:K:169:HIS:CD2	2.47	0.49
1:Q:188:ALA:HA	1:Q:218:GLN:OE1	2.11	0.49
1:Q:193:ASP:CA	1:Q:196:ASP:HB2	2.42	0.49
1:T:147:ILE:HG21	1:T:169:HIS:CD2	2.47	0.49
1:U:352:GLU:HB2	1:W:272:GLU:HG3	1.94	0.49
1:D:147:ILE:HG21	1:D:169:HIS:CD2	2.46	0.49
1:F:49:ARG:NE	1:F:83:ASP:OD2	2.33	0.49
1:G:193:ASP:O	1:G:196:ASP:N	2.44	0.49
1:H:147:ILE:HG21	1:H:169:HIS:NE2	2.26	0.49
1:M:147:ILE:HG21	1:M:169:HIS:NE2	2.26	0.49
1:N:51:ASN:HA	1:N:83:ASP:HB3	1.94	0.49
1:R:147:ILE:HG21	1:R:169:HIS:CD2	2.46	0.49
1:U:456:ARG:HH22	2:U:700:FDP:P1	2.34	0.49
1:U:456:ARG:NH1	2:U:700:FDP:O2P	2.35	0.49
1:U:383:SER:HB2	1:V:383:SER:CB	2.42	0.49
1:A:147:ILE:HG21	1:A:169:HIS:CD2	2.46	0.49
1:A:51:ASN:HA	1:A:83:ASP:HB3	1.95	0.49
1:F:456:ARG:HH22	2:F:700:FDP:P1	2.34	0.49
1:H:51:ASN:HA	1:H:83:ASP:HB3	1.94	0.49
1:O:211:SER:HA	1:O:238:LYS:HD3	1.93	0.49
1:Q:51:ASN:HA	1:Q:83:ASP:HB3	1.94	0.49
1:W:390:GLU:OE1	1:X:379:ALA:CA	2.60	0.49
1:H:147:ILE:HG21	1:H:169:HIS:CD2	2.46	0.49
1:I:49:ARG:NE	1:I:83:ASP:OD2	2.33	0.49
1:L:147:ILE:HG21	1:L:169:HIS:NE2	2.27	0.49
1:Q:471:GLN:O	1:Q:497:VAL:HG22	2.13	0.49
1:R:11:ILE:HG12	1:R:12:PHE:CD2	2.47	0.49
1:U:270:PRO:HG2	1:U:273:LYS:HD2	1.92	0.49
1:V:273:LYS:CD	1:X:11:ILE:HB	2.43	0.49
1:V:283:SER:HB3	1:X:3:LEU:HD23	1.93	0.49
1:W:147:ILE:HG21	1:W:169:HIS:CD2	2.46	0.49
1:X:270:PRO:O	1:X:273:LYS:HB2	2.12	0.49
1:B:270:PRO:HD2	1:B:273:LYS:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:ASN:HA	1:E:83:ASP:HB3	1.94	0.49
1:A:391:THR:O	1:J:373:PRO:HB3	2.11	0.49
1:L:51:ASN:HA	1:L:83:ASP:HB3	1.94	0.49
1:M:19:ARG:NH1	1:M:21:ALA:O	2.46	0.49
1:L:12:PHE:CZ	1:N:242:HIS:NE2	2.80	0.49
1:P:147:ILE:HG21	1:P:169:HIS:CD2	2.46	0.49
1:Q:147:ILE:HG21	1:Q:169:HIS:CD2	2.46	0.49
1:Q:284:LYS:HG3	1:S:7:LEU:HD22	1.93	0.49
1:S:147:ILE:HG21	1:S:169:HIS:CD2	2.46	0.49
1:U:471:GLN:O	1:U:497:VAL:HG22	2.13	0.49
1:A:19:ARG:NH1	1:A:21:ALA:O	2.46	0.49
1:C:471:GLN:O	1:C:497:VAL:HG22	2.13	0.49
1:E:147:ILE:HG21	1:E:169:HIS:CD2	2.46	0.49
1:E:372:ILE:HD11	1:E:374:MET:HE1	1.93	0.49
1:G:147:ILE:HG21	1:G:169:HIS:CD2	2.47	0.49
1:G:19:ARG:NH1	1:G:21:ALA:O	2.46	0.49
1:H:272:GLU:C	1:J:352:GLU:HG2	2.32	0.49
1:I:456:ARG:HH22	2:I:700:FDP:P1	2.34	0.49
1:L:284:LYS:HG3	1:N:7:LEU:HD22	1.92	0.49
1:L:487:GLY:CA	1:S:229:LYS:CG	2.76	0.49
1:I:229:LYS:HD2	1:M:487:GLY:CA	2.41	0.49
1:M:391:THR:HA	1:N:373:PRO:HB3	1.94	0.49
1:Q:193:ASP:O	1:Q:197:LEU:N	2.38	0.49
1:Q:7:LEU:CD2	1:S:284:LYS:HG3	2.43	0.49
1:U:147:ILE:HG21	1:U:169:HIS:NE2	2.26	0.49
1:V:19:ARG:NH1	1:V:21:ALA:O	2.46	0.49
1:A:193:ASP:CA	1:A:196:ASP:HB2	2.41	0.49
1:B:471:GLN:O	1:B:497:VAL:HG22	2.13	0.49
1:C:147:ILE:HG21	1:C:169:HIS:CD2	2.47	0.49
1:F:193:ASP:CA	1:F:196:ASP:HB2	2.42	0.49
1:H:19:ARG:NH1	1:H:21:ALA:O	2.46	0.49
1:I:147:ILE:HG21	1:I:169:HIS:NE2	2.26	0.49
1:I:51:ASN:HA	1:I:83:ASP:HB3	1.94	0.49
1:N:270:PRO:O	1:N:273:LYS:HB2	2.12	0.49
1:L:3:LEU:CD2	1:N:283:SER:HB3	2.42	0.49
1:T:270:PRO:O	1:T:273:LYS:HB2	2.12	0.49
1:T:471:GLN:O	1:T:497:VAL:HG22	2.13	0.49
1:U:51:ASN:HA	1:U:83:ASP:HB3	1.94	0.49
1:V:482:ASP:H	1:V:490:ASN:HD21	1.61	0.49
1:D:51:ASN:HA	1:D:83:ASP:HB3	1.94	0.49
1:F:372:ILE:HD11	1:F:374:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:ASN:HA	1:F:83:ASP:HB3	1.95	0.49
1:G:471:GLN:O	1:G:497:VAL:HG22	2.13	0.49
1:G:49:ARG:NE	1:G:83:ASP:OD2	2.33	0.49
1:H:311:ALA:HA	1:J:315:ASP:CB	2.43	0.49
1:H:352:GLU:CB	1:J:272:GLU:HB2	2.42	0.49
1:K:51:ASN:HA	1:K:83:ASP:HB3	1.94	0.49
1:N:49:ARG:NE	1:N:83:ASP:OD2	2.33	0.49
1:O:471:GLN:O	1:O:497:VAL:HG22	2.13	0.49
1:S:471:GLN:O	1:S:497:VAL:HG22	2.13	0.49
1:U:482:ASP:H	1:U:490:ASN:HD21	1.61	0.49
1:V:471:GLN:O	1:V:497:VAL:HG22	2.13	0.49
1:V:51:ASN:HA	1:V:83:ASP:HB3	1.94	0.49
1:X:51:ASN:HA	1:X:83:ASP:HB3	1.94	0.49
1:A:270:PRO:HD2	1:A:273:LYS:HD3	1.95	0.49
1:F:482:ASP:H	1:F:490:ASN:HD21	1.61	0.49
1:E:273:LYS:HB3	1:G:11:ILE:HB	1.95	0.49
1:F:391:THR:C	1:G:373:PRO:HB3	2.33	0.49
1:C:216:ALA:CB	1:N:446:LYS:CE	2.81	0.49
1:N:482:ASP:H	1:N:490:ASN:HD21	1.61	0.49
1:S:482:ASP:H	1:S:490:ASN:HD21	1.61	0.49
1:V:276:VAL:C	1:V:280:ILE:HD12	2.33	0.49
1:W:51:ASN:HA	1:W:83:ASP:HB3	1.95	0.49
1:B:19:ARG:NH1	1:B:21:ALA:O	2.46	0.49
1:C:19:ARG:NH1	1:C:21:ALA:O	2.46	0.49
1:F:471:GLN:O	1:F:497:VAL:HG22	2.13	0.49
1:A:12:PHE:CE2	1:I:242:HIS:CE1	3.00	0.49
1:K:310:ARG:CG	1:M:297:GLN:HB2	2.43	0.49
1:L:11:ILE:HG13	1:L:12:PHE:HD2	1.72	0.49
1:L:482:ASP:H	1:L:490:ASN:HD21	1.61	0.49
1:M:482:ASP:H	1:M:490:ASN:HD21	1.61	0.49
1:M:471:GLN:O	1:M:497:VAL:HG22	2.13	0.49
1:O:270:PRO:HD2	1:O:273:LYS:HD3	1.95	0.49
1:U:352:GLU:HG2	1:W:272:GLU:O	2.13	0.49
1:C:482:ASP:H	1:C:490:ASN:HD21	1.61	0.48
1:D:193:ASP:CA	1:D:196:ASP:HB2	2.41	0.48
1:D:482:ASP:H	1:D:490:ASN:HD21	1.61	0.48
1:G:90:ARG:HD3	1:G:174:ARG:O	2.13	0.48
1:G:270:PRO:O	1:G:273:LYS:HB2	2.12	0.48
1:G:51:ASN:HA	1:G:83:ASP:HB3	1.94	0.48
1:J:471:GLN:O	1:J:497:VAL:HG22	2.13	0.48
1:L:11:ILE:HG12	1:L:12:PHE:CD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:471:GLN:O	1:L:497:VAL:HG22	2.13	0.48
1:P:471:GLN:O	1:P:497:VAL:HG22	2.13	0.48
1:R:90:ARG:HD3	1:R:174:ARG:O	2.13	0.48
1:T:90:ARG:HD3	1:T:174:ARG:O	2.14	0.48
1:U:310:ARG:CB	1:W:297:GLN:HB2	2.42	0.48
1:W:482:ASP:H	1:W:490:ASN:HD21	1.61	0.48
1:B:283:SER:CB	1:C:3:LEU:CD2	2.91	0.48
1:B:297:GLN:OE1	1:C:310:ARG:NH2	2.45	0.48
1:C:270:PRO:HD2	1:C:273:LYS:HD3	1.95	0.48
1:C:270:PRO:HG2	1:C:273:LYS:HD2	1.92	0.48
1:H:482:ASP:H	1:H:490:ASN:HD21	1.61	0.48
1:J:90:ARG:HD3	1:J:174:ARG:O	2.13	0.48
1:K:472:THR:CG2	1:K:498:GLU:HA	2.18	0.48
1:L:90:ARG:HD3	1:L:174:ARG:O	2.13	0.48
1:L:272:GLU:HB2	1:N:352:GLU:HG2	1.94	0.48
1:P:90:ARG:HD3	1:P:174:ARG:O	2.14	0.48
1:P:89:ILE:HG21	1:P:177:VAL:HG22	1.96	0.48
1:R:12:PHE:N	1:R:12:PHE:CD2	2.79	0.48
1:S:90:ARG:HD3	1:S:174:ARG:O	2.13	0.48
1:V:284:LYS:HG3	1:X:7:LEU:HD23	1.80	0.48
1:A:482:ASP:H	1:A:490:ASN:HD21	1.61	0.48
1:B:272:GLU:HG3	1:C:352:GLU:CG	2.43	0.48
1:D:391:THR:C	1:E:373:PRO:HB3	2.34	0.48
1:E:482:ASP:H	1:E:490:ASN:HD21	1.61	0.48
1:E:471:GLN:O	1:E:497:VAL:HG22	2.13	0.48
1:H:471:GLN:O	1:H:497:VAL:HG22	2.13	0.48
1:I:89:ILE:HG21	1:I:177:VAL:HG22	1.96	0.48
1:I:90:ARG:HD3	1:I:174:ARG:O	2.13	0.48
1:K:89:ILE:HG21	1:K:177:VAL:HG22	1.96	0.48
1:M:89:ILE:HG21	1:M:177:VAL:HG22	1.96	0.48
1:O:90:ARG:HD3	1:O:174:ARG:O	2.13	0.48
1:O:51:ASN:HA	1:O:83:ASP:HB3	1.94	0.48
1:Q:3:LEU:CD2	1:S:283:SER:CB	2.91	0.48
1:U:90:ARG:HD3	1:U:174:ARG:O	2.13	0.48
1:D:19:ARG:NH1	1:D:21:ALA:O	2.46	0.48
1:F:90:ARG:HD3	1:F:174:ARG:O	2.13	0.48
1:H:90:ARG:HD3	1:H:174:ARG:O	2.13	0.48
1:H:372:ILE:HD11	1:I:390:GLU:HG2	1.94	0.48
1:K:471:GLN:O	1:K:497:VAL:HG22	2.13	0.48
1:M:90:ARG:HD3	1:M:174:ARG:O	2.13	0.48
1:R:273:LYS:CB	1:T:11:ILE:HB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:19:ARG:NH1	1:T:21:ALA:O	2.46	0.48
1:T:51:ASN:HA	1:T:83:ASP:HB3	1.94	0.48
1:U:19:ARG:NH1	1:U:21:ALA:O	2.46	0.48
1:V:284:LYS:HE2	1:X:7:LEU:HD22	1.95	0.48
1:U:11:ILE:HB	1:W:273:LYS:HB3	1.93	0.48
1:A:89:ILE:HG21	1:A:177:VAL:HG22	1.96	0.48
1:B:456:ARG:NH1	2:B:700:FDP:O2P	2.34	0.48
1:D:212:PHE:HD2	1:D:214:ARG:HH21	1.62	0.48
1:J:51:ASN:HA	1:J:83:ASP:HB3	1.94	0.48
1:Q:270:PRO:HD2	1:Q:273:LYS:HD3	1.95	0.48
1:R:482:ASP:H	1:R:490:ASN:HD21	1.61	0.48
1:U:311:ALA:HB3	1:W:312:GLU:HG3	1.95	0.48
1:V:89:ILE:HG21	1:V:177:VAL:HG22	1.96	0.48
1:W:193:ASP:CA	1:W:196:ASP:HB2	2.42	0.48
1:X:90:ARG:HD3	1:X:174:ARG:O	2.13	0.48
1:A:90:ARG:HD3	1:A:174:ARG:O	2.14	0.48
1:D:242:HIS:CE1	1:F:12:PHE:CE2	3.02	0.48
1:F:472:THR:CG2	1:F:498:GLU:HA	2.18	0.48
1:H:483:HIS:CD2	1:I:483:HIS:CD2	3.01	0.48
1:J:19:ARG:NH1	1:J:21:ALA:O	2.46	0.48
1:H:272:GLU:HG3	1:J:352:GLU:HB2	1.95	0.48
1:L:19:ARG:NH1	1:L:21:ALA:O	2.46	0.48
1:M:51:ASN:HA	1:M:83:ASP:HB3	1.94	0.48
1:M:376:ALA:HA	1:N:494:ILE:HD12	1.96	0.48
1:Q:482:ASP:H	1:Q:490:ASN:HD21	1.61	0.48
1:U:297:GLN:HB3	1:W:310:ARG:H	1.77	0.48
1:W:90:ARG:HD3	1:W:174:ARG:O	2.13	0.48
1:E:90:ARG:HD3	1:E:174:ARG:O	2.13	0.48
1:E:212:PHE:HD2	1:E:214:ARG:HH21	1.62	0.48
1:F:89:ILE:HG21	1:F:177:VAL:HG22	1.96	0.48
1:G:193:ASP:CA	1:G:196:ASP:HB2	2.41	0.48
1:H:89:ILE:HG21	1:H:177:VAL:HG22	1.96	0.48
1:I:195:VAL:CG2	1:N:496:LEU:HG	2.43	0.48
1:C:390:GLU:O	1:P:372:ILE:HG13	2.14	0.48
1:Q:212:PHE:HD2	1:Q:214:ARG:HH21	1.62	0.48
1:Q:276:VAL:CG1	1:S:9:LEU:HB3	2.43	0.48
1:Q:379:ALA:CB	1:R:390:GLU:OE1	2.62	0.48
1:V:279:LYS:HB3	1:X:6:ASN:OD1	2.13	0.48
1:W:372:ILE:HD11	1:X:390:GLU:HG2	1.96	0.48
1:V:9:LEU:CB	1:X:280:ILE:HD11	2.42	0.48
1:B:402:THR:OG1	1:B:404:ARG:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:GLN:O	1:D:497:VAL:HG22	2.13	0.48
1:I:193:ASP:CA	1:I:196:ASP:HB2	2.41	0.48
1:K:272:GLU:CG	1:M:352:GLU:HG2	2.44	0.48
1:M:49:ARG:NE	1:M:83:ASP:OD2	2.33	0.48
1:M:373:PRO:CA	1:N:390:GLU:O	2.46	0.48
1:N:90:ARG:HD3	1:N:174:ARG:O	2.13	0.48
1:Q:193:ASP:O	1:Q:196:ASP:HB2	2.14	0.48
1:R:51:ASN:HA	1:R:83:ASP:HB3	1.94	0.48
1:Q:297:GLN:CD	1:S:310:ARG:HG2	2.24	0.48
1:S:372:ILE:CG1	1:T:390:GLU:CG	2.91	0.48
1:S:372:ILE:HG23	1:T:390:GLU:C	2.33	0.48
1:U:89:ILE:HG21	1:U:177:VAL:HG22	1.96	0.48
1:V:212:PHE:HD2	1:V:214:ARG:HH21	1.62	0.48
1:W:471:GLN:O	1:W:497:VAL:HG22	2.13	0.48
1:X:212:PHE:HD2	1:X:214:ARG:HH21	1.62	0.48
1:X:471:GLN:O	1:X:497:VAL:HG22	2.13	0.48
1:E:402:THR:OG1	1:E:404:ARG:HB2	2.14	0.48
1:F:270:PRO:O	1:F:273:LYS:HB2	2.14	0.48
1:F:390:GLU:HG2	1:G:372:ILE:HD11	1.94	0.48
1:G:193:ASP:O	1:G:196:ASP:HB2	2.14	0.48
1:I:402:THR:OG1	1:I:404:ARG:HB2	2.14	0.48
1:J:402:THR:OG1	1:J:404:ARG:HB2	2.14	0.48
1:J:482:ASP:H	1:J:490:ASN:HD21	1.61	0.48
1:M:212:PHE:HD2	1:M:214:ARG:HH21	1.62	0.48
1:O:49:ARG:NE	1:O:83:ASP:OD2	2.33	0.48
1:P:270:PRO:O	1:P:273:LYS:HB2	2.14	0.48
1:Q:311:ALA:CB	1:S:312:GLU:HA	2.43	0.48
1:T:49:ARG:NE	1:T:83:ASP:OD2	2.33	0.48
1:T:89:ILE:HG21	1:T:177:VAL:HG22	1.96	0.48
1:V:12:PHE:CD2	1:V:12:PHE:N	2.79	0.48
1:V:402:THR:OG1	1:V:404:ARG:HB2	2.14	0.48
1:X:19:ARG:NH1	1:X:21:ALA:O	2.46	0.48
1:G:212:PHE:HD2	1:G:214:ARG:HH21	1.62	0.48
1:I:471:GLN:O	1:I:497:VAL:HG22	2.13	0.48
1:J:212:PHE:HD2	1:J:214:ARG:HH21	1.62	0.48
1:K:19:ARG:NH1	1:K:21:ALA:O	2.46	0.48
1:M:193:ASP:O	1:M:196:ASP:HB2	2.14	0.48
1:N:471:GLN:O	1:N:497:VAL:HG22	2.13	0.48
1:O:193:ASP:O	1:O:196:ASP:HB2	2.14	0.48
1:P:402:THR:OG1	1:P:404:ARG:HB2	2.14	0.48
1:P:51:ASN:HA	1:P:83:ASP:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:19:ARG:NH1	1:R:21:ALA:O	2.46	0.48
1:S:193:ASP:O	1:S:196:ASP:HB2	2.14	0.48
1:R:297:GLN:CD	1:T:310:ARG:HG2	2.34	0.48
1:D:270:PRO:HD2	1:D:273:LYS:HD3	1.95	0.47
1:D:402:THR:OG1	1:D:404:ARG:HB2	2.14	0.47
1:E:89:ILE:HG21	1:E:177:VAL:HG22	1.96	0.47
1:H:311:ALA:O	1:J:311:ALA:O	2.31	0.47
1:I:11:ILE:HG12	1:I:12:PHE:CD2	2.47	0.47
1:J:193:ASP:O	1:J:196:ASP:HB2	2.14	0.47
1:J:270:PRO:O	1:J:273:LYS:HB2	2.14	0.47
1:L:273:LYS:HG2	1:N:11:ILE:CA	2.44	0.47
1:L:372:ILE:HD12	1:L:374:MET:HG3	1.96	0.47
1:O:89:ILE:HG21	1:O:177:VAL:HG22	1.96	0.47
1:Q:19:ARG:NH1	1:Q:21:ALA:O	2.46	0.47
1:Q:402:THR:OG1	1:Q:404:ARG:HB2	2.14	0.47
1:S:19:ARG:NH1	1:S:21:ALA:O	2.46	0.47
1:S:402:THR:OG1	1:S:404:ARG:HB2	2.14	0.47
1:V:90:ARG:HD3	1:V:174:ARG:O	2.13	0.47
1:X:193:ASP:O	1:X:196:ASP:HB2	2.14	0.47
1:X:402:THR:OG1	1:X:404:ARG:HB2	2.14	0.47
1:X:89:ILE:HG21	1:X:177:VAL:HG22	1.96	0.47
1:B:89:ILE:HG21	1:B:177:VAL:HG22	1.96	0.47
1:C:49:ARG:NE	1:C:83:ASP:OD2	2.33	0.47
1:H:371:HIS:C	1:H:372:ILE:HD13	2.34	0.47
1:N:89:ILE:HG21	1:N:177:VAL:HG22	1.95	0.47
1:R:471:GLN:O	1:R:497:VAL:HG22	2.13	0.47
1:S:384:ALA:O	1:S:387:SER:HB2	2.14	0.47
1:U:193:ASP:O	1:U:196:ASP:HB2	2.14	0.47
1:A:193:ASP:O	1:A:196:ASP:HB2	2.14	0.47
1:A:471:GLN:O	1:A:497:VAL:HG22	2.13	0.47
1:C:402:THR:OG1	1:C:404:ARG:HB2	2.14	0.47
1:D:472:THR:CG2	1:D:498:GLU:HA	2.18	0.47
1:K:193:ASP:CA	1:K:196:ASP:HB2	2.41	0.47
1:K:270:PRO:HD2	1:K:273:LYS:HD3	1.95	0.47
1:L:89:ILE:HG21	1:L:177:VAL:HG22	1.95	0.47
1:O:315:ASP:CB	1:P:311:ALA:HA	2.42	0.47
1:O:365:SER:CB	1:P:3:LEU:HD12	2.45	0.47
1:R:212:PHE:HD2	1:R:214:ARG:HH21	1.62	0.47
1:T:193:ASP:O	1:T:196:ASP:HB2	2.14	0.47
1:U:6:ASN:OD1	1:W:279:LYS:CE	2.51	0.47
1:C:193:ASP:O	1:C:196:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:ALA:O	1:D:387:SER:HB2	2.14	0.47
1:E:103:ARG:HG3	1:E:167:ASN:HA	1.97	0.47
1:H:270:PRO:HD2	1:H:273:LYS:HD3	1.95	0.47
1:I:193:ASP:O	1:I:196:ASP:HB2	2.14	0.47
1:I:482:ASP:H	1:I:490:ASN:HD21	1.61	0.47
1:P:384:ALA:O	1:P:387:SER:HB2	2.15	0.47
1:Q:49:ARG:NE	1:Q:83:ASP:OD2	2.33	0.47
1:T:212:PHE:HD2	1:T:214:ARG:HH21	1.62	0.47
1:R:11:ILE:HB	1:T:273:LYS:HG2	1.95	0.47
1:T:402:THR:OG1	1:T:404:ARG:HB2	2.14	0.47
1:W:19:ARG:NH1	1:W:21:ALA:O	2.46	0.47
1:X:482:ASP:H	1:X:490:ASN:HD21	1.61	0.47
1:C:193:ASP:CA	1:C:196:ASP:HB2	2.41	0.47
1:C:90:ARG:HD3	1:C:174:ARG:O	2.13	0.47
1:D:456:ARG:NH1	2:D:700:FDP:O2P	2.34	0.47
1:G:482:ASP:H	1:G:490:ASN:HD21	1.61	0.47
1:H:384:ALA:O	1:H:387:SER:HB2	2.14	0.47
1:J:384:ALA:O	1:J:387:SER:HB2	2.14	0.47
1:O:19:ARG:NH1	1:O:21:ALA:O	2.46	0.47
1:O:310:ARG:NH2	1:P:297:GLN:OE1	2.47	0.47
1:Q:90:ARG:HD3	1:Q:174:ARG:O	2.14	0.47
1:C:496:LEU:CG	1:V:195:VAL:CG2	2.80	0.47
1:V:193:ASP:O	1:V:196:ASP:HB2	2.14	0.47
1:X:193:ASP:CA	1:X:196:ASP:HB2	2.41	0.47
1:X:384:ALA:O	1:X:387:SER:HB2	2.14	0.47
1:C:384:ALA:O	1:C:387:SER:HB2	2.14	0.47
1:D:90:ARG:HD3	1:D:174:ARG:O	2.13	0.47
1:D:89:ILE:HG21	1:D:177:VAL:HG22	1.96	0.47
1:F:193:ASP:O	1:F:196:ASP:HB2	2.14	0.47
1:K:482:ASP:H	1:K:490:ASN:HD21	1.61	0.47
1:L:384:ALA:O	1:L:387:SER:HB2	2.14	0.47
1:M:193:ASP:CA	1:M:196:ASP:HB2	2.41	0.47
1:N:193:ASP:O	1:N:196:ASP:HB2	2.14	0.47
1:N:224:LYS:HE3	1:N:224:LYS:HB3	1.81	0.47
1:O:270:PRO:CG	1:O:273:LYS:HD2	2.45	0.47
1:O:310:ARG:HG2	1:P:297:GLN:CB	2.42	0.47
1:P:212:PHE:HD2	1:P:214:ARG:HH21	1.62	0.47
1:P:19:ARG:NH1	1:P:21:ALA:O	2.46	0.47
1:S:89:ILE:HG21	1:S:177:VAL:HG22	1.96	0.47
1:U:270:PRO:HD2	1:U:273:LYS:HD3	1.95	0.47
1:C:250:SER:HB2	1:N:446:LYS:CD	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ASP:O	1:D:196:ASP:HB2	2.14	0.47
1:F:384:ALA:O	1:F:387:SER:HB2	2.14	0.47
1:H:193:ASP:O	1:H:196:ASP:HB2	2.14	0.47
1:I:384:ALA:O	1:I:387:SER:HB2	2.14	0.47
1:L:193:ASP:CA	1:L:196:ASP:HB2	2.41	0.47
1:N:402:THR:OG1	1:N:404:ARG:HB2	2.14	0.47
1:O:384:ALA:O	1:O:387:SER:HB2	2.14	0.47
1:O:482:ASP:H	1:O:490:ASN:HD21	1.61	0.47
1:Q:297:GLN:HB2	1:S:310:ARG:HG2	1.95	0.47
1:S:493:ARG:HG2	1:T:482:ASP:OD2	2.15	0.47
1:Q:284:LYS:CG	1:S:7:LEU:CD2	2.90	0.47
1:U:212:PHE:HD2	1:U:214:ARG:HH21	1.62	0.47
1:U:310:ARG:HB2	1:W:297:GLN:HB2	1.97	0.47
1:U:372:ILE:HD12	1:U:374:MET:HG2	1.97	0.47
1:W:212:PHE:HD2	1:W:214:ARG:HH21	1.62	0.47
1:W:89:ILE:HG21	1:W:177:VAL:HG22	1.96	0.47
1:G:384:ALA:O	1:G:387:SER:HB2	2.15	0.47
1:G:402:THR:OG1	1:G:404:ARG:HB2	2.15	0.47
1:G:89:ILE:HG21	1:G:177:VAL:HG22	1.96	0.47
1:H:270:PRO:CG	1:H:273:LYS:HD2	2.45	0.47
1:J:89:ILE:HG21	1:J:177:VAL:HG22	1.96	0.47
1:K:193:ASP:O	1:K:196:ASP:HB2	2.14	0.47
1:K:193:ASP:O	1:K:197:LEU:N	2.38	0.47
1:L:12:PHE:CD2	1:L:12:PHE:N	2.79	0.47
1:O:212:PHE:HD2	1:O:214:ARG:HH21	1.62	0.47
1:O:365:SER:HB3	1:P:3:LEU:HD12	1.95	0.47
1:W:384:ALA:O	1:W:387:SER:HB2	2.14	0.47
1:B:482:ASP:H	1:B:490:ASN:HD21	1.61	0.47
1:E:384:ALA:O	1:E:387:SER:HB2	2.14	0.47
1:F:402:THR:OG1	1:F:404:ARG:HB2	2.14	0.47
1:H:11:ILE:HG13	1:H:12:PHE:HD2	1.80	0.47
1:H:242:HIS:NE2	1:J:12:PHE:HE2	2.11	0.47
1:I:212:PHE:HD2	1:I:214:ARG:HH21	1.62	0.47
1:I:456:ARG:NH1	2:I:700:FDP:O2P	2.34	0.47
1:J:224:LYS:HB3	1:J:224:LYS:HE3	1.82	0.47
1:K:90:ARG:HD3	1:K:174:ARG:O	2.13	0.47
1:M:270:PRO:O	1:M:273:LYS:HB2	2.14	0.47
1:P:193:ASP:O	1:P:196:ASP:HB2	2.14	0.47
1:P:49:ARG:NE	1:P:83:ASP:OD2	2.33	0.47
1:R:89:ILE:HG21	1:R:177:VAL:HG22	1.96	0.47
1:C:89:ILE:HG21	1:C:177:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:ILE:O	1:F:273:LYS:HE3	2.15	0.47
1:D:270:PRO:CG	1:D:273:LYS:HD2	2.45	0.47
1:E:193:ASP:O	1:E:196:ASP:HB2	2.14	0.47
1:F:212:PHE:HD2	1:F:214:ARG:HH21	1.62	0.47
1:H:193:ASP:CA	1:H:196:ASP:HB2	2.42	0.47
1:K:297:GLN:CB	1:M:310:ARG:HG2	2.44	0.47
1:N:19:ARG:NH1	1:N:21:ALA:O	2.46	0.47
1:Q:89:ILE:HG21	1:Q:177:VAL:HG22	1.96	0.47
1:U:384:ALA:O	1:U:387:SER:HB2	2.14	0.47
1:V:193:ASP:CA	1:V:196:ASP:HB2	2.41	0.47
1:V:370:GLN:CB	1:V:374:MET:SD	3.03	0.47
1:A:270:PRO:CG	1:A:273:LYS:HD2	2.45	0.47
1:A:370:GLN:CB	1:A:374:MET:SD	3.03	0.47
1:B:270:PRO:CG	1:B:273:LYS:HD2	2.45	0.47
1:B:384:ALA:O	1:B:387:SER:HB2	2.14	0.47
1:D:373:PRO:HB3	1:E:391:THR:HA	1.97	0.47
1:I:19:ARG:NH1	1:I:21:ALA:O	2.46	0.47
1:L:212:PHE:HD2	1:L:214:ARG:HH21	1.62	0.47
1:L:231:ARG:HH21	1:S:231:ARG:HH21	1.62	0.47
1:M:402:THR:OG1	1:M:404:ARG:HB2	2.14	0.47
1:L:273:LYS:HG2	1:N:11:ILE:HB	1.96	0.47
1:N:384:ALA:O	1:N:387:SER:HB2	2.14	0.47
1:O:11:ILE:HB	1:P:273:LYS:CB	2.45	0.47
1:S:270:PRO:O	1:S:273:LYS:HB2	2.14	0.47
1:T:384:ALA:O	1:T:387:SER:HB2	2.14	0.47
1:W:193:ASP:O	1:W:196:ASP:HB2	2.14	0.47
1:A:283:SER:HB3	1:I:3:LEU:HD21	1.96	0.46
1:A:402:THR:OG1	1:A:404:ARG:HB2	2.14	0.46
1:B:193:ASP:CA	1:B:196:ASP:HB2	2.41	0.46
1:B:193:ASP:O	1:B:196:ASP:HB2	2.14	0.46
1:C:212:PHE:HD2	1:C:214:ARG:HH21	1.62	0.46
1:E:12:PHE:N	1:E:12:PHE:CD2	2.79	0.46
1:H:311:ALA:CB	1:J:312:GLU:HG2	2.44	0.46
1:P:482:ASP:H	1:P:490:ASN:HD21	1.61	0.46
1:U:193:ASP:CA	1:U:196:ASP:HB2	2.41	0.46
1:A:384:ALA:O	1:A:387:SER:HB2	2.14	0.46
1:B:311:ALA:HA	1:C:315:ASP:HB2	1.97	0.46
1:D:272:GLU:HG3	1:F:352:GLU:HB2	1.97	0.46
1:L:193:ASP:O	1:L:196:ASP:HB2	2.14	0.46
1:M:384:ALA:O	1:M:387:SER:HB2	2.14	0.46
1:O:424:ARG:CG	1:O:424:ARG:NH1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:193:ASP:CA	1:P:196:ASP:HB2	2.42	0.46
1:Q:284:LYS:CG	1:S:7:LEU:HD22	2.46	0.46
1:T:372:ILE:HD12	1:T:374:MET:CG	2.46	0.46
1:V:384:ALA:O	1:V:387:SER:HB2	2.14	0.46
1:X:370:GLN:CB	1:X:374:MET:SD	3.03	0.46
1:A:273:LYS:NZ	1:I:352:GLU:OE1	2.48	0.46
1:C:270:PRO:CG	1:C:273:LYS:HD2	2.45	0.46
1:A:369:LEU:CD1	1:I:3:LEU:HD13	2.45	0.46
1:K:372:ILE:HD12	1:K:374:MET:CG	2.46	0.46
1:I:229:LYS:CG	1:M:487:GLY:HA3	2.25	0.46
1:Q:370:GLN:CB	1:Q:374:MET:SD	3.03	0.46
1:R:11:ILE:HG13	1:R:12:PHE:HD2	1.72	0.46
1:R:193:ASP:O	1:R:196:ASP:HB2	2.14	0.46
1:R:297:GLN:HB3	1:R:297:GLN:HE21	1.50	0.46
1:R:384:ALA:O	1:R:387:SER:HB2	2.15	0.46
1:W:270:PRO:O	1:W:273:LYS:HB2	2.14	0.46
1:A:372:ILE:HD11	1:A:374:MET:HE2	1.96	0.46
1:B:276:VAL:CG1	1:C:9:LEU:HB3	2.45	0.46
1:B:370:GLN:CB	1:B:374:MET:SD	3.03	0.46
1:E:370:GLN:CB	1:E:374:MET:SD	3.03	0.46
1:E:297:GLN:HB2	1:G:310:ARG:CG	2.46	0.46
1:K:212:PHE:HD2	1:K:214:ARG:HH21	1.62	0.46
1:K:270:PRO:CG	1:K:273:LYS:HD2	2.45	0.46
1:K:384:ALA:O	1:K:387:SER:HB2	2.14	0.46
1:K:390:GLU:HG2	1:L:374:MET:CE	2.45	0.46
1:M:391:THR:HA	1:N:373:PRO:CB	2.45	0.46
1:O:311:ALA:HB3	1:P:312:GLU:HG3	1.97	0.46
1:Q:270:PRO:CG	1:Q:273:LYS:HD2	2.45	0.46
1:Q:384:ALA:O	1:Q:387:SER:HB2	2.14	0.46
1:X:372:ILE:HD12	1:X:374:MET:CG	2.46	0.46
1:B:212:PHE:HD2	1:B:214:ARG:HH21	1.62	0.46
1:E:19:ARG:NH1	1:E:21:ALA:O	2.46	0.46
1:H:372:ILE:HG13	1:I:390:GLU:O	2.15	0.46
1:J:372:ILE:HD12	1:J:374:MET:CG	2.46	0.46
1:N:193:ASP:CA	1:N:196:ASP:HB2	2.42	0.46
1:N:372:ILE:HD12	1:N:372:ILE:HA	1.73	0.46
1:O:370:GLN:CB	1:O:374:MET:SD	3.03	0.46
1:T:364:ASN:O	1:T:368:LYS:HG2	2.16	0.46
1:T:482:ASP:H	1:T:490:ASN:HD21	1.61	0.46
1:W:372:ILE:HD12	1:W:374:MET:CG	2.46	0.46
1:X:424:ARG:CG	1:X:424:ARG:NH1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:THR:O	1:P:373:PRO:HB3	2.16	0.46
1:F:370:GLN:CB	1:F:374:MET:SD	3.03	0.46
1:L:364:ASN:O	1:L:368:LYS:HG2	2.16	0.46
1:L:273:LYS:HG2	1:N:11:ILE:HA	1.96	0.46
1:N:370:GLN:CB	1:N:374:MET:SD	3.03	0.46
1:O:297:GLN:OE1	1:P:310:ARG:NH2	2.49	0.46
1:O:402:THR:OG1	1:O:404:ARG:HB2	2.15	0.46
1:R:297:GLN:HB2	1:T:310:ARG:CB	2.36	0.46
1:U:270:PRO:CG	1:U:273:LYS:HD2	2.45	0.46
1:A:362:PHE:HD2	1:A:366:ILE:HD12	1.81	0.46
1:B:364:ASN:O	1:B:368:LYS:HG2	2.16	0.46
1:C:364:ASN:O	1:C:368:LYS:HG2	2.16	0.46
1:C:370:GLN:CB	1:C:374:MET:SD	3.03	0.46
1:D:370:GLN:CB	1:D:374:MET:SD	3.03	0.46
1:D:424:ARG:NH1	1:D:424:ARG:CG	2.41	0.46
1:F:19:ARG:NH1	1:F:21:ALA:O	2.46	0.46
1:F:372:ILE:HD12	1:F:374:MET:CG	2.46	0.46
1:G:372:ILE:HD12	1:G:374:MET:CG	2.46	0.46
1:A:12:PHE:HE2	1:I:242:HIS:CE1	2.34	0.46
1:A:297:GLN:OE1	1:I:310:ARG:HG2	2.15	0.46
1:H:390:GLU:O	1:I:373:PRO:CB	2.63	0.46
1:K:272:GLU:HG3	1:M:352:GLU:CB	2.43	0.46
1:L:276:VAL:CG1	1:N:9:LEU:CB	2.92	0.46
1:L:310:ARG:CZ	1:N:297:GLN:OE1	2.64	0.46
1:N:212:PHE:HD2	1:N:214:ARG:HH21	1.62	0.46
1:M:483:HIS:HD2	1:N:483:HIS:NE2	2.13	0.46
1:A:364:ASN:O	1:A:368:LYS:HG2	2.16	0.46
1:B:90:ARG:HD3	1:B:174:ARG:O	2.13	0.46
1:K:364:ASN:O	1:K:368:LYS:HG2	2.16	0.46
1:M:364:ASN:O	1:M:368:LYS:HG2	2.16	0.46
1:O:362:PHE:HD2	1:O:366:ILE:HD12	1.81	0.46
1:Q:472:THR:CG2	1:Q:498:GLU:HA	2.18	0.46
1:S:212:PHE:HD2	1:S:214:ARG:HH21	1.62	0.46
1:V:287:VAL:CG2	1:X:3:LEU:HD22	2.46	0.46
1:V:297:GLN:NE2	1:V:300:GLU:HB3	2.24	0.46
1:A:472:THR:CG2	1:A:498:GLU:HA	2.18	0.46
1:B:79:ALA:HB2	1:B:429:ARG:O	2.16	0.46
1:E:79:ALA:HB2	1:E:429:ARG:O	2.16	0.46
1:I:364:ASN:O	1:I:368:LYS:HG2	2.16	0.46
1:J:362:PHE:HD2	1:J:366:ILE:HD12	1.81	0.46
1:M:472:THR:CG2	1:M:498:GLU:CA	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:79:ALA:HB2	1:M:429:ARG:O	2.16	0.46
1:Q:193:ASP:C	1:Q:196:ASP:H	2.20	0.46
1:R:364:ASN:O	1:R:368:LYS:HG2	2.16	0.46
1:W:402:THR:OG1	1:W:404:ARG:HB2	2.16	0.46
1:A:224:LYS:HB3	1:A:224:LYS:HE3	1.82	0.46
1:C:362:PHE:HD2	1:C:366:ILE:HD12	1.81	0.46
1:D:193:ASP:C	1:D:196:ASP:H	2.20	0.46
1:E:11:ILE:HG12	1:E:12:PHE:CD2	2.47	0.46
1:H:212:PHE:HD2	1:H:214:ARG:HH21	1.62	0.46
1:Q:362:PHE:HD2	1:Q:366:ILE:HD12	1.81	0.46
1:W:370:GLN:CB	1:W:374:MET:SD	3.03	0.46
1:X:364:ASN:O	1:X:368:LYS:HG2	2.16	0.46
1:B:193:ASP:C	1:B:196:ASP:H	2.20	0.45
1:C:372:ILE:HD12	1:C:374:MET:CG	2.46	0.45
1:E:372:ILE:HD12	1:E:374:MET:CG	2.46	0.45
1:G:364:ASN:O	1:G:368:LYS:HG2	2.16	0.45
1:F:373:PRO:CB	1:G:390:GLU:O	2.64	0.45
1:H:193:ASP:C	1:H:196:ASP:H	2.20	0.45
1:H:79:ALA:HB2	1:H:429:ARG:O	2.16	0.45
1:S:362:PHE:HD2	1:S:366:ILE:HD12	1.81	0.45
1:S:364:ASN:O	1:S:368:LYS:HG2	2.16	0.45
1:V:193:ASP:C	1:V:196:ASP:H	2.20	0.45
1:V:79:ALA:HB2	1:V:429:ARG:O	2.16	0.45
1:X:193:ASP:C	1:X:196:ASP:H	2.20	0.45
1:A:212:PHE:HD2	1:A:214:ARG:HH21	1.62	0.45
1:A:372:ILE:HD12	1:A:374:MET:CG	2.46	0.45
1:B:224:LYS:HE3	1:B:224:LYS:HB3	1.82	0.45
1:D:372:ILE:HD12	1:D:374:MET:CG	2.46	0.45
1:F:362:PHE:HD2	1:F:366:ILE:HD12	1.81	0.45
1:G:370:GLN:CB	1:G:374:MET:SD	3.03	0.45
1:H:297:GLN:HG3	1:J:310:ARG:CG	2.43	0.45
1:H:364:ASN:O	1:H:368:LYS:HG2	2.16	0.45
1:I:79:ALA:HB2	1:I:429:ARG:O	2.16	0.45
1:H:376:ALA:HA	1:I:494:ILE:HD12	1.98	0.45
1:H:352:GLU:OE1	1:J:272:GLU:HG2	2.16	0.45
1:K:12:PHE:CE2	1:M:242:HIS:NE2	2.77	0.45
1:L:193:ASP:C	1:L:196:ASP:H	2.20	0.45
1:L:272:GLU:C	1:N:352:GLU:HG2	2.36	0.45
1:N:362:PHE:HD2	1:N:366:ILE:HD12	1.81	0.45
1:Q:456:ARG:NH1	2:Q:700:FDP:O2P	2.34	0.45
1:R:79:ALA:HB2	1:R:429:ARG:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:362:PHE:HD2	1:T:366:ILE:HD12	1.81	0.45
1:V:372:ILE:HD12	1:V:374:MET:CG	2.46	0.45
1:C:168:SER:O	1:C:169:HIS:HB2	2.17	0.45
1:D:364:ASN:O	1:D:368:LYS:HG2	2.16	0.45
1:E:193:ASP:C	1:E:196:ASP:H	2.20	0.45
1:E:193:ASP:CA	1:E:196:ASP:HB2	2.41	0.45
1:G:79:ALA:HB2	1:G:429:ARG:O	2.16	0.45
1:I:195:VAL:HG22	1:N:496:LEU:CD2	2.46	0.45
1:J:364:ASN:O	1:J:368:LYS:HG2	2.16	0.45
1:K:49:ARG:NE	1:K:83:ASP:OD2	2.33	0.45
1:L:168:SER:O	1:L:169:HIS:HB2	2.17	0.45
1:H:496:LEU:HD21	1:M:195:VAL:HG23	1.97	0.45
1:N:79:ALA:HB2	1:N:429:ARG:O	2.16	0.45
1:O:193:ASP:CA	1:O:196:ASP:HB2	2.41	0.45
1:O:79:ALA:HB2	1:O:429:ARG:O	2.16	0.45
1:C:383:SER:CB	1:P:383:SER:HB2	2.45	0.45
1:Q:79:ALA:HB2	1:Q:429:ARG:O	2.16	0.45
1:S:168:SER:O	1:S:169:HIS:HB2	2.17	0.45
1:Q:272:GLU:HG3	1:S:352:GLU:CG	2.45	0.45
1:U:168:SER:O	1:U:169:HIS:HB2	2.17	0.45
1:A:193:ASP:C	1:A:196:ASP:H	2.20	0.45
1:B:280:ILE:CG1	1:C:6:ASN:O	2.64	0.45
1:G:193:ASP:O	1:G:197:LEU:N	2.38	0.45
1:N:193:ASP:C	1:N:196:ASP:H	2.20	0.45
1:N:364:ASN:O	1:N:368:LYS:HG2	2.16	0.45
1:O:372:ILE:HD12	1:O:374:MET:CG	2.46	0.45
1:P:193:ASP:C	1:P:196:ASP:H	2.20	0.45
1:P:364:ASN:O	1:P:368:LYS:HG2	2.16	0.45
1:O:279:LYS:HE3	1:P:6:ASN:OD1	2.15	0.45
1:Q:372:ILE:HD12	1:Q:374:MET:CG	2.46	0.45
1:S:456:ARG:NH1	2:S:700:FDP:O2P	2.34	0.45
1:V:364:ASN:O	1:V:368:LYS:HG2	2.16	0.45
1:W:79:ALA:HB2	1:W:429:ARG:O	2.16	0.45
1:V:284:LYS:HG2	1:X:7:LEU:CD2	2.38	0.45
1:D:79:ALA:HB2	1:D:429:ARG:O	2.16	0.45
1:D:272:GLU:CG	1:F:352:GLU:HG2	2.47	0.45
1:F:79:ALA:HB2	1:F:429:ARG:O	2.16	0.45
1:G:168:SER:O	1:G:169:HIS:HB2	2.17	0.45
1:H:311:ALA:CB	1:J:312:GLU:CA	2.72	0.45
1:J:370:GLN:CB	1:J:374:MET:SD	3.03	0.45
1:K:370:GLN:CB	1:K:374:MET:SD	3.03	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:168:SER:O	1:Q:169:HIS:HB2	2.17	0.45
1:R:273:LYS:HD3	1:T:11:ILE:C	2.33	0.45
1:R:362:PHE:HD2	1:R:366:ILE:HD12	1.81	0.45
1:T:193:ASP:C	1:T:196:ASP:H	2.20	0.45
1:U:193:ASP:O	1:U:197:LEU:N	2.38	0.45
1:A:79:ALA:HB2	1:A:429:ARG:O	2.16	0.45
1:C:494:ILE:HD12	1:P:376:ALA:HA	1.97	0.45
1:F:456:ARG:NH1	2:F:700:FDP:O2P	2.34	0.45
1:G:193:ASP:C	1:G:196:ASP:H	2.20	0.45
1:G:362:PHE:HD2	1:G:366:ILE:HD12	1.81	0.45
1:H:242:HIS:NE2	1:J:12:PHE:CE2	2.79	0.45
1:J:193:ASP:C	1:J:196:ASP:H	2.20	0.45
1:M:168:SER:O	1:M:169:HIS:HB2	2.17	0.45
1:N:168:SER:O	1:N:169:HIS:HB2	2.17	0.45
1:N:372:ILE:HD12	1:N:374:MET:CG	2.46	0.45
1:O:193:ASP:C	1:O:196:ASP:H	2.20	0.45
1:O:11:ILE:O	1:P:273:LYS:CD	2.65	0.45
1:S:193:ASP:C	1:S:196:ASP:H	2.20	0.45
1:R:311:ALA:CB	1:T:315:ASP:HB2	2.46	0.45
1:U:364:ASN:O	1:U:368:LYS:HG2	2.16	0.45
1:W:362:PHE:HD2	1:W:366:ILE:HD12	1.81	0.45
1:X:401:ASN:N	2:X:700:FDP:O5P	2.50	0.45
1:B:168:SER:O	1:B:169:HIS:HB2	2.17	0.45
1:C:79:ALA:HB2	1:C:429:ARG:O	2.16	0.45
1:D:168:SER:O	1:D:169:HIS:HB2	2.17	0.45
1:E:11:ILE:HG13	1:E:12:PHE:HD2	1.72	0.45
1:H:315:ASP:CB	1:J:311:ALA:CA	2.89	0.45
1:I:168:SER:O	1:I:169:HIS:HB2	2.17	0.45
1:K:362:PHE:HD2	1:K:366:ILE:HD12	1.81	0.45
1:O:168:SER:O	1:O:169:HIS:HB2	2.17	0.45
1:O:472:THR:CG2	1:O:498:GLU:CA	2.84	0.45
1:R:193:ASP:C	1:R:196:ASP:H	2.20	0.45
1:W:193:ASP:C	1:W:196:ASP:H	2.20	0.45
1:A:223:ARG:NH1	1:A:223:ARG:HG2	2.25	0.45
1:F:168:SER:O	1:F:169:HIS:HB2	2.17	0.45
1:F:193:ASP:C	1:F:196:ASP:H	2.20	0.45
1:E:242:HIS:NE2	1:G:12:PHE:HE2	2.15	0.45
1:J:79:ALA:HB2	1:J:429:ARG:O	2.16	0.45
1:P:362:PHE:HD2	1:P:366:ILE:HD12	1.81	0.45
1:R:311:ALA:HB1	1:T:311:ALA:O	2.16	0.45
1:U:193:ASP:C	1:U:196:ASP:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:168:SER:O	1:V:169:HIS:HB2	2.17	0.45
1:C:193:ASP:C	1:C:196:ASP:H	2.20	0.45
1:C:178:ASN:OD1	1:C:268:GLU:OE2	2.35	0.45
1:H:270:PRO:CG	1:H:273:LYS:CD	2.94	0.45
1:I:193:ASP:C	1:I:196:ASP:H	2.20	0.45
1:L:178:ASN:OD1	1:L:268:GLU:OE2	2.35	0.45
1:L:272:GLU:O	1:N:352:GLU:HG2	2.17	0.45
1:K:297:GLN:OE1	1:M:310:ARG:CZ	2.65	0.45
1:O:372:ILE:HD11	1:O:374:MET:HE2	1.98	0.45
1:S:79:ALA:HB2	1:S:429:ARG:O	2.16	0.45
1:S:494:ILE:HD12	1:T:376:ALA:CB	2.44	0.45
1:U:188:ALA:CB	1:U:218:GLN:HG2	2.21	0.45
1:U:372:ILE:HA	1:U:372:ILE:HD12	1.78	0.45
1:V:273:LYS:CG	1:X:11:ILE:HB	2.47	0.45
1:V:9:LEU:HB2	1:X:280:ILE:CD1	2.42	0.45
1:W:364:ASN:O	1:W:368:LYS:HG2	2.16	0.45
1:X:178:ASN:OD1	1:X:268:GLU:OE2	2.35	0.45
1:F:364:ASN:O	1:F:368:LYS:HG2	2.16	0.45
1:F:372:ILE:HA	1:F:372:ILE:HD12	1.73	0.45
1:H:9:LEU:CB	1:J:276:VAL:HG13	2.46	0.45
1:P:178:ASN:OD1	1:P:268:GLU:OE2	2.35	0.45
1:Q:11:ILE:CB	1:S:273:LYS:HG2	2.46	0.45
1:W:168:SER:O	1:W:169:HIS:HB2	2.17	0.45
1:B:362:PHE:HD2	1:B:366:ILE:HD12	1.81	0.44
1:D:224:LYS:HB3	1:D:224:LYS:HE3	1.82	0.44
1:E:364:ASN:O	1:E:368:LYS:HG2	2.16	0.44
1:H:311:ALA:HB3	1:J:312:GLU:HG2	1.98	0.44
1:I:178:ASN:OD1	1:I:268:GLU:OE2	2.35	0.44
1:I:362:PHE:HD2	1:I:366:ILE:HD12	1.81	0.44
1:N:178:ASN:OD1	1:N:268:GLU:OE2	2.35	0.44
1:Q:352:GLU:HG2	1:S:272:GLU:O	2.16	0.44
1:P:487:GLY:N	1:V:229:LYS:HE3	2.29	0.44
1:U:372:ILE:CG1	1:V:390:GLU:O	2.65	0.44
1:C:270:PRO:CG	1:C:273:LYS:CD	2.94	0.44
1:D:178:ASN:OD1	1:D:268:GLU:OE2	2.35	0.44
1:E:283:SER:OG	1:G:3:LEU:CD2	2.64	0.44
1:G:372:ILE:HD12	1:G:372:ILE:HA	1.73	0.44
1:H:362:PHE:HD2	1:H:366:ILE:HD12	1.81	0.44
1:J:17:ASN:HD22	1:J:17:ASN:C	2.21	0.44
1:M:472:THR:CG2	1:M:498:GLU:HA	2.18	0.44
1:Q:178:ASN:OD1	1:Q:268:GLU:OE2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:193:ASP:CA	1:S:196:ASP:HB2	2.42	0.44
1:T:188:ALA:CB	1:T:218:GLN:HG2	2.21	0.44
1:U:491:GLN:OE1	1:U:493:ARG:HD2	2.18	0.44
1:U:390:GLU:HG2	1:V:374:MET:HE2	1.99	0.44
1:B:372:ILE:HD12	1:B:374:MET:CG	2.46	0.44
1:D:17:ASN:C	1:D:17:ASN:HD22	2.21	0.44
1:F:178:ASN:OD1	1:F:268:GLU:OE2	2.35	0.44
1:J:491:GLN:OE1	1:J:493:ARG:HD2	2.18	0.44
1:K:193:ASP:C	1:K:196:ASP:H	2.20	0.44
1:K:491:GLN:OE1	1:K:493:ARG:HD2	2.18	0.44
1:L:17:ASN:C	1:L:17:ASN:HD22	2.21	0.44
1:M:483:HIS:CD2	1:N:483:HIS:NE2	2.85	0.44
1:O:178:ASN:OD1	1:O:268:GLU:OE2	2.35	0.44
1:Q:270:PRO:CG	1:Q:273:LYS:CD	2.94	0.44
1:T:168:SER:O	1:T:169:HIS:HB2	2.17	0.44
1:S:376:ALA:HB1	1:T:494:ILE:HB	1.99	0.44
1:V:17:ASN:C	1:V:17:ASN:HD22	2.21	0.44
1:X:362:PHE:HD2	1:X:366:ILE:HD12	1.81	0.44
1:X:79:ALA:HB2	1:X:429:ARG:O	2.16	0.44
1:A:17:ASN:HD22	1:A:17:ASN:C	2.21	0.44
1:B:178:ASN:OD1	1:B:268:GLU:OE2	2.35	0.44
1:C:17:ASN:C	1:C:17:ASN:HD22	2.21	0.44
1:K:79:ALA:HB2	1:K:429:ARG:O	2.17	0.44
1:M:193:ASP:C	1:M:196:ASP:H	2.20	0.44
1:M:373:PRO:HB3	1:N:391:THR:CA	2.45	0.44
1:O:398:VAL:HG13	1:O:479:ILE:HB	2.00	0.44
1:P:168:SER:O	1:P:169:HIS:HB2	2.17	0.44
1:T:178:ASN:OD1	1:T:268:GLU:OE2	2.35	0.44
1:R:284:LYS:CG	1:T:7:LEU:HD21	2.38	0.44
1:U:362:PHE:HD2	1:U:366:ILE:HD12	1.81	0.44
1:V:178:ASN:OD1	1:V:268:GLU:OE2	2.35	0.44
1:X:17:ASN:HD22	1:X:17:ASN:C	2.21	0.44
1:B:372:ILE:HD11	1:B:374:MET:HE1	1.98	0.44
1:B:280:ILE:HD11	1:C:9:LEU:HB2	1.99	0.44
1:J:178:ASN:OD1	1:J:268:GLU:OE2	2.35	0.44
1:K:372:ILE:HD11	1:K:374:MET:HE2	2.00	0.44
1:K:391:THR:C	1:L:373:PRO:HB3	2.37	0.44
1:L:491:GLN:OE1	1:L:493:ARG:HD2	2.18	0.44
1:M:483:HIS:NE2	1:N:483:HIS:CD2	2.86	0.44
1:L:3:LEU:HD23	1:N:283:SER:HB3	1.98	0.44
1:N:451:GLU:H	1:N:451:GLU:HG2	1.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:6:ASN:OD1	1:P:279:LYS:CE	2.54	0.44
1:P:224:LYS:HB3	1:P:224:LYS:HE3	1.82	0.44
1:R:491:GLN:OE1	1:R:493:ARG:HD2	2.18	0.44
1:U:79:ALA:HB2	1:U:429:ARG:O	2.16	0.44
1:V:362:PHE:HD2	1:V:366:ILE:HD12	1.81	0.44
1:V:491:GLN:OE1	1:V:493:ARG:HD2	2.18	0.44
1:U:11:ILE:HG13	1:W:273:LYS:HD3	1.99	0.44
1:A:168:SER:O	1:A:169:HIS:HB2	2.17	0.44
1:A:178:ASN:OD1	1:A:268:GLU:OE2	2.35	0.44
1:B:398:VAL:HG13	1:B:479:ILE:HB	2.00	0.44
1:D:491:GLN:HG3	1:E:491:GLN:HG3	1.99	0.44
1:E:491:GLN:OE1	1:E:493:ARG:HD2	2.18	0.44
1:J:168:SER:O	1:J:169:HIS:HB2	2.17	0.44
1:K:17:ASN:C	1:K:17:ASN:HD22	2.21	0.44
1:L:79:ALA:HB2	1:L:429:ARG:O	2.16	0.44
1:O:352:GLU:HB2	1:P:272:GLU:HG3	1.99	0.44
1:P:17:ASN:C	1:P:17:ASN:HD22	2.21	0.44
1:P:79:ALA:HB2	1:P:429:ARG:O	2.16	0.44
1:Q:383:SER:CB	1:R:383:SER:HB2	2.46	0.44
1:Q:374:MET:HE2	1:R:390:GLU:HG2	1.99	0.44
1:U:372:ILE:HD12	1:U:374:MET:HG3	1.99	0.44
1:V:372:ILE:HD12	1:V:372:ILE:HA	1.73	0.44
1:X:372:ILE:HA	1:X:372:ILE:HD12	1.73	0.44
1:X:491:GLN:OE1	1:X:493:ARG:HD2	2.18	0.44
1:D:362:PHE:HD2	1:D:366:ILE:HD12	1.81	0.44
1:D:398:VAL:HG13	1:D:479:ILE:HB	2.00	0.44
1:E:398:VAL:HG13	1:E:479:ILE:HB	2.00	0.44
1:H:17:ASN:C	1:H:17:ASN:HD22	2.21	0.44
1:H:491:GLN:OE1	1:H:493:ARG:HD2	2.18	0.44
1:J:101:MET:HE1	1:J:124:PHE:CE1	2.53	0.44
1:K:168:SER:O	1:K:169:HIS:HB2	2.17	0.44
1:L:401:ASN:N	2:L:700:FDP:O5P	2.50	0.44
1:O:17:ASN:HD22	1:O:17:ASN:C	2.21	0.44
1:O:364:ASN:O	1:O:368:LYS:HG2	2.16	0.44
1:P:424:ARG:CG	1:P:424:ARG:NH1	2.41	0.44
1:Q:297:GLN:HB2	1:S:310:ARG:HB2	2.00	0.44
1:Q:364:ASN:O	1:Q:368:LYS:HG2	2.16	0.44
1:T:3:LEU:HD23	1:T:4:ALA:N	2.24	0.44
1:T:491:GLN:OE1	1:T:493:ARG:HD2	2.18	0.44
1:T:79:ALA:HB2	1:T:429:ARG:O	2.16	0.44
1:U:17:ASN:HD22	1:U:17:ASN:C	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:178:ASN:OD1	1:W:268:GLU:OE2	2.35	0.44
1:W:398:VAL:HG13	1:W:479:ILE:HB	2.00	0.44
1:E:17:ASN:C	1:E:17:ASN:HD22	2.21	0.44
1:E:362:PHE:HD2	1:E:366:ILE:HD12	1.81	0.44
1:H:312:GLU:CG	1:J:311:ALA:HB3	2.48	0.44
1:J:398:VAL:HG13	1:J:479:ILE:HB	2.00	0.44
1:L:352:GLU:HG2	1:N:272:GLU:C	2.38	0.44
1:O:401:ASN:N	2:O:700:FDP:O5P	2.50	0.44
1:Q:451:GLU:H	1:Q:451:GLU:HG2	1.59	0.44
1:Q:491:GLN:OE1	1:Q:493:ARG:HD2	2.18	0.44
1:W:17:ASN:HD22	1:W:17:ASN:C	2.21	0.44
1:W:49:ARG:NE	1:W:83:ASP:OD2	2.33	0.44
1:X:168:SER:O	1:X:169:HIS:HB2	2.17	0.44
1:C:491:GLN:OE1	1:C:493:ARG:HD2	2.18	0.44
1:D:491:GLN:OE1	1:D:493:ARG:HD2	2.18	0.44
1:D:6:ASN:OD1	1:F:279:LYS:HE3	2.17	0.44
1:H:398:VAL:HG13	1:H:479:ILE:HB	2.00	0.44
1:K:101:MET:HE1	1:K:124:PHE:CE1	2.53	0.44
1:K:178:ASN:OD1	1:K:268:GLU:OE2	2.35	0.44
1:M:362:PHE:HD2	1:M:366:ILE:HD12	1.81	0.44
1:M:491:GLN:OE1	1:M:493:ARG:HD2	2.18	0.44
1:C:483:HIS:CD2	1:P:483:HIS:CD2	3.06	0.44
1:Q:17:ASN:HD22	1:Q:17:ASN:C	2.21	0.44
1:U:472:THR:CG2	1:U:498:GLU:CA	2.84	0.44
1:W:401:ASN:N	2:W:700:FDP:O5P	2.50	0.44
1:B:491:GLN:OE1	1:B:493:ARG:HD2	2.18	0.43
1:D:242:HIS:HE1	1:F:12:PHE:CE2	2.36	0.43
1:F:17:ASN:HD22	1:F:17:ASN:C	2.21	0.43
1:G:178:ASN:OD1	1:G:268:GLU:OE2	2.35	0.43
1:H:168:SER:O	1:H:169:HIS:HB2	2.17	0.43
1:H:178:ASN:OD1	1:H:268:GLU:OE2	2.35	0.43
1:K:270:PRO:CG	1:K:273:LYS:CD	2.94	0.43
1:M:17:ASN:HD22	1:M:17:ASN:C	2.21	0.43
1:R:178:ASN:OD1	1:R:268:GLU:OE2	2.35	0.43
1:R:193:ASP:CA	1:R:196:ASP:HB2	2.41	0.43
1:R:371:HIS:CD2	1:R:373:PRO:O	2.71	0.43
1:S:178:ASN:OD1	1:S:268:GLU:OE2	2.35	0.43
1:X:398:VAL:HG13	1:X:479:ILE:HB	2.00	0.43
1:A:369:LEU:HD12	1:I:3:LEU:HD13	2.00	0.43
1:B:17:ASN:HD22	1:B:17:ASN:C	2.21	0.43
1:E:310:ARG:HG2	1:G:297:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:398:VAL:HG13	1:G:479:ILE:HB	2.00	0.43
1:G:491:GLN:OE1	1:G:493:ARG:HD2	2.18	0.43
1:L:362:PHE:HD2	1:L:366:ILE:HD12	1.81	0.43
1:O:372:ILE:HA	1:O:372:ILE:HD12	1.73	0.43
1:R:168:SER:O	1:R:169:HIS:HB2	2.17	0.43
1:R:272:GLU:HG2	1:T:352:GLU:CD	2.39	0.43
1:S:17:ASN:C	1:S:17:ASN:HD22	2.21	0.43
1:W:491:GLN:OE1	1:W:493:ARG:HD2	2.18	0.43
1:A:372:ILE:HA	1:A:372:ILE:HD12	1.73	0.43
1:A:398:VAL:HG13	1:A:479:ILE:HB	2.00	0.43
1:D:273:LYS:HG2	1:F:11:ILE:HB	1.99	0.43
1:E:311:ALA:CB	1:G:312:GLU:HA	2.47	0.43
1:P:491:GLN:OE1	1:P:493:ARG:HD2	2.18	0.43
1:T:3:LEU:CD2	1:T:4:ALA:N	2.80	0.43
1:A:270:PRO:CG	1:A:273:LYS:CD	2.94	0.43
1:B:372:ILE:HD12	1:B:372:ILE:HA	1.73	0.43
1:B:3:LEU:HD13	1:C:369:LEU:CD1	2.48	0.43
1:C:398:VAL:HG13	1:C:479:ILE:HB	2.00	0.43
1:E:272:GLU:CB	1:G:352:GLU:HG2	2.49	0.43
1:K:11:ILE:HB	1:M:273:LYS:CG	2.43	0.43
1:M:178:ASN:OD1	1:M:268:GLU:OE2	2.35	0.43
1:N:398:VAL:HG13	1:N:479:ILE:HB	2.00	0.43
1:Q:224:LYS:HB3	1:Q:224:LYS:HE3	1.81	0.43
1:Q:398:VAL:HG13	1:Q:479:ILE:HB	2.00	0.43
1:R:402:THR:OG1	1:R:404:ARG:HB2	2.19	0.43
1:T:17:ASN:HD22	1:T:17:ASN:C	2.21	0.43
1:U:178:ASN:OD1	1:U:268:GLU:OE2	2.35	0.43
1:A:491:GLN:OE1	1:A:493:ARG:HD2	2.18	0.43
1:B:272:GLU:O	1:C:352:GLU:CG	2.66	0.43
1:E:168:SER:O	1:E:169:HIS:HB2	2.17	0.43
1:I:491:GLN:OE1	1:I:493:ARG:HD2	2.18	0.43
1:N:491:GLN:OE1	1:N:493:ARG:HD2	2.18	0.43
1:R:276:VAL:CG1	1:T:9:LEU:HB2	2.45	0.43
1:V:273:LYS:HD3	1:X:11:ILE:HB	1.99	0.43
1:V:287:VAL:HG23	1:X:3:LEU:HD21	2.00	0.43
1:W:390:GLU:HG2	1:X:374:MET:HE2	1.99	0.43
1:C:496:LEU:CD2	1:V:195:VAL:CG2	2.93	0.43
1:E:101:MET:HE1	1:E:124:PHE:CE1	2.54	0.43
1:I:17:ASN:C	1:I:17:ASN:HD22	2.21	0.43
1:I:487:GLY:HA2	1:M:229:LYS:CD	2.42	0.43
1:O:451:GLU:HG2	1:O:451:GLU:H	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:491:GLN:OE1	1:O:493:ARG:HD2	2.18	0.43
1:R:280:ILE:HD11	1:T:9:LEU:CB	2.40	0.43
1:R:424:ARG:NH1	1:R:424:ARG:CG	2.41	0.43
1:R:398:VAL:HG13	1:R:479:ILE:HB	2.00	0.43
1:S:398:VAL:HG13	1:S:479:ILE:HB	2.00	0.43
1:E:178:ASN:OD1	1:E:268:GLU:OE2	2.35	0.43
1:F:398:VAL:HG13	1:F:479:ILE:HB	2.00	0.43
1:I:224:LYS:HE3	1:I:224:LYS:HB3	1.81	0.43
1:L:398:VAL:HG13	1:L:479:ILE:HB	2.00	0.43
1:M:398:VAL:HG13	1:M:479:ILE:HB	2.00	0.43
1:N:17:ASN:C	1:N:17:ASN:HD22	2.21	0.43
1:O:429:ARG:O	1:O:432:ASN:HB2	2.19	0.43
1:U:402:THR:OG1	1:U:404:ARG:HB2	2.18	0.43
1:V:287:VAL:HG23	1:X:3:LEU:HD22	2.01	0.43
1:F:491:GLN:OE1	1:F:493:ARG:HD2	2.18	0.43
1:G:224:LYS:HB3	1:G:224:LYS:HE3	1.82	0.43
1:G:429:ARG:O	1:G:432:ASN:HB2	2.19	0.43
1:F:483:HIS:CD2	1:G:483:HIS:NE2	2.86	0.43
1:H:401:ASN:N	2:H:700:FDP:O5P	2.50	0.43
1:K:283:SER:HB3	1:M:3:LEU:CD2	2.49	0.43
1:L:279:LYS:HB3	1:N:6:ASN:CG	2.39	0.43
1:T:429:ARG:O	1:T:432:ASN:HB2	2.19	0.43
1:T:398:VAL:HG13	1:T:479:ILE:HB	2.00	0.43
1:G:17:ASN:C	1:G:17:ASN:HD22	2.21	0.43
1:J:429:ARG:O	1:J:432:ASN:HB2	2.19	0.43
1:L:293:ILE:HG12	1:L:326:CYS:HB2	2.01	0.43
1:S:429:ARG:O	1:S:432:ASN:HB2	2.19	0.43
1:S:491:GLN:OE1	1:S:493:ARG:HD2	2.18	0.43
1:V:424:ARG:NH1	1:V:424:ARG:CG	2.41	0.43
1:W:293:ILE:HG12	1:W:326:CYS:HB2	2.01	0.43
1:C:429:ARG:O	1:C:432:ASN:HB2	2.19	0.43
1:D:188:ALA:CB	1:D:218:GLN:HG2	2.21	0.43
1:D:429:ARG:O	1:D:432:ASN:HB2	2.19	0.43
1:H:293:ILE:HG12	1:H:326:CYS:HB2	2.01	0.43
1:K:6:ASN:OD1	1:M:279:LYS:HE3	2.18	0.43
1:L:276:VAL:HG13	1:N:9:LEU:HD13	2.01	0.43
1:O:377:ASP:OD2	1:O:377:ASP:N	2.52	0.43
1:P:293:ILE:HG12	1:P:326:CYS:HB2	2.01	0.43
1:C:373:PRO:HD3	1:P:392:LYS:HD2	2.01	0.43
1:R:371:HIS:C	1:R:372:ILE:HD13	2.39	0.43
1:S:451:GLU:HG2	1:S:451:GLU:H	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:242:HIS:CE1	1:T:12:PHE:CE2	3.07	0.43
1:V:293:ILE:HG12	1:V:326:CYS:HB2	2.01	0.43
1:V:79:ALA:HA	1:V:429:ARG:HB3	2.01	0.43
1:W:362:PHE:O	1:W:366:ILE:HD12	2.19	0.43
1:W:429:ARG:O	1:W:432:ASN:HB2	2.19	0.43
1:V:272:GLU:CB	1:X:352:GLU:HG2	2.49	0.43
1:B:79:ALA:HA	1:B:429:ARG:HB3	2.01	0.42
1:E:377:ASP:OD2	1:E:377:ASP:N	2.52	0.42
1:F:362:PHE:O	1:F:366:ILE:HD12	2.19	0.42
1:K:398:VAL:HG13	1:K:479:ILE:HB	2.00	0.42
1:H:498:GLU:HG2	1:M:195:VAL:HG11	2.01	0.42
1:M:390:GLU:HA	1:N:372:ILE:HG13	2.01	0.42
1:P:362:PHE:O	1:P:366:ILE:HD12	2.19	0.42
1:P:429:ARG:O	1:P:432:ASN:HB2	2.19	0.42
1:Q:297:GLN:OE1	1:S:310:ARG:CZ	2.67	0.42
1:U:138:GLY:HA2	1:U:151:GLN:HE21	1.84	0.42
1:U:279:LYS:HE3	1:W:6:ASN:OD1	2.19	0.42
1:U:398:VAL:HG13	1:U:479:ILE:HB	2.00	0.42
1:X:293:ILE:HG12	1:X:326:CYS:HB2	2.01	0.42
1:A:429:ARG:O	1:A:432:ASN:HB2	2.19	0.42
1:A:6:ASN:O	1:I:280:ILE:HG12	2.19	0.42
1:E:429:ARG:O	1:E:432:ASN:HB2	2.19	0.42
1:F:212:PHE:CD2	1:F:214:ARG:NE	2.88	0.42
1:F:472:THR:CG2	1:F:498:GLU:CA	2.84	0.42
1:G:79:ALA:HA	1:G:429:ARG:HB3	2.02	0.42
1:H:138:GLY:HA2	1:H:151:GLN:HE21	1.85	0.42
1:H:312:GLU:HG3	1:J:311:ALA:HB3	2.00	0.42
1:H:451:GLU:HG2	1:H:451:GLU:H	1.59	0.42
1:H:496:LEU:HG	1:M:195:VAL:HG21	1.89	0.42
1:H:79:ALA:HA	1:H:429:ARG:HB3	2.01	0.42
1:K:293:ILE:HG12	1:K:326:CYS:HB2	2.01	0.42
1:K:451:GLU:H	1:K:451:GLU:HG2	1.59	0.42
1:L:362:PHE:O	1:L:366:ILE:HD12	2.19	0.42
1:M:293:ILE:HG12	1:M:326:CYS:HB2	2.01	0.42
1:O:79:ALA:HA	1:O:429:ARG:HB3	2.01	0.42
1:P:138:GLY:HA2	1:P:151:GLN:HE21	1.84	0.42
1:R:17:ASN:C	1:R:17:ASN:HD22	2.21	0.42
1:S:293:ILE:HG12	1:S:326:CYS:HB2	2.01	0.42
1:T:224:LYS:HB3	1:T:224:LYS:HE3	1.81	0.42
1:T:474:ASP:O	1:T:497:VAL:HG13	2.20	0.42
1:U:293:ILE:HG12	1:U:326:CYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:451:GLU:HG2	1:U:451:GLU:H	1.59	0.42
1:U:6:ASN:CG	1:W:279:LYS:HE3	2.36	0.42
1:W:79:ALA:HA	1:W:429:ARG:HB3	2.01	0.42
1:C:138:GLY:HA2	1:C:151:GLN:HE21	1.85	0.42
1:C:293:ILE:HG12	1:C:326:CYS:HB2	2.01	0.42
1:H:362:PHE:O	1:H:366:ILE:HD12	2.19	0.42
1:M:491:GLN:HG3	1:N:491:GLN:CG	2.47	0.42
1:N:293:ILE:HG12	1:N:326:CYS:HB2	2.01	0.42
1:N:362:PHE:O	1:N:366:ILE:HD12	2.19	0.42
1:P:398:VAL:HG13	1:P:479:ILE:HB	2.00	0.42
1:Q:242:HIS:NE2	1:S:12:PHE:CE2	2.85	0.42
1:Q:310:ARG:HG2	1:S:297:GLN:HB2	2.00	0.42
1:T:212:PHE:CD2	1:T:214:ARG:NE	2.88	0.42
1:T:472:THR:CG2	1:T:498:GLU:CA	2.84	0.42
1:T:79:ALA:HA	1:T:429:ARG:HB3	2.01	0.42
1:V:212:PHE:CD2	1:V:214:ARG:NE	2.88	0.42
1:V:429:ARG:O	1:V:432:ASN:HB2	2.19	0.42
1:B:352:GLU:HG2	1:C:272:GLU:O	2.18	0.42
1:C:377:ASP:OD2	1:C:377:ASP:N	2.52	0.42
1:E:293:ILE:HG12	1:E:326:CYS:HB2	2.01	0.42
1:E:362:PHE:O	1:E:366:ILE:HD12	2.19	0.42
1:E:49:ARG:NE	1:E:83:ASP:OD2	2.33	0.42
1:F:483:HIS:NE2	1:G:483:HIS:CD2	2.86	0.42
1:G:212:PHE:CD2	1:G:214:ARG:NE	2.88	0.42
1:I:293:ILE:HG12	1:I:326:CYS:HB2	2.01	0.42
1:I:429:ARG:O	1:I:432:ASN:HB2	2.19	0.42
1:K:12:PHE:HE2	1:M:242:HIS:NE2	2.08	0.42
1:M:362:PHE:O	1:M:366:ILE:HD12	2.19	0.42
1:N:429:ARG:O	1:N:432:ASN:HB2	2.19	0.42
1:R:429:ARG:O	1:R:432:ASN:HB2	2.19	0.42
1:S:362:PHE:O	1:S:366:ILE:HD12	2.19	0.42
1:S:474:ASP:O	1:S:497:VAL:HG13	2.20	0.42
1:Q:276:VAL:HG13	1:S:9:LEU:HB3	2.02	0.42
1:T:293:ILE:HG12	1:T:326:CYS:HB2	2.01	0.42
1:U:377:ASP:N	1:U:377:ASP:OD2	2.52	0.42
1:U:491:GLN:HG3	1:V:491:GLN:HG3	2.01	0.42
1:U:79:ALA:HA	1:U:429:ARG:HB3	2.01	0.42
1:V:276:VAL:HG13	1:X:9:LEU:CD1	2.48	0.42
1:U:372:ILE:CD1	1:V:390:GLU:HG2	2.45	0.42
1:V:398:VAL:HG13	1:V:479:ILE:HB	2.00	0.42
1:A:352:GLU:HG2	1:I:272:GLU:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ALA:HA	1:A:429:ARG:HB3	2.01	0.42
1:B:138:GLY:HA2	1:B:151:GLN:HE21	1.85	0.42
1:B:429:ARG:O	1:B:432:ASN:HB2	2.19	0.42
1:D:138:GLY:HA2	1:D:151:GLN:HE21	1.85	0.42
1:D:79:ALA:HA	1:D:429:ARG:HB3	2.01	0.42
1:F:138:GLY:HA2	1:F:151:GLN:HE21	1.84	0.42
1:H:297:GLN:HB2	1:J:310:ARG:HB2	1.99	0.42
1:H:429:ARG:O	1:H:432:ASN:HB2	2.19	0.42
1:I:398:VAL:HG13	1:I:479:ILE:HB	2.00	0.42
1:J:79:ALA:HA	1:J:429:ARG:HB3	2.01	0.42
1:K:474:ASP:O	1:K:497:VAL:HG13	2.20	0.42
1:L:474:ASP:O	1:L:497:VAL:HG13	2.20	0.42
1:N:474:ASP:O	1:N:497:VAL:HG13	2.20	0.42
1:O:212:PHE:CD2	1:O:214:ARG:NE	2.88	0.42
1:O:474:ASP:O	1:O:497:VAL:HG13	2.20	0.42
1:R:138:GLY:HA2	1:R:151:GLN:HE21	1.85	0.42
1:R:212:PHE:CD2	1:R:214:ARG:NE	2.88	0.42
1:R:377:ASP:OD2	1:R:377:ASP:N	2.52	0.42
1:U:270:PRO:CG	1:U:273:LYS:CD	2.94	0.42
1:V:224:LYS:HE3	1:V:224:LYS:HB3	1.81	0.42
1:W:138:GLY:HA2	1:W:151:GLN:HE21	1.84	0.42
1:D:270:PRO:CG	1:D:273:LYS:CD	2.94	0.42
1:G:293:ILE:HG12	1:G:326:CYS:HB2	2.01	0.42
1:H:212:PHE:CD2	1:H:214:ARG:NE	2.88	0.42
1:J:474:ASP:O	1:J:497:VAL:HG13	2.20	0.42
1:K:312:GLU:HA	1:M:311:ALA:CB	2.35	0.42
1:K:377:ASP:OD2	1:K:377:ASP:N	2.52	0.42
1:L:79:ALA:HA	1:L:429:ARG:HB3	2.01	0.42
1:M:429:ARG:O	1:M:432:ASN:HB2	2.19	0.42
1:R:79:ALA:HA	1:R:429:ARG:HB3	2.01	0.42
1:S:79:ALA:HA	1:S:429:ARG:HB3	2.01	0.42
1:T:138:GLY:HA2	1:T:151:GLN:HE21	1.85	0.42
1:V:472:THR:CG2	1:V:498:GLU:HA	2.18	0.42
1:W:372:ILE:HD11	1:W:374:MET:HE1	2.01	0.42
1:X:212:PHE:CD2	1:X:214:ARG:NE	2.88	0.42
1:F:429:ARG:O	1:F:432:ASN:HB2	2.19	0.42
1:H:424:ARG:CG	1:H:424:ARG:NH1	2.41	0.42
1:J:362:PHE:O	1:J:366:ILE:HD12	2.19	0.42
1:K:362:PHE:O	1:K:366:ILE:HD12	2.20	0.42
1:K:372:ILE:HD12	1:K:372:ILE:HA	1.73	0.42
1:K:79:ALA:HA	1:K:429:ARG:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:424:ARG:NH1	1:M:424:ARG:CG	2.41	0.42
1:M:79:ALA:HA	1:M:429:ARG:HB3	2.02	0.42
1:M:474:ASP:O	1:M:497:VAL:HG13	2.20	0.42
1:L:283:SER:CA	1:N:3:LEU:HD21	2.49	0.42
1:T:53:SER:HA	1:T:85:LYS:CG	2.50	0.42
1:V:11:ILE:HD12	1:X:269:ILE:HG12	2.02	0.42
1:X:79:ALA:HA	1:X:429:ARG:HB3	2.01	0.42
1:B:276:VAL:HG13	1:C:9:LEU:CB	2.49	0.42
1:E:3:LEU:HD13	1:G:369:LEU:HD12	2.01	0.42
1:F:474:ASP:O	1:F:497:VAL:HG13	2.20	0.42
1:J:138:GLY:HA2	1:J:151:GLN:HE21	1.85	0.42
1:L:212:PHE:CD2	1:L:214:ARG:NE	2.88	0.42
1:L:224:LYS:HE3	1:L:224:LYS:HB3	1.82	0.42
1:O:362:PHE:O	1:O:366:ILE:HD12	2.19	0.42
1:O:263:GLY:HA2	1:P:310:ARG:HH11	1.84	0.42
1:P:53:SER:HA	1:P:85:LYS:CG	2.50	0.42
1:Q:270:PRO:CB	1:Q:273:LYS:HD2	2.50	0.42
1:S:189:VAL:HG13	1:S:193:ASP:HB2	2.02	0.42
1:L:487:GLY:CA	1:S:229:LYS:CD	2.94	0.42
1:R:11:ILE:O	1:T:273:LYS:HE3	2.20	0.42
1:U:424:ARG:NH1	1:U:424:ARG:CG	2.41	0.42
1:U:429:ARG:O	1:U:432:ASN:HB2	2.19	0.42
1:A:189:VAL:HG13	1:A:193:ASP:HB2	2.02	0.42
1:A:293:ILE:HG12	1:A:326:CYS:HB2	2.01	0.42
1:A:371:HIS:O	1:A:374:MET:CG	2.57	0.42
1:B:293:ILE:HG12	1:B:326:CYS:HB2	2.01	0.42
1:C:53:SER:HA	1:C:85:LYS:CG	2.50	0.42
1:D:270:PRO:CB	1:D:273:LYS:HD2	2.50	0.42
1:E:138:GLY:HA2	1:E:151:GLN:HE21	1.85	0.42
1:G:362:PHE:O	1:G:366:ILE:HD12	2.19	0.42
1:I:362:PHE:O	1:I:366:ILE:HD12	2.19	0.42
1:I:372:ILE:HD12	1:I:374:MET:HG3	2.00	0.42
1:J:189:VAL:HG13	1:J:193:ASP:HB2	2.02	0.42
1:K:401:ASN:N	2:K:700:FDP:O5P	2.50	0.42
1:N:79:ALA:HA	1:N:429:ARG:HB3	2.01	0.42
1:P:474:ASP:O	1:P:497:VAL:HG13	2.20	0.42
1:Q:429:ARG:O	1:Q:432:ASN:HB2	2.19	0.42
1:Q:79:ALA:HA	1:Q:429:ARG:HB3	2.01	0.42
1:R:272:GLU:HB2	1:T:352:GLU:HG2	1.94	0.42
1:U:362:PHE:O	1:U:366:ILE:HD12	2.19	0.42
1:W:189:VAL:HG13	1:W:193:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:212:PHE:CD2	1:W:214:ARG:NE	2.88	0.42
1:A:270:PRO:CB	1:A:273:LYS:HD2	2.50	0.42
1:B:362:PHE:O	1:B:366:ILE:HD12	2.19	0.42
1:B:373:PRO:HB3	1:O:391:THR:CA	2.49	0.42
1:C:474:ASP:O	1:C:497:VAL:HG13	2.20	0.42
1:D:293:ILE:HG12	1:D:326:CYS:HB2	2.01	0.42
1:D:372:ILE:HD11	1:D:374:MET:HE1	2.01	0.42
1:E:53:SER:HA	1:E:85:LYS:CG	2.50	0.42
1:F:371:HIS:O	1:F:374:MET:CG	2.57	0.42
1:H:402:THR:OG1	1:H:404:ARG:HB2	2.20	0.42
1:M:189:VAL:HG13	1:M:193:ASP:HB2	2.02	0.42
1:O:53:SER:HA	1:O:85:LYS:CG	2.50	0.42
1:P:401:ASN:N	2:P:700:FDP:O5P	2.50	0.42
1:U:352:GLU:CG	1:W:272:GLU:CG	2.98	0.42
1:V:138:GLY:HA2	1:V:151:GLN:HE21	1.85	0.42
1:W:474:ASP:O	1:W:497:VAL:HG13	2.20	0.42
1:B:212:PHE:CD2	1:B:214:ARG:NE	2.88	0.41
1:B:53:SER:HA	1:B:85:LYS:CG	2.50	0.41
1:C:212:PHE:CD2	1:C:214:ARG:NE	2.88	0.41
1:C:270:PRO:CB	1:C:273:LYS:HD2	2.50	0.41
1:C:79:ALA:HA	1:C:429:ARG:HB3	2.01	0.41
1:D:362:PHE:O	1:D:366:ILE:HD12	2.19	0.41
1:F:293:ILE:HG12	1:F:326:CYS:HB2	2.01	0.41
1:G:53:SER:HA	1:G:85:LYS:CG	2.50	0.41
1:H:53:SER:HA	1:H:85:LYS:CG	2.50	0.41
1:L:311:ALA:HA	1:N:315:ASP:HB2	2.01	0.41
1:L:472:THR:CG2	1:L:498:GLU:CA	2.84	0.41
1:M:138:GLY:HA2	1:M:151:GLN:HE21	1.85	0.41
1:P:212:PHE:CD2	1:P:214:ARG:NE	2.88	0.41
1:P:371:HIS:C	1:P:372:ILE:HD13	2.40	0.41
1:Q:474:ASP:O	1:Q:497:VAL:HG13	2.20	0.41
1:S:138:GLY:HA2	1:S:151:GLN:HE21	1.84	0.41
1:U:11:ILE:HB	1:W:273:LYS:CD	2.42	0.41
1:U:212:PHE:CD2	1:U:214:ARG:NE	2.88	0.41
1:U:311:ALA:HB3	1:W:312:GLU:CG	2.49	0.41
1:X:362:PHE:O	1:X:366:ILE:HD12	2.19	0.41
1:D:474:ASP:O	1:D:497:VAL:HG13	2.20	0.41
1:E:272:GLU:HG3	1:G:352:GLU:CB	2.50	0.41
1:I:474:ASP:O	1:I:497:VAL:HG13	2.20	0.41
1:L:429:ARG:O	1:L:432:ASN:HB2	2.19	0.41
1:K:242:HIS:NE2	1:M:12:PHE:CE2	2.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:284:LYS:CG	1:N:7:LEU:HD22	2.50	0.41
1:O:135:VAL:HG12	1:O:136:ARG:N	2.35	0.41
1:O:293:ILE:HG12	1:O:326:CYS:HB2	2.01	0.41
1:O:315:ASP:HB2	1:P:311:ALA:CA	2.48	0.41
1:P:189:VAL:HG13	1:P:193:ASP:HB2	2.02	0.41
1:P:79:ALA:HA	1:P:429:ARG:HB3	2.02	0.41
1:Q:293:ILE:HG12	1:Q:326:CYS:HB2	2.01	0.41
1:Q:362:PHE:O	1:Q:366:ILE:HD12	2.19	0.41
1:R:362:PHE:O	1:R:366:ILE:HD12	2.19	0.41
1:X:474:ASP:O	1:X:497:VAL:HG13	2.20	0.41
1:A:138:GLY:HA2	1:A:151:GLN:HE21	1.85	0.41
1:A:362:PHE:O	1:A:366:ILE:HD12	2.19	0.41
1:B:188:ALA:CB	1:B:218:GLN:HG2	2.21	0.41
1:B:270:PRO:CB	1:B:273:LYS:HD2	2.50	0.41
1:B:474:ASP:O	1:B:497:VAL:HG13	2.20	0.41
1:C:223:ARG:NH1	1:C:223:ARG:HG2	2.26	0.41
1:E:189:VAL:HG13	1:E:193:ASP:HB2	2.02	0.41
1:E:474:ASP:O	1:E:497:VAL:HG13	2.20	0.41
1:G:189:VAL:HG13	1:G:193:ASP:HB2	2.02	0.41
1:H:189:VAL:HG13	1:H:193:ASP:HB2	2.02	0.41
1:H:296:THR:O	1:J:310:ARG:HG3	2.20	0.41
1:I:53:SER:HA	1:I:85:LYS:CG	2.50	0.41
1:K:212:PHE:CD2	1:K:214:ARG:NE	2.88	0.41
1:L:53:SER:HA	1:L:85:LYS:CG	2.50	0.41
1:N:138:GLY:HA2	1:N:151:GLN:HE21	1.85	0.41
1:O:101:MET:HE1	1:O:124:PHE:CE1	2.55	0.41
1:O:270:PRO:CB	1:O:273:LYS:HD2	2.50	0.41
1:Q:212:PHE:CD2	1:Q:214:ARG:NE	2.88	0.41
1:Q:390:GLU:O	1:R:372:ILE:HG13	2.20	0.41
1:R:474:ASP:O	1:R:497:VAL:HG13	2.20	0.41
1:U:474:ASP:O	1:U:497:VAL:HG13	2.20	0.41
1:V:401:ASN:N	2:V:700:FDP:O5P	2.50	0.41
1:X:138:GLY:HA2	1:X:151:GLN:HE21	1.84	0.41
1:F:189:VAL:HG13	1:F:193:ASP:HB2	2.02	0.41
1:G:474:ASP:O	1:G:497:VAL:HG13	2.20	0.41
1:I:212:PHE:CD2	1:I:214:ARG:NE	2.88	0.41
1:I:79:ALA:HA	1:I:429:ARG:HB3	2.01	0.41
1:J:293:ILE:HG12	1:J:326:CYS:HB2	2.01	0.41
1:K:297:GLN:HB2	1:M:310:ARG:HB2	2.01	0.41
1:N:189:VAL:HG13	1:N:193:ASP:HB2	2.02	0.41
1:P:214:ARG:HH11	1:P:214:ARG:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:467:LYS:HE2	1:Q:467:LYS:HB3	1.86	0.41
1:T:362:PHE:O	1:T:366:ILE:HD12	2.19	0.41
1:S:491:GLN:NE2	1:T:491:GLN:NE2	2.68	0.41
1:U:214:ARG:HH11	1:U:214:ARG:HG3	1.86	0.41
1:V:189:VAL:HG13	1:V:193:ASP:HB2	2.02	0.41
1:B:214:ARG:HG3	1:B:214:ARG:HH11	1.86	0.41
1:B:49:ARG:NE	1:B:83:ASP:OD2	2.33	0.41
1:C:214:ARG:HH11	1:C:214:ARG:HG3	1.86	0.41
1:C:362:PHE:O	1:C:366:ILE:HD12	2.20	0.41
1:H:474:ASP:O	1:H:497:VAL:HG13	2.20	0.41
1:K:138:GLY:HA2	1:K:151:GLN:HE21	1.84	0.41
1:K:429:ARG:O	1:K:432:ASN:HB2	2.19	0.41
1:L:138:GLY:HA2	1:L:151:GLN:HE21	1.84	0.41
1:N:101:MET:HE1	1:N:124:PHE:CE1	2.55	0.41
1:N:212:PHE:CD2	1:N:214:ARG:NE	2.88	0.41
1:T:424:ARG:NH1	1:T:424:ARG:CG	2.41	0.41
1:U:189:VAL:HG13	1:U:193:ASP:HB2	2.02	0.41
1:V:362:PHE:O	1:V:366:ILE:HD12	2.19	0.41
1:W:223:ARG:HG2	1:W:223:ARG:NH1	2.25	0.41
1:H:310:ARG:H	1:J:297:GLN:HB3	1.86	0.41
1:K:270:PRO:CB	1:K:273:LYS:HD2	2.50	0.41
1:L:310:ARG:NH2	1:N:297:GLN:OE1	2.53	0.41
1:P:377:ASP:OD2	1:P:377:ASP:N	2.52	0.41
1:U:311:ALA:CB	1:W:312:GLU:CG	2.99	0.41
1:V:474:ASP:O	1:V:497:VAL:HG13	2.20	0.41
1:W:53:SER:HA	1:W:85:LYS:CG	2.50	0.41
1:X:429:ARG:O	1:X:432:ASN:HB2	2.19	0.41
1:B:272:GLU:CG	1:C:352:GLU:CB	2.98	0.41
1:E:79:ALA:HA	1:E:429:ARG:HB3	2.01	0.41
1:F:214:ARG:HG3	1:F:214:ARG:HH11	1.86	0.41
1:F:79:ALA:HA	1:F:429:ARG:HB3	2.01	0.41
1:G:138:GLY:HA2	1:G:151:GLN:HE21	1.85	0.41
1:F:373:PRO:HB2	1:G:391:THR:HA	1.95	0.41
1:H:270:PRO:CB	1:H:273:LYS:HD2	2.50	0.41
1:I:138:GLY:HA2	1:I:151:GLN:HE21	1.84	0.41
1:A:272:GLU:HA	1:I:313:VAL:CG1	2.51	0.41
1:I:451:GLU:HG2	1:I:451:GLU:H	1.59	0.41
1:J:212:PHE:CD2	1:J:214:ARG:NE	2.88	0.41
1:H:310:ARG:H	1:J:297:GLN:CB	2.34	0.41
1:K:214:ARG:HH11	1:K:214:ARG:HG3	1.86	0.41
1:K:283:SER:OG	1:M:3:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:402:THR:OG1	1:L:404:ARG:HB2	2.20	0.41
1:O:214:ARG:HG3	1:O:214:ARG:HH11	1.86	0.41
1:P:467:LYS:HB3	1:P:467:LYS:HE2	1.87	0.41
1:V:53:SER:HA	1:V:85:LYS:CG	2.50	0.41
1:U:315:ASP:CB	1:W:311:ALA:CB	2.99	0.41
1:X:189:VAL:HG13	1:X:193:ASP:HB2	2.02	0.41
1:X:214:ARG:HH11	1:X:214:ARG:HG3	1.86	0.41
1:D:214:ARG:HG3	1:D:214:ARG:HH11	1.86	0.41
1:G:214:ARG:HH11	1:G:214:ARG:HG3	1.86	0.41
1:K:189:VAL:HG13	1:K:193:ASP:HB2	2.02	0.41
1:N:472:THR:CG2	1:N:498:GLU:CA	2.84	0.41
1:N:53:SER:HA	1:N:85:LYS:CG	2.50	0.41
1:O:138:GLY:HA2	1:O:151:GLN:HE21	1.84	0.41
1:O:224:LYS:HB3	1:O:224:LYS:HE3	1.82	0.41
1:Q:444:ALA:O	1:Q:448:GLY:N	2.54	0.41
1:R:293:ILE:HG12	1:R:326:CYS:HB2	2.01	0.41
1:R:279:LYS:CE	1:T:6:ASN:OD1	2.63	0.41
1:U:376:ALA:HA	1:V:494:ILE:HD12	2.03	0.41
1:A:214:ARG:HH11	1:A:214:ARG:HG3	1.86	0.41
1:A:474:ASP:O	1:A:497:VAL:HG13	2.20	0.41
1:E:212:PHE:CD2	1:E:214:ARG:NE	2.88	0.41
1:I:189:VAL:HG13	1:I:193:ASP:HB2	2.02	0.41
1:H:390:GLU:O	1:I:373:PRO:HB3	2.21	0.41
1:I:444:ALA:O	1:I:448:GLY:N	2.54	0.41
1:J:214:ARG:HG3	1:J:214:ARG:HH11	1.86	0.41
1:K:11:ILE:O	1:M:273:LYS:HE3	2.21	0.41
1:Q:189:VAL:HG13	1:Q:193:ASP:HB2	2.02	0.41
1:Q:374:MET:HB2	1:Q:375:SER:H	1.78	0.41
1:S:212:PHE:CD2	1:S:214:ARG:NE	2.88	0.41
1:S:214:ARG:HG3	1:S:214:ARG:HH11	1.86	0.41
1:T:189:VAL:HG13	1:T:193:ASP:HB2	2.02	0.41
1:U:101:MET:CE	1:U:124:PHE:CE1	3.04	0.41
1:W:377:ASP:OD2	1:W:377:ASP:N	2.52	0.41
1:W:424:ARG:NH1	1:W:424:ARG:CG	2.41	0.41
1:B:101:MET:CE	1:B:124:PHE:CE1	3.04	0.41
1:C:189:VAL:HG13	1:C:193:ASP:HB2	2.02	0.41
1:D:444:ALA:O	1:D:448:GLY:N	2.54	0.41
1:E:242:HIS:CE1	1:G:12:PHE:HZ	2.34	0.41
1:H:352:GLU:CG	1:J:272:GLU:CG	2.99	0.41
1:M:101:MET:CE	1:M:124:PHE:CE1	3.04	0.41
1:M:444:ALA:O	1:M:448:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:297:GLN:HB2	1:P:310:ARG:CG	2.44	0.41
1:O:312:GLU:CA	1:P:311:ALA:HB1	2.33	0.41
1:Q:284:LYS:HG3	1:S:7:LEU:HD21	2.00	0.41
1:Q:310:ARG:CG	1:S:297:GLN:HB2	2.51	0.41
1:V:101:MET:CE	1:V:124:PHE:CE1	3.04	0.41
1:C:389:TYR:O	1:P:372:ILE:HG21	2.21	0.41
1:D:212:PHE:CD2	1:D:214:ARG:NE	2.88	0.41
1:E:372:ILE:HA	1:E:372:ILE:HD12	1.73	0.41
1:H:444:ALA:O	1:H:448:GLY:N	2.54	0.41
1:O:189:VAL:HG13	1:O:193:ASP:HB2	2.02	0.41
1:P:101:MET:CE	1:P:124:PHE:CE1	3.04	0.41
1:P:372:ILE:HA	1:P:372:ILE:HD12	1.80	0.41
1:S:223:ARG:HG2	1:S:223:ARG:NH1	2.26	0.41
1:S:472:THR:CG2	1:S:498:GLU:CA	2.84	0.41
1:L:195:VAL:HG11	1:T:498:GLU:HG2	2.02	0.41
1:U:277:ALA:HB2	1:W:11:ILE:HG21	2.03	0.41
1:A:212:PHE:CD2	1:A:214:ARG:NE	2.88	0.40
1:A:444:ALA:O	1:A:448:GLY:N	2.54	0.40
1:A:53:SER:HA	1:A:85:LYS:CG	2.50	0.40
1:B:110:THR:O	1:B:125:TYR:HA	2.22	0.40
1:B:189:VAL:HG13	1:B:193:ASP:HB2	2.02	0.40
1:B:270:PRO:CG	1:B:273:LYS:CD	2.94	0.40
1:H:101:MET:CE	1:H:124:PHE:CE1	3.04	0.40
1:I:101:MET:CE	1:I:124:PHE:CE1	3.04	0.40
1:K:188:ALA:CB	1:K:218:GLN:HG2	2.21	0.40
1:K:53:SER:HA	1:K:85:LYS:CG	2.50	0.40
1:L:214:ARG:HH11	1:L:214:ARG:HG3	1.86	0.40
1:L:451:GLU:H	1:L:451:GLU:HG2	1.59	0.40
1:N:101:MET:CE	1:N:124:PHE:CE1	3.04	0.40
1:O:444:ALA:O	1:O:448:GLY:N	2.54	0.40
1:Q:110:THR:O	1:Q:125:TYR:HA	2.22	0.40
1:Q:138:GLY:HA2	1:Q:151:GLN:HE21	1.85	0.40
1:Q:273:LYS:HG2	1:S:11:ILE:O	2.21	0.40
1:R:53:SER:HA	1:R:85:LYS:CG	2.50	0.40
1:L:229:LYS:CG	1:S:487:GLY:CA	2.84	0.40
1:U:53:SER:HA	1:U:85:LYS:CG	2.50	0.40
1:W:214:ARG:HG3	1:W:214:ARG:HH11	1.86	0.40
1:A:101:MET:CE	1:A:124:PHE:CE1	3.04	0.40
1:A:110:THR:O	1:A:125:TYR:HA	2.22	0.40
1:A:12:PHE:CE2	1:I:242:HIS:HE1	2.38	0.40
1:B:451:GLU:O	1:B:453:LYS:HE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:GLU:O	1:C:453:LYS:HE2	2.22	0.40
1:E:110:THR:O	1:E:125:TYR:HA	2.22	0.40
1:F:101:MET:HE1	1:F:124:PHE:CE1	2.56	0.40
1:F:188:ALA:CB	1:F:218:GLN:HG2	2.21	0.40
1:G:110:THR:O	1:G:125:TYR:HA	2.21	0.40
1:H:101:MET:HE1	1:H:124:PHE:CE1	2.56	0.40
1:I:110:THR:O	1:I:125:TYR:HA	2.21	0.40
1:H:494:ILE:HD12	1:I:376:ALA:HB1	2.03	0.40
1:J:110:THR:O	1:J:125:TYR:HA	2.22	0.40
1:M:110:THR:O	1:M:125:TYR:HA	2.22	0.40
1:N:424:ARG:NH1	1:N:424:ARG:CG	2.41	0.40
1:O:310:ARG:CG	1:P:297:GLN:OE1	2.60	0.40
1:Q:101:MET:HE1	1:Q:124:PHE:CE1	2.56	0.40
1:Q:53:SER:HA	1:Q:85:LYS:CG	2.50	0.40
1:R:189:VAL:HG13	1:R:193:ASP:HB2	2.02	0.40
1:R:444:ALA:O	1:R:448:GLY:N	2.54	0.40
1:Q:276:VAL:HG13	1:S:9:LEU:HD13	2.04	0.40
1:T:214:ARG:HH11	1:T:214:ARG:HG3	1.86	0.40
1:U:310:ARG:CG	1:W:297:GLN:OE1	2.59	0.40
1:X:110:THR:O	1:X:125:TYR:HA	2.22	0.40
1:A:451:GLU:O	1:A:453:LYS:HE2	2.22	0.40
1:B:371:HIS:O	1:B:374:MET:CG	2.57	0.40
1:C:110:THR:O	1:C:125:TYR:HA	2.21	0.40
1:C:451:GLU:HG2	1:C:451:GLU:H	1.59	0.40
1:D:189:VAL:HG13	1:D:193:ASP:HB2	2.02	0.40
1:E:214:ARG:HH11	1:E:214:ARG:HG3	1.86	0.40
1:H:110:THR:O	1:H:125:TYR:HA	2.22	0.40
1:I:451:GLU:O	1:I:453:LYS:HE2	2.22	0.40
1:J:372:ILE:HD12	1:J:372:ILE:HA	1.73	0.40
1:K:110:THR:O	1:K:125:TYR:HA	2.22	0.40
1:L:312:GLU:HG3	1:N:311:ALA:HB3	2.03	0.40
1:K:273:LYS:HG2	1:M:11:ILE:O	2.22	0.40
1:O:270:PRO:CG	1:O:273:LYS:CD	2.94	0.40
1:O:467:LYS:HE2	1:O:467:LYS:HB3	1.86	0.40
1:Q:101:MET:CE	1:Q:124:PHE:CE1	3.04	0.40
1:Q:214:ARG:HG3	1:Q:214:ARG:HH11	1.86	0.40
1:R:110:THR:O	1:R:125:TYR:HA	2.22	0.40
1:T:401:ASN:N	2:T:700:FDP:O5P	2.50	0.40
1:V:371:HIS:O	1:V:374:MET:CG	2.57	0.40
1:A:467:LYS:HB3	1:A:467:LYS:HE2	1.86	0.40
1:A:472:THR:CG2	1:A:498:GLU:CA	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:ILE:HA	1:C:372:ILE:HD12	1.73	0.40
1:F:101:MET:CE	1:F:124:PHE:CE1	3.04	0.40
1:H:318:ASN:CG	1:J:318:ASN:ND2	2.75	0.40
1:K:310:ARG:NH2	1:M:297:GLN:OE1	2.54	0.40
1:M:451:GLU:O	1:M:453:LYS:HE2	2.22	0.40
1:M:53:SER:HA	1:M:85:LYS:CG	2.50	0.40
1:R:101:MET:HE1	1:R:124:PHE:CE1	2.57	0.40
1:R:451:GLU:O	1:R:453:LYS:HE2	2.22	0.40
1:R:401:ASN:N	2:R:700:FDP:O5P	2.54	0.40
1:S:110:THR:O	1:S:125:TYR:HA	2.22	0.40
1:U:110:THR:O	1:U:125:TYR:HA	2.22	0.40
1:U:372:ILE:HD11	1:U:374:MET:CE	2.51	0.40
1:B:482:ASP:HB3	1:B:491:GLN:HE21	1.87	0.40
1:H:451:GLU:O	1:H:453:LYS:HE2	2.22	0.40
1:K:297:GLN:HB2	1:M:310:ARG:CB	2.51	0.40
1:M:372:ILE:HD12	1:M:374:MET:HG3	2.04	0.40
1:O:101:MET:CE	1:O:124:PHE:CE1	3.04	0.40
1:Q:451:GLU:O	1:Q:453:LYS:HE2	2.22	0.40
1:R:101:MET:CE	1:R:124:PHE:CE1	3.04	0.40
1:S:482:ASP:HB3	1:S:491:GLN:HE21	1.87	0.40
1:U:270:PRO:CB	1:U:273:LYS:HD2	2.50	0.40
1:V:214:ARG:HG3	1:V:214:ARG:HH11	1.86	0.40
1:W:101:MET:HE1	1:W:124:PHE:CE1	2.57	0.40

All (4) 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:J:103:ARG:CD	1:T:58:GLU:OE1[5_545]	1.91	0.29
1:F:229:LYS:CE	1:W:487:GLY:CA[5_545]	2.08	0.12
1:F:229:LYS:CD	1:W:487:GLY:CA[5_545]	2.15	0.05
1:F:229:LYS:CG	1:W:487:GLY:CA[5_545]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	B	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	C	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	D	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	E	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	F	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	G	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	H	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	I	496/499 (99%)	485 (98%)	10 (2%)	1 (0%)	51	85
1	J	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	K	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	L	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	M	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	N	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	O	496/499 (99%)	485 (98%)	10 (2%)	1 (0%)	51	85
1	P	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	Q	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	R	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	S	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	T	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	U	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	V	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	W	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
1	X	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	51	85
All	All	11904/11976 (99%)	11662 (98%)	218 (2%)	24 (0%)	51	85

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	THR
1	B	296	THR
1	C	296	THR

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Mol	Chain	Res	Type
1	D	296	THR
1	E	296	THR
1	F	296	THR
1	G	296	THR
1	H	296	THR
1	I	296	THR
1	J	296	THR
1	K	296	THR
1	L	296	THR
1	M	296	THR
1	N	296	THR
1	O	296	THR
1	P	296	THR
1	Q	296	THR
1	R	296	THR
1	S	296	THR
1	T	296	THR
1	U	296	THR
1	V	296	THR
1	W	296	THR
1	X	296	THR

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	416/417 (100%)	376 (90%)	40 (10%)	10	36
1	B	416/417 (100%)	375 (90%)	41 (10%)	9	35
1	C	416/417 (100%)	374 (90%)	42 (10%)	9	34
1	D	416/417 (100%)	375 (90%)	41 (10%)	9	35
1	E	416/417 (100%)	376 (90%)	40 (10%)	10	36
1	F	416/417 (100%)	375 (90%)	41 (10%)	9	35
1	G	416/417 (100%)	375 (90%)	41 (10%)	9	35
1	H	416/417 (100%)	375 (90%)	41 (10%)	9	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	416/417 (100%)	375 (90%)	41 (10%)	9	35
1	J	416/417 (100%)	375 (90%)	41 (10%)	9	35
1	K	416/417 (100%)	376 (90%)	40 (10%)	10	36
1	L	416/417 (100%)	376 (90%)	40 (10%)	10	36
1	M	416/417 (100%)	376 (90%)	40 (10%)	10	36
1	N	416/417 (100%)	376 (90%)	40 (10%)	10	36
1	O	416/417 (100%)	375 (90%)	41 (10%)	9	35
1	P	416/417 (100%)	376 (90%)	40 (10%)	10	36
1	Q	416/417 (100%)	375 (90%)	41 (10%)	9	35
1	R	416/417 (100%)	376 (90%)	40 (10%)	10	36
1	S	416/417 (100%)	376 (90%)	40 (10%)	10	36
1	T	416/417 (100%)	376 (90%)	40 (10%)	10	36
1	U	416/417 (100%)	376 (90%)	40 (10%)	10	36
1	V	416/417 (100%)	376 (90%)	40 (10%)	10	36
1	W	416/417 (100%)	374 (90%)	42 (10%)	9	34
1	X	416/417 (100%)	377 (91%)	39 (9%)	10	38
All	All	9984/10008 (100%)	9012 (90%)	972 (10%)	9	36

All (972) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	17	ASN
1	A	31	THR
1	A	38	LYS
1	A	40	LEU
1	A	118	LYS
1	A	175	ARG
1	A	177	VAL
1	A	179	LEU
1	A	194	ARG
1	A	214	ARG
1	A	223	ARG
1	A	265	LEU
1	A	267	VAL
1	A	269	ILE

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Mol	Chain	Res	Type
1	A	304	TYR
1	A	335	LYS
1	A	345	TYR
1	A	362	PHE
1	A	372	ILE
1	A	374	MET
1	A	382	SER
1	A	383	SER
1	A	394	LYS
1	A	396	MET
1	A	398	VAL
1	A	424	ARG
1	A	435	GLN
1	A	446	LYS
1	A	451	GLU
1	A	453	LYS
1	A	454	GLU
1	A	466	SER
1	A	467	LYS
1	A	471	GLN
1	A	472	THR
1	A	490	ASN
1	A	495	LEU
1	A	497	VAL
1	A	498	GLU
1	B	3	LEU
1	B	17	ASN
1	B	31	THR
1	B	38	LYS
1	B	40	LEU
1	B	103	ARG
1	B	118	LYS
1	B	175	ARG
1	B	177	VAL
1	B	179	LEU
1	B	194	ARG
1	B	214	ARG
1	B	223	ARG
1	B	265	LEU
1	B	267	VAL
1	B	269	ILE
1	B	304	TYR

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Mol	Chain	Res	Type
1	B	335	LYS
1	B	345	TYR
1	B	362	PHE
1	B	372	ILE
1	B	374	MET
1	B	382	SER
1	B	383	SER
1	B	394	LYS
1	B	396	MET
1	B	398	VAL
1	B	424	ARG
1	B	435	GLN
1	B	446	LYS
1	B	451	GLU
1	B	453	LYS
1	B	454	GLU
1	B	466	SER
1	B	467	LYS
1	B	471	GLN
1	B	472	THR
1	B	490	ASN
1	B	495	LEU
1	B	497	VAL
1	B	498	GLU
1	C	3	LEU
1	C	12	PHE
1	C	17	ASN
1	C	31	THR
1	C	38	LYS
1	C	40	LEU
1	C	58	GLU
1	C	118	LYS
1	C	175	ARG
1	C	177	VAL
1	C	179	LEU
1	C	194	ARG
1	C	214	ARG
1	C	223	ARG
1	C	265	LEU
1	C	267	VAL
1	C	269	ILE
1	C	304	TYR

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Mol	Chain	Res	Type
1	C	335	LYS
1	C	345	TYR
1	C	362	PHE
1	C	372	ILE
1	C	374	MET
1	C	382	SER
1	C	383	SER
1	C	394	LYS
1	C	396	MET
1	C	398	VAL
1	C	424	ARG
1	C	435	GLN
1	C	446	LYS
1	C	451	GLU
1	C	453	LYS
1	C	454	GLU
1	C	466	SER
1	C	467	LYS
1	C	471	GLN
1	C	472	THR
1	C	490	ASN
1	C	495	LEU
1	C	497	VAL
1	C	498	GLU
1	D	3	LEU
1	D	17	ASN
1	D	31	THR
1	D	38	LYS
1	D	40	LEU
1	D	118	LYS
1	D	175	ARG
1	D	177	VAL
1	D	179	LEU
1	D	194	ARG
1	D	214	ARG
1	D	223	ARG
1	D	265	LEU
1	D	267	VAL
1	D	269	ILE
1	D	304	TYR
1	D	335	LYS
1	D	345	TYR

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Mol	Chain	Res	Type
1	D	362	PHE
1	D	372	ILE
1	D	374	MET
1	D	382	SER
1	D	383	SER
1	D	394	LYS
1	D	396	MET
1	D	398	VAL
1	D	404	ARG
1	D	424	ARG
1	D	435	GLN
1	D	446	LYS
1	D	451	GLU
1	D	453	LYS
1	D	454	GLU
1	D	466	SER
1	D	467	LYS
1	D	471	GLN
1	D	472	THR
1	D	490	ASN
1	D	495	LEU
1	D	497	VAL
1	D	498	GLU
1	E	3	LEU
1	E	17	ASN
1	E	31	THR
1	E	38	LYS
1	E	40	LEU
1	E	118	LYS
1	E	175	ARG
1	E	177	VAL
1	E	179	LEU
1	E	194	ARG
1	E	214	ARG
1	E	223	ARG
1	E	265	LEU
1	E	267	VAL
1	E	269	ILE
1	E	304	TYR
1	E	335	LYS
1	E	345	TYR
1	E	362	PHE

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Mol	Chain	Res	Type
1	E	372	ILE
1	E	374	MET
1	E	382	SER
1	E	383	SER
1	E	394	LYS
1	E	396	MET
1	E	398	VAL
1	E	424	ARG
1	E	435	GLN
1	E	446	LYS
1	E	451	GLU
1	E	453	LYS
1	E	454	GLU
1	E	466	SER
1	E	467	LYS
1	E	471	GLN
1	E	472	THR
1	E	490	ASN
1	E	495	LEU
1	E	497	VAL
1	E	498	GLU
1	F	3	LEU
1	F	12	PHE
1	F	17	ASN
1	F	31	THR
1	F	38	LYS
1	F	40	LEU
1	F	118	LYS
1	F	175	ARG
1	F	177	VAL
1	F	179	LEU
1	F	194	ARG
1	F	214	ARG
1	F	223	ARG
1	F	265	LEU
1	F	267	VAL
1	F	269	ILE
1	F	304	TYR
1	F	335	LYS
1	F	345	TYR
1	F	362	PHE
1	F	372	ILE

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Mol	Chain	Res	Type
1	F	374	MET
1	F	382	SER
1	F	383	SER
1	F	394	LYS
1	F	396	MET
1	F	398	VAL
1	F	424	ARG
1	F	435	GLN
1	F	446	LYS
1	F	451	GLU
1	F	453	LYS
1	F	454	GLU
1	F	466	SER
1	F	467	LYS
1	F	471	GLN
1	F	472	THR
1	F	490	ASN
1	F	495	LEU
1	F	497	VAL
1	F	498	GLU
1	G	3	LEU
1	G	17	ASN
1	G	31	THR
1	G	38	LYS
1	G	40	LEU
1	G	118	LYS
1	G	175	ARG
1	G	177	VAL
1	G	179	LEU
1	G	194	ARG
1	G	214	ARG
1	G	223	ARG
1	G	265	LEU
1	G	267	VAL
1	G	269	ILE
1	G	304	TYR
1	G	335	LYS
1	G	345	TYR
1	G	362	PHE
1	G	372	ILE
1	G	374	MET
1	G	382	SER

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Mol	Chain	Res	Type
1	G	383	SER
1	G	394	LYS
1	G	396	MET
1	G	398	VAL
1	G	404	ARG
1	G	424	ARG
1	G	435	GLN
1	G	446	LYS
1	G	451	GLU
1	G	453	LYS
1	G	454	GLU
1	G	466	SER
1	G	467	LYS
1	G	471	GLN
1	G	472	THR
1	G	490	ASN
1	G	495	LEU
1	G	497	VAL
1	G	498	GLU
1	H	3	LEU
1	H	17	ASN
1	H	31	THR
1	H	38	LYS
1	H	40	LEU
1	H	118	LYS
1	H	175	ARG
1	H	177	VAL
1	H	179	LEU
1	H	194	ARG
1	H	214	ARG
1	H	223	ARG
1	H	265	LEU
1	H	267	VAL
1	H	269	ILE
1	H	297	GLN
1	H	304	TYR
1	H	335	LYS
1	H	345	TYR
1	H	362	PHE
1	H	371	HIS
1	H	372	ILE
1	H	382	SER

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Mol	Chain	Res	Type
1	H	383	SER
1	H	394	LYS
1	H	396	MET
1	H	398	VAL
1	H	424	ARG
1	H	435	GLN
1	H	446	LYS
1	H	451	GLU
1	H	453	LYS
1	H	454	GLU
1	H	466	SER
1	H	467	LYS
1	H	471	GLN
1	H	472	THR
1	H	490	ASN
1	H	495	LEU
1	H	497	VAL
1	H	498	GLU
1	I	3	LEU
1	I	17	ASN
1	I	31	THR
1	I	38	LYS
1	I	40	LEU
1	I	118	LYS
1	I	175	ARG
1	I	177	VAL
1	I	179	LEU
1	I	194	ARG
1	I	214	ARG
1	I	223	ARG
1	I	265	LEU
1	I	267	VAL
1	I	269	ILE
1	I	304	TYR
1	I	335	LYS
1	I	345	TYR
1	I	362	PHE
1	I	371	HIS
1	I	372	ILE
1	I	382	SER
1	I	383	SER
1	I	394	LYS

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Mol	Chain	Res	Type
1	I	396	MET
1	I	398	VAL
1	I	404	ARG
1	I	424	ARG
1	I	435	GLN
1	I	446	LYS
1	I	451	GLU
1	I	453	LYS
1	I	454	GLU
1	I	466	SER
1	I	467	LYS
1	I	471	GLN
1	I	472	THR
1	I	490	ASN
1	I	495	LEU
1	I	497	VAL
1	I	498	GLU
1	J	3	LEU
1	J	12	PHE
1	J	17	ASN
1	J	31	THR
1	J	38	LYS
1	J	40	LEU
1	J	118	LYS
1	J	175	ARG
1	J	177	VAL
1	J	179	LEU
1	J	194	ARG
1	J	214	ARG
1	J	223	ARG
1	J	265	LEU
1	J	267	VAL
1	J	269	ILE
1	J	304	TYR
1	J	335	LYS
1	J	345	TYR
1	J	362	PHE
1	J	372	ILE
1	J	374	MET
1	J	382	SER
1	J	383	SER
1	J	394	LYS

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Mol	Chain	Res	Type
1	J	396	MET
1	J	398	VAL
1	J	424	ARG
1	J	435	GLN
1	J	446	LYS
1	J	451	GLU
1	J	453	LYS
1	J	454	GLU
1	J	466	SER
1	J	467	LYS
1	J	471	GLN
1	J	472	THR
1	J	490	ASN
1	J	495	LEU
1	J	497	VAL
1	J	498	GLU
1	K	3	LEU
1	K	17	ASN
1	K	31	THR
1	K	38	LYS
1	K	40	LEU
1	K	118	LYS
1	K	175	ARG
1	K	177	VAL
1	K	179	LEU
1	K	194	ARG
1	K	214	ARG
1	K	223	ARG
1	K	265	LEU
1	K	267	VAL
1	K	269	ILE
1	K	304	TYR
1	K	335	LYS
1	K	345	TYR
1	K	362	PHE
1	K	372	ILE
1	K	374	MET
1	K	382	SER
1	K	383	SER
1	K	394	LYS
1	K	396	MET
1	K	398	VAL

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Mol	Chain	Res	Type
1	K	424	ARG
1	K	435	GLN
1	K	446	LYS
1	K	451	GLU
1	K	453	LYS
1	K	454	GLU
1	K	466	SER
1	K	467	LYS
1	K	471	GLN
1	K	472	THR
1	K	490	ASN
1	K	495	LEU
1	K	497	VAL
1	K	498	GLU
1	L	3	LEU
1	L	17	ASN
1	L	31	THR
1	L	38	LYS
1	L	40	LEU
1	L	118	LYS
1	L	175	ARG
1	L	177	VAL
1	L	179	LEU
1	L	194	ARG
1	L	214	ARG
1	L	223	ARG
1	L	265	LEU
1	L	267	VAL
1	L	269	ILE
1	L	304	TYR
1	L	335	LYS
1	L	337	LYS
1	L	345	TYR
1	L	362	PHE
1	L	372	ILE
1	L	382	SER
1	L	383	SER
1	L	394	LYS
1	L	396	MET
1	L	398	VAL
1	L	424	ARG
1	L	435	GLN

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Mol	Chain	Res	Type
1	L	446	LYS
1	L	451	GLU
1	L	453	LYS
1	L	454	GLU
1	L	466	SER
1	L	467	LYS
1	L	471	GLN
1	L	472	THR
1	L	490	ASN
1	L	495	LEU
1	L	497	VAL
1	L	498	GLU
1	M	3	LEU
1	M	12	PHE
1	M	17	ASN
1	M	31	THR
1	M	38	LYS
1	M	40	LEU
1	M	118	LYS
1	M	175	ARG
1	M	177	VAL
1	M	179	LEU
1	M	194	ARG
1	M	214	ARG
1	M	223	ARG
1	M	265	LEU
1	M	267	VAL
1	M	269	ILE
1	M	304	TYR
1	M	335	LYS
1	M	345	TYR
1	M	362	PHE
1	M	372	ILE
1	M	382	SER
1	M	383	SER
1	M	394	LYS
1	M	396	MET
1	M	398	VAL
1	M	424	ARG
1	M	435	GLN
1	M	446	LYS
1	M	451	GLU

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Mol	Chain	Res	Type
1	M	453	LYS
1	M	454	GLU
1	M	466	SER
1	M	467	LYS
1	M	471	GLN
1	M	472	THR
1	M	490	ASN
1	M	495	LEU
1	M	497	VAL
1	M	498	GLU
1	N	3	LEU
1	N	17	ASN
1	N	31	THR
1	N	38	LYS
1	N	40	LEU
1	N	118	LYS
1	N	175	ARG
1	N	177	VAL
1	N	179	LEU
1	N	194	ARG
1	N	214	ARG
1	N	223	ARG
1	N	265	LEU
1	N	267	VAL
1	N	269	ILE
1	N	304	TYR
1	N	335	LYS
1	N	345	TYR
1	N	362	PHE
1	N	372	ILE
1	N	374	MET
1	N	382	SER
1	N	383	SER
1	N	394	LYS
1	N	396	MET
1	N	398	VAL
1	N	424	ARG
1	N	435	GLN
1	N	446	LYS
1	N	451	GLU
1	N	453	LYS
1	N	454	GLU

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Mol	Chain	Res	Type
1	N	466	SER
1	N	467	LYS
1	N	471	GLN
1	N	472	THR
1	N	490	ASN
1	N	495	LEU
1	N	497	VAL
1	N	498	GLU
1	O	3	LEU
1	O	17	ASN
1	O	31	THR
1	O	38	LYS
1	O	40	LEU
1	O	118	LYS
1	O	175	ARG
1	O	177	VAL
1	O	179	LEU
1	O	194	ARG
1	O	214	ARG
1	O	223	ARG
1	O	265	LEU
1	O	267	VAL
1	O	269	ILE
1	O	304	TYR
1	O	335	LYS
1	O	345	TYR
1	O	362	PHE
1	O	372	ILE
1	O	374	MET
1	O	382	SER
1	O	383	SER
1	O	394	LYS
1	O	396	MET
1	O	398	VAL
1	O	404	ARG
1	O	424	ARG
1	O	435	GLN
1	O	446	LYS
1	O	451	GLU
1	O	453	LYS
1	O	454	GLU
1	O	466	SER

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Mol	Chain	Res	Type
1	O	467	LYS
1	O	471	GLN
1	O	472	THR
1	O	490	ASN
1	O	495	LEU
1	O	497	VAL
1	O	498	GLU
1	P	3	LEU
1	P	12	PHE
1	P	17	ASN
1	P	31	THR
1	P	38	LYS
1	P	40	LEU
1	P	118	LYS
1	P	175	ARG
1	P	177	VAL
1	P	179	LEU
1	P	194	ARG
1	P	214	ARG
1	P	223	ARG
1	P	265	LEU
1	P	267	VAL
1	P	269	ILE
1	P	304	TYR
1	P	335	LYS
1	P	345	TYR
1	P	362	PHE
1	P	372	ILE
1	P	382	SER
1	P	383	SER
1	P	394	LYS
1	P	396	MET
1	P	398	VAL
1	P	424	ARG
1	P	435	GLN
1	P	446	LYS
1	P	451	GLU
1	P	453	LYS
1	P	454	GLU
1	P	466	SER
1	P	467	LYS
1	P	471	GLN

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Mol	Chain	Res	Type
1	P	472	THR
1	P	490	ASN
1	P	495	LEU
1	P	497	VAL
1	P	498	GLU
1	Q	3	LEU
1	Q	12	PHE
1	Q	17	ASN
1	Q	31	THR
1	Q	38	LYS
1	Q	40	LEU
1	Q	118	LYS
1	Q	175	ARG
1	Q	177	VAL
1	Q	179	LEU
1	Q	194	ARG
1	Q	214	ARG
1	Q	223	ARG
1	Q	265	LEU
1	Q	267	VAL
1	Q	269	ILE
1	Q	304	TYR
1	Q	335	LYS
1	Q	345	TYR
1	Q	362	PHE
1	Q	372	ILE
1	Q	374	MET
1	Q	382	SER
1	Q	383	SER
1	Q	394	LYS
1	Q	396	MET
1	Q	398	VAL
1	Q	424	ARG
1	Q	435	GLN
1	Q	446	LYS
1	Q	451	GLU
1	Q	453	LYS
1	Q	454	GLU
1	Q	466	SER
1	Q	467	LYS
1	Q	471	GLN
1	Q	472	THR

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Mol	Chain	Res	Type
1	Q	490	ASN
1	Q	495	LEU
1	Q	497	VAL
1	Q	498	GLU
1	R	3	LEU
1	R	17	ASN
1	R	31	THR
1	R	38	LYS
1	R	40	LEU
1	R	118	LYS
1	R	175	ARG
1	R	177	VAL
1	R	179	LEU
1	R	194	ARG
1	R	214	ARG
1	R	223	ARG
1	R	265	LEU
1	R	267	VAL
1	R	269	ILE
1	R	297	GLN
1	R	304	TYR
1	R	335	LYS
1	R	345	TYR
1	R	362	PHE
1	R	372	ILE
1	R	382	SER
1	R	383	SER
1	R	394	LYS
1	R	396	MET
1	R	398	VAL
1	R	424	ARG
1	R	435	GLN
1	R	446	LYS
1	R	451	GLU
1	R	453	LYS
1	R	454	GLU
1	R	466	SER
1	R	467	LYS
1	R	471	GLN
1	R	472	THR
1	R	490	ASN
1	R	495	LEU

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Mol	Chain	Res	Type
1	R	497	VAL
1	R	498	GLU
1	S	3	LEU
1	S	12	PHE
1	S	17	ASN
1	S	31	THR
1	S	38	LYS
1	S	40	LEU
1	S	118	LYS
1	S	175	ARG
1	S	177	VAL
1	S	179	LEU
1	S	194	ARG
1	S	214	ARG
1	S	223	ARG
1	S	265	LEU
1	S	267	VAL
1	S	269	ILE
1	S	304	TYR
1	S	335	LYS
1	S	345	TYR
1	S	362	PHE
1	S	374	MET
1	S	382	SER
1	S	383	SER
1	S	394	LYS
1	S	396	MET
1	S	398	VAL
1	S	424	ARG
1	S	435	GLN
1	S	446	LYS
1	S	451	GLU
1	S	453	LYS
1	S	454	GLU
1	S	466	SER
1	S	467	LYS
1	S	471	GLN
1	S	472	THR
1	S	490	ASN
1	S	495	LEU
1	S	497	VAL
1	S	498	GLU

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Mol	Chain	Res	Type
1	T	3	LEU
1	T	12	PHE
1	T	17	ASN
1	T	31	THR
1	T	38	LYS
1	T	40	LEU
1	T	118	LYS
1	T	175	ARG
1	T	177	VAL
1	T	179	LEU
1	T	194	ARG
1	T	214	ARG
1	T	223	ARG
1	T	265	LEU
1	T	267	VAL
1	T	269	ILE
1	T	304	TYR
1	T	335	LYS
1	T	345	TYR
1	T	362	PHE
1	T	372	ILE
1	T	382	SER
1	T	383	SER
1	T	394	LYS
1	T	396	MET
1	T	398	VAL
1	T	424	ARG
1	T	435	GLN
1	T	446	LYS
1	T	451	GLU
1	T	453	LYS
1	T	454	GLU
1	T	466	SER
1	T	467	LYS
1	T	471	GLN
1	T	472	THR
1	T	490	ASN
1	T	495	LEU
1	T	497	VAL
1	T	498	GLU
1	U	3	LEU
1	U	17	ASN

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Mol	Chain	Res	Type
1	U	31	THR
1	U	38	LYS
1	U	40	LEU
1	U	118	LYS
1	U	175	ARG
1	U	177	VAL
1	U	179	LEU
1	U	194	ARG
1	U	214	ARG
1	U	223	ARG
1	U	265	LEU
1	U	267	VAL
1	U	269	ILE
1	U	304	TYR
1	U	335	LYS
1	U	345	TYR
1	U	362	PHE
1	U	372	ILE
1	U	382	SER
1	U	383	SER
1	U	394	LYS
1	U	396	MET
1	U	398	VAL
1	U	404	ARG
1	U	424	ARG
1	U	435	GLN
1	U	446	LYS
1	U	451	GLU
1	U	453	LYS
1	U	454	GLU
1	U	466	SER
1	U	467	LYS
1	U	471	GLN
1	U	472	THR
1	U	490	ASN
1	U	495	LEU
1	U	497	VAL
1	U	498	GLU
1	V	3	LEU
1	V	17	ASN
1	V	31	THR
1	V	38	LYS

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Mol	Chain	Res	Type
1	V	40	LEU
1	V	118	LYS
1	V	175	ARG
1	V	177	VAL
1	V	179	LEU
1	V	194	ARG
1	V	214	ARG
1	V	223	ARG
1	V	265	LEU
1	V	267	VAL
1	V	269	ILE
1	V	304	TYR
1	V	335	LYS
1	V	345	TYR
1	V	362	PHE
1	V	372	ILE
1	V	374	MET
1	V	382	SER
1	V	383	SER
1	V	394	LYS
1	V	396	MET
1	V	398	VAL
1	V	424	ARG
1	V	435	GLN
1	V	446	LYS
1	V	451	GLU
1	V	453	LYS
1	V	454	GLU
1	V	466	SER
1	V	467	LYS
1	V	471	GLN
1	V	472	THR
1	V	490	ASN
1	V	495	LEU
1	V	497	VAL
1	V	498	GLU
1	W	3	LEU
1	W	12	PHE
1	W	17	ASN
1	W	31	THR
1	W	38	LYS
1	W	40	LEU

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Mol	Chain	Res	Type
1	W	118	LYS
1	W	175	ARG
1	W	177	VAL
1	W	179	LEU
1	W	194	ARG
1	W	214	ARG
1	W	223	ARG
1	W	265	LEU
1	W	267	VAL
1	W	269	ILE
1	W	304	TYR
1	W	335	LYS
1	W	345	TYR
1	W	362	PHE
1	W	372	ILE
1	W	374	MET
1	W	382	SER
1	W	383	SER
1	W	394	LYS
1	W	396	MET
1	W	398	VAL
1	W	404	ARG
1	W	424	ARG
1	W	435	GLN
1	W	446	LYS
1	W	451	GLU
1	W	453	LYS
1	W	454	GLU
1	W	466	SER
1	W	467	LYS
1	W	471	GLN
1	W	472	THR
1	W	490	ASN
1	W	495	LEU
1	W	497	VAL
1	W	498	GLU
1	X	17	ASN
1	X	31	THR
1	X	38	LYS
1	X	40	LEU
1	X	118	LYS
1	X	175	ARG

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Mol	Chain	Res	Type
1	X	177	VAL
1	X	179	LEU
1	X	194	ARG
1	X	214	ARG
1	X	223	ARG
1	X	265	LEU
1	X	267	VAL
1	X	269	ILE
1	X	304	TYR
1	X	335	LYS
1	X	345	TYR
1	X	362	PHE
1	X	372	ILE
1	X	374	MET
1	X	382	SER
1	X	383	SER
1	X	394	LYS
1	X	396	MET
1	X	398	VAL
1	X	424	ARG
1	X	435	GLN
1	X	446	LYS
1	X	451	GLU
1	X	453	LYS
1	X	454	GLU
1	X	466	SER
1	X	467	LYS
1	X	471	GLN
1	X	472	THR
1	X	490	ASN
1	X	495	LEU
1	X	497	VAL
1	X	498	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (267) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	139	ASN
1	A	151	GLN
1	A	178	ASN
1	A	218	GLN

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Mol	Chain	Res	Type
1	A	286	ASN
1	A	305	ASN
1	A	371	HIS
1	A	490	ASN
1	B	17	ASN
1	B	139	ASN
1	B	151	GLN
1	B	178	ASN
1	B	218	GLN
1	B	242	HIS
1	B	286	ASN
1	B	305	ASN
1	B	371	HIS
1	B	490	ASN
1	C	17	ASN
1	C	139	ASN
1	C	151	GLN
1	C	178	ASN
1	C	218	GLN
1	C	242	HIS
1	C	286	ASN
1	C	305	ASN
1	C	371	HIS
1	C	483	HIS
1	C	490	ASN
1	D	17	ASN
1	D	139	ASN
1	D	151	GLN
1	D	178	ASN
1	D	218	GLN
1	D	242	HIS
1	D	286	ASN
1	D	305	ASN
1	D	371	HIS
1	D	483	HIS
1	D	490	ASN
1	E	17	ASN
1	E	139	ASN
1	E	151	GLN
1	E	178	ASN
1	E	218	GLN
1	E	242	HIS

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Mol	Chain	Res	Type
1	E	286	ASN
1	E	305	ASN
1	E	371	HIS
1	E	483	HIS
1	E	490	ASN
1	F	17	ASN
1	F	139	ASN
1	F	151	GLN
1	F	178	ASN
1	F	218	GLN
1	F	242	HIS
1	F	286	ASN
1	F	305	ASN
1	F	371	HIS
1	F	483	HIS
1	F	490	ASN
1	G	17	ASN
1	G	139	ASN
1	G	151	GLN
1	G	178	ASN
1	G	218	GLN
1	G	286	ASN
1	G	305	ASN
1	G	371	HIS
1	G	483	HIS
1	G	490	ASN
1	H	17	ASN
1	H	139	ASN
1	H	151	GLN
1	H	178	ASN
1	H	218	GLN
1	H	242	HIS
1	H	286	ASN
1	H	305	ASN
1	H	318	ASN
1	H	371	HIS
1	H	483	HIS
1	H	490	ASN
1	I	17	ASN
1	I	139	ASN
1	I	151	GLN
1	I	178	ASN

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Mol	Chain	Res	Type
1	I	218	GLN
1	I	242	HIS
1	I	286	ASN
1	I	305	ASN
1	I	371	HIS
1	I	483	HIS
1	I	490	ASN
1	J	17	ASN
1	J	139	ASN
1	J	151	GLN
1	J	178	ASN
1	J	218	GLN
1	J	242	HIS
1	J	286	ASN
1	J	305	ASN
1	J	318	ASN
1	J	371	HIS
1	J	490	ASN
1	K	17	ASN
1	K	139	ASN
1	K	151	GLN
1	K	178	ASN
1	K	218	GLN
1	K	242	HIS
1	K	286	ASN
1	K	305	ASN
1	K	318	ASN
1	K	371	HIS
1	K	483	HIS
1	K	490	ASN
1	L	17	ASN
1	L	139	ASN
1	L	151	GLN
1	L	178	ASN
1	L	218	GLN
1	L	242	HIS
1	L	286	ASN
1	L	305	ASN
1	L	371	HIS
1	L	483	HIS
1	L	490	ASN
1	M	17	ASN

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Mol	Chain	Res	Type
1	M	139	ASN
1	M	151	GLN
1	M	178	ASN
1	M	218	GLN
1	M	242	HIS
1	M	286	ASN
1	M	305	ASN
1	M	318	ASN
1	M	371	HIS
1	M	483	HIS
1	M	490	ASN
1	N	17	ASN
1	N	139	ASN
1	N	151	GLN
1	N	178	ASN
1	N	218	GLN
1	N	242	HIS
1	N	286	ASN
1	N	305	ASN
1	N	371	HIS
1	N	483	HIS
1	N	490	ASN
1	O	17	ASN
1	O	139	ASN
1	O	151	GLN
1	O	178	ASN
1	O	218	GLN
1	O	242	HIS
1	O	286	ASN
1	O	305	ASN
1	O	318	ASN
1	O	371	HIS
1	O	490	ASN
1	P	17	ASN
1	P	139	ASN
1	P	151	GLN
1	P	178	ASN
1	P	218	GLN
1	P	242	HIS
1	P	286	ASN
1	P	305	ASN
1	P	318	ASN

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Mol	Chain	Res	Type
1	P	371	HIS
1	P	483	HIS
1	P	490	ASN
1	Q	17	ASN
1	Q	139	ASN
1	Q	151	GLN
1	Q	178	ASN
1	Q	218	GLN
1	Q	242	HIS
1	Q	286	ASN
1	Q	305	ASN
1	Q	371	HIS
1	Q	483	HIS
1	Q	490	ASN
1	R	17	ASN
1	R	139	ASN
1	R	151	GLN
1	R	178	ASN
1	R	218	GLN
1	R	242	HIS
1	R	286	ASN
1	R	297	GLN
1	R	305	ASN
1	R	371	HIS
1	R	483	HIS
1	R	490	ASN
1	S	17	ASN
1	S	139	ASN
1	S	151	GLN
1	S	178	ASN
1	S	218	GLN
1	S	242	HIS
1	S	286	ASN
1	S	305	ASN
1	S	371	HIS
1	S	490	ASN
1	T	17	ASN
1	T	139	ASN
1	T	151	GLN
1	T	178	ASN
1	T	218	GLN
1	T	286	ASN

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Mol	Chain	Res	Type
1	T	305	ASN
1	T	371	HIS
1	T	483	HIS
1	T	490	ASN
1	T	491	GLN
1	U	17	ASN
1	U	139	ASN
1	U	151	GLN
1	U	178	ASN
1	U	218	GLN
1	U	242	HIS
1	U	286	ASN
1	U	305	ASN
1	U	318	ASN
1	U	371	HIS
1	U	483	HIS
1	U	490	ASN
1	V	17	ASN
1	V	139	ASN
1	V	151	GLN
1	V	178	ASN
1	V	218	GLN
1	V	242	HIS
1	V	286	ASN
1	V	297	GLN
1	V	305	ASN
1	V	371	HIS
1	V	483	HIS
1	V	490	ASN
1	W	17	ASN
1	W	139	ASN
1	W	151	GLN
1	W	178	ASN
1	W	218	GLN
1	W	242	HIS
1	W	286	ASN
1	W	305	ASN
1	W	318	ASN
1	W	371	HIS
1	W	483	HIS
1	W	490	ASN
1	X	17	ASN

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Mol	Chain	Res	Type
1	X	139	ASN
1	X	151	GLN
1	X	178	ASN
1	X	218	GLN
1	X	242	HIS
1	X	286	ASN
1	X	305	ASN
1	X	371	HIS
1	X	483	HIS
1	X	490	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FDP	A	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	B	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	C	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FDP	D	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	E	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	F	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	G	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	H	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	I	700	-	20,20,20	1.05	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	J	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	K	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	L	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	M	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	N	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	O	700	-	20,20,20	1.05	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	P	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	Q	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	R	700	-	20,20,20	1.05	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	S	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	T	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	U	700	-	20,20,20	1.05	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	V	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	W	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)
2	FDP	X	700	-	20,20,20	1.06	2 (10%)	30,32,32	1.33	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FDP	A	700	-	-	0/12/34/34	0/1/1/1
2	FDP	B	700	-	-	0/12/34/34	0/1/1/1
2	FDP	C	700	-	-	0/12/34/34	0/1/1/1
2	FDP	D	700	-	-	0/12/34/34	0/1/1/1
2	FDP	E	700	-	-	0/12/34/34	0/1/1/1
2	FDP	F	700	-	-	0/12/34/34	0/1/1/1
2	FDP	G	700	-	-	0/12/34/34	0/1/1/1
2	FDP	H	700	-	-	0/12/34/34	0/1/1/1
2	FDP	I	700	-	-	0/12/34/34	0/1/1/1
2	FDP	J	700	-	-	0/12/34/34	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FDP	K	700	-	-	0/12/34/34	0/1/1/1
2	FDP	L	700	-	-	0/12/34/34	0/1/1/1
2	FDP	M	700	-	-	0/12/34/34	0/1/1/1
2	FDP	N	700	-	-	0/12/34/34	0/1/1/1
2	FDP	O	700	-	-	0/12/34/34	0/1/1/1
2	FDP	P	700	-	-	0/12/34/34	0/1/1/1
2	FDP	Q	700	-	-	0/12/34/34	0/1/1/1
2	FDP	R	700	-	-	0/12/34/34	0/1/1/1
2	FDP	S	700	-	-	0/12/34/34	0/1/1/1
2	FDP	T	700	-	-	0/12/34/34	0/1/1/1
2	FDP	U	700	-	-	0/12/34/34	0/1/1/1
2	FDP	V	700	-	-	0/12/34/34	0/1/1/1
2	FDP	W	700	-	-	0/12/34/34	0/1/1/1
2	FDP	X	700	-	-	0/12/34/34	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	700	FDP	O4-C4	-2.52	1.37	1.43
2	X	700	FDP	O4-C4	-2.52	1.37	1.43
2	A	700	FDP	O4-C4	-2.52	1.37	1.43
2	W	700	FDP	O4-C4	-2.51	1.37	1.43
2	E	700	FDP	O4-C4	-2.51	1.37	1.43
2	C	700	FDP	O4-C4	-2.50	1.37	1.43
2	V	700	FDP	O4-C4	-2.50	1.37	1.43
2	M	700	FDP	O4-C4	-2.50	1.37	1.43
2	N	700	FDP	O4-C4	-2.50	1.37	1.43
2	D	700	FDP	O4-C4	-2.50	1.37	1.43
2	F	700	FDP	O4-C4	-2.50	1.37	1.43
2	L	700	FDP	O4-C4	-2.50	1.37	1.43
2	B	700	FDP	O4-C4	-2.49	1.37	1.43
2	P	700	FDP	O4-C4	-2.48	1.37	1.43
2	J	700	FDP	O4-C4	-2.48	1.37	1.43
2	I	700	FDP	O4-C4	-2.48	1.37	1.43
2	Q	700	FDP	O4-C4	-2.48	1.37	1.43
2	O	700	FDP	O4-C4	-2.48	1.37	1.43
2	G	700	FDP	O4-C4	-2.48	1.37	1.43
2	S	700	FDP	O4-C4	-2.47	1.37	1.43
2	U	700	FDP	O4-C4	-2.47	1.37	1.43
2	T	700	FDP	O4-C4	-2.47	1.37	1.43
2	H	700	FDP	O4-C4	-2.47	1.37	1.43
2	R	700	FDP	O4-C4	-2.46	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	700	FDP	P2-O5P	-2.09	1.46	1.54
2	E	700	FDP	P2-O5P	-2.09	1.46	1.54
2	H	700	FDP	P2-O5P	-2.08	1.46	1.54
2	P	700	FDP	P2-O5P	-2.08	1.46	1.54
2	Q	700	FDP	P2-O5P	-2.08	1.46	1.54
2	T	700	FDP	P2-O5P	-2.07	1.46	1.54
2	W	700	FDP	P2-O5P	-2.07	1.46	1.54
2	A	700	FDP	P2-O5P	-2.07	1.46	1.54
2	U	700	FDP	P2-O5P	-2.07	1.46	1.54
2	M	700	FDP	P2-O5P	-2.07	1.46	1.54
2	K	700	FDP	P2-O5P	-2.07	1.46	1.54
2	X	700	FDP	P2-O5P	-2.07	1.46	1.54
2	I	700	FDP	P2-O5P	-2.07	1.46	1.54
2	G	700	FDP	P2-O5P	-2.07	1.46	1.54
2	V	700	FDP	P2-O5P	-2.06	1.46	1.54
2	C	700	FDP	P2-O5P	-2.06	1.46	1.54
2	J	700	FDP	P2-O5P	-2.06	1.46	1.54
2	S	700	FDP	P2-O5P	-2.06	1.46	1.54
2	R	700	FDP	P2-O5P	-2.06	1.46	1.54
2	O	700	FDP	P2-O5P	-2.06	1.46	1.54
2	D	700	FDP	P2-O5P	-2.06	1.46	1.54
2	L	700	FDP	P2-O5P	-2.06	1.46	1.54
2	B	700	FDP	P2-O5P	-2.06	1.46	1.54
2	F	700	FDP	P2-O5P	-2.06	1.46	1.54

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	700	FDP	C6-C5-C4	-2.63	105.28	115.29
2	X	700	FDP	C6-C5-C4	-2.62	105.29	115.29
2	W	700	FDP	C6-C5-C4	-2.62	105.30	115.29
2	O	700	FDP	C6-C5-C4	-2.62	105.30	115.29
2	Q	700	FDP	C6-C5-C4	-2.62	105.31	115.29
2	R	700	FDP	C6-C5-C4	-2.62	105.31	115.29
2	U	700	FDP	C6-C5-C4	-2.62	105.32	115.29
2	D	700	FDP	C6-C5-C4	-2.62	105.32	115.29
2	C	700	FDP	C6-C5-C4	-2.62	105.32	115.29
2	B	700	FDP	C6-C5-C4	-2.61	105.32	115.29
2	T	700	FDP	C6-C5-C4	-2.61	105.32	115.29
2	N	700	FDP	C6-C5-C4	-2.61	105.32	115.29
2	K	700	FDP	C6-C5-C4	-2.61	105.33	115.29
2	J	700	FDP	C6-C5-C4	-2.61	105.33	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	FDP	C6-C5-C4	-2.61	105.33	115.29
2	I	700	FDP	C6-C5-C4	-2.61	105.33	115.29
2	P	700	FDP	C6-C5-C4	-2.61	105.34	115.29
2	G	700	FDP	C6-C5-C4	-2.61	105.34	115.29
2	M	700	FDP	C6-C5-C4	-2.61	105.34	115.29
2	E	700	FDP	C6-C5-C4	-2.61	105.35	115.29
2	S	700	FDP	C6-C5-C4	-2.61	105.35	115.29
2	L	700	FDP	C6-C5-C4	-2.61	105.36	115.29
2	H	700	FDP	C6-C5-C4	-2.60	105.38	115.29
2	V	700	FDP	C6-C5-C4	-2.60	105.38	115.29
2	R	700	FDP	O5-C2-C3	-2.16	100.88	105.57
2	A	700	FDP	O5-C2-C3	-2.16	100.89	105.57
2	O	700	FDP	O5-C2-C3	-2.15	100.90	105.57
2	L	700	FDP	O5-C2-C3	-2.15	100.90	105.57
2	P	700	FDP	O5-C2-C3	-2.15	100.91	105.57
2	B	700	FDP	O5-C2-C3	-2.15	100.91	105.57
2	Q	700	FDP	O5-C2-C3	-2.14	100.92	105.57
2	I	700	FDP	O5-C2-C3	-2.14	100.92	105.57
2	K	700	FDP	O5-C2-C3	-2.14	100.93	105.57
2	V	700	FDP	O5-C2-C3	-2.14	100.93	105.57
2	F	700	FDP	O5-C2-C3	-2.14	100.93	105.57
2	U	700	FDP	O5-C2-C3	-2.13	100.94	105.57
2	S	700	FDP	O5-C2-C3	-2.13	100.94	105.57
2	T	700	FDP	O5-C2-C3	-2.13	100.94	105.57
2	M	700	FDP	O5-C2-C3	-2.13	100.95	105.57
2	N	700	FDP	O5-C2-C3	-2.13	100.95	105.57
2	H	700	FDP	O5-C2-C3	-2.13	100.95	105.57
2	E	700	FDP	O5-C2-C3	-2.12	100.96	105.57
2	J	700	FDP	O5-C2-C3	-2.12	100.96	105.57
2	D	700	FDP	O5-C2-C3	-2.12	100.96	105.57
2	C	700	FDP	O5-C2-C3	-2.12	100.97	105.57
2	G	700	FDP	O5-C2-C3	-2.12	100.97	105.57
2	X	700	FDP	O5-C2-C3	-2.12	100.97	105.57
2	W	700	FDP	O5-C2-C3	-2.12	100.97	105.57
2	D	700	FDP	O2-C2-C3	3.00	118.43	108.22
2	N	700	FDP	O2-C2-C3	3.00	118.43	108.22
2	P	700	FDP	O2-C2-C3	3.01	118.44	108.22
2	U	700	FDP	O2-C2-C3	3.01	118.45	108.22
2	L	700	FDP	O2-C2-C3	3.01	118.45	108.22
2	X	700	FDP	O2-C2-C3	3.01	118.46	108.22
2	S	700	FDP	O2-C2-C3	3.01	118.46	108.22
2	M	700	FDP	O2-C2-C3	3.01	118.46	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	FDP	O2-C2-C3	3.01	118.46	108.22
2	H	700	FDP	O2-C2-C3	3.02	118.48	108.22
2	O	700	FDP	O2-C2-C3	3.02	118.48	108.22
2	B	700	FDP	O2-C2-C3	3.02	118.48	108.22
2	Q	700	FDP	O2-C2-C3	3.02	118.49	108.22
2	C	700	FDP	O2-C2-C3	3.02	118.49	108.22
2	G	700	FDP	O2-C2-C3	3.02	118.49	108.22
2	K	700	FDP	O2-C2-C3	3.02	118.50	108.22
2	V	700	FDP	O2-C2-C3	3.02	118.50	108.22
2	W	700	FDP	O2-C2-C3	3.02	118.50	108.22
2	J	700	FDP	O2-C2-C3	3.03	118.50	108.22
2	I	700	FDP	O2-C2-C3	3.03	118.51	108.22
2	F	700	FDP	O2-C2-C3	3.03	118.52	108.22
2	R	700	FDP	O2-C2-C3	3.03	118.52	108.22
2	E	700	FDP	O2-C2-C3	3.03	118.52	108.22
2	T	700	FDP	O2-C2-C3	3.03	118.53	108.22
2	W	700	FDP	O6-P2-O4P	3.04	115.00	106.47
2	N	700	FDP	O6-P2-O4P	3.04	115.00	106.47
2	C	700	FDP	O6-P2-O4P	3.04	115.01	106.47
2	H	700	FDP	O6-P2-O4P	3.04	115.01	106.47
2	P	700	FDP	O6-P2-O4P	3.05	115.02	106.47
2	D	700	FDP	O6-P2-O4P	3.05	115.03	106.47
2	K	700	FDP	O6-P2-O4P	3.05	115.03	106.47
2	E	700	FDP	O6-P2-O4P	3.05	115.03	106.47
2	U	700	FDP	O6-P2-O4P	3.05	115.03	106.47
2	A	700	FDP	O6-P2-O4P	3.05	115.03	106.47
2	T	700	FDP	O6-P2-O4P	3.05	115.04	106.47
2	J	700	FDP	O6-P2-O4P	3.05	115.04	106.47
2	R	700	FDP	O6-P2-O4P	3.06	115.05	106.47
2	L	700	FDP	O6-P2-O4P	3.06	115.06	106.47
2	G	700	FDP	O6-P2-O4P	3.06	115.06	106.47
2	Q	700	FDP	O6-P2-O4P	3.06	115.06	106.47
2	B	700	FDP	O6-P2-O4P	3.06	115.07	106.47
2	S	700	FDP	O6-P2-O4P	3.06	115.07	106.47
2	I	700	FDP	O6-P2-O4P	3.07	115.07	106.47
2	F	700	FDP	O6-P2-O4P	3.07	115.08	106.47
2	M	700	FDP	O6-P2-O4P	3.07	115.09	106.47
2	X	700	FDP	O6-P2-O4P	3.07	115.09	106.47
2	O	700	FDP	O6-P2-O4P	3.07	115.09	106.47
2	V	700	FDP	O6-P2-O4P	3.08	115.10	106.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 106 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	FDP	4	0
2	B	700	FDP	4	0
2	C	700	FDP	4	0
2	D	700	FDP	4	0
2	E	700	FDP	4	0
2	F	700	FDP	4	0
2	G	700	FDP	4	0
2	H	700	FDP	5	0
2	I	700	FDP	4	0
2	J	700	FDP	4	0
2	K	700	FDP	5	0
2	L	700	FDP	5	0
2	M	700	FDP	4	0
2	N	700	FDP	4	0
2	O	700	FDP	5	0
2	P	700	FDP	5	0
2	Q	700	FDP	4	0
2	R	700	FDP	5	0
2	S	700	FDP	4	0
2	T	700	FDP	5	0
2	U	700	FDP	4	0
2	V	700	FDP	5	0
2	W	700	FDP	5	0
2	X	700	FDP	5	0

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	498/499 (99%)	0.52	28 (5%) 25 23	13, 23, 36, 46	0
1	B	498/499 (99%)	0.35	16 (3%) 48 41	13, 23, 36, 46	0
1	C	498/499 (99%)	0.38	11 (2%) 62 56	13, 23, 36, 46	0
1	D	498/499 (99%)	0.42	19 (3%) 41 36	13, 23, 36, 46	0
1	E	498/499 (99%)	0.39	14 (2%) 53 47	13, 23, 36, 46	0
1	F	498/499 (99%)	0.40	14 (2%) 53 47	13, 23, 36, 46	0
1	G	498/499 (99%)	0.37	14 (2%) 53 47	13, 23, 36, 46	0
1	H	498/499 (99%)	0.34	15 (3%) 51 44	13, 23, 36, 46	0
1	I	498/499 (99%)	0.36	12 (2%) 59 53	13, 23, 36, 46	0
1	J	498/499 (99%)	0.42	19 (3%) 41 36	13, 23, 36, 46	0
1	K	498/499 (99%)	0.38	17 (3%) 46 40	13, 23, 36, 46	0
1	L	498/499 (99%)	0.41	11 (2%) 62 56	13, 23, 36, 46	0
1	M	498/499 (99%)	0.32	5 (1%) 82 76	13, 23, 36, 46	0
1	N	498/499 (99%)	0.40	14 (2%) 53 47	13, 23, 36, 46	0
1	O	498/499 (99%)	0.47	30 (6%) 23 21	13, 23, 36, 46	0
1	P	498/499 (99%)	0.37	16 (3%) 48 41	13, 23, 36, 46	0
1	Q	498/499 (99%)	0.34	7 (1%) 75 68	13, 23, 36, 46	0
1	R	498/499 (99%)	0.38	14 (2%) 53 47	13, 23, 36, 46	0
1	S	498/499 (99%)	0.33	7 (1%) 75 68	13, 23, 36, 46	0
1	T	498/499 (99%)	0.43	21 (4%) 37 33	13, 23, 36, 46	0
1	U	498/499 (99%)	0.37	10 (2%) 65 59	13, 23, 36, 46	0
1	V	498/499 (99%)	0.41	8 (1%) 72 65	13, 23, 36, 46	0
1	W	498/499 (99%)	0.41	14 (2%) 53 47	13, 23, 36, 46	0
1	X	498/499 (99%)	0.50	28 (5%) 25 23	13, 23, 36, 46	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	11952/11976 (99%)	0.40	364 (3%)	51	44	13, 23, 36, 46	0

All (364) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	VAL	6.1
1	O	163	CYS	5.7
1	A	132	SER	5.4
1	A	131	LEU	5.2
1	T	116	ALA	5.1
1	A	134	VAL	5.0
1	S	49	ARG	4.9
1	A	100	VAL	4.8
1	O	162	GLU	4.5
1	X	95	VAL	4.3
1	I	124	PHE	4.3
1	G	105	ALA	4.2
1	L	141	ILE	4.2
1	Q	87	PRO	4.2
1	R	498	GLU	4.2
1	U	498	GLU	4.1
1	P	260	VAL	4.1
1	O	92	GLY	3.9
1	B	493	ARG	3.8
1	H	101	MET	3.8
1	O	91	THR	3.7
1	X	96	GLY	3.7
1	I	123	LYS	3.7
1	G	171	ILE	3.7
1	J	346	MET	3.7
1	H	498	GLU	3.6
1	L	135	VAL	3.5
1	A	332	GLU	3.5
1	T	117	ASP	3.4
1	A	109	VAL	3.4
1	O	99	ALA	3.4
1	K	172	SER	3.4
1	E	328	MET	3.3
1	A	440	VAL	3.3
1	E	172	SER	3.3
1	K	169	HIS	3.3
1	G	102	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	188	ALA	3.3
1	F	342	VAL	3.3
1	K	171	ILE	3.3
1	W	184	VAL	3.3
1	A	439	SER	3.2
1	P	173	ASP	3.2
1	S	50	MET	3.2
1	A	38	LYS	3.2
1	O	184	VAL	3.2
1	X	120	THR	3.2
1	X	170	THR	3.2
1	G	101	MET	3.2
1	T	106	THR	3.2
1	H	93	GLN	3.1
1	G	106	THR	3.1
1	A	494	ILE	3.1
1	I	106	THR	3.1
1	Q	161	LEU	3.1
1	B	396	MET	3.1
1	N	124	PHE	3.1
1	J	106	THR	3.1
1	K	155	HIS	3.1
1	D	96	GLY	3.1
1	E	131	LEU	3.0
1	Q	494	ILE	3.0
1	T	165	VAL	3.0
1	E	100	VAL	3.0
1	T	93	GLN	3.0
1	X	171	ILE	3.0
1	O	101	MET	3.0
1	K	141	ILE	3.0
1	W	102	GLU	3.0
1	T	184	VAL	3.0
1	U	494	ILE	3.0
1	W	49	ARG	3.0
1	D	370	GLN	2.9
1	D	88	GLU	2.9
1	X	143	ILE	2.9
1	O	259	MET	2.9
1	L	140	TYR	2.9
1	R	320	VAL	2.9
1	O	154	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	150	LEU	2.9
1	B	367	LYS	2.9
1	D	97	GLY	2.9
1	D	101	MET	2.9
1	P	381	CYS	2.9
1	P	258	ILE	2.8
1	V	85	LYS	2.8
1	R	106	THR	2.8
1	Q	162	GLU	2.8
1	P	57	HIS	2.8
1	B	240	GLU	2.8
1	O	129	GLN	2.8
1	K	214	ARG	2.8
1	R	99	ALA	2.8
1	C	171	ILE	2.8
1	G	165	VAL	2.8
1	V	396	MET	2.8
1	G	27	ILE	2.7
1	M	346	MET	2.7
1	J	207	MET	2.7
1	T	232	ASP	2.7
1	A	184	VAL	2.7
1	C	188	ALA	2.7
1	O	153	GLN	2.7
1	H	92	GLY	2.7
1	D	259	MET	2.7
1	G	197	LEU	2.7
1	P	439	SER	2.7
1	F	96	GLY	2.7
1	U	93	GLN	2.7
1	H	166	THR	2.7
1	X	316	VAL	2.7
1	P	261	ALA	2.7
1	H	124	PHE	2.7
1	C	390	GLU	2.7
1	B	327	VAL	2.7
1	G	100	VAL	2.7
1	H	165	VAL	2.7
1	K	161	LEU	2.7
1	A	27	ILE	2.7
1	B	478	VAL	2.7
1	J	397	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	327	VAL	2.6
1	C	101	MET	2.6
1	F	124	PHE	2.6
1	O	398	VAL	2.6
1	B	449	HIS	2.6
1	K	170	THR	2.6
1	B	328	MET	2.6
1	C	150	LEU	2.6
1	C	396	MET	2.6
1	X	135	VAL	2.6
1	K	143	ILE	2.6
1	W	124	PHE	2.6
1	A	407	ARG	2.6
1	N	239	ILE	2.6
1	I	259	MET	2.6
1	T	101	MET	2.6
1	X	306	PRO	2.6
1	O	126	ILE	2.6
1	J	479	ILE	2.6
1	G	376	ALA	2.6
1	J	476	CYS	2.5
1	H	161	LEU	2.5
1	J	150	LEU	2.5
1	O	182	CYS	2.5
1	O	298	MET	2.5
1	K	156	GLU	2.5
1	T	102	GLU	2.5
1	W	412	TYR	2.5
1	E	335	LYS	2.5
1	I	91	THR	2.5
1	F	346	MET	2.5
1	I	101	MET	2.5
1	K	45	MET	2.5
1	N	49	ARG	2.5
1	O	479	ILE	2.5
1	F	353	ALA	2.5
1	B	409	VAL	2.5
1	I	150	LEU	2.5
1	D	209	PHE	2.5
1	I	377	ASP	2.5
1	F	476	CYS	2.5
1	A	46	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	381	CYS	2.5
1	E	170	THR	2.5
1	I	299	LEU	2.5
1	N	131	LEU	2.5
1	S	48	ALA	2.5
1	J	163	CYS	2.5
1	X	209	PHE	2.5
1	A	412	TYR	2.4
1	X	486	LYS	2.4
1	D	239	ILE	2.4
1	P	434	THR	2.4
1	L	352	GLU	2.4
1	D	188	ALA	2.4
1	E	180	PRO	2.4
1	Q	486	LYS	2.4
1	W	493	ARG	2.4
1	D	412	TYR	2.4
1	W	99	ALA	2.4
1	E	184	VAL	2.4
1	B	294	CYS	2.4
1	T	50	MET	2.4
1	C	287	VAL	2.4
1	J	11	ILE	2.4
1	O	128	TYR	2.4
1	F	492	THR	2.4
1	P	143	ILE	2.4
1	T	164	THR	2.4
1	X	488	TYR	2.4
1	K	367	LYS	2.4
1	W	123	LYS	2.4
1	K	137	PRO	2.4
1	E	135	VAL	2.4
1	T	105	ALA	2.4
1	H	430	GLN	2.4
1	D	122	ASP	2.4
1	O	433	ILE	2.4
1	A	299	LEU	2.4
1	X	214	ARG	2.3
1	E	390	GLU	2.3
1	F	49	ARG	2.3
1	L	439	SER	2.3
1	W	183	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	V	184	VAL	2.3
1	V	437	VAL	2.3
1	W	377	ASP	2.3
1	B	492	THR	2.3
1	A	479	ILE	2.3
1	J	446	LYS	2.3
1	A	302	MET	2.3
1	N	50	MET	2.3
1	O	189	VAL	2.3
1	M	96	GLY	2.3
1	X	198	GLN	2.3
1	W	19	ARG	2.3
1	D	261	ALA	2.3
1	I	476	CYS	2.3
1	H	126	ILE	2.3
1	H	494	ILE	2.3
1	T	376	ALA	2.3
1	A	185	ASP	2.3
1	O	87	PRO	2.3
1	M	325	ASP	2.3
1	X	183	ASP	2.3
1	J	107	CYS	2.3
1	T	316	VAL	2.3
1	G	239	ILE	2.3
1	O	345	TYR	2.3
1	J	268	GLU	2.3
1	H	476	CYS	2.3
1	V	84	THR	2.3
1	X	119	GLY	2.3
1	K	154	SER	2.2
1	F	328	MET	2.2
1	T	100	VAL	2.2
1	N	150	LEU	2.2
1	L	346	MET	2.2
1	T	492	THR	2.2
1	P	171	ILE	2.2
1	A	124	PHE	2.2
1	L	298	MET	2.2
1	U	154	SER	2.2
1	V	390	GLU	2.2
1	O	18	TYR	2.2
1	X	492	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	98	ASP	2.2
1	O	183	ASP	2.2
1	H	312	GLU	2.2
1	D	258	ILE	2.2
1	J	478	VAL	2.2
1	J	73	GLU	2.2
1	A	152	VAL	2.2
1	N	165	VAL	2.2
1	X	157	ASP	2.2
1	P	406	ALA	2.2
1	X	399	LEU	2.2
1	B	435	GLN	2.2
1	N	162	GLU	2.2
1	S	359	GLU	2.2
1	R	148	LEU	2.2
1	X	494	ILE	2.2
1	R	261	ALA	2.2
1	C	419	VAL	2.2
1	F	480	HIS	2.2
1	J	396	MET	2.2
1	I	118	LYS	2.2
1	R	346	MET	2.2
1	P	239	ILE	2.2
1	M	150	LEU	2.2
1	A	126	ILE	2.2
1	F	327	VAL	2.2
1	F	350	CYS	2.2
1	A	408	LEU	2.1
1	A	475	TYR	2.1
1	U	73	GLU	2.1
1	L	149	ILE	2.1
1	T	494	ILE	2.1
1	N	91	THR	2.1
1	T	173	ASP	2.1
1	N	82	LEU	2.1
1	D	19	ARG	2.1
1	Q	476	CYS	2.1
1	B	184	VAL	2.1
1	H	102	GLU	2.1
1	W	169	HIS	2.1
1	X	239	ILE	2.1
1	R	49	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	124	PHE	2.1
1	D	494	ILE	2.1
1	K	241	ASN	2.1
1	O	434	THR	2.1
1	T	49	ARG	2.1
1	D	414	PRO	2.1
1	X	201	VAL	2.1
1	L	294	CYS	2.1
1	W	476	CYS	2.1
1	H	207	MET	2.1
1	I	438	GLU	2.1
1	K	244	GLY	2.1
1	E	490	ASN	2.1
1	Q	134	VAL	2.1
1	P	213	ILE	2.1
1	T	412	TYR	2.1
1	X	409	VAL	2.1
1	R	171	ILE	2.1
1	U	412	TYR	2.1
1	G	135	VAL	2.1
1	P	104	GLY	2.1
1	R	316	VAL	2.1
1	S	399	LEU	2.1
1	G	124	PHE	2.1
1	O	174	ARG	2.1
1	X	237	CYS	2.1
1	U	117	ASP	2.1
1	X	136	ARG	2.1
1	O	176	GLY	2.1
1	V	17	ASN	2.1
1	B	293	ILE	2.1
1	C	50	MET	2.1
1	B	421	VAL	2.1
1	K	40	LEU	2.1
1	V	131	LEU	2.1
1	C	149	ILE	2.1
1	E	336	GLY	2.1
1	U	232	ASP	2.0
1	N	85	LYS	2.0
1	A	110	THR	2.0
1	N	238	LYS	2.0
1	U	367	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	U	124	PHE	2.0
1	W	203	GLN	2.0
1	T	9	LEU	2.0
1	J	294	CYS	2.0
1	B	93	GLN	2.0
1	S	126	ILE	2.0
1	F	494	ILE	2.0
1	X	456	ARG	2.0
1	X	313	VAL	2.0
1	C	456	ARG	2.0
1	D	128	TYR	2.0
1	D	289	GLY	2.0
1	F	381	CYS	2.0
1	N	52	PHE	2.0
1	R	242	HIS	2.0
1	O	89	ILE	2.0
1	O	359	GLU	2.0
1	L	406	ALA	2.0
1	X	339	PRO	2.0
1	A	367	LYS	2.0
1	N	161	LEU	2.0
1	P	244	GLY	2.0
1	M	152	VAL	2.0
1	P	291	PRO	2.0
1	J	460	GLY	2.0
1	R	105	ALA	2.0
1	R	495	LEU	2.0
1	O	100	VAL	2.0
1	S	57	HIS	2.0
1	D	89	ILE	2.0
1	O	131	LEU	2.0
1	R	184	VAL	2.0
1	G	93	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	FDP	C	700	20/20	0.64	0.32	-0.43	25,32,34,35	0
2	FDP	H	700	20/20	0.71	0.31	-0.57	25,32,34,35	0
2	FDP	V	700	20/20	0.79	0.30	-0.61	25,32,34,35	0
2	FDP	S	700	20/20	0.70	0.33	-0.65	25,32,34,35	0
2	FDP	F	700	20/20	0.78	0.31	-0.72	25,32,34,35	0
2	FDP	G	700	20/20	0.76	0.31	-0.74	25,32,34,35	0
2	FDP	E	700	20/20	0.74	0.24	-0.76	25,32,34,35	0
2	FDP	X	700	20/20	0.63	0.34	-0.79	25,32,34,35	0
2	FDP	K	700	20/20	0.73	0.27	-0.79	25,32,34,35	0
2	FDP	U	700	20/20	0.73	0.32	-0.82	25,32,34,35	0
2	FDP	P	700	20/20	0.66	0.29	-0.83	25,32,34,35	0
2	FDP	T	700	20/20	0.67	0.25	-0.85	25,32,34,35	0
2	FDP	Q	700	20/20	0.74	0.30	-0.86	25,32,34,35	0
2	FDP	J	700	20/20	0.64	0.37	-0.86	25,32,34,35	0
2	FDP	W	700	20/20	0.80	0.32	-0.98	25,32,34,35	0
2	FDP	L	700	20/20	0.64	0.30	-1.05	25,32,34,35	0
2	FDP	A	700	20/20	0.81	0.19	-1.06	25,32,34,35	0
2	FDP	N	700	20/20	0.80	0.26	-1.08	25,32,34,35	0
2	FDP	B	700	20/20	0.78	0.19	-1.18	25,32,34,35	0
2	FDP	O	700	20/20	0.82	0.26	-1.18	25,32,34,35	0
2	FDP	D	700	20/20	0.87	0.23	-1.20	25,32,34,35	0
2	FDP	M	700	20/20	0.82	0.22	-1.27	25,32,34,35	0
2	FDP	R	700	20/20	0.75	0.23	-1.34	25,32,34,35	0
2	FDP	I	700	20/20	0.81	0.25	-1.56	25,32,34,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.