



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:12 am BST

PDB ID : 5WMH  
Title : Arabidopsis thaliana prephenate aminotransferase  
Authors : Holland, C.K.; Jez, J.M.  
Deposited on : 2017-07-28  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

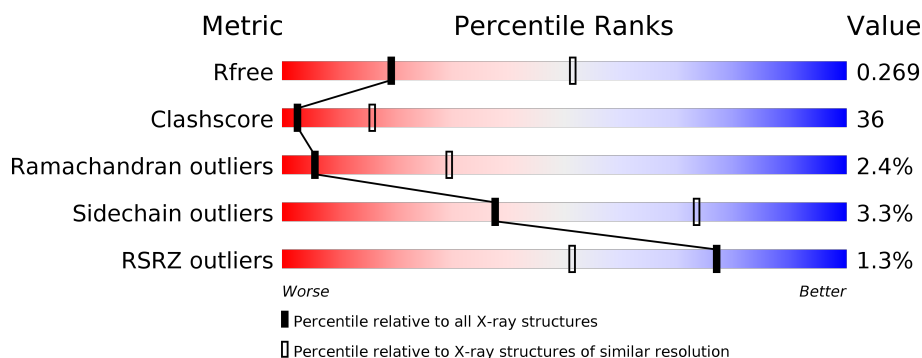
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	475	<div> <div>%</div> <div> <div></div> <div>57%</div> <div>24%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	475	<div> <div>%</div> <div> <div></div> <div>57%</div> <div>24%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	475	<div> <div>%</div> <div> <div></div> <div>57%</div> <div>25%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	475	<div> <div></div> <div> <div>53%</div> <div>28%</div> <div>••</div> <div>16%</div> </div> </div>
1	E	475	<div> <div>%</div> <div> <div></div> <div>34%</div> <div>46%</div> <div>•</div> <div>16%</div> </div> </div>
1	F	475	<div> <div>3%</div> <div> <div></div> <div>22%</div> <div>48%</div> <div>10%</div> <div>•</div> <div>16%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 18299 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Bifunctional aspartate aminotransferase and glutamate/aspartate-prephenate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	1	0
			3034	1941	507	576	10			
1	B	399	Total	C	N	O	S	0	0	0
			3027	1936	505	576	10			
1	C	401	Total	C	N	O	S	0	0	0
			3038	1940	507	580	11			
1	D	400	Total	C	N	O	S	0	0	0
			3035	1941	506	577	11			
1	E	399	Total	C	N	O	S	0	0	0
			3027	1936	505	576	10			
1	F	397	Total	C	N	O	S	0	0	0
			3007	1921	501	574	11			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).




Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	14	Total	O	0	0
			14	14		
3	C	8	Total	O	0	0
			8	8		
3	D	11	Total	O	0	0
			11	11		
3	E	1	Total	O	0	0
			1	1		
3	F	3	Total	O	0	0
			3	3		

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

- Chain A: 

- Chain B:

57% 24% 16%

Amino Acid	Percentage (%)
ALA	0.1
GLU	0.1
THR	0.1
LEU	0.1
SER	0.1
VAL	0.1
ASP	0.1
GLY	0.1
ARG	0.1
ILE	0.1
ASP	0.1
GLY	0.1
GLU	0.1
VAL	0.1
ASP	0.1
GLY	0.1
ARG	0.1
ILE	0.1
ASP	0.1
GLY	0.1
GLU	0.1
VAL	0.1
ASP	0.1
GLY	0.1
ARG	0.1
ILE	0.1
ASP	0.1
GLY	0.1
GLU	0.1
VAL	0.1
ASP	0.1
GLY	0.1
ARG	0.1
ILE	0.1
ASP	0.1
GLY	0.1
GLU	0.1
VAL	0.1
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GLU	0.1
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ASP	0.1
GLY	0.1
ARG	0.1
ILE	0.1
ASP	0.1
GLY	0.1
GLU	0.1
VAL	0.1
ASP	0.1
GLY	0.1
ARG	0.1
ILE	0.1
ASP	0.1
GLY	





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.34Å 111.58Å 141.78Å 90.00° 90.37° 90.00°	Depositor
Resolution (Å)	33.27 – 3.00 33.27 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.27-3.00) 99.7 (33.27-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.14 (at 3.00Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, $R_{free}$	0.210 , 0.270 0.210 , 0.269	Depositor DCC
$R_{free}$ test set	2515 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.5	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	18299	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.66	1/3096 (0.0%)	0.85	7/4203 (0.2%)
1	B	0.67	1/3085 (0.0%)	0.98	6/4187 (0.1%)
1	C	0.66	2/3096 (0.1%)	0.85	6/4201 (0.1%)
1	D	0.67	1/3093 (0.0%)	0.90	8/4197 (0.2%)
1	E	0.62	1/3085 (0.0%)	0.93	10/4187 (0.2%)
1	F	0.82	16/3063 (0.5%)	1.52	58/4155 (1.4%)
All	All	0.68	22/18518 (0.1%)	1.03	95/25130 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	10
All	All	0	20

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	372	ARG	NE-CZ	9.56	1.45	1.33
1	C	180	CYS	CB-SG	-7.90	1.68	1.82
1	F	448	TYR	CD2-CE2	-7.68	1.27	1.39
1	F	372	ARG	CD-NE	7.30	1.58	1.46
1	F	366	LYS	CB-CG	6.98	1.71	1.52
1	F	372	ARG	CZ-NH2	-6.97	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	CYS	CB-SG	-6.96	1.70	1.82
1	F	370	GLU	CB-CG	6.96	1.65	1.52
1	F	448	TYR	CE2-CZ	-6.23	1.30	1.38
1	E	266	ARG	CG-CD	5.97	1.66	1.51
1	F	369	ARG	CB-CG	-5.78	1.36	1.52
1	F	404	TYR	CD2-CE2	-5.71	1.30	1.39
1	D	466	LEU	CG-CD1	-5.58	1.31	1.51
1	F	448	TYR	CD1-CE1	-5.55	1.31	1.39
1	C	328	CYS	CB-SG	-5.51	1.72	1.81
1	F	369	ARG	CA-C	5.49	1.67	1.52
1	F	369	ARG	C-N	5.43	1.46	1.34
1	B	95	VAL	CB-CG2	-5.37	1.41	1.52
1	F	90	LEU	CG-CD2	-5.24	1.32	1.51
1	F	224	ASP	CB-CG	-5.21	1.40	1.51
1	F	370	GLU	N-CA	5.15	1.56	1.46
1	F	369	ARG	CG-CD	-5.02	1.39	1.51

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	372	ARG	NE-CZ-NH1	36.16	138.38	120.30
1	B	166	ASN	CB-CG-OD1	25.46	172.53	121.60
1	F	372	ARG	NH1-CZ-NH2	-17.13	100.56	119.40
1	B	166	ASN	CB-CG-ND2	-16.95	76.02	116.70
1	F	372	ARG	CD-NE-CZ	15.84	145.77	123.60
1	F	369	ARG	NE-CZ-NH2	-14.94	112.83	120.30
1	F	366	LYS	CA-CB-CG	13.04	142.09	113.40
1	F	264	HIS	N-CA-CB	12.93	133.87	110.60
1	F	372	ARG	CG-CD-NE	12.19	137.40	111.80
1	F	147	ARG	CG-CD-NE	12.09	137.19	111.80
1	F	264	HIS	CB-CA-C	-11.88	86.63	110.40
1	F	366	LYS	CB-CG-CD	11.28	140.92	111.60
1	F	314	ARG	NE-CZ-NH1	-11.25	114.67	120.30
1	E	253	LEU	CA-CB-CG	11.15	140.96	115.30
1	F	146	CYS	CA-CB-SG	10.75	133.35	114.00
1	E	466	LEU	CB-CG-CD2	-10.73	92.77	111.00
1	F	90	LEU	CB-CG-CD2	-10.19	93.68	111.00
1	F	147	ARG	CD-NE-CZ	9.98	137.58	123.60
1	F	217	ASN	CB-CG-ND2	-9.27	94.46	116.70
1	D	466	LEU	CB-CG-CD1	-9.05	95.62	111.00
1	F	369	ARG	CG-CD-NE	-8.94	93.02	111.80
1	D	466	LEU	CB-CG-CD2	8.93	126.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	234	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	F	123	ASN	N-CA-CB	8.88	126.59	110.60
1	F	318	LEU	CA-CB-CG	-8.68	95.33	115.30
1	B	166	ASN	OD1-CG-ND2	-8.67	101.96	121.90
1	F	122	ILE	C-N-CA	-8.28	101.00	121.70
1	F	147	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	F	369	ARG	C-N-CA	8.03	141.77	121.70
1	F	460	GLU	OE1-CD-OE2	-7.97	113.73	123.30
1	F	368	TYR	C-N-CA	7.89	141.43	121.70
1	D	94	LEU	CA-CB-CG	7.88	133.43	115.30
1	F	173	LEU	CA-CB-CG	7.62	132.84	115.30
1	B	469	LEU	CB-CG-CD2	-7.54	98.19	111.00
1	C	96	GLN	CA-CB-CG	7.46	129.82	113.40
1	F	452	LEU	CB-CG-CD2	-7.20	98.77	111.00
1	F	452	LEU	CB-CG-CD1	7.03	122.96	111.00
1	C	96	GLN	CG-CD-NE2	-6.81	100.35	116.70
1	F	217	ASN	N-CA-CB	6.80	122.84	110.60
1	F	466	LEU	CB-CG-CD2	-6.77	99.50	111.00
1	A	410	GLY	C-N-CA	6.75	138.59	121.70
1	F	448	TYR	CB-CG-CD2	-6.74	116.96	121.00
1	F	369	ARG	CB-CG-CD	-6.58	94.49	111.60
1	A	415	ASN	CB-CA-C	-6.55	97.29	110.40
1	F	425	LEU	CB-CG-CD2	-6.42	100.09	111.00
1	E	291	LEU	CB-CG-CD2	-6.39	100.14	111.00
1	F	314	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	E	75	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	F	147	ARG	NH1-CZ-NH2	-6.11	112.68	119.40
1	F	229	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	238	LEU	CB-CG-CD2	-6.05	100.71	111.00
1	E	266	ARG	CG-CD-NE	5.98	124.35	111.80
1	F	94	LEU	CA-CB-CG	5.96	129.00	115.30
1	A	415	ASN	N-CA-CB	-5.95	99.88	110.60
1	C	71	SER	C-N-CA	5.92	136.49	121.70
1	F	246	GLY	N-CA-C	-5.89	98.36	113.10
1	A	425	LEU	CA-CB-CG	5.82	128.68	115.30
1	F	371	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	F	254	LEU	CA-CB-CG	5.76	128.54	115.30
1	E	266	ARG	CA-CB-CG	5.75	126.04	113.40
1	F	238	LEU	CB-CG-CD1	-5.73	101.26	111.00
1	F	223	LYS	CB-CG-CD	5.72	126.47	111.60
1	C	318	LEU	CA-CB-CG	5.70	128.42	115.30
1	F	217	ASN	CB-CA-C	-5.68	99.04	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	375	LEU	CA-CB-CG	5.65	128.29	115.30
1	F	371	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	F	228	LYS	N-CA-C	-5.62	95.82	111.00
1	F	330	LYS	N-CA-CB	5.62	120.71	110.60
1	F	146	CYS	CB-CA-C	-5.59	99.21	110.40
1	F	142	ARG	CB-CG-CD	-5.54	97.20	111.60
1	B	80	LYS	N-CA-C	-5.50	96.14	111.00
1	D	427	LYS	CD-CE-NZ	-5.50	99.04	111.70
1	D	466	LEU	CA-CB-CG	5.47	127.88	115.30
1	F	144	ALA	C-N-CA	5.37	135.13	121.70
1	F	361	VAL	CG1-CB-CG2	5.36	119.48	110.90
1	F	369	ARG	N-CA-C	5.35	125.44	111.00
1	F	249	TYR	CA-CB-CG	5.34	123.55	113.40
1	E	234	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	225	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	D	422	LEU	CA-CB-CG	5.30	127.50	115.30
1	D	90	LEU	CA-CB-CG	5.29	127.47	115.30
1	F	460	GLU	CG-CD-OE1	5.29	128.88	118.30
1	E	254	LEU	CA-CB-CG	5.29	127.46	115.30
1	F	448	TYR	CB-CG-CD1	5.21	124.12	121.00
1	B	142	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	F	315	LEU	CA-CB-CG	-5.13	103.49	115.30
1	A	134	LEU	CA-CB-CG	5.11	127.04	115.30
1	C	306	LYS	CD-CE-NZ	-5.09	100.00	111.70
1	F	369	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	E	260	ILE	CG1-CB-CG2	-5.07	100.24	111.40
1	F	219	LEU	CB-CG-CD1	5.06	119.61	111.00
1	F	257	ILE	CG1-CB-CG2	-5.06	100.27	111.40
1	F	391	GLN	CA-CB-CG	5.06	124.53	113.40
1	C	427	LYS	CD-CE-NZ	-5.04	100.12	111.70
1	F	94	LEU	CB-CG-CD1	5.04	119.56	111.00

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	TYR	Peptide
1	A	410	GLY	Peptide
1	A	71	SER	Peptide
1	B	280	TYR	Peptide
1	C	405	GLY	Peptide
1	C	96	GLN	Sidechain

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Mol	Chain	Res	Type	Group
1	D	92	ALA	Peptide
1	D	94	LEU	Peptide
1	E	381	ASP	Peptide
1	E	80	LYS	Peptide
1	F	123	ASN	Sidechain
1	F	216	ASN	Peptide
1	F	217	ASN	Sidechain
1	F	227	SER	Peptide
1	F	228	LYS	Mainchain,Peptide
1	F	246	GLY	Peptide
1	F	264	HIS	Sidechain,Mainchain
1	F	369	ARG	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3034	0	3097	123	1
1	B	3027	0	3090	131	0
1	C	3038	0	3087	124	0
1	D	3035	0	3099	159	1
1	E	3027	0	3090	294	0
1	F	3007	0	3048	539	0
2	A	15	0	7	1	0
2	B	15	0	7	1	0
2	C	15	0	7	2	0
2	D	15	0	7	3	0
2	E	15	0	7	1	0
2	F	15	0	7	4	0
3	A	4	0	0	0	0
3	B	14	0	0	2	1
3	C	8	0	0	0	0
3	D	11	0	0	0	1
3	E	1	0	0	0	0
3	F	3	0	0	1	0
All	All	18299	0	18553	1320	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 36.

All (1320) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:GLU:N	1:F:147:ARG:HH12	1.13	1.45
1:B:102:ILE:HD12	1:B:103:ARG:N	1.37	1.34
1:F:143:GLU:CA	1:F:147:ARG:CZ	2.05	1.33
1:F:143:GLU:N	1:F:147:ARG:NH1	1.74	1.33
1:C:96:GLN:CA	1:C:96:GLN:HE21	1.34	1.29
1:E:253:LEU:CD1	1:E:254:LEU:HG	1.62	1.28
1:F:143:GLU:HA	1:F:147:ARG:CZ	1.62	1.28
1:F:317:TYR:O	1:F:318:LEU:HD22	1.24	1.28
1:F:317:TYR:C	1:F:318:LEU:HD22	1.58	1.22
1:F:143:GLU:CA	1:F:147:ARG:NH1	2.02	1.22
1:C:96:GLN:HA	1:C:96:GLN:NE2	1.44	1.21
1:F:300:THR:O	1:F:318:LEU:HD12	1.42	1.17
1:F:372:ARG:HB3	1:F:448:TYR:OH	1.43	1.15
1:E:196:TYR:OH	1:E:239:CYS:SG	2.05	1.14
1:F:142:ARG:C	1:F:147:ARG:HH12	1.49	1.13
1:F:223:LYS:HG3	1:F:226:GLU:N	1.64	1.12
1:F:223:LYS:HD3	1:F:224:ASP:CA	1.80	1.12
1:F:144:ALA:N	1:F:147:ARG:HH11	1.45	1.11
1:F:143:GLU:C	1:F:147:ARG:NH1	2.05	1.10
1:F:144:ALA:N	1:F:147:ARG:NH1	1.98	1.10
1:F:372:ARG:HD2	1:F:373:ASP:N	1.66	1.09
1:F:226:GLU:HA	1:F:228:LYS:O	1.51	1.09
1:F:87:ILE:HA	1:F:90:LEU:HD21	1.14	1.09
1:F:162:ILE:HD13	1:F:319:ALA:HB2	1.35	1.08
1:F:371:ARG:HB3	1:F:448:TYR:HE1	1.16	1.07
1:F:223:LYS:HG2	1:F:225:LEU:N	1.70	1.07
1:F:356:ALA:HB1	1:F:361:VAL:H	0.97	1.06
1:E:254:LEU:HB3	1:E:291:LEU:HD21	1.36	1.06
1:F:225:LEU:HD12	1:F:229:LEU:CD1	1.85	1.06
1:F:372:ARG:CD	1:F:373:ASP:H	1.67	1.06
1:E:136:ALA:HB3	1:E:142:ARG:HH21	1.08	1.05
1:C:267:LEU:O	1:C:297:ARG:NH1	1.87	1.05
1:E:80:LYS:HG3	1:E:81:PRO:HD3	1.32	1.05
1:E:253:LEU:HD12	1:E:254:LEU:HG	1.33	1.05
1:F:409:GLU:OE1	1:F:415:ASN:ND2	1.90	1.04
1:F:223:LYS:HE3	1:F:226:GLU:C	1.78	1.04
1:E:249:TYR:O	1:E:253:LEU:HD23	1.58	1.03
1:F:143:GLU:C	1:F:147:ARG:CZ	2.25	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:ALA:HB2	1:D:425:LEU:HD21	1.41	1.02
1:D:466:LEU:HD13	1:D:466:LEU:H	1.20	1.02
1:F:371:ARG:HA	1:F:374:PHE:CD1	1.94	1.02
1:F:223:LYS:HD3	1:F:224:ASP:HA	1.02	1.01
1:F:281:ALA:HB2	1:F:369:ARG:HH22	1.23	1.01
1:E:258:ALA:HB2	1:E:291:LEU:HD13	1.43	1.00
1:F:356:ALA:HB1	1:F:361:VAL:N	1.76	1.00
1:D:80:LYS:HD2	1:D:81:PRO:HD2	1.43	0.99
1:F:397:PHE:CE1	1:F:443:CYS:HB2	1.96	0.99
1:A:111:PHE:CG	1:A:364:MET:HE3	1.96	0.99
1:F:251:LYS:O	1:F:255:GLU:N	1.96	0.99
1:A:111:PHE:CD2	1:A:364:MET:HE3	1.97	0.99
1:F:223:LYS:CD	1:F:224:ASP:HA	1.92	0.99
1:A:111:PHE:CD2	1:A:364:MET:CE	2.45	0.98
1:F:372:ARG:HD2	1:F:373:ASP:H	0.81	0.98
1:C:102:ILE:HD12	1:C:103:ARG:N	1.78	0.98
1:F:356:ALA:CB	1:F:361:VAL:H	1.77	0.98
1:E:267:LEU:O	1:E:297:ARG:NH1	1.98	0.97
1:F:143:GLU:HA	1:F:147:ARG:NH2	1.79	0.97
1:C:133:THR:HG21	1:C:344:GLN:HE22	1.30	0.97
1:B:102:ILE:CD1	1:B:103:ARG:N	2.28	0.96
1:F:104:LEU:HB3	1:F:446:ILE:HG23	1.45	0.96
1:F:371:ARG:HB3	1:F:448:TYR:CE1	2.00	0.95
1:F:371:ARG:HA	1:F:374:PHE:CE1	2.02	0.95
1:F:460:GLU:H	1:F:460:GLU:CD	1.65	0.95
1:F:403:TYR:OH	1:F:467:GLU:OE2	1.84	0.95
1:E:335:VAL:HA	1:F:173:LEU:HD11	1.47	0.94
1:F:317:TYR:O	1:F:318:LEU:CD2	2.13	0.94
1:D:408:ALA:HB2	1:D:413:LEU:HA	1.46	0.94
1:F:460:GLU:OE2	1:F:460:GLU:N	2.01	0.94
1:F:87:ILE:HA	1:F:90:LEU:CD2	1.99	0.93
1:F:247:SER:OG	1:F:391:GLN:N	2.03	0.92
1:B:102:ILE:HD12	1:B:103:ARG:H	1.12	0.91
1:B:398:ILE:HD12	1:B:446:ILE:HD12	1.50	0.91
1:E:190:ALA:O	1:E:212:THR:OG1	1.86	0.91
1:F:371:ARG:H	1:F:372:ARG:HH21	1.15	0.91
1:F:148:LYS:NZ	1:F:351:LEU:O	2.03	0.91
1:F:405:GLY:N	1:F:415:ASN:OD1	2.05	0.90
1:B:91:ALA:HB2	1:B:425:LEU:HD21	1.53	0.90
1:F:170:GLN:OE1	1:F:336:SER:HB2	1.72	0.90
1:F:458:ALA:N	1:F:460:GLU:OE1	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:386:LYS:NZ	1:F:399:ASP:OD2	2.06	0.89
1:F:153:ASN:HD22	1:F:287:SER:HB3	1.34	0.89
1:F:164:VAL:HG23	1:F:317:TYR:HB3	1.54	0.89
1:F:225:LEU:HD12	1:F:229:LEU:HD12	1.53	0.89
1:F:144:ALA:C	1:F:147:ARG:HD3	1.92	0.89
1:F:166:ASN:ND2	1:F:336:SER:OG	2.06	0.88
1:E:76:VAL:HG21	1:F:178:ALA:HA	1.55	0.88
1:F:371:ARG:N	1:F:372:ARG:HH21	1.71	0.88
1:F:370:GLU:C	1:F:372:ARG:HE	1.73	0.88
1:D:281:ALA:HB2	1:D:369:ARG:NH2	1.88	0.88
1:C:409:GLU:HB2	1:C:411:PHE:H	1.39	0.88
1:F:301:VAL:HA	1:F:318:LEU:CD1	2.04	0.88
1:F:258:ALA:HB2	1:F:291:LEU:HD13	1.57	0.87
1:C:102:ILE:HD13	1:C:104:LEU:HG	1.56	0.87
1:E:136:ALA:HB3	1:E:142:ARG:NH2	1.90	0.87
1:F:133:THR:HG21	1:F:344:GLN:HE22	1.38	0.87
1:E:218:PHE:HB2	1:E:245:THR:HG21	1.57	0.86
1:F:173:LEU:HG	1:F:199:GLN:HG2	1.57	0.86
1:D:102:ILE:HG12	1:D:430:VAL:HA	1.55	0.86
1:F:147:ARG:HD2	1:F:147:ARG:N	1.91	0.86
1:F:301:VAL:O	1:F:302:ASN:ND2	2.08	0.86
1:B:264:HIS:O	1:B:297:ARG:NH2	2.08	0.86
1:C:424:PHE:HB3	1:C:430:VAL:HG12	1.58	0.86
1:B:413:LEU:HD12	1:B:415:ASN:OD1	1.75	0.85
1:E:338:GLY:O	1:F:314:ARG:NH1	2.09	0.85
1:F:373:ASP:HA	1:F:376:VAL:HG12	1.59	0.85
1:E:102:ILE:HD13	1:E:104:LEU:HG	1.59	0.85
1:A:102:ILE:HD12	1:A:103:ARG:N	1.92	0.85
1:F:406:SER:OG	1:F:407:GLU:OE1	1.92	0.85
1:B:403:TYR:CZ	1:B:466:LEU:HD21	2.12	0.84
1:C:102:ILE:HD12	1:C:103:ARG:H	1.43	0.84
1:F:326:ALA:O	1:F:330:LYS:NZ	2.11	0.84
1:C:214:ILE:HD12	1:C:215:SER:N	1.93	0.84
1:E:409:GLU:OE1	1:E:410:GLY:N	2.11	0.84
1:F:264:HIS:CD2	1:F:265:PRO:HD2	2.13	0.84
1:A:452:LEU:H	1:A:452:LEU:HD12	1.42	0.83
1:F:223:LYS:HE2	1:F:225:LEU:O	1.78	0.83
1:B:267:LEU:O	1:B:297:ARG:NH1	2.12	0.83
1:E:253:LEU:CD1	1:E:254:LEU:CG	2.53	0.82
1:D:458:ALA:O	1:D:462:ILE:N	2.10	0.82
1:D:462:ILE:O	1:D:466:LEU:HD11	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:229:LEU:HB3	1:F:233:SER:HB3	1.60	0.82
1:F:229:LEU:HB3	1:F:233:SER:CB	2.08	0.82
1:F:386:LYS:NZ	1:F:401:SER:OG	2.11	0.82
1:D:105:ALA:HB1	1:D:433:VAL:HG23	1.61	0.82
1:D:459:VAL:O	1:D:463:ARG:N	2.10	0.82
1:E:234:ARG:HH22	1:F:70:MET:HG3	1.43	0.82
1:E:125:ILE:HD12	1:E:126:ARG:H	1.44	0.82
1:E:276:GLU:O	1:E:279:ILE:HD11	1.78	0.81
1:F:172:LEU:HG	1:F:301:VAL:HG11	1.62	0.81
1:F:164:VAL:HA	1:F:317:TYR:HA	1.60	0.81
1:E:258:ALA:H	1:E:261:ILE:HG12	1.45	0.81
1:F:460:GLU:CD	1:F:460:GLU:N	2.33	0.81
1:F:184:ASP:OD1	1:F:266:ARG:NH2	2.15	0.80
1:F:300:THR:C	1:F:318:LEU:HD12	2.01	0.80
1:F:229:LEU:HD23	1:F:233:SER:HB2	1.62	0.80
1:E:106:ALA:O	1:E:447:SER:OG	1.99	0.80
1:F:129:PHE:O	1:F:341:SER:OG	1.98	0.80
1:E:80:LYS:CG	1:E:81:PRO:HD3	2.12	0.80
1:F:221:ASP:HB3	1:F:224:ASP:OD2	1.82	0.80
1:A:111:PHE:CD2	1:A:364:MET:HE2	2.15	0.80
1:E:368:TYR:HB3	1:E:448:TYR:HE1	1.46	0.80
1:B:96:GLN:O	1:B:99:VAL:N	2.16	0.79
1:E:361:VAL:O	1:E:365:VAL:N	2.15	0.79
1:F:301:VAL:HA	1:F:318:LEU:HD11	1.62	0.79
1:F:363:GLU:HA	1:F:366:LYS:HD2	1.63	0.79
1:B:93:THR:HG22	1:B:94:LEU:HD23	1.64	0.79
1:F:123:ASN:O	1:F:127:GLU:N	2.14	0.79
1:E:102:ILE:HD12	1:E:103:ARG:N	1.98	0.79
1:F:223:LYS:CG	1:F:226:GLU:N	2.45	0.79
1:A:102:ILE:HD12	1:A:103:ARG:H	1.48	0.79
1:D:281:ALA:HB2	1:D:369:ARG:HH22	1.44	0.79
1:D:460:GLU:HA	1:D:463:ARG:HB2	1.63	0.79
1:E:273:GLU:OE1	1:E:285:HIS:NE2	2.16	0.78
1:F:302:ASN:H	1:F:318:LEU:HD21	1.48	0.78
1:F:142:ARG:C	1:F:147:ARG:NH1	2.18	0.78
1:C:409:GLU:H	1:C:410:GLY:HA2	1.48	0.78
1:E:322:LYS:HD3	1:E:322:LYS:N	1.95	0.78
1:F:243:ASN:OD1	1:F:445:ARG:NH1	2.16	0.78
1:A:102:ILE:HD13	1:A:104:LEU:HG	1.66	0.78
1:F:301:VAL:C	1:F:302:ASN:HD22	1.87	0.78
1:C:420:LEU:HD22	1:C:424:PHE:HE1	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:ASP:HB2	1:C:419:SER:OG	1.84	0.77
1:B:408:ALA:HB1	1:B:469:LEU:HD21	1.64	0.77
1:F:104:LEU:O	1:F:447:SER:N	2.14	0.77
1:F:264:HIS:CD2	1:F:266:ARG:H	2.02	0.77
1:C:420:LEU:HD22	1:C:424:PHE:CE1	2.20	0.77
1:E:173:LEU:HG	1:E:177:LEU:HD11	1.66	0.77
1:F:169:LYS:HG3	1:F:193:TRP:HH2	1.47	0.77
1:F:300:THR:O	1:F:318:LEU:CD1	2.30	0.77
1:B:416:ASP:HB3	1:B:419:SER:H	1.50	0.77
1:E:199:GLN:HA	1:E:202:LEU:HD12	1.65	0.77
1:F:147:ARG:HD2	1:F:147:ARG:H	1.50	0.76
1:F:274:ILE:HG23	1:F:275:TYR:HD1	1.49	0.76
1:D:407:GLU:HG3	1:D:408:ALA:N	1.98	0.76
1:D:411:PHE:O	1:D:413:LEU:N	2.18	0.76
1:F:281:ALA:HB2	1:F:369:ARG:NH2	1.98	0.76
1:F:401:SER:O	1:F:403:TYR:N	2.18	0.76
1:F:195:SER:HB3	1:F:199:GLN:OE1	1.86	0.76
1:F:361:VAL:O	1:F:365:VAL:N	2.19	0.76
1:E:357:GLY:N	1:E:361:VAL:HG11	2.01	0.75
1:F:382:ILE:HD11	1:F:385:VAL:HG13	1.66	0.75
1:A:91:ALA:HB2	1:A:425:LEU:HD11	1.69	0.75
1:F:144:ALA:H	1:F:147:ARG:NH1	1.84	0.75
1:C:96:GLN:HA	1:C:96:GLN:HE21	0.60	0.75
1:F:370:GLU:CB	1:F:372:ARG:NH2	2.42	0.75
1:F:280:TYR:OH	1:F:372:ARG:HG3	1.87	0.75
1:E:85:MET:O	1:E:89:ASP:N	2.18	0.75
1:F:223:LYS:HG2	1:F:224:ASP:C	2.06	0.75
1:A:76:VAL:HG21	1:B:178:ALA:HA	1.68	0.75
1:C:264:HIS:O	1:C:297:ARG:NH2	2.19	0.75
1:C:424:PHE:HB3	1:C:430:VAL:CG1	2.17	0.75
1:F:147:ARG:CD	1:F:147:ARG:H	2.00	0.75
1:B:87:ILE:HG13	1:B:425:LEU:HD23	1.68	0.74
1:E:181:SER:N	1:E:184:ASP:OD2	2.20	0.74
1:E:356:ALA:N	1:E:357:GLY:HA2	2.02	0.74
1:F:384:GLY:HA3	1:F:403:TYR:HE1	1.50	0.74
1:E:122:ILE:HD12	1:F:122:ILE:HG23	1.68	0.74
1:F:372:ARG:HD3	1:F:373:ASP:OD2	1.87	0.74
1:A:229:LEU:HD13	1:A:264[B]:HIS:CD2	2.23	0.74
1:F:110:ASP:HB3	1:F:371:ARG:HH12	1.51	0.74
1:F:229:LEU:HD21	1:F:267:LEU:HD22	1.68	0.74
1:F:304:PHE:HZ	1:F:315:LEU:HD23	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:ALA:HB2	1:D:432:MET:HA	1.69	0.74
1:F:111:PHE:HD2	1:F:364:MET:HG3	1.51	0.74
1:F:452:LEU:HD21	1:F:456:GLN:NE2	2.03	0.74
1:F:154:GLY:O	1:F:155:LEU:HD12	1.88	0.73
1:D:87:ILE:HA	1:D:90:LEU:HD22	1.69	0.73
1:E:102:ILE:HD11	1:E:430:VAL:HG13	1.70	0.73
1:F:163:LEU:O	1:F:318:LEU:N	2.17	0.73
1:E:125:ILE:HD12	1:E:126:ARG:N	2.01	0.73
1:F:304:PHE:CZ	1:F:315:LEU:HD23	2.24	0.73
1:F:169:LYS:HG3	1:F:193:TRP:CH2	2.22	0.73
1:F:242:SER:HB2	1:F:246:GLY:HA3	1.69	0.73
1:F:254:LEU:O	1:F:257:ILE:HG22	1.89	0.73
1:F:92:ALA:O	1:F:93:THR:OG1	2.03	0.73
1:D:462:ILE:O	1:D:466:LEU:CD1	2.37	0.73
1:B:411:PHE:CE2	1:B:422:LEU:HB3	2.25	0.72
1:E:264:HIS:O	1:E:297:ARG:NH2	2.22	0.72
1:A:111:PHE:HB2	1:A:364:MET:HE1	1.71	0.72
1:C:95:VAL:CB	1:C:99:VAL:HB	2.19	0.72
1:F:239:CYS:O	1:F:242:SER:OG	2.04	0.72
1:A:111:PHE:HB2	1:A:364:MET:CE	2.20	0.72
1:C:404:TYR:O	1:C:406:SER:N	2.22	0.72
1:D:82:SER:O	1:D:85:MET:HG2	1.90	0.72
1:E:75:ARG:NH2	1:E:204:ASP:N	2.37	0.72
1:F:331:LEU:O	1:F:335:VAL:HG12	1.89	0.72
1:F:353:LEU:HB3	1:F:357:GLY:C	2.09	0.72
1:F:397:PHE:CD1	1:F:443:CYS:HB2	2.24	0.72
1:A:111:PHE:CG	1:A:364:MET:CE	2.70	0.72
1:E:340:SER:HB3	1:E:343:ALA:HB3	1.72	0.72
1:F:181:SER:N	1:F:184:ASP:OD2	2.21	0.72
1:F:264:HIS:CD2	1:F:265:PRO:CD	2.73	0.72
1:A:111:PHE:HD2	1:A:364:MET:HE2	1.53	0.72
1:B:387:ILE:HD11	1:B:398:ILE:HG12	1.71	0.72
1:F:396:LEU:HD11	1:F:446:ILE:HD12	1.70	0.72
1:E:365:VAL:O	1:E:369:ARG:NE	2.22	0.72
1:F:356:ALA:H	1:F:357:GLY:HA2	1.53	0.72
1:A:376:VAL:HG13	1:A:387:ILE:HG21	1.72	0.72
1:F:371:ARG:N	1:F:372:ARG:HE	1.86	0.72
1:F:119:GLU:OE2	1:F:123:ASN:ND2	2.22	0.71
1:E:254:LEU:HB3	1:E:291:LEU:CD2	2.18	0.71
1:F:225:LEU:CD1	1:F:229:LEU:CD1	2.65	0.71
1:F:301:VAL:CA	1:F:318:LEU:HD11	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:CB	1:A:364:MET:CE	2.67	0.71
1:F:198:GLU:N	1:F:198:GLU:OE2	2.22	0.71
1:F:382:ILE:CD1	1:F:385:VAL:HG13	2.19	0.71
1:F:223:LYS:HG3	1:F:226:GLU:H	1.53	0.71
1:B:196:TYR:OH	1:B:272:ASP:OD2	2.08	0.71
1:E:253:LEU:HD11	1:E:254:LEU:HG	1.68	0.71
1:C:373:ASP:O	1:C:377:LYS:HG2	1.90	0.71
1:F:370:GLU:C	1:F:372:ARG:NE	2.43	0.71
1:D:93:THR:HA	1:D:96:GLN:HB3	1.72	0.71
1:F:264:HIS:HD2	1:F:265:PRO:N	1.88	0.70
1:D:102:ILE:HD11	1:D:430:VAL:HG13	1.73	0.70
1:F:239:CYS:SG	1:F:242:SER:HA	2.31	0.70
1:F:368:TYR:O	1:F:448:TYR:OH	2.10	0.70
1:F:432:MET:HG2	1:F:446:ILE:HG12	1.71	0.70
1:B:91:ALA:CB	1:B:425:LEU:HD21	2.22	0.70
1:E:394:PHE:HA	1:E:448:TYR:CZ	2.27	0.70
1:D:466:LEU:HD13	1:D:466:LEU:N	1.93	0.70
1:C:95:VAL:O	1:C:99:VAL:N	2.24	0.70
1:F:267:LEU:O	1:F:297:ARG:NH1	2.24	0.70
1:F:374:PHE:O	1:F:375:LEU:HD23	1.92	0.70
1:E:181:SER:HB3	1:F:74:PRO:HD2	1.74	0.70
1:A:74:PRO:O	1:A:75:ARG:HB3	1.92	0.70
1:F:144:ALA:H	1:F:147:ARG:HH11	1.35	0.69
1:E:73:SER:OG	1:F:178:ALA:O	2.07	0.69
1:F:264:HIS:CD2	1:F:265:PRO:N	2.60	0.69
1:F:370:GLU:HG2	1:F:372:ARG:NH2	2.07	0.69
1:A:86:VAL:O	1:A:90:LEU:HB2	1.92	0.69
1:C:467:GLU:N	1:C:467:GLU:OE1	2.24	0.69
1:B:102:ILE:HD12	1:B:103:ARG:CA	2.22	0.69
1:F:165:SER:OG	1:F:332:GLN:OE1	2.08	0.69
1:F:84:THR:HB	1:F:88:THR:CG2	2.22	0.69
1:B:428:PHE:CE2	1:B:465:ALA:HA	2.27	0.69
1:C:409:GLU:N	1:C:410:GLY:HA2	2.06	0.69
1:E:335:VAL:HA	1:F:173:LEU:CD1	2.23	0.69
1:F:191:PRO:HB2	1:F:244:PRO:HG2	1.73	0.69
1:F:275:TYR:HE1	1:F:306:LYS:HZ2	1.38	0.69
1:A:230:THR:O	1:A:264[A]:HIS:NE2	2.26	0.69
1:D:422:LEU:O	1:D:427:LYS:NZ	2.26	0.69
1:E:368:TYR:HB3	1:E:448:TYR:CE1	2.28	0.69
1:E:401:SER:HA	1:E:404:TYR:CD2	2.26	0.69
1:F:225:LEU:CD1	1:F:229:LEU:HD11	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:THR:HG22	1:B:232:LYS:H	1.57	0.69
1:B:413:LEU:HD23	1:B:413:LEU:H	1.56	0.69
1:B:80:LYS:HG3	1:B:81:PRO:HD2	1.74	0.69
1:E:361:VAL:HA	1:E:364:MET:HE2	1.74	0.68
1:D:464:LYS:HA	1:D:467:GLU:HG3	1.74	0.68
1:F:168:ALA:O	1:F:172:LEU:HD12	1.93	0.68
1:F:306:LYS:HZ3	2:F:701:PLP:C4	2.06	0.68
1:F:400:PHE:HE1	1:F:466:LEU:HD21	1.58	0.68
1:D:424:PHE:HB3	1:D:430:VAL:HB	1.75	0.68
1:E:222:PRO:HB3	1:E:256:GLU:HG2	1.76	0.68
1:F:281:ALA:CB	1:F:369:ARG:HH22	2.04	0.68
1:D:406:SER:OG	1:D:407:GLU:N	2.13	0.68
1:E:90:LEU:O	1:E:94:LEU:HB2	1.94	0.68
1:D:408:ALA:HB2	1:D:413:LEU:CA	2.22	0.68
1:E:114:PRO:HB2	1:E:117:VAL:HG23	1.76	0.68
1:B:133:THR:HG21	1:B:344:GLN:HE22	1.58	0.68
1:B:372:ARG:O	1:B:376:VAL:HG23	1.92	0.68
1:F:409:GLU:O	1:F:414:ILE:HG21	1.92	0.68
1:E:249:TYR:HB3	1:E:253:LEU:HB3	1.75	0.68
1:C:96:GLN:CA	1:C:96:GLN:NE2	2.14	0.68
1:D:407:GLU:HG3	1:D:408:ALA:H	1.57	0.67
1:C:152:GLU:OE1	1:C:277:HIS:NE2	2.26	0.67
1:E:222:PRO:HD3	1:E:256:GLU:OE1	1.94	0.67
1:F:225:LEU:HD12	1:F:229:LEU:HD11	1.75	0.67
1:F:374:PHE:CD1	1:F:452:LEU:HD12	2.28	0.67
1:F:371:ARG:HG3	1:F:374:PHE:CZ	2.30	0.67
1:F:455:LEU:O	1:F:459:VAL:HG12	1.94	0.67
1:F:301:VAL:HA	1:F:318:LEU:HG	1.76	0.67
1:F:356:ALA:HB3	1:F:357:GLY:C	2.15	0.67
1:F:223:LYS:CD	1:F:224:ASP:CA	2.61	0.67
1:A:76:VAL:HG11	1:B:327:ALA:HB1	1.75	0.67
1:E:158:ALA:H	1:E:161:GLN:CD	1.97	0.67
1:F:273:GLU:HB2	1:F:302:ASN:HD21	1.59	0.67
1:B:417:SER:OG	1:B:441:ASP:O	2.13	0.67
1:C:404:TYR:O	1:C:415:ASN:ND2	2.28	0.67
1:A:80:LYS:H	1:A:81:PRO:HD3	1.59	0.67
1:E:155:LEU:HD21	1:E:289:ALA:HB3	1.77	0.67
1:E:413:LEU:HD22	1:E:414:ILE:H	1.60	0.66
1:C:133:THR:HG21	1:C:344:GLN:NE2	2.09	0.66
1:F:144:ALA:O	1:F:148:LYS:HB2	1.94	0.66
1:F:222:PRO:HA	1:F:223:LYS:C	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:HIS:HD2	1:F:265:PRO:CD	2.07	0.66
1:C:387:ILE:HD11	1:C:396:LEU:HD11	1.78	0.66
1:E:356:ALA:C	1:E:361:VAL:HG11	2.15	0.66
1:E:362:ALA:HA	1:E:365:VAL:HB	1.76	0.66
1:C:131:ARG:HH11	1:C:131:ARG:HG3	1.59	0.66
1:C:455:LEU:O	1:C:459:VAL:HG23	1.95	0.66
1:E:170:GLN:NE2	1:E:336:SER:OG	2.24	0.66
1:F:230:THR:O	1:F:233:SER:OG	2.13	0.66
1:F:324:ILE:O	1:F:328:CYS:N	2.27	0.66
1:A:420:LEU:HG	1:A:424:PHE:HE2	1.59	0.66
1:B:94:LEU:O	1:B:97:SER:OG	2.13	0.66
1:D:93:THR:HG22	1:D:96:GLN:HG2	1.77	0.66
1:E:258:ALA:HB2	1:E:291:LEU:CD1	2.23	0.66
1:A:356:ALA:N	1:A:357:GLY:HA2	2.10	0.66
1:A:95:VAL:O	1:A:97:SER:N	2.27	0.66
1:E:338:GLY:C	1:F:314:ARG:HH12	1.99	0.66
1:D:168:ALA:HB3	2:D:701:PLP:H5A2	1.78	0.66
1:E:455:LEU:O	1:E:459:VAL:HG23	1.95	0.66
1:D:90:LEU:O	1:D:93:THR:O	2.14	0.66
1:F:301:VAL:HA	1:F:318:LEU:CG	2.26	0.65
1:F:317:TYR:C	1:F:318:LEU:CD2	2.51	0.65
1:F:407:GLU:OE1	1:F:407:GLU:N	2.30	0.65
1:B:80:LYS:HB2	1:B:198:GLU:OE1	1.95	0.65
1:D:423:TYR:HA	1:D:427:LYS:NZ	2.12	0.65
1:E:79:LEU:O	1:E:80:LYS:HG2	1.95	0.65
1:F:371:ARG:H	1:F:372:ARG:NH2	1.92	0.65
1:D:466:LEU:H	1:D:466:LEU:CD1	2.02	0.65
1:E:253:LEU:HD12	1:E:254:LEU:CG	2.17	0.65
1:F:451:SER:O	1:F:454:VAL:HG22	1.97	0.65
1:E:276:GLU:OE1	1:E:302:ASN:ND2	2.30	0.65
1:A:261:ILE:HD11	1:A:294:MET:SD	2.37	0.65
1:E:269:VAL:HG21	1:E:288:PHE:CE2	2.32	0.65
1:A:111:PHE:CB	1:A:364:MET:HE3	2.27	0.65
1:B:403:TYR:O	1:B:406:SER:OG	2.14	0.65
1:E:265:PRO:O	1:F:69:ASP:N	2.30	0.65
1:E:90:LEU:HA	1:E:94:LEU:HD12	1.78	0.65
1:C:371:ARG:HG2	1:C:455:LEU:CD1	2.27	0.64
1:D:306:LYS:HZ1	2:D:701:PLP:C4A	2.10	0.64
1:F:370:GLU:HG2	1:F:372:ARG:HH21	1.60	0.64
1:F:86:VAL:O	1:F:90:LEU:HD23	1.95	0.64
1:F:188:ILE:HD11	1:F:209:VAL:HG22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:LYS:HE2	1:F:224:ASP:O	1.97	0.64
1:D:453:ASP:OD1	1:D:454:VAL:N	2.29	0.64
1:E:250:PRO:O	1:E:252:SER:N	2.26	0.64
1:F:294:MET:HA	1:F:294:MET:HE3	1.79	0.64
1:C:102:ILE:HG12	1:C:430:VAL:HG23	1.79	0.64
1:F:70:MET:SD	1:F:71:SER:N	2.71	0.64
1:F:233:SER:O	1:F:235:LEU:N	2.29	0.64
1:F:318:LEU:N	1:F:318:LEU:HD22	2.09	0.64
1:F:278:ILE:HG23	1:F:368:TYR:HD2	1.62	0.64
1:F:84:THR:HB	1:F:88:THR:HG23	1.78	0.64
1:E:258:ALA:CB	1:E:291:LEU:HD13	2.23	0.64
1:C:214:ILE:HD12	1:C:215:SER:H	1.62	0.64
1:E:405:GLY:N	1:E:414:ILE:O	2.20	0.64
1:D:102:ILE:HG13	1:D:103:ARG:N	2.13	0.64
1:E:249:TYR:HB3	1:E:253:LEU:CB	2.28	0.64
1:E:253:LEU:HD13	1:E:254:LEU:CD2	2.27	0.64
1:F:243:ASN:HD21	1:F:445:ARG:HH22	1.46	0.64
1:F:399:ASP:O	1:F:442:SER:O	2.16	0.63
1:C:89:ASP:O	1:C:93:THR:HG22	1.98	0.63
1:E:339:ALA:O	1:E:344:GLN:NE2	2.24	0.63
1:C:404:TYR:HE1	1:C:420:LEU:HD12	1.63	0.63
1:B:387:ILE:CD1	1:B:398:ILE:HG12	2.28	0.63
1:C:458:ALA:O	1:C:462:ILE:HG13	1.99	0.63
1:F:144:ALA:CA	1:F:147:ARG:HD3	2.28	0.63
1:F:189:PRO:HD2	1:F:237:ILE:O	1.99	0.63
1:F:153:ASN:ND2	1:F:287:SER:HB3	2.11	0.63
1:F:356:ALA:HA	1:F:361:VAL:HG13	1.80	0.63
1:F:405:GLY:O	1:F:406:SER:HB3	1.98	0.63
1:E:260:ILE:HD12	1:E:261:ILE:N	2.14	0.63
1:F:288:PHE:HB3	1:F:298:THR:HG21	1.79	0.63
1:C:333:GLY:C	1:C:334:GLN:HE21	2.02	0.62
1:F:274:ILE:HG23	1:F:275:TYR:CD1	2.32	0.62
1:F:398:ILE:O	1:F:443:CYS:HB3	1.99	0.62
1:F:374:PHE:CG	1:F:452:LEU:HD12	2.33	0.62
1:A:80:LYS:N	1:A:81:PRO:HD3	2.15	0.62
1:C:173:LEU:HD22	1:D:335:VAL:HG22	1.81	0.62
1:F:150:LYS:HA	1:F:155:LEU:H	1.64	0.62
1:F:219:LEU:HG	1:F:249:TYR:CD2	2.34	0.62
1:F:375:LEU:O	1:F:379:LEU:N	2.33	0.62
1:F:408:ALA:H	1:F:409:GLU:HA	1.65	0.62
1:D:401:SER:HB3	1:D:404:TYR:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:LYS:HG3	1:F:226:GLU:CA	2.30	0.62
1:E:173:LEU:O	1:E:177:LEU:HD12	1.99	0.62
1:F:187:ILE:HD12	1:F:229:LEU:HG	1.79	0.62
1:F:370:GLU:HG3	1:F:374:PHE:HE1	1.63	0.62
1:F:372:ARG:HB3	1:F:448:TYR:CZ	2.34	0.62
1:A:83:LYS:HE3	1:A:418:SER:HB3	1.82	0.62
1:E:302:ASN:HB3	1:E:317:TYR:CZ	2.34	0.62
1:F:373:ASP:HA	1:F:376:VAL:CG1	2.29	0.62
1:C:420:LEU:O	1:C:424:PHE:HD1	1.83	0.62
1:E:304:PHE:HB3	1:E:308:PHE:CD1	2.35	0.62
1:E:299:LEU:HD21	1:E:324:ILE:HG21	1.80	0.62
1:F:165:SER:HB3	1:F:170:GLN:NE2	2.14	0.62
1:F:227:SER:O	1:F:228:LYS:HG2	1.99	0.62
1:E:248:VAL:HG23	1:E:391:GLN:HB2	1.82	0.62
1:D:306:LYS:NZ	2:D:701:PLP:C4A	2.63	0.61
1:F:145:ILE:O	1:F:149:LEU:N	2.29	0.61
1:E:155:LEU:CD2	1:E:289:ALA:HB3	2.30	0.61
1:E:327:ALA:HB1	1:F:76:VAL:HG11	1.82	0.61
1:F:229:LEU:CD2	1:F:267:LEU:HD22	2.29	0.61
1:F:340:SER:O	1:F:344:GLN:HG3	1.99	0.61
1:F:466:LEU:O	1:F:469:LEU:HD12	2.00	0.61
1:C:126:ARG:HH22	1:D:126:ARG:HH22	1.47	0.61
1:E:220:LEU:H	1:E:249:TYR:HE1	1.48	0.61
1:E:153:ASN:ND2	1:E:276:GLU:OE2	2.19	0.61
1:F:247:SER:O	1:F:391:GLN:HB2	2.00	0.61
1:F:335:VAL:HG13	1:F:336:SER:H	1.66	0.61
1:F:371:ARG:HA	1:F:374:PHE:CG	2.34	0.61
1:D:110:ASP:HB3	1:D:449:ALA:O	2.00	0.61
1:E:92:ALA:O	1:E:94:LEU:N	2.33	0.61
1:F:223:LYS:HE3	1:F:226:GLU:O	2.01	0.61
1:E:340:SER:HA	1:F:314:ARG:CZ	2.30	0.61
1:F:452:LEU:HA	1:F:455:LEU:HD13	1.82	0.61
1:D:102:ILE:HD12	1:D:104:LEU:HG	1.82	0.61
1:A:102:ILE:HD11	1:A:430:VAL:HA	1.83	0.61
1:C:281:ALA:HB2	1:C:369:ARG:HH22	1.65	0.61
1:F:188:ILE:HG22	1:F:237:ILE:HB	1.83	0.61
1:F:356:ALA:O	1:F:361:VAL:HG13	2.01	0.61
1:F:124:ALA:HB2	1:F:345:LYS:HD3	1.81	0.61
1:E:455:LEU:O	1:E:459:VAL:N	2.30	0.61
1:F:150:LYS:HB2	1:F:155:LEU:O	2.01	0.61
1:F:223:LYS:CD	1:F:224:ASP:C	2.68	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:GLU:O	1:A:363:GLU:HG2	2.01	0.61
1:E:281:ALA:HB3	1:E:282:PRO:HD3	1.83	0.61
1:F:221:ASP:O	1:F:224:ASP:N	2.33	0.61
1:D:356:ALA:N	1:D:357:GLY:HA2	2.15	0.61
1:D:404:TYR:HA	1:D:415:ASN:OD1	2.01	0.61
1:E:179:VAL:HG12	1:E:324:ILE:HD12	1.83	0.61
1:F:222:PRO:HD3	1:F:253:LEU:HD21	1.83	0.61
1:F:462:ILE:HG22	1:F:466:LEU:HD22	1.83	0.61
1:D:80:LYS:HD2	1:D:81:PRO:CD	2.24	0.60
1:C:399:ASP:OD1	1:C:401:SER:OG	2.16	0.60
1:C:406:SER:OG	1:C:408:ALA:HB2	1.99	0.60
1:E:257:ILE:H	1:E:257:ILE:HD12	1.65	0.60
1:F:371:ARG:CA	1:F:374:PHE:CD1	2.78	0.60
1:B:386:LYS:NZ	1:B:387:ILE:O	2.29	0.60
1:F:384:GLY:HA3	1:F:403:TYR:CE1	2.36	0.60
1:F:456:GLN:C	1:F:460:GLU:OE1	2.40	0.60
1:A:411:PHE:HE2	1:A:423:TYR:HA	1.66	0.60
1:D:427:LYS:N	1:D:427:LYS:HD3	2.17	0.60
1:F:382:ILE:CG1	1:F:385:VAL:HG13	2.31	0.60
1:D:426:ASP:HB3	1:D:427:LYS:HD3	1.82	0.60
1:A:411:PHE:CE2	1:A:423:TYR:HD1	2.19	0.60
1:C:356:ALA:N	1:C:357:GLY:HA2	2.16	0.60
1:E:219:LEU:HD22	1:E:249:TYR:CD1	2.37	0.60
1:F:346:ALA:O	1:F:350:ALA:N	2.29	0.60
1:D:261:ILE:HD12	1:D:267:LEU:HD12	1.84	0.60
1:E:261:ILE:HA	1:E:267:LEU:HD23	1.83	0.60
1:F:147:ARG:O	1:F:151:GLU:HG2	2.00	0.60
1:F:163:LEU:N	1:F:318:LEU:O	2.32	0.60
1:D:264:HIS:O	1:D:297:ARG:NH2	2.35	0.60
1:E:122:ILE:HD11	1:F:125:ILE:HB	1.83	0.60
1:F:173:LEU:CG	1:F:199:GLN:HG2	2.31	0.60
1:F:289:ALA:O	1:F:295:TYR:HB2	2.02	0.60
1:A:428:PHE:O	1:A:461:LYS:HD3	2.02	0.60
1:A:95:VAL:HG21	1:A:101:VAL:HG12	1.83	0.59
1:B:168:ALA:HB3	2:B:701:PLP:H5A2	1.82	0.59
1:D:281:ALA:CB	1:D:369:ARG:HH22	2.13	0.59
1:F:239:CYS:HA	1:F:272:ASP:HB3	1.83	0.59
1:F:371:ARG:CA	1:F:374:PHE:CE1	2.83	0.59
1:F:382:ILE:HG12	1:F:385:VAL:HG13	1.83	0.59
1:A:194:VAL:HG12	1:A:437:ALA:O	2.02	0.59
1:F:133:THR:HG21	1:F:344:GLN:NE2	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:LEU:HD13	1:E:254:LEU:HD23	1.82	0.59
1:C:194:VAL:HG12	1:C:437:ALA:O	2.02	0.59
1:E:261:ILE:HD12	1:E:267:LEU:HD21	1.82	0.59
1:F:356:ALA:HA	1:F:361:VAL:CG1	2.33	0.59
1:F:356:ALA:H	1:F:357:GLY:CA	2.15	0.59
1:F:74:PRO:O	1:F:76:VAL:N	2.32	0.59
1:A:420:LEU:HG	1:A:424:PHE:CE2	2.38	0.59
1:C:302:ASN:HB3	1:C:317:TYR:CZ	2.38	0.59
1:D:100:PRO:O	1:D:429:GLN:HG3	2.02	0.59
1:F:85:MET:SD	1:F:88:THR:OG1	2.59	0.59
1:B:356:ALA:H	1:B:358:GLY:H	1.50	0.59
1:E:387:ILE:HD11	1:E:396:LEU:HD11	1.84	0.59
1:F:118:ALA:O	1:F:122:ILE:HD12	2.01	0.59
1:F:370:GLU:CG	1:F:372:ARG:HH21	2.16	0.59
1:F:283:ALA:HB2	1:F:391:GLN:HB3	1.85	0.59
1:A:95:VAL:CG2	1:A:101:VAL:HG12	2.32	0.59
1:E:78:SER:O	1:E:80:LYS:HD2	2.01	0.59
1:F:229:LEU:CD2	1:F:233:SER:HB2	2.31	0.59
1:A:102:ILE:HD11	1:A:431:ALA:H	1.66	0.59
1:E:150:LYS:HG2	1:E:155:LEU:O	2.02	0.59
1:E:75:ARG:NH2	1:E:204:ASP:H	2.01	0.59
1:F:355:LYS:N	1:F:358:GLY:H	2.01	0.59
1:F:370:GLU:CG	1:F:372:ARG:NH2	2.65	0.59
1:E:75:ARG:NH1	1:E:202:LEU:O	2.36	0.59
1:E:428:PHE:CZ	1:E:465:ALA:HA	2.37	0.59
1:F:273:GLU:CB	1:F:302:ASN:HD21	2.16	0.59
1:A:131:ARG:NH2	1:B:110:ASP:O	2.36	0.58
1:E:222:PRO:HG2	1:E:223:LYS:H	1.68	0.58
1:B:356:ALA:HB3	1:B:358:GLY:N	2.18	0.58
1:B:455:LEU:O	1:B:459:VAL:HG23	2.03	0.58
1:D:88:THR:HB	1:D:89:ASP:OD1	2.02	0.58
1:E:234:ARG:HH22	1:F:70:MET:CG	2.14	0.58
1:E:253:LEU:HD11	1:E:286:THR:HB	1.85	0.58
1:F:214:ILE:HD12	1:F:214:ILE:H	1.66	0.58
1:E:71:SER:O	1:F:234:ARG:NH2	2.37	0.58
1:F:445:ARG:HG2	1:F:446:ILE:N	2.18	0.58
1:E:195:SER:O	1:E:199:GLN:HG3	2.04	0.58
1:B:93:THR:O	1:B:96:GLN:HG3	2.03	0.58
1:D:455:LEU:O	1:D:459:VAL:HG23	2.03	0.58
1:E:254:LEU:HD13	1:E:291:LEU:HG	1.85	0.58
1:E:280:TYR:CZ	1:E:282:PRO:HD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:THR:C	1:F:318:LEU:CD1	2.72	0.58
1:D:170:GLN:O	1:D:174:GLN:HG3	2.03	0.58
1:E:260:ILE:HD12	1:E:261:ILE:HD13	1.84	0.58
1:A:372:ARG:HB2	1:A:448:TYR:CZ	2.39	0.58
1:F:90:LEU:HD23	1:F:90:LEU:H	1.68	0.58
1:A:80:LYS:H	1:A:81:PRO:CD	2.17	0.57
1:D:190:ALA:O	1:D:212:THR:OG1	2.14	0.57
1:F:279:ILE:HG22	1:F:280:TYR:H	1.68	0.57
1:F:371:ARG:N	1:F:372:ARG:NH2	2.48	0.57
1:F:369:ARG:O	1:F:372:ARG:HD3	2.03	0.57
1:B:450:THR:OG1	1:B:454:VAL:HG21	2.04	0.57
1:F:442:SER:OG	1:F:443:CYS:SG	2.53	0.57
1:A:287:SER:O	1:A:290:SER:OG	2.21	0.57
1:A:408:ALA:O	1:A:412:GLY:N	2.37	0.57
1:A:411:PHE:CE2	1:A:423:TYR:HA	2.39	0.57
1:C:230:THR:HG22	1:C:232:LYS:H	1.69	0.57
1:B:102:ILE:C	1:B:102:ILE:HD12	2.18	0.57
1:B:281:ALA:HB1	1:B:282:PRO:CD	2.34	0.57
1:C:76:VAL:HG11	1:D:327:ALA:HB1	1.86	0.57
1:E:401:SER:HA	1:E:404:TYR:CE2	2.38	0.57
1:F:372:ARG:CG	1:F:373:ASP:N	2.68	0.57
1:A:75:ARG:NH1	1:B:177:LEU:HD22	2.20	0.57
1:B:305:SER:HB3	1:B:311:THR:HG22	1.85	0.57
1:E:258:ALA:N	1:E:261:ILE:HG12	2.17	0.57
1:E:356:ALA:HB3	1:E:358:GLY:N	2.19	0.57
1:A:102:ILE:HD11	1:A:431:ALA:N	2.20	0.57
1:F:223:LYS:HD3	1:F:224:ASP:C	2.24	0.57
1:F:223:LYS:HE2	1:F:225:LEU:C	2.23	0.57
1:B:91:ALA:HA	1:B:95:VAL:HG21	1.87	0.57
1:E:79:LEU:C	1:E:80:LYS:HG2	2.24	0.57
1:E:125:ILE:HD13	1:F:122:ILE:HD11	1.86	0.57
1:F:223:LYS:O	1:F:225:LEU:HD23	2.04	0.56
1:C:337:SER:HB2	1:D:169:LYS:HE3	1.85	0.56
1:A:122:ILE:HG23	1:B:122:ILE:HG23	1.86	0.56
1:B:91:ALA:HA	1:B:95:VAL:CG2	2.35	0.56
1:E:230:THR:HG22	1:E:232:LYS:H	1.70	0.56
1:F:115:LYS:O	1:F:119:GLU:N	2.30	0.56
1:B:409:GLU:OE2	1:B:410:GLY:N	2.39	0.56
1:E:135:ASN:HD22	1:E:135:ASN:C	2.08	0.56
1:A:345:LYS:O	1:A:348:VAL:HG22	2.05	0.56
1:B:181:SER:N	1:B:184:ASP:OD2	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ARG:HB3	1:D:108:GLU:OE1	2.05	0.56
1:F:372:ARG:CG	1:F:373:ASP:H	2.18	0.56
1:C:463:ARG:O	1:C:467:GLU:OE1	2.24	0.56
1:D:423:TYR:HD1	1:D:427:LYS:HE3	1.71	0.56
1:F:353:LEU:HB3	1:F:357:GLY:O	2.05	0.56
1:E:304:PHE:HB3	1:E:308:PHE:HD1	1.69	0.56
1:F:185:GLU:O	1:F:233:SER:O	2.24	0.56
1:F:243:ASN:OD1	1:F:244:PRO:HA	2.06	0.56
1:F:219:LEU:HG	1:F:249:TYR:HD2	1.71	0.56
1:F:353:LEU:HD13	1:F:357:GLY:O	2.06	0.56
1:A:87:ILE:HG23	1:A:88:THR:H	1.71	0.56
1:F:229:LEU:CD2	1:F:267:LEU:HD13	2.36	0.56
1:F:291:LEU:HB2	1:F:294:MET:HB2	1.88	0.56
1:B:408:ALA:CB	1:B:469:LEU:HD21	2.34	0.56
1:D:281:ALA:CB	1:D:282:PRO:CD	2.83	0.56
1:F:372:ARG:CB	1:F:448:TYR:OH	2.36	0.56
1:C:72:LEU:HD21	1:D:324:ILE:HD13	1.88	0.55
1:D:160:ASP:OD2	1:D:322:LYS:HE3	2.05	0.55
1:D:93:THR:HA	1:D:96:GLN:CB	2.34	0.55
1:B:102:ILE:HG12	1:B:430:VAL:HG13	1.88	0.55
1:D:73:SER:O	1:D:76:VAL:HG12	2.07	0.55
1:F:78:SER:OG	1:F:79:LEU:HD23	2.05	0.55
1:A:404:TYR:HA	1:A:414:ILE:O	2.07	0.55
1:F:265:PRO:HA	1:F:297:ARG:NH2	2.21	0.55
1:D:408:ALA:CB	1:D:413:LEU:HA	2.30	0.55
1:E:249:TYR:CB	1:E:253:LEU:HB3	2.36	0.55
1:E:254:LEU:HA	1:E:291:LEU:HD11	1.88	0.55
1:F:188:ILE:HD12	1:F:209:VAL:HA	1.88	0.55
1:B:133:THR:HG22	1:B:134:LEU:O	2.07	0.55
1:E:434:PRO:HA	1:E:444:ILE:HG22	1.88	0.55
1:F:448:TYR:CD1	1:F:448:TYR:O	2.59	0.55
1:C:337:SER:HB2	1:D:169:LYS:CE	2.36	0.55
1:E:117:VAL:HG13	1:E:346:ALA:O	2.06	0.55
1:F:394:PHE:O	1:F:448:TYR:HD2	1.89	0.55
1:C:133:THR:HG22	1:C:134:LEU:O	2.07	0.55
1:C:281:ALA:HB2	1:C:369:ARG:HH12	1.72	0.55
1:C:372:ARG:NH2	1:C:389:GLU:OE2	2.39	0.55
1:D:399:ASP:OD1	1:D:401:SER:OG	2.24	0.55
1:F:114:PRO:HB2	1:F:117:VAL:HG23	1.87	0.55
1:B:151:GLU:HG2	1:B:355:LYS:HE3	1.88	0.55
1:B:81:PRO:O	1:B:82:SER:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:LYS:HD2	1:F:337:SER:HB2	1.89	0.55
1:E:197:THR:HG22	1:E:201:ARG:HE	1.72	0.55
1:E:143:GLU:O	1:E:147:ARG:HG3	2.07	0.55
1:E:373:ASP:O	1:E:377:LYS:HG2	2.07	0.55
1:B:356:ALA:N	1:B:357:GLY:HA2	2.22	0.55
1:E:403:TYR:CE2	1:E:466:LEU:HD21	2.42	0.55
1:F:396:LEU:O	1:F:396:LEU:HD12	2.06	0.55
1:B:463:ARG:NH1	1:B:464:LYS:HD2	2.23	0.54
1:C:254:LEU:HB3	1:C:291:LEU:HD11	1.89	0.54
1:F:261:ILE:HG23	1:F:267:LEU:CD2	2.37	0.54
1:A:153:ASN:ND2	1:A:276:GLU:OE2	2.30	0.54
1:D:82:SER:HB2	1:D:85:MET:HE3	1.88	0.54
1:D:75:ARG:HA	1:D:78:SER:HB3	1.90	0.54
1:E:74:PRO:O	1:E:76:VAL:N	2.36	0.54
1:F:119:GLU:CD	1:F:123:ASN:ND2	2.60	0.54
1:F:143:GLU:O	1:F:147:ARG:HG3	2.08	0.54
1:F:257:ILE:O	1:F:261:ILE:HD12	2.07	0.54
1:B:406:SER:HB3	1:B:408:ALA:HB2	1.89	0.54
1:C:234:ARG:NH1	1:C:266:ARG:O	2.37	0.54
1:F:261:ILE:HG23	1:F:267:LEU:HD23	1.90	0.54
1:F:280:TYR:OH	1:F:372:ARG:CG	2.56	0.54
1:C:372:ARG:O	1:C:376:VAL:HG23	2.08	0.54
1:D:84:THR:C	1:D:88:THR:HG23	2.28	0.54
1:D:405:GLY:N	1:D:415:ASN:OD1	2.41	0.54
1:E:115:LYS:HA	1:E:118:ALA:HB3	1.89	0.54
1:E:378:SER:HB2	1:E:459:VAL:HG11	1.90	0.54
1:F:115:LYS:N	3:F:801:HOH:O	2.39	0.54
1:F:356:ALA:HB2	1:F:361:VAL:HG22	1.90	0.54
1:D:123:ASN:O	1:D:127:GLU:HG3	2.08	0.54
1:E:275:TYR:CZ	1:E:306:LYS:HD2	2.43	0.54
1:F:409:GLU:C	1:F:414:ILE:HG21	2.27	0.54
1:B:281:ALA:HB1	1:B:282:PRO:HD2	1.90	0.53
1:C:281:ALA:H	1:C:369:ARG:NH2	2.06	0.53
1:E:269:VAL:HG21	1:E:288:PHE:HE2	1.71	0.53
1:E:452:LEU:HD12	1:E:452:LEU:H	1.72	0.53
1:F:223:LYS:HE3	1:F:227:SER:N	2.21	0.53
1:F:229:LEU:HD21	1:F:267:LEU:CD2	2.38	0.53
1:B:463:ARG:HH11	1:B:464:LYS:HD2	1.73	0.53
1:B:90:LEU:O	1:B:95:VAL:HG21	2.08	0.53
1:D:409:GLU:N	1:D:410:GLY:HA3	2.23	0.53
1:E:222:PRO:HB3	1:E:256:GLU:CG	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:ALA:O	1:F:212:THR:OG1	2.20	0.53
1:B:169:LYS:HE3	1:B:193:TRP:CH2	2.43	0.53
1:B:409:GLU:CG	1:B:410:GLY:H	2.22	0.53
1:D:92:ALA:O	1:D:96:GLN:HB3	2.08	0.53
1:E:122:ILE:HA	1:E:125:ILE:HD11	1.90	0.53
1:B:93:THR:O	1:B:96:GLN:N	2.22	0.53
1:D:394:PHE:HA	1:D:448:TYR:CE1	2.43	0.53
1:D:420:LEU:O	1:D:423:TYR:N	2.41	0.53
1:E:102:ILE:CD1	1:E:104:LEU:HG	2.35	0.53
1:F:146:CYS:SG	1:F:147:ARG:NH2	2.79	0.53
1:F:261:ILE:HG12	1:F:269:VAL:HG21	1.90	0.53
1:E:375:LEU:HD11	1:E:455:LEU:HB3	1.91	0.53
1:E:406:SER:O	1:E:406:SER:OG	2.26	0.53
1:F:459:VAL:O	1:F:462:ILE:HB	2.08	0.53
1:C:321:PRO:HG2	1:C:324:ILE:HD12	1.90	0.53
1:F:459:VAL:HG13	1:F:460:GLU:OE2	2.08	0.53
1:F:462:ILE:O	1:F:466:LEU:N	2.42	0.53
1:F:84:THR:HB	1:F:88:THR:HG21	1.91	0.53
1:A:248:VAL:HG23	1:A:391:GLN:HB2	1.90	0.53
1:A:414:ILE:O	1:A:414:ILE:HG22	2.08	0.53
1:C:153:ASN:ND2	1:C:276:GLU:OE2	2.33	0.53
1:F:273:GLU:HB2	1:F:302:ASN:ND2	2.21	0.53
1:C:114:PRO:HB2	1:C:117:VAL:HG23	1.91	0.53
1:C:133:THR:HG23	1:C:138:ILE:HG23	1.90	0.53
1:D:302:ASN:HB3	1:D:317:TYR:CE1	2.44	0.53
1:E:131:ARG:HG2	1:F:108:GLU:CG	2.39	0.53
1:F:244:PRO:HG3	1:F:438:PHE:HB3	1.89	0.53
1:F:353:LEU:HB3	1:F:357:GLY:CA	2.39	0.53
1:F:460:GLU:HG2	1:F:461:LYS:H	1.72	0.53
1:B:79:LEU:HB2	1:B:198:GLU:OE1	2.09	0.53
1:D:254:LEU:HB3	1:D:291:LEU:HD11	1.91	0.53
1:E:440:ASP:OD1	1:E:442:SER:OG	2.25	0.53
1:F:273:GLU:CA	1:F:302:ASN:HD21	2.21	0.53
1:F:273:GLU:C	1:F:302:ASN:HD21	2.12	0.53
1:E:372:ARG:NH2	1:E:373:ASP:OD1	2.41	0.52
1:F:240:SER:HB2	1:F:248:VAL:HA	1.91	0.52
1:F:345:LYS:O	1:F:348:VAL:HG22	2.09	0.52
1:A:408:ALA:HB3	1:A:411:PHE:O	2.09	0.52
1:D:426:ASP:HB3	1:D:427:LYS:HZ2	1.74	0.52
1:E:148:LYS:HE2	1:E:152:GLU:OE1	2.08	0.52
1:E:458:ALA:O	1:E:462:ILE:HG13	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:SER:OG	1:A:338:GLY:N	2.41	0.52
1:B:302:ASN:HB3	1:B:317:TYR:CZ	2.44	0.52
1:D:401:SER:O	1:D:403:TYR:N	2.39	0.52
1:F:374:PHE:CZ	1:F:452:LEU:HB2	2.44	0.52
1:C:372:ARG:NH2	1:C:373:ASP:OD1	2.42	0.52
1:F:440:ASP:OD1	1:F:442:SER:OG	2.27	0.52
1:F:143:GLU:C	1:F:147:ARG:NE	2.61	0.52
1:A:356:ALA:C	1:A:361:VAL:HG11	2.29	0.52
1:B:403:TYR:CZ	1:B:466:LEU:CD2	2.88	0.52
1:E:260:ILE:CD1	1:E:261:ILE:HD13	2.39	0.52
1:F:236:LEU:HB3	1:F:269:VAL:HG22	1.92	0.52
1:F:460:GLU:HG2	1:F:461:LYS:N	2.24	0.52
1:B:463:ARG:HG3	1:B:464:LYS:N	2.24	0.52
1:E:110:ASP:OD1	1:E:110:ASP:N	2.41	0.52
1:E:253:LEU:HD21	1:E:286:THR:HB	1.92	0.52
1:E:269:VAL:HG11	1:E:288:PHE:CD2	2.45	0.52
1:F:138:ILE:HG13	1:F:141:LEU:HB2	1.92	0.52
1:F:166:ASN:H	1:F:170:GLN:NE2	2.08	0.52
1:F:192:TYR:HE2	1:F:197:THR:HG1	1.56	0.52
1:D:414:ILE:HG21	1:D:423:TYR:CD2	2.45	0.52
1:D:423:TYR:HA	1:D:427:LYS:CE	2.40	0.52
1:F:225:LEU:HD12	1:F:229:LEU:CG	2.38	0.52
1:F:382:ILE:O	1:F:385:VAL:HG22	2.09	0.52
1:F:382:ILE:HG12	1:F:385:VAL:CG1	2.39	0.52
1:A:411:PHE:CD2	1:A:423:TYR:HD1	2.28	0.52
1:C:131:ARG:O	1:C:341:SER:OG	2.27	0.52
1:E:394:PHE:HA	1:E:448:TYR:CE2	2.45	0.52
1:B:436:ASP:HA	1:F:413:LEU:HD21	1.92	0.52
1:D:428:PHE:CZ	1:D:465:ALA:HA	2.44	0.52
1:E:401:SER:HA	1:E:404:TYR:HD2	1.73	0.52
1:F:304:PHE:CZ	1:F:347:GLY:HA2	2.45	0.52
1:C:240:SER:HB2	1:C:249:TYR:HD1	1.73	0.51
1:D:356:ALA:HB3	1:D:358:GLY:N	2.25	0.51
1:D:413:LEU:CD1	1:D:415:ASN:HB2	2.41	0.51
1:E:254:LEU:HD22	1:E:291:LEU:HG	1.91	0.51
1:F:455:LEU:H	1:F:455:LEU:HD12	1.75	0.51
1:B:386:LYS:HB3	1:B:399:ASP:HB3	1.92	0.51
1:D:226:GLU:HG3	1:D:260:ILE:HD13	1.93	0.51
1:E:252:SER:HA	1:E:255:GLU:HB2	1.92	0.51
1:E:467:GLU:C	1:E:469:LEU:H	2.14	0.51
1:C:404:TYR:CE1	1:C:420:LEU:HD12	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:SER:HB2	1:D:85:MET:CE	2.40	0.51
1:D:86:VAL:HG13	1:D:87:ILE:HG13	1.91	0.51
1:E:304:PHE:CE2	1:E:315:LEU:HD23	2.45	0.51
1:E:372:ARG:O	1:E:376:VAL:HG23	2.09	0.51
1:F:225:LEU:HA	1:F:228:LYS:HB2	1.92	0.51
1:E:222:PRO:HD3	1:E:256:GLU:CD	2.30	0.51
1:F:102:ILE:HG22	1:F:104:LEU:HG	1.92	0.51
1:F:146:CYS:HB3	1:F:157:TYR:O	2.10	0.51
1:A:452:LEU:H	1:A:452:LEU:CD1	2.16	0.51
1:F:223:LYS:CG	1:F:224:ASP:C	2.77	0.51
1:F:372:ARG:N	1:F:448:TYR:CE1	2.78	0.51
1:B:91:ALA:O	1:B:93:THR:N	2.34	0.51
1:F:196:TYR:OH	1:F:272:ASP:OD2	2.27	0.51
1:B:241:PRO:HB3	1:B:248:VAL:HG22	1.92	0.51
1:B:276:GLU:HG3	1:B:285:HIS:ND1	2.26	0.51
1:C:261:ILE:HD11	1:C:294:MET:SD	2.50	0.51
1:E:417:SER:OG	1:E:436:ASP:HB2	2.11	0.51
1:E:460:GLU:HA	1:E:463:ARG:HG3	1.93	0.51
1:F:140:GLU:O	1:F:144:ALA:N	2.44	0.51
1:F:223:LYS:HG2	1:F:224:ASP:CA	2.41	0.51
1:C:459:VAL:O	1:C:463:ARG:HG3	2.11	0.51
1:D:114:PRO:HB2	1:D:117:VAL:HG23	1.93	0.51
1:D:302:ASN:HB3	1:D:317:TYR:CZ	2.46	0.51
1:F:173:LEU:O	1:F:177:LEU:HD12	2.10	0.51
1:F:264:HIS:O	1:F:297:ARG:NH2	2.43	0.51
1:F:91:ALA:O	1:F:103:ARG:NH2	2.44	0.51
1:D:83:LYS:HD2	1:D:436:ASP:CG	2.32	0.51
1:E:87:ILE:HG13	1:E:425:LEU:HD22	1.93	0.51
1:F:129:PHE:CD2	1:F:345:LYS:HD2	2.45	0.51
1:F:145:ILE:N	1:F:147:ARG:HD3	2.25	0.51
1:F:467:GLU:C	1:F:469:LEU:H	2.14	0.51
1:C:356:ALA:HB3	1:C:358:GLY:N	2.25	0.51
1:E:231:GLU:O	1:E:266:ARG:HD3	2.11	0.51
1:F:370:GLU:HG3	1:F:374:PHE:CE1	2.46	0.51
1:C:114:PRO:HB3	1:C:360:THR:HG21	1.93	0.50
1:E:131:ARG:HH22	1:F:112:ASP:HA	1.76	0.50
1:F:119:GLU:CD	1:F:123:ASN:HD21	2.13	0.50
1:F:235:LEU:HA	1:F:268:LEU:O	2.11	0.50
1:B:222:PRO:HG2	1:B:256:GLU:OE1	2.11	0.50
1:C:371:ARG:HG2	1:C:455:LEU:HD13	1.91	0.50
1:E:255:GLU:HA	1:E:255:GLU:OE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:353:LEU:HB3	1:F:357:GLY:HA3	1.93	0.50
1:B:426:ASP:O	1:B:427:LYS:HB2	2.12	0.50
1:E:165:SER:OG	1:E:332:GLN:OE1	2.15	0.50
1:B:80:LYS:HD2	1:F:411:PHE:HD2	1.77	0.50
1:A:425:LEU:HA	1:A:430:VAL:H	1.77	0.50
1:E:199:GLN:O	1:E:202:LEU:HB2	2.11	0.50
1:F:381:ASP:CG	1:F:382:ILE:N	2.64	0.50
1:F:409:GLU:O	1:F:469:LEU:CD2	2.59	0.50
1:A:416:ASP:OD1	1:A:441:ASP:OD2	2.29	0.50
1:D:281:ALA:HB1	1:D:282:PRO:CD	2.41	0.50
1:D:419:SER:O	1:D:422:LEU:HB3	2.12	0.50
1:A:302:ASN:HB3	1:A:317:TYR:CZ	2.47	0.50
1:D:387:ILE:HG12	1:D:398:ILE:HG23	1.94	0.50
1:F:409:GLU:O	1:F:469:LEU:HD22	2.11	0.50
1:D:237:ILE:O	1:D:238:LEU:HD23	2.12	0.50
1:F:194:VAL:O	1:F:198:GLU:OE2	2.29	0.50
1:F:187:ILE:HD11	1:F:229:LEU:HA	1.93	0.50
1:A:81:PRO:O	1:A:82:SER:HB3	2.12	0.50
1:C:281:ALA:H	1:C:369:ARG:HH22	1.60	0.50
1:D:90:LEU:O	1:D:94:LEU:O	2.29	0.50
1:F:155:LEU:HD23	1:F:295:TYR:CD2	2.47	0.50
1:F:386:LYS:NZ	1:F:401:SER:HG	2.06	0.50
1:C:172:LEU:HD23	1:C:301:VAL:HG21	1.94	0.50
1:C:400:PHE:O	1:C:403:TYR:HB2	2.12	0.50
1:A:111:PHE:CB	1:A:364:MET:HE1	2.36	0.49
1:A:234:ARG:HH22	1:B:71:SER:HA	1.76	0.49
1:E:222:PRO:HG2	1:E:223:LYS:HD3	1.93	0.49
1:E:75:ARG:HH21	1:E:204:ASP:N	2.06	0.49
1:A:75:ARG:HH12	1:B:177:LEU:HD22	1.76	0.49
1:D:123:ASN:OD1	1:D:127:GLU:OE2	2.31	0.49
1:E:218:PHE:CB	1:E:245:THR:HG21	2.36	0.49
1:F:457:ALA:N	1:F:460:GLU:OE1	2.45	0.49
1:C:452:LEU:HA	1:C:455:LEU:HD12	1.93	0.49
1:E:75:ARG:HH21	1:E:204:ASP:H	1.60	0.49
1:E:249:TYR:C	1:E:253:LEU:HB3	2.33	0.49
1:E:273:GLU:O	1:E:276:GLU:HB2	2.12	0.49
1:E:356:ALA:N	1:E:357:GLY:CA	2.73	0.49
1:F:264:HIS:O	1:F:297:ARG:NH1	2.42	0.49
1:F:302:ASN:N	1:F:318:LEU:HD21	2.23	0.49
1:A:386:LYS:HB3	1:A:399:ASP:HB3	1.94	0.49
1:B:102:ILE:CD1	1:B:104:LEU:N	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:VAL:HG22	1:D:437:ALA:O	2.13	0.49
1:F:226:GLU:HG2	1:F:229:LEU:HD12	1.93	0.49
1:F:78:SER:C	1:F:79:LEU:HD23	2.33	0.49
1:C:409:GLU:HB3	1:C:411:PHE:CE2	2.47	0.49
1:D:111:PHE:CD2	1:D:364:MET:HG2	2.48	0.49
1:D:153:ASN:ND2	1:D:276:GLU:OE2	2.30	0.49
1:E:179:VAL:HG21	1:E:235:LEU:HD13	1.95	0.49
1:E:403:TYR:CE2	1:E:466:LEU:CD2	2.95	0.49
1:D:361:VAL:O	1:D:365:VAL:HG23	2.12	0.49
1:E:304:PHE:HE2	1:E:315:LEU:HD23	1.78	0.49
1:E:361:VAL:HG22	1:E:365:VAL:HG23	1.95	0.49
1:F:147:ARG:H	1:F:147:ARG:NE	2.11	0.49
1:B:403:TYR:CE2	1:B:466:LEU:CD2	2.96	0.49
1:F:305:SER:HB3	1:F:311:THR:HG22	1.94	0.49
1:F:367:ALA:O	1:F:368:TYR:HD1	1.95	0.49
1:C:90:LEU:HB3	1:C:425:LEU:HD23	1.95	0.49
1:C:306:LYS:NZ	2:C:701:PLP:C4A	2.76	0.49
1:D:93:THR:HA	1:D:96:GLN:CG	2.43	0.49
1:F:163:LEU:HD13	1:F:329:SER:HB2	1.93	0.49
1:F:404:TYR:OH	1:F:417:SER:CA	2.61	0.49
1:C:109:PRO:HB3	1:C:368:TYR:OH	2.12	0.49
1:C:387:ILE:HD11	1:C:396:LEU:CD1	2.42	0.49
1:E:161:GLN:HG2	1:E:322:LYS:HD2	1.93	0.49
1:F:133:THR:HG23	1:F:138:ILE:HG23	1.95	0.49
1:F:299:LEU:HD23	1:F:320:GLY:HA3	1.94	0.49
1:F:90:LEU:O	1:F:94:LEU:HD23	2.12	0.49
1:D:413:LEU:HD13	1:D:415:ASN:HB2	1.94	0.48
1:E:253:LEU:CD1	1:E:254:LEU:CD2	2.90	0.48
1:D:90:LEU:HD23	1:D:91:ALA:N	2.28	0.48
1:E:153:ASN:HB2	1:E:155:LEU:CD1	2.43	0.48
1:E:189:PRO:O	1:E:192:TYR:HB3	2.13	0.48
1:F:143:GLU:O	1:F:147:ARG:CD	2.61	0.48
1:F:150:LYS:O	1:F:154:GLY:N	2.45	0.48
1:F:269:VAL:O	1:F:298:THR:HA	2.13	0.48
1:C:314:ARG:NH1	1:D:132:TYR:HE1	2.11	0.48
1:C:378:SER:HB2	1:C:459:VAL:HG11	1.95	0.48
1:C:93:THR:HG23	1:C:94:LEU:H	1.78	0.48
1:D:103:ARG:HA	1:D:431:ALA:HB3	1.96	0.48
1:D:269:VAL:HG21	1:D:288:PHE:CE2	2.46	0.48
1:F:188:ILE:O	1:F:188:ILE:HD12	2.14	0.48
1:F:280:TYR:CD1	1:F:369:ARG:HD3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:LYS:HZ2	2:C:701:PLP:C4A	2.25	0.48
1:D:419:SER:O	1:D:423:TYR:N	2.47	0.48
1:F:139:THR:O	1:F:143:GLU:HB2	2.13	0.48
1:E:75:ARG:NH2	1:E:202:LEU:C	2.67	0.48
1:E:254:LEU:CA	1:E:291:LEU:HD11	2.43	0.48
1:F:356:ALA:HB3	1:F:358:GLY:N	2.29	0.48
1:A:416:ASP:OD2	1:A:441:ASP:OD1	2.31	0.48
1:C:404:TYR:OH	1:C:441:ASP:O	2.18	0.48
1:E:109:PRO:HB3	1:E:368:TYR:OH	2.13	0.48
1:E:274:ILE:HG23	1:E:275:TYR:CD1	2.49	0.48
1:F:328:CYS:O	1:F:331:LEU:HB2	2.13	0.48
1:F:371:ARG:HA	1:F:374:PHE:CZ	2.44	0.48
1:A:178:ALA:HA	1:B:76:VAL:HG11	1.96	0.48
1:C:416:ASP:HB3	1:C:419:SER:H	1.77	0.48
1:E:75:ARG:HH22	1:E:204:ASP:N	2.11	0.48
1:E:302:ASN:HB3	1:E:317:TYR:OH	2.14	0.48
1:A:230:THR:HG22	1:A:231:GLU:HG2	1.96	0.48
1:A:299:LEU:HD21	1:A:324:ILE:HG21	1.95	0.48
1:F:139:THR:O	1:F:143:GLU:N	2.46	0.48
1:F:438:PHE:CZ	1:F:445:ARG:NH2	2.81	0.48
1:E:291:LEU:CD2	1:E:292:PRO:HD2	2.44	0.48
1:E:129:PHE:CE2	1:E:345:LYS:HE2	2.49	0.48
1:F:367:ALA:O	1:F:371:ARG:HD2	2.14	0.48
1:F:408:ALA:N	1:F:409:GLU:HA	2.29	0.48
1:D:281:ALA:HB2	1:D:369:ARG:CZ	2.41	0.47
1:E:189:PRO:HD2	1:E:237:ILE:O	2.14	0.47
1:A:249:TYR:HB3	1:A:254:LEU:HG	1.96	0.47
1:B:173:LEU:HD13	1:B:199:GLN:HG2	1.95	0.47
1:B:275:TYR:OH	1:B:306:LYS:NZ	2.47	0.47
1:F:257:ILE:HG13	1:F:261:ILE:HD11	1.97	0.47
1:F:375:LEU:HB3	1:F:378:SER:HB3	1.96	0.47
1:E:214:ILE:HG12	1:E:218:PHE:CZ	2.49	0.47
1:E:386:LYS:HB2	1:E:399:ASP:HB3	1.95	0.47
1:F:145:ILE:HG22	1:F:146:CYS:N	2.29	0.47
1:F:163:LEU:HB2	1:F:325:VAL:HG13	1.96	0.47
1:F:229:LEU:HD21	1:F:267:LEU:HD13	1.96	0.47
1:F:356:ALA:N	1:F:357:GLY:HA2	2.26	0.47
1:B:129:PHE:CD1	1:B:345:LYS:NZ	2.79	0.47
1:B:356:ALA:N	1:B:358:GLY:H	2.11	0.47
1:F:301:VAL:CA	1:F:318:LEU:CD1	2.82	0.47
1:F:371:ARG:O	1:F:374:PHE:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:LEU:HD21	1:C:324:ILE:HG21	1.97	0.47
1:D:412:GLY:O	1:D:414:ILE:N	2.31	0.47
1:D:102:ILE:CG1	1:D:430:VAL:HA	2.35	0.47
1:F:305:SER:HB3	1:F:311:THR:HA	1.95	0.47
1:F:315:LEU:HA	1:F:315:LEU:HD12	1.50	0.47
1:F:404:TYR:OH	1:F:417:SER:N	2.47	0.47
1:B:434:PRO:HB2	1:B:436:ASP:HB3	1.96	0.47
1:B:92:ALA:HA	1:B:103:ARG:NH2	2.29	0.47
1:F:164:VAL:HG23	1:F:317:TYR:CB	2.34	0.47
1:D:96:GLN:NE2	1:D:97:SER:OG	2.48	0.47
1:E:102:ILE:HD12	1:E:103:ARG:H	1.76	0.47
1:E:249:TYR:CB	1:E:253:LEU:CB	2.91	0.47
1:E:361:VAL:HG13	1:E:362:ALA:N	2.30	0.47
1:E:80:LYS:HE2	1:E:80:LYS:HB3	1.49	0.47
1:F:145:ILE:HD13	1:F:317:TYR:CD2	2.49	0.47
1:F:158:ALA:HB3	1:F:160:ASP:OD1	2.14	0.47
1:F:275:TYR:HH	1:F:395:TYR:HE2	1.63	0.47
1:B:376:VAL:HG13	1:B:387:ILE:HG21	1.96	0.47
1:C:189:PRO:O	1:C:192:TYR:HB3	2.15	0.47
1:D:102:ILE:HG23	1:D:429:GLN:O	2.15	0.47
1:E:459:VAL:O	1:E:463:ARG:HG3	2.15	0.47
1:F:150:LYS:HA	1:F:155:LEU:N	2.29	0.47
1:F:165:SER:N	1:F:316:GLY:O	2.30	0.47
1:B:332:GLN:O	1:B:336:SER:O	2.33	0.47
1:E:121:GLY:O	1:E:125:ILE:HG13	2.15	0.47
1:E:252:SER:C	1:E:254:LEU:N	2.67	0.47
1:C:82:SER:OG	1:C:84:THR:HG22	2.15	0.47
1:C:90:LEU:O	1:C:94:LEU:N	2.48	0.47
1:E:195:SER:HA	1:E:198:GLU:OE1	2.15	0.47
1:E:86:VAL:HA	1:E:89:ASP:HB2	1.96	0.47
1:F:101:VAL:HG23	1:F:429:GLN:C	2.36	0.47
1:B:281:ALA:CB	1:B:282:PRO:CD	2.93	0.47
1:B:406:SER:HB2	1:B:414:ILE:HD13	1.97	0.47
1:C:95:VAL:O	1:C:98:GLY:N	2.48	0.47
1:D:396:LEU:HB3	1:D:398:ILE:HD11	1.96	0.47
1:F:138:ILE:HG13	1:F:141:LEU:CB	2.45	0.47
1:B:102:ILE:HD13	1:B:104:LEU:HG	1.96	0.46
1:B:399:ASP:OD1	1:B:401:SER:OG	2.17	0.46
1:E:115:LYS:O	1:E:119:GLU:N	2.29	0.46
1:E:124:ALA:HB1	1:E:129:PHE:HB2	1.96	0.46
1:E:280:TYR:CE1	1:E:282:PRO:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:ALA:HB1	1:E:433:VAL:HG23	1.97	0.46
1:E:258:ALA:O	1:E:262:ALA:N	2.45	0.46
1:D:281:ALA:HB1	1:D:282:PRO:HD3	1.96	0.46
1:D:95:VAL:O	1:D:99:VAL:O	2.33	0.46
1:F:223:LYS:CG	1:F:224:ASP:CA	2.93	0.46
1:F:251:LYS:O	1:F:255:GLU:HB2	2.15	0.46
1:B:172:LEU:O	1:B:176:VAL:HG23	2.15	0.46
1:A:131:ARG:HB3	1:B:108:GLU:OE1	2.15	0.46
1:B:240:SER:HB2	1:B:249:TYR:HD2	1.81	0.46
1:B:87:ILE:HG13	1:B:425:LEU:CD2	2.42	0.46
1:D:85:MET:HA	1:D:88:THR:OG1	2.15	0.46
1:D:97:SER:HA	1:D:98:GLY:HA2	1.62	0.46
1:E:365:VAL:HG12	1:E:365:VAL:O	2.16	0.46
1:F:106:ALA:O	1:F:447:SER:OG	2.17	0.46
1:A:383:LYS:N	1:A:383:LYS:HD2	2.31	0.46
1:B:413:LEU:C	1:B:414:ILE:HD12	2.36	0.46
1:B:411:PHE:O	1:B:414:ILE:HG13	2.15	0.46
1:D:401:SER:C	1:D:403:TYR:N	2.69	0.46
1:E:230:THR:HG22	1:E:231:GLU:N	2.30	0.46
1:E:258:ALA:HA	1:E:294:MET:SD	2.55	0.46
1:F:264:HIS:CG	1:F:266:ARG:H	2.31	0.46
1:F:417:SER:C	1:F:434:PRO:HB3	2.35	0.46
1:E:132:TYR:OH	2:F:701:PLP:O1P	2.27	0.46
1:A:102:ILE:HG12	1:A:430:VAL:HG22	1.97	0.46
1:E:173:LEU:HB2	1:E:199:GLN:OE1	2.16	0.46
1:E:131:ARG:HG2	1:F:108:GLU:HG2	1.97	0.46
1:F:214:ILE:HG13	1:F:218:PHE:CZ	2.51	0.46
1:F:155:LEU:HD23	1:F:295:TYR:HD2	1.81	0.46
1:A:264[A]:HIS:CE1	1:A:266:ARG:HB2	2.51	0.46
1:A:457:ALA:O	1:A:461:LYS:HG3	2.16	0.46
1:D:411:PHE:CE1	1:D:414:ILE:HD11	2.50	0.46
1:F:247:SER:OG	1:F:391:GLN:CD	2.54	0.46
1:F:276:GLU:HG3	1:F:277:HIS:N	2.30	0.46
1:E:322:LYS:N	1:E:322:LYS:CD	2.72	0.46
1:F:223:LYS:C	1:F:225:LEU:HD23	2.36	0.46
1:B:411:PHE:HE2	1:B:422:LEU:HB3	1.80	0.46
1:E:174:GLN:OE1	1:E:332:GLN:HG2	2.16	0.46
1:F:115:LYS:HA	1:F:118:ALA:HB3	1.98	0.46
1:F:318:LEU:N	1:F:318:LEU:CD2	2.76	0.46
1:D:107:GLY:O	1:D:306:LYS:HE3	2.16	0.45
1:F:317:TYR:CD2	1:F:317:TYR:O	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:GLU:OE1	1:C:285:HIS:NE2	2.33	0.45
1:D:364:MET:HE2	1:D:364:MET:HB2	1.78	0.45
1:F:225:LEU:O	1:F:227:SER:C	2.54	0.45
1:F:238:LEU:HD12	1:F:238:LEU:N	2.30	0.45
1:F:265:PRO:HA	1:F:297:ARG:HH22	1.79	0.45
1:F:275:TYR:HE1	1:F:306:LYS:NZ	2.12	0.45
1:B:241:PRO:HG2	1:B:275:TYR:HB2	1.97	0.45
1:B:409:GLU:CD	1:B:410:GLY:H	2.19	0.45
1:E:133:THR:HG22	1:E:134:LEU:N	2.31	0.45
1:E:359:GLU:HG3	1:E:360:THR:N	2.30	0.45
1:F:223:LYS:HE2	1:F:224:ASP:C	2.37	0.45
1:F:302:ASN:N	1:F:318:LEU:HD11	2.31	0.45
1:A:451:SER:O	1:A:454:VAL:HG22	2.17	0.45
1:D:423:TYR:O	1:D:423:TYR:CD1	2.69	0.45
1:F:216:ASN:O	1:F:219:LEU:HD13	2.16	0.45
1:A:413:LEU:O	1:A:413:LEU:HD12	2.16	0.45
1:F:405:GLY:O	1:F:406:SER:CB	2.64	0.45
1:B:94:LEU:H	1:B:94:LEU:HD23	1.81	0.45
1:D:179:VAL:HG12	1:D:324:ILE:HD12	1.97	0.45
1:D:423:TYR:O	1:D:423:TYR:CG	2.69	0.45
1:C:327:ALA:HB1	1:D:76:VAL:HG21	1.98	0.45
1:E:236:LEU:HD21	1:E:238:LEU:HG	1.99	0.45
1:E:234:ARG:HD3	1:E:266:ARG:HB3	1.98	0.45
1:E:340:SER:HB3	1:E:343:ALA:CB	2.44	0.45
1:F:149:LEU:HD11	1:F:157:TYR:HD1	1.82	0.45
1:F:281:ALA:HB3	1:F:282:PRO:HD3	1.98	0.45
1:F:413:LEU:C	1:F:414:ILE:HG22	2.37	0.45
1:F:244:PRO:HB3	1:F:445:ARG:NH2	2.30	0.45
1:B:281:ALA:CB	1:B:282:PRO:HD2	2.47	0.45
1:C:405:GLY:HA2	1:C:415:ASN:HD21	1.82	0.45
1:C:427:LYS:HD3	1:C:427:LYS:HA	1.56	0.45
1:E:409:GLU:C	1:E:411:PHE:H	2.19	0.45
1:F:239:CYS:HA	1:F:272:ASP:CB	2.46	0.45
1:F:330:LYS:HZ1	1:F:330:LYS:H	1.63	0.45
1:D:417:SER:HB3	1:D:441:ASP:O	2.17	0.45
1:E:161:GLN:CD	1:E:322:LYS:HZ1	2.20	0.45
1:F:259:ARG:HG3	1:F:259:ARG:H	1.44	0.45
1:F:330:LYS:HB3	1:F:330:LYS:HE3	1.48	0.45
1:F:383:LYS:HG3	1:F:383:LYS:H	1.48	0.45
1:B:80:LYS:HG3	1:B:81:PRO:CD	2.43	0.45
1:D:432:MET:CE	1:D:462:ILE:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:LEU:CD2	1:E:288:PHE:HA	2.47	0.45
1:E:403:TYR:N	1:E:403:TYR:CD1	2.85	0.45
1:E:457:ALA:HA	1:E:460:GLU:HG2	1.98	0.45
1:F:214:ILE:HG13	1:F:218:PHE:CE2	2.52	0.45
1:F:234:ARG:NH1	1:F:268:LEU:HD13	2.32	0.45
1:F:243:ASN:ND2	1:F:445:ARG:HH22	2.12	0.45
1:F:92:ALA:O	1:F:93:THR:CB	2.65	0.45
1:A:102:ILE:HG13	1:A:102:ILE:H	1.51	0.44
1:A:79:LEU:O	1:A:80:LYS:HD2	2.17	0.44
1:B:403:TYR:OH	1:B:466:LEU:HD21	2.17	0.44
1:D:423:TYR:HA	1:D:427:LYS:HZ1	1.82	0.44
1:D:428:PHE:O	1:D:430:VAL:HG23	2.17	0.44
1:E:291:LEU:HA	1:E:291:LEU:HD23	1.64	0.44
1:A:83:LYS:HZ1	1:A:418:SER:HA	1.82	0.44
1:E:157:TYR:HA	1:E:161:GLN:OE1	2.17	0.44
1:E:253:LEU:HD12	1:E:254:LEU:CB	2.46	0.44
1:F:264:HIS:C	1:F:297:ARG:HH22	2.21	0.44
1:F:356:ALA:CB	1:F:361:VAL:HG22	2.47	0.44
1:F:401:SER:C	1:F:403:TYR:N	2.70	0.44
1:B:345:LYS:O	1:B:348:VAL:HG22	2.17	0.44
1:D:332:GLN:O	1:D:336:SER:O	2.35	0.44
1:E:361:VAL:HA	1:E:364:MET:HB2	1.99	0.44
1:E:335:VAL:O	1:F:169:LYS:HB3	2.17	0.44
1:F:226:GLU:CA	1:F:228:LYS:O	2.42	0.44
1:C:414:ILE:HA	1:C:419:SER:HB2	1.98	0.44
1:E:118:ALA:O	1:E:122:ILE:HG12	2.17	0.44
1:E:372:ARG:HG3	1:E:390:PRO:HG2	1.99	0.44
1:F:225:LEU:HD11	1:F:229:LEU:HD11	2.00	0.44
1:F:288:PHE:HD2	1:F:298:THR:OG1	2.00	0.44
1:A:83:LYS:NZ	1:A:434:PRO:HG2	2.32	0.44
1:E:153:ASN:HB2	1:E:155:LEU:HD13	2.00	0.44
1:A:269:VAL:HG21	1:A:288:PHE:CE2	2.52	0.44
1:C:299:LEU:HB3	1:C:318:LEU:HD21	2.00	0.44
1:E:158:ALA:HB3	1:E:161:GLN:HG3	2.00	0.44
1:F:462:ILE:O	1:F:466:LEU:HB2	2.17	0.44
1:A:111:PHE:CE2	1:A:364:MET:HB3	2.52	0.44
1:E:150:LYS:HE3	1:E:156:SER:HA	2.00	0.44
1:E:257:ILE:O	1:E:258:ALA:HB3	2.18	0.44
1:E:278:ILE:HD12	1:E:368:TYR:HE2	1.83	0.44
1:E:361:VAL:O	1:E:365:VAL:HG23	2.18	0.44
1:E:432:MET:HE2	1:E:446:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:370:GLU:O	1:F:374:PHE:HD1	2.01	0.44
1:F:414:ILE:HD13	1:F:423:TYR:HB2	1.99	0.44
1:D:424:PHE:O	1:D:428:PHE:HB2	2.18	0.44
1:E:413:LEU:HD22	1:E:414:ILE:N	2.30	0.44
1:E:415:ASN:N	1:E:415:ASN:OD1	2.50	0.44
1:F:150:LYS:HE3	1:F:154:GLY:O	2.17	0.44
1:F:270:LEU:HD21	1:F:301:VAL:HG21	1.99	0.44
1:F:450:THR:OG1	1:F:455:LEU:HD11	2.18	0.44
1:F:306:LYS:NZ	2:F:701:PLP:C4	2.79	0.44
1:A:83:LYS:CE	1:A:418:SER:HB3	2.47	0.44
1:B:97:SER:HA	1:B:98:GLY:HA2	1.52	0.44
1:C:411:PHE:CE2	1:C:427:LYS:NZ	2.86	0.44
1:C:102:ILE:HD11	1:C:431:ALA:H	1.83	0.44
1:C:90:LEU:HD12	1:C:90:LEU:HA	1.83	0.44
1:D:404:TYR:OH	1:D:417:SER:HA	2.17	0.44
1:D:90:LEU:O	1:D:94:LEU:C	2.56	0.44
1:D:94:LEU:HA	1:D:95:VAL:HA	1.84	0.44
1:F:254:LEU:HD11	1:F:288:PHE:CE1	2.53	0.44
1:B:230:THR:HG22	1:B:231:GLU:N	2.33	0.43
1:C:102:ILE:CD1	1:C:103:ARG:N	2.67	0.43
1:E:234:ARG:CD	1:E:266:ARG:HB3	2.48	0.43
1:E:95:VAL:HG13	1:E:99:VAL:HB	2.00	0.43
1:F:257:ILE:HG23	1:F:258:ALA:N	2.33	0.43
1:F:261:ILE:HG12	1:F:269:VAL:CG2	2.48	0.43
1:F:274:ILE:HD13	1:F:303:GLY:N	2.33	0.43
1:A:150:LYS:HZ1	1:A:156:SER:HG	1.65	0.43
1:A:72:LEU:HD13	1:B:327:ALA:HB2	1.99	0.43
1:C:184:ASP:OD1	1:C:266:ARG:NH2	2.51	0.43
1:C:414:ILE:HD13	1:C:419:SER:HB3	2.00	0.43
1:F:408:ALA:N	1:F:409:GLU:HG2	2.33	0.43
1:F:110:ASP:N	1:F:449:ALA:HB1	2.34	0.43
1:F:90:LEU:HD23	1:F:90:LEU:N	2.33	0.43
1:A:150:LYS:NZ	1:A:156:SER:OG	2.50	0.43
1:C:79:LEU:HA	1:C:79:LEU:HD23	1.86	0.43
1:D:269:VAL:HG11	1:D:288:PHE:CD2	2.53	0.43
1:D:401:SER:HA	1:D:404:TYR:CG	2.53	0.43
1:D:401:SER:C	1:D:403:TYR:H	2.20	0.43
1:F:99:VAL:HG11	1:F:429:GLN:HE21	1.83	0.43
1:A:306:LYS:NZ	2:A:701:PLP:C4A	2.81	0.43
1:B:467:GLU:O	1:B:469:LEU:N	2.44	0.43
1:E:102:ILE:HG13	1:E:430:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:225:LEU:H	1:F:225:LEU:HD23	1.83	0.43
1:F:223:LYS:CG	1:F:226:GLU:H	2.23	0.43
1:F:303:GLY:HA2	1:F:317:TYR:CE1	2.53	0.43
1:F:278:ILE:CG2	1:F:368:TYR:HD2	2.30	0.43
1:A:383:LYS:O	1:A:403:TYR:OH	2.27	0.43
1:A:425:LEU:O	1:A:427:LYS:N	2.49	0.43
1:B:81:PRO:O	3:B:801:HOH:O	2.21	0.43
1:C:281:ALA:HB3	1:C:282:PRO:CD	2.48	0.43
1:C:356:ALA:HB3	1:C:358:GLY:O	2.19	0.43
1:C:375:LEU:HG	1:C:455:LEU:HD22	2.01	0.43
1:E:251:LYS:HD3	1:E:252:SER:N	2.33	0.43
1:E:252:SER:C	1:E:254:LEU:H	2.20	0.43
1:E:339:ALA:C	1:F:314:ARG:NH1	2.71	0.43
1:F:299:LEU:HD21	1:F:324:ILE:HG21	2.01	0.43
1:D:398:ILE:HD13	1:D:446:ILE:HD12	1.99	0.43
1:F:150:LYS:O	1:F:154:GLY:HA2	2.18	0.43
1:A:233:SER:HB3	1:A:267:LEU:HD13	2.00	0.43
1:A:80:LYS:N	1:A:81:PRO:CD	2.79	0.43
1:B:436:ASP:OD1	1:F:413:LEU:HG	2.19	0.43
1:C:405:GLY:O	1:C:407:GLU:HG2	2.19	0.43
1:E:254:LEU:HD13	1:E:291:LEU:CG	2.47	0.43
1:E:234:ARG:CD	1:E:266:ARG:HE	2.32	0.43
1:E:334:GLN:O	1:F:173:LEU:HD11	2.19	0.43
1:F:105:ALA:HB1	1:F:433:VAL:CG2	2.48	0.43
1:E:225:LEU:O	1:E:229:LEU:HG	2.18	0.43
1:F:223:LYS:CG	1:F:225:LEU:C	2.86	0.43
1:F:235:LEU:HD23	1:F:236:LEU:N	2.33	0.43
1:F:191:PRO:CB	1:F:244:PRO:HG2	2.44	0.43
1:F:110:ASP:CG	1:F:371:ARG:HH22	2.20	0.43
1:F:394:PHE:HB2	1:F:448:TYR:CD2	2.54	0.43
1:F:306:LYS:HZ3	2:F:701:PLP:C3	2.32	0.43
1:C:404:TYR:C	1:C:406:SER:H	2.17	0.43
1:E:79:LEU:HD21	1:E:198:GLU:HG2	2.01	0.43
1:F:256:GLU:O	1:F:260:ILE:HG12	2.18	0.43
1:F:409:GLU:HB2	1:F:414:ILE:HG23	2.01	0.43
1:A:225:LEU:O	1:A:229:LEU:HG	2.18	0.42
1:A:386:LYS:O	1:A:387:ILE:HD12	2.19	0.42
1:A:460:GLU:O	1:A:464:LYS:HG3	2.19	0.42
1:A:90:LEU:HD13	1:A:90:LEU:HA	1.88	0.42
1:B:91:ALA:C	1:B:93:THR:H	2.17	0.42
1:E:135:ASN:HD21	1:E:332:GLN:HE21	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:SER:HA	1:E:255:GLU:CB	2.49	0.42
1:E:75:ARG:NE	1:E:201:ARG:O	2.52	0.42
1:F:428:PHE:CG	1:F:465:ALA:HB2	2.54	0.42
1:F:457:ALA:C	1:F:460:GLU:OE1	2.56	0.42
1:A:411:PHE:CE2	1:A:423:TYR:CD1	3.03	0.42
1:A:420:LEU:HD12	1:A:420:LEU:HA	1.77	0.42
1:A:102:ILE:CD1	1:A:431:ALA:H	2.31	0.42
1:A:87:ILE:HG23	1:A:88:THR:N	2.32	0.42
1:D:85:MET:HE2	1:D:85:MET:HB3	1.95	0.42
1:E:292:PRO:O	1:E:293:ASP:HB2	2.19	0.42
1:A:425:LEU:HD23	1:A:426:ASP:HB2	2.01	0.42
1:E:83:LYS:HD2	1:E:436:ASP:OD2	2.19	0.42
1:F:399:ASP:O	1:F:401:SER:N	2.52	0.42
1:A:366:LYS:HB2	1:A:366:LYS:HE3	1.73	0.42
1:A:409:GLU:HA	1:A:410:GLY:HA2	1.23	0.42
1:B:386:LYS:HD2	1:B:387:ILE:H	1.85	0.42
1:C:420:LEU:O	1:C:424:PHE:CD1	2.70	0.42
1:D:396:LEU:HD23	1:D:396:LEU:HA	1.65	0.42
1:D:414:ILE:O	1:D:415:ASN:ND2	2.51	0.42
1:E:254:LEU:HD11	1:E:286:THR:HG22	2.01	0.42
1:E:398:ILE:HG21	1:E:446:ILE:HD11	2.02	0.42
1:A:274:ILE:HG23	1:A:275:TYR:CD2	2.54	0.42
1:B:425:LEU:HG	1:B:426:ASP:OD1	2.20	0.42
1:D:425:LEU:HA	1:D:430:VAL:H	1.82	0.42
1:E:280:TYR:N	1:E:391:GLN:O	2.51	0.42
1:E:97:SER:HA	1:E:98:GLY:HA2	1.46	0.42
1:A:84:THR:O	1:A:88:THR:HG22	2.19	0.42
1:C:122:ILE:HG23	1:D:122:ILE:HD13	2.01	0.42
1:D:466:LEU:N	1:D:466:LEU:CD1	2.70	0.42
1:D:80:LYS:HE3	1:D:81:PRO:O	2.19	0.42
1:E:168:ALA:HB3	2:E:701:PLP:H5A2	2.02	0.42
1:E:275:TYR:CE2	1:E:306:LYS:HD2	2.53	0.42
1:E:359:GLU:HG2	1:E:359:GLU:H	1.63	0.42
1:E:448:TYR:HD1	1:E:448:TYR:O	2.03	0.42
1:F:356:ALA:N	1:F:357:GLY:CA	2.80	0.42
1:A:356:ALA:N	1:A:357:GLY:CA	2.81	0.42
1:A:450:THR:OG1	1:A:454:VAL:HG21	2.19	0.42
1:B:398:ILE:HD12	1:B:446:ILE:CD1	2.36	0.42
1:B:410:GLY:HA3	3:B:802:HOH:O	2.20	0.42
1:C:406:SER:OG	1:C:469:LEU:HD23	2.20	0.42
1:C:466:LEU:HD23	1:C:466:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:VAL:HA	1:D:429:GLN:HG2	2.02	0.42
1:D:267:LEU:HA	1:D:267:LEU:HD22	1.75	0.42
1:F:102:ILE:HG21	1:F:458:ALA:HB2	2.02	0.42
1:F:228:LYS:C	1:F:229:LEU:O	2.56	0.42
1:F:359:GLU:O	1:F:362:ALA:HB3	2.20	0.42
1:A:86:VAL:HA	1:A:90:LEU:HD23	2.01	0.42
1:B:335:VAL:HG12	1:B:336:SER:N	2.34	0.42
1:D:191:PRO:HA	1:D:438:PHE:O	2.20	0.42
1:D:95:VAL:HB	1:D:99:VAL:CG1	2.49	0.42
1:A:229:LEU:HD13	1:A:264[B]:HIS:NE2	2.35	0.42
1:A:458:ALA:O	1:A:462:ILE:HG13	2.19	0.42
1:B:456:GLN:HG3	1:B:457:ALA:N	2.35	0.42
1:E:138:ILE:HG12	1:E:344:GLN:OE1	2.19	0.42
1:E:404:TYR:HE1	1:E:416:ASP:O	2.02	0.42
1:F:403:TYR:HE2	1:F:466:LEU:O	2.02	0.42
1:B:83:LYS:NZ	1:F:412:GLY:HA3	2.35	0.42
1:B:102:ILE:C	1:B:102:ILE:CD1	2.79	0.42
1:B:177:LEU:HD23	1:B:203:ALA:HB2	2.02	0.42
1:E:105:ALA:HB1	1:E:433:VAL:CG2	2.50	0.42
1:E:102:ILE:HG12	1:E:430:VAL:HG22	2.02	0.42
1:F:356:ALA:HA	1:F:361:VAL:CB	2.50	0.42
1:F:372:ARG:CB	1:F:448:TYR:CZ	3.01	0.42
1:F:379:LEU:HD21	1:F:459:VAL:HG23	2.02	0.42
1:A:414:ILE:HD11	1:A:423:TYR:CG	2.54	0.41
1:B:93:THR:O	1:B:95:VAL:N	2.53	0.41
1:E:243:ASN:OD1	1:E:244:PRO:HA	2.19	0.41
1:F:214:ILE:N	1:F:214:ILE:HD12	2.33	0.41
1:F:381:ASP:OD1	1:F:382:ILE:N	2.53	0.41
1:F:414:ILE:O	1:F:414:ILE:HG13	2.20	0.41
1:B:91:ALA:C	1:B:93:THR:N	2.74	0.41
1:D:99:VAL:HG22	1:D:100:PRO:O	2.20	0.41
1:E:99:VAL:HG12	1:E:100:PRO:HD2	2.02	0.41
1:E:131:ARG:O	1:E:341:SER:OG	2.29	0.41
1:E:222:PRO:HG2	1:E:223:LYS:N	2.35	0.41
1:E:399:ASP:OD1	1:E:401:SER:HB3	2.20	0.41
1:A:79:LEU:HD22	1:A:198:GLU:OE1	2.20	0.41
1:B:102:ILE:HD13	1:B:104:LEU:N	2.35	0.41
1:D:398:ILE:N	1:D:398:ILE:HD12	2.35	0.41
1:E:158:ALA:H	1:E:161:GLN:CG	2.33	0.41
1:E:161:GLN:CD	1:E:322:LYS:NZ	2.74	0.41
1:E:194:VAL:HG22	1:E:198:GLU:CD	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:LEU:HD23	1:E:292:PRO:HD2	2.01	0.41
1:F:101:VAL:HG21	1:F:425:LEU:CD1	2.50	0.41
1:F:372:ARG:CD	1:F:373:ASP:OD2	2.65	0.41
1:A:230:THR:HG22	1:A:231:GLU:N	2.35	0.41
1:B:133:THR:HG22	1:B:134:LEU:N	2.35	0.41
1:B:355:LYS:C	1:B:357:GLY:HA2	2.41	0.41
1:C:138:ILE:HG12	1:C:344:GLN:OE1	2.20	0.41
1:C:188:ILE:O	1:C:209:VAL:HA	2.21	0.41
1:F:143:GLU:O	1:F:147:ARG:CG	2.69	0.41
1:F:189:PRO:HG3	1:F:220:LEU:HG	2.01	0.41
1:F:230:THR:HG22	1:F:231:GLU:H	1.85	0.41
1:F:353:LEU:HD23	1:F:353:LEU:HA	1.81	0.41
1:F:370:GLU:O	1:F:374:PHE:CD1	2.74	0.41
1:E:234:ARG:HD3	1:E:266:ARG:HE	1.85	0.41
1:E:420:LEU:O	1:E:423:TYR:HB3	2.20	0.41
1:F:147:ARG:HE	1:F:147:ARG:H	1.68	0.41
1:D:453:ASP:OD1	1:D:454:VAL:HG23	2.20	0.41
1:F:188:ILE:CD1	1:F:209:VAL:HA	2.49	0.41
1:F:318:LEU:HA	1:F:318:LEU:HD13	1.79	0.41
1:F:105:ALA:HB1	1:F:433:VAL:HG23	2.02	0.41
1:F:451:SER:O	1:F:455:LEU:HD12	2.21	0.41
1:A:102:ILE:HD11	1:A:430:VAL:CA	2.48	0.41
1:A:455:LEU:O	1:A:459:VAL:HG23	2.20	0.41
1:C:281:ALA:HB3	1:C:282:PRO:HD3	2.02	0.41
1:C:466:LEU:HA	1:C:469:LEU:HD13	2.02	0.41
1:C:314:ARG:HH12	1:D:132:TYR:HE1	1.67	0.41
1:D:421:ALA:HB3	1:D:434:PRO:HG3	2.02	0.41
1:F:317:TYR:CG	1:F:317:TYR:O	2.74	0.41
1:F:374:PHE:CE1	1:F:452:LEU:HD12	2.56	0.41
1:D:275:TYR:OH	1:D:306:LYS:HE2	2.21	0.41
1:E:72:LEU:HD13	1:F:327:ALA:CB	2.51	0.41
1:E:79:LEU:O	1:E:79:LEU:HD23	2.21	0.41
1:F:124:ALA:HB2	1:F:345:LYS:CD	2.47	0.41
1:F:201:ARG:HH11	1:F:201:ARG:HG2	1.86	0.41
1:F:244:PRO:HG3	1:F:438:PHE:CB	2.51	0.41
1:F:310:MET:HE2	1:F:310:MET:HB3	1.85	0.41
1:A:102:ILE:CG1	1:A:430:VAL:HA	2.51	0.41
1:E:149:LEU:HD13	1:E:157:TYR:CD2	2.56	0.41
1:F:361:VAL:O	1:F:362:ALA:C	2.59	0.41
1:A:467:GLU:HB2	1:A:468:PRO:HD3	2.02	0.41
1:E:257:ILE:H	1:E:257:ILE:CD1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:LEU:HD12	1:E:315:LEU:HA	1.86	0.41
1:F:110:ASP:H	1:F:449:ALA:HB1	1.86	0.41
1:F:149:LEU:HD12	1:F:150:LYS:N	2.35	0.41
1:F:162:ILE:CD1	1:F:319:ALA:HB2	2.26	0.41
1:A:466:LEU:HD23	1:A:466:LEU:HA	1.86	0.41
1:C:279:ILE:HG21	1:C:279:ILE:HD13	1.88	0.41
1:D:464:LYS:CA	1:D:467:GLU:HG3	2.47	0.41
1:E:254:LEU:HD21	1:E:288:PHE:HA	2.03	0.41
1:E:279:ILE:HG22	1:E:280:TYR:N	2.35	0.41
1:F:90:LEU:HD11	1:F:425:LEU:HD23	2.03	0.41
1:F:86:VAL:O	1:F:90:LEU:CD2	2.67	0.41
1:B:403:TYR:CE2	1:B:466:LEU:HG	2.56	0.40
1:B:102:ILE:HG13	1:B:430:VAL:HA	2.03	0.40
1:D:102:ILE:HG12	1:D:429:GLN:O	2.21	0.40
1:D:463:ARG:HA	1:D:466:LEU:HD11	2.03	0.40
1:E:237:ILE:O	1:E:238:LEU:HD23	2.21	0.40
1:E:261:ILE:HD12	1:E:267:LEU:CD2	2.48	0.40
1:E:357:GLY:O	1:E:361:VAL:HG12	2.21	0.40
1:E:417:SER:HG	1:E:436:ASP:HB2	1.86	0.40
1:E:75:ARG:HA	1:E:78:SER:OG	2.21	0.40
1:F:117:VAL:HG12	1:F:346:ALA:HB1	2.03	0.40
1:F:133:THR:HG22	1:F:134:LEU:O	2.21	0.40
1:F:195:SER:HA	1:F:198:GLU:OE1	2.20	0.40
1:F:335:VAL:HG13	1:F:336:SER:N	2.33	0.40
1:F:454:VAL:O	1:F:458:ALA:N	2.55	0.40
1:B:378:SER:HB3	1:B:459:VAL:HG11	2.03	0.40
1:E:222:PRO:HG2	1:E:223:LYS:CD	2.51	0.40
1:E:435:GLY:N	1:E:443:CYS:O	2.48	0.40
1:F:269:VAL:HG11	1:F:288:PHE:CZ	2.56	0.40
1:F:375:LEU:HD12	1:F:459:VAL:HG11	2.03	0.40
1:F:278:ILE:HB	1:F:393:ALA:HA	2.02	0.40
1:B:142:ARG:HH11	1:B:142:ARG:HD2	1.62	0.40
1:C:356:ALA:N	1:C:357:GLY:CA	2.83	0.40
1:D:104:LEU:HD11	1:D:458:ALA:HB1	2.02	0.40
1:F:147:ARG:HD2	1:F:148:LYS:H	1.86	0.40
1:F:280:TYR:CE1	1:F:369:ARG:HD3	2.56	0.40
1:F:356:ALA:HB3	1:F:358:GLY:C	2.42	0.40
1:F:400:PHE:CE1	1:F:466:LEU:HD21	2.48	0.40
1:A:235:LEU:HD11	1:A:270:LEU:HB2	2.02	0.40
1:A:425:LEU:HD23	1:A:426:ASP:N	2.37	0.40
1:F:111:PHE:HE2	1:F:367:ALA:HB3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:378:SER:O	1:F:381:ASP:OD1	2.39	0.40
1:F:445:ARG:HD3	1:F:445:ARG:HH11	1.70	0.40
1:C:131:ARG:HG3	1:C:131:ARG:NH1	2.33	0.40
1:C:394:PHE:CE1	1:C:395:TYR:CZ	3.10	0.40
1:E:403:TYR:N	1:E:403:TYR:HD1	2.20	0.40
1:F:202:LEU:HA	1:F:202:LEU:HD23	1.88	0.40
1:F:275:TYR:CE2	1:F:395:TYR:HE2	2.39	0.40
1:F:294:MET:CE	1:F:297:ARG:HD2	2.52	0.40
1:F:452:LEU:HA	1:F:455:LEU:CD1	2.51	0.40
1:E:178:ALA:HA	1:F:76:VAL:HG21	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ASN:ND2	1:D:416:ASP:OD1[2_555]	2.00	0.20
3:B:812:HOH:O	3:D:809:HOH:O[1_665]	2.03	0.17

## 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	398/475 (84%)	378 (95%)	13 (3%)	7 (2%)	8	37
1	B	397/475 (84%)	374 (94%)	13 (3%)	10 (2%)	5	28
1	C	399/475 (84%)	378 (95%)	17 (4%)	4 (1%)	15	53
1	D	398/475 (84%)	371 (93%)	18 (4%)	9 (2%)	6	30
1	E	397/475 (84%)	368 (93%)	21 (5%)	8 (2%)	7	34
1	F	393/475 (83%)	353 (90%)	22 (6%)	18 (5%)	2	14
All	All	2382/2850 (84%)	2222 (93%)	104 (4%)	56 (2%)	6	29

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
1	A	81	PRO
1	A	97	SER
1	B	72	LEU
1	B	281	ALA
1	B	406	SER
1	B	427	LYS
1	C	72	LEU
1	C	281	ALA
1	D	88	THR
1	D	281	ALA
1	D	412	GLY
1	D	413	LEU
1	E	80	LYS
1	E	253	LEU
1	F	217	ASN
1	F	229	LEU
1	F	234	ARG
1	F	245	THR
1	F	248	VAL
1	F	395	TYR
1	F	402	ALA
1	F	406	SER
1	A	96	GLN
1	A	402	ALA
1	B	92	ALA
1	B	94	LEU
1	B	409	GLU
1	B	412	GLY
1	C	95	VAL
1	C	405	GLY
1	D	75	ARG
1	D	92	ALA
1	D	468	PRO
1	E	93	THR
1	E	250	PRO
1	F	75	ARG
1	F	93	THR
1	F	226	GLU
1	A	75	ARG
1	A	82	SER
1	D	401	SER

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Mol	Chain	Res	Type
1	D	402	ALA
1	F	154	GLY
1	F	225	LEU
1	F	401	SER
1	E	251	LYS
1	E	406	SER
1	E	409	GLU
1	F	74	PRO
1	F	400	PHE
1	B	337	SER
1	B	335	VAL
1	F	145	ILE
1	F	468	PRO
1	E	265	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	327/390 (84%)	319 (98%)	8 (2%)	49	79
1	B	326/390 (84%)	319 (98%)	7 (2%)	53	82
1	C	326/390 (84%)	321 (98%)	5 (2%)	65	87
1	D	327/390 (84%)	318 (97%)	9 (3%)	43	77
1	E	326/390 (84%)	315 (97%)	11 (3%)	37	72
1	F	322/390 (83%)	298 (92%)	24 (8%)	13	43
All	All	1954/2340 (84%)	1890 (97%)	64 (3%)	38	73

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	A	96	GLN
1	A	337	SER
1	A	383	LYS

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Mol	Chain	Res	Type
1	A	397	PHE
1	A	411	PHE
1	A	415	ASN
1	A	416	ASP
1	B	94	LEU
1	B	103	ARG
1	B	156	SER
1	B	242	SER
1	B	397	PHE
1	B	413	LEU
1	B	463	ARG
1	C	85	MET
1	C	126	ARG
1	C	217	ASN
1	C	394	PHE
1	C	397	PHE
1	D	75	ARG
1	D	90	LEU
1	D	148	LYS
1	D	192	TYR
1	D	217	ASN
1	D	397	PHE
1	D	452	LEU
1	D	464	LYS
1	D	466	LEU
1	E	71	SER
1	E	80	LYS
1	E	96	GLN
1	E	115	LYS
1	E	135	ASN
1	E	226	GLU
1	E	231	GLU
1	E	253	LEU
1	E	397	PHE
1	E	401	SER
1	E	424	PHE
1	F	72	LEU
1	F	79	LEU
1	F	90	LEU
1	F	103	ARG
1	F	112	ASP
1	F	147	ARG

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Mol	Chain	Res	Type
1	F	149	LEU
1	F	169	LYS
1	F	216	ASN
1	F	223	LYS
1	F	225	LEU
1	F	280	TYR
1	F	295	TYR
1	F	302	ASN
1	F	314	ARG
1	F	323	HIS
1	F	330	LYS
1	F	340	SER
1	F	366	LYS
1	F	372	ARG
1	F	374	PHE
1	F	378	SER
1	F	397	PHE
1	F	448	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	166	ASN
1	C	96	GLN
1	C	415	ASN
1	E	135	ASN
1	F	123	ASN
1	F	153	ASN
1	F	166	ASN
1	F	170	GLN
1	F	217	ASN
1	F	264	HIS
1	F	302	ASN
1	F	391	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	PLP	E	701	-	15,15,16	0.99	0	20,22,23	0.94	0
2	PLP	D	701	-	15,15,16	1.72	1 (6%)	20,22,23	1.42	4 (20%)
2	PLP	F	701	-	15,15,16	1.20	1 (6%)	20,22,23	1.16	2 (10%)
2	PLP	A	701	-	15,15,16	1.48	2 (13%)	20,22,23	1.74	8 (40%)
2	PLP	C	701	-	15,15,16	1.59	2 (13%)	20,22,23	1.29	3 (15%)
2	PLP	B	701	-	15,15,16	1.27	1 (6%)	20,22,23	1.48	2 (10%)

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	PLP	E	701	-	-	3/6/6/8	0/1/1/1
2	PLP	D	701	-	-	5/6/6/8	0/1/1/1
2	PLP	F	701	-	-	3/6/6/8	0/1/1/1
2	PLP	A	701	-	-	3/6/6/8	0/1/1/1
2	PLP	C	701	-	-	3/6/6/8	0/1/1/1
2	PLP	B	701	-	-	5/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	PLP	C3-C2	-4.69	1.36	1.40
2	A	701	PLP	C3-C2	-3.79	1.37	1.40
2	C	701	PLP	C3-C2	-3.24	1.37	1.40
2	B	701	PLP	C2A-C2	2.35	1.54	1.50
2	F	701	PLP	C3-C2	-2.30	1.38	1.40
2	C	701	PLP	C5-C4	-2.12	1.38	1.40
2	A	701	PLP	C5-C4	-2.11	1.38	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	PLP	C4A-C4-C5	-3.62	117.21	120.94
2	D	701	PLP	O4P-C5A-C5	3.43	115.89	109.35
2	B	701	PLP	O3P-P-O4P	3.24	115.36	106.73
2	C	701	PLP	C5-C6-N1	-2.60	119.49	123.82
2	B	701	PLP	C6-N1-C2	2.51	123.82	119.17
2	A	701	PLP	C2A-C2-C3	-2.47	117.83	120.89
2	A	701	PLP	O3-C3-C4	2.38	124.36	118.10
2	A	701	PLP	O2P-P-O4P	2.36	113.00	106.73
2	A	701	PLP	C5-C6-N1	-2.33	119.94	123.82
2	C	701	PLP	C6-C5-C4	2.26	119.94	118.16
2	A	701	PLP	O4P-C5A-C5	2.25	113.64	109.35
2	F	701	PLP	C2A-C2-C3	-2.24	118.12	120.89
2	D	701	PLP	O3-C3-C4	2.22	123.96	118.10
2	D	701	PLP	C5-C6-N1	-2.19	120.18	123.82
2	D	701	PLP	C6-N1-C2	2.16	123.18	119.17
2	A	701	PLP	C2A-C2-N1	2.15	121.86	117.67
2	C	701	PLP	C2A-C2-C3	-2.14	118.24	120.89
2	F	701	PLP	C5-C6-N1	-2.06	120.39	123.82
2	A	701	PLP	C6-N1-C2	2.02	122.91	119.17

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	701	PLP	C5A-O4P-P-O2P
2	E	701	PLP	C5A-O4P-P-O3P
2	D	701	PLP	C6-C5-C5A-O4P
2	D	701	PLP	C5A-O4P-P-O3P
2	F	701	PLP	C5A-O4P-P-O3P
2	A	701	PLP	C5A-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
2	A	701	PLP	C5A-O4P-P-O3P
2	C	701	PLP	C5A-O4P-P-O1P
2	C	701	PLP	C5A-O4P-P-O2P
2	C	701	PLP	C5A-O4P-P-O3P
2	B	701	PLP	C4-C5-C5A-O4P
2	B	701	PLP	C6-C5-C5A-O4P
2	B	701	PLP	C5A-O4P-P-O3P
2	E	701	PLP	C5A-O4P-P-O1P
2	F	701	PLP	C5A-O4P-P-O1P
2	A	701	PLP	C5A-O4P-P-O1P
2	B	701	PLP	C5A-O4P-P-O1P
2	D	701	PLP	C5A-O4P-P-O2P
2	F	701	PLP	C5A-O4P-P-O2P
2	B	701	PLP	C5A-O4P-P-O2P
2	D	701	PLP	C5A-O4P-P-O1P
2	D	701	PLP	C4-C5-C5A-O4P

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	701	PLP	1	0
2	D	701	PLP	3	0
2	F	701	PLP	4	0
2	A	701	PLP	1	0
2	C	701	PLP	2	0
2	B	701	PLP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	399/475 (84%)	-0.42	3 (0%) 86 65	37, 50, 99, 172	0
1	B	399/475 (84%)	-0.42	3 (0%) 86 65	37, 47, 98, 162	0
1	C	401/475 (84%)	-0.51	3 (0%) 87 69	38, 53, 96, 185	0
1	D	400/475 (84%)	-0.45	2 (0%) 91 75	37, 49, 107, 195	0
1	E	399/475 (84%)	-0.08	4 (1%) 82 59	57, 88, 133, 173	0
1	F	397/475 (83%)	0.24	15 (3%) 40 16	60, 107, 167, 235	0
All	All	2395/2850 (84%)	-0.27	30 (1%) 77 51	37, 63, 134, 235	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	408	ALA	6.7
1	F	357	GLY	3.8
1	F	91	ALA	3.7
1	C	409	GLU	3.3
1	E	93	THR	3.2
1	A	80	LYS	3.2
1	F	96	GLN	3.0
1	B	426	ASP	2.8
1	C	410	GLY	2.7
1	F	89	ASP	2.6
1	F	296	GLU	2.6
1	F	220	LEU	2.5
1	B	94	LEU	2.5
1	A	384	GLY	2.4
1	F	406	SER	2.4
1	D	89	ASP	2.3
1	F	368	TYR	2.3
1	F	263	LYS	2.3
1	F	272	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	412	GLY	2.2
1	F	374	PHE	2.2
1	E	89	ASP	2.2
1	A	410	GLY	2.2
1	E	406	SER	2.2
1	F	253	LEU	2.1
1	F	245	THR	2.1
1	C	413	LEU	2.1
1	B	81	PRO	2.1
1	E	407	GLU	2.1
1	F	93	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PLP	F	701	15/16	0.91	0.32	97,115,123,125	0
2	PLP	E	701	15/16	0.94	0.27	80,86,96,101	0
2	PLP	D	701	15/16	0.95	0.23	39,40,66,69	0
2	PLP	A	701	15/16	0.95	0.21	37,50,56,62	0
2	PLP	C	701	15/16	0.95	0.26	41,48,59,65	0
2	PLP	B	701	15/16	0.97	0.25	38,47,56,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.