



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:20 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 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/ValidationPDFNotes.html>

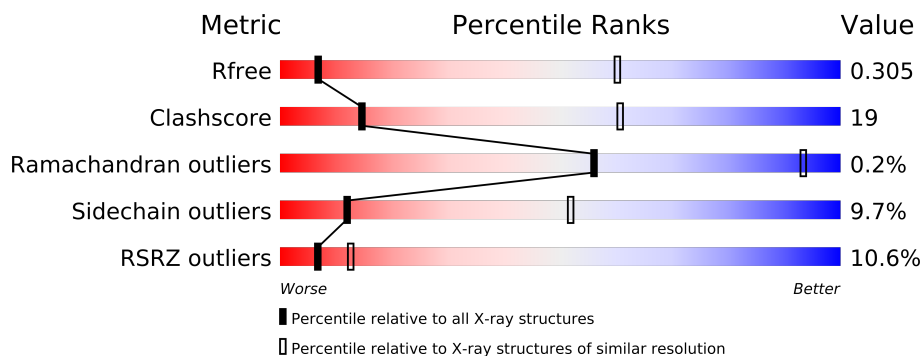
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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.












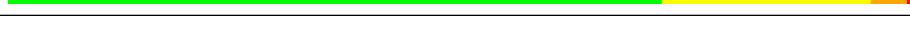
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1054 (6.62-3.50)
Clashscore	79885	1330 (6.62-3.50)
Ramachandran outliers	78287	1245 (6.62-3.50)
Sidechain outliers	78261	1223 (6.60-3.50)
RSRZ outliers	66119	1053 (6.62-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	499	
1	B	499	
1	C	499	
1	D	499	
1	E	499	
1	F	499	
1	G	499	
1	H	499	
1	I	499	
1	J	499	
1	K	499	
1	L	499	
1	M	499	
1	N	499	

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Mol	Chain	Length	Quality of chain
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 hydrogen and 0 are deuterium.

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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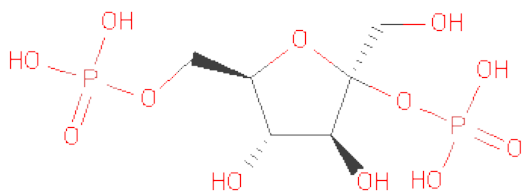
Chain	Residue	Modelled	Actual	Comment	Reference
F	405	SER	GLY	SEE REMARK 999	UNP Q27686
G	382	SER	GLY	SEE REMARK 999	UNP Q27686
G	389	TYR	SER	SEE REMARK 999	UNP Q27686
G	404	ARG	ALA	SEE REMARK 999	UNP Q27686
G	405	SER	GLY	SEE REMARK 999	UNP Q27686
H	382	SER	GLY	SEE REMARK 999	UNP Q27686
H	389	TYR	SER	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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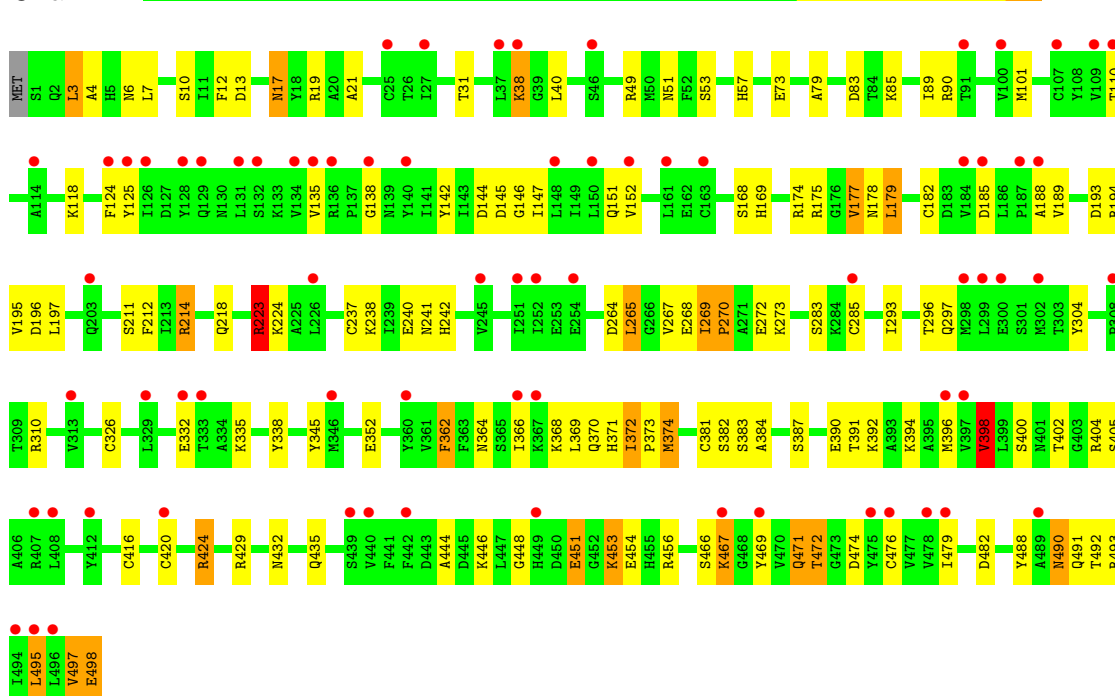
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total 20	C 6	O 12	P 2	0	0
2	P	1	Total 20	C 6	O 12	P 2	0	0
2	Q	1	Total 20	C 6	O 12	P 2	0	0
2	R	1	Total 20	C 6	O 12	P 2	0	0
2	S	1	Total 20	C 6	O 12	P 2	0	0
2	T	1	Total 20	C 6	O 12	P 2	0	0
2	U	1	Total 20	C 6	O 12	P 2	0	0
2	V	1	Total 20	C 6	O 12	P 2	0	0
2	W	1	Total 20	C 6	O 12	P 2	0	0
2	X	1	Total 20	C 6	O 12	P 2	0	0

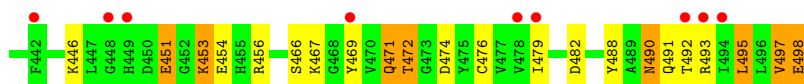
3 Residue-property plots

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

• Molecule 1: Pyruvate kinase

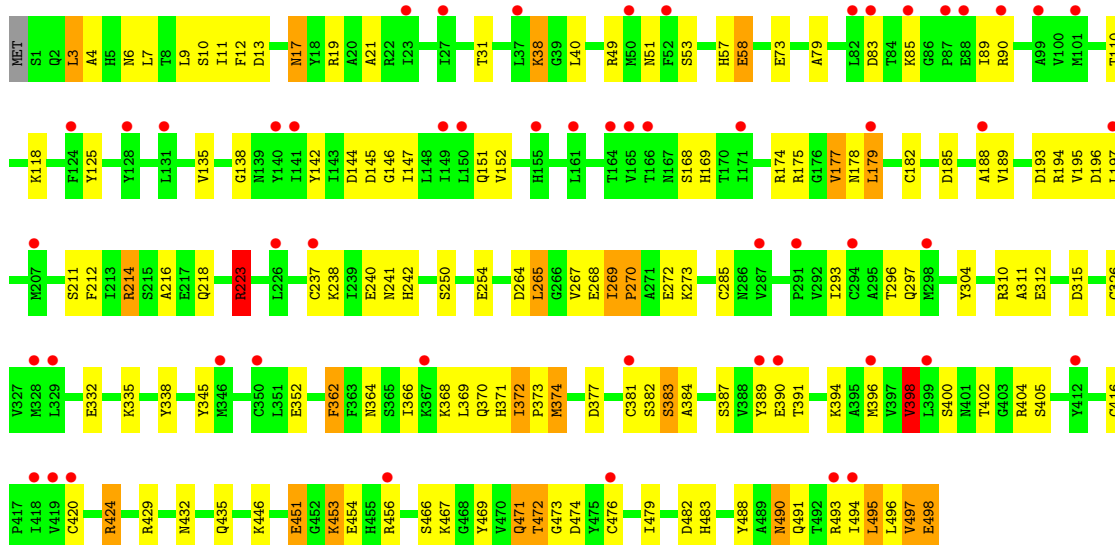
Chain A:





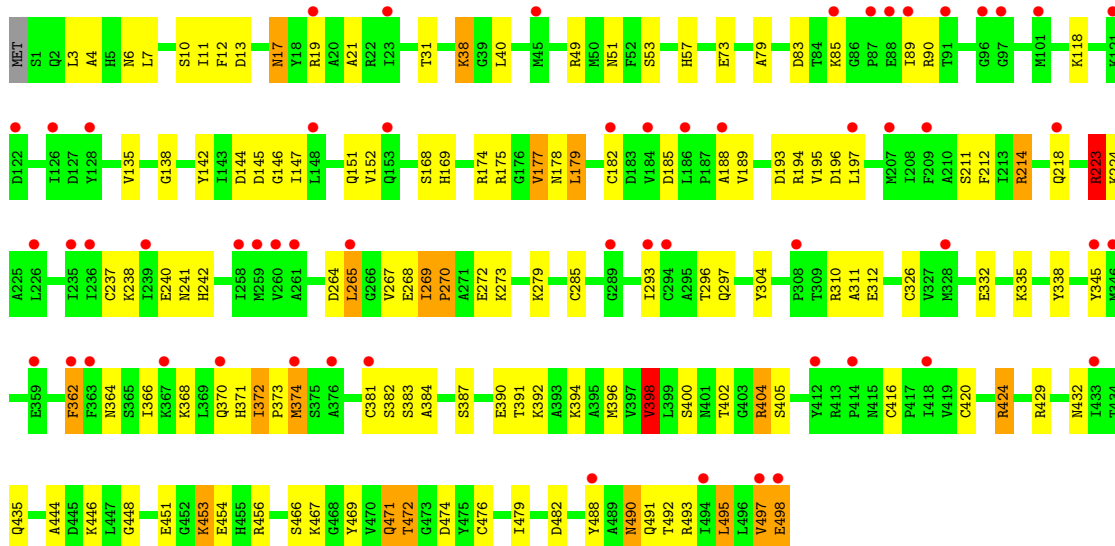
• Molecule 1: Pyruvate kinase

Chain C:



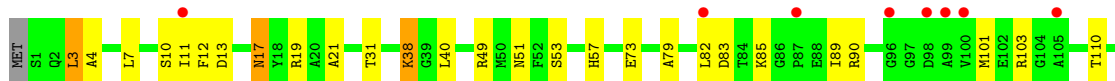
• Molecule 1: Pyruvate kinase

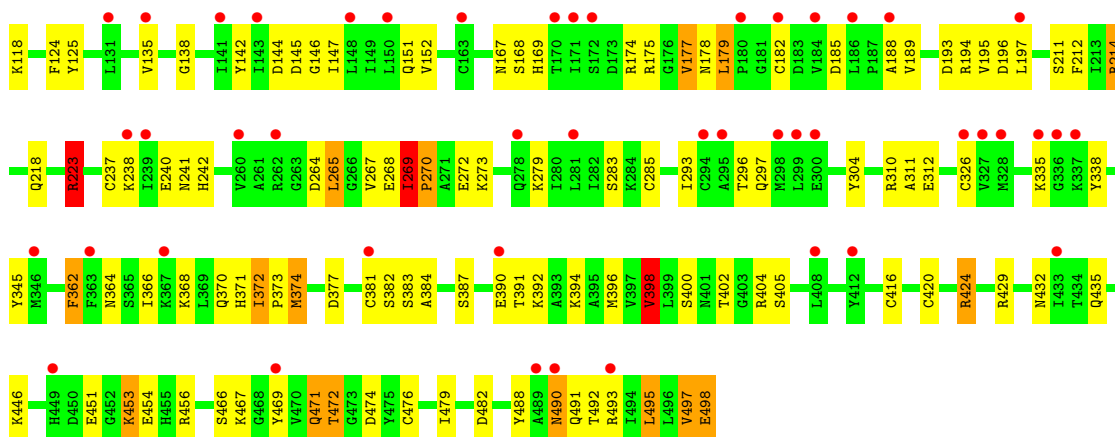
Chain D:



• Molecule 1: Pyruvate kinase

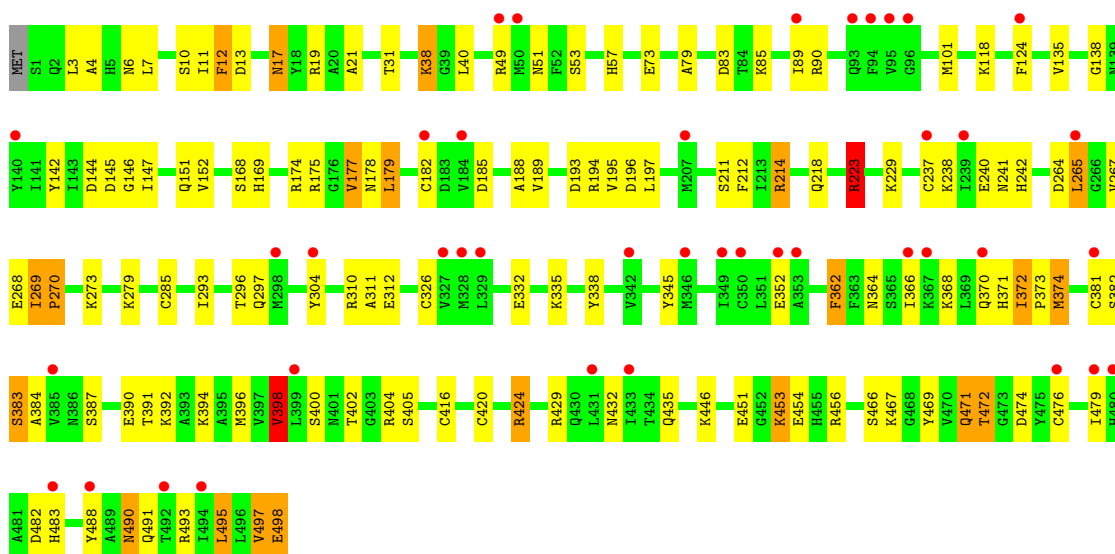
Chain E:





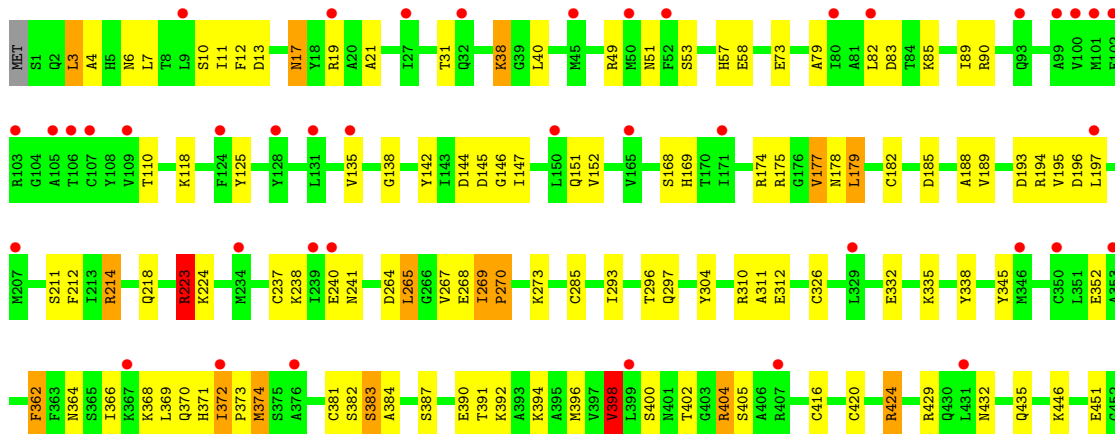
• Molecule 1: Pyruvate kinase

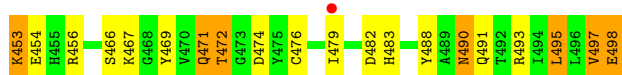
Chain F:



• Molecule 1: Pyruvate kinase

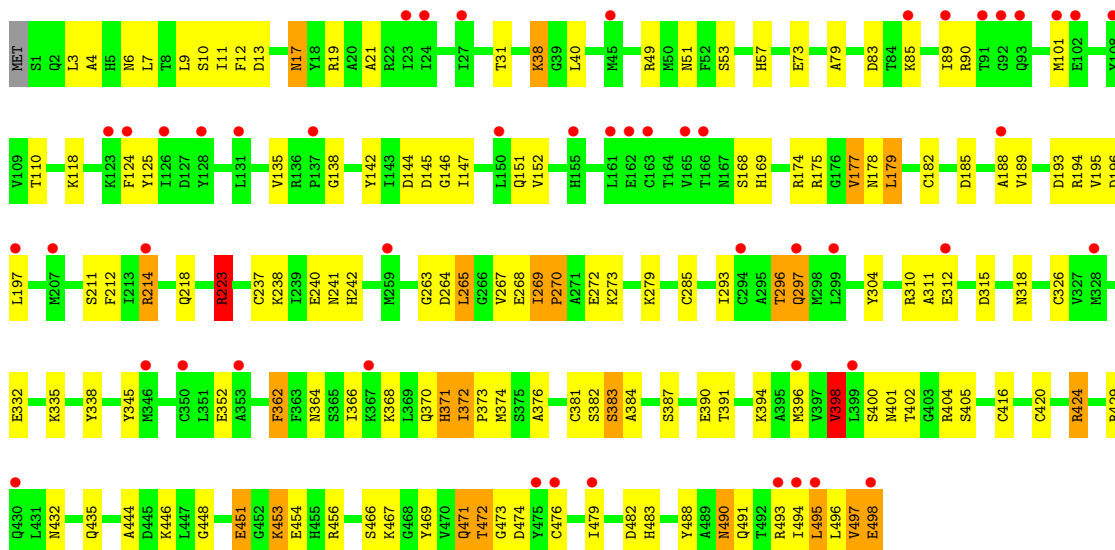
Chain G:





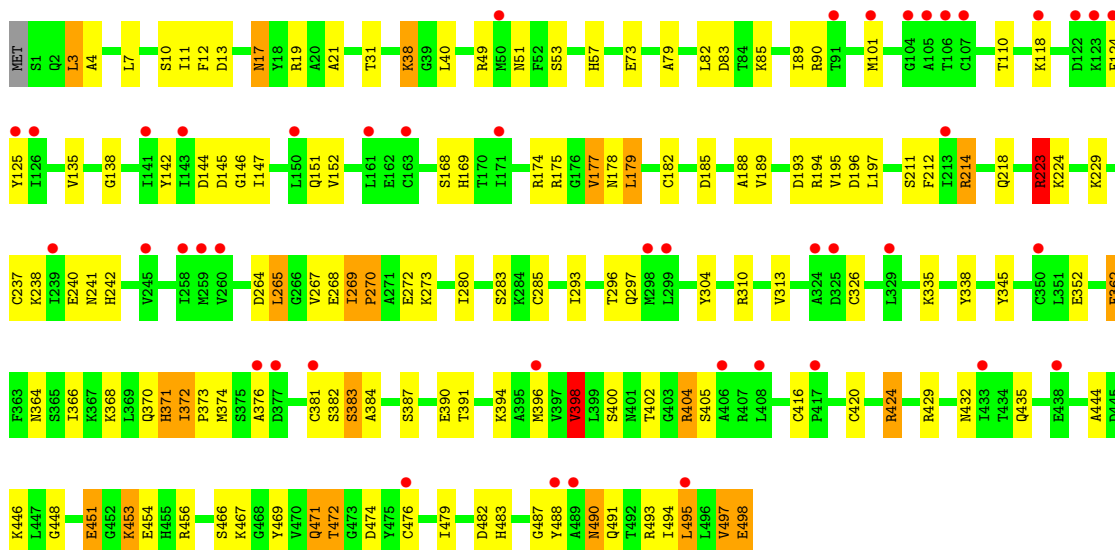
• Molecule 1: Pyruvate kinase

Chain H:



• Molecule 1: Pyruvate kinase

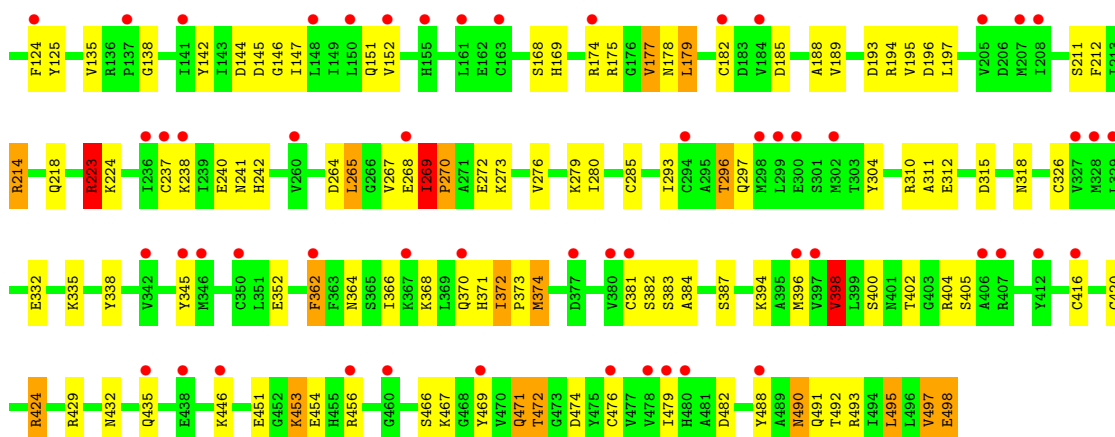
Chain I:



• Molecule 1: Pyruvate kinase

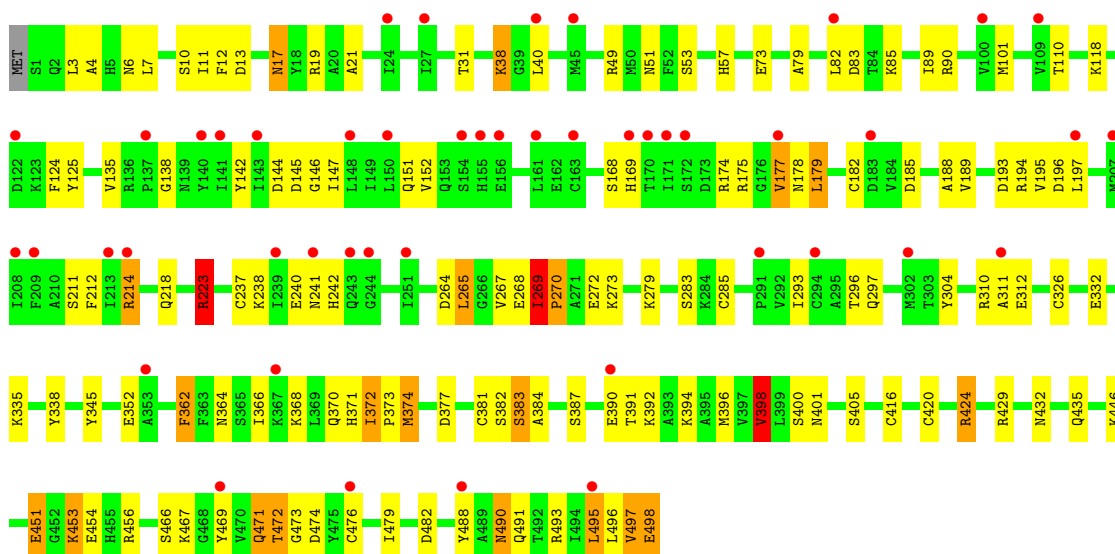
Chain J:





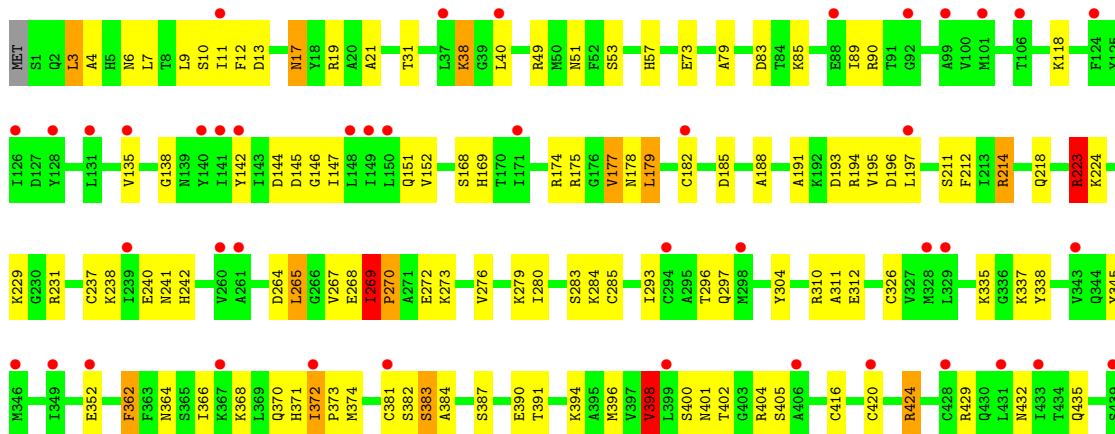
• Molecule 1: Pyruvate kinase

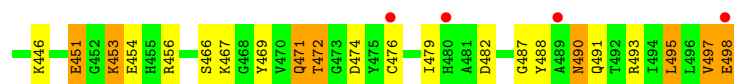
Chain K:



• Molecule 1: Pyruvate kinase

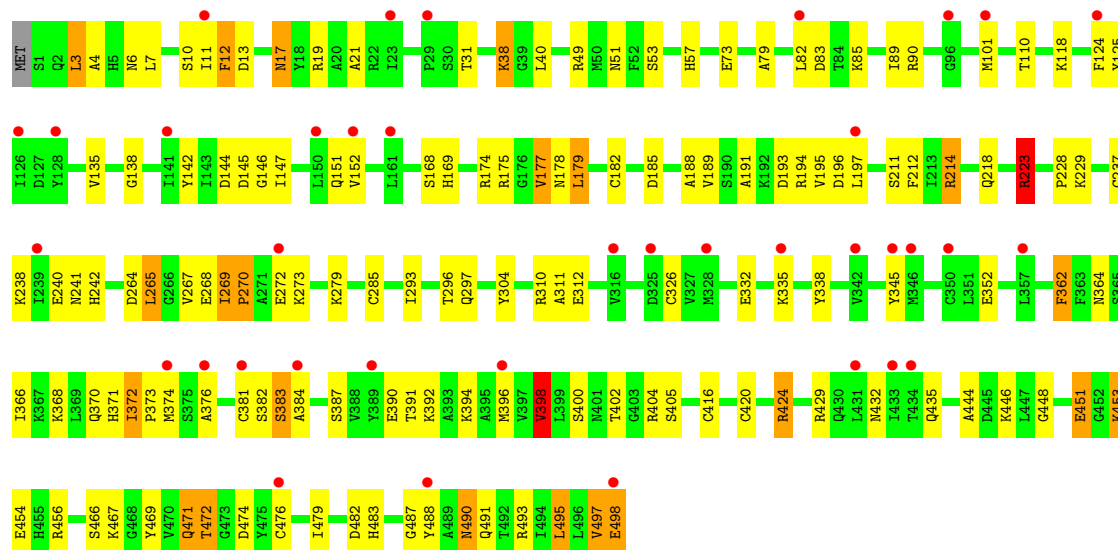
Chain L:





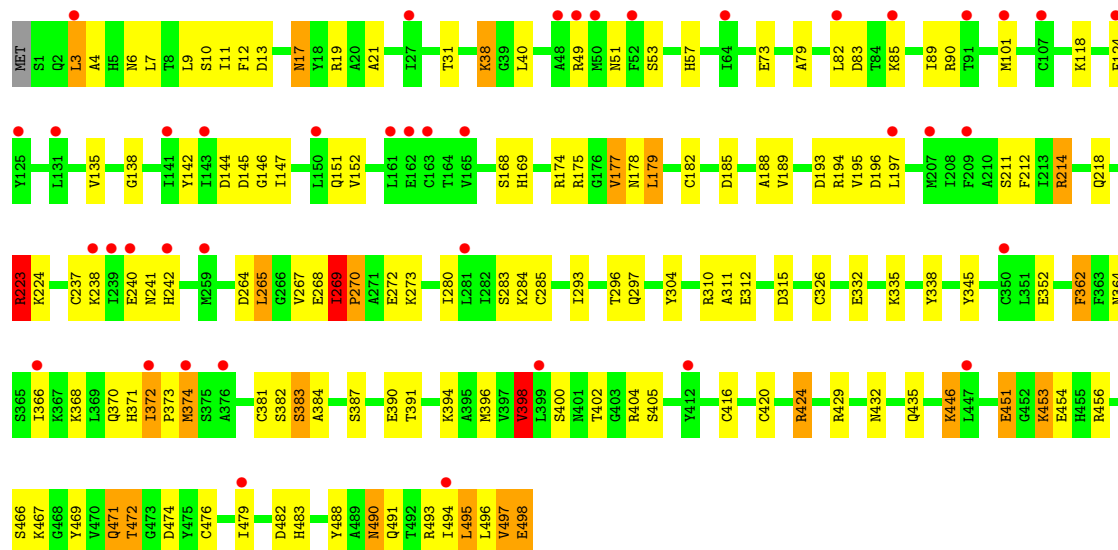
• Molecule 1: Pyruvate kinase

Chain M:



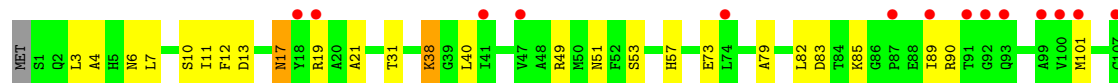
• Molecule 1: Pyruvate kinase

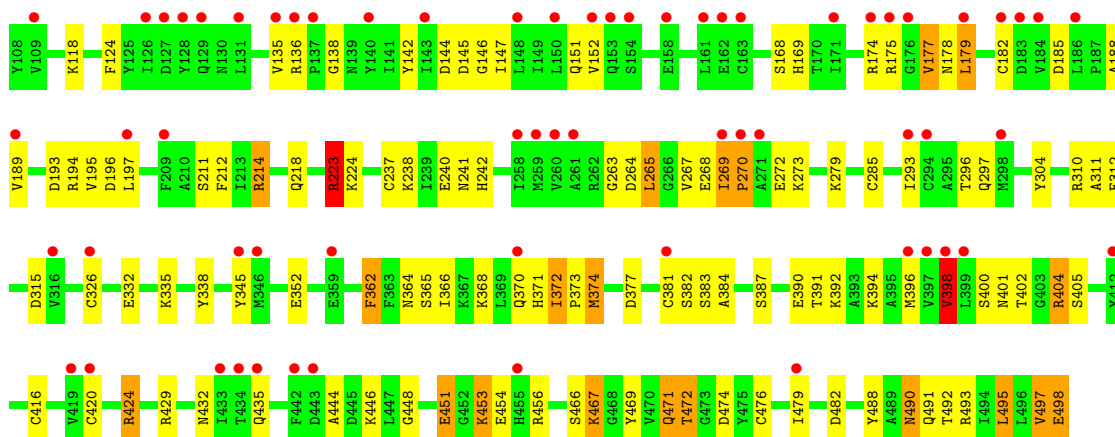
Chain N:



• Molecule 1: Pyruvate kinase

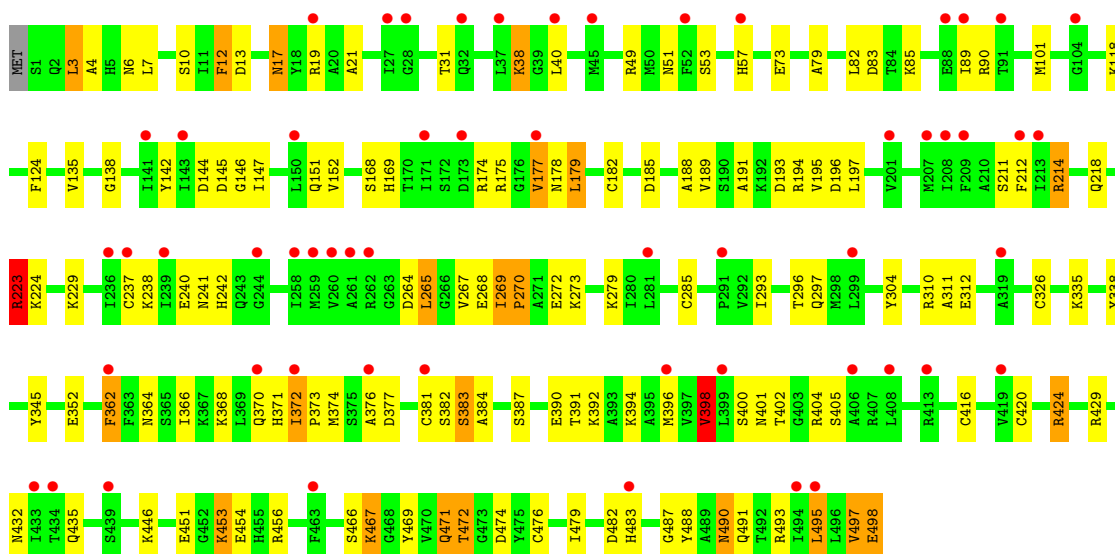
Chain O:





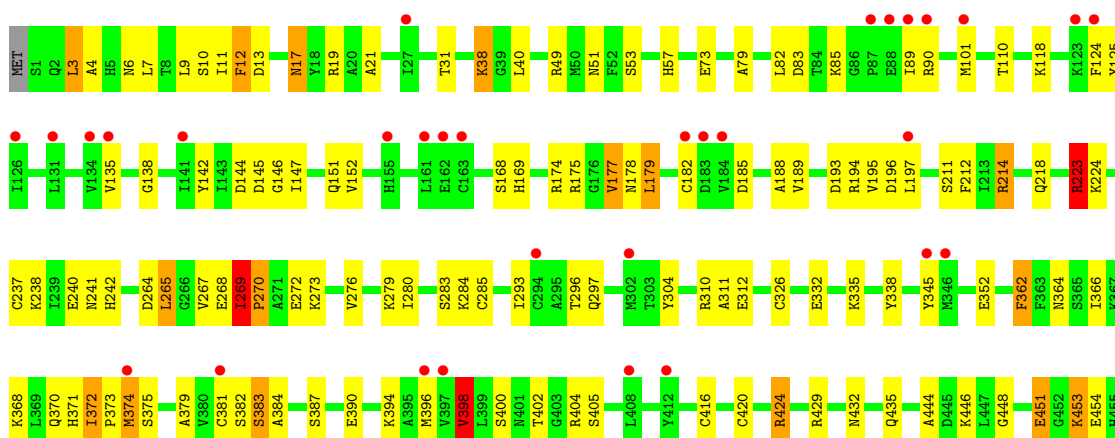
• Molecule 1: Pyruvate kinase

Chain P:



• Molecule 1: Pyruvate kinase

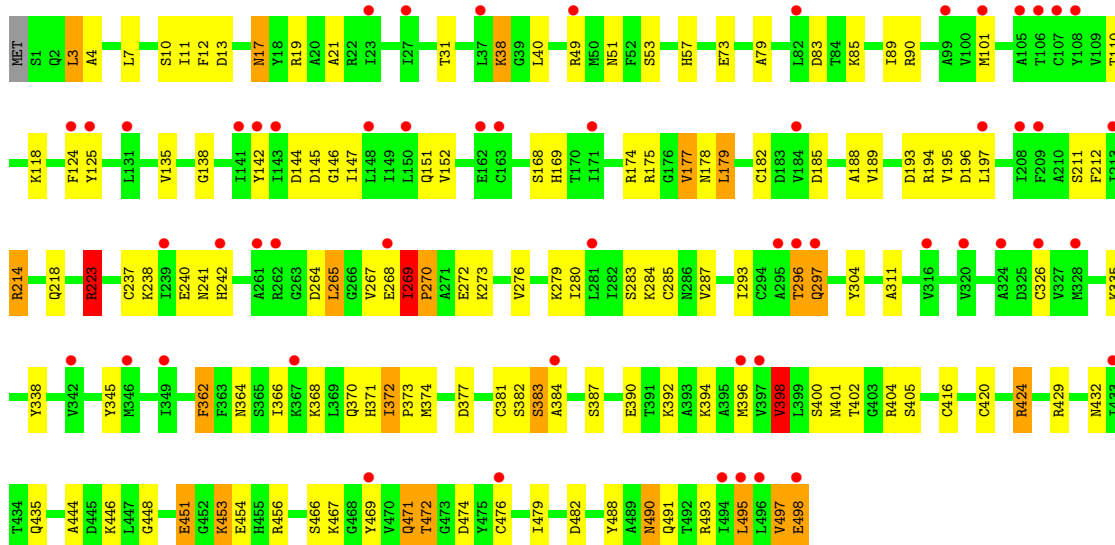
Chain Q:





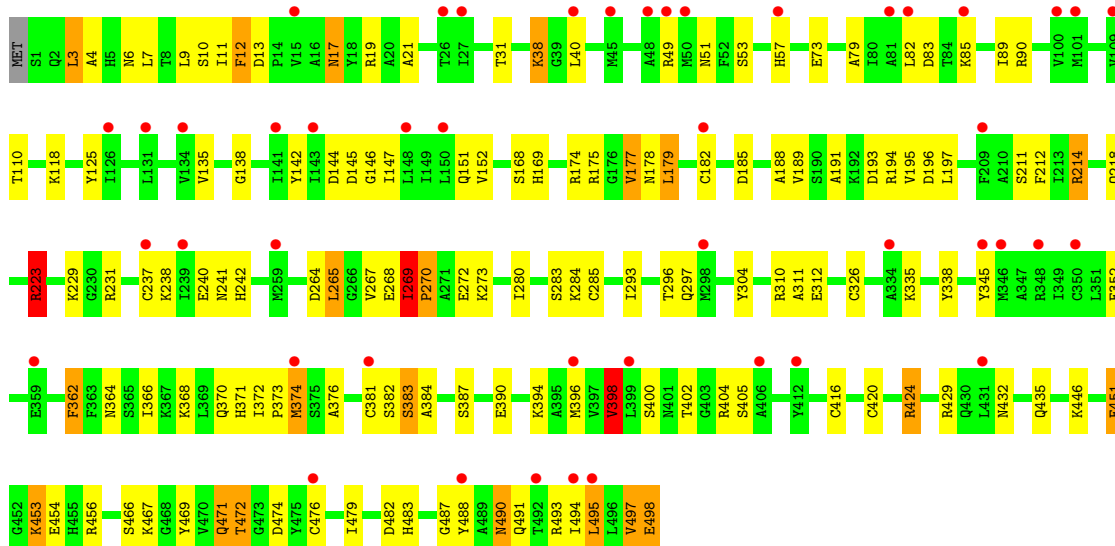
• Molecule 1: Pyruvate kinase

Chain R:



• Molecule 1: Pyruvate kinase

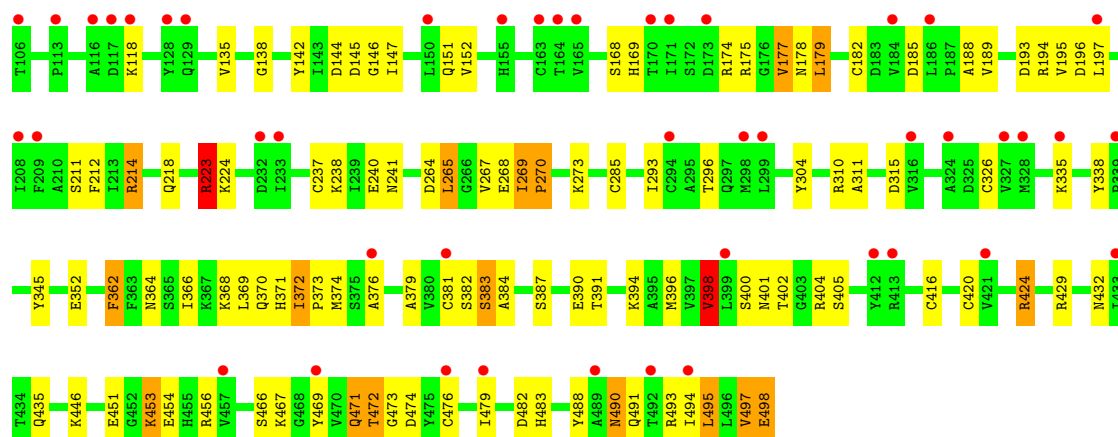
Chain S:



• Molecule 1: Pyruvate kinase

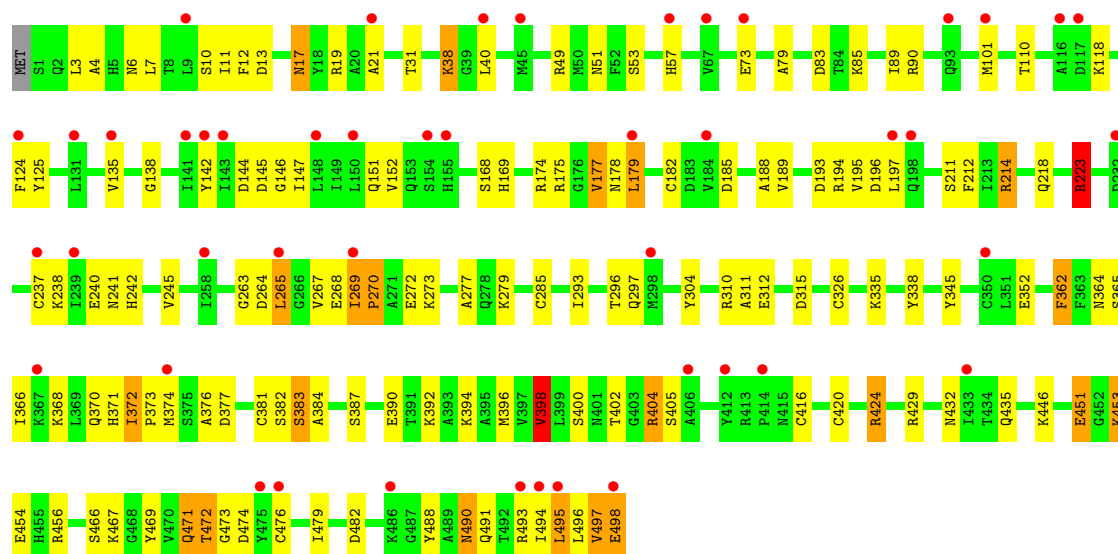
Chain T:





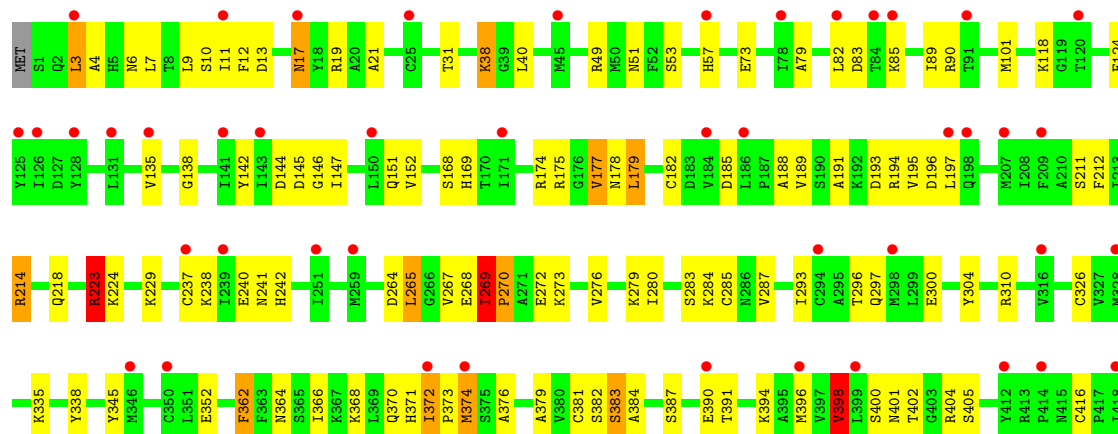
- Molecule 1: Pyruvate kinase

Chain U:



- Molecule 1: Pyruvate kinase

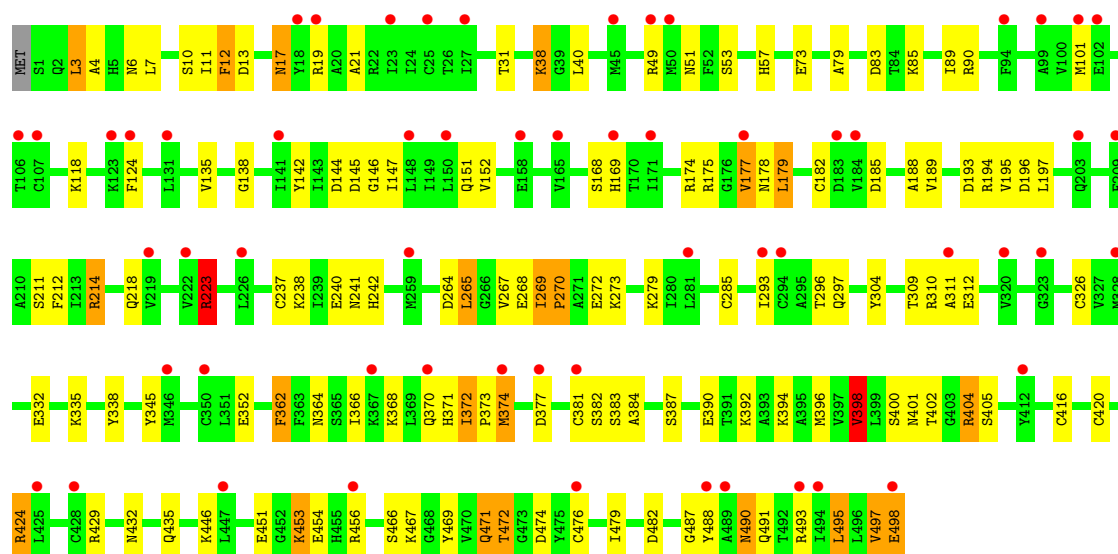
Chain V:





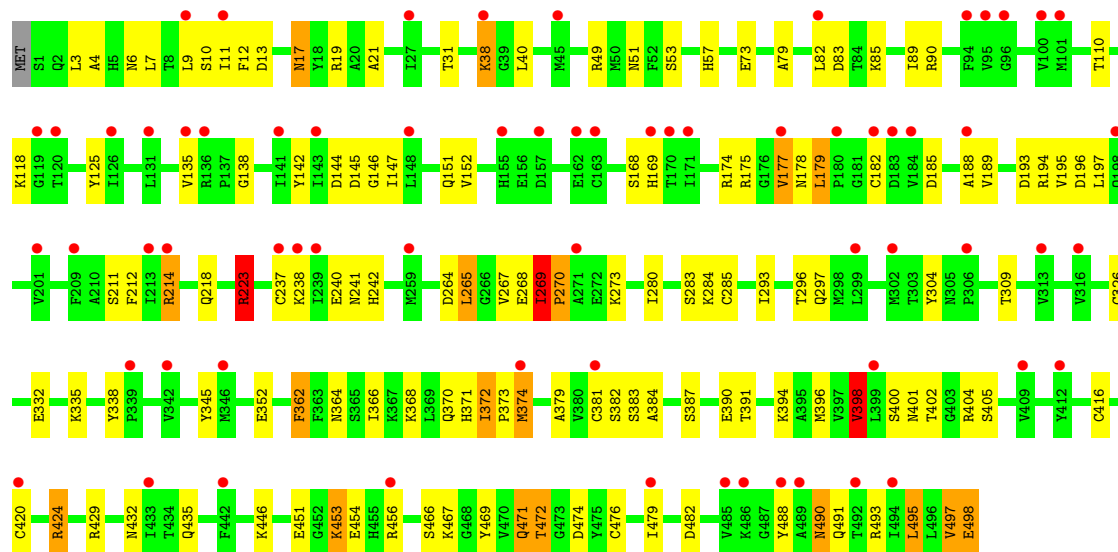
• Molecule 1: Pyruvate kinase

Chain W:



• Molecule 1: Pyruvate kinase

Chain X:



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 0.308 , 0.305	Depositor DCC
R_{free} test set	5652 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	131.8	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.4	EDS
Estimated twinning fraction	0.118 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 112779 reflections	Xtriage
F_o, F_c correlation	0.77	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (3536) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:V:284:LYS:HG3	1:X:7:LEU:CD2	1.60	1.28
1:K:188:ALA:CB	1:K:218:GLN:HG3	1.62	1.28
1:L:188:ALA:CB	1:L:218:GLN:HG3	1.62	1.28
1:T:188:ALA:CB	1:T:218:GLN:HG3	1.62	1.28
1:N:188:ALA:CB	1:N:218:GLN:HG3	1.62	1.28
1:U:242:HIS:CE1	1:W:12:PHE:CZ	2.20	1.28
1:E:188:ALA:CB	1:E:218:GLN:HG3	1.62	1.28
1:W:188:ALA:CB	1:W:218:GLN:HG3	1.62	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:S:188:ALA:CB	1:S:218:GLN:HG3	1.62	1.28
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:A:188:ALA:CB	1:A:218:GLN:HG3	1.62	1.27

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:L:242:HIS:HE1	1:N:12:PHE:CE2	1.51	1.27
1:H:188:ALA:CB	1:H:218:GLN:HG3	1.62	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:H:310:ARG:HG2	1:J:297:GLN:CB	1.73	1.17
1:C:390:GLU:HA	1:P:372:ILE:HG13	1.23	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:I:487:GLY:HA2	1:M:229:LYS:CG	1.76	1.15
1:F:373:PRO:HA	1:G:390:GLU:O	1.40	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:P:487:GLY:HA2	1:V:229:LYS:CD	1.77	1.13
1:S:372:ILE:HD11	1:T:390:GLU:HG2	1.29	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:U:242:HIS:CE1	1:W:12:PHE:CE2	2.37	1.13
1:S:372:ILE:CG1	1:T:390:GLU:HA	1.77	1.13
1:Q:297:GLN:OE1	1:S:310:ARG:HG2	1.43	1.13
1:K:12:PHE:CZ	1:M:242:HIS:CE1	2.36	1.12
1:U:11:ILE:HB	1:W:273:LYS:CG	1.77	1.12

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:312:GLU:HA	1:J:311:ALA:CB	1.78	1.12
1:K:12:PHE:CE2	1:M:242:HIS:HE1	1.65	1.12
1:W:472:THR:HG22	1:W:498:GLU:HA	1.25	1.12
1:U:297:GLN:HB2	1:W:310:ARG:HG2	1.32	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:U:472:THR:HG22	1:U:498:GLU:HA	1.25	1.12
1:F:188:ALA:CB	1:F:218:GLN:CG	2.28	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:O:472:THR:HG22	1:O:498:GLU:HA	1.25	1.11
1:M:188:ALA:CB	1:M:218:GLN:CG	2.28	1.11
1:H:188:ALA:CB	1:H:218:GLN:CG	2.28	1.11
1:C:472:THR:HG22	1:C:498:GLU:HA	1.25	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:I:188:ALA:CB	1:I:218:GLN:CG	2.28	1.11
1:Q:188:ALA:CB	1:Q:218:GLN:CG	2.28	1.11
1:F:472:THR:HG22	1:F:498:GLU:HA	1.25	1.11
1:C:188:ALA:CB	1:C:218:GLN:CG	2.28	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:H:242:HIS:CE1	1:J:12:PHE:CE2	2.39	1.11
1:X:472:THR:HG22	1:X:498:GLU:HA	1.25	1.11
1:V:188:ALA:CB	1:V:218:GLN:CG	2.29	1.10
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: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:W:188:ALA:CB	1:W:218:GLN:CG	2.28	1.10
1:U:11:ILE:CB	1:W:273:LYS:HG2	1.81	1.10
1:P:487:GLY:CA	1:V:229:LYS:HE3	1.82	1.10
1:J:188:ALA:CB	1:J:218:GLN:CG	2.28	1.10
1:A:188:ALA:CB	1:A:218:GLN:CG	2.28	1.10
1:A:392:LYS:HD2	1:J:373:PRO:HD3	1.34	1.10
1:K:188:ALA:CB	1:K:218:GLN:CG	2.28	1.10
1:E:188:ALA:CB	1:E:218:GLN:CG	2.28	1.10
1:P:188:ALA:CB	1:P:218:GLN:CG	2.28	1.10
1:G:472:THR:HG22	1:G:498:GLU:HA	1.25	1.10

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:188:ALA:CB	1:D:218:GLN:CG	2.28	1.09
1:R:188:ALA:CB	1:R:218:GLN:CG	2.28	1.09
1:N:188:ALA:CB	1:N:218:GLN:CG	2.28	1.09
1:S:188:ALA:HB2	1:S:218:GLN:CG	1.82	1.09
1:I:188:ALA:HB2	1:I:218:GLN:CG	1.82	1.09
1:E:472:THR:HG22	1:E:498:GLU:HA	1.25	1.09
1:O:12:PHE:CE2	1:P:242:HIS:HE1	1.69	1.09
1:I:472:THR:HG22	1:I:498:GLU:HA	1.25	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:G:188:ALA:CB	1:G:218:GLN:CG	2.28	1.09
1:A:188:ALA:HB2	1:A:218:GLN:CG	1.83	1.09
1:M:188:ALA:HB2	1:M:218:GLN:CG	1.82	1.09
1:G:188:ALA:HB2	1:G: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:R:272:GLU:CG	1:T:352:GLU:HG2	1.80	1.09
1:F:390:GLU:O	1:G:373:PRO:HA	1.52	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: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:R:270:PRO:HG2	1:R:273:LYS:HE2	1.36	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:B:188:ALA:HB2	1:B:218:GLN:CG	1.83	1.08
1:O:188:ALA:HB2	1:O:218:GLN:CG	1.82	1.08
1:H:188:ALA:HB2	1:H:218:GLN:CG	1.83	1.08
1:L:424:ARG:NH1	1:L:424:ARG:HG2	1.55	1.08
1:C:216:ALA:HB3	1:N:446:LYS:HD3	1.28	1.08
1:F:188:ALA:HB2	1:F:218:GLN:CG	1.83	1.08
1:U:371:HIS:O	1:U:374:MET:HG2	1.54	1.08
1:T:472:THR:HG22	1:T:498:GLU:HA	1.25	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

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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:12:PHE:HE2	1:W:242:HIS:CE1	1.75	1.04
1:H:312:GLU:HA	1:J:311:ALA:HB1	1.06	1.04
1:O:12:PHE:CE2	1:P:242:HIS:CE1	2.45	1.04
1:H:496:LEU:CG	1:M:195:VAL:HG22	1.85	1.04
1:G:424:ARG:CG	1:G:424:ARG:HH11	1.68	1.04
1:L:371:HIS:O	1:L:374:MET:HG2	1.58	1.04
1:V:424:ARG:HH11	1:V:424:ARG:CG	1.68	1.04
1:K:424:ARG:HH11	1:K:424:ARG:CG	1.68	1.04
1:R:284:LYS:HG3	1:T:7:LEU:HD22	1.36	1.04
1:H:372:ILE:HG23	1:I:390:GLU:O	1.57	1.04
1:M:373:PRO:HA	1:N:390:GLU:O	1.58	1.04
1:L:424:ARG:CG	1:L:424:ARG:HH11	1.68	1.04
1:M:424:ARG:HH11	1:M:424:ARG:CG	1.68	1.04
1:V:242:HIS:HE1	1:X:12:PHE:CE2	1.74	1.03
1:X:424:ARG:CG	1:X:424:ARG:HH11	1.68	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:W:424:ARG:HH11	1:W:424:ARG:CG	1.68	1.03
1:M:372:ILE:HG13	1:N:390:GLU:HA	1.36	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:373:PRO:HA	1:V:390:GLU:O	1.59	1.02
1:F:424:ARG:HH11	1:F:424:ARG:CG	1.69	1.02
1:U:424:ARG:CG	1:U:424:ARG:HH11	1.68	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:P:487:GLY:HA2	1:V:229:LYS:HE3	1.06	1.02
1:H:372:ILE:HG13	1:I:390:GLU:HA	1.40	1.02
1:S:372:ILE:HG13	1:T:390:GLU:O	1.59	1.01
1:H:310:ARG:HG2	1:J:297:GLN:HB2	1.30	1.01
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:U:12:PHE:CE2	1:W:242:HIS:CE1	2.49	1.01
1:M:371:HIS:O	1:M:374:MET:HG2	1.60	1.01

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:242:HIS:HE1	1:G:12:PHE:CZ	1.77	1.01
1:V:284:LYS:CG	1:X:7:LEU:CD2	2.37	1.00
1:W:372:ILE:HG13	1:X:390:GLU:HA	1.39	1.00
1:T:371:HIS:O	1:T:374:MET:HG2	1.61	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:H:311:ALA:HB1	1:J:312:GLU:CA	1.90	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: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:HG2	1:D:424:ARG:NH1	1.55	0.99
1:U:372:ILE:HG23	1:V:390:GLU:O	1.62	0.99
1:H:496:LEU:HG	1:M:195:VAL:HG22	1.39	0.99
1:H:12:PHE:CE2	1:J:242:HIS:HE1	1.80	0.99
1:K:12:PHE:HE2	1:M:242:HIS:CE1	1.75	0.99
1:I:229:LYS:HG3	1:M:487:GLY:CA	1.91	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:NH1	1:J:424:ARG:HG2	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:NH1	1:A:424:ARG:HG2	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
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:HG2	1:S:424:ARG:NH1	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:F:472:THR:HG22	1:F:498:GLU:CA	1.96	0.96
1:V:424:ARG:NH1	1:V:424:ARG:HG2	1.56	0.96
1:Q:472:THR:HG22	1:Q:498:GLU:CA	1.96	0.96
1:L:472:THR:HG22	1:L:498:GLU:CA	1.96	0.96
1:B:472:THR:HG22	1:B: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:K:472:THR:HG22	1:K:498:GLU:CA	1.96	0.95
1:F:372:ILE:HG13	1:G:390:GLU:HA	1.48	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:B:373:PRO:HD3	1:O:392:LYS:HD2	1.45	0.95
1:P:195:VAL:HG22	1:U:496:LEU:CG	1.95	0.95
1:V:472:THR:HG22	1:V:498:GLU:CA	1.96	0.95
1:U:472:THR:HG22	1:U: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:W:472:THR:HG22	1:W:498:GLU:CA	1.96	0.94
1:G:472:THR:HG22	1:G:498:GLU:CA	1.96	0.94
1:P:472:THR:HG22	1:P:498:GLU:CA	1.96	0.94
1:C:373:PRO:HA	1:P:390:GLU:O	1.66	0.94
1:E:472:THR:HG22	1:E:498:GLU:CA	1.96	0.94
1:N:472:THR:HG22	1:N:498:GLU:CA	1.96	0.94
1:D:12:PHE:CZ	1:F:242:HIS:HE1	1.84	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:N:424:ARG:HG2	1:N:424:ARG:NH1	1.55	0.93
1:E:242:HIS:CE1	1:G:12:PHE:CE2	2.56	0.93
1:B:12:PHE:CE2	1:C:242:HIS:CE1	2.56	0.93
1:R:370:GLN:HB3	1:R:374:MET:SD	2.08	0.93
1:J:472:THR:HG22	1:J:498:GLU:CA	1.96	0.93
1:D:392:LYS:HD2	1:E:373:PRO:HD3	1.51	0.93
1:E:242:HIS:HE1	1:G:12:PHE:CE2	1.86	0.93
1:W:188:ALA:HB1	1:W:218:GLN:CG	1.98	0.93
1:I:487:GLY:HA2	1:M:229:LYS:HG3	0.93	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:M:188:ALA:HB1	1:M:218:GLN:CG	1.98	0.93
1:G:188:ALA:HB1	1:G: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:R:188:ALA:HB1	1:R:218:GLN:CG	1.98	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: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
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:J:188:ALA:HB1	1:J:218:GLN:CG	1.98	0.92
1:H:242:HIS:CE1	1:J:12:PHE:CZ	2.55	0.92
1:R:272:GLU:CG	1:T:352:GLU:CG	2.46	0.92
1:D:12:PHE:CE2	1:F:242:HIS:HE1	1.88	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:M:188:ALA:HB2	1:M:218:GLN:HG3	0.91	0.91
1:L:188:ALA:HB2	1:L:218:GLN:HG3	0.91	0.91
1:X:188:ALA:HB2	1:X:218:GLN:HG3	0.91	0.91
1:L:242:HIS:CE1	1:N:12:PHE:HE2	1.81	0.91
1:L:188:ALA:HB1	1:L:218:GLN:CG	1.98	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: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:S:372:ILE:CD1	1:T:390:GLU:HG2	2.00	0.91
1:O:424:ARG:HG2	1:O:424:ARG:NH1	1.55	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:C:216:ALA:HB2	1:N:446:LYS:HD3	1.52	0.91
1:M:390:GLU:O	1:N:373:PRO:HA	1.69	0.91
1:P:487:GLY:CA	1:V:229:LYS:HG3	2.00	0.91
1:E:188:ALA:HB1	1:E:218:GLN:CG	1.98	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:O:371:HIS:O	1:O:374:MET:HG2	1.71	0.91
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:K:242:HIS:HE1	1:M:12:PHE:CE2	1.89	0.90
1:G:371:HIS:O	1:G:374:MET:HG2	1.71	0.90
1:G:188:ALA:HB2	1:G:218:GLN:HG3	0.91	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
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:P:487:GLY:CA	1:V:229:LYS:CD	2.50	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:S:372:ILE:HG23	1:T:390:GLU:O	1.70	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:296:THR:HG22	1:R:297:GLN:HG2	1.54	0.90
1:I:229:LYS:CG	1:M:487:GLY:HA2	2.02	0.90
1:V:188:ALA:HB2	1:V:218:GLN:HG3	0.91	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:K:371:HIS:O	1:K:374:MET:HG2	1.71	0.90
1:E:371:HIS:O	1:E: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: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:T:188:ALA:HB2	1:T:218:GLN:HG3	0.91	0.89
1:R:276:VAL:CG1	1:T:9:LEU:HB3	2.02	0.89
1:F:188:ALA:HB2	1:F:218:GLN:HG3	0.91	0.89
1:W:373:PRO:HA	1:X:390:GLU:O	1.72	0.89
1:D:11:ILE:HB	1:F:273:LYS:HG2	1.52	0.89
1:K:12:PHE:HZ	1:M:242:HIS:HE1	1.20	0.89
1:R:284:LYS:CG	1:T:7:LEU:HD22	2.01	0.89
1:O:11:ILE:CB	1:P:273:LYS:HG2	2.03	0.89
1:U:312:GLU:HA	1:W:311:ALA:CB	2.01	0.89
1:S:144:ASP:O	1:S:145:ASP:HB2	1.73	0.89
1:P:144:ASP:O	1:P:145:ASP:HB2	1.73	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:F:144:ASP:O	1:F:145:ASP:HB2	1.72	0.89
1:E:144:ASP:O	1:E:145:ASP:HB2	1.72	0.89
1:C:216:ALA:HB1	1:N:446:LYS:HE2	1.54	0.89
1:S:188:ALA:HB2	1:S:218:GLN:HG3	0.91	0.89
1:L:487:GLY:HA2	1:S:229:LYS:HE3	1.53	0.89
1:W:144:ASP:O	1:W:145:ASP:HB2	1.72	0.89
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: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:Q:144:ASP:O	1:Q: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:K:144:ASP:O	1:K:145:ASP:HB2	1.72	0.89
1:V:284:LYS:CG	1:X:7:LEU:HD22	2.01	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:371:HIS:O	1:W:374:MET:HG2	1.71	0.88
1:D:144:ASP:O	1:D:145:ASP:HB2	1.72	0.88
1:R:188:ALA:HB2	1:R:218:GLN:HG3	0.91	0.88
1:E:188:ALA:HB2	1:E: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:H:383:SER:HB2	1:I:383:SER:HB2	1.54	0.88
1:B:144:ASP:O	1:B:145:ASP:HB2	1.72	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:373:PRO:CA	1:G:390:GLU:O	2.20	0.88
1:F:371:HIS:O	1:F:374:MET:HG2	1.71	0.88
1:U:144:ASP:O	1:U:145:ASP:HB2	1.72	0.88
1:D:371:HIS:O	1:D:374:MET:HG2	1.71	0.88
1:C:144:ASP:O	1:C:145:ASP:HB2	1.72	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:Q:242:HIS:HE1	1:S:12:PHE:CE2	1.87	0.87
1:L:144:ASP:O	1:L:145:ASP:HB2	1.72	0.87
1:H:144:ASP:O	1:H:145:ASP:HB2	1.72	0.87
1:B:272:GLU:HG3	1:C:352:GLU:HB2	1.55	0.87
1:H:188:ALA:HB1	1:H:218:GLN:HG2	1.56	0.87
1:C:496:LEU:HG	1:V:195:VAL:CG2	2.05	0.87
1:V:144:ASP:O	1:V:145:ASP:HB2	1.72	0.87
1:L:229:LYS:HG3	1:S:487:GLY:CA	2.05	0.87
1:I:404:ARG:NH2	1:M:228:PRO:HG2	1.89	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:C:188:ALA:HB2	1:C:218:GLN:HG3	0.91	0.87
1:T:3:LEU:CD2	1:T:3:LEU:C	2.42	0.87
1:R:272:GLU:HG3	1:T:352:GLU:CG	2.05	0.87
1:W:372:ILE:HG23	1:X:390:GLU:O	1.75	0.87
1:B:312:GLU:HA	1:C:311:ALA:HB1	1.56	0.87
1:L:269:ILE:HG12	1:N:11:ILE:HD12	1.57	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:I:144:ASP:O	1:I:145:ASP:HB2	1.72	0.86
1:K:311:ALA:HB1	1:M:312:GLU:HA	1.57	0.86
1:U:188:ALA:HB1	1:U:218:GLN:HG2	1.56	0.86
1:U:11:ILE:CA	1:W:273:LYS:HG2	2.05	0.86
1:S:390:GLU:OE1	1:T:379:ALA:CB	2.23	0.86
1:A:144:ASP:O	1:A:145:ASP:HB2	1.72	0.86
1:D:188:ALA:HB1	1:D:218:GLN:HG2	1.57	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:H:310:ARG:HB2	1:J:297:GLN:HB2	1.58	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: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:E:11:ILE:CG1	1:E:12:PHE:CE2	2.60	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:HG2	1:V:424:ARG:HH11	0.74	0.85
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: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:M:383:SER:HB2	1:N:383:SER:HB2	1.59	0.85
1:O:188:ALA:HB1	1:O:218:GLN:HG2	1.56	0.85
1:X:188:ALA:HB1	1:X:218:GLN:HG2	1.56	0.85
1:K:496:LEU:CG	1:S:195:VAL:HG22	2.06	0.85
1:I:188:ALA:HB1	1:I:218:GLN:HG2	1.56	0.85
1:I:11:ILE:CG1	1:I:12:PHE:CE2	2.60	0.85
1:H:352:GLU:HG2	1:J:272:GLU:O	1.77	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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: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:V:188:ALA:HB1	1:V:218:GLN:HG2	1.56	0.84
1:L:11:ILE:HG13	1:L:12:PHE:CD2	2.12	0.84
1:S:483:HIS:CD2	1:T:483:HIS:NE2	2.44	0.84
1:O:12:PHE:CZ	1:P:242:HIS:CE1	2.64	0.84
1:K:390:GLU:HA	1:L:372:ILE:HG13	1.60	0.84
1:I:11:ILE:HG13	1:I:12:PHE:CD2	2.13	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:S:188:ALA:HB1	1:S:218:GLN:HG2	1.57	0.84
1:L:297:GLN:HB2	1:N:310:ARG:HG3	1.59	0.84
1:L:11:ILE:HD11	1:L:12:PHE:CE2	2.12	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:W:188:ALA:HB1	1:W:218:GLN:HG2	1.56	0.84
1:E:424:ARG:HG2	1:E:424:ARG:HH11	0.74	0.84
1:U:310:ARG:HG2	1:W:297:GLN:HB2	1.59	0.84
1:K:297:GLN:OE1	1:M:310:ARG:HG2	1.77	0.84
1:W:373:PRO:HB3	1:X:391:THR:CA	2.07	0.84
1:U:297:GLN:HB2	1:W:310:ARG:CG	2.08	0.83
1:R:272:GLU:CB	1:T:352:GLU:HG2	2.08	0.83
1:E:11:ILE:HG13	1:E:12:PHE:CD2	2.12	0.83
1:S:10:SER:HB3	1:S:13:ASP:OD1	1.79	0.83
1:H:10:SER:HB3	1:H:13:ASP:OD1	1.78	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:V:11:ILE:HG13	1:V:12:PHE:CD2	2.12	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:H:496:LEU:CD2	1:M:195:VAL:CG2	2.56	0.83
1:L:10:SER:HB3	1:L:13:ASP:OD1	1.78	0.83
1:B:279:LYS:HE3	1:C:6:ASN:OD1	1.78	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:254:GLU:HG2	1:N:446:LYS:HE2	1.60	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:M:10:SER:HB3	1:M:13:ASP:OD1	1.79	0.83
1:G:10:SER:HB3	1:G:13:ASP:OD1	1.79	0.83
1:O:10:SER:HB3	1:O:13:ASP:OD1	1.78	0.83
1:H:315:ASP:HB2	1:J:311:ALA:HA	1.61	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:M:390:GLU:O	1:N:373:PRO:CB	2.27	0.83
1:E:279:LYS:HE3	1:G:6:ASN:OD1	1.76	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:M:390:GLU:O	1:N:373:PRO:CA	2.26	0.83
1:V:3:LEU:HD23	1:X:283:SER:HB3	1.61	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:U:10:SER:HB3	1:U:13:ASP:OD1	1.78	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: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: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: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:H:310:ARG:CG	1:J:297:GLN:CG	2.57	0.82
1:A:3:LEU:HD21	1:I:283:SER:HB3	1.61	0.82
1:E:10:SER:HB3	1:E:13:ASP:OD1	1.79	0.82
1:C:10:SER:HB3	1:C:13:ASP:OD1	1.78	0.82
1:V:284:LYS:CG	1:X:7:LEU:HD21	2.07	0.82
1:F:390:GLU:O	1:G:373:PRO:CA	2.26	0.82
1:F:373:PRO:CB	1:G:391:THR:HA	2.09	0.82
1:B:10:SER:HB3	1:B:13:ASP:OD1	1.79	0.82
1:O:424:ARG:HG2	1:O:424:ARG:HH11	0.74	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:H:11:ILE:CA	1:J:273:LYS:HG2	2.08	0.82
1:C:496:LEU:CG	1:V:195:VAL:HG22	2.10	0.82
1:Q:310:ARG:HG2	1:S:297:GLN:OE1	1.80	0.82
1:D:10:SER:HB3	1:D:13:ASP:OD1	1.79	0.82
1:I:424:ARG:HH11	1:I:424:ARG:HG2	0.74	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:F:453:LYS:NZ	2:F:700:FDP:O1P	2.13	0.82
1:A:424:ARG:HH11	1:A:424:ARG:HG2	0.74	0.82
1:Q:283:SER:CB	1:S:3:LEU:HD23	2.09	0.82
1:Q:283:SER:CB	1:S:3:LEU:CD2	2.57	0.82
1:X:10:SER:HB3	1:X:13:ASP:OD1	1.78	0.82
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:L:11:ILE:O	1:N:273:LYS:HE3	1.79	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:B:453:LYS:NZ	2:B:700:FDP:O1P	2.13	0.81
1:H:496:LEU:CG	1:M:195:VAL:CG2	2.52	0.81
1:L:487:GLY:HA2	1:S:229:LYS:HG3	1.59	0.81
1:Q:10:SER:HB3	1:Q:13:ASP:OD1	1.78	0.81
1:N:453:LYS:NZ	2:N:700:FDP:O1P	2.13	0.81
1:J:453:LYS:NZ	2:J:700:FDP:O1P	2.13	0.81
1:D:453:LYS:NZ	2:D:700:FDP:O1P	2.13	0.81
1:C:424:ARG:HH11	1:C:424:ARG:HG2	0.74	0.81
1:Q:453:LYS:NZ	2:Q:700:FDP:O1P	2.13	0.81
1:N:446:LYS:O	1:N:446:LYS:HD2	1.81	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:S:453:LYS:NZ	2:S:700:FDP:O1P	2.13	0.81
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:V:12:PHE:CE2	1:X:242:HIS:CE1	2.69	0.81
1:L:311:ALA:HB1	1:N:312:GLU:HA	1.63	0.81
1:T:424:ARG:HG2	1:T:424:ARG:HH11	0.74	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:D:12:PHE:CZ	1:F:242:HIS:CE1	2.69	0.81
1:L:487:GLY:HA2	1:S:229:LYS:CE	2.09	0.81
1:W:390:GLU:OE1	1:X:379:ALA:CB	2.29	0.81
1:L:229:LYS:HE3	1:S:487:GLY:HA2	1.61	0.81
1:S:483:HIS:CD2	1:T:483:HIS:CD2	2.69	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:I:453:LYS:NZ	2:I:700:FDP:O1P	2.13	0.81
1:K:372:ILE:HG13	1:L:390:GLU:HA	1.61	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:R:280:ILE:CG1	1:T:6:ASN:O	2.26	0.80
1:H:315:ASP:CB	1:J:311:ALA:HA	2.12	0.80
1:E:270:PRO:HG2	1:E:273:LYS:CE	2.11	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: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:H:390:GLU:O	1:I:373:PRO:HA	1.79	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:K:453:LYS:NZ	2:K:700:FDP:O1P	2.15	0.79
1:H:453:LYS:NZ	2:H:700:FDP:O1P	2.15	0.79
1:O:453:LYS:NZ	2:O:700:FDP:O1P	2.14	0.79
1:U:242:HIS:NE2	1:W:12:PHE:CE2	2.49	0.79
1:N:142:TYR:HB3	1:N:146:GLY:HA2	1.65	0.79
1:H:11:ILE:O	1:J:273:LYS:CG	2.30	0.79
1:V:276:VAL:CG1	1:V:280:ILE:HD11	2.11	0.79
1:H:496:LEU:HD23	1:M:195:VAL:HG22	1.64	0.79
1:B:372:ILE:HG13	1:O:390:GLU:HA	1.64	0.79
1:L:487:GLY:HA2	1:S:229:LYS:CG	2.11	0.79
1:W:390:GLU:OE1	1:X:379:ALA:HB1	1.82	0.79
1:L:142:TYR:HB3	1:L:146:GLY:HA2	1.65	0.79
1:N:446:LYS:O	1:N:446:LYS:CD	2.30	0.79
1:P:370:GLN:HB3	1:P:374:MET:SD	2.22	0.79
1:H:424:ARG:HH11	1:H:424:ARG:HG2	0.74	0.79
1:O:312:GLU:HA	1:P:311:ALA:CB	2.13	0.79
1:P:453:LYS:NZ	2:P:700:FDP:O1P	2.15	0.79
1:V:242:HIS:HE1	1:X:12:PHE:CZ	2.00	0.79
1:G:142:TYR:HB3	1:G:146:GLY:HA2	1.65	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:L:312:GLU:HA	1:N:311:ALA:HB1	1.64	0.79
1:P:487:GLY:CA	1:V:229:LYS:CG	2.61	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:280:ILE:HD11	1:S:9:LEU:HB2	1.65	0.79
1:Q:142:TYR:HB3	1:Q:146:GLY:HA2	1.65	0.79
1:K:142:TYR:HB3	1:K: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: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: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:H:11:ILE:CB	1:J:273:LYS:HG2	2.13	0.78
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:C:216:ALA:HB1	1:N:446:LYS:CE	2.13	0.78
1:L:270:PRO:HG2	1:L:273:LYS:CE	2.11	0.78
1:H:142:TYR:HB3	1:H:146:GLY:HA2	1.64	0.78
1:S:4:ALA:O	1:S:7:LEU:HB2	1.83	0.78
1:L:284:LYS:HG3	1:N:7:LEU:CD2	2.13	0.78
1:B:4:ALA:O	1:B:7:LEU:HB2	1.84	0.78
1:R:284:LYS:HG3	1:T:7:LEU:HD21	1.59	0.78
1:T:4:ALA:O	1:T:7:LEU:HB2	1.84	0.78
1:N:424:ARG:HG2	1:N:424:ARG:HH11	0.74	0.78
1:W:373:PRO:CB	1:X:391:THR:HA	2.12	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:D:142:TYR:HB3	1:D:146:GLY:HA2	1.65	0.78
1:N:4:ALA:O	1:N:7:LEU:HB2	1.84	0.78
1:I:4:ALA:O	1:I:7:LEU:HB2	1.84	0.78
1:U:142:TYR:HB3	1:U:146:GLY:HA2	1.65	0.78
1:R:142:TYR:HB3	1:R:146:GLY:HA2	1.65	0.78
1:G:453:LYS:NZ	2:G:700:FDP:O1P	2.15	0.78
1:J:142:TYR:HB3	1:J:146:GLY:HA2	1.65	0.78
1:R:284:LYS:CG	1:T:7:LEU:CD2	2.56	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:F:424:ARG:HG2	1:F:424:ARG:HH11	0.74	0.78
1:Q:283:SER:HB3	1:S:3:LEU:HD23	1.65	0.78
1:C:223:ARG:HG2	1:C:223:ARG:HH11	1.49	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:223:ARG:HH11	1:P:223:ARG:HG2	1.49	0.78
1:L:272:GLU:CG	1:N:352:GLU:HG2	2.13	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: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:B:223:ARG:HG2	1:B:223:ARG:HH11	1.49	0.78
1:W:223:ARG:HG2	1:W:223:ARG:HH11	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: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:P:142:TYR:HB3	1:P:146:GLY:HA2	1.65	0.78
1:L:4:ALA:O	1:L:7:LEU:HB2	1.83	0.78
1:X:4:ALA:O	1:X:7:LEU:HB2	1.84	0.77
1:F:223:ARG:HH11	1:F:223:ARG:HG2	1.49	0.77
1:C:142:TYR:HB3	1:C:146:GLY:HA2	1.65	0.77
1:P:424:ARG:HG2	1:P:424:ARG:HH11	0.74	0.77
1:L:487:GLY:HA3	1:S:229:LYS:HG3	1.64	0.77
1:J:223:ARG:HG2	1:J:223:ARG:HH11	1.49	0.77
1:I:142:TYR:HB3	1:I:146:GLY:HA2	1.65	0.77
1:G:4:ALA:O	1:G:7:LEU:HB2	1.83	0.77
1:A:4:ALA:O	1:A:7:LEU:HB2	1.84	0.77
1:X:142:TYR:HB3	1:X:146:GLY:HA2	1.64	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:Q:424:ARG:HG2	1:Q:424:ARG:HH11	0.74	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:H:297:GLN:CG	1:J:310:ARG:HG2	2.15	0.77
1:A:223:ARG:HG2	1:A:223:ARG:HH11	1.49	0.77
1:V:142:TYR:HB3	1:V:146:GLY:HA2	1.65	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:S:223:ARG:HG2	1:S:223:ARG:HH11	1.49	0.77
1:Q:223:ARG:HH11	1:Q:223:ARG:HG2	1.49	0.77
1:B:311:ALA:HB1	1:C:312:GLU:HA	1.65	0.77
1:F:4:ALA:O	1:F:7:LEU:HB2	1.83	0.77
1:E:142:TYR:HB3	1:E:146:GLY:HA2	1.65	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:4:ALA:O	1:M:7:LEU:HB2	1.84	0.77
1:H:4:ALA:O	1:H:7:LEU:HB2	1.84	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:HH11	1:U:223:ARG:HG2	1.49	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:V:283:SER:HB3	1:X:3:LEU:HG	1.66	0.77
1:U:4:ALA:O	1:U:7:LEU:HB2	1.84	0.77
1:M:214:ARG:H	1:M:218:GLN:HE22	1.33	0.76
1:V:12:PHE:CZ	1:X:242:HIS:CE1	2.72	0.76
1:G:223:ARG:HH11	1:G:223:ARG:HG2	1.49	0.76
1:H:223:ARG:HH11	1:H:223:ARG:HG2	1.49	0.76
1:S:142:TYR:HB3	1:S:146:GLY:HA2	1.64	0.76
1:Q:4:ALA:O	1:Q:7:LEU:HB2	1.84	0.76
1:V:283:SER:HB3	1:X:3:LEU:CD2	2.15	0.76
1:V:214:ARG:H	1:V:218:GLN:HE22	1.33	0.76
1:Q:390:GLU:O	1:R:372:ILE:HG23	1.86	0.76
1:A:392:LYS:CD	1:J:373:PRO:HD3	2.13	0.76
1:L:269:ILE:HG12	1:N:11:ILE:CD1	2.15	0.76
1:K:223:ARG:HG2	1:K:223:ARG:HH11	1.49	0.76
1:X:223:ARG:HG2	1:X:223:ARG:HH11	1.49	0.76
1:K:214:ARG:H	1:K:218:GLN:HE22	1.34	0.76
1:B:373:PRO:HB3	1:O:391:THR:C	2.06	0.76
1:N:223:ARG:HH11	1:N:223:ARG:HG2	1.49	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:L:229:LYS:HG3	1:S:487:GLY:HA3	1.67	0.76
1:O:223:ARG:HG2	1:O:223:ARG:HH11	1.49	0.76
1:I:223:ARG:HG2	1:I:223:ARG:HH11	1.49	0.76
1:R:223:ARG:HG2	1:R:223:ARG:HH11	1.49	0.76
1:L:229:LYS:HG3	1:S:487:GLY:HA2	1.66	0.76
1:C:373:PRO:CA	1:P:390:GLU:O	2.34	0.76
1:M:223:ARG:HG2	1:M:223:ARG:HH11	1.49	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:V:4:ALA:O	1:V:7:LEU:HB2	1.84	0.75
1:V:223:ARG:HG2	1:V:223:ARG:HH11	1.49	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:383:SER:HB2	1:G:383:SER:HB2	1.69	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:O:214:ARG:H	1:O:218:GLN:HE22	1.34	0.75
1:E:214:ARG:H	1:E:218:GLN:HE22	1.33	0.75
1:A:214:ARG:H	1:A:218:GLN:HE22	1.33	0.75
1:L:214:ARG:H	1:L:218:GLN:HE22	1.33	0.74
1:R:276:VAL:CG1	1:T:9:LEU:CB	2.64	0.74
1:K:272:GLU:HG3	1:M:352:GLU:HB2	1.68	0.74
1:U:242:HIS:CE1	1:W:12:PHE:HZ	2.00	0.74
1:H:297:GLN:HG3	1:J:310:ARG:HG2	1.69	0.74
1:V:280:ILE:HD11	1:X:9:LEU:HB2	1.68	0.74
1:E:223:ARG:HG2	1:E:223:ARG:HH11	1.49	0.74
1:S:491:GLN:HG3	1:T:491:GLN:HG3	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
1:U:214:ARG:H	1:U:218:GLN:HE22	1.33	0.74
1:F:390:GLU:HA	1:G:372:ILE:HG13	1.69	0.74
1:P:229:LYS:HG3	1:V:487:GLY:HA3	1.69	0.74
1:K:11:ILE:HB	1:M:273:LYS:HG2	1.68	0.74
1:L:191:ALA:HB1	1:T:473:GLY:HA3	1.69	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: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:C:373:PRO:HB3	1:P:391:THR:HA	1.69	0.74
1:I:193:ASP:HA	1:I:196:ASP:HB2	1.70	0.74
1:J:214:ARG:H	1:J:218:GLN:HE22	1.33	0.74
1:Q:214:ARG:H	1:Q:218:GLN:HE22	1.33	0.74
1:F:391:THR:HA	1:G:373:PRO:HB3	1.70	0.74
1:Q:12:PHE:CE2	1:S:242:HIS:HE1	2.06	0.74
1:K:193:ASP:HA	1:K:196:ASP:HB2	1.70	0.74
1:W:193:ASP:HA	1:W:196:ASP:HB2	1.70	0.74
1:M:193:ASP:HA	1:M:196:ASP:HB2	1.70	0.74
1:R:276:VAL:HG13	1:T:9:LEU:CB	2.18	0.74
1:V:297:GLN:OE1	1:X:309:THR:HB	1.88	0.74
1:W:392:LYS:HD2	1:X:373:PRO:HD3	1.69	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:9:LEU:HB2	1:X:280:ILE:HD11	1.68	0.74
1:O:193:ASP:HA	1:O:196:ASP:HB2	1.70	0.74
1:L:283:SER:CB	1:N:3:LEU:HD21	2.17	0.73
1:L:193:ASP:HA	1:L:196:ASP:HB2	1.70	0.73
1:S:494:ILE:HD12	1:T:376:ALA:HB1	1.68	0.73
1:S:214:ARG:H	1:S:218:GLN:HE22	1.33	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:E:11:ILE:CG1	1:E:12:PHE:CD2	2.71	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:F:193:ASP:HA	1:F:196:ASP:HB2	1.70	0.73
1:A:179:LEU:HB3	1:A:182:CYS:HB2	1.71	0.73
1:V:310:ARG:HG2	1:X:297:GLN:OE1	1.88	0.73
1:N:179:LEU:HB3	1:N:182:CYS:HB2	1.70	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
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:R:214:ARG:H	1:R:218:GLN:HE22	1.33	0.73
1:Q:297:GLN:OE1	1:S:310:ARG:CG	2.31	0.73
1:L:424:ARG:HH11	1:L:424:ARG:HG2	0.74	0.73
1:K:242:HIS:CE1	1:M:12:PHE:CZ	2.75	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: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:N:214:ARG:H	1:N:218:GLN:HE22	1.33	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:D:179:LEU:HB3	1:D:182:CYS:HB2	1.70	0.73
1:Q:312:GLU:HA	1:S:311:ALA:HB1	1.70	0.73
1:D:193:ASP:HA	1:D:196:ASP:HB2	1.70	0.73
1:N:193:ASP:HA	1:N:196:ASP:HB2	1.70	0.73
1:C:179:LEU:HB3	1:C:182:CYS:HB2	1.70	0.73
1:I:179:LEU:HB3	1:I:182:CYS:HB2	1.70	0.73
1:W:214:ARG:H	1:W:218:GLN:HE22	1.33	0.73
1:C:496:LEU:CD2	1:V:195:VAL:HG22	2.19	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:370:GLN:HB3	1:T:374:MET:SD	2.29	0.73
1:O:179:LEU:HB3	1:O:182:CYS:HB2	1.71	0.73
1:U:424:ARG:HH11	1:U:424:ARG:HG2	0.74	0.72
1:L:11:ILE:CG1	1:L:12:PHE:CD2	2.71	0.72
1:X:179:LEU:HB3	1:X:182:CYS:HB2	1.70	0.72
1:Q:193:ASP:HA	1:Q:196:ASP:HB2	1.70	0.72
1:A:193:ASP:HA	1:A:196:ASP: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:U:370:GLN:HB3	1:U:374:MET:SD	2.29	0.72
1:L:229:LYS:CE	1:S:487:GLY:HA2	2.19	0.72
1:P:191:ALA:HB1	1:U:473:GLY:HA3	1.69	0.72
1:R:193:ASP:HA	1:R:196:ASP:HB2	1.70	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:V:193:ASP:HA	1:V:196:ASP:HB2	1.70	0.72
1:Q:179:LEU:HB3	1:Q:182:CYS:HB2	1.71	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:J:193:ASP:HA	1:J:196:ASP:HB2	1.70	0.72
1:C:193:ASP:HA	1:C:196:ASP:HB2	1.70	0.72
1:Q:11:ILE:HB	1:S:273:LYS:HG2	1.72	0.72
1:S:179:LEU:HB3	1:S:182:CYS:HB2	1.70	0.72
1:Q:3:LEU:CD2	1:S:283:SER:HB3	2.20	0.72
1:U:373:PRO:HB3	1:V:391:THR:CA	2.19	0.72
1:Q:373:PRO:HD3	1:R:392:LYS:HD2	1.72	0.72
1:L:272:GLU:HG3	1:N:352:GLU:HB2	1.70	0.72
1:F:179:LEU:HB3	1:F:182:CYS:HB2	1.70	0.72
1:U:372:ILE:HD11	1:V:390:GLU:HG2	1.71	0.72
1:A:390:GLU:HA	1:J:372:ILE:HG13	1.70	0.72
1:J:424:ARG:HH11	1:J:424:ARG:HG2	0.74	0.72
1:E:193:ASP:HA	1:E:196:ASP:HB2	1.70	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:F:491:GLN:HG3	1:G:491:GLN:HG3	1.72	0.72
1:H:11:ILE:O	1:J:273:LYS:HG2	1.90	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:M:179:LEU:HB3	1:M:182:CYS: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:193:ASP:HA	1:B:196:ASP:HB2	1.70	0.72
1:H:193:ASP:HA	1:H:196:ASP:HB2	1.70	0.71
1:K:179:LEU:HB3	1:K:182:CYS:HB2	1.70	0.71
1:H:179:LEU:HB3	1:H:182:CYS:HB2	1.70	0.71
1:H:11:ILE:O	1:J:273:LYS:CE	2.37	0.71
1:G:179:LEU:HB3	1:G:182:CYS:HB2	1.70	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:Q:272:GLU:CG	1:S:352:GLU:HG2	2.21	0.71
1:A:283:SER:HB3	1:I:3:LEU:CD2	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:P:487:GLY:CA	1:V:229:LYS:CE	2.49	0.71
1:R:276:VAL:HG12	1:R:280:ILE:CD1	2.21	0.71
1:U:315:ASP:CB	1:W:311:ALA:HA	2.21	0.71
1:L:273:LYS:HD3	1:N:11:ILE:O	1.90	0.71
1:C:254:GLU:CG	1:N:446:LYS:HE2	2.21	0.71
1:L:229:LYS:CG	1:S:487:GLY:HA2	2.20	0.71
1:O:310:ARG:HG2	1:P:297:GLN:HB2	1.72	0.71
1:E:179:LEU:HB3	1:E:182:CYS:HB2	1.70	0.71
1:X:193:ASP:HA	1:X:196:ASP:HB2	1.70	0.71
1:G:193:ASP:HA	1:G:196:ASP:HB2	1.70	0.71
1:L:273:LYS:CG	1:N:11:ILE:HB	2.21	0.70
1:B:179:LEU:HB3	1:B:182:CYS:HB2	1.70	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:C:270:PRO:HG2	1:C:273:LYS:CD	2.21	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:V:7:LEU:HD22	1:X:284:LYS:HG2	1.74	0.70
1:T:193:ASP:HA	1:T:196:ASP:HB2	1.70	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:M:491:GLN:HG3	1:N:491:GLN:HG3	1.72	0.70
1:A:270:PRO:HG2	1:A:273:LYS:CD	2.21	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:11:ILE:CD1	1:R:12:PHE:CE2	2.75	0.70
1:R:280:ILE:HG23	1:T:7:LEU:HA	1.74	0.70
1:B:373:PRO:HD3	1:O:392:LYS:CD	2.22	0.70
1:I:11:ILE:CD1	1:I:12:PHE:CE2	2.75	0.70
1:A:135:VAL:HG11	1:A:152:VAL:HG21	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: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: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:X:135:VAL:HG11	1:X:152:VAL:HG21	1.74	0.70
1:T:38:LYS:HE3	1:T:73:GLU:OE1	1.92	0.70
1:V:11:ILE:CD1	1:V:12:PHE:CE2	2.75	0.69
1:I:38:LYS:HE3	1:I:73:GLU:OE1	1.92	0.69
1:L:11:ILE:CD1	1:L:12:PHE:CE2	2.75	0.69
1:B:270:PRO:HG2	1:B:273:LYS:CD	2.22	0.69
1:E:38:LYS:HE3	1:E:73:GLU:OE1	1.92	0.69
1:C:58:GLU:CD	1:E:103:ARG:HD2	2.12	0.69
1:F:38:LYS:HE3	1:F:73:GLU:OE1	1.92	0.69
1:M:135:VAL:HG11	1:M:152:VAL:HG21	1.74	0.69
1:R:276:VAL:HG11	1:T:9:LEU:HB3	1.74	0.69
1:A:391:THR:C	1:J:373:PRO:HB3	2.13	0.69
1:V:272:GLU:HG3	1:X:352:GLU:HB2	1.73	0.69
1:N:38:LYS:HE3	1:N:73:GLU: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:D:310:ARG:HG2	1:F:297:GLN:OE1	1.92	0.69
1:U:38:LYS:HE3	1:U:73:GLU:OE1	1.92	0.69
1:F:373:PRO:HD3	1:G:392:LYS:HD2	1.75	0.69
1:H:456:ARG:NH2	2:H:700:FDP:O1P	2.25	0.69
1:A:38:LYS:HE3	1:A:73:GLU:OE1	1.92	0.69
1:X:38:LYS:HE3	1:X:73:GLU:OE1	1.92	0.69
1:H:270:PRO:HG2	1:H:273:LYS:CD	2.22	0.69
1:O:297:GLN:HB2	1:P:310:ARG:HG2	1.74	0.69
1:L:38:LYS:HE3	1:L: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:V:135:VAL:HG11	1:V:152:VAL:HG21	1.74	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:270:PRO:HG2	1:U:273:LYS:CD	2.22	0.69
1:H:12:PHE:HZ	1:J:242:HIS:CE1	2.02	0.69
1:U:297:GLN:CB	1:W:310:ARG:HG2	2.17	0.69
1:V:276:VAL:HG13	1:X:9:LEU:HD13	1.75	0.69
1:M:456:ARG:NH2	2:M:700:FDP:O1P	2.25	0.69
1:K:272:GLU:O	1:M:352:GLU:HG2	1.92	0.69
1:W:38:LYS:HE3	1:W:73:GLU:OE1	1.92	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:J:135:VAL:HG11	1:J:152:VAL:HG21	1.74	0.69
1:W:372:ILE:HG13	1:X:390:GLU:O	1.93	0.69
1:W:456:ARG:NH2	2:W:700:FDP:O1P	2.25	0.69
1:P:456:ARG:NH2	2:P:700:FDP:O1P	2.25	0.69
1:H:38:LYS:HE3	1:H:73:GLU:OE1	1.92	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
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:H:11:ILE:HD12	1:J:269:ILE:HG12	1.74	0.69
1:H:11:ILE:HB	1:J:273:LYS:HB3	1.74	0.69
1:H:311:ALA:HB3	1:J:312:GLU:CG	2.23	0.69
1:V:272:GLU:HG2	1:X:352:GLU:HG2	1.73	0.69
1:P:38:LYS:HE3	1:P:73:GLU:OE1	1.92	0.69
1:M:38:LYS:HE3	1:M:73:GLU:OE1	1.92	0.69
1:G:38:LYS:HE3	1:G:73:GLU:OE1	1.92	0.69
1:O:456:ARG:NH2	2:O:700:FDP:O1P	2.25	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:V:38:LYS:HE3	1:V:73:GLU:OE1	1.92	0.69
1:S:372:ILE:CG2	1:T:390:GLU:O	2.42	0.68
1:L:297:GLN:HB2	1:N:310:ARG:CG	2.24	0.68
1:E:135:VAL:HG11	1:E:152:VAL:HG21	1.74	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:V:297:GLN:HE21	1:V:300:GLU:CD	1.97	0.68
1:K:297:GLN:HB2	1:M:310:ARG:CG	2.23	0.68
1:B:273:LYS:HB3	1:C:11:ILE:HB	1.75	0.68
1:P:135:VAL:HG11	1:P:152:VAL:HG21	1.74	0.68
1:L:456:ARG:NH2	2:L:700:FDP:O1P	2.25	0.68
1:B:38:LYS:HE3	1:B:73:GLU:OE1	1.92	0.68
1:Q:135:VAL:HG11	1:Q:152:VAL:HG21	1.74	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:242:HIS:CE1	1:X:12:PHE:HE2	2.06	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:R:372:ILE:HD12	1:R:374:MET:HG3	1.75	0.68
1:L:11:ILE:HG13	1:L:12:PHE:CE2	2.29	0.68
1:K:456:ARG:NH2	2:K:700:FDP:O1P	2.25	0.68
1:W:135:VAL:HG11	1:W:152:VAL:HG21	1.74	0.68
1:C:390:GLU:O	1:P:372:ILE:HG23	1.92	0.68
1:I:135:VAL:HG11	1:I:152:VAL:HG21	1.74	0.68
1:F:135:VAL:HG11	1:F:152:VAL:HG21	1.74	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: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:U:135:VAL:HG11	1:U:152:VAL:HG21	1.74	0.68
1:K:279:LYS:HE3	1:M:6:ASN:OD1	1.94	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:L:135:VAL:HG11	1:L:152:VAL:HG21	1.74	0.68
1:U:242:HIS:NE2	1:W:12:PHE:HE2	1.93	0.67
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: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:L:12:PHE:CE2	1:N:242:HIS:CE1	2.82	0.67
1:Q:12:PHE:HE2	1:S:242:HIS:HE1	1.40	0.67
1:C:391:THR:HA	1:P:373:PRO:HB3	1.75	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:135:VAL:HG11	1:C:152:VAL:HG21	1.74	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: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:D:390:GLU:O	1:E:373:PRO:HA	1.94	0.67
1:A:371:HIS:CD2	1:A:373:PRO:O	2.48	0.67
1:X:371:HIS:CD2	1:X: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: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:C:254:GLU:HG2	1:N:446:LYS:CE	2.24	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:263:GLY:HA2	1:J:310:ARG:HH11	1.60	0.67
1:V:283:SER:HB3	1:X:3:LEU:CG	2.25	0.67
1:R:11:ILE:HG13	1:R:12:PHE:CE2	2.29	0.67
1:J:371:HIS:CD2	1:J:373:PRO:O	2.48	0.67
1:L:280:ILE:HD11	1:N:9:LEU:HB2	1.76	0.67
1:D:373:PRO:HD3	1:E:392:LYS:HD2	1.76	0.67
1:K:135:VAL:HG11	1:K:152:VAL:HG21	1.74	0.67
1:U:311:ALA:CB	1:W:312:GLU:HA	2.19	0.66
1:N:371:HIS:CD2	1:N:373:PRO:O	2.48	0.66
1:V:371:HIS:CD2	1:V:373:PRO:O	2.48	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:K:371:HIS:CD2	1:K:373:PRO:O	2.48	0.66
1:H:53:SER:OG	1:H:85:LYS:HA	1.96	0.66
1:U:242:HIS:HE1	1:W:12:PHE:CE2	1.85	0.66
1:S:373:PRO:HB3	1:T:391:THR:C	2.16	0.66
1:H:310:ARG:CG	1:J:297:GLN:HG3	2.22	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:L:53:SER:OG	1:L: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: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:O:12:PHE:HZ	1:P:242:HIS:HE1	1.42	0.66
1:E:371:HIS:CD2	1:E:373:PRO:O	2.48	0.66
1:Q:371:HIS:CD2	1:Q:373:PRO:O	2.48	0.66
1:L:352:GLU:HG2	1:N:272:GLU:O	1.96	0.66
1:X:53:SER:OG	1:X:85:LYS:HA	1.96	0.66
1:D:53:SER:OG	1:D:85:LYS:HA	1.96	0.66
1:F:53:SER:OG	1:F:85:LYS:HA	1.96	0.66
1:O:371:HIS:CD2	1:O:373:PRO:O	2.48	0.66
1:D:371:HIS:CD2	1:D:373:PRO:O	2.48	0.66
1:F:373:PRO:HB3	1:G:391:THR:C	2.16	0.66
1:L:279:LYS:HE3	1:N:6:ASN:OD1	1.96	0.66
1:H:352:GLU:HG2	1:J:272:GLU:C	2.16	0.66
1:S:53:SER:OG	1:S:85:LYS:HA	1.96	0.66
1:C:53:SER:OG	1:C:85:LYS:HA	1.96	0.66
1:R:283:SER:HB3	1:T:3:LEU:HG	1.77	0.66
1:C:250:SER:HB3	1:N:446:LYS:HG2	1.71	0.66
1:A:53:SER:OG	1:A:85:LYS:HA	1.96	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:11:ILE:O	1:W:273:LYS:CD	2.45	0.65
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:V:269:ILE:HG12	1:X:11:ILE:CD1	2.27	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:N:53:SER:OG	1:N:85:LYS:HA	1.96	0.65
1:W:53:SER:OG	1:W:85:LYS:HA	1.96	0.65
1:E:53:SER:OG	1:E:85:LYS:HA	1.96	0.65
1:A:242:HIS:HE1	1:I:12:PHE:CE2	2.10	0.65
1:U:390:GLU:O	1:V:373:PRO:CA	2.44	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
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:A:3:LEU:CD2	1:I:283:SER:CB	2.74	0.65
1:W:144:ASP:O	1:W:145:ASP:CB	2.45	0.65
1:V:144:ASP:O	1:V:145:ASP:CB	2.45	0.65
1:U:315:ASP:CG	1:W:311:ALA:HA	2.16	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:O:242:HIS:CE1	1:P:12:PHE:CE2	2.84	0.65
1:E:312:GLU:HA	1:G:311:ALA:HB1	1.78	0.65
1:J:53:SER:OG	1:J:85:LYS:HA	1.96	0.65
1:R:269:ILE:CG1	1:T:11:ILE:CD1	2.65	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:V:297:GLN:HE22	1:V:300:GLU:HG2	1.62	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:K:53:SER:OG	1:K:85:LYS:HA	1.96	0.65
1:U:372:ILE:CG2	1:V:390:GLU:O	2.43	0.65
1:O:311:ALA:CB	1:P:312:GLU:HA	2.23	0.65
1:D:144:ASP:O	1:D:145:ASP:CB	2.45	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:H:11:ILE:HB	1:J:273:LYS:CB	2.27	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:R:3:LEU:HD13	1:T:369:LEU:CD1	2.26	0.65
1:B:53:SER:OG	1:B:85:LYS:HA	1.96	0.65
1:Q:390:GLU:CA	1:R:372:ILE:HG13	2.24	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:269:ILE:CG1	1:X:11:ILE:HD12	2.27	0.64
1:U:53:SER:OG	1:U:85:LYS:HA	1.96	0.64
1:T:214:ARG:N	1:T:218:GLN:HE22	1.96	0.64
1:X:370:GLN:HB3	1:X:374:MET:SD	2.37	0.64
1:R:144:ASP:O	1:R:145:ASP:CB	2.45	0.64
1:Q:383:SER:HB2	1:R:383:SER:HB2	1.79	0.64
1:G:370:GLN:HB3	1:G:374:MET:SD	2.38	0.64
1:L:269:ILE:CG1	1:N:11:ILE:HD12	2.27	0.64
1:K:370:GLN:HB3	1:K:374:MET:SD	2.37	0.64
1:F:144:ASP:O	1:F:145:ASP:CB	2.45	0.64
1:U:245:VAL:HG11	1:W:11:ILE:HD13	1.79	0.64
1:M:214:ARG:N	1:M:218:GLN:HE22	1.96	0.64
1:X:214:ARG:N	1:X:218:GLN:HE22	1.96	0.64
1:Q:370:GLN:HB3	1:Q:374:MET:SD	2.38	0.64
1:B:272:GLU:HG3	1:C:352:GLU:CB	2.26	0.64
1:L:310:ARG:HG2	1:N:297:GLN:HB2	1.78	0.64
1:C:214:ARG:N	1:C:218:GLN:HE22	1.96	0.64
1:U:11:ILE:HB	1:W:273:LYS:CB	2.27	0.64
1:R:273:LYS:CD	1:T:11:ILE:O	2.42	0.64
1:W:370:GLN:HB3	1:W:374:MET:SD	2.37	0.64
1:B:370:GLN:HB3	1:B:374:MET:SD	2.38	0.64
1:N:370:GLN:HB3	1:N:374:MET:SD	2.37	0.64
1:Q:373:PRO:CA	1:R:390:GLU:O	2.46	0.64
1:D:370:GLN:HB3	1:D:374:MET:SD	2.38	0.64
1:Q:272:GLU:HG3	1:S:352:GLU:CB	2.27	0.64
1:V:53:SER:OG	1:V:85:LYS:HA	1.96	0.64
1:S:390:GLU:OE1	1:T:379:ALA:HB2	1.98	0.64
1:O:370:GLN:HB3	1:O:374:MET:SD	2.37	0.64
1:U:310:ARG:NH2	1:W:297:GLN:OE1	2.30	0.64
1:I:371:HIS:CD2	1:I:373:PRO:O	2.50	0.64
1:E:370:GLN:HB3	1:E:374:MET:SD	2.37	0.64
1:W:214:ARG:N	1:W:218:GLN:HE22	1.96	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:E:144:ASP:O	1:E:145:ASP:CB	2.45	0.64
1:B:214:ARG:N	1:B:218:GLN:HE22	1.96	0.64
1:J:214:ARG:N	1:J:218:GLN:HE22	1.96	0.64
1:U:214:ARG:N	1:U:218:GLN:HE22	1.96	0.64
1:H:214:ARG:N	1:H:218:GLN:HE22	1.96	0.64
1:C:370:GLN:HB3	1:C:374:MET:SD	2.37	0.64
1:A:370:GLN:HB3	1:A:374:MET:SD	2.38	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:6:ASN:O	1:S:280:ILE:HG12	1.98	0.64
1:T:144:ASP:O	1:T:145:ASP:CB	2.45	0.63
1:Q:214:ARG:N	1:Q:218:GLN:HE22	1.95	0.63
1:E:297:GLN:OE1	1:G:310:ARG:CG	2.35	0.63
1:V:214:ARG:N	1:V:218:GLN:HE22	1.96	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:F:214:ARG:N	1:F:218:GLN:HE22	1.96	0.63
1:H:297:GLN:HB2	1:J:310:ARG:CB	2.28	0.63
1:F:391:THR:CA	1:G:373:PRO:HB3	2.29	0.63
1:L:311:ALA:CB	1:N:312:GLU:HA	2.28	0.63
1:A:492:THR:HG22	1:J:492:THR:HG22	1.79	0.63
1:G:214:ARG:N	1:G:218:GLN:HE22	1.96	0.63
1:R:214:ARG:N	1:R:218:GLN:HE22	1.96	0.63
1:J:370:GLN:HB3	1:J:374:MET:SD	2.37	0.63
1:I:371:HIS:O	1:I:374:MET:CG	2.41	0.63
1:M:370:GLN:CB	1:M:374:MET:SD	2.86	0.63
1:P:195:VAL:CG2	1:U:496:LEU:CD2	2.73	0.63
1:P:214:ARG:N	1:P:218:GLN:HE22	1.96	0.63
1:L:272:GLU:CG	1:N:352:GLU:CG	2.76	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:X:144:ASP:O	1:X:145:ASP:CB	2.45	0.63
1:L:11:ILE:HD12	1:N:269:ILE:HG12	1.80	0.63
1:L:9:LEU:HB2	1:N:280:ILE:HD11	1.81	0.63
1:P:487:GLY:CA	1:V:229:LYS:HD2	2.27	0.63
1:O:214:ARG:N	1:O:218:GLN:HE22	1.96	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:V:7:LEU:HD23	1:X:284:LYS:HG3	1.80	0.63
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:B:272:GLU:C	1:C:352:GLU:HG2	2.20	0.62
1:I:214:ARG:N	1:I:218:GLN:HE22	1.96	0.62
1:M:373:PRO:HB3	1:N:391:THR:HA	1.80	0.62
1:I:11:ILE:HG13	1:I:12:PHE:CE2	2.29	0.62
1:P:144:ASP:O	1:P:145:ASP:CB	2.45	0.62
1:E:11:ILE:CD1	1:E:12:PHE:HE2	2.12	0.62
1:K:456:ARG:NH1	2:K:700:FDP:O2P	2.28	0.62
1:H:372:ILE:HD12	1:H:374:MET:HG3	1.81	0.62
1:F:372:ILE:HD11	1:G:390:GLU:HG2	1.81	0.62
1:G:144:ASP:O	1:G:145:ASP:CB	2.45	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:P:371:HIS:CD2	1:P:373:PRO:O	2.53	0.62
1:O:315:ASP:HB2	1:P:311:ALA:HA	1.82	0.62
1:P:456:ARG:NH1	2:P:700:FDP:O2P	2.28	0.62
1:H:273:LYS:HB3	1:J:11:ILE:HB	1.82	0.62
1:L:310:ARG:HG2	1:N:297:GLN:OE1	1.99	0.62
1:N:214:ARG:N	1:N:218:GLN:HE22	1.96	0.62
1:R:276:VAL:CG1	1:R:280:ILE:HD11	2.27	0.62
1:Q:372:ILE:HD11	1:Q:374:MET:HE1	1.81	0.62
1:L:144:ASP:O	1:L:145:ASP:CB	2.45	0.62
1:L:242:HIS:NE2	1:N:12:PHE:HE2	1.98	0.61
1:S:144:ASP:O	1:S:145:ASP:CB	2.45	0.61
1:K:269:ILE:HG12	1:M:11:ILE:HD12	1.82	0.61
1:B:283:SER:OG	1:C:3:LEU:HD23	1.99	0.61
1:L:283:SER:HB3	1:N:3:LEU:HD22	1.79	0.61
1:C:250:SER:HB2	1:N:446:LYS:HG2	0.69	0.61
1:H:315:ASP:HB2	1:J:311:ALA:CA	2.30	0.61
1:V:456:ARG:NH1	2:V:700:FDP:O2P	2.28	0.61
1:D:492:THR:HG22	1:E:492:THR:HG22	1.83	0.61
1:E:214:ARG:N	1:E:218:GLN:HE22	1.96	0.61
1:C:390:GLU:HA	1:P:372:ILE:CG1	2.15	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:S:373:PRO:CA	1:T:390:GLU:O	2.37	0.61
1:H:352:GLU:CG	1:J:272:GLU:O	2.49	0.61
1:V:297:GLN:NE2	1:V:300:GLU:CD	2.53	0.61
1:S:491:GLN:HG3	1:T:491:GLN:CD	2.21	0.61
1:C:250:SER:CB	1:N:446:LYS:CG	2.46	0.61
1:P:370:GLN:CB	1:P:374:MET:SD	2.88	0.61
1:U:310:ARG:CZ	1:W:297:GLN:OE1	2.49	0.61
1:L:11:ILE:CD1	1:L:12:PHE:HE2	2.12	0.61
1:B:270:PRO:HG2	1:B:273:LYS:HE2	1.83	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:R:287:VAL:HG23	1:T:3:LEU:HD11	1.83	0.61
1:K:373:PRO:HB3	1:L:391:THR:CA	2.26	0.61
1:J:144:ASP:O	1:J:145:ASP:CB	2.45	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:11:ILE:HB	1:G:273:LYS:HG2	1.82	0.61
1:O:456:ARG:NH1	2:O:700:FDP:O2P	2.28	0.61
1:H:279:LYS:HE3	1:J:6:ASN:OD1	2.01	0.61
1:T:456:ARG:NH1	2:T:700:FDP:O2P	2.28	0.61
1:M:456:ARG:NH1	2:M:700:FDP:O2P	2.28	0.61
1:Q:456:ARG:NH2	2:Q:700:FDP:O1P	2.34	0.60
1:B:103:ARG:HD2	1:G:58:GLU:OE1	2.01	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:H:270:PRO:HG2	1:H:273:LYS:HE2	1.83	0.60
1:E:311:ALA:HB1	1:G:312:GLU:HA	1.82	0.60
1:D:400:SER:HB2	1:D:405:SER:HB2	1.84	0.60
1:N:456:ARG:NH2	2:N:700:FDP:O1P	2.34	0.60
1:D:270:PRO:HG2	1:D:273:LYS:HE2	1.83	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:O:270:PRO:HG2	1:O:273:LYS:HE2	1.83	0.60
1:M:400:SER:HB2	1:M:405:SER:HB2	1.83	0.60
1:U:372:ILE:HG13	1:V:390:GLU:O	2.01	0.60
1:H:296:THR:HG22	1:H:297:GLN:HG2	1.83	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:E:472:THR:CG2	1:E:498:GLU:C	2.70	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: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:242:HIS:CE1	1:G:12:PHE:HE2	2.17	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: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:F:490:ASN:H	1:F:490:ASN:HD22	1.50	0.60
1:L:400:SER:HB2	1:L:405:SER:HB2	1.84	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:W:212:PHE:CE1	1:W:241:ASN:ND2	2.70	0.60
1:A:472:THR:CG2	1:A:498:GLU:C	2.70	0.60
1:W:472:THR:CG2	1:W:498:GLU:C	2.70	0.60
1:G:472:THR:CG2	1:G:498:GLU:C	2.70	0.60

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

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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:472:THR:HG22	1:Q:498:GLU:C	2.23	0.59
1:S:370:GLN:CB	1:S:374:MET:SD	2.90	0.59
1:M:472:THR:CG2	1:M:498:GLU:C	2.70	0.59
1:K:472:THR:CG2	1:K:498:GLU:C	2.70	0.59
1:I:11:ILE:CD1	1:I:12:PHE:HE2	2.12	0.59
1:B:272:GLU:CG	1:C:352:GLU:CG	2.79	0.59
1:H:352:GLU:HG2	1:J:272:GLU:CB	2.32	0.59
1:A:456:ARG:NH2	2:A:700:FDP:O1P	2.34	0.59
1:U:456:ARG:NH2	2:U:700:FDP:O1P	2.35	0.59
1:G:456:ARG:NH1	2:G:700:FDP:O2P	2.28	0.59
1:K:352:GLU:HG2	1:M:272:GLU:O	2.03	0.59
1:A:147:ILE:CG2	1:A:169:HIS:CD2	2.85	0.59
1:S:147:ILE:CG2	1:S:169:HIS:CD2	2.85	0.59
1:L:490:ASN:HD22	1:L:490:ASN:H	1.50	0.59
1:Q:147:ILE:CG2	1:Q:169:HIS:CD2	2.85	0.59
1:K:212:PHE:CE1	1:K:241:ASN:ND2	2.70	0.59
1:H:371:HIS:O	1:H:374:MET:CG	2.36	0.59
1:L:472:THR:HG22	1:L:498:GLU:C	2.22	0.59
1:X:472:THR:HG22	1:X:498:GLU:C	2.23	0.59
1:K:311:ALA:CB	1:M:312:GLU:HA	2.32	0.59
1:E:456:ARG:NH2	2:E:700:FDP:O1P	2.34	0.59
1:K:456:ARG:HH22	2:K:700:FDP:P1	2.26	0.59
1:O:456:ARG:HH22	2:O:700:FDP:P1	2.25	0.59
1:P:456:ARG:HH22	2:P:700:FDP:P1	2.26	0.59
1:L:272:GLU:HG3	1:N:352:GLU:CG	2.33	0.59
1:B:311:ALA:CB	1:C:312:GLU:HA	2.32	0.59
1:A:400:SER:HB2	1:A:405:SER:HB2	1.83	0.59
1:W:147:ILE:CG2	1:W:169:HIS:CD2	2.85	0.59
1:R:147:ILE:CG2	1:R:169:HIS:CD2	2.85	0.59
1:L:147:ILE:CG2	1:L:169:HIS:CD2	2.86	0.59
1:F:147:ILE:CG2	1:F:169:HIS:CD2	2.85	0.59
1:P:147:ILE:CG2	1:P:169:HIS:CD2	2.86	0.59
1:W:472:THR:HG22	1:W:498:GLU:C	2.23	0.59
1:L:270:PRO:CG	1:L:273:LYS:HE2	2.23	0.59
1:L:273:LYS:CB	1:N:11:ILE:HB	2.33	0.59
1:C:373:PRO:CB	1:P:390:GLU:O	2.51	0.59
1:Q:372:ILE:HD11	1:Q:374:MET:CE	2.33	0.59
1:H:383:SER:HB2	1:I:383:SER:CB	2.29	0.59
1:O:242:HIS:HE1	1:P:12:PHE:CE2	2.20	0.59
1:S:491:GLN:CD	1:T:491:GLN:NE2	2.56	0.59
1:T:490:ASN:H	1:T:490:ASN:HD22	1.50	0.59
1:S:400:SER:HB2	1:S:405:SER:HB2	1.84	0.59

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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:490:ASN:H	1:N:490:ASN:HD22	1.50	0.58
1:M:212:PHE:CE1	1:M:241:ASN:ND2	2.70	0.58
1:L:297:GLN:HB2	1:N:310:ARG:HB2	1.84	0.58
1:Q:242:HIS:CE1	1:S:12:PHE:CZ	2.91	0.58
1:V:283:SER:O	1:X:3:LEU:HD21	2.03	0.58
1:A:372:ILE:HD11	1:A:374:MET:CE	2.33	0.58
1:N:144:ASP:O	1:N:145:ASP:CB	2.45	0.58
1:X:372:ILE:HD11	1:X:374:MET:CE	2.33	0.58
1:L:456:ARG:HH22	2:L:700:FDP:P1	2.26	0.58
1:K:57:HIS:HE1	1:K:195:VAL:HG12	1.69	0.58
1:T:147:ILE:CG2	1:T:169:HIS:CD2	2.85	0.58
1:T:212:PHE:CE1	1:T:241:ASN:ND2	2.70	0.58
1:I:212:PHE:CE1	1:I:241:ASN:ND2	2.70	0.58
1:F:372:ILE:HD11	1:F:374:MET:CE	2.33	0.58
1:M:57:HIS:HE1	1:M:195:VAL:HG12	1.69	0.58
1:H:456:ARG:NH1	2:H:700:FDP:O2P	2.29	0.58
1:N:400:SER:HB2	1:N:405:SER:HB2	1.84	0.58
1:X:57:HIS:HE1	1:X:195:VAL:HG12	1.69	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:H:11:ILE:C	1:J:273:LYS:HG2	2.23	0.58
1:Q:212:PHE:CE1	1:Q:241:ASN:ND2	2.70	0.58
1:H:371:HIS:CD2	1:H:373:PRO:O	2.57	0.58
1:K:472:THR:HG22	1:K:498:GLU:C	2.23	0.58
1:V:57:HIS:HE1	1:V:195:VAL:HG12	1.69	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:B:283:SER:HB3	1:C:3:LEU:CD2	2.34	0.58
1:O:57:HIS:HE1	1:O:195:VAL:HG12	1.69	0.58
1:X:147:ILE:CG2	1:X:169:HIS:CD2	2.86	0.58
1:U:490:ASN:H	1:U:490:ASN:HD22	1.50	0.58
1:I:400:SER:HB2	1:I:405:SER:HB2	1.84	0.58
1:H:57:HIS:HE1	1:H:195:VAL:HG12	1.69	0.58
1:A:212:PHE:CE1	1:A:241:ASN:ND2	2.70	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:A:242:HIS:CE1	1:I:12:PHE:HE2	2.18	0.58
1:D:11:ILE:HB	1:F:273:LYS:CG	2.31	0.58
1:C:147:ILE:CG2	1:C:169:HIS:CD2	2.86	0.58
1:H:11:ILE:HA	1:J:273:LYS:HG2	1.86	0.58
1:B:212:PHE:CE1	1:B:241:ASN:ND2	2.70	0.58
1:L:212:PHE:CE1	1:L:241:ASN:ND2	2.70	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:472:THR:HG22	1:B:498:GLU:C	2.22	0.58
1:D:372:ILE:HD11	1:D:374:MET:CE	2.33	0.58
1:I:456:ARG:NH2	2:I:700:FDP:O1P	2.34	0.58
1:H:490:ASN:H	1:H:490:ASN:HD22	1.50	0.58
1:X:490:ASN:H	1:X:490:ASN:HD22	1.50	0.58
1:F:483:HIS:CD2	1:G:483:HIS:CD2	2.92	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:H:11:ILE:O	1:J:273:LYS:HD3	2.04	0.58
1:N:212:PHE:CE1	1:N:241:ASN:ND2	2.70	0.58
1:M:472:THR:HA	1:M:497:VAL:O	2.04	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:U:372:ILE:HG13	1:V:390:GLU:C	2.24	0.58
1:C:391:THR:CA	1:P:373:PRO:HB3	2.33	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:T:472:THR:HA	1:T:497:VAL:O	2.04	0.58
1:U:310:ARG:HG2	1:W:297:GLN:CB	2.30	0.58
1:H:456:ARG:HH22	2:H:700:FDP:P1	2.26	0.58
1:T:456:ARG:HH22	2:T:700:FDP:P1	2.26	0.58
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:G:472:THR:HA	1:G:497:VAL:O	2.04	0.57
1:U:272:GLU:HG3	1:W:352:GLU:HB2	1.86	0.57
1:H:9:LEU:HB3	1:J:276:VAL:HG13	1.85	0.57
1:F:57:HIS:HE1	1:F:195:VAL:HG12	1.69	0.57
1:G:212:PHE:CE1	1:G:241:ASN:ND2	2.70	0.57
1:R:472:THR:HG22	1:R:498:GLU:C	2.23	0.57
1:E:472:THR:HG22	1:E:498:GLU:C	2.23	0.57
1:P:472:THR:HA	1:P:497:VAL:O	2.04	0.57
1:N:57:HIS:HE1	1:N:195:VAL:HG12	1.69	0.57
1:C:472:THR:HA	1:C:497:VAL:O	2.04	0.57
1:I:472:THR:HA	1:I:497:VAL:O	2.05	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:U:57:HIS:HE1	1:U:195:VAL:HG12	1.69	0.57
1:R:280:ILE:CD1	1:T:9:LEU:HB2	2.32	0.57
1:L:472:THR:HA	1:L:497:VAL:O	2.04	0.57
1:B:456:ARG:NH2	2:B:700:FDP:O1P	2.34	0.57
1:L:272:GLU:HG3	1:N:352:GLU:CB	2.33	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:57:HIS:HE1	1:C:195:VAL:HG12	1.69	0.57
1:Q:490:ASN:HD22	1:Q:490:ASN:H	1.50	0.57
1:H:212:PHE:CE1	1:H:241:ASN:ND2	2.70	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:P:57:HIS:HE1	1:P:195:VAL:HG12	1.69	0.57
1:C:372:ILE:HG13	1:P:390:GLU:HA	1.85	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:E:57:HIS:HE1	1:E: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: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:G:490:ASN:H	1:G:490:ASN:HD22	1.50	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:W:472:THR:HA	1:W: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:E:472:THR:HA	1:E:497:VAL:O	2.04	0.57
1:L:57:HIS:HE1	1:L:195:VAL:HG12	1.69	0.57
1:B:373:PRO:HB3	1:O:391:THR:O	2.03	0.57
1:I:57:HIS:HE1	1:I:195:VAL:HG12	1.69	0.57
1:Q:11:ILE:O	1:S:273:LYS:HE3	2.05	0.57
1:L:6:ASN:O	1:N:280:ILE:HG12	2.04	0.57
1:D:57:HIS:HE1	1:D:195:VAL:HG12	1.69	0.57
1:Q:57:HIS:HE1	1:Q:195:VAL:HG12	1.69	0.57
1:S:212:PHE:CE1	1:S:241:ASN:ND2	2.70	0.57
1:G:472:THR:HG22	1:G:498:GLU:C	2.23	0.57
1:C:373:PRO:CB	1:P:391:THR:HA	2.33	0.57
1:L:280:ILE:HG13	1:N:6:ASN:O	2.03	0.57
1:R:11:ILE:HG12	1:R:12:PHE:CE2	2.40	0.57
1:E:283:SER:HB3	1:G:3:LEU:CD2	2.35	0.57
1:R:57:HIS:HE1	1:R:195:VAL:HG12	1.69	0.57
1:G:57:HIS:HE1	1:G:195:VAL:HG12	1.69	0.57
1:V:472:THR:HA	1:V:497:VAL:O	2.04	0.57
1:R:273:LYS:HB3	1:T:11:ILE:HB	1.85	0.57
1:H:472:THR:HA	1:H:497:VAL:O	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:273:LYS:CD	1:N:11:ILE:O	2.53	0.57
1:R:456:ARG:NH2	2:R:700:FDP:O1P	2.34	0.57
1:Q:12:PHE:CE2	1:S:242:HIS:CE1	2.86	0.57
1:J:212:PHE:CE1	1:J:241:ASN:ND2	2.70	0.57
1:G:372:ILE:HD11	1:G:374:MET:HE1	1.86	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: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:J:472:THR:HA	1:J:497:VAL:O	2.04	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:A:3:LEU:HD23	1:I:283:SER:CB	2.34	0.56
1:A:57:HIS:HE1	1:A:195:VAL:HG12	1.69	0.56
1:X:212:PHE:CE1	1:X:241:ASN:ND2	2.70	0.56
1:I:229:LYS:HE3	1:M:487:GLY:N	2.19	0.56
1:U:11:ILE:HA	1:W:273:LYS:HG2	1.85	0.56
1:O:472:THR:HA	1:O:497:VAL:O	2.04	0.56
1:C:498:GLU:HG2	1:V:195:VAL:HG11	1.87	0.56
1:U:315:ASP:HB2	1:W:311:ALA:CA	2.34	0.56
1:M:372:ILE:HD11	1:N:390:GLU:HG2	1.87	0.56
1:P:195:VAL:HG22	1:U:496:LEU:HD23	1.85	0.56
1:D:373:PRO:HB3	1:E:391:THR:C	2.25	0.56
1:Q:272:GLU:HG2	1:S:352:GLU:HG2	1.85	0.56
1:U:223:ARG:HH11	1:U:223:ARG:CG	2.19	0.56
1:S:493:ARG:NE	1:T:482:ASP:OD2	2.34	0.56
1:K:310:ARG:HG2	1:M:297:GLN:OE1	2.05	0.56
1:X:57:HIS:CE1	1:X:195:VAL:HG12	2.41	0.56
1:F:57:HIS:CE1	1:F:195:VAL:HG12	2.41	0.56
1:C:57:HIS:CE1	1:C:195:VAL:HG12	2.41	0.56
1:V:57:HIS:CE1	1:V:195:VAL:HG12	2.41	0.56
1:G:472:THR:CG2	1:G:498:GLU:HA	2.18	0.56
1:P:223:ARG:HH11	1:P:223:ARG:CG	2.19	0.56
1:L:352:GLU:HB2	1:N:272:GLU:HG3	1.87	0.56
1:O:57:HIS:CE1	1:O:195:VAL:HG12	2.41	0.56
1:N:57:HIS:CE1	1:N:195:VAL:HG12	2.41	0.56
1:U:57:HIS:CE1	1:U:195:VAL:HG12	2.41	0.56
1:K:491:GLN:HG3	1:L:491:GLN:HG3	1.87	0.56
1:S:57:HIS:HE1	1:S:195:VAL:HG12	1.69	0.56
1:L:11:ILE:HG12	1:L:12:PHE:CE2	2.40	0.56
1:E:57:HIS:CE1	1:E:195:VAL:HG12	2.41	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:57:HIS:CE1	1:G:195:VAL:HG12	2.41	0.56
1:D:312:GLU:HA	1:F:311:ALA:HB1	1.87	0.56
1:H:390:GLU:HA	1:I:372:ILE:HG13	1.88	0.56
1:S:57:HIS:CE1	1:S:195:VAL:HG12	2.41	0.56
1:Q:272:GLU:CG	1:S:352:GLU:CG	2.83	0.56
1:A:223:ARG:CG	1:A:223:ARG:HH11	2.19	0.56
1:K:57:HIS:CE1	1:K:195:VAL:HG12	2.41	0.56
1:Q:57:HIS:CE1	1:Q: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:B:57:HIS:CE1	1:B:195:VAL:HG12	2.41	0.56
1:T:370:GLN:CB	1:T:374:MET:SD	2.94	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: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:L:297:GLN:CB	1:N:310:ARG:HG3	2.33	0.56
1:A:3:LEU:HD21	1:I:283:SER:CB	2.34	0.56
1:U:392:LYS:HD2	1:V:373:PRO:HD3	1.87	0.56
1:B:269:ILE:HG12	1:C:11:ILE:CD1	2.35	0.56
1:T:223:ARG:HH11	1:T:223:ARG:CG	2.19	0.56
1:X:223:ARG:CG	1:X:223:ARG:HH11	2.19	0.56
1:K:144:ASP:O	1:K:145:ASP:CB	2.45	0.55
1:W:456:ARG:NH1	2:W:700:FDP:O2P	2.28	0.55
1:W:223:ARG:CG	1:W:223:ARG:HH11	2.19	0.55
1:D:311:ALA:HB1	1:F:312:GLU:HA	1.88	0.55
1:U:370:GLN:CB	1:U:374:MET:SD	2.94	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:E:223:ARG:CG	1:E:223:ARG:HH11	2.19	0.55
1:P:57:HIS:CE1	1:P: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:Q:9:LEU:HB2	1:S:280:ILE:HD11	1.88	0.55
1:H:57:HIS:CE1	1:H:195:VAL:HG12	2.41	0.55
1:D:57:HIS:CE1	1:D:195:VAL:HG12	2.41	0.55
1:W:57:HIS:CE1	1:W:195:VAL:HG12	2.41	0.55
1:N:446:LYS:C	1:N:446:LYS:CD	2.72	0.55

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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:147:ILE:HG22	1:L:169:HIS:CD2	2.42	0.54
1:D:147:ILE:HG22	1:D:169:HIS:CD2	2.42	0.54
1:Q:223:ARG:HH11	1:Q:223:ARG:CG	2.19	0.54
1:V:147:ILE:HG22	1:V:169:HIS:CD2	2.42	0.54
1:Q:147:ILE:HG22	1:Q:169:HIS:CD2	2.42	0.54
1:X:49:ARG:NE	1:X:83:ASP:OD2	2.33	0.54
1:G:372:ILE:HD12	1:G:374:MET:HG2	1.89	0.54
1:O:372:ILE:HD12	1:O:374:MET:HG2	1.89	0.54
1:A:53:SER:HA	1:A:85:LYS:HG3	1.89	0.54
1:O:147:ILE:HG22	1:O:169:HIS:CD2	2.42	0.54
1:A:147:ILE:HG22	1:A:169:HIS:CD2	2.42	0.54
1:J:372:ILE:HD12	1:J:374:MET:HG2	1.89	0.54
1:R:270:PRO:CG	1:R:273:LYS:HE2	2.23	0.54
1:K:372:ILE:HD12	1:K:374:MET:HG2	1.89	0.54
1:V:272:GLU:HG3	1:X:352:GLU:CG	2.37	0.54
1:L:284:LYS:HG3	1:N:7:LEU:HD21	1.89	0.54
1:J:53:SER:HA	1:J:85:LYS:HG3	1.89	0.54
1:K:53:SER:HA	1:K:85:LYS:HG3	1.89	0.54
1:T:147:ILE:HG22	1:T:169:HIS:CD2	2.42	0.54
1:C:147:ILE:HG22	1:C:169:HIS:CD2	2.42	0.54
1:V:276:VAL:O	1:V:280:ILE:CD1	2.54	0.54
1:E:11:ILE:HG12	1:E:12:PHE:CE2	2.40	0.54
1:R:456:ARG:NH1	2:R:700:FDP:O2P	2.34	0.54
1:Q:11:ILE:HB	1:S:273:LYS:CG	2.37	0.54
1:B:147:ILE:HG22	1:B:169:HIS:CD2	2.42	0.54
1:M:147:ILE:HG22	1:M:169:HIS:CD2	2.42	0.54
1:V:273:LYS:HD3	1:X:11:ILE:O	2.08	0.54
1:K:390:GLU:HG2	1:L:374:MET:HE2	1.89	0.54
1:K:223:ARG:CG	1:K:223:ARG:HH11	2.19	0.54
1:O:223:ARG:CG	1:O:223:ARG:HH11	2.19	0.54
1:T:53:SER:HA	1:T:85:LYS:HG3	1.89	0.54
1:O:53:SER:HA	1:O:85:LYS:HG3	1.89	0.54
1:U:53:SER:HA	1:U:85:LYS:HG3	1.89	0.54
1:S:147:ILE:HG22	1:S:169:HIS:CD2	2.42	0.54
1:H:9:LEU:O	1:J:280:ILE:HD11	2.07	0.54
1:V:279:LYS:HB3	1:X:6:ASN:CG	2.28	0.54
1:C:373:PRO:HB3	1:P:391:THR:CA	2.38	0.54
1:I:144:ASP:O	1:I:145:ASP:CB	2.45	0.54
1:H:223:ARG:HH11	1:H:223:ARG:CG	2.19	0.54
1:F:193:ASP:O	1:F:197:LEU:N	2.38	0.54
1:J:147:ILE:HG22	1:J:169:HIS:CD2	2.42	0.54
1:E:472:THR:CG2	1:E:498:GLU:HA	2.18	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:270:PRO:CG	1:V:273:LYS:HE2	2.24	0.54
1:J:456:ARG:NH1	2:J:700:FDP:O2P	2.34	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:S:53:SER:HA	1:S:85:LYS:HG3	1.89	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:G:147:ILE:HG22	1:G:169:HIS:CD2	2.42	0.54
1:F:147:ILE:HG22	1:F:169:HIS:CD2	2.42	0.54
1:R:49:ARG:NE	1:R:83:ASP:OD2	2.33	0.54
1:X:472:THR:CG2	1:X:498:GLU:HA	2.18	0.54
1:V:276:VAL:CG1	1:X:9:LEU:HB3	2.37	0.54
1:Q:283:SER:CB	1:S:3:LEU:HD21	2.38	0.54
1:E:372:ILE:HD12	1:E:374:MET:HG2	1.89	0.54
1:Q:273:LYS:HB3	1:S:11:ILE:HB	1.88	0.54
1:H:270:PRO:HB2	1:H:273:LYS:HD2	1.90	0.54
1:W:53:SER:HA	1:W:85:LYS:HG3	1.89	0.54
1:P:53:SER:HA	1:P:85:LYS:HG3	1.89	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:V:11:ILE:HG12	1:V:12:PHE:CE2	2.40	0.54
1:B:273:LYS:HG2	1:C:11:ILE:O	2.07	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:H:11:ILE:CD1	1:J:269:ILE:HG12	2.38	0.53
1:U:297:GLN:OE1	1:W:310:ARG:NH2	2.41	0.53
1:R:273:LYS:CD	1:T:11:ILE:HB	2.39	0.53
1:L:276:VAL:HG13	1:N:9:LEU:HB3	1.90	0.53
1:S:223:ARG:CG	1:S:223:ARG:HH11	2.19	0.53
1:I:195:VAL:HG22	1:N:496:LEU:CG	2.36	0.53
1:C:270:PRO:HB2	1:C:273:LYS:HD2	1.90	0.53
1:A:270:PRO:HG2	1:A:273:LYS:CE	2.38	0.53
1:E:53:SER:HA	1:E:85:LYS:HG3	1.89	0.53
1:E:147:ILE:HG22	1:E:169:HIS:CD2	2.42	0.53
1:O:272:GLU:O	1:P:352:GLU:HG2	2.08	0.53
1:K:147:ILE:HG22	1:K:169:HIS:CD2	2.42	0.53
1:O:12:PHE:HZ	1:P:242:HIS:CE1	2.21	0.53
1:F:390:GLU:O	1:G:373:PRO:CB	2.56	0.53
1:W:373:PRO:HB3	1:X:391:THR:C	2.28	0.53
1:L:229:LYS:CD	1:S:487:GLY:HA2	2.38	0.53
1:B:270:PRO:HB2	1:B:273:LYS:HD2	1.90	0.53
1:I:53:SER:HA	1:I:85:LYS:HG3	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:472:THR:CG2	1:R:498:GLU:HA	2.18	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: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:U:494:ILE:HD12	1:V:376:ALA:HB1	1.89	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:L:223:ARG:CG	1:L:223:ARG:HH11	2.19	0.53
1:D:270:PRO:HG2	1:D:273:LYS:CE	2.38	0.53
1:B:297:GLN:CD	1:C:310:ARG:HG2	2.26	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:223:ARG:CG	1:G:223:ARG:HH11	2.19	0.53
1:F:483:HIS:NE2	1:G:483:HIS:HD2	2.07	0.53
1:O:472:THR:CG2	1:O:498:GLU:HA	2.18	0.53
1:R:273:LYS:CG	1:T:11:ILE:HB	2.39	0.53
1:Q:270:PRO:HB2	1:Q:273:LYS:HD2	1.90	0.53
1:R:193:ASP:O	1:R:197:LEU:N	2.38	0.53
1:K:270:PRO:HG2	1:K:273:LYS:CE	2.38	0.53
1:O:270:PRO:HB2	1:O:273:LYS:HD2	1.90	0.53
1:G:53:SER:HA	1:G:85:LYS:HG3	1.89	0.53
1:L:310:ARG:CG	1:N:297:GLN:HB2	2.37	0.53
1:Q:352:GLU:HB2	1:S:272:GLU:HG3	1.89	0.53
1:P:472:THR:CG2	1:P:498:GLU:HA	2.18	0.53
1:B:372:ILE:HD12	1:B:374:MET:HG2	1.89	0.53
1:M:392:LYS:HD2	1:N:373:PRO:HD3	1.91	0.53
1:H:53:SER:HA	1:H:85:LYS:HG3	1.89	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:C:89:ILE:CG2	1:C:177:VAL:HG22	2.39	0.53
1:P:89:ILE:CG2	1:P:177:VAL:HG22	2.39	0.53
1:B:297:GLN:CB	1:C:310:ARG:HG2	2.38	0.53
1:O:311:ALA:HB1	1:P:312:GLU:CA	2.26	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:K:89:ILE:CG2	1:K:177:VAL:HG22	2.39	0.53
1:N:89:ILE:CG2	1:N:177:VAL:HG22	2.39	0.53
1:S:89:ILE:CG2	1:S:177:VAL:HG22	2.39	0.53
1:D:89:ILE:CG2	1:D: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	Distance(Å)	Clash(Å)
1:H:296:THR:HG22	1:H:297:GLN:CG	2.39	0.53
1:R:270:PRO:O	1:R:273:LYS:HB2	2.09	0.53
1:B:297:GLN:HB2	1:C:310:ARG:CB	2.39	0.53
1:C:193:ASP:O	1:C:197:LEU:N	2.38	0.53
1:A:270:PRO:HB2	1:A:273:LYS:HD2	1.90	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:M:240:GLU:HB3	1:M:264:ASP:HB2	1.91	0.53
1:B:89:ILE:CG2	1:B:177:VAL:HG22	2.39	0.53
1:F:89:ILE:CG2	1:F:177:VAL:HG22	2.39	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:J:240:GLU:HB3	1:J:264:ASP:HB2	1.91	0.53
1:B:3:LEU:HD13	1:C:369:LEU:HD12	1.90	0.53
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:L:276:VAL:HG13	1:N:9:LEU:CB	2.39	0.52
1:A:372:ILE:HD12	1:A:374:MET:HG2	1.89	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:A:240:GLU:HB3	1:A:264:ASP:HB2	1.91	0.52
1:C:390:GLU:HG2	1:P:372:ILE:HD11	1.91	0.52
1:L:273:LYS:CD	1:N:11:ILE:HB	2.39	0.52
1:N:193:ASP:O	1:N:197:LEU:N	2.38	0.52
1:C:270:PRO:HG2	1:C:273:LYS:CE	2.38	0.52
1:C:53:SER:HA	1:C:85:LYS:HG3	1.90	0.52
1:M:53:SER:HA	1:M:85:LYS:HG3	1.89	0.52
1:S:240:GLU:HB3	1:S:264:ASP:HB2	1.91	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:S:372:ILE:CG1	1:T:390:GLU:CB	2.87	0.52
1:H:372:ILE:HD12	1:H:374:MET:CG	2.38	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:U:49:ARG:NE	1:U:83:ASP:OD2	2.33	0.52
1:I:89:ILE:CG2	1:I:177:VAL:HG22	2.39	0.52
1:X:89:ILE:CG2	1:X:177:VAL:HG22	2.39	0.52
1:W:240:GLU:HB3	1:W:264:ASP:HB2	1.91	0.52
1:V:270:PRO:O	1:V:273:LYS:HB2	2.09	0.52
1:H:352:GLU:HG2	1:J:272:GLU:HB2	1.92	0.52
1:M:223:ARG:HH11	1:M:223:ARG:CG	2.19	0.52
1:M:193:ASP:O	1:M:197:LEU:N	2.38	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:193:ASP:O	1:X:197:LEU:N	2.38	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:V:240:GLU:HB3	1:V:264:ASP:HB2	1.91	0.52
1:H:270:PRO:HG2	1:H:273:LYS:CE	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:V:287:VAL:HG23	1:X:3:LEU:CD2	2.40	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:Q:471:GLN:O	1:Q:497:VAL:CG2	2.58	0.52
1:U:471:GLN:O	1:U:497:VAL:CG2	2.58	0.52
1:V:280:ILE:HA	1:X:6:ASN:HB3	1.90	0.52
1:J:372:ILE:HD11	1:J:374:MET:HE1	1.92	0.52
1:H:391:THR:HA	1:I:373:PRO:HB3	1.91	0.52
1:M:373:PRO:CB	1:N:391:THR:HA	2.39	0.52
1:S:390:GLU:O	1:T:373:PRO:HB3	2.09	0.52
1:D:12:PHE:HZ	1:F:242:HIS:HE1	1.51	0.52
1:J:223:ARG:CG	1:J:223:ARG:HH11	2.19	0.52
1:O:193:ASP:O	1:O:197:LEU:N	2.38	0.52
1:P:193:ASP:O	1:P:197:LEU:N	2.38	0.52
1:D:270:PRO:HB2	1:D:273:LYS:HD2	1.90	0.52
1:O:270:PRO:HG2	1:O:273:LYS:HD2	1.92	0.52
1:X:240:GLU:HB3	1:X:264:ASP:HB2	1.91	0.52
1:U:240:GLU:HB3	1:U:264:ASP:HB2	1.91	0.52
1:B:193:ASP:O	1:B:197:LEU:N	2.38	0.52
1:H:193:ASP:O	1:H:197:LEU:N	2.38	0.52
1:A:89:ILE:CG2	1:A:177:VAL:HG22	2.39	0.52
1:Q:89:ILE:CG2	1:Q:177:VAL:HG22	2.39	0.52
1:H:89:ILE:CG2	1:H:177:VAL:HG22	2.39	0.52
1:N:240:GLU:HB3	1:N:264:ASP:HB2	1.91	0.52
1:V:89:ILE:CG2	1:V:177:VAL:HG22	2.39	0.52
1:H:240:GLU:HB3	1:H:264:ASP:HB2	1.91	0.52
1:M:471:GLN:O	1:M:497:VAL:CG2	2.58	0.52
1:C:471:GLN:O	1:C:497:VAL:CG2	2.58	0.52
1:X:471:GLN:O	1:X:497:VAL:CG2	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:O:310:ARG:CZ	1:P:297:GLN:OE1	2.58	0.52
1:W:471:GLN:O	1:W:497:VAL:CG2	2.58	0.52
1:O:471:GLN:O	1:O:497:VAL:CG2	2.58	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:373:PRO:HB3	1:R:390:GLU:O	2.09	0.52
1:U:272:GLU:C	1:W:352:GLU:HG2	2.29	0.52
1:S:193:ASP:O	1:S:197:LEU:N	2.38	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:D:471:GLN:O	1:D:497:VAL:CG2	2.58	0.51
1:N:471:GLN:O	1:N:497:VAL:CG2	2.58	0.51
1:E:456:ARG:HH22	2:E:700:FDP:P1	2.33	0.51
1:L:193:ASP:O	1:L:197:LEU:N	2.38	0.51
1:G:240:GLU:HB3	1:G:264:ASP:HB2	1.91	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:R:471:GLN:O	1:R:497:VAL:CG2	2.58	0.51
1:L:471:GLN:O	1:L:497:VAL:CG2	2.58	0.51
1:L:270:PRO:O	1:L:273:LYS:HB2	2.09	0.51
1:B:280:ILE:HG12	1:C:6:ASN:O	2.10	0.51
1:B:223:ARG:CG	1:B:223:ARG:HH11	2.19	0.51
1:R:223:ARG:CG	1:R:223:ARG:HH11	2.19	0.51
1:D:270:PRO:HG2	1:D:273:LYS:HD2	1.92	0.51
1:C:240:GLU:HB3	1:C:264:ASP:HB2	1.91	0.51
1:R:240:GLU:HB3	1:R:264:ASP:HB2	1.91	0.51
1:W:188:ALA:HA	1:W:218:GLN:OE1	2.11	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:V:471:GLN:O	1:V:497:VAL:CG2	2.58	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:T:471:GLN:O	1:T:497:VAL:CG2	2.58	0.51
1:H:471:GLN:O	1:H:497:VAL:CG2	2.58	0.51
1:B:297:GLN:OE1	1:C:310:ARG:CZ	2.58	0.51
1:H:270:PRO:HG2	1:H:273:LYS:HD2	1.92	0.51
1:E:89:ILE:CG2	1:E:177:VAL:HG22	2.39	0.51
1:P:240:GLU:HB3	1:P:264:ASP:HB2	1.92	0.51
1:B:471:GLN:O	1:B:497:VAL:CG2	2.58	0.51
1:P:471:GLN:O	1:P:497:VAL:CG2	2.58	0.51
1:L:372:ILE:HD12	1:L:374:MET:CG	2.41	0.51
1:Q:279:LYS:HE3	1:S:6:ASN:OD1	2.10	0.51
1:V:352:GLU:OE1	1:X:273:LYS:NZ	2.43	0.51
1:N:456:ARG:HH22	2:N:700:FDP:P1	2.34	0.51
1:V:223:ARG:CG	1:V:223:ARG:HH11	2.19	0.51
1:I:193:ASP:O	1:I:197:LEU:N	2.38	0.51
1:M:188:ALA:HA	1:M:218:GLN:OE1	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:S:471:GLN:O	1:S:497:VAL:CG2	2.58	0.51
1:N:456:ARG:NH1	2:N:700:FDP:O2P	2.34	0.51
1:Q:3:LEU:HD23	1:S:283:SER:CB	2.41	0.51
1:C:491:GLN:HG3	1:P:491:GLN:HG3	1.93	0.51
1:I:188:ALA:HA	1:I:218:GLN:OE1	2.11	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:B:270:PRO:HG2	1:B:273:LYS:HD2	1.92	0.51
1:B:103:ARG:CB	1:G:58:GLU:OE1	2.59	0.51
1:B:492:THR:HG22	1:O:492:THR:HG22	1.92	0.51
1:M:483:HIS:NE2	1:N:483:HIS:HD2	2.09	0.51
1:T:240:GLU:HB3	1:T:264:ASP:HB2	1.91	0.51
1:P:211:SER:HA	1:P:238:LYS:HD3	1.93	0.51
1:U:372:ILE:HG23	1:V:390:GLU:C	2.29	0.51
1:I:471:GLN:O	1:I:497:VAL:CG2	2.58	0.51
1:W:372:ILE:CG1	1:X:390:GLU:O	2.58	0.51
1:B:276:VAL:HG13	1:C:9:LEU:HB3	1.93	0.51
1:C:456:ARG:NH1	2:C:700:FDP:O2P	2.34	0.51
1:F:240:GLU:HB3	1:F:264:ASP:HB2	1.91	0.51
1:Q:240:GLU:HB3	1:Q:264:ASP:HB2	1.91	0.51
1:D:188:ALA:HA	1:D:218:GLN:OE1	2.11	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:P:372:ILE:HD12	1:P:374:MET:CG	2.40	0.51
1:E:471:GLN:O	1:E:497:VAL:CG2	2.58	0.51
1:J:471:GLN:O	1:J:497:VAL:CG2	2.58	0.51
1:I:270:PRO:HD2	1:I:273:LYS:HD2	1.93	0.51
1:D:193:ASP:O	1:D:197:LEU:N	2.38	0.51
1:V:193:ASP:O	1:V:196:ASP:N	2.44	0.51
1:J:193:ASP:O	1:J:196:ASP:N	2.44	0.51
1:E:193:ASP:O	1:E:196:ASP:N	2.44	0.51
1:H:193:ASP:O	1:H:196:ASP:N	2.44	0.51
1:K:240:GLU:HB3	1:K:264:ASP:HB2	1.91	0.51
1:V:49:ARG:NE	1:V:83:ASP:OD2	2.33	0.51
1:J:49:ARG:NE	1:J:83:ASP:OD2	2.33	0.51
1:C:211:SER:HA	1:C:238:LYS:HD3	1.93	0.51
1:D:211:SER:HA	1:D:238:LYS:HD3	1.93	0.51
1:K:211:SER:HA	1:K:238:LYS:HD3	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:49:ARG:NE	1:L:83:ASP:OD2	2.33	0.51
1:V:284:LYS:HG2	1:X:7:LEU:HD22	1.86	0.51
1:K:188:ALA:HA	1:K:218:GLN:OE1	2.11	0.51
1:H:373:PRO:HB3	1:I:391:THR:HA	1.92	0.51
1:E:269:ILE:HG12	1:G:11:ILE:HD12	1.93	0.51
1:V:270:PRO:HD2	1:V:273:LYS:HD2	1.93	0.51
1:R:456:ARG:HH22	2:R:700:FDP:P1	2.34	0.51
1:Q:193:ASP:O	1:Q:196:ASP:N	2.44	0.51
1:U:352:GLU:HG2	1:W:272:GLU:CG	2.40	0.51
1:I:147:ILE:HG21	1:I:169:HIS:CD2	2.46	0.51
1:S:147:ILE:HG21	1:S:169:HIS:NE2	2.26	0.51
1:M:483:HIS:CD2	1:N:483:HIS:CD2	2.98	0.51
1:U:211:SER:HA	1:U:238:LYS:HD3	1.93	0.51
1:I:240:GLU:HB3	1:I:264:ASP:HB2	1.91	0.51
1:O:188:ALA:HA	1:O:218:GLN:OE1	2.11	0.51
1:O:11:ILE:O	1:P:273:LYS:CE	2.56	0.51
1:Q:270:PRO:O	1:Q:273:LYS:HB2	2.11	0.51
1:B:272:GLU:HG2	1:C:352:GLU:HG2	1.93	0.51
1:E:456:ARG:NH1	2:E:700:FDP:O2P	2.34	0.51
1:Q:456:ARG:HH22	2:Q:700:FDP:P1	2.34	0.51
1:B:270:PRO:O	1:B:273:LYS:HB2	2.11	0.51
1:M:193:ASP:O	1:M:196:ASP:N	2.44	0.51
1:S:193:ASP:O	1:S:196:ASP:N	2.44	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:V:193:ASP:O	1:V:197:LEU:N	2.38	0.51
1:X:193:ASP:O	1:X:196:ASP:N	2.44	0.51
1:C:270:PRO:O	1:C:273:LYS:HB2	2.11	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:F:483:HIS:HD2	1:G:483:HIS:NE2	2.08	0.51
1:S:49:ARG:NE	1:S:83:ASP:OD2	2.33	0.51
1:O:240:GLU:HB3	1:O:264:ASP:HB2	1.91	0.51
1:W:211:SER:HA	1:W:238:LYS:HD3	1.93	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:U:188:ALA:HA	1:U:218:GLN:OE1	2.11	0.50
1:E:188:ALA:HA	1:E:218:GLN:OE1	2.11	0.50
1:K:471:GLN:O	1:K:497:VAL:CG2	2.58	0.50
1:P:195:VAL:CG2	1:U:496:LEU:HD21	2.40	0.50
1:K:193:ASP:O	1:K:196:ASP:N	2.44	0.50
1:W:193:ASP:O	1:W:197:LEU:N	2.38	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:193:ASP:O	1:U:196:ASP:N	2.44	0.50
1:D:193:ASP:O	1:D:196:ASP:N	2.44	0.50
1:O:270:PRO:O	1:O:273:LYS:HB2	2.11	0.50
1:E:283:SER:CB	1:G:3:LEU:CD2	2.89	0.50
1:O:147:ILE:HG21	1:O:169:HIS:NE2	2.26	0.50
1:V:147:ILE:HG21	1:V:169:HIS:NE2	2.26	0.50
1:E:147:ILE:HG21	1:E:169:HIS:NE2	2.27	0.50
1:B:310:ARG:HG2	1:C:297:GLN:HB2	1.92	0.50
1:R:188:ALA:HA	1:R:218:GLN:OE1	2.11	0.50
1:P:188:ALA:HA	1:P:218:GLN:OE1	2.11	0.50
1:H:311:ALA:HA	1:J:315:ASP:HB2	1.93	0.50
1:E:270:PRO:HD2	1:E:273:LYS:HD2	1.93	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:J:472:THR:CG2	1:J:498:GLU:HA	2.18	0.50
1:C:456:ARG:HH22	2:C:700:FDP:P1	2.34	0.50
1:J:456:ARG:HH22	2:J:700:FDP:P1	2.34	0.50
1:O:193:ASP:O	1:O:196:ASP:N	2.44	0.50
1:L:193:ASP:O	1:L:196:ASP:N	2.44	0.50
1:F:193:ASP:O	1:F:196:ASP:N	2.44	0.50
1:N:193:ASP:O	1:N:196:ASP:N	2.44	0.50
1:R:193:ASP:O	1:R:196:ASP:N	2.44	0.50
1:B:193:ASP:O	1:B:196:ASP:N	2.44	0.50
1:T:193:ASP:O	1:T:196:ASP:N	2.44	0.50
1:A:270:PRO:O	1:A:273:LYS:HB2	2.11	0.50
1:F:147:ILE:HG21	1:F:169:HIS:NE2	2.26	0.50
1:P:147:ILE:HG21	1:P:169:HIS:NE2	2.27	0.50
1:N:147:ILE:HG21	1:N:169:HIS:NE2	2.27	0.50
1:T:147:ILE:HG21	1:T:169:HIS:NE2	2.27	0.50
1:X:147:ILE:HG21	1:X:169:HIS:CD2	2.47	0.50
1:C:147:ILE:HG21	1:C:169:HIS:NE2	2.27	0.50
1:L:240:GLU:HB3	1:L:264:ASP:HB2	1.91	0.50
1:I:211:SER:HA	1:I:238:LYS:HD3	1.93	0.50
1:N:211:SER:HA	1:N:238:LYS:HD3	1.93	0.50
1:H:49:ARG:NE	1:H:83:ASP:OD2	2.33	0.50
1:M:211:SER:HA	1:M:238:LYS:HD3	1.93	0.50
1:J:188:ALA:HA	1:J:218:GLN:OE1	2.11	0.50
1:R:270:PRO:HD2	1:R:273:LYS:HD2	1.93	0.50
1:E:273:LYS:HG2	1:G:11:ILE:HB	1.92	0.50
1:C:372:ILE:HD11	1:C:374:MET:HE1	1.92	0.50
1:A:456:ARG:HH22	2:A:700:FDP:P1	2.33	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:193:ASP:O	1:P:196:ASP:N	2.44	0.50
1:D:270:PRO:O	1:D:273:LYS:HB2	2.11	0.50
1:B:147:ILE:HG21	1:B:169:HIS:CD2	2.46	0.50
1:A:147:ILE:HG21	1:A:169:HIS:NE2	2.27	0.50
1:F:147:ILE:HG21	1:F:169:HIS:CD2	2.46	0.50
1:S:211:SER:HA	1:S:238:LYS:HD3	1.93	0.50
1:H:211:SER:HA	1:H:238:LYS:HD3	1.93	0.50
1:A:211:SER:HA	1:A:238:LYS:HD3	1.93	0.50
1:V:211:SER:HA	1:V:238:LYS:HD3	1.93	0.50
1:N:188:ALA:HA	1:N:218:GLN:OE1	2.11	0.50
1:V:280:ILE:CD1	1:X:9:LEU:HB2	2.40	0.50
1:I:472:THR:CG2	1:I:498:GLU:HA	2.18	0.50
1:D:456:ARG:HH22	2:D:700:FDP:P1	2.34	0.50
1:W:193:ASP:O	1:W:196:ASP:N	2.44	0.50
1:J:193:ASP:CA	1:J:196:ASP:HB2	2.41	0.50
1:U:270:PRO:O	1:U:273:LYS:HB2	2.11	0.50
1:U:147:ILE:HG21	1:U:169:HIS:CD2	2.46	0.50
1:Q:147:ILE:HG21	1:Q:169:HIS:NE2	2.26	0.50
1:W:147:ILE:HG21	1:W:169:HIS:NE2	2.26	0.50
1:N:147:ILE:HG21	1:N:169:HIS:CD2	2.46	0.50
1:D:240:GLU:HB3	1:D:264:ASP:HB2	1.91	0.50
1:G:188:ALA:HA	1:G:218:GLN:OE1	2.11	0.50
1:U:11:ILE:O	1:W:273:LYS:CG	2.60	0.50
1:H:312:GLU:CA	1:J:311:ALA:CB	2.71	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:T:193:ASP:CA	1:T:196:ASP:HB2	2.42	0.50
1:B:147:ILE:HG21	1:B:169:HIS:NE2	2.27	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:R:147:ILE:HG21	1:R:169:HIS:NE2	2.26	0.50
1:B:211:SER:HA	1:B:238:LYS:HD3	1.93	0.50
1:O:352:GLU:HG2	1:P:272:GLU:O	2.11	0.50
1:C:188:ALA:HA	1:C:218:GLN:OE1	2.11	0.50
1:U:263:GLY:HA2	1:W:310:ARG:NH1	2.16	0.50
1:K:372:ILE:HD11	1:L:390:GLU:HG2	1.93	0.50
1:X:372:ILE:HD11	1:X:374:MET:HE2	1.93	0.50
1:K:297:GLN:OE1	1:M:310:ARG:NH2	2.45	0.50
1:B:456:ARG:HH22	2:B:700:FDP:P1	2.34	0.50
1:O:147:ILE:HG21	1:O:169:HIS:CD2	2.46	0.50
1:J:147:ILE:HG21	1:J:169:HIS:NE2	2.26	0.50
1:J:147:ILE:HG21	1:J:169:HIS:CD2	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:R:211:SER:HA	1:R:238:LYS:HD3	1.93	0.50
1:H:188:ALA:HA	1:H:218:GLN:OE1	2.11	0.50
1:B:472:THR:CG2	1:B:498:GLU:HA	2.18	0.50
1:I:11:ILE:HG13	1:I:12:PHE:HD2	1.72	0.50
1:V:11:ILE:HG12	1:V:12:PHE:CD2	2.47	0.50
1:L:7:LEU:CD2	1:N:284:LYS:HG3	2.42	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:270:PRO:O	1:H:273:LYS:HB2	2.11	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: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:P:372:ILE:HD12	1:P:374:MET:HG3	1.92	0.50
1:G:147:ILE:HG21	1:G:169:HIS:NE2	2.27	0.50
1:S:51:ASN:HA	1:S:83:ASP:HB3	1.94	0.50
1:G:211:SER:HA	1:G:238:LYS:HD3	1.93	0.50
1:Q:491:GLN:HG3	1:R:491:GLN:HG3	1.93	0.50
1:A:49:ARG:NE	1:A:83:ASP:OD2	2.33	0.50
1:L:211:SER:HA	1:L:238:LYS:HD3	1.93	0.50
1:Q:211:SER:HA	1:Q:238:LYS:HD3	1.93	0.50
1:W:472:THR:CG2	1:W:498:GLU:HA	2.18	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:I:193:ASP:O	1:I:196:ASP:N	2.44	0.50
1:V:147:ILE:HG21	1:V:169:HIS:CD2	2.46	0.50
1:K:147:ILE:HG21	1:K:169:HIS:NE2	2.27	0.50
1:X:147:ILE:HG21	1:X:169:HIS:NE2	2.27	0.50
1:C:51:ASN:HA	1:C:83:ASP:HB3	1.94	0.50
1:B:51:ASN:HA	1:B:83:ASP:HB3	1.94	0.50
1:D:49:ARG:NE	1:D:83:ASP:OD2	2.33	0.50
1:J:211:SER:HA	1:J:238:LYS:HD3	1.93	0.50
1:Q:188:ALA:HA	1:Q:218:GLN:OE1	2.11	0.49
1:I:12:PHE:N	1:I:12:PHE:CD2	2.79	0.49
1:Q:193:ASP:CA	1:Q:196:ASP:HB2	2.42	0.49
1:U:352:GLU:HB2	1:W:272:GLU:HG3	1.94	0.49
1:K:147:ILE:HG21	1:K:169:HIS:CD2	2.47	0.49
1:T:147:ILE:HG21	1:T:169:HIS:CD2	2.47	0.49
1:F:211:SER:HA	1:F:238:LYS:HD3	1.93	0.49
1:U:456:ARG:HH22	2:U:700:FDP:P1	2.34	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:456:ARG:NH1	2:U:700:FDP:O2P	2.35	0.49
1:G:193:ASP:O	1:G:196:ASP:N	2.44	0.49
1:U:383:SER:HB2	1:V:383:SER:CB	2.42	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:R:147:ILE:HG21	1:R:169:HIS:CD2	2.46	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:N:51:ASN:HA	1:N:83:ASP:HB3	1.94	0.49
1:W:390:GLU:OE1	1:X:379:ALA:CA	2.60	0.49
1:F:456:ARG:HH22	2:F:700:FDP:P1	2.34	0.49
1:A:147:ILE:HG21	1:A:169:HIS:CD2	2.46	0.49
1:H:51:ASN:HA	1:H:83:ASP:HB3	1.94	0.49
1:A:51:ASN:HA	1:A:83:ASP:HB3	1.95	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:Q:471:GLN:O	1:Q:497:VAL:HG22	2.13	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:R:11:ILE:HG12	1:R:12:PHE:CD2	2.47	0.49
1:X:270:PRO:O	1:X:273:LYS:HB2	2.12	0.49
1:U:270:PRO:HG2	1:U:273:LYS:HD2	1.92	0.49
1:H:147:ILE:HG21	1:H:169:HIS:CD2	2.46	0.49
1:W:147:ILE:HG21	1:W:169:HIS:CD2	2.46	0.49
1:L:147:ILE:HG21	1:L:169:HIS:NE2	2.27	0.49
1:I:49:ARG:NE	1:I:83:ASP:OD2	2.33	0.49
1:U:471:GLN:O	1:U:497:VAL:HG22	2.13	0.49
1:A:391:THR:O	1:J:373:PRO:HB3	2.11	0.49
1:L:12:PHE:CZ	1:N:242:HIS:NE2	2.80	0.49
1:B:270:PRO:HD2	1:B:273:LYS:HD3	1.95	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:Q:147:ILE:HG21	1:Q:169:HIS:CD2	2.46	0.49
1:P:147:ILE:HG21	1:P:169:HIS:CD2	2.46	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:E:51:ASN:HA	1:E:83:ASP:HB3	1.94	0.49
1:I:229:LYS:HD2	1:M:487:GLY:CA	2.41	0.49
1:C:471:GLN:O	1:C:497:VAL:HG22	2.13	0.49
1:E:372:ILE:HD11	1:E:374:MET:HE1	1.93	0.49
1:L:487:GLY:CA	1:S:229:LYS:CG	2.76	0.49
1:M:391:THR:HA	1:N:373:PRO:HB3	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:Q:7:LEU:CD2	1:S:284:LYS:HG3	2.43	0.49
1:Q:193:ASP:O	1:Q:197:LEU:N	2.38	0.49
1:G:147:ILE:HG21	1:G:169:HIS:CD2	2.47	0.49
1:U:147:ILE:HG21	1:U:169:HIS:NE2	2.26	0.49
1:E:147:ILE:HG21	1:E:169:HIS:CD2	2.46	0.49
1:G:19:ARG:NH1	1:G:21:ALA:O	2.46	0.49
1:A:19:ARG:NH1	1:A:21:ALA:O	2.46	0.49
1:V:19:ARG:NH1	1:V:21:ALA:O	2.46	0.49
1:B:471:GLN:O	1:B:497:VAL:HG22	2.13	0.49
1:T:471:GLN:O	1:T:497:VAL:HG22	2.13	0.49
1:N:270:PRO:O	1:N:273:LYS:HB2	2.12	0.49
1:T:270:PRO:O	1:T:273:LYS:HB2	2.12	0.49
1:F:193:ASP:CA	1:F:196:ASP:HB2	2.42	0.49
1:A:193:ASP:CA	1:A:196:ASP:HB2	2.41	0.49
1:V:482:ASP:H	1:V:490:ASN:HD21	1.61	0.49
1:I:147:ILE:HG21	1:I:169:HIS:NE2	2.26	0.49
1:C:147:ILE:HG21	1:C:169:HIS:CD2	2.47	0.49
1:U:51:ASN:HA	1:U:83:ASP:HB3	1.94	0.49
1:I:51:ASN:HA	1:I:83:ASP:HB3	1.94	0.49
1:H:19:ARG:NH1	1:H:21:ALA:O	2.46	0.49
1:L:3:LEU:CD2	1:N:283:SER:HB3	2.42	0.49
1:F:372:ILE:HD11	1:F:374:MET:HE1	1.94	0.49
1:S:471:GLN:O	1:S:497:VAL:HG22	2.13	0.49
1:V:471:GLN:O	1:V:497:VAL:HG22	2.13	0.49
1:H:311:ALA:HA	1:J:315:ASP:CB	2.43	0.49
1:O:471:GLN:O	1:O:497:VAL:HG22	2.13	0.49
1:G:471:GLN:O	1:G:497:VAL:HG22	2.13	0.49
1:H:352:GLU:CB	1:J:272:GLU:HB2	2.42	0.49
1:U:482:ASP:H	1:U:490:ASN:HD21	1.61	0.49
1:X:51:ASN:HA	1:X:83:ASP:HB3	1.94	0.49
1:V:51:ASN:HA	1:V:83:ASP:HB3	1.94	0.49
1:D:51:ASN:HA	1:D:83:ASP:HB3	1.94	0.49
1:F:51:ASN:HA	1:F:83:ASP:HB3	1.95	0.49
1:N:49:ARG:NE	1:N:83:ASP:OD2	2.33	0.49
1:K:51:ASN:HA	1:K:83:ASP:HB3	1.94	0.49
1:G:49:ARG:NE	1:G:83:ASP:OD2	2.33	0.49
1:C:216:ALA:CB	1:N:446:LYS:CE	2.81	0.49
1:V:276:VAL:C	1:V:280:ILE:HD12	2.33	0.49
1:F:391:THR:C	1:G:373:PRO:HB3	2.33	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:273:LYS:HB3	1:G:11:ILE:HB	1.95	0.49
1:S:482:ASP:H	1:S:490:ASN:HD21	1.61	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:N:482:ASP:H	1:N:490:ASN:HD21	1.61	0.49
1:W:51:ASN:HA	1:W:83:ASP:HB3	1.95	0.49
1:M:471:GLN:O	1:M:497:VAL:HG22	2.13	0.49
1:F:471:GLN:O	1:F:497:VAL:HG22	2.13	0.49
1:L:11:ILE:HG13	1:L:12:PHE:HD2	1.72	0.49
1:O:270:PRO:HD2	1:O:273:LYS:HD3	1.95	0.49
1:K:310:ARG:CG	1:M:297:GLN:HB2	2.43	0.49
1:U:352:GLU:HG2	1:W:272:GLU:O	2.13	0.49
1:M:482:ASP:H	1:M:490:ASN:HD21	1.61	0.49
1:L:482:ASP:H	1:L:490:ASN:HD21	1.61	0.49
1:A:12:PHE:CE2	1:I:242:HIS:CE1	3.00	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: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:J:471:GLN:O	1:J:497:VAL:HG22	2.13	0.48
1:G:270:PRO:O	1:G:273:LYS:HB2	2.12	0.48
1:U:310:ARG:CB	1:W:297:GLN:HB2	2.42	0.48
1:L:11:ILE:HG12	1:L:12:PHE:CD2	2.47	0.48
1:D:193:ASP:CA	1:D:196:ASP:HB2	2.41	0.48
1:W:482:ASP:H	1:W:490:ASN:HD21	1.61	0.48
1:C:482:ASP:H	1:C:490:ASN:HD21	1.61	0.48
1:D:482:ASP:H	1:D:490:ASN:HD21	1.61	0.48
1:G:51:ASN:HA	1:G:83:ASP:HB3	1.94	0.48
1:G:90:ARG:HD3	1:G:174:ARG:O	2.13	0.48
1:T:90:ARG:HD3	1:T:174:ARG:O	2.14	0.48
1:R:90:ARG:HD3	1:R:174:ARG:O	2.13	0.48
1:V:284:LYS:HG3	1:X:7:LEU:HD23	1.80	0.48
1:K:472:THR:CG2	1:K:498:GLU:HA	2.18	0.48
1:B:297:GLN:OE1	1:C:310:ARG:NH2	2.45	0.48
1:R:12:PHE:CD2	1:R:12:PHE:N	2.79	0.48
1:L:272:GLU:HB2	1:N:352:GLU:HG2	1.94	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:B:283:SER:CB	1:C:3:LEU:CD2	2.91	0.48
1:H:482:ASP:H	1:H:490:ASN:HD21	1.61	0.48
1:P:89:ILE:HG21	1:P:177:VAL:HG22	1.96	0.48
1:S:90:ARG:HD3	1:S:174:ARG:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:90:ARG:HD3	1:P:174:ARG:O	2.14	0.48
1:L:90:ARG:HD3	1:L:174:ARG:O	2.13	0.48
1:J:90:ARG:HD3	1:J:174:ARG:O	2.13	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:D:391:THR:C	1:E:373:PRO:HB3	2.34	0.48
1:B:272:GLU:HG3	1:C:352:GLU:CG	2.43	0.48
1:Q:3:LEU:CD2	1:S:283:SER:CB	2.91	0.48
1:A:482:ASP:H	1:A:490:ASN:HD21	1.61	0.48
1:E:482:ASP:H	1:E:490:ASN:HD21	1.61	0.48
1:K:89:ILE:HG21	1:K:177:VAL:HG22	1.96	0.48
1:I:89:ILE:HG21	1:I:177:VAL:HG22	1.96	0.48
1:M:89:ILE:HG21	1:M:177:VAL:HG22	1.96	0.48
1:O:51:ASN:HA	1:O:83:ASP:HB3	1.94	0.48
1:O:90:ARG:HD3	1:O:174:ARG:O	2.13	0.48
1:I:90:ARG:HD3	1:I:174:ARG:O	2.13	0.48
1:U:90:ARG:HD3	1:U:174:ARG:O	2.13	0.48
1:V:284:LYS:HE2	1:X:7:LEU:HD22	1.95	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:U:11:ILE:HB	1:W:273:LYS:HB3	1.93	0.48
1:R:273:LYS:CB	1:T:11:ILE:HB	2.43	0.48
1:M:90:ARG:HD3	1:M:174:ARG:O	2.13	0.48
1:H:90:ARG:HD3	1:H:174:ARG:O	2.13	0.48
1:F:90:ARG:HD3	1:F:174:ARG:O	2.13	0.48
1:T:19:ARG:NH1	1:T:21:ALA:O	2.46	0.48
1:U:19:ARG:NH1	1:U:21:ALA:O	2.46	0.48
1:T:51:ASN:HA	1:T:83:ASP:HB3	1.94	0.48
1:D:19:ARG:NH1	1:D:21:ALA:O	2.46	0.48
1:D:212:PHE:HD2	1:D:214:ARG:HH21	1.62	0.48
1:U:311:ALA:HB3	1:W:312:GLU:HG3	1.95	0.48
1:Q:270:PRO:HD2	1:Q:273:LYS:HD3	1.95	0.48
1:B:456:ARG:NH1	2:B:700:FDP:O2P	2.34	0.48
1:W:193:ASP:CA	1:W:196:ASP:HB2	2.42	0.48
1:R:482:ASP:H	1:R:490:ASN:HD21	1.61	0.48
1:A:89:ILE:HG21	1:A:177:VAL:HG22	1.96	0.48
1:V:89:ILE:HG21	1:V:177:VAL:HG22	1.96	0.48
1:J:51:ASN:HA	1:J:83:ASP:HB3	1.94	0.48
1:X:90:ARG:HD3	1:X:174:ARG:O	2.13	0.48
1:U:297:GLN:HB3	1:W:310:ARG:H	1.77	0.48
1:F:472:THR:CG2	1:F:498:GLU:HA	2.18	0.48
1:H:272:GLU:HG3	1:J:352:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:482:ASP:H	1:Q:490:ASN:HD21	1.61	0.48
1:W:90:ARG:HD3	1:W:174:ARG:O	2.13	0.48
1:H:483:HIS:CD2	1:I:483:HIS:CD2	3.01	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: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:J:19:ARG:NH1	1:J:21:ALA:O	2.46	0.48
1:E:212:PHE:HD2	1:E:214:ARG:HH21	1.62	0.48
1:Q:212:PHE:HD2	1:Q:214:ARG:HH21	1.62	0.48
1:C:390:GLU:O	1:P:372:ILE:HG13	2.14	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:Q:379:ALA:CB	1:R:390:GLU:OE1	2.62	0.48
1:Q:276:VAL:CG1	1:S:9:LEU:HB3	2.43	0.48
1:I:195:VAL:CG2	1:N:496:LEU:HG	2.43	0.48
1:V:9:LEU:CB	1:X:280:ILE:HD11	2.42	0.48
1:G:193:ASP:CA	1:G:196:ASP:HB2	2.41	0.48
1:F:89:ILE:HG21	1:F:177:VAL:HG22	1.96	0.48
1:H:89:ILE:HG21	1:H:177:VAL:HG22	1.96	0.48
1:E:90:ARG:HD3	1:E:174:ARG:O	2.13	0.48
1:V:212:PHE:HD2	1:V:214:ARG:HH21	1.62	0.48
1:X:212:PHE:HD2	1:X:214:ARG:HH21	1.62	0.48
1:D:471:GLN:O	1:D:497:VAL:HG22	2.13	0.48
1:S:372:ILE:HG23	1:T:390:GLU:C	2.33	0.48
1:S:372:ILE:CG1	1:T:390:GLU:CG	2.91	0.48
1:Q:297:GLN:CD	1:S:310:ARG:HG2	2.24	0.48
1:W:471:GLN:O	1:W:497:VAL:HG22	2.13	0.48
1:X:471:GLN:O	1:X:497:VAL:HG22	2.13	0.48
1:M:373:PRO:CA	1:N:390:GLU:O	2.46	0.48
1:K:272:GLU:CG	1:M:352:GLU:HG2	2.44	0.48
1:I:193:ASP:CA	1:I:196:ASP:HB2	2.41	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:U:89:ILE:HG21	1:U:177:VAL:HG22	1.96	0.48
1:M:49:ARG:NE	1:M:83:ASP:OD2	2.33	0.48
1:B:402:THR:OG1	1:B:404:ARG:HB2	2.14	0.48
1:N:90:ARG:HD3	1:N:174:ARG:O	2.13	0.48
1:M:212:PHE:HD2	1:M:214:ARG:HH21	1.62	0.48
1:P:270:PRO:O	1:P:273:LYS:HB2	2.14	0.48
1:F:390:GLU:HG2	1:G:372:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:270:PRO:O	1:F:273:LYS:HB2	2.14	0.48
1:I:402:THR:OG1	1:I:404:ARG:HB2	2.14	0.48
1:V:12:PHE:CD2	1:V:12:PHE:N	2.79	0.48
1:G:193:ASP:O	1:G:196:ASP:HB2	2.14	0.48
1:Q:311:ALA:CB	1:S:312:GLU:HA	2.43	0.48
1:J:482:ASP:H	1:J:490:ASN:HD21	1.61	0.48
1:T:89:ILE:HG21	1:T:177:VAL:HG22	1.96	0.48
1:O:49:ARG:NE	1:O:83:ASP:OD2	2.33	0.48
1:T:49:ARG:NE	1:T:83:ASP:OD2	2.33	0.48
1:X:19:ARG:NH1	1:X:21:ALA:O	2.46	0.48
1:V:402:THR:OG1	1:V:404:ARG:HB2	2.14	0.48
1:J:402:THR:OG1	1:J:404:ARG:HB2	2.14	0.48
1:E:402:THR:OG1	1:E:404:ARG:HB2	2.14	0.48
1:J:212:PHE:HD2	1:J:214:ARG:HH21	1.62	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:N:471:GLN:O	1:N:497:VAL:HG22	2.13	0.48
1:R:297:GLN:CD	1:T:310:ARG:HG2	2.34	0.48
1:M:193:ASP:O	1:M:196:ASP:HB2	2.14	0.48
1:O:193:ASP:O	1:O:196:ASP:HB2	2.14	0.48
1:S:193:ASP:O	1:S:196:ASP:HB2	2.14	0.48
1:K:19:ARG:NH1	1:K:21:ALA:O	2.46	0.48
1:R:19:ARG:NH1	1:R:21:ALA:O	2.46	0.48
1:P:51:ASN:HA	1:P:83:ASP:HB3	1.94	0.48
1:P:402:THR:OG1	1:P:404:ARG:HB2	2.14	0.48
1:J:270:PRO:O	1:J:273:LYS:HB2	2.14	0.47
1:H:311:ALA:O	1:J:311:ALA:O	2.31	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: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:X:193:ASP:O	1:X:196:ASP:HB2	2.14	0.47
1:D:270:PRO:HD2	1:D:273:LYS:HD3	1.95	0.47
1:X:89:ILE:HG21	1:X:177:VAL:HG22	1.96	0.47
1:O:89:ILE:HG21	1:O:177:VAL:HG22	1.96	0.47
1:E:89:ILE:HG21	1:E:177:VAL:HG22	1.96	0.47
1:Q:19:ARG:NH1	1:Q:21:ALA:O	2.46	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:D:402:THR:OG1	1:D:404:ARG:HB2	2.14	0.47
1:Q:402:THR:OG1	1:Q:404:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:402:THR:OG1	1:X:404:ARG:HB2	2.14	0.47
1:H:371:HIS:C	1:H:372:ILE:HD13	2.34	0.47
1:R:471:GLN:O	1:R:497:VAL:HG22	2.13	0.47
1:U:193:ASP:O	1:U:196:ASP:HB2	2.14	0.47
1:N:89:ILE:HG21	1:N:177:VAL:HG22	1.95	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:S:384:ALA:O	1:S:387:SER:HB2	2.14	0.47
1:R:212:PHE:HD2	1:R:214:ARG:HH21	1.62	0.47
1:D:472:THR:CG2	1:D:498:GLU:HA	2.18	0.47
1:A:471:GLN:O	1:A:497:VAL:HG22	2.13	0.47
1:O:315:ASP:CB	1:P:311:ALA:HA	2.42	0.47
1:U:6:ASN:OD1	1:W:279:LYS:CE	2.51	0.47
1:K:193:ASP:CA	1:K:196:ASP:HB2	2.41	0.47
1:A:193:ASP:O	1:A:196:ASP:HB2	2.14	0.47
1:T:193:ASP:O	1:T:196:ASP:HB2	2.14	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:C:402:THR:OG1	1:C:404:ARG:HB2	2.14	0.47
1:O:365:SER:CB	1:P:3:LEU:HD12	2.45	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:I:193:ASP:O	1:I:196:ASP:HB2	2.14	0.47
1:C:193:ASP:O	1:C:196:ASP: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:482:ASP:H	1:I:490:ASN:HD21	1.61	0.47
1:X:482:ASP:H	1:X:490:ASN:HD21	1.61	0.47
1:Q:49:ARG:NE	1:Q:83:ASP:OD2	2.33	0.47
1:W:19:ARG:NH1	1:W:21:ALA:O	2.46	0.47
1:T:402:THR:OG1	1:T:404:ARG:HB2	2.14	0.47
1:P:384:ALA:O	1:P:387:SER:HB2	2.15	0.47
1:D:384:ALA:O	1:D:387:SER:HB2	2.14	0.47
1:C:496:LEU:CG	1:V:195:VAL:CG2	2.80	0.47
1:O:310:ARG:NH2	1:P:297:GLN:OE1	2.47	0.47
1:D:456:ARG:NH1	2:D:700:FDP:O2P	2.34	0.47
1:V:193:ASP:O	1:V:196:ASP:HB2	2.14	0.47
1:C:193:ASP:CA	1:C:196:ASP:HB2	2.41	0.47
1:X:193:ASP:CA	1:X:196:ASP:HB2	2.41	0.47
1:G:482:ASP:H	1:G:490:ASN:HD21	1.61	0.47
1:Q:90:ARG:HD3	1:Q:174:ARG:O	2.14	0.47
1:J:384:ALA:O	1:J:387:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:384:ALA:O	1:X:387:SER:HB2	2.14	0.47
1:O:19:ARG:NH1	1:O:21:ALA:O	2.46	0.47
1:C:90:ARG:HD3	1:C:174:ARG:O	2.13	0.47
1:H:384:ALA:O	1:H:387:SER:HB2	2.14	0.47
1:P:212:PHE:HD2	1:P:214:ARG:HH21	1.62	0.47
1:O:310:ARG:HG2	1:P:297:GLN:CB	2.42	0.47
1:M:193:ASP:CA	1:M:196:ASP:HB2	2.41	0.47
1:F:193:ASP:O	1:F:196:ASP:HB2	2.14	0.47
1:N:193:ASP:O	1:N:196:ASP:HB2	2.14	0.47
1:U:270:PRO:HD2	1:U:273:LYS:HD3	1.95	0.47
1:O:270:PRO:CG	1:O:273:LYS:HD2	2.45	0.47
1:K:482:ASP:H	1:K:490:ASN:HD21	1.61	0.47
1:S:89:ILE:HG21	1:S:177:VAL:HG22	1.96	0.47
1:D:89:ILE:HG21	1:D:177:VAL:HG22	1.96	0.47
1:N:224:LYS:HE3	1:N:224:LYS:HB3	1.81	0.47
1:C:384:ALA:O	1:C:387:SER:HB2	2.14	0.47
1:L:384:ALA:O	1:L:387:SER:HB2	2.14	0.47
1:D:90:ARG:HD3	1:D:174:ARG:O	2.13	0.47
1:P:19:ARG:NH1	1:P:21:ALA:O	2.46	0.47
1:C:250:SER:HB2	1:N:446:LYS:CD	2.37	0.47
1:U:212:PHE:HD2	1:U:214:ARG:HH21	1.62	0.47
1:O:212:PHE:HD2	1:O:214:ARG:HH21	1.62	0.47
1:W:212:PHE:HD2	1:W:214:ARG:HH21	1.62	0.47
1:U:372:ILE:HD12	1:U:374:MET:HG2	1.97	0.47
1:Q:297:GLN:HB2	1:S:310:ARG:HG2	1.95	0.47
1:U:310:ARG:HB2	1:W:297:GLN:HB2	1.97	0.47
1:L:12:PHE:N	1:L:12:PHE:CD2	2.79	0.47
1:Q:284:LYS:CG	1:S:7:LEU:CD2	2.90	0.47
1:S:493:ARG:HG2	1:T:482:ASP:OD2	2.15	0.47
1:K:193:ASP:O	1:K:197:LEU:N	2.38	0.47
1:K:193:ASP:O	1:K:196:ASP:HB2	2.14	0.47
1:L:193:ASP:CA	1:L:196:ASP:HB2	2.41	0.47
1:D:193:ASP:O	1:D:196:ASP:HB2	2.14	0.47
1:H:193:ASP:O	1:H:196:ASP:HB2	2.14	0.47
1:H:270:PRO:CG	1:H:273:LYS:HD2	2.45	0.47
1:O:482:ASP:H	1:O:490:ASN:HD21	1.61	0.47
1:W:89:ILE:HG21	1:W:177:VAL:HG22	1.96	0.47
1:G:89:ILE:HG21	1:G:177:VAL:HG22	1.96	0.47
1:J:89:ILE:HG21	1:J:177:VAL:HG22	1.96	0.47
1:O:365:SER:HB3	1:P:3:LEU:HD12	1.95	0.47
1:I:384:ALA:O	1:I:387:SER:HB2	2.14	0.47
1:N:402:THR:OG1	1:N:404:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:384:ALA:O	1:F:387:SER:HB2	2.14	0.47
1:O:384:ALA:O	1:O:387:SER:HB2	2.14	0.47
1:G:402:THR:OG1	1:G:404:ARG:HB2	2.15	0.47
1:W:384:ALA:O	1:W:387:SER:HB2	2.14	0.47
1:G:384:ALA:O	1:G:387:SER:HB2	2.15	0.47
1:H:11:ILE:HG13	1:H:12:PHE:HD2	1.80	0.47
1:I:212:PHE:HD2	1:I:214:ARG:HH21	1.62	0.47
1:H:242:HIS:NE2	1:J:12:PHE:HE2	2.11	0.47
1:I:456:ARG:NH1	2:I:700:FDP:O2P	2.34	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:B:482:ASP:H	1:B:490:ASN:HD21	1.61	0.47
1:R:89:ILE:HG21	1:R:177:VAL:HG22	1.96	0.47
1:P:49:ARG:NE	1:P:83:ASP:OD2	2.33	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: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:F:212:PHE:HD2	1:F:214:ARG:HH21	1.62	0.47
1:D:11:ILE:O	1:F:273:LYS:HE3	2.15	0.47
1:V:370:GLN:CB	1:V:374:MET:SD	3.03	0.47
1:K:297:GLN:CB	1:M:310:ARG:HG2	2.44	0.47
1:V:193:ASP:CA	1:V:196:ASP:HB2	2.41	0.47
1:E:193:ASP:O	1:E:196:ASP:HB2	2.14	0.47
1:H:193:ASP:CA	1:H:196:ASP:HB2	2.42	0.47
1:D:270:PRO:CG	1:D:273:LYS:HD2	2.45	0.47
1:C:89:ILE:HG21	1:C:177:VAL:HG22	1.96	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:N:19:ARG:NH1	1:N:21:ALA:O	2.46	0.47
1:L:212:PHE:HD2	1:L:214:ARG:HH21	1.62	0.47
1:O:11:ILE:HB	1:P:273:LYS:CB	2.45	0.47
1:L:273:LYS:HG2	1:N:11:ILE:HB	1.96	0.47
1:A:370:GLN:CB	1:A:374:MET:SD	3.03	0.47
1:D:373:PRO:HB3	1:E:391:THR:HA	1.97	0.47
1:B:270:PRO:CG	1:B:273:LYS:HD2	2.45	0.47
1:W:193:ASP:O	1:W:196:ASP:HB2	2.14	0.47
1:S:270:PRO:O	1:S:273:LYS:HB2	2.14	0.47
1:A:270:PRO:CG	1:A:273:LYS:HD2	2.45	0.47
1:L:231:ARG:HH21	1:S:231:ARG:HH21	1.62	0.47
1:I:19:ARG:NH1	1:I:21:ALA:O	2.46	0.47
1:M:402:THR:OG1	1:M:404:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:384:ALA:O	1:T:387:SER:HB2	2.14	0.47
1:N:384:ALA:O	1:N:387:SER:HB2	2.14	0.47
1:B:384:ALA:O	1:B:387:SER:HB2	2.14	0.47
1:C:212:PHE:HD2	1:C:214:ARG:HH21	1.62	0.46
1:H:311:ALA:CB	1:J:312:GLU:HG2	2.44	0.46
1:E:12:PHE:N	1:E:12:PHE:CD2	2.79	0.46
1:U:193:ASP:CA	1:U:196:ASP:HB2	2.41	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:A:283:SER:HB3	1:I:3:LEU:HD21	1.96	0.46
1:P:482:ASP:H	1:P:490:ASN:HD21	1.61	0.46
1:A:402:THR:OG1	1:A:404:ARG:HB2	2.14	0.46
1:O:424:ARG:CG	1:O:424:ARG:NH1	2.41	0.46
1:T:372:ILE:HD12	1:T:374:MET:CG	2.46	0.46
1:X:370:GLN:CB	1:X:374:MET:SD	3.03	0.46
1:Q:284:LYS:CG	1:S:7:LEU:HD22	2.46	0.46
1:B:311:ALA:HA	1:C:315:ASP:HB2	1.97	0.46
1:L:193:ASP:O	1:L:196:ASP:HB2	2.14	0.46
1:P:193:ASP:CA	1:P:196:ASP:HB2	2.42	0.46
1:V:384:ALA:O	1:V:387:SER:HB2	2.14	0.46
1:D:272:GLU:HG3	1:F:352:GLU:HB2	1.97	0.46
1:M:384:ALA:O	1:M:387:SER:HB2	2.14	0.46
1:A:384:ALA:O	1:A:387:SER:HB2	2.14	0.46
1:I:229:LYS:CG	1:M:487:GLY:HA3	2.25	0.46
1:W:270:PRO:O	1:W:273:LYS:HB2	2.14	0.46
1:R:297:GLN:HB3	1:R:297:GLN:HE21	1.50	0.46
1:K:372:ILE:HD12	1:K:374:MET:CG	2.46	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:A:369:LEU:CD1	1:I:3:LEU:HD13	2.45	0.46
1:C:270:PRO:CG	1:C:273:LYS:HD2	2.45	0.46
1:A:273:LYS:NZ	1:I:352:GLU:OE1	2.48	0.46
1:R:384:ALA:O	1:R:387:SER:HB2	2.15	0.46
1:K:212:PHE:HD2	1:K:214:ARG:HH21	1.62	0.46
1:E:297:GLN:HB2	1:G:310:ARG:CG	2.46	0.46
1:K:390:GLU:HG2	1:L:374:MET:CE	2.45	0.46
1:O:311:ALA:HB3	1:P:312:GLU:HG3	1.97	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:Q:270:PRO:CG	1:Q:273:LYS:HD2	2.45	0.46
1:M:391:THR:HA	1:N:373:PRO:CB	2.45	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:372:ILE:HD11	1:A:374:MET:HE2	1.96	0.46
1:X:372:ILE:HD12	1:X:374:MET:CG	2.46	0.46
1:B:276:VAL:CG1	1:C:9:LEU:HB3	2.45	0.46
1:K:270:PRO:CG	1:K:273:LYS:HD2	2.45	0.46
1:Q:384:ALA:O	1:Q:387:SER:HB2	2.14	0.46
1:K:384:ALA:O	1:K:387:SER:HB2	2.14	0.46
1:B:212:PHE:HD2	1:B:214:ARG:HH21	1.62	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:X:424:ARG:CG	1:X:424:ARG:NH1	2.41	0.46
1:W:372:ILE:HD12	1:W:374:MET:CG	2.46	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:482:ASP:H	1:T:490:ASN:HD21	1.61	0.46
1:N:193:ASP:CA	1:N:196:ASP:HB2	2.42	0.46
1:E:19:ARG:NH1	1:E:21:ALA:O	2.46	0.46
1:T:364:ASN:O	1:T:368:LYS:HG2	2.16	0.46
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:273:LYS:HG2	1:N:11:ILE:HA	1.96	0.46
1:R:297:GLN:HB2	1:T:310:ARG:CB	2.36	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:U:270:PRO:CG	1:U:273:LYS:HD2	2.45	0.46
1:L:364:ASN:O	1:L:368:LYS:HG2	2.16	0.46
1:O:402:THR:OG1	1:O:404:ARG:HB2	2.15	0.46
1:N:212:PHE:HD2	1:N:214:ARG:HH21	1.62	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:D:424:ARG:CG	1:D:424:ARG:NH1	2.41	0.46
1:H:390:GLU:O	1:I:373:PRO:CB	2.63	0.46
1:C:370:GLN:CB	1:C:374:MET:SD	3.03	0.46
1:L:276:VAL:CG1	1:N:9:LEU:CB	2.92	0.46
1:D:370:GLN:CB	1:D:374:MET:SD	3.03	0.46
1:K:272:GLU:HG3	1:M:352:GLU:CB	2.43	0.46
1:L:310:ARG:CZ	1:N:297:GLN:OE1	2.64	0.46
1:M:483:HIS:HD2	1:N:483:HIS:NE2	2.13	0.46
1:A:12:PHE:HE2	1:I:242:HIS:CE1	2.34	0.46
1:F:19:ARG:NH1	1:F:21:ALA:O	2.46	0.46
1:A:297:GLN:OE1	1:I:310:ARG:HG2	2.15	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:364:ASN:O	1:C:368:LYS:HG2	2.16	0.46
1:S:212:PHE:HD2	1:S:214:ARG:HH21	1.62	0.46
1:Q:472:THR:CG2	1:Q:498:GLU:HA	2.18	0.46
1:V:297:GLN:NE2	1:V:300:GLU:HB3	2.24	0.46
1:V:287:VAL:CG2	1:X:3:LEU:HD22	2.46	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: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:O:362:PHE:HD2	1:O:366:ILE:HD12	1.81	0.46
1:M:472:THR:CG2	1:M:498:GLU:CA	2.84	0.46
1:A:472:THR:CG2	1:A:498:GLU:HA	2.18	0.46
1:Q:193:ASP:C	1:Q:196:ASP:H	2.20	0.46
1:B:79:ALA:HB2	1:B:429:ARG:O	2.16	0.46
1:M:79:ALA:HB2	1:M:429:ARG:O	2.16	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:J:362:PHE:HD2	1:J:366:ILE:HD12	1.81	0.46
1:I:364:ASN:O	1:I:368:LYS:HG2	2.16	0.46
1:E:79:ALA:HB2	1:E:429:ARG:O	2.16	0.46
1:H:212:PHE:HD2	1:H:214:ARG:HH21	1.62	0.46
1:W:370:GLN:CB	1:W:374:MET:SD	3.03	0.46
1:E:11:ILE:HG12	1:E:12:PHE:CD2	2.47	0.46
1:D:193:ASP:C	1:D:196:ASP:H	2.20	0.46
1:A:224:LYS:HB3	1:A:224:LYS:HE3	1.82	0.46
1:Q:362:PHE:HD2	1:Q:366:ILE:HD12	1.81	0.46
1:X:364:ASN:O	1:X:368:LYS:HG2	2.16	0.46
1:C:362:PHE:HD2	1:C:366:ILE:HD12	1.81	0.46
1:F:373:PRO:CB	1:G:390:GLU:O	2.64	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:V:193:ASP:C	1:V:196:ASP:H	2.20	0.45
1:B:193:ASP:C	1:B:196:ASP:H	2.20	0.45
1:H:193:ASP:C	1:H:196:ASP:H	2.20	0.45
1:X:193:ASP:C	1:X:196:ASP:H	2.20	0.45
1:H:79:ALA:HB2	1:H:429:ARG:O	2.16	0.45
1:V:79:ALA:HB2	1:V:429:ARG:O	2.16	0.45
1:S:364:ASN:O	1:S:368:LYS:HG2	2.16	0.45
1:S:362:PHE:HD2	1:S:366:ILE:HD12	1.81	0.45
1:G:364:ASN:O	1:G:368:LYS:HG2	2.16	0.45
1:K:12:PHE:CE2	1:M:242:HIS:NE2	2.77	0.45
1:A:212:PHE:HD2	1:A:214:ARG:HH21	1.62	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:297:GLN:HG3	1:J:310:ARG:CG	2.43	0.45
1:G:370:GLN:CB	1:G:374:MET:SD	3.03	0.45
1:A:372:ILE:HD12	1:A:374:MET:CG	2.46	0.45
1:V:372:ILE:HD12	1:V:374:MET:CG	2.46	0.45
1:D:372:ILE:HD12	1:D:374:MET:CG	2.46	0.45
1:H:352:GLU:OE1	1:J:272:GLU:HG2	2.16	0.45
1:Q:456:ARG:NH1	2:Q:700:FDP:O2P	2.34	0.45
1:L:272:GLU:C	1:N:352:GLU:HG2	2.36	0.45
1:L:193:ASP:C	1:L:196:ASP:H	2.20	0.45
1:B:224:LYS:HB3	1:B:224:LYS:HE3	1.82	0.45
1:H:376:ALA:HA	1:I:494:ILE:HD12	1.98	0.45
1:F:362:PHE:HD2	1:F:366:ILE:HD12	1.81	0.45
1:I:79:ALA:HB2	1:I:429:ARG:O	2.16	0.45
1:T:362:PHE:HD2	1:T:366:ILE:HD12	1.81	0.45
1:N:362:PHE:HD2	1:N:366:ILE:HD12	1.81	0.45
1:H:364:ASN:O	1:H:368:LYS:HG2	2.16	0.45
1:R:79:ALA:HB2	1:R:429:ARG:O	2.16	0.45
1:H:496:LEU:HD21	1:M:195:VAL:HG23	1.97	0.45
1:Q:272:GLU:HG3	1:S:352:GLU:CG	2.45	0.45
1:I:195:VAL:HG22	1:N:496:LEU:CD2	2.46	0.45
1:O:193:ASP:CA	1:O:196:ASP:HB2	2.41	0.45
1:C:383:SER:CB	1:P:383:SER:HB2	2.45	0.45
1:E:193:ASP:CA	1:E:196:ASP:HB2	2.41	0.45
1:E:193:ASP:C	1:E:196:ASP:H	2.20	0.45
1:U:168:SER:O	1:U:169:HIS:HB2	2.17	0.45
1:S:168:SER:O	1:S:169:HIS:HB2	2.17	0.45
1:L:168:SER:O	1:L:169:HIS:HB2	2.17	0.45
1:C:168:SER:O	1:C:169:HIS:HB2	2.17	0.45
1:K:49:ARG:NE	1:K:83:ASP:OD2	2.33	0.45
1:N:79:ALA:HB2	1:N:429:ARG:O	2.16	0.45
1:Q:79:ALA:HB2	1:Q:429:ARG:O	2.16	0.45
1:O:79:ALA:HB2	1:O:429:ARG:O	2.16	0.45
1:G:79:ALA:HB2	1:G:429:ARG:O	2.16	0.45
1:J:364:ASN:O	1:J:368:LYS:HG2	2.16	0.45
1:D:364:ASN:O	1:D:368:LYS:HG2	2.16	0.45
1:V:284:LYS:HG2	1:X:7:LEU:CD2	2.38	0.45
1:O:372:ILE:HD12	1:O:374:MET:CG	2.46	0.45
1:Q:372:ILE:HD12	1:Q:374:MET:CG	2.46	0.45
1:B:280:ILE:CG1	1:C:6:ASN:O	2.64	0.45
1:S:456:ARG:NH1	2:S:700:FDP:O2P	2.34	0.45
1:P:193:ASP:C	1:P:196:ASP:H	2.20	0.45
1:N:193:ASP:C	1:N:196:ASP:H	2.20	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:193:ASP:C	1:A:196:ASP:H	2.20	0.45
1:G:193:ASP:O	1:G:197:LEU:N	2.38	0.45
1:O:279:LYS:HE3	1:P:6:ASN:OD1	2.15	0.45
1:V:364:ASN:O	1:V:368:LYS:HG2	2.16	0.45
1:P:364:ASN:O	1:P:368:LYS:HG2	2.16	0.45
1:N:364:ASN:O	1:N:368:LYS:HG2	2.16	0.45
1:W:79:ALA:HB2	1:W:429:ARG:O	2.16	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:R:273:LYS:HD3	1:T:11:ILE:C	2.33	0.45
1:K:370:GLN:CB	1:K:374:MET:SD	3.03	0.45
1:U:193:ASP:O	1:U:197:LEU:N	2.38	0.45
1:T:193:ASP:C	1:T:196:ASP:H	2.20	0.45
1:G:168:SER:O	1:G:169:HIS:HB2	2.17	0.45
1:Q:168:SER:O	1:Q:169:HIS:HB2	2.17	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:R:362:PHE:HD2	1:R:366:ILE:HD12	1.81	0.45
1:D:79:ALA:HB2	1:D:429:ARG:O	2.16	0.45
1:H:242:HIS:NE2	1:J:12:PHE:CE2	2.79	0.45
1:O:11:ILE:O	1:P:273:LYS:CD	2.65	0.45
1:N:372:ILE:HD12	1:N:374:MET:CG	2.46	0.45
1:F:456:ARG:NH1	2:F:700:FDP:O2P	2.34	0.45
1:X:401:ASN:N	2:X:700:FDP:O5P	2.50	0.45
1:O:193:ASP:C	1:O:196:ASP:H	2.20	0.45
1:S:193:ASP:C	1:S:196:ASP:H	2.20	0.45
1:J:193:ASP:C	1:J:196:ASP:H	2.20	0.45
1:G:193:ASP:C	1:G: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:R:311:ALA:CB	1:T:315:ASP:HB2	2.46	0.45
1:W:362:PHE:HD2	1:W:366:ILE:HD12	1.81	0.45
1:C:494:ILE:HD12	1:P:376:ALA:HA	1.97	0.45
1:A:79:ALA:HB2	1:A:429:ARG:O	2.16	0.45
1:G:362:PHE:HD2	1:G:366:ILE:HD12	1.81	0.45
1:U:364:ASN:O	1:U:368:LYS:HG2	2.16	0.45
1:H:315:ASP:CB	1:J:311:ALA:CA	2.89	0.45
1:O:472:THR:CG2	1:O:498:GLU:CA	2.84	0.45
1:E:11:ILE:HG13	1:E:12:PHE:HD2	1.72	0.45
1:W:193:ASP:C	1:W:196:ASP:H	2.20	0.45
1:R:193:ASP:C	1:R:196:ASP:H	2.20	0.45
1:B:168:SER:O	1:B:169:HIS:HB2	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:168:SER:O	1:O:169:HIS:HB2	2.17	0.45
1:I:168:SER:O	1:I:169:HIS:HB2	2.17	0.45
1:D:168:SER:O	1:D:169:HIS:HB2	2.17	0.45
1:K:362:PHE:HD2	1:K:366:ILE:HD12	1.81	0.45
1:C:79:ALA:HB2	1:C:429:ARG:O	2.16	0.45
1:E:242:HIS:NE2	1:G:12:PHE:HE2	2.15	0.45
1:A:223:ARG:NH1	1:A:223:ARG:HG2	2.25	0.45
1:F:193:ASP:C	1:F:196:ASP:H	2.20	0.45
1:U:193:ASP:C	1:U:196:ASP:H	2.20	0.45
1:V:168:SER:O	1:V:169:HIS:HB2	2.17	0.45
1:F:168:SER:O	1:F:169:HIS:HB2	2.17	0.45
1:R:311:ALA:HB1	1:T:311:ALA:O	2.16	0.45
1:P:362:PHE:HD2	1:P:366:ILE:HD12	1.81	0.45
1:J:79:ALA:HB2	1:J:429:ARG:O	2.16	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:O:372:ILE:HD11	1:O:374:MET:HE2	1.98	0.45
1:K:297:GLN:OE1	1:M:310:ARG:CZ	2.65	0.45
1:L:272:GLU:O	1:N:352:GLU:HG2	2.17	0.45
1:I:193:ASP:C	1:I:196:ASP:H	2.20	0.45
1:V:9:LEU:HB2	1:X:280:ILE:CD1	2.42	0.45
1:S:494:ILE:HD12	1:T:376:ALA:CB	2.44	0.45
1:C:193:ASP:C	1:C:196:ASP:H	2.20	0.45
1:H:270:PRO:CG	1:H:273:LYS:CD	2.94	0.45
1:W:364:ASN:O	1:W:368:LYS:HG2	2.16	0.45
1:S:79:ALA:HB2	1:S:429:ARG:O	2.16	0.45
1:X:178:ASN:OD1	1:X:268:GLU:OE2	2.35	0.45
1:L:178:ASN:OD1	1:L:268:GLU:OE2	2.35	0.45
1:C:178:ASN:OD1	1:C:268:GLU:OE2	2.35	0.45
1:F:372:ILE:HA	1:F:372:ILE:HD12	1.73	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:H:9:LEU:CB	1:J:276:VAL:HG13	2.46	0.45
1:F:364:ASN:O	1:F:368:LYS:HG2	2.16	0.45
1:P:178:ASN:OD1	1:P:268:GLU:OE2	2.35	0.45
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:H:311:ALA:HB3	1:J:312:GLU:HG2	1.98	0.44
1:Q:352:GLU:HG2	1:S:272:GLU:O	2.16	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:178:ASN:OD1	1:N:268:GLU:OE2	2.35	0.44
1:B:362:PHE:HD2	1:B:366:ILE:HD12	1.81	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:T:188:ALA:CB	1:T:218:GLN:HG2	2.21	0.44
1:M:472:THR:CG2	1:M:498:GLU:HA	2.18	0.44
1:G:372:ILE:HD12	1:G:372:ILE:HA	1.73	0.44
1:U:390:GLU:HG2	1:V:374:MET:HE2	1.99	0.44
1:S:193:ASP:CA	1:S:196:ASP:HB2	2.42	0.44
1:C:270:PRO:CG	1:C:273:LYS:CD	2.94	0.44
1:E:283:SER:OG	1:G:3:LEU:CD2	2.64	0.44
1:J:17:ASN:HD22	1:J:17:ASN:C	2.21	0.44
1:Q:178:ASN:OD1	1:Q:268:GLU:OE2	2.35	0.44
1:D:178:ASN:OD1	1:D:268:GLU:OE2	2.35	0.44
1:U:491:GLN:OE1	1:U:493:ARG:HD2	2.18	0.44
1:H:362:PHE:HD2	1:H:366:ILE:HD12	1.81	0.44
1:B:372:ILE:HD12	1:B:374:MET:CG	2.46	0.44
1:Q:270:PRO:CG	1:Q:273:LYS:CD	2.94	0.44
1:K:193:ASP:C	1:K:196:ASP:H	2.20	0.44
1:S:376:ALA:HB1	1:T:494:ILE:HB	1.99	0.44
1:T:168:SER:O	1:T:169:HIS:HB2	2.17	0.44
1:K:491:GLN:OE1	1:K:493:ARG:HD2	2.18	0.44
1:M:483:HIS:CD2	1:N:483:HIS:NE2	2.85	0.44
1:L:17:ASN:C	1:L:17:ASN:HD22	2.21	0.44
1:V:17:ASN:C	1:V:17:ASN:HD22	2.21	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:X:362:PHE:HD2	1:X:366:ILE:HD12	1.81	0.44
1:J:491:GLN:OE1	1:J:493:ARG:HD2	2.18	0.44
1:X:79:ALA:HB2	1:X:429:ARG:O	2.16	0.44
1:O:178:ASN:OD1	1:O:268:GLU:OE2	2.35	0.44
1:R:284:LYS:CG	1:T:7:LEU:HD21	2.38	0.44
1:M:373:PRO:HB3	1:N:391:THR:CA	2.45	0.44
1:M:193:ASP:C	1:M:196:ASP:H	2.20	0.44
1:P:168:SER:O	1:P:169:HIS:HB2	2.17	0.44
1:X:17:ASN:HD22	1:X:17:ASN:C	2.21	0.44
1:A:17:ASN:HD22	1:A:17:ASN:C	2.21	0.44
1:C:17:ASN:HD22	1:C:17:ASN:C	2.21	0.44
1:T:178:ASN:OD1	1:T:268:GLU:OE2	2.35	0.44
1:B:178:ASN:OD1	1:B:268:GLU:OE2	2.35	0.44
1:O:398:VAL:HG13	1:O:479:ILE:HB	2.00	0.44
1:U:362:PHE:HD2	1:U:366:ILE:HD12	1.81	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:178:ASN:OD1	1:V:268:GLU:OE2	2.35	0.44
1:K:79:ALA:HB2	1:K:429:ARG:O	2.17	0.44
1:U:11:ILE:HG13	1:W:273:LYS:HD3	1.99	0.44
1:K:391:THR:C	1:L:373:PRO:HB3	2.37	0.44
1:K:372:ILE:HD11	1:K:374:MET:HE2	2.00	0.44
1:B:372:ILE:HD11	1:B:374:MET:HE1	1.98	0.44
1:O:6:ASN:OD1	1:P:279:LYS:CE	2.54	0.44
1:B:280:ILE:HD11	1:C:9:LEU:HB2	1.99	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:R:491:GLN:OE1	1:R:493:ARG:HD2	2.18	0.44
1:L:3:LEU:HD23	1:N:283:SER:HB3	1.98	0.44
1:V:491:GLN:OE1	1:V:493:ARG:HD2	2.18	0.44
1:P:224:LYS:HB3	1:P:224:LYS:HE3	1.82	0.44
1:N:451:GLU:H	1:N:451:GLU:HG2	1.59	0.44
1:V:362:PHE:HD2	1:V:366:ILE:HD12	1.81	0.44
1:U:79:ALA:HB2	1:U:429:ARG:O	2.16	0.44
1:J:178:ASN:OD1	1:J:268:GLU:OE2	2.35	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:Q:374:MET:HE2	1:R:390:GLU:HG2	1.99	0.44
1:Q:383:SER:CB	1:R:383:SER:HB2	2.46	0.44
1:A:168:SER:O	1:A:169:HIS:HB2	2.17	0.44
1:J:168:SER:O	1:J:169:HIS:HB2	2.17	0.44
1:O:352:GLU:HB2	1:P:272:GLU:HG3	1.99	0.44
1:K:17:ASN:C	1:K:17:ASN:HD22	2.21	0.44
1:P:17:ASN:C	1:P:17:ASN:HD22	2.21	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:A:178:ASN:OD1	1:A:268:GLU:OE2	2.35	0.44
1:X:491:GLN:OE1	1:X:493:ARG:HD2	2.18	0.44
1:P:79:ALA:HB2	1:P:429:ARG:O	2.16	0.44
1:L:79:ALA:HB2	1:L:429:ARG:O	2.16	0.44
1:B:398:VAL:HG13	1:B:479:ILE:HB	2.00	0.44
1:T:3:LEU:HD23	1:T:4:ALA:N	2.24	0.44
1:Q:297:GLN:HB2	1:S:310:ARG:HB2	2.00	0.44
1:P:424:ARG:NH1	1:P:424:ARG:CG	2.41	0.44
1:L:401:ASN:N	2:L:700:FDP:O5P	2.50	0.44
1:T:491:GLN:OE1	1:T:493:ARG:HD2	2.18	0.44
1:K:168:SER:O	1:K:169:HIS:HB2	2.17	0.44
1:H:491:GLN:OE1	1:H:493:ARG:HD2	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:178:ASN:OD1	1:W:268:GLU:OE2	2.35	0.44
1:H:17:ASN:C	1:H:17:ASN:HD22	2.21	0.44
1:U:17:ASN:HD22	1:U:17:ASN:C	2.21	0.44
1:O:17:ASN:HD22	1:O:17:ASN:C	2.21	0.44
1:Q:364:ASN:O	1:Q:368:LYS:HG2	2.16	0.44
1:D:398:VAL:HG13	1:D:479:ILE:HB	2.00	0.44
1:W:398:VAL:HG13	1:W:479:ILE:HB	2.00	0.44
1:T:79:ALA:HB2	1:T:429:ARG:O	2.16	0.44
1:J:101:MET:HE1	1:J:124:PHE:CE1	2.53	0.44
1:E:398:VAL:HG13	1:E:479:ILE:HB	2.00	0.44
1:O:364:ASN:O	1:O:368:LYS:HG2	2.16	0.44
1:D:362:PHE:HD2	1:D:366:ILE:HD12	1.81	0.44
1:H:312:GLU:CG	1:J:311:ALA:HB3	2.48	0.44
1:Q:451:GLU:H	1:Q:451:GLU:HG2	1.59	0.44
1:O:401:ASN:N	2:O:700:FDP:O5P	2.50	0.44
1:L:352:GLU:HG2	1:N:272:GLU:C	2.38	0.44
1:X:168:SER:O	1:X:169:HIS:HB2	2.17	0.44
1:Q:491:GLN:OE1	1:Q:493:ARG:HD2	2.18	0.44
1:W:49:ARG:NE	1:W:83:ASP:OD2	2.33	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:J:398:VAL:HG13	1:J:479:ILE:HB	2.00	0.44
1:W:17:ASN:HD22	1:W: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:M:491:GLN:OE1	1:M:493:ARG:HD2	2.18	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:K:178:ASN:OD1	1:K:268:GLU:OE2	2.35	0.44
1:D:6:ASN:OD1	1:F:279:LYS:HE3	2.17	0.44
1:C:483:HIS:CD2	1:P:483:HIS:CD2	3.06	0.44
1:M:362:PHE:HD2	1:M:366:ILE:HD12	1.81	0.44
1:K:101:MET:HE1	1:K:124:PHE:CE1	2.53	0.44
1:H:398:VAL:HG13	1:H:479:ILE:HB	2.00	0.44
1:Q:17:ASN:HD22	1:Q:17:ASN:C	2.21	0.44
1:R:371:HIS:CD2	1:R:373:PRO:O	2.71	0.43
1:R:193:ASP:CA	1:R:196:ASP:HB2	2.41	0.43
1:K:270:PRO:CG	1:K:273:LYS:CD	2.94	0.43
1:H:168:SER:O	1:H:169:HIS:HB2	2.17	0.43
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:S:178:ASN:OD1	1:S:268:GLU:OE2	2.35	0.43
1:G:178:ASN:OD1	1:G:268:GLU:OE2	2.35	0.43
1:X:398:VAL:HG13	1:X:479:ILE:HB	2.00	0.43
1:H:178:ASN:OD1	1:H:268:GLU:OE2	2.35	0.43
1:R:272:GLU:HG2	1:T:352:GLU:CD	2.39	0.43
1:O:372:ILE:HA	1:O:372:ILE:HD12	1.73	0.43
1:G:491:GLN:OE1	1:G:493:ARG:HD2	2.18	0.43
1:A:369:LEU:HD12	1:I:3:LEU:HD13	2.00	0.43
1:R:168:SER:O	1:R:169:HIS:HB2	2.17	0.43
1:S:17:ASN:C	1:S:17:ASN:HD22	2.21	0.43
1:B:17:ASN:C	1:B:17:ASN:HD22	2.21	0.43
1:L:362:PHE:HD2	1:L:366:ILE:HD12	1.81	0.43
1:W:491:GLN:OE1	1:W:493:ARG:HD2	2.18	0.43
1:E:310:ARG:HG2	1:G:297:GLN:OE1	2.19	0.43
1:G:398:VAL:HG13	1:G:479:ILE:HB	2.00	0.43
1:T:3:LEU:CD2	1:T:4:ALA:N	2.80	0.43
1:A:372:ILE:HA	1:A:372:ILE:HD12	1.73	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:A:398:VAL:HG13	1:A:479:ILE:HB	2.00	0.43
1:B:372:ILE:HD12	1:B:372:ILE:HA	1.73	0.43
1:K:11:ILE:HB	1:M:273:LYS:CG	2.43	0.43
1:A:270:PRO:CG	1:A:273:LYS:CD	2.94	0.43
1:E:272:GLU:CB	1:G:352:GLU:HG2	2.49	0.43
1:B:3:LEU:HD13	1:C:369:LEU:CD1	2.48	0.43
1:T:17:ASN:HD22	1:T:17:ASN:C	2.21	0.43
1:Q:224:LYS:HB3	1:Q:224:LYS:HE3	1.81	0.43
1:C:398:VAL:HG13	1:C:479:ILE:HB	2.00	0.43
1:N:398:VAL:HG13	1:N:479:ILE:HB	2.00	0.43
1:M:178:ASN:OD1	1:M:268:GLU:OE2	2.35	0.43
1:Q:398:VAL:HG13	1:Q:479:ILE:HB	2.00	0.43
1:U:178:ASN:OD1	1:U:268:GLU:OE2	2.35	0.43
1:R:402:THR:OG1	1:R:404:ARG:HB2	2.19	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:B:272:GLU:O	1:C:352:GLU:CG	2.66	0.43
1:N:491:GLN:OE1	1:N:493:ARG:HD2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:491:GLN:OE1	1:A:493:ARG:HD2	2.18	0.43
1:R:280:ILE:HD11	1:T:9:LEU:CB	2.40	0.43
1:I:487:GLY:HA2	1:M:229:LYS:CD	2.42	0.43
1:C:496:LEU:CD2	1:V:195:VAL:CG2	2.93	0.43
1:R:424:ARG:NH1	1:R:424:ARG:CG	2.41	0.43
1:I:17:ASN:C	1:I:17:ASN:HD22	2.21	0.43
1:O:451:GLU:HG2	1:O:451:GLU:H	1.59	0.43
1:O:491:GLN:OE1	1:O:493:ARG:HD2	2.18	0.43
1:R:398:VAL:HG13	1:R:479:ILE:HB	2.00	0.43
1:E:101:MET:HE1	1:E:124:PHE:CE1	2.54	0.43
1:S:398:VAL:HG13	1:S:479:ILE:HB	2.00	0.43
1:V:287:VAL:HG23	1:X:3:LEU:HD22	2.01	0.43
1:O:429:ARG:O	1:O:432:ASN:HB2	2.19	0.43
1:I:224:LYS:HE3	1:I:224:LYS:HB3	1.81	0.43
1:N:17:ASN:C	1:N:17:ASN:HD22	2.21	0.43
1:E:178:ASN:OD1	1:E:268:GLU:OE2	2.35	0.43
1:U:402:THR:OG1	1:U:404:ARG:HB2	2.18	0.43
1:L:398:VAL:HG13	1:L:479:ILE:HB	2.00	0.43
1:F:398:VAL:HG13	1:F:479:ILE:HB	2.00	0.43
1:M:398:VAL:HG13	1:M:479:ILE:HB	2.00	0.43
1:L:279:LYS:HB3	1:N:6:ASN:CG	2.39	0.43
1:H:401:ASN:N	2:H:700:FDP:O5P	2.50	0.43
1:F:491:GLN:OE1	1:F:493:ARG:HD2	2.18	0.43
1:F:483:HIS:CD2	1:G:483:HIS:NE2	2.86	0.43
1:G:429:ARG:O	1:G:432:ASN:HB2	2.19	0.43
1:T:429:ARG:O	1:T:432:ASN:HB2	2.19	0.43
1:G:224:LYS:HB3	1:G:224:LYS:HE3	1.82	0.43
1:K:283:SER:HB3	1:M:3:LEU:CD2	2.49	0.43
1:T:398:VAL:HG13	1:T:479:ILE:HB	2.00	0.43
1:V:424:ARG:NH1	1:V:424:ARG:CG	2.41	0.43
1:S:491:GLN:OE1	1:S:493:ARG:HD2	2.18	0.43
1:J:429:ARG:O	1:J:432:ASN:HB2	2.19	0.43
1:S:429:ARG:O	1:S:432:ASN:HB2	2.19	0.43
1:G:17:ASN:HD22	1:G:17:ASN:C	2.21	0.43
1:L:293:ILE:HG12	1:L:326:CYS:HB2	2.01	0.43
1:W:293:ILE:HG12	1:W:326:CYS:HB2	2.01	0.43
1:D:188:ALA:CB	1:D:218:GLN:HG2	2.21	0.43
1:R:371:HIS:C	1:R:372:ILE:HD13	2.39	0.43
1:C:373:PRO:HD3	1:P:392:LYS:HD2	2.01	0.43
1:L:276:VAL:HG13	1:N:9:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:272:GLU:CB	1:X:352:GLU:HG2	2.49	0.43
1:V:79:ALA:HA	1:V:429:ARG:HB3	2.01	0.43
1:W:429:ARG:O	1:W:432:ASN:HB2	2.19	0.43
1:D:429:ARG:O	1:D:432:ASN:HB2	2.19	0.43
1:W:362:PHE:O	1:W:366:ILE:HD12	2.19	0.43
1:C:429:ARG:O	1:C:432:ASN:HB2	2.19	0.43
1:S:451:GLU:H	1:S:451:GLU:HG2	1.59	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:H:293:ILE:HG12	1:H:326:CYS:HB2	2.01	0.43
1:R:242:HIS:CE1	1:T:12:PHE:CE2	3.07	0.43
1:K:6:ASN:OD1	1:M:279:LYS:HE3	2.18	0.43
1:V:293:ILE:HG12	1:V:326:CYS:HB2	2.01	0.43
1:Q:297:GLN:OE1	1:S:310:ARG:CZ	2.67	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:B:79:ALA:HA	1:B:429:ARG:HB3	2.01	0.42
1:F:362:PHE:O	1:F:366:ILE:HD12	2.19	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:E:377:ASP:OD2	1:E:377:ASP:N	2.52	0.42
1:U:398:VAL:HG13	1:U:479:ILE:HB	2.00	0.42
1:U:138:GLY:HA2	1:U:151:GLN:HE21	1.84	0.42
1:K:398:VAL:HG13	1:K:479:ILE:HB	2.00	0.42
1:X:293:ILE:HG12	1:X:326:CYS:HB2	2.01	0.42
1:U:279:LYS:HE3	1:W:6:ASN:OD1	2.19	0.42
1:F:212:PHE:CD2	1:F:214:ARG:NE	2.88	0.42
1:H:312:GLU:HG3	1:J:311:ALA:HB3	2.00	0.42
1:F:472:THR:CG2	1:F:498:GLU:CA	2.84	0.42
1:T:474:ASP:O	1:T:497:VAL:HG13	2.20	0.42
1:H:496:LEU:HG	1:M:195:VAL:HG21	1.89	0.42
1:U:6:ASN:CG	1:W:279:LYS:HE3	2.36	0.42
1:H:451:GLU:H	1:H:451:GLU:HG2	1.59	0.42
1:E:429:ARG:O	1:E:432:ASN:HB2	2.19	0.42
1:H:79:ALA:HA	1:H:429:ARG:HB3	2.01	0.42
1:O:79:ALA:HA	1:O:429:ARG:HB3	2.01	0.42
1:G:79:ALA:HA	1:G:429:ARG:HB3	2.02	0.42
1:W:79:ALA:HA	1:W:429:ARG:HB3	2.01	0.42
1:A:429:ARG:O	1:A:432:ASN:HB2	2.19	0.42
1:L:362:PHE:O	1:L:366:ILE:HD12	2.19	0.42
1:R:17:ASN:C	1:R:17:ASN:HD22	2.21	0.42
1:K:451:GLU:H	1:K:451:GLU:HG2	1.59	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:224:LYS:HB3	1:T:224:LYS:HE3	1.81	0.42
1:U:451:GLU:HG2	1:U:451:GLU:H	1.59	0.42
1:K:293:ILE:HG12	1:K:326:CYS:HB2	2.01	0.42
1:H:138:GLY:HA2	1:H:151:GLN:HE21	1.85	0.42
1:U:293:ILE:HG12	1:U:326:CYS:HB2	2.01	0.42
1:P:138:GLY:HA2	1:P:151:GLN:HE21	1.84	0.42
1:S:293:ILE:HG12	1:S:326:CYS:HB2	2.01	0.42
1:M:293:ILE:HG12	1:M:326:CYS:HB2	2.01	0.42
1:A:6:ASN:O	1:I:280:ILE:HG12	2.19	0.42
1:T:212:PHE:CD2	1:T:214:ARG:NE	2.88	0.42
1:V:212:PHE:CD2	1:V:214:ARG:NE	2.88	0.42
1:T:472:THR:CG2	1:T:498:GLU:CA	2.84	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:M:491:GLN:HG3	1:N:491:GLN:CG	2.47	0.42
1:V:429:ARG:O	1:V:432:ASN:HB2	2.19	0.42
1:N:362:PHE:O	1:N:366:ILE:HD12	2.19	0.42
1:H:362:PHE:O	1:H:366:ILE:HD12	2.19	0.42
1:T:79:ALA:HA	1:T:429:ARG:HB3	2.01	0.42
1:C:293:ILE:HG12	1:C:326:CYS:HB2	2.01	0.42
1:P:398:VAL:HG13	1:P:479:ILE:HB	2.00	0.42
1:N:293:ILE:HG12	1:N:326:CYS:HB2	2.01	0.42
1:C:138:GLY:HA2	1:C:151:GLN:HE21	1.85	0.42
1:K:12:PHE:HE2	1:M:242:HIS:NE2	2.08	0.42
1:G:212:PHE:CD2	1:G:214:ARG:NE	2.88	0.42
1:U:372:ILE:CD1	1:V:390:GLU:HG2	2.45	0.42
1:S:474:ASP:O	1:S:497:VAL:HG13	2.20	0.42
1:V:276:VAL:HG13	1:X:9:LEU:CD1	2.48	0.42
1:Q:276:VAL:HG13	1:S:9:LEU:HB3	2.02	0.42
1:F:483:HIS:NE2	1:G:483:HIS:CD2	2.86	0.42
1:E:49:ARG:NE	1:E:83:ASP:OD2	2.33	0.42
1:S:362:PHE:O	1:S:366:ILE:HD12	2.19	0.42
1:I:429:ARG:O	1:I:432:ASN:HB2	2.19	0.42
1:R:429:ARG:O	1:R:432:ASN:HB2	2.19	0.42
1:N:429:ARG:O	1:N:432:ASN:HB2	2.19	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:E:362:PHE:O	1:E:366:ILE:HD12	2.19	0.42
1:M:362:PHE:O	1:M:366:ILE:HD12	2.19	0.42
1:U:377:ASP:N	1:U:377:ASP:OD2	2.52	0.42
1:I:293:ILE:HG12	1:I:326:CYS:HB2	2.01	0.42
1:V:398:VAL:HG13	1:V:479:ILE:HB	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:293:ILE:HG12	1:E:326:CYS:HB2	2.01	0.42
1:T:293:ILE:HG12	1:T:326:CYS:HB2	2.01	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:O:212:PHE:CD2	1:O:214:ARG:NE	2.88	0.42
1:R:212:PHE:CD2	1:R:214:ARG:NE	2.88	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:H:297:GLN:HB2	1:J:310:ARG:HB2	1.99	0.42
1:O:474:ASP:O	1:O:497:VAL:HG13	2.20	0.42
1:N:474:ASP:O	1:N:497:VAL:HG13	2.20	0.42
1:U:270:PRO:CG	1:U:273:LYS:CD	2.94	0.42
1:B:429:ARG:O	1:B:432:ASN:HB2	2.19	0.42
1:H:429:ARG:O	1:H:432:ASN:HB2	2.19	0.42
1:D:79:ALA:HA	1:D:429:ARG:HB3	2.01	0.42
1:A:79:ALA:HA	1:A:429:ARG:HB3	2.01	0.42
1:J:79:ALA:HA	1:J:429:ARG:HB3	2.01	0.42
1:R:377:ASP:N	1:R:377:ASP:OD2	2.52	0.42
1:V:224:LYS:HE3	1:V:224:LYS:HB3	1.81	0.42
1:I:398:VAL:HG13	1:I:479:ILE:HB	2.00	0.42
1:F:138:GLY:HA2	1:F:151:GLN:HE21	1.84	0.42
1:B:138:GLY:HA2	1:B:151:GLN:HE21	1.85	0.42
1:D:138:GLY:HA2	1:D:151:GLN:HE21	1.85	0.42
1:W:138:GLY:HA2	1:W:151:GLN:HE21	1.84	0.42
1:R:138:GLY:HA2	1:R:151:GLN:HE21	1.85	0.42
1:A:352:GLU:HG2	1:I:272:GLU:CG	2.50	0.42
1:X:212:PHE:CD2	1:X:214:ARG:NE	2.88	0.42
1:H:212:PHE:CD2	1:H:214:ARG:NE	2.88	0.42
1:V:472:THR:CG2	1:V:498:GLU:HA	2.18	0.42
1:J:474:ASP:O	1:J:497:VAL:HG13	2.20	0.42
1:W:372:ILE:HD11	1:W:374:MET:HE1	2.01	0.42
1:K:312:GLU:HA	1:M:311:ALA:CB	2.35	0.42
1:D:270:PRO:CG	1:D:273:LYS:CD	2.94	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:L:79:ALA:HA	1:L:429:ARG:HB3	2.01	0.42
1:K:377:ASP:OD2	1:K:377:ASP:N	2.52	0.42
1:T:138:GLY:HA2	1:T:151:GLN:HE21	1.85	0.42
1:G:293:ILE:HG12	1:G:326:CYS:HB2	2.01	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:424:ARG:NH1	1:M:424:ARG:CG	2.41	0.42
1:H:424:ARG:CG	1:H:424:ARG:NH1	2.41	0.42
1:K:372:ILE:HD12	1:K:372:ILE:HA	1.73	0.42
1:V:11:ILE:HD12	1:X:269:ILE:HG12	2.02	0.42
1:T:53:SER:HA	1:T:85:LYS:CG	2.50	0.42
1:M:79:ALA:HA	1:M:429:ARG:HB3	2.02	0.42
1:J:362:PHE:O	1:J:366:ILE:HD12	2.19	0.42
1:F:429:ARG:O	1:F:432:ASN:HB2	2.19	0.42
1:K:362:PHE:O	1:K:366:ILE:HD12	2.20	0.42
1:X:79:ALA:HA	1:X:429:ARG:HB3	2.01	0.42
1:K:79:ALA:HA	1:K:429:ARG:HB3	2.02	0.42
1:L:212:PHE:CD2	1:L:214:ARG:NE	2.88	0.42
1:F:474:ASP:O	1:F:497:VAL:HG13	2.20	0.42
1:U:424:ARG:NH1	1:U:424:ARG:CG	2.41	0.42
1:Q:270:PRO:CB	1:Q:273:LYS:HD2	2.50	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:B:276:VAL:HG13	1:C:9:LEU:CB	2.49	0.42
1:S:189:VAL:HG13	1:S:193:ASP:HB2	2.02	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:O:362:PHE:O	1:O:366:ILE:HD12	2.19	0.42
1:U:429:ARG:O	1:U:432:ASN:HB2	2.19	0.42
1:L:224:LYS:HE3	1:L:224:LYS:HB3	1.82	0.42
1:E:3:LEU:HD13	1:G:369:LEU:HD12	2.01	0.42
1:J:138:GLY:HA2	1:J:151:GLN:HE21	1.85	0.42
1:W:212:PHE:CD2	1:W:214:ARG:NE	2.88	0.42
1:R:272:GLU:HB2	1:T:352:GLU:HG2	1.94	0.42
1:P:474:ASP:O	1:P:497:VAL:HG13	2.20	0.42
1:I:372:ILE:HD12	1:I:374:MET:HG3	2.00	0.42
1:A:371:HIS:O	1:A:374:MET:CG	2.57	0.42
1:K:401:ASN:N	2:K:700:FDP:O5P	2.50	0.42
1:W:189:VAL:HG13	1:W:193:ASP:HB2	2.02	0.42
1:A:189:VAL:HG13	1:A:193:ASP:HB2	2.02	0.42
1:J:189:VAL:HG13	1:J:193:ASP:HB2	2.02	0.42
1:D:270:PRO:CB	1:D:273:LYS:HD2	2.50	0.42
1:C:53:SER:HA	1:C:85:LYS:CG	2.50	0.42
1:N:79:ALA:HA	1:N:429:ARG:HB3	2.01	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: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

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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:315:ASP:HB2	1:P:311:ALA:CA	2.48	0.41
1:K:242:HIS:NE2	1:M:12:PHE:CE2	2.85	0.41
1:L:284:LYS:CG	1:N:7:LEU:HD22	2.50	0.41
1:P:189:VAL:HG13	1:P:193:ASP:HB2	2.02	0.41
1:O:135:VAL:HG12	1:O:136:ARG:N	2.35	0.41
1:E:272:GLU:HG3	1:G:352:GLU:CB	2.50	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:P:79:ALA:HA	1:P:429:ARG:HB3	2.02	0.41
1:L:429:ARG:O	1:L:432:ASN:HB2	2.19	0.41
1:Q:293:ILE:HG12	1:Q:326:CYS:HB2	2.01	0.41
1:O:293:ILE:HG12	1:O:326:CYS:HB2	2.01	0.41
1:B:188:ALA:CB	1:B:218:GLN:HG2	2.21	0.41
1:K:212:PHE:CD2	1:K:214:ARG:NE	2.88	0.41
1:Q:212:PHE:CD2	1:Q:214:ARG:NE	2.88	0.41
1:R:474:ASP:O	1:R:497:VAL:HG13	2.20	0.41
1:B:474:ASP:O	1:B:497:VAL:HG13	2.20	0.41
1:H:296:THR:O	1:J:310:ARG:HG3	2.20	0.41
1:U:474:ASP:O	1:U:497:VAL:HG13	2.20	0.41
1:Q:390:GLU:O	1:R:372:ILE:HG13	2.20	0.41
1:E:474:ASP:O	1:E:497:VAL:HG13	2.20	0.41
1:V:401:ASN:N	2:V:700:FDP:O5P	2.50	0.41
1:B:270:PRO:CB	1:B:273:LYS:HD2	2.50	0.41
1:C:223:ARG:HG2	1:C:223:ARG:NH1	2.26	0.41
1:E:189:VAL:HG13	1:E:193:ASP:HB2	2.02	0.41
1:H:189:VAL:HG13	1:H:193:ASP:HB2	2.02	0.41
1:G:189:VAL:HG13	1:G:193:ASP:HB2	2.02	0.41
1:O:270:PRO:CB	1:O:273:LYS:HD2	2.50	0.41
1:L:53:SER:HA	1:L:85:LYS:CG	2.50	0.41
1:I:53:SER:HA	1:I:85:LYS:CG	2.50	0.41
1:A:362:PHE:O	1:A:366:ILE:HD12	2.19	0.41
1:O:101:MET:HE1	1:O:124:PHE:CE1	2.55	0.41
1:A:138:GLY:HA2	1:A:151:GLN:HE21	1.85	0.41
1:N:138:GLY:HA2	1:N:151:GLN:HE21	1.85	0.41
1:X:138:GLY:HA2	1:X:151:GLN:HE21	1.84	0.41
1:U:214:ARG:HG3	1:U:214:ARG:HH11	1.86	0.41
1:I:212:PHE:CD2	1:I:214:ARG:NE	2.88	0.41
1:P:214:ARG:HH11	1:P:214:ARG:HG3	1.86	0.41
1:G:474:ASP:O	1:G:497:VAL:HG13	2.20	0.41
1:K:297:GLN:HB2	1:M:310:ARG:HB2	2.01	0.41
1:S:491:GLN:NE2	1:T:491:GLN:NE2	2.68	0.41
1:F:189:VAL:HG13	1:F:193:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:189:VAL:HG13	1:N:193:ASP:HB2	2.02	0.41
1:V:189:VAL:HG13	1:V:193:ASP:HB2	2.02	0.41
1:I:79:ALA:HA	1:I:429:ARG:HB3	2.01	0.41
1:T:362:PHE:O	1:T:366:ILE:HD12	2.19	0.41
1:Q:467:LYS:HE2	1:Q:467:LYS:HB3	1.86	0.41
1:J:293:ILE:HG12	1:J:326:CYS:HB2	2.01	0.41
1:B:214:ARG:HH11	1:B:214:ARG:HG3	1.86	0.41
1:N:212:PHE:CD2	1:N:214:ARG:NE	2.88	0.41
1:C:214:ARG:HH11	1:C:214:ARG:HG3	1.86	0.41
1:H:474:ASP:O	1:H:497:VAL:HG13	2.20	0.41
1:T:424:ARG:NH1	1:T:424:ARG:CG	2.41	0.41
1:W:223:ARG:HG2	1:W:223:ARG:NH1	2.25	0.41
1:U:189:VAL:HG13	1:U:193:ASP:HB2	2.02	0.41
1:B:49:ARG:NE	1:B:83:ASP:OD2	2.33	0.41
1:C:362:PHE:O	1:C:366:ILE:HD12	2.20	0.41
1:K:429:ARG:O	1:K:432:ASN:HB2	2.19	0.41
1:V:362:PHE:O	1:V:366:ILE:HD12	2.19	0.41
1:K:138:GLY:HA2	1:K:151:GLN:HE21	1.84	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:H:310:ARG:H	1:J:297:GLN:HB3	1.86	0.41
1:V:474:ASP:O	1:V:497:VAL:HG13	2.20	0.41
1:U:311:ALA:CB	1:W:312:GLU:CG	2.99	0.41
1:K:270:PRO:CB	1:K:273:LYS:HD2	2.50	0.41
1:W:53:SER:HA	1:W:85:LYS:CG	2.50	0.41
1:L:310:ARG:NH2	1:N:297:GLN:OE1	2.53	0.41
1:X:429:ARG:O	1:X:432:ASN:HB2	2.19	0.41
1:P:377:ASP:N	1:P:377:ASP:OD2	2.52	0.41
1:F:214:ARG:HG3	1:F:214:ARG:HH11	1.86	0.41
1:J:212:PHE:CD2	1:J:214:ARG:NE	2.88	0.41
1:O:214:ARG:HH11	1:O:214:ARG:HG3	1.86	0.41
1:K:214:ARG:HH11	1:K:214:ARG:HG3	1.86	0.41
1:X:214:ARG:HG3	1:X:214:ARG:HH11	1.86	0.41
1:H:310:ARG:H	1:J:297:GLN:CB	2.34	0.41
1:F:373:PRO:HB2	1:G:391:THR:HA	1.95	0.41
1:U:315:ASP:CB	1:W:311:ALA:CB	2.99	0.41
1:B:272:GLU:CG	1:C:352:GLU:CB	2.98	0.41
1:I:451:GLU:H	1:I:451:GLU:HG2	1.59	0.41
1:X:189:VAL:HG13	1:X:193:ASP:HB2	2.02	0.41
1:H:270:PRO:CB	1:H:273:LYS:HD2	2.50	0.41
1:V:53:SER:HA	1:V:85:LYS:CG	2.50	0.41
1:E:79:ALA:HA	1:E:429:ARG:HB3	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:79:ALA:HA	1:F:429:ARG:HB3	2.01	0.41
1:K:283:SER:OG	1:M:3:LEU:HD23	2.21	0.41
1:P:467:LYS:HE2	1:P:467:LYS:HB3	1.87	0.41
1:G:138:GLY:HA2	1:G:151:GLN:HE21	1.85	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:L:402:THR:OG1	1:L:404:ARG:HB2	2.20	0.41
1:D:214:ARG:HG3	1:D:214:ARG:HH11	1.86	0.41
1:G:214:ARG:HG3	1:G:214:ARG:HH11	1.86	0.41
1:R:279:LYS:CE	1:T:6:ASN:OD1	2.63	0.41
1:N:472:THR:CG2	1:N:498:GLU:CA	2.84	0.41
1:K:189:VAL:HG13	1:K:193:ASP:HB2	2.02	0.41
1:N:53:SER:HA	1:N:85:LYS:CG	2.50	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:U:376:ALA:HA	1:V:494:ILE:HD12	2.03	0.41
1:O:138:GLY:HA2	1:O:151:GLN:HE21	1.84	0.41
1:J:214:ARG:HH11	1:J:214:ARG:HG3	1.86	0.41
1:E:212:PHE:CD2	1:E:214:ARG:NE	2.88	0.41
1:S:212:PHE:CD2	1:S:214:ARG:NE	2.88	0.41
1:S:214:ARG:HH11	1:S:214:ARG:HG3	1.86	0.41
1:A:214:ARG:HG3	1:A:214:ARG:HH11	1.86	0.41
1:A:474:ASP:O	1:A:497:VAL:HG13	2.20	0.41
1:H:390:GLU:O	1:I:373:PRO:HB3	2.21	0.41
1:W:424:ARG:NH1	1:W:424:ARG:CG	2.41	0.41
1:E:242:HIS:CE1	1:G:12:PHE:HZ	2.34	0.41
1:O:312:GLU:CA	1:P:311:ALA:HB1	2.33	0.41
1:Q:374:MET:HB2	1:Q:375:SER:H	1.78	0.41
1:H:352:GLU:CG	1:J:272:GLU:CG	2.99	0.41
1:Q:310:ARG:CG	1:S:297:GLN:HB2	2.51	0.41
1:Q:284:LYS:HG3	1:S:7:LEU:HD21	2.00	0.41
1:K:11:ILE:O	1:M:273:LYS:HE3	2.21	0.41
1:I:189:VAL:HG13	1:I:193:ASP:HB2	2.02	0.41
1:Q:189:VAL:HG13	1:Q:193:ASP:HB2	2.02	0.41
1:C:189:VAL:HG13	1:C:193:ASP:HB2	2.02	0.41
1:T:189:VAL:HG13	1:T:193:ASP:HB2	2.02	0.41
1:O:297:GLN:HB2	1:P:310:ARG:CG	2.44	0.41
1:W:377:ASP:OD2	1:W:377:ASP:N	2.52	0.41
1:U:101:MET:CE	1:U:124:PHE:CE1	3.04	0.41
1:I:444:ALA:O	1:I:448:GLY:N	2.54	0.41
1:B:101:MET:CE	1:B:124:PHE:CE1	3.04	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:444:ALA:O	1:D:448:GLY:N	2.54	0.41
1:M:444:ALA:O	1:M:448:GLY:N	2.54	0.41
1:V:101:MET:CE	1:V:124:PHE:CE1	3.04	0.41
1:M:101:MET:CE	1:M:124:PHE:CE1	3.04	0.41
1:D:212:PHE:CD2	1:D:214:ARG:NE	2.88	0.41
1:P:372:ILE:HD12	1:P:372:ILE:HA	1.80	0.41
1:C:389:TYR:O	1:P:372:ILE:HG21	2.21	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:E:372:ILE:HD12	1:E:372:ILE:HA	1.73	0.41
1:S:223:ARG:HG2	1:S:223:ARG:NH1	2.26	0.41
1:O:189:VAL:HG13	1:O:193:ASP:HB2	2.02	0.41
1:U:277:ALA:HB2	1:W:11:ILE:HG21	2.03	0.41
1:P:101:MET:CE	1:P:124:PHE:CE1	3.04	0.41
1:H:444:ALA:O	1:H:448:GLY:N	2.54	0.41
1:K:188:ALA:CB	1:K:218:GLN:HG2	2.21	0.40
1:L:214:ARG:HH11	1:L:214:ARG:HG3	1.86	0.40
1:W:214:ARG:HG3	1:W:214:ARG:HH11	1.86	0.40
1:A:212:PHE:CD2	1:A:214:ARG:NE	2.88	0.40
1:Q:273:LYS:HG2	1:S:11:ILE:O	2.21	0.40
1:L:229:LYS:CG	1:S:487:GLY:CA	2.84	0.40
1:B:270:PRO:CG	1:B:273:LYS:CD	2.94	0.40
1:B:189:VAL:HG13	1:B:193:ASP:HB2	2.02	0.40
1:R:53:SER:HA	1:R:85:LYS:CG	2.50	0.40
1:A:53:SER:HA	1:A:85:LYS:CG	2.50	0.40
1:K:53:SER:HA	1:K:85:LYS:CG	2.50	0.40
1:U:53:SER:HA	1:U:85:LYS:CG	2.50	0.40
1:N:101:MET:CE	1:N:124:PHE:CE1	3.04	0.40
1:L:451:GLU:HG2	1:L:451:GLU:H	1.59	0.40
1:I:101:MET:CE	1:I:124:PHE:CE1	3.04	0.40
1:H:101:MET:CE	1:H:124:PHE:CE1	3.04	0.40
1:B:110:THR:O	1:B:125:TYR:HA	2.22	0.40
1:A:444:ALA:O	1:A: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:O:444:ALA:O	1:O:448:GLY:N	2.54	0.40
1:F:188:ALA:CB	1:F:218:GLN:HG2	2.21	0.40
1:T:214:ARG:HH11	1:T:214:ARG:HG3	1.86	0.40
1:N:424:ARG:NH1	1:N:424:ARG:CG	2.41	0.40
1:Q:276:VAL:HG13	1:S:9:LEU:HD13	2.04	0.40
1:O:310:ARG:CG	1:P:297:GLN:OE1	2.60	0.40
1:U:310:ARG:CG	1:W:297:GLN:OE1	2.59	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:451:GLU:O	1:C:453:LYS:HE2	2.22	0.40
1:B:451:GLU:O	1:B:453:LYS:HE2	2.21	0.40
1:R:189:VAL:HG13	1:R:193:ASP:HB2	2.02	0.40
1:Q:53:SER:HA	1:Q:85:LYS:CG	2.50	0.40
1:A:12:PHE:CE2	1:I:242:HIS:HE1	2.38	0.40
1:H:101:MET:HE1	1:H:124:PHE:CE1	2.56	0.40
1:H:494:ILE:HD12	1:I:376:ALA:HB1	2.03	0.40
1:I:110:THR:O	1:I:125:TYR:HA	2.21	0.40
1:R:444:ALA:O	1:R:448:GLY:N	2.54	0.40
1:J:110:THR:O	1:J:125:TYR:HA	2.22	0.40
1:Q:101:MET:HE1	1:Q:124:PHE:CE1	2.56	0.40
1:F:101:MET:HE1	1:F:124:PHE:CE1	2.56	0.40
1:E:110:THR:O	1:E:125:TYR:HA	2.22	0.40
1:X:110:THR:O	1:X:125:TYR:HA	2.22	0.40
1:M:110:THR:O	1:M:125:TYR:HA	2.22	0.40
1:A:101:MET:CE	1:A:124:PHE:CE1	3.04	0.40
1:G:110:THR:O	1:G:125:TYR:HA	2.21	0.40
1:A:110:THR:O	1:A:125:TYR:HA	2.22	0.40
1:E:214:ARG:HG3	1:E:214:ARG:HH11	1.86	0.40
1:Q:214:ARG:HH11	1:Q:214:ARG:HG3	1.86	0.40
1:J:372:ILE:HA	1:J:372:ILE:HD12	1.73	0.40
1:B:371:HIS:O	1:B:374:MET:CG	2.57	0.40
1:V:371:HIS:O	1:V:374:MET:CG	2.57	0.40
1:A:451:GLU:O	1:A:453:LYS:HE2	2.22	0.40
1:C:451:GLU:HG2	1:C:451:GLU:H	1.59	0.40
1:I:451:GLU:O	1:I:453:LYS:HE2	2.22	0.40
1:T:401:ASN:N	2:T:700:FDP:O5P	2.50	0.40
1:L:312:GLU:HG3	1:N:311:ALA:HB3	2.03	0.40
1:D:189:VAL:HG13	1:D:193:ASP:HB2	2.02	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:Q:101:MET:CE	1:Q:124:PHE:CE1	3.04	0.40
1:O:467:LYS:HB3	1:O:467:LYS:HE2	1.86	0.40
1:C:110:THR:O	1:C:125:TYR:HA	2.21	0.40
1:K:110:THR:O	1:K:125:TYR:HA	2.22	0.40
1:R:110:THR:O	1:R:125:TYR:HA	2.22	0.40
1:H:110:THR:O	1:H:125:TYR:HA	2.22	0.40
1:U:372:ILE:HD11	1:U:374:MET:CE	2.51	0.40
1:A:472:THR:CG2	1:A:498:GLU:CA	2.84	0.40
1:C:372:ILE:HD12	1:C:372:ILE:HA	1.73	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:K:310:ARG:NH2	1:M:297:GLN:OE1	2.54	0.40
1:H:318:ASN:CG	1:J:318:ASN:ND2	2.75	0.40
1:F:101:MET:CE	1:F:124:PHE:CE1	3.04	0.40
1:A:467:LYS:HE2	1:A:467:LYS:HB3	1.86	0.40
1:U:110:THR:O	1:U:125:TYR:HA	2.22	0.40
1:R:101:MET:HE1	1:R:124:PHE:CE1	2.57	0.40
1:S:110:THR:O	1:S:125:TYR:HA	2.22	0.40
1:V:214:ARG:HG3	1:V:214:ARG:HH11	1.86	0.40
1:M:372:ILE:HD12	1:M:374:MET:HG3	2.04	0.40
1:K:297:GLN:HB2	1:M:310:ARG:CB	2.51	0.40
1:Q:451:GLU:O	1:Q:453:LYS:HE2	2.22	0.40
1:H:451:GLU:O	1:H:453:LYS:HE2	2.22	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:B:482:ASP:HB3	1:B:491:GLN:HE21	1.87	0.40
1:O:101:MET:CE	1:O:124:PHE:CE1	3.04	0.40
1:R:101:MET:CE	1:R:124:PHE:CE1	3.04	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	Distance(Å)	Clash(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

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56 93

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	C	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	D	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	E	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	F	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	G	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	H	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	I	496/499 (99%)	485 (98%)	10 (2%)	1 (0%)	56	93
1	J	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	K	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	L	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	M	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	N	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	O	496/499 (99%)	485 (98%)	10 (2%)	1 (0%)	56	93
1	P	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	Q	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	R	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	S	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	T	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	U	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	V	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	W	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
1	X	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	56	93
All	All	11904/11976 (99%)	11662 (98%)	218 (2%)	24 (0%)	56	93

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	THR
1	B	296	THR
1	C	296	THR
1	D	296	THR
1	E	296	THR
1	F	296	THR

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Mol	Chain	Res	Type
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%)	12	52
1	B	416/417 (100%)	375 (90%)	41 (10%)	11	51
1	C	416/417 (100%)	374 (90%)	42 (10%)	11	50
1	D	416/417 (100%)	375 (90%)	41 (10%)	11	51
1	E	416/417 (100%)	376 (90%)	40 (10%)	12	52
1	F	416/417 (100%)	375 (90%)	41 (10%)	11	51
1	G	416/417 (100%)	375 (90%)	41 (10%)	11	51
1	H	416/417 (100%)	375 (90%)	41 (10%)	11	51
1	I	416/417 (100%)	375 (90%)	41 (10%)	11	51
1	J	416/417 (100%)	375 (90%)	41 (10%)	11	51
1	K	416/417 (100%)	376 (90%)	40 (10%)	12	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	416/417 (100%)	376 (90%)	40 (10%)	12	52
1	M	416/417 (100%)	376 (90%)	40 (10%)	12	52
1	N	416/417 (100%)	376 (90%)	40 (10%)	12	52
1	O	416/417 (100%)	375 (90%)	41 (10%)	11	51
1	P	416/417 (100%)	376 (90%)	40 (10%)	12	52
1	Q	416/417 (100%)	375 (90%)	41 (10%)	11	51
1	R	416/417 (100%)	376 (90%)	40 (10%)	12	52
1	S	416/417 (100%)	376 (90%)	40 (10%)	12	52
1	T	416/417 (100%)	376 (90%)	40 (10%)	12	52
1	U	416/417 (100%)	376 (90%)	40 (10%)	12	52
1	V	416/417 (100%)	376 (90%)	40 (10%)	12	52
1	W	416/417 (100%)	374 (90%)	42 (10%)	11	50
1	X	416/417 (100%)	377 (91%)	39 (9%)	13	53
All	All	9984/10008 (100%)	9012 (90%)	972 (10%)	12	52

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
1	A	304	TYR
1	A	335	LYS
1	A	345	TYR
1	A	362	PHE

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Mol	Chain	Res	Type
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
1	B	335	LYS
1	B	345	TYR
1	B	362	PHE
1	B	372	ILE

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Mol	Chain	Res	Type
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
1	C	335	LYS
1	C	345	TYR
1	C	362	PHE
1	C	372	ILE

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Mol	Chain	Res	Type
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
1	D	362	PHE
1	D	372	ILE
1	D	374	MET
1	D	382	SER

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Mol	Chain	Res	Type
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
1	E	372	ILE
1	E	374	MET
1	E	382	SER
1	E	383	SER

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Mol	Chain	Res	Type
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
1	F	374	MET
1	F	382	SER
1	F	383	SER
1	F	394	LYS

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Mol	Chain	Res	Type
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
1	G	383	SER
1	G	394	LYS
1	G	396	MET
1	G	398	VAL

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Mol	Chain	Res	Type
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
1	H	383	SER
1	H	394	LYS
1	H	396	MET
1	H	398	VAL

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Mol	Chain	Res	Type
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
1	I	396	MET
1	I	398	VAL
1	I	404	ARG
1	I	424	ARG

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Mol	Chain	Res	Type
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
1	J	396	MET
1	J	398	VAL
1	J	424	ARG
1	J	435	GLN

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Mol	Chain	Res	Type
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
1	K	424	ARG
1	K	435	GLN
1	K	446	LYS
1	K	451	GLU

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Mol	Chain	Res	Type
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
1	L	446	LYS
1	L	451	GLU
1	L	453	LYS
1	L	454	GLU

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Mol	Chain	Res	Type
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
1	M	453	LYS
1	M	454	GLU
1	M	466	SER
1	M	467	LYS

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Mol	Chain	Res	Type
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
1	N	466	SER
1	N	467	LYS
1	N	471	GLN
1	N	472	THR

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Mol	Chain	Res	Type
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
1	O	467	LYS
1	O	471	GLN
1	O	472	THR
1	O	490	ASN

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Mol	Chain	Res	Type
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
1	P	472	THR
1	P	490	ASN
1	P	495	LEU
1	P	497	VAL

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Mol	Chain	Res	Type
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
1	Q	490	ASN
1	Q	495	LEU
1	Q	497	VAL
1	Q	498	GLU

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Mol	Chain	Res	Type
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
1	R	497	VAL
1	R	498	GLU
1	S	3	LEU
1	S	12	PHE

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Mol	Chain	Res	Type
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
1	T	3	LEU
1	T	12	PHE
1	T	17	ASN
1	T	31	THR

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Mol	Chain	Res	Type
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
1	U	31	THR
1	U	38	LYS
1	U	40	LEU
1	U	118	LYS

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Mol	Chain	Res	Type
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
1	V	40	LEU
1	V	118	LYS
1	V	175	ARG
1	V	177	VAL

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Mol	Chain	Res	Type
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
1	W	118	LYS
1	W	175	ARG
1	W	177	VAL
1	W	179	LEU

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Mol	Chain	Res	Type
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
1	X	177	VAL
1	X	179	LEU
1	X	194	ARG
1	X	214	ARG

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Mol	Chain	Res	Type
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
1	A	286	ASN
1	A	305	ASN
1	A	371	HIS
1	A	490	ASN

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Mol	Chain	Res	Type
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
1	E	286	ASN
1	E	305	ASN
1	E	371	HIS
1	E	483	HIS

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Mol	Chain	Res	Type
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
1	I	218	GLN
1	I	242	HIS
1	I	286	ASN
1	I	305	ASN

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Mol	Chain	Res	Type
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
1	M	139	ASN
1	M	151	GLN
1	M	178	ASN
1	M	218	GLN

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Mol	Chain	Res	Type
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
1	P	371	HIS
1	P	483	HIS
1	P	490	ASN
1	Q	17	ASN

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Mol	Chain	Res	Type
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
1	T	305	ASN
1	T	371	HIS
1	T	483	HIS
1	T	490	ASN

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Mol	Chain	Res	Type
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
1	X	139	ASN
1	X	151	GLN
1	X	178	ASN
1	X	218	GLN

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Mol	Chain	Res	Type
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 chains 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	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	B	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	C	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	D	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	E	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	F	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FDP	G	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	H	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	I	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	J	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	K	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	L	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	M	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	N	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	O	700	-	20,20,20	1.08	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	P	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	Q	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	R	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	6 (18%)
2	FDP	S	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	T	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	U	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	V	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	W	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)
2	FDP	X	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)

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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-2.41	1.37	1.43
2	X	700	FDP	O4-C4	-2.41	1.37	1.43
2	A	700	FDP	O4-C4	-2.40	1.37	1.43
2	W	700	FDP	O4-C4	-2.40	1.37	1.43
2	E	700	FDP	O4-C4	-2.40	1.37	1.43
2	C	700	FDP	O4-C4	-2.39	1.37	1.43
2	V	700	FDP	O4-C4	-2.39	1.37	1.43
2	N	700	FDP	O4-C4	-2.38	1.37	1.43
2	M	700	FDP	O4-C4	-2.39	1.37	1.43
2	F	700	FDP	O4-C4	-2.38	1.37	1.43
2	D	700	FDP	O4-C4	-2.38	1.37	1.43
2	L	700	FDP	O4-C4	-2.38	1.37	1.43
2	B	700	FDP	O4-C4	-2.37	1.37	1.43
2	P	700	FDP	O4-C4	-2.37	1.37	1.43
2	J	700	FDP	O4-C4	-2.37	1.37	1.43
2	Q	700	FDP	O4-C4	-2.37	1.37	1.43
2	I	700	FDP	O4-C4	-2.37	1.37	1.43
2	O	700	FDP	O4-C4	-2.37	1.37	1.43
2	G	700	FDP	O4-C4	-2.36	1.37	1.43
2	S	700	FDP	O4-C4	-2.36	1.37	1.43
2	U	700	FDP	O4-C4	-2.36	1.37	1.43
2	T	700	FDP	O4-C4	-2.36	1.37	1.43
2	H	700	FDP	O4-C4	-2.36	1.37	1.43
2	R	700	FDP	O4-C4	-2.35	1.37	1.43
2	N	700	FDP	P2-O5P	-2.32	1.46	1.54
2	E	700	FDP	P2-O5P	-2.32	1.46	1.54
2	H	700	FDP	P2-O5P	-2.31	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	700	FDP	P2-O5P	-2.31	1.46	1.54
2	Q	700	FDP	P2-O5P	-2.31	1.46	1.54
2	T	700	FDP	P2-O5P	-2.30	1.46	1.54
2	W	700	FDP	P2-O5P	-2.30	1.46	1.54
2	A	700	FDP	P2-O5P	-2.30	1.46	1.54
2	U	700	FDP	P2-O5P	-2.30	1.46	1.54
2	M	700	FDP	P2-O5P	-2.30	1.46	1.54
2	K	700	FDP	P2-O5P	-2.29	1.46	1.54
2	I	700	FDP	P2-O5P	-2.29	1.46	1.54
2	X	700	FDP	P2-O5P	-2.29	1.46	1.54
2	G	700	FDP	P2-O5P	-2.29	1.46	1.54
2	V	700	FDP	P2-O5P	-2.29	1.46	1.54
2	J	700	FDP	P2-O5P	-2.29	1.46	1.54
2	C	700	FDP	P2-O5P	-2.29	1.46	1.54
2	S	700	FDP	P2-O5P	-2.29	1.46	1.54
2	O	700	FDP	P2-O5P	-2.29	1.46	1.54
2	R	700	FDP	P2-O5P	-2.29	1.46	1.54
2	D	700	FDP	P2-O5P	-2.29	1.46	1.54
2	L	700	FDP	P2-O5P	-2.29	1.46	1.54
2	B	700	FDP	P2-O5P	-2.29	1.46	1.54
2	F	700	FDP	P2-O5P	-2.28	1.46	1.54

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	700	FDP	O6-P2-O4P	2.86	115.10	106.71
2	O	700	FDP	O6-P2-O4P	2.86	115.09	106.71
2	M	700	FDP	O6-P2-O4P	2.86	115.09	106.71
2	X	700	FDP	O6-P2-O4P	2.86	115.09	106.71
2	F	700	FDP	O6-P2-O4P	2.86	115.08	106.71
2	I	700	FDP	O6-P2-O4P	2.85	115.07	106.71
2	S	700	FDP	O6-P2-O4P	2.85	115.07	106.71
2	Q	700	FDP	O6-P2-O4P	2.85	115.06	106.71
2	B	700	FDP	O6-P2-O4P	2.85	115.07	106.71
2	L	700	FDP	O6-P2-O4P	2.85	115.06	106.71
2	G	700	FDP	O6-P2-O4P	2.85	115.06	106.71
2	R	700	FDP	O6-P2-O4P	2.84	115.05	106.71
2	T	700	FDP	O6-P2-O4P	2.84	115.04	106.71
2	J	700	FDP	O6-P2-O4P	2.84	115.04	106.71
2	A	700	FDP	O6-P2-O4P	2.84	115.03	106.71
2	U	700	FDP	O6-P2-O4P	2.84	115.03	106.71
2	K	700	FDP	O6-P2-O4P	2.84	115.03	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	700	FDP	O6-P2-O4P	2.84	115.03	106.71
2	D	700	FDP	O6-P2-O4P	2.84	115.03	106.71
2	P	700	FDP	O6-P2-O4P	2.84	115.02	106.71
2	H	700	FDP	O6-P2-O4P	2.83	115.01	106.71
2	C	700	FDP	O6-P2-O4P	2.83	115.01	106.71
2	N	700	FDP	O6-P2-O4P	2.83	115.00	106.71
2	W	700	FDP	O6-P2-O4P	2.83	115.00	106.71
2	H	700	FDP	O2-P1-O1P	2.73	114.41	106.79
2	R	700	FDP	O2-P1-O1P	2.73	114.41	106.79
2	Q	700	FDP	O2-P1-O1P	2.72	114.39	106.79
2	T	700	FDP	O2-P1-O1P	2.72	114.38	106.79
2	M	700	FDP	O2-P1-O1P	2.72	114.38	106.79
2	K	700	FDP	O2-P1-O1P	2.71	114.36	106.79
2	X	700	FDP	O2-P1-O1P	2.71	114.36	106.79
2	I	700	FDP	O2-P1-O1P	2.71	114.36	106.79
2	A	700	FDP	O2-P1-O1P	2.71	114.35	106.79
2	D	700	FDP	O2-P1-O1P	2.71	114.35	106.79
2	N	700	FDP	O2-P1-O1P	2.71	114.35	106.79
2	W	700	FDP	O2-P1-O1P	2.71	114.35	106.79
2	O	700	FDP	O2-P1-O1P	2.71	114.35	106.79
2	F	700	FDP	O2-P1-O1P	2.70	114.34	106.79
2	P	700	FDP	O2-P1-O1P	2.70	114.34	106.79
2	U	700	FDP	O2-P1-O1P	2.70	114.33	106.79
2	J	700	FDP	O2-P1-O1P	2.70	114.33	106.79
2	L	700	FDP	O2-P1-O1P	2.70	114.33	106.79
2	V	700	FDP	O2-P1-O1P	2.70	114.33	106.79
2	B	700	FDP	O2-P1-O1P	2.69	114.32	106.79
2	G	700	FDP	O2-P1-O1P	2.70	114.32	106.79
2	S	700	FDP	O2-P1-O1P	2.69	114.31	106.79
2	E	700	FDP	O2-P1-O1P	2.69	114.31	106.79
2	C	700	FDP	O2-P1-O1P	2.69	114.31	106.79
2	F	700	FDP	C6-C5-C4	-2.48	105.28	115.21
2	X	700	FDP	C6-C5-C4	-2.48	105.29	115.21
2	W	700	FDP	C6-C5-C4	-2.47	105.30	115.21
2	O	700	FDP	C6-C5-C4	-2.47	105.30	115.21
2	Q	700	FDP	C6-C5-C4	-2.47	105.31	115.21
2	R	700	FDP	C6-C5-C4	-2.47	105.31	115.21
2	T	700	FDP	C6-C5-C4	-2.47	105.32	115.21
2	N	700	FDP	C6-C5-C4	-2.47	105.32	115.21
2	U	700	FDP	C6-C5-C4	-2.47	105.32	115.21
2	B	700	FDP	C6-C5-C4	-2.47	105.32	115.21
2	D	700	FDP	C6-C5-C4	-2.47	105.32	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	700	FDP	C6-C5-C4	-2.47	105.32	115.21
2	K	700	FDP	C6-C5-C4	-2.47	105.33	115.21
2	J	700	FDP	C6-C5-C4	-2.47	105.33	115.21
2	I	700	FDP	C6-C5-C4	-2.47	105.33	115.21
2	A	700	FDP	C6-C5-C4	-2.47	105.33	115.21
2	P	700	FDP	C6-C5-C4	-2.46	105.34	115.21
2	M	700	FDP	C6-C5-C4	-2.46	105.34	115.21
2	G	700	FDP	C6-C5-C4	-2.46	105.34	115.21
2	S	700	FDP	C6-C5-C4	-2.46	105.35	115.21
2	E	700	FDP	C6-C5-C4	-2.46	105.35	115.21
2	L	700	FDP	C6-C5-C4	-2.46	105.36	115.21
2	H	700	FDP	C6-C5-C4	-2.46	105.38	115.21
2	V	700	FDP	C6-C5-C4	-2.45	105.38	115.21
2	O	700	FDP	O2P-P1-O2	-2.40	100.18	107.09
2	J	700	FDP	O2P-P1-O2	-2.40	100.18	107.09
2	V	700	FDP	O2P-P1-O2	-2.40	100.18	107.09
2	D	700	FDP	O2P-P1-O2	-2.40	100.19	107.09
2	X	700	FDP	O2P-P1-O2	-2.39	100.20	107.09
2	H	700	FDP	O2P-P1-O2	-2.39	100.21	107.09
2	N	700	FDP	O2P-P1-O2	-2.39	100.21	107.09
2	T	700	FDP	O2P-P1-O2	-2.39	100.21	107.09
2	L	700	FDP	O2P-P1-O2	-2.39	100.22	107.09
2	A	700	FDP	O2P-P1-O2	-2.39	100.21	107.09
2	G	700	FDP	O2P-P1-O2	-2.39	100.22	107.09
2	E	700	FDP	O2P-P1-O2	-2.39	100.22	107.09
2	U	700	FDP	O2P-P1-O2	-2.38	100.22	107.09
2	M	700	FDP	O2P-P1-O2	-2.38	100.23	107.09
2	Q	700	FDP	O2P-P1-O2	-2.38	100.23	107.09
2	K	700	FDP	O2P-P1-O2	-2.38	100.23	107.09
2	F	700	FDP	O2P-P1-O2	-2.38	100.23	107.09
2	S	700	FDP	O2P-P1-O2	-2.38	100.25	107.09
2	P	700	FDP	O2P-P1-O2	-2.38	100.24	107.09
2	R	700	FDP	O2P-P1-O2	-2.37	100.25	107.09
2	B	700	FDP	O2P-P1-O2	-2.37	100.26	107.09
2	I	700	FDP	O2P-P1-O2	-2.37	100.26	107.09
2	W	700	FDP	O2P-P1-O2	-2.37	100.26	107.09
2	C	700	FDP	O2P-P1-O2	-2.37	100.26	107.09
2	T	700	FDP	O2-C2-C3	2.33	118.53	108.39
2	E	700	FDP	O2-C2-C3	2.33	118.52	108.39
2	F	700	FDP	O2-C2-C3	2.32	118.52	108.39
2	R	700	FDP	O2-C2-C3	2.32	118.52	108.39
2	I	700	FDP	O2-C2-C3	2.32	118.51	108.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	700	FDP	O2-C2-C3	2.32	118.50	108.39
2	K	700	FDP	O2-C2-C3	2.32	118.50	108.39
2	J	700	FDP	O2-C2-C3	2.32	118.50	108.39
2	V	700	FDP	O2-C2-C3	2.32	118.50	108.39
2	Q	700	FDP	O2-C2-C3	2.32	118.49	108.39
2	C	700	FDP	O2-C2-C3	2.32	118.49	108.39
2	G	700	FDP	O2-C2-C3	2.32	118.49	108.39
2	B	700	FDP	O2-C2-C3	2.32	118.48	108.39
2	H	700	FDP	O2-C2-C3	2.32	118.48	108.39
2	O	700	FDP	O2-C2-C3	2.32	118.48	108.39
2	S	700	FDP	O2-C2-C3	2.31	118.46	108.39
2	M	700	FDP	O2-C2-C3	2.31	118.46	108.39
2	X	700	FDP	O2-C2-C3	2.31	118.46	108.39
2	A	700	FDP	O2-C2-C3	2.31	118.46	108.39
2	U	700	FDP	O2-C2-C3	2.31	118.45	108.39
2	L	700	FDP	O2-C2-C3	2.31	118.45	108.39
2	P	700	FDP	O2-C2-C3	2.31	118.44	108.39
2	N	700	FDP	O2-C2-C3	2.31	118.43	108.39
2	D	700	FDP	O2-C2-C3	2.30	118.43	108.39
2	R	700	FDP	O5-C2-C3	-2.01	100.88	105.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	1.07	72 (14%) 3 7	13, 23, 36, 46	0
1	B	498/499 (99%)	0.91	59 (11%) 5 11	13, 23, 36, 46	0
1	C	498/499 (99%)	0.93	54 (10%) 6 12	13, 23, 36, 46	0
1	D	498/499 (99%)	0.97	57 (11%) 6 11	13, 23, 36, 46	0
1	E	498/499 (99%)	0.93	54 (10%) 6 12	13, 23, 36, 46	0
1	F	498/499 (99%)	0.96	41 (8%) 12 17	13, 23, 36, 46	0
1	G	498/499 (99%)	0.92	42 (8%) 11 17	13, 23, 36, 46	0
1	H	498/499 (99%)	0.89	49 (9%) 8 14	13, 23, 36, 46	0
1	I	498/499 (99%)	0.90	44 (8%) 10 16	13, 23, 36, 46	0
1	J	498/499 (99%)	0.97	65 (13%) 4 9	13, 23, 36, 46	0
1	K	498/499 (99%)	0.93	47 (9%) 9 15	13, 23, 36, 46	0
1	L	498/499 (99%)	0.96	47 (9%) 9 15	13, 23, 36, 46	0
1	M	498/499 (99%)	0.86	37 (7%) 14 19	13, 23, 36, 46	0
1	N	498/499 (99%)	0.95	41 (8%) 12 17	13, 23, 36, 46	0
1	O	498/499 (99%)	1.03	77 (15%) 3 7	13, 23, 36, 46	0
1	P	498/499 (99%)	0.92	56 (11%) 6 11	13, 23, 36, 46	0
1	Q	498/499 (99%)	0.88	41 (8%) 12 17	13, 23, 36, 46	0
1	R	498/499 (99%)	0.93	55 (11%) 6 12	13, 23, 36, 46	0
1	S	498/499 (99%)	0.88	46 (9%) 9 15	13, 23, 36, 46	0
1	T	498/499 (99%)	0.98	60 (12%) 5 11	13, 23, 36, 46	0
1	U	498/499 (99%)	0.91	46 (9%) 9 15	13, 23, 36, 46	0
1	V	498/499 (99%)	0.96	52 (10%) 7 13	13, 23, 36, 46	0
1	W	498/499 (99%)	0.96	58 (11%) 5 11	13, 23, 36, 46	0
1	X	498/499 (99%)	1.05	67 (13%) 4 8	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%)	0.94	1267 (10%) 7 12	13, 23, 36, 46	0

All (1267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	163	CYS	9.0
1	A	131	LEU	7.0
1	A	135	VAL	6.6
1	T	116	ALA	6.1
1	S	49	ARG	5.8
1	H	101	MET	5.8
1	J	346	MET	5.4
1	L	141	ILE	5.4
1	A	134	VAL	5.4
1	O	162	GLU	5.4
1	G	105	ALA	5.3
1	A	100	VAL	5.2
1	R	498	GLU	5.0
1	U	498	GLU	5.0
1	E	328	MET	5.0
1	S	50	MET	4.9
1	X	95	VAL	4.9
1	Q	87	PRO	4.9
1	I	124	PHE	4.9
1	P	381	CYS	4.8
1	G	171	ILE	4.8
1	G	101	MET	4.8
1	B	396	MET	4.8
1	B	493	ARG	4.7
1	O	101	MET	4.7
1	O	259	MET	4.7
1	L	140	TYR	4.5
1	D	101	MET	4.5
1	A	132	SER	4.5
1	K	169	HIS	4.5
1	Q	161	LEU	4.5
1	P	260	VAL	4.5
1	E	131	LEU	4.4
1	J	476	CYS	4.4
1	J	381	CYS	4.4
1	J	163	CYS	4.4
1	H	498	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	I	123	LYS	4.4
1	J	207	MET	4.4
1	K	171	ILE	4.4
1	V	396	MET	4.4
1	F	476	CYS	4.3
1	D	259	MET	4.3
1	B	294	CYS	4.3
1	T	101	MET	4.3
1	A	332	GLU	4.3
1	M	346	MET	4.3
1	A	494	ILE	4.3
1	O	182	CYS	4.3
1	C	101	MET	4.2
1	L	150	LEU	4.2
1	O	91	THR	4.2
1	A	188	ALA	4.2
1	K	155	HIS	4.2
1	B	328	MET	4.2
1	O	92	GLY	4.1
1	C	396	MET	4.1
1	X	171	ILE	4.1
1	I	259	MET	4.1
1	K	141	ILE	4.1
1	O	99	ALA	4.1
1	Q	494	ILE	4.1
1	K	45	MET	4.1
1	X	96	GLY	4.1
1	G	102	GLU	4.1
1	H	476	CYS	4.1
1	I	476	CYS	4.0
1	O	298	MET	4.0
1	I	101	MET	4.0
1	U	494	ILE	4.0
1	F	346	MET	4.0
1	X	143	ILE	4.0
1	L	135	VAL	4.0
1	G	197	LEU	4.0
1	A	440	VAL	3.9
1	J	107	CYS	3.9
1	K	161	LEU	3.9
1	A	38	LYS	3.9
1	A	109	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	T	50	MET	3.9
1	H	93	GLN	3.9
1	P	258	ILE	3.9
1	A	302	MET	3.9
1	W	412	TYR	3.9
1	X	488	TYR	3.8
1	C	150	LEU	3.8
1	F	350	CYS	3.8
1	F	381	CYS	3.8
1	O	128	TYR	3.8
1	C	171	ILE	3.8
1	Q	476	CYS	3.8
1	G	27	ILE	3.8
1	F	342	VAL	3.8
1	A	412	TYR	3.8
1	J	150	LEU	3.8
1	H	161	LEU	3.8
1	D	370	GLN	3.7
1	D	412	TYR	3.7
1	J	294	CYS	3.7
1	L	294	CYS	3.7
1	W	476	CYS	3.7
1	N	50	MET	3.7
1	W	102	GLU	3.7
1	I	150	LEU	3.7
1	L	298	MET	3.7
1	P	57	HIS	3.7
1	X	237	CYS	3.7
1	N	131	LEU	3.7
1	F	328	MET	3.7
1	W	49	ARG	3.7
1	T	93	GLN	3.7
1	I	106	THR	3.7
1	W	184	VAL	3.7
1	G	106	THR	3.7
1	N	124	PHE	3.7
1	O	345	TYR	3.7
1	R	346	MET	3.7
1	A	27	ILE	3.7
1	B	367	LYS	3.7
1	I	299	LEU	3.7
1	X	170	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	449	HIS	3.6
1	L	346	MET	3.6
1	D	88	GLU	3.6
1	X	120	THR	3.6
1	J	396	MET	3.6
1	T	106	THR	3.6
1	C	188	ALA	3.6
1	O	184	VAL	3.6
1	N	239	ILE	3.6
1	O	18	TYR	3.6
1	T	165	VAL	3.6
1	K	143	ILE	3.6
1	H	207	MET	3.6
1	K	214	ARG	3.6
1	J	479	ILE	3.6
1	O	126	ILE	3.6
1	V	85	LYS	3.5
1	A	299	LEU	3.5
1	Q	162	GLU	3.5
1	A	475	TYR	3.5
1	J	106	THR	3.5
1	R	99	ALA	3.5
1	O	129	GLN	3.5
1	T	117	ASP	3.5
1	E	100	VAL	3.5
1	U	93	GLN	3.5
1	T	184	VAL	3.5
1	B	240	GLU	3.5
1	N	150	LEU	3.5
1	L	420	CYS	3.5
1	X	182	CYS	3.4
1	C	50	MET	3.4
1	O	479	ILE	3.4
1	T	412	TYR	3.4
1	D	239	ILE	3.4
1	O	433	ILE	3.4
1	P	143	ILE	3.4
1	K	163	CYS	3.4
1	O	153	GLN	3.4
1	H	124	PHE	3.4
1	O	326	CYS	3.4
1	R	320	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	P	261	ALA	3.4
1	D	96	GLY	3.4
1	U	412	TYR	3.4
1	C	350	CYS	3.3
1	J	11	ILE	3.3
1	M	150	LEU	3.3
1	R	148	LEU	3.3
1	X	399	LEU	3.3
1	Q	396	MET	3.3
1	X	306	PRO	3.3
1	C	207	MET	3.3
1	D	128	TYR	3.3
1	G	376	ALA	3.3
1	C	390	GLU	3.3
1	A	408	LEU	3.3
1	N	82	LEU	3.3
1	F	124	PHE	3.3
1	D	97	GLY	3.3
1	H	494	ILE	3.3
1	K	156	GLU	3.3
1	S	399	LEU	3.3
1	A	407	ARG	3.3
1	T	102	GLU	3.3
1	H	126	ILE	3.3
1	A	479	ILE	3.3
1	X	374	MET	3.2
1	G	165	VAL	3.2
1	R	106	THR	3.2
1	P	173	ASP	3.2
1	V	131	LEU	3.2
1	J	397	VAL	3.2
1	R	495	LEU	3.2
1	G	100	VAL	3.2
1	S	48	ALA	3.2
1	C	476	CYS	3.2
1	X	163	CYS	3.2
1	K	140	TYR	3.2
1	B	478	VAL	3.2
1	F	353	ALA	3.2
1	B	327	VAL	3.2
1	K	40	LEU	3.2
1	O	148	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	O	107	CYS	3.2
1	P	213	ILE	3.2
1	H	165	VAL	3.2
1	O	398	VAL	3.2
1	W	124	PHE	3.2
1	D	261	ALA	3.2
1	X	101	MET	3.2
1	A	184	VAL	3.2
1	M	374	MET	3.2
1	E	335	LYS	3.2
1	W	99	ALA	3.2
1	Q	182	CYS	3.2
1	U	101	MET	3.2
1	W	101	MET	3.2
1	W	493	ARG	3.2
1	N	101	MET	3.2
1	L	352	GLU	3.1
1	G	239	ILE	3.1
1	P	171	ILE	3.1
1	B	298	MET	3.1
1	N	161	LEU	3.1
1	D	381	CYS	3.1
1	B	50	MET	3.1
1	K	137	PRO	3.1
1	O	294	CYS	3.1
1	D	188	ALA	3.1
1	O	131	LEU	3.1
1	N	49	ARG	3.1
1	X	316	VAL	3.1
1	X	486	LYS	3.1
1	S	346	MET	3.1
1	F	49	ARG	3.1
1	R	131	LEU	3.1
1	T	105	ALA	3.1
1	D	258	ILE	3.1
1	L	101	MET	3.1
1	H	166	THR	3.1
1	H	92	GLY	3.1
1	P	259	MET	3.1
1	D	209	PHE	3.1
1	E	327	VAL	3.1
1	X	494	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	R	197	LEU	3.1
1	P	239	ILE	3.1
1	S	101	MET	3.1
1	K	367	LYS	3.1
1	G	107	CYS	3.1
1	A	161	LEU	3.1
1	K	170	THR	3.1
1	X	209	PHE	3.1
1	I	107	CYS	3.1
1	A	128	TYR	3.1
1	S	126	ILE	3.1
1	D	346	MET	3.1
1	F	480	HIS	3.1
1	T	9	LEU	3.1
1	A	125	TYR	3.1
1	F	431	LEU	3.0
1	Q	163	CYS	3.1
1	P	396	MET	3.0
1	T	494	ILE	3.0
1	X	214	ARG	3.0
1	R	82	LEU	3.0
1	W	169	HIS	3.0
1	T	376	ALA	3.0
1	X	135	VAL	3.0
1	C	131	LEU	3.0
1	E	180	PRO	3.0
1	A	126	ILE	3.0
1	G	128	TYR	3.0
1	J	328	MET	3.0
1	W	19	ARG	3.0
1	C	389	TYR	3.0
1	E	346	MET	3.0
1	G	399	LEU	3.0
1	J	299	LEU	3.0
1	Q	486	LYS	3.0
1	O	412	TYR	3.0
1	H	430	GLN	3.0
1	J	446	LYS	3.0
1	W	123	LYS	3.0
1	X	198	GLN	3.0
1	B	150	LEU	3.0
1	E	197	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	476	CYS	3.0
1	B	409	VAL	3.0
1	F	96	GLY	3.0
1	L	148	LEU	3.0
1	B	293	ILE	3.0
1	L	149	ILE	3.0
1	X	239	ILE	3.0
1	D	494	ILE	3.0
1	R	476	CYS	3.0
1	N	162	GLU	3.0
1	V	237	CYS	3.0
1	T	232	ASP	3.0
1	C	381	CYS	3.0
1	O	87	PRO	3.0
1	N	125	TYR	3.0
1	X	45	MET	3.0
1	I	91	THR	3.0
1	O	89	ILE	3.0
1	R	242	HIS	3.0
1	R	328	MET	3.0
1	E	390	GLU	3.0
1	H	350	CYS	3.0
1	V	390	GLU	3.0
1	C	399	LEU	3.0
1	J	268	GLU	3.0
1	J	161	LEU	2.9
1	J	237	CYS	2.9
1	W	107	CYS	2.9
1	F	50	MET	2.9
1	R	171	ILE	2.9
1	H	312	GLU	2.9
1	U	495	LEU	2.9
1	C	149	ILE	2.9
1	G	50	MET	2.9
1	S	57	HIS	2.9
1	R	261	ALA	2.9
1	R	107	CYS	2.9
1	C	128	TYR	2.9
1	L	480	HIS	2.9
1	J	73	GLU	2.9
1	S	374	MET	2.9
1	A	495	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	494	ILE	2.9
1	E	172	SER	2.9
1	P	406	ALA	2.9
1	K	172	SER	2.9
1	D	19	ARG	2.9
1	H	102	GLU	2.9
1	E	326	CYS	2.9
1	M	239	ILE	2.9
1	O	420	CYS	2.9
1	H	155	HIS	2.9
1	A	396	MET	2.9
1	E	150	LEU	2.9
1	J	412	TYR	2.9
1	U	148	LEU	2.9
1	N	163	CYS	2.9
1	E	135	VAL	2.9
1	D	433	ILE	2.9
1	E	170	THR	2.9
1	V	45	MET	2.9
1	V	184	VAL	2.9
1	V	437	VAL	2.9
1	M	23	ILE	2.9
1	B	131	LEU	2.9
1	U	73	GLU	2.9
1	L	399	LEU	2.9
1	O	189	VAL	2.9
1	U	197	LEU	2.9
1	D	374	MET	2.9
1	B	494	ILE	2.9
1	D	89	ILE	2.9
1	K	82	LEU	2.9
1	S	131	LEU	2.9
1	T	299	LEU	2.9
1	A	124	PHE	2.9
1	B	435	GLN	2.9
1	G	207	MET	2.8
1	I	126	ILE	2.8
1	U	141	ILE	2.8
1	V	294	CYS	2.8
1	X	126	ILE	2.8
1	X	169	HIS	2.8
1	E	184	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	299	LEU	2.8
1	K	294	CYS	2.8
1	C	287	VAL	2.8
1	S	359	GLU	2.8
1	P	434	THR	2.8
1	X	148	LEU	2.8
1	B	237	CYS	2.8
1	C	346	MET	2.8
1	R	49	ARG	2.8
1	W	148	LEU	2.8
1	H	23	ILE	2.8
1	R	141	ILE	2.8
1	U	433	ILE	2.8
1	B	492	THR	2.8
1	T	49	ARG	2.8
1	A	439	SER	2.8
1	X	155	HIS	2.8
1	F	237	CYS	2.8
1	A	37	LEU	2.8
1	F	492	THR	2.8
1	S	298	MET	2.8
1	T	298	MET	2.8
1	M	488	TYR	2.8
1	W	141	ILE	2.8
1	A	163	CYS	2.8
1	G	82	LEU	2.8
1	W	150	LEU	2.8
1	E	299	LEU	2.8
1	I	438	GLU	2.8
1	T	164	THR	2.8
1	R	143	ILE	2.8
1	X	136	ARG	2.8
1	N	165	VAL	2.8
1	G	150	LEU	2.8
1	M	381	CYS	2.8
1	J	124	PHE	2.8
1	P	236	ILE	2.8
1	I	118	LYS	2.8
1	T	27	ILE	2.8
1	T	100	VAL	2.8
1	U	476	CYS	2.8
1	O	161	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	T	399	LEU	2.8
1	W	328	MET	2.8
1	V	498	GLU	2.8
1	X	456	ARG	2.8
1	E	469	TYR	2.7
1	G	45	MET	2.7
1	T	316	VAL	2.7
1	V	143	ILE	2.7
1	U	131	LEU	2.7
1	B	101	MET	2.7
1	C	141	ILE	2.7
1	D	414	PRO	2.7
1	J	148	LEU	2.7
1	C	456	ARG	2.7
1	O	346	MET	2.7
1	N	85	LYS	2.7
1	L	406	ALA	2.7
1	V	197	LEU	2.7
1	O	136	ARG	2.7
1	R	262	ARG	2.7
1	R	469	TYR	2.7
1	O	359	GLU	2.7
1	V	84	THR	2.7
1	H	475	TYR	2.7
1	N	238	LYS	2.7
1	B	188	ALA	2.7
1	Q	495	LEU	2.7
1	N	64	ILE	2.7
1	O	174	ARG	2.7
1	V	433	ILE	2.7
1	W	428	CYS	2.7
1	A	346	MET	2.7
1	W	171	ILE	2.7
1	I	141	ILE	2.7
1	J	478	VAL	2.7
1	S	239	ILE	2.7
1	E	300	GLU	2.7
1	N	242	HIS	2.7
1	R	105	ALA	2.7
1	H	131	LEU	2.7
1	S	150	LEU	2.7
1	W	447	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	93	GLN	2.7
1	W	203	GLN	2.7
1	N	52	PHE	2.7
1	X	302	MET	2.7
1	O	269	ILE	2.7
1	X	27	ILE	2.7
1	F	327	VAL	2.7
1	T	492	THR	2.7
1	V	346	MET	2.7
1	A	496	LEU	2.7
1	B	24	ILE	2.7
1	L	142	TYR	2.7
1	R	125	TYR	2.7
1	C	419	VAL	2.7
1	C	420	CYS	2.7
1	J	141	ILE	2.7
1	N	141	ILE	2.7
1	P	399	LEU	2.7
1	X	259	MET	2.7
1	K	488	TYR	2.7
1	N	412	TYR	2.7
1	U	155	HIS	2.7
1	X	9	LEU	2.7
1	X	339	PRO	2.7
1	B	261	ALA	2.7
1	D	186	LEU	2.7
1	I	239	ILE	2.7
1	K	239	ILE	2.7
1	Q	197	LEU	2.7
1	U	124	PHE	2.7
1	X	409	VAL	2.7
1	G	479	ILE	2.7
1	M	197	LEU	2.7
1	K	476	CYS	2.6
1	L	428	CYS	2.6
1	O	140	TYR	2.6
1	F	265	LEU	2.6
1	G	93	GLN	2.6
1	P	291	PRO	2.6
1	E	143	ILE	2.6
1	M	11	ILE	2.6
1	G	124	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	P	376	ALA	2.6
1	X	201	VAL	2.6
1	X	492	THR	2.6
1	B	239	ILE	2.6
1	O	158	GLU	2.6
1	O	271	ALA	2.6
1	S	396	MET	2.6
1	U	367	LYS	2.6
1	B	87	PRO	2.6
1	D	376	ALA	2.6
1	F	304	TYR	2.6
1	G	32	GLN	2.6
1	M	96	GLY	2.6
1	V	150	LEU	2.6
1	X	82	LEU	2.6
1	A	152	VAL	2.6
1	L	124	PHE	2.6
1	Q	134	VAL	2.6
1	H	399	LEU	2.6
1	Q	488	TYR	2.6
1	B	184	VAL	2.6
1	W	23	ILE	2.6
1	R	150	LEU	2.6
1	V	57	HIS	2.6
1	B	259	MET	2.6
1	I	213	ILE	2.6
1	I	377	ASP	2.6
1	N	209	PHE	2.6
1	W	494	ILE	2.6
1	J	350	CYS	2.6
1	P	37	LEU	2.6
1	B	27	ILE	2.6
1	P	141	ILE	2.6
1	V	412	TYR	2.6
1	C	291	PRO	2.6
1	T	197	LEU	2.6
1	X	131	LEU	2.6
1	K	390	GLU	2.6
1	S	237	CYS	2.6
1	U	237	CYS	2.6
1	W	25	CYS	2.6
1	M	128	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	Q	479	ILE	2.6
1	R	23	ILE	2.6
1	F	207	MET	2.6
1	J	302	MET	2.6
1	R	316	VAL	2.6
1	E	489	ALA	2.6
1	K	243	GLN	2.6
1	B	346	MET	2.6
1	B	421	VAL	2.6
1	C	329	LEU	2.6
1	T	479	ILE	2.6
1	U	142	TYR	2.6
1	G	135	VAL	2.6
1	L	433	ILE	2.6
1	N	91	THR	2.6
1	Q	88	GLU	2.6
1	R	162	GLU	2.6
1	S	143	ILE	2.6
1	J	81	ALA	2.6
1	S	209	PHE	2.6
1	C	82	LEU	2.6
1	A	367	LYS	2.6
1	G	407	ARG	2.6
1	O	171	ILE	2.6
1	T	163	CYS	2.6
1	V	374	MET	2.6
1	I	406	ALA	2.6
1	W	18	TYR	2.6
1	A	110	THR	2.6
1	C	87	PRO	2.6
1	F	298	MET	2.6
1	U	374	MET	2.6
1	H	163	CYS	2.6
1	I	381	CYS	2.6
1	C	197	LEU	2.6
1	S	495	LEU	2.6
1	B	335	LYS	2.5
1	O	154	SER	2.5
1	T	209	PHE	2.5
1	U	239	ILE	2.5
1	W	50	MET	2.5
1	K	197	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	40	LEU	2.5
1	E	294	CYS	2.5
1	H	91	THR	2.5
1	O	434	THR	2.5
1	V	25	CYS	2.5
1	E	99	ALA	2.5
1	X	183	ASP	2.5
1	D	367	LYS	2.5
1	P	89	ILE	2.5
1	V	126	ILE	2.5
1	E	381	CYS	2.5
1	R	163	CYS	2.5
1	X	442	PHE	2.5
1	D	45	MET	2.5
1	I	171	ILE	2.5
1	M	126	ILE	2.5
1	W	209	PHE	2.5
1	Q	131	LEU	2.5
1	V	399	LEU	2.5
1	D	126	ILE	2.5
1	C	52	PHE	2.5
1	V	463	PHE	2.5
1	A	187	PRO	2.5
1	L	239	ILE	2.5
1	N	107	CYS	2.5
1	P	27	ILE	2.5
1	C	99	ALA	2.5
1	F	488	TYR	2.5
1	U	9	LEU	2.5
1	D	498	GLU	2.5
1	W	177	VAL	2.5
1	W	381	CYS	2.5
1	L	349	ILE	2.5
1	V	207	MET	2.5
1	L	329	LEU	2.5
1	C	328	MET	2.5
1	Q	345	TYR	2.5
1	R	184	VAL	2.5
1	G	372	ILE	2.5
1	B	420	CYS	2.5
1	O	175	ARG	2.5
1	U	406	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	V	438	GLU	2.5
1	B	412	TYR	2.5
1	C	412	TYR	2.5
1	J	469	TYR	2.5
1	M	152	VAL	2.5
1	X	313	VAL	2.5
1	J	155	HIS	2.5
1	W	377	ASP	2.5
1	B	381	CYS	2.5
1	D	153	GLN	2.5
1	D	182	CYS	2.5
1	V	298	MET	2.5
1	D	121	LYS	2.5
1	H	123	LYS	2.5
1	M	376	ALA	2.5
1	O	100	VAL	2.5
1	W	367	LYS	2.5
1	E	412	TYR	2.5
1	K	24	ILE	2.5
1	R	37	LEU	2.5
1	R	297	GLN	2.5
1	V	141	ILE	2.5
1	K	207	MET	2.5
1	A	254	GLU	2.5
1	A	129	GLN	2.5
1	R	496	LEU	2.5
1	X	184	VAL	2.5
1	P	19	ARG	2.5
1	D	418	ILE	2.5
1	F	370	GLN	2.5
1	O	143	ILE	2.5
1	W	106	THR	2.5
1	I	396	MET	2.5
1	W	346	MET	2.5
1	A	25	CYS	2.5
1	S	476	CYS	2.5
1	L	489	ALA	2.5
1	R	124	PHE	2.5
1	B	242	HIS	2.5
1	U	493	ARG	2.5
1	O	370	GLN	2.5
1	M	350	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	374	MET	2.5
1	F	94	PHE	2.5
1	W	183	ASP	2.5
1	V	467	LYS	2.5
1	W	219	VAL	2.5
1	A	107	CYS	2.5
1	B	479	ILE	2.5
1	D	122	ASP	2.4
1	E	98	ASP	2.4
1	R	433	ILE	2.5
1	V	78	ILE	2.5
1	F	329	LEU	2.4
1	O	419	VAL	2.4
1	Q	155	HIS	2.4
1	P	32	GLN	2.4
1	P	209	PHE	2.4
1	Q	89	ILE	2.4
1	M	357	LEU	2.4
1	M	476	CYS	2.4
1	P	237	CYS	2.4
1	T	489	ALA	2.4
1	X	119	GLY	2.4
1	U	269	ILE	2.4
1	B	37	LEU	2.4
1	K	148	LEU	2.4
1	P	362	PHE	2.4
1	C	27	ILE	2.4
1	Q	27	ILE	2.4
1	Q	381	CYS	2.4
1	C	493	ARG	2.4
1	O	176	GLY	2.4
1	V	186	LEU	2.4
1	T	88	GLU	2.4
1	M	141	ILE	2.4
1	V	171	ILE	2.4
1	H	396	MET	2.4
1	M	325	ASP	2.4
1	X	141	ILE	2.4
1	E	408	LEU	2.4
1	E	105	ALA	2.4
1	P	201	VAL	2.4
1	R	324	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	U	184	VAL	2.4
1	K	291	PRO	2.4
1	S	148	LEU	2.4
1	T	113	PRO	2.4
1	D	289	GLY	2.4
1	F	89	ILE	2.4
1	J	80	ILE	2.4
1	N	372	ILE	2.4
1	T	171	ILE	2.4
1	U	198	GLN	2.4
1	A	226	LEU	2.4
1	U	298	MET	2.4
1	I	376	ALA	2.4
1	V	128	TYR	2.4
1	B	258	ILE	2.4
1	D	235	ILE	2.4
1	E	171	ILE	2.4
1	H	495	LEU	2.4
1	J	82	LEU	2.4
1	M	342	VAL	2.4
1	Q	302	MET	2.4
1	S	81	ALA	2.4
1	U	350	CYS	2.4
1	S	494	ILE	2.4
1	P	439	SER	2.4
1	U	150	LEU	2.4
1	E	336	GLY	2.4
1	K	244	GLY	2.4
1	T	324	ALA	2.4
1	A	442	PHE	2.4
1	D	148	LEU	2.4
1	J	362	PHE	2.4
1	A	185	ASP	2.4
1	M	328	MET	2.4
1	J	416	CYS	2.4
1	O	381	CYS	2.4
1	O	399	LEU	2.4
1	V	198	GLN	2.4
1	W	294	CYS	2.4
1	I	298	MET	2.4
1	T	433	ILE	2.4
1	H	137	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	P	419	VAL	2.4
1	D	85	LYS	2.4
1	H	89	ILE	2.4
1	H	128	TYR	2.4
1	A	136	ARG	2.4
1	C	179	LEU	2.4
1	D	260	VAL	2.4
1	M	431	LEU	2.4
1	Q	90	ARG	2.4
1	P	372	ILE	2.4
1	X	489	ALA	2.4
1	Q	123	LYS	2.4
1	A	333	THR	2.4
1	Q	346	MET	2.4
1	T	45	MET	2.4
1	T	128	TYR	2.4
1	O	150	LEU	2.4
1	K	208	ILE	2.4
1	C	164	THR	2.4
1	D	497	VAL	2.4
1	P	104	GLY	2.4
1	H	346	MET	2.4
1	X	299	LEU	2.4
1	X	412	TYR	2.4
1	R	326	CYS	2.4
1	G	367	LYS	2.4
1	J	460	GLY	2.4
1	L	106	THR	2.4
1	M	396	MET	2.4
1	T	339	PRO	2.4
1	B	448	GLY	2.4
1	J	152	VAL	2.4
1	S	82	LEU	2.4
1	F	95	VAL	2.4
1	L	498	GLU	2.4
1	N	494	ILE	2.4
1	U	414	PRO	2.4
1	V	11	ILE	2.4
1	E	363	PHE	2.4
1	U	486	LYS	2.4
1	E	182	CYS	2.3
1	N	3	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	N	447	LEU	2.3
1	T	294	CYS	2.3
1	V	350	CYS	2.3
1	A	308	PRO	2.3
1	A	449	HIS	2.3
1	B	469	TYR	2.3
1	E	11	ILE	2.3
1	J	407	ARG	2.3
1	J	184	VAL	2.3
1	P	40	LEU	2.3
1	P	150	LEU	2.3
1	O	442	PHE	2.3
1	R	239	ILE	2.3
1	C	23	ILE	2.3
1	L	11	ILE	2.3
1	P	281	LEU	2.3
1	E	298	MET	2.3
1	P	244	GLY	2.3
1	E	87	PRO	2.3
1	O	270	PRO	2.3
1	B	260	VAL	2.3
1	J	300	GLU	2.3
1	M	498	GLU	2.3
1	X	157	ASP	2.3
1	B	234	MET	2.3
1	E	239	ILE	2.3
1	L	126	ILE	2.3
1	V	239	ILE	2.3
1	O	19	ARG	2.3
1	C	161	LEU	2.3
1	G	234	MET	2.3
1	I	50	MET	2.3
1	X	100	VAL	2.3
1	J	50	MET	2.3
1	O	258	ILE	2.3
1	O	397	VAL	2.3
1	Q	124	PHE	2.3
1	B	107	CYS	2.3
1	D	184	VAL	2.3
1	E	367	LYS	2.3
1	S	350	CYS	2.3
1	R	494	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	251	ILE	2.3
1	D	226	LEU	2.3
1	E	281	LEU	2.3
1	P	299	LEU	2.3
1	I	163	CYS	2.3
1	T	381	CYS	2.3
1	H	45	MET	2.3
1	J	367	LYS	2.3
1	O	260	VAL	2.3
1	A	150	LEU	2.3
1	J	329	LEU	2.3
1	P	52	PHE	2.3
1	A	478	VAL	2.3
1	C	298	MET	2.3
1	Q	492	THR	2.3
1	S	109	VAL	2.3
1	E	238	LYS	2.3
1	W	374	MET	2.3
1	A	329	LEU	2.3
1	I	125	TYR	2.3
1	N	143	ILE	2.3
1	A	469	TYR	2.3
1	E	163	CYS	2.3
1	K	311	ALA	2.3
1	U	135	VAL	2.3
1	U	265	LEU	2.3
1	W	27	ILE	2.3
1	W	498	GLU	2.3
1	A	298	MET	2.3
1	I	104	GLY	2.3
1	U	117	ASP	2.3
1	H	162	GLU	2.3
1	W	320	VAL	2.3
1	C	237	CYS	2.3
1	Q	294	CYS	2.3
1	E	96	GLY	2.3
1	Q	184	VAL	2.3
1	C	88	GLU	2.3
1	S	141	ILE	2.3
1	S	348	ARG	2.3
1	X	381	CYS	2.3
1	X	177	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	208	ILE	2.3
1	R	27	ILE	2.3
1	U	143	ILE	2.3
1	R	384	ALA	2.3
1	S	40	LEU	2.3
1	A	245	VAL	2.3
1	B	11	ILE	2.3
1	H	24	ILE	2.3
1	O	183	ASP	2.3
1	Q	141	ILE	2.3
1	T	129	GLN	2.3
1	L	431	LEU	2.3
1	X	271	ALA	2.3
1	F	366	ILE	2.3
1	I	350	CYS	2.3
1	N	259	MET	2.3
1	W	350	CYS	2.3
1	A	397	VAL	2.3
1	O	186	LEU	2.3
1	U	21	ALA	2.3
1	D	345	TYR	2.2
1	M	272	GLU	2.3
1	I	433	ILE	2.2
1	V	372	ILE	2.2
1	O	152	VAL	2.2
1	Q	397	VAL	2.2
1	K	209	PHE	2.2
1	A	300	GLU	2.2
1	D	293	ILE	2.2
1	D	359	GLU	2.2
1	T	31	THR	2.2
1	J	174	ARG	2.2
1	J	380	VAL	2.2
1	O	435	GLN	2.2
1	F	483	HIS	2.2
1	L	476	CYS	2.2
1	G	431	LEU	2.2
1	M	434	THR	2.2
1	P	433	ILE	2.2
1	R	208	ILE	2.2
1	I	161	LEU	2.2
1	K	150	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	T	118	LYS	2.2
1	R	213	ILE	2.2
1	H	150	LEU	2.2
1	L	197	LEU	2.2
1	N	399	LEU	2.2
1	H	328	MET	2.2
1	U	232	ASP	2.2
1	V	259	MET	2.2
1	T	155	HIS	2.2
1	E	148	LEU	2.2
1	F	140	TYR	2.2
1	H	197	LEU	2.2
1	M	161	LEU	2.2
1	S	488	TYR	2.2
1	T	186	LEU	2.2
1	W	281	LEU	2.2
1	A	91	THR	2.2
1	C	418	ILE	2.2
1	K	251	ILE	2.2
1	R	349	ILE	2.2
1	W	259	MET	2.2
1	F	385	VAL	2.2
1	A	46	SER	2.2
1	J	238	LYS	2.2
1	S	406	ALA	2.2
1	T	327	VAL	2.2
1	V	3	LEU	2.2
1	X	238	LYS	2.2
1	A	203	GLN	2.2
1	E	278	GLN	2.2
1	R	101	MET	2.2
1	S	259	MET	2.2
1	T	233	ILE	2.2
1	C	90	ARG	2.2
1	I	495	LEU	2.2
1	J	480	HIS	2.2
1	P	88	GLU	2.2
1	S	85	LYS	2.2
1	T	173	ASP	2.2
1	A	366	ILE	2.2
1	D	91	THR	2.2
1	R	108	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	82	LEU	2.2
1	G	9	LEU	2.2
1	L	88	GLU	2.2
1	J	137	PRO	2.2
1	J	327	VAL	2.2
1	L	381	CYS	2.2
1	V	414	PRO	2.2
1	W	488	TYR	2.2
1	M	101	MET	2.2
1	F	352	GLU	2.2
1	N	197	LEU	2.2
1	P	413	ARG	2.2
1	J	342	VAL	2.2
1	D	308	PRO	2.2
1	J	406	ALA	2.2
1	N	48	ALA	2.2
1	O	455	HIS	2.2
1	Q	477	VAL	2.2
1	R	396	MET	2.2
1	W	311	ALA	2.2
1	T	150	LEU	2.2
1	D	363	PHE	2.2
1	T	170	THR	2.2
1	U	67	VAL	2.2
1	H	27	ILE	2.2
1	U	258	ILE	2.2
1	V	120	THR	2.2
1	A	138	GLY	2.2
1	P	319	ALA	2.2
1	L	343	VAL	2.2
1	U	179	LEU	2.2
1	X	346	MET	2.2
1	S	27	ILE	2.2
1	U	40	LEU	2.2
1	V	316	VAL	2.2
1	X	485	VAL	2.2
1	H	214	ARG	2.2
1	Q	101	MET	2.2
1	Q	493	ARG	2.2
1	G	80	ILE	2.2
1	K	213	ILE	2.2
1	A	140	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	316	VAL	2.2
1	Q	135	VAL	2.2
1	S	345	TYR	2.2
1	V	82	LEU	2.2
1	N	479	ILE	2.2
1	I	417	PRO	2.2
1	K	100	VAL	2.2
1	K	109	VAL	2.2
1	U	57	HIS	2.2
1	V	135	VAL	2.2
1	K	353	ALA	2.2
1	K	469	TYR	2.2
1	E	262	ARG	2.2
1	I	260	VAL	2.2
1	J	298	MET	2.2
1	B	148	LEU	2.2
1	J	345	TYR	2.2
1	J	236	ILE	2.2
1	K	183	ASP	2.2
1	O	41	ILE	2.2
1	S	182	CYS	2.2
1	W	94	PHE	2.2
1	H	259	MET	2.2
1	H	353	ALA	2.2
1	N	281	LEU	2.2
1	J	456	ARG	2.2
1	N	27	ILE	2.2
1	Q	126	ILE	2.2
1	T	90	ARG	2.2
1	C	294	CYS	2.2
1	J	438	GLU	2.2
1	D	207	MET	2.2
1	Q	489	ALA	2.2
1	M	345	TYR	2.2
1	O	74	LEU	2.2
1	O	135	VAL	2.2
1	U	45	MET	2.2
1	D	87	PRO	2.1
1	S	134	VAL	2.1
1	V	209	PHE	2.1
1	W	158	GLU	2.1
1	O	293	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	207	MET	2.1
1	G	19	ARG	2.1
1	L	128	TYR	2.1
1	P	483	HIS	2.1
1	V	125	TYR	2.1
1	X	213	ILE	2.1
1	G	52	PHE	2.1
1	G	353	ALA	2.1
1	O	197	LEU	2.1
1	R	268	GLU	2.1
1	C	367	LYS	2.1
1	F	367	LYS	2.1
1	I	122	ASP	2.1
1	X	433	ILE	2.1
1	A	285	CYS	2.1
1	D	362	PHE	2.1
1	P	463	PHE	2.1
1	R	397	VAL	2.1
1	S	100	VAL	2.1
1	C	85	LYS	2.1
1	E	337	LYS	2.1
1	H	85	LYS	2.1
1	L	171	ILE	2.1
1	B	209	PHE	2.1
1	D	488	TYR	2.1
1	H	108	TYR	2.1
1	I	488	TYR	2.1
1	O	47	VAL	2.1
1	S	381	CYS	2.1
1	C	166	THR	2.1
1	E	186	LEU	2.1
1	P	208	ILE	2.1
1	J	435	GLN	2.1
1	X	94	PHE	2.1
1	E	295	ALA	2.1
1	M	29	PRO	2.1
1	X	180	PRO	2.1
1	A	252	ILE	2.1
1	C	165	VAL	2.1
1	P	494	ILE	2.1
1	R	342	VAL	2.1
1	X	11	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	346	MET	2.1
1	C	37	LEU	2.1
1	D	265	LEU	2.1
1	D	218	GLN	2.1
1	P	28	GLY	2.1
1	P	370	GLN	2.1
1	H	188	ALA	2.1
1	B	23	ILE	2.1
1	B	141	ILE	2.1
1	C	83	ASP	2.1
1	G	329	LEU	2.1
1	N	366	ILE	2.1
1	R	296	THR	2.1
1	A	114	ALA	2.1
1	K	177	VAL	2.1
1	B	329	LEU	2.1
1	C	155	HIS	2.1
1	C	494	ILE	2.1
1	T	469	TYR	2.1
1	V	418	ILE	2.1
1	W	131	LEU	2.1
1	N	376	ALA	2.1
1	P	177	VAL	2.1
1	P	262	ARG	2.1
1	T	457	VAL	2.1
1	W	456	ARG	2.1
1	I	143	ILE	2.1
1	R	281	LEU	2.1
1	S	45	MET	2.1
1	G	109	VAL	2.1
1	A	467	LYS	2.1
1	J	205	VAL	2.1
1	W	165	VAL	2.1
1	E	188	ALA	2.1
1	F	182	CYS	2.1
1	G	99	ALA	2.1
1	H	294	CYS	2.1
1	O	93	GLN	2.1
1	S	334	ALA	2.1
1	T	476	CYS	2.1
1	J	488	TYR	2.1
1	L	37	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	377	ASP	2.1
1	W	45	MET	2.1
1	E	141	ILE	2.1
1	L	439	SER	2.1
1	A	420	CYS	2.1
1	E	490	ASN	2.1
1	I	329	LEU	2.1
1	M	316	VAL	2.1
1	O	109	VAL	2.1
1	J	182	CYS	2.1
1	M	335	LYS	2.1
1	T	335	LYS	2.1
1	V	17	ASN	2.1
1	I	325	ASP	2.1
1	H	493	ARG	2.1
1	O	261	ALA	2.1
1	P	91	THR	2.1
1	W	293	ILE	2.1
1	W	226	LEU	2.1
1	W	370	GLN	2.1
1	X	479	ILE	2.1
1	Q	183	ASP	2.1
1	D	328	MET	2.1
1	J	109	VAL	2.1
1	U	116	ALA	2.1
1	X	342	VAL	2.1
1	T	89	ILE	2.1
1	J	370	GLN	2.1
1	B	124	PHE	2.1
1	S	15	VAL	2.1
1	F	479	ILE	2.1
1	S	492	THR	2.1
1	T	328	MET	2.1
1	A	148	LEU	2.1
1	D	236	ILE	2.1
1	O	137	PRO	2.1
1	T	413	ARG	2.1
1	X	162	GLU	2.1
1	P	408	LEU	2.1
1	Q	408	LEU	2.1
1	D	294	CYS	2.1
1	R	367	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	V	420	CYS	2.1
1	M	389	TYR	2.1
1	C	226	LEU	2.1
1	I	245	VAL	2.1
1	H	297	GLN	2.1
1	K	154	SER	2.1
1	K	302	MET	2.1
1	K	495	LEU	2.1
1	O	209	PHE	2.1
1	R	209	PHE	2.1
1	T	92	GLY	2.1
1	A	489	ALA	2.1
1	F	349	ILE	2.1
1	G	350	CYS	2.1
1	M	433	ILE	2.1
1	U	475	TYR	2.1
1	W	222	VAL	2.1
1	B	179	LEU	2.1
1	D	197	LEU	2.1
1	F	399	LEU	2.1
1	L	131	LEU	2.1
1	B	94	PHE	2.0
1	C	124	PHE	2.0
1	I	489	ALA	2.0
1	L	367	LYS	2.0
1	V	328	MET	2.0
1	A	360	TYR	2.0
1	C	140	TYR	2.0
1	F	239	ILE	2.0
1	G	103	ARG	2.0
1	V	91	THR	2.0
1	B	350	CYS	2.0
1	K	241	ASN	2.0
1	F	93	GLN	2.0
1	B	189	VAL	2.0
1	B	437	VAL	2.0
1	D	23	ILE	2.0
1	H	479	ILE	2.0
1	L	261	ALA	2.0
1	T	208	ILE	2.0
1	G	131	LEU	2.0
1	K	122	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	N	240	GLU	2.0
1	E	260	VAL	2.0
1	K	27	ILE	2.0
1	L	372	ILE	2.0
1	N	207	MET	2.0
1	N	350	CYS	2.0
1	O	443	ASP	2.0
1	P	495	LEU	2.0
1	S	26	THR	2.0
1	B	397	VAL	2.0
1	G	240	GLU	2.0
1	I	105	ALA	2.0
1	M	384	ALA	2.0
1	M	82	LEU	2.0
1	M	124	PHE	2.0
1	P	45	MET	2.0
1	W	425	LEU	2.0
1	I	258	ILE	2.0
1	O	127	ASP	2.0
1	P	212	PHE	2.0
1	I	324	ALA	2.0
1	X	188	ALA	2.0
1	B	419	VAL	2.0
1	J	260	VAL	2.0
1	L	260	VAL	2.0
1	O	396	MET	2.0
1	Q	374	MET	2.0
1	S	412	TYR	2.0
1	B	442	PHE	2.0
1	E	433	ILE	2.0
1	F	433	ILE	2.0
1	T	421	VAL	2.0
1	V	251	ILE	2.0
1	W	489	ALA	2.0
1	X	38	LYS	2.0
1	L	182	CYS	2.0
1	X	420	CYS	2.0
1	I	408	LEU	2.0
1	L	328	MET	2.0
1	S	431	LEU	2.0
1	W	323	GLY	2.0
1	F	184	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	70	ALA	2.0
1	L	99	ALA	2.0
1	Q	412	TYR	2.0
1	R	142	TYR	2.0
1	R	295	ALA	2.0
1	U	154	SER	2.0
1	E	449	HIS	2.0
1	E	493	ARG	2.0
1	O	179	LEU	2.0
1	A	313	VAL	2.0
1	H	367	LYS	2.0
1	L	92	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FDP	C	700	20/20	0.33	-0.42	25,32,34,35	0
2	FDP	H	700	20/20	0.32	-0.53	25,32,34,35	0
2	FDP	V	700	20/20	0.30	-0.62	25,32,34,35	0
2	FDP	S	700	20/20	0.33	-0.63	25,32,34,35	0
2	FDP	F	700	20/20	0.31	-0.72	25,32,34,35	0
2	FDP	G	700	20/20	0.31	-0.74	25,32,34,35	0
2	FDP	E	700	20/20	0.24	-0.76	25,32,34,35	0
2	FDP	K	700	20/20	0.27	-0.78	25,32,34,35	0
2	FDP	X	700	20/20	0.34	-0.79	25,32,34,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FDP	U	700	20/20	0.32	-0.80	25,32,34,35	0
2	FDP	P	700	20/20	0.29	-0.84	25,32,34,35	0
2	FDP	T	700	20/20	0.25	-0.85	25,32,34,35	0
2	FDP	Q	700	20/20	0.30	-0.89	25,32,34,35	0
2	FDP	J	700	20/20	0.37	-0.89	25,32,34,35	0
2	FDP	W	700	20/20	0.33	-0.98	25,32,34,35	0
2	FDP	A	700	20/20	0.19	-1.05	25,32,34,35	0
2	FDP	L	700	20/20	0.30	-1.06	25,32,34,35	0
2	FDP	N	700	20/20	0.26	-1.07	25,32,34,35	0
2	FDP	B	700	20/20	0.19	-1.17	25,32,34,35	0
2	FDP	D	700	20/20	0.24	-1.19	25,32,34,35	0
2	FDP	O	700	20/20	0.26	-1.20	25,32,34,35	0
2	FDP	M	700	20/20	0.22	-1.27	25,32,34,35	0
2	FDP	R	700	20/20	0.23	-1.35	25,32,34,35	0
2	FDP	I	700	20/20	0.25	-1.57	25,32,34,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.