



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 01:50 AM UTC

PDB ID : 5WMH / pdb_00005wmh
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

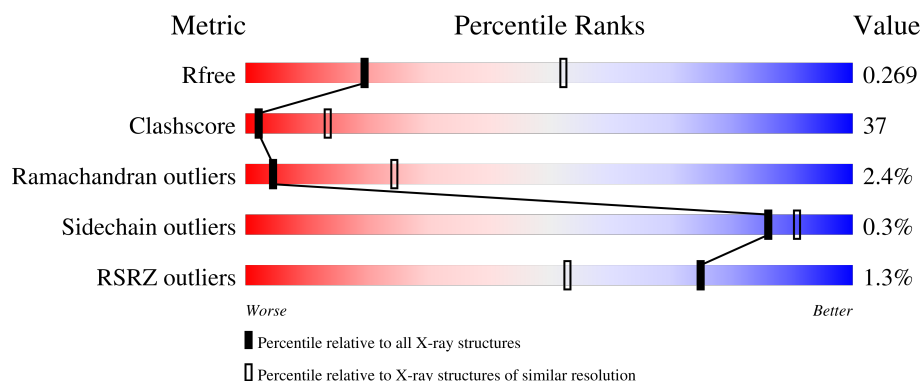
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	475	0% 58% 24% • 16%
1	B	475	0% 58% 24% • 16%
1	C	475	0% 57% 26% •• 16%
1	D	475	0% 53% 28% • 16%
1	E	475	2% 34% 47% • 16%

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Mol	Chain	Length	Quality of chain
1	F	475	2% 23% 52% 7% 16%

2 Entry composition [i](#)

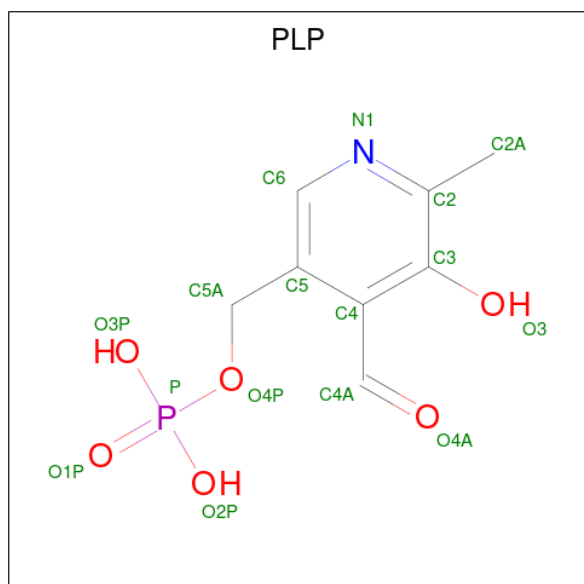
There are 3 unique types of molecules in this entry. The entry contains 18299 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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		

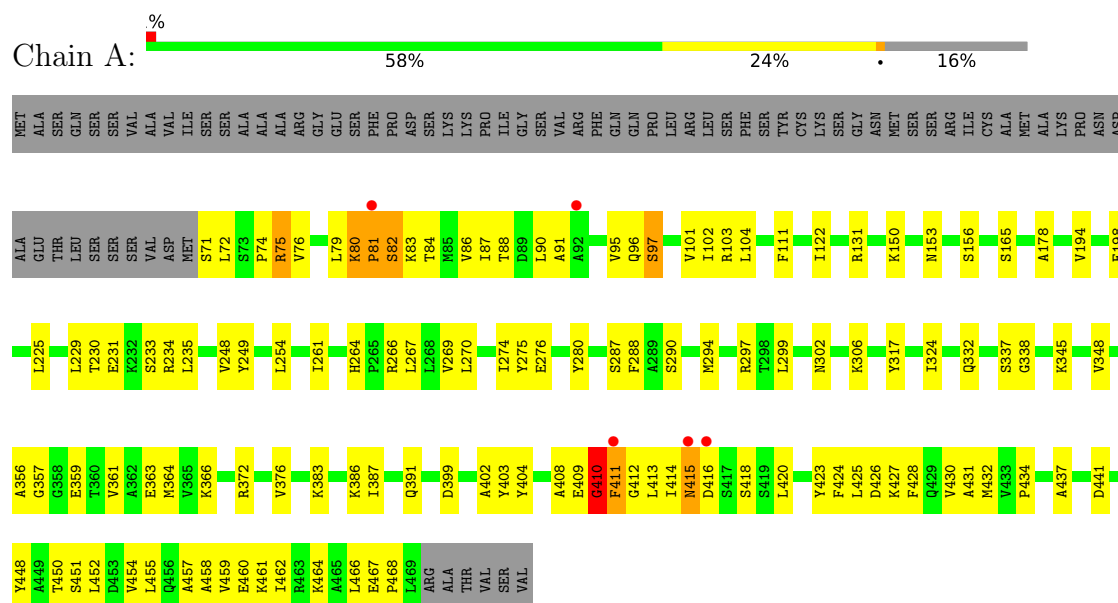
- Molecule 3 is water.

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		

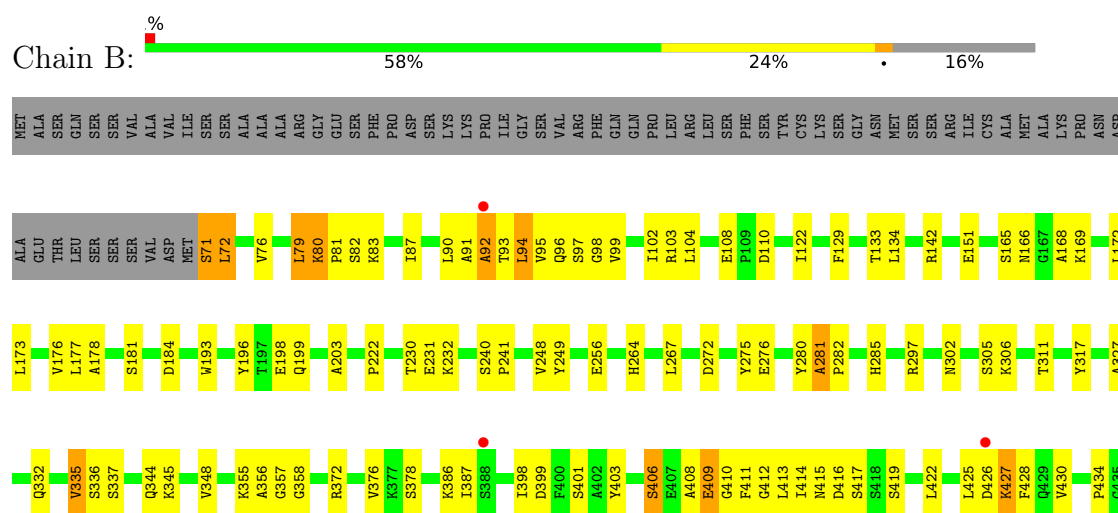
3 Residue-property plots

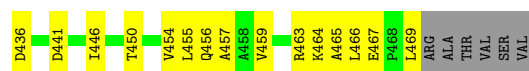
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Bifunctional aspartate aminotransferase and glutamate/aspartate-prephenate aminotransferase

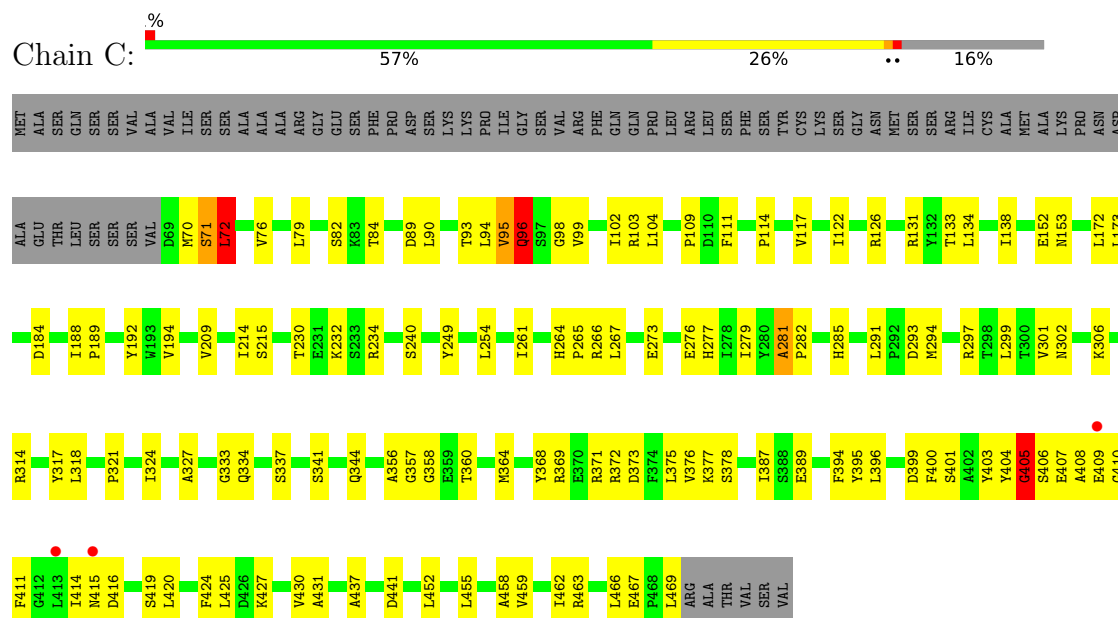


- Molecule 1: Bifunctional aspartate aminotransferase and glutamate/aspartate-prephenate aminotransferase

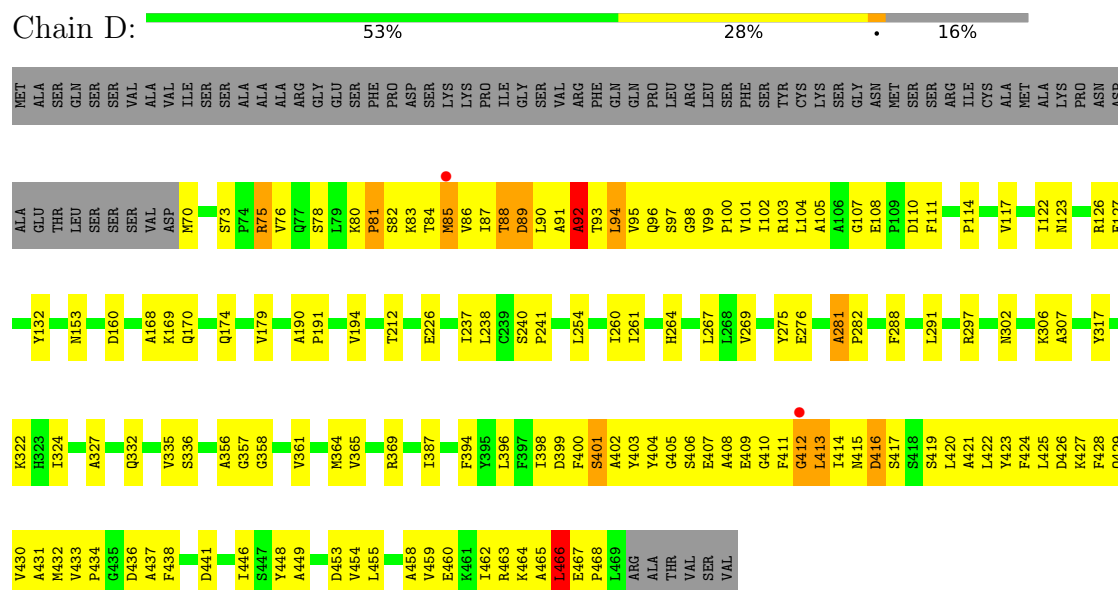




- Molecule 1: Bifunctional aspartate aminotransferase and glutamate/aspartate-prephenate aminotransferase



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MET	Y385	S329	I260	V194	R126	ALA
	L396	K330	I261	Y196	E127	GLU
	F397	L331		Y196	S128	THR
	I398	Q332	R264	T197	LEU	GLN
	D399		R266	E198	SER	SER
	F400	V335	R267	Q199	SER	VAL
	S401	S336	L267	A200	VAL	
	A402	S337	L268	L202		
	Y403		V269	L270	I138	D69
	Y404	S340	L270		T139	M70
G405	S341		V209	E140		
S406		S271		I141	S71	
E407	Q344	E273	T212	R142	P74	
A408	K345	I274	K213	E143	R75	
A409	A346	Y275	I214	A144	V76	
G410	G347	E276	S215	R145	Q77	
F411	V348	H277	N216	G146	GLY	
G412	A349	I278	M217	R147	S78	
L413	K350	I279	F218	K148	L79	
L414	L351	Y280	L219	L149	LHS	
N415	K352	A281	L220	K150	PRO	
D416	L353	P282	D221	E151	ASP	
S417	G354	A283	P222	E152	LVS	
	K355		K223	M153	T84	
Y423	A356	S287	D224	G154	M85	
F424	G357	F288	L225	L155	V86	
L425	G358	A289	E226	S156	I87	
	E359	S290	S227	Y157	T88	
F428	T360	L291	K228	A158	D89	
Q429	V361		L229	P159	L90	
V430	A362	M294	E231	D160	A91	
A431	K363	Y295	K232	I162	A92	
M432	V364	E296	K233	L163	T93	
V433	V365	R297	S233		O94	
P434	K366	T298	R234	V164		
	A367	L299	L235	S165	V99	
F438	V368	T300	L236	M166	P100	
Q439	R369	V301	L237	G167	V101	
D440	E370	N302	L238	A168	I102	
D441	R371	G303	C239	K169	R103	
S442	R372	F304	S240	Q170	PHE	
C443	D373	S305	P241	S171	A105	
L444	F374	K306	S242	G107	A106	
R445	L375		N243	E108	CYS	
L446	V376	M310	P244	L173	GLY	
S447	K377	T311	T245	L177	ASN	
Y448	S378		G246	A178	MET	
A449	L379	R314	S247		SER	
T450	G380	L315	V248	S181	SER	
S451	D381	G316	Y249		ARG	
L452	T382	Y317	P250	D184	K115	
D453	K383	L318	K251	E185	V116	
V454	G384	A319	S252	V186	CYS	
L455	V385	G320	L253	I187	V117	
Q456	K386		L254	L188	ALA	
A457		I324	E255	P189	MET	
A458		V325	E256	A190	LYS	
V459	G392	A326	T257	P191	LYS	
E460	A393	A327	A258	Y192	ASN	
F461	F204	P268	P259	H102	ASN	

L462	
A465	
L466	
E467	
P468	
L469	
ARG	
ALA	
THR	
VAL	
SER	
VAL	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 99.6 (33.27-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.14 (at 3.00Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.210 , 0.270 0.211 , 0.269	Depositor DCC
R_{free} test set	4326 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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%)	0.92	6/4203 (0.1%)
1	B	0.67	0/3085	1.13	12/4187 (0.3%)
1	C	0.65	0/3096	0.95	7/4201 (0.2%)
1	D	0.69	1/3093 (0.0%)	0.96	8/4197 (0.2%)
1	E	0.61	0/3085	0.95	7/4187 (0.2%)
1	F	0.89	12/3063 (0.4%)	1.63	69/4155 (1.7%)
All	All	0.70	14/18518 (0.1%)	1.12	109/25130 (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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	372	ARG	NE-CZ	11.30	1.45	1.33
1	F	369	ARG	CA-C	10.58	1.67	1.52
1	F	369	ARG	C-N	10.33	1.46	1.33
1	F	372	ARG	CD-NE	9.01	1.58	1.46
1	F	370	GLU	N-CA	8.80	1.56	1.46
1	F	372	ARG	CZ-NH2	-7.28	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	369	ARG	N-CA	7.28	1.55	1.46
1	F	370	GLU	CA-C	6.58	1.61	1.52
1	D	466	LEU	CG-CD1	-6.46	1.31	1.52
1	F	366	LYS	CB-CG	6.31	1.71	1.52
1	A	415	ASN	CA-C	-6.28	1.44	1.52
1	F	90	LEU	CG-CD2	-6.09	1.32	1.52
1	F	369	ARG	CD-NE	-5.33	1.38	1.46
1	F	369	ARG	CB-CG	-5.17	1.36	1.52

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	ASN	CB-CG-ND2	-26.92	76.02	116.40
1	B	166	ASN	CB-CG-OD1	25.86	172.53	120.80
1	B	166	ASN	OD1-CG-ND2	-20.64	101.96	122.60
1	F	372	ARG	NE-CZ-NH1	16.88	138.38	121.50
1	F	369	ARG	CA-C-N	16.00	141.77	120.65
1	F	369	ARG	C-N-CA	16.00	141.77	120.65
1	F	264	HIS	CB-CA-C	-15.86	86.63	108.68
1	F	372	ARG	CD-NE-CZ	15.26	145.77	124.40
1	F	217	ASN	CB-CG-ND2	-14.63	94.46	116.40
1	F	372	ARG	NH1-CZ-NH2	-14.42	100.56	119.30
1	F	264	HIS	N-CA-CB	14.40	133.87	110.11
1	F	366	LYS	CA-CB-CG	13.99	142.09	114.10
1	F	366	LYS	CB-CG-CD	12.88	140.92	111.30
1	F	368	TYR	CA-C-N	12.21	141.43	120.68
1	F	368	TYR	C-N-CA	12.21	141.43	120.68
1	C	96	GLN	OE1-CD-NE2	-12.18	110.42	122.60
1	F	122	ILE	CA-C-N	-11.74	101.00	121.66
1	F	122	ILE	C-N-CA	-11.74	101.00	121.66
1	F	372	ARG	CG-CD-NE	11.54	137.40	112.00
1	F	147	ARG	CG-CD-NE	11.45	137.19	112.00
1	F	217	ASN	OD1-CG-ND2	-10.97	111.63	122.60
1	C	96	GLN	CG-CD-NE2	-10.70	100.35	116.40
1	F	369	ARG	N-CA-C	10.48	125.44	112.23
1	F	123	ASN	N-CA-CB	10.35	126.59	110.44
1	F	264	HIS	CB-CG-CD2	-10.07	118.11	131.20
1	F	370	GLU	N-CA-C	9.57	121.40	110.97
1	F	147	ARG	CD-NE-CZ	9.41	137.58	124.40
1	A	410	GLY	CA-C-N	9.38	138.59	121.70
1	A	410	GLY	C-N-CA	9.38	138.59	121.70
1	F	369	ARG	CG-CD-NE	-8.63	93.02	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	370	GLU	CA-C-N	8.26	131.69	120.54
1	F	370	GLU	C-N-CA	8.26	131.69	120.54
1	F	146	CYS	CA-CB-SG	8.24	133.35	114.40
1	C	96	GLN	CB-CG-CD	-7.92	99.14	112.60
1	C	96	GLN	CA-CB-CG	7.86	129.82	114.10
1	C	71	SER	CA-C-N	7.83	136.49	121.54
1	C	71	SER	C-N-CA	7.83	136.49	121.54
1	F	123	ASN	N-CA-C	-7.61	103.80	113.23
1	F	123	ASN	OD1-CG-ND2	-7.34	115.26	122.60
1	A	415	ASN	CB-CA-C	-7.33	97.29	110.70
1	F	144	ALA	CA-C-N	7.31	135.13	121.97
1	F	144	ALA	C-N-CA	7.31	135.13	121.97
1	F	369	ARG	CB-CG-CD	-7.31	94.49	111.30
1	F	217	ASN	N-CA-CB	7.31	122.84	110.49
1	F	217	ASN	CA-CB-CG	7.08	119.68	112.60
1	F	369	ARG	NE-CZ-NH2	-7.08	112.83	119.20
1	E	253	LEU	CA-CB-CG	7.04	140.96	116.30
1	F	228	LYS	N-CA-C	-7.03	95.82	110.80
1	F	146	CYS	CB-CA-C	-6.94	99.21	110.74
1	A	415	ASN	N-CA-CB	-6.92	99.88	110.20
1	F	314	ARG	NE-CZ-NH1	-6.83	114.67	121.50
1	F	145	ILE	N-CA-C	6.64	123.16	109.34
1	F	123	ASN	CB-CG-ND2	-6.63	106.45	116.40
1	F	223	LYS	CB-CG-CD	6.59	126.47	111.30
1	F	264	HIS	ND1-CG-CD2	-6.54	99.56	106.10
1	F	226	GLU	CA-C-N	6.45	133.30	121.70
1	F	226	GLU	C-N-CA	6.45	133.30	121.70
1	F	223	LYS	CA-C-N	6.33	133.10	121.70
1	F	223	LYS	C-N-CA	6.33	133.10	121.70
1	F	142	ARG	CB-CG-CD	-6.13	97.20	111.30
1	F	318	LEU	CA-CB-CG	-5.99	95.33	116.30
1	F	363	GLU	CB-CG-CD	5.99	122.77	112.60
1	E	466	LEU	CB-CG-CD2	-5.98	92.77	110.70
1	E	266	ARG	CA-CB-CG	5.97	126.04	114.10
1	F	330	LYS	N-CA-CB	5.90	120.71	110.39
1	B	79	LEU	CA-C-N	5.75	132.05	121.70
1	B	79	LEU	C-N-CA	5.75	132.05	121.70
1	B	165	SER	CA-C-N	-5.74	114.32	122.41
1	B	165	SER	C-N-CA	-5.74	114.32	122.41
1	F	217	ASN	CB-CA-C	-5.72	99.04	110.42
1	B	166	ASN	CB-CA-C	-5.68	103.42	112.05
1	F	90	LEU	CB-CG-CD2	-5.67	93.68	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	266	ARG	CG-CD-NE	5.62	124.35	112.00
1	F	369	ARG	N-CA-CB	-5.59	101.69	110.30
1	F	393	ALA	CA-C-N	-5.50	112.56	122.46
1	F	393	ALA	C-N-CA	-5.50	112.56	122.46
1	E	256	GLU	CB-CG-CD	-5.48	103.29	112.60
1	F	249	TYR	CA-CB-CG	5.36	123.55	113.90
1	F	234	ARG	N-CA-C	5.34	122.17	110.80
1	B	80	LYS	N-CA-C	-5.31	96.14	111.00
1	C	72	LEU	N-CA-C	5.31	122.10	110.80
1	D	89	ASP	CA-C-N	-5.23	112.36	120.31
1	D	89	ASP	C-N-CA	-5.23	112.36	120.31
1	F	391	GLN	CA-CB-CG	5.21	124.53	114.10
1	F	147	ARG	CB-CG-CD	-5.19	99.36	111.30
1	A	411	PHE	CA-C-N	5.17	131.01	121.70
1	A	411	PHE	C-N-CA	5.17	131.01	121.70
1	F	361	VAL	CB-CA-C	-5.16	105.17	112.14
1	D	466	LEU	CB-CG-CD2	5.16	126.18	110.70
1	F	246	GLY	N-CA-C	-5.15	98.36	113.30
1	D	416	ASP	N-CA-C	-5.14	101.90	110.17
1	F	361	VAL	N-CA-CB	5.13	117.52	110.54
1	F	146	CYS	CA-C-N	5.12	127.14	120.28
1	F	146	CYS	C-N-CA	5.12	127.14	120.28
1	F	448	TYR	N-CA-CB	-5.12	102.78	111.17
1	E	81	PRO	CA-N-CD	-5.10	104.86	112.00
1	B	71	SER	CA-C-N	5.09	131.26	121.54
1	B	71	SER	C-N-CA	5.09	131.26	121.54
1	E	256	GLU	CA-CB-CG	5.09	124.28	114.10
1	F	147	ARG	NH1-CZ-NH2	-5.09	112.68	119.30
1	F	448	TYR	CB-CA-C	5.09	119.32	111.13
1	B	72	LEU	N-CA-C	5.09	121.64	110.80
1	F	330	LYS	CG-CD-CE	-5.08	99.62	111.30
1	F	314	ARG	CA-C-N	-5.07	114.93	122.74
1	F	314	ARG	C-N-CA	-5.07	114.93	122.74
1	D	466	LEU	CB-CG-CD1	-5.03	95.62	110.70
1	D	81	PRO	CA-C-N	-5.01	114.12	122.64
1	D	81	PRO	C-N-CA	-5.01	114.12	122.64
1	D	85	MET	CB-CG-SD	-5.01	97.66	112.70

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
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	Peptide,Mainchain
1	F	246	GLY	Peptide
1	F	264	HIS	Mainchain,Sidechain
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	135	0
1	C	3038	0	3087	132	0
1	D	3035	0	3099	168	1
1	E	3027	0	3090	306	0
1	F	3007	0	3048	553	0
2	A	15	0	7	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	F	3	0	0	1	0
All	All	18299	0	18553	1365	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 37.

All (1365) 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:HE21	1:C:96:GLN:CA	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	1.27
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:142:ARG:C	1:F:147:ARG:HH12	1.49	1.18
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:F:143:GLU:C	1:F:147:ARG:NH1	2.05	1.15
1:E:196:TYR:OH	1:E:239:CYS:SG	2.05	1.14
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:A:111:PHE:CD2	1:A:364:MET:HE2	1.83	1.12
1:F:144:ALA:N	1:F:147:ARG:HH11	1.45	1.11
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:223:LYS:HE3	1:F:226:GLU:C	1.78	1.09
1:F:143:GLU:C	1:F:147:ARG:CZ	2.25	1.08
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:249:TYR:O	1:E:253:LEU:HD23	1.58	1.03
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:F:460:GLU:H	1:F:460:GLU:CD	1.65	0.99
1:F:251:LYS:O	1:F:255:GLU:N	1.96	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: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:144:ALA:C	1:F:147:ARG:HD3	1.92	0.93
1:F:370:GLU:C	1:F:372:ARG:HE	1.73	0.92
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:82:SER:HB2	1:D:85:MET:HE3	1.53	0.90
1:F:458:ALA:N	1:F:460:GLU:OE1	2.05	0.90
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:E:76:VAL:HG21	1:F:178:ALA:HA	1.55	0.88
1:F:166:ASN:ND2	1:F:336:SER:OG	2.06	0.88
1:F:371:ARG:N	1:F:372:ARG:HH21	1.71	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:A:111:PHE:CG	1:A:364:MET:HE3	2.09	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:A:111:PHE:HD2	1:A:364:MET:HE2	1.38	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:F:460:GLU:CD	1:F:460:GLU:N	2.33	0.85
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:F:300:THR:C	1:F:318:LEU:HD12	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:A:452:LEU:H	1.42	0.83
1:F:223:LYS:HE2	1:F:225:LEU:O	1.78	0.83
1:F:142:ARG:C	1:F:147:ARG:NH1	2.18	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:F:301:VAL:C	1:F:302:ASN:HD22	1.87	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
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:A:111:PHE:CB	1:A:364:MET:HE3	2.09	0.81
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:184:ASP:OD1	1:F:266:ARG:NH2	2.15	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:E:368:TYR:HB3	1:E:448:TYR:HE1	1.46	0.80
1:F:223:LYS:HG2	1:F:224:ASP:C	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:420:LEU:HD22	1:C:424:PHE:HE1	1.49	0.78
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:353:LEU:HB3	1:F:357:GLY:C	2.09	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:D:423:TYR:HA	1:D:427:LYS:HZ1	1.50	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:HE21	1:C:96:GLN:HA	0.60	0.75
1:F:280:TYR:OH	1:F:372:ARG:HG3	1.87	0.75
1:F:370:GLU:CB	1:F:372:ARG:NH2	2.42	0.75
1:E:85:MET:O	1:E:89:ASP:N	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:ARG:H	1:F:147:ARG:CD	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
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:370:GLU:C	1:F:372:ARG:NE	2.43	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:D:306:LYS:HZ1	2:D:701:PLP:C4A	2.01	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:A:111:PHE:CG	1:A:364:MET:CE	2.70	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: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:397:PHE:CD1	1:F:443:CYS:HB2	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB3	1:F:357:GLY:C	2.15	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:E:158:ALA:H	1:E:161:GLN:CD	1.97	0.71
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
1:A:111:PHE:CB	1:A:364:MET:CE	2.67	0.71
1:F:198:GLU:OE2	1:F:198:GLU:N	2.22	0.71
1:F:382:ILE:CD1	1:F:385:VAL:HG13	2.19	0.71
1:F:222:PRO:HA	1:F:223:LYS:C	2.14	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:E:356:ALA:C	1:E:361:VAL:HG11	2.15	0.71
1:C:373:ASP:O	1:C:377:LYS:HG2	1.90	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:E:338:GLY:C	1:F:314:ARG:HH12	1.99	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:E:181:SER:HB3	1:F:74:PRO:HD2	1.74	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:F:317:TYR:C	1:F:318:LEU:CD2	2.51	0.70
1:A:74:PRO:O	1:A:75:ARG:HB3	1.92	0.70
1:E:73:SER:OG	1:F:178:ALA:O	2.07	0.69
1:F:144:ALA:H	1:F:147:ARG:HH11	1.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:84:THR:HB	1:F:88:THR:CG2	2.22	0.69
1:F:165:SER:OG	1:F:332:GLN:OE1	2.08	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
1:B:80:LYS:HG3	1:B:81:PRO:HD2	1.74	0.69
1:B:230:THR:HG22	1:B:232:LYS:H	1.57	0.69
1:B:413:LEU:H	1:B:413:LEU:HD23	1.56	0.69
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:371:ARG:HG3	1:F:374:PHE:CZ	2.30	0.67
1:F:374:PHE:CD1	1:F:452:LEU:HD12	2.28	0.67
1:F:455:LEU:O	1:F:459:VAL:HG12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:GLY:C	1:C:334:GLN:HE21	2.02	0.67
1:F:301:VAL:HA	1:F:318:LEU:HG	1.76	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: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: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:362:ALA:HA	1:E:365:VAL:HB	1.76	0.66
1:C:131:ARG:HG3	1:C:131:ARG:HH11	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:294:MET:HE3	1:F:294:MET:HA	1.78	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:95:VAL:O	1:A:97:SER:N	2.27	0.66
1:A:356:ALA:N	1:A:357:GLY:HA2	2.10	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:223:LYS:CD	1:F:224:ASP:C	2.68	0.65
1:F:301:VAL:HA	1:F:318:LEU:CG	2.26	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: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:456:GLN:C	1:F:460:GLU:OE1	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ILE:HD11	1:A:294:MET:SD	2.37	0.65
1:D:423:TYR:HA	1:D:427:LYS:NZ	2.12	0.65
1:E:269:VAL:HG21	1:E:288:PHE:CE2	2.32	0.65
1:B:403:TYR:O	1:B:406:SER:OG	2.14	0.65
1:E:90:LEU:HA	1:E:94:LEU:HD12	1.78	0.65
1:E:265:PRO:O	1:F:69:ASP:N	2.30	0.65
1:C:371:ARG:HG2	1:C:455:LEU:CD1	2.27	0.64
1:F:86:VAL:O	1:F:90:LEU:HD23	1.95	0.64
1:F:370:GLU:HG2	1:F:372:ARG:HH21	1.60	0.64
1:F:188:ILE:HD11	1:F:209:VAL:HG22	1.78	0.64
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: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:84:THR:HB	1:F:88:THR:HG23	1.78	0.64
1:F:233:SER:O	1:F:235:LEU:N	2.29	0.64
1:F:278:ILE:HG23	1:F:368:TYR:HD2	1.62	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:432:MET:HE2	1:E:446:ILE:HG12	1.80	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:153:ASN:ND2	1:F:287:SER:HB3	2.11	0.63
1:F:189:PRO:HD2	1:F:237:ILE:O	1.99	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:C:70:MET:HE3	1:C:71:SER:O	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:F:300:THR:C	1:F:318:LEU:CD1	2.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:ILE:HG23	1:F:275:TYR:CD1	2.32	0.62
1:F:374:PHE:CG	1:F:452:LEU:HD12	2.33	0.62
1:F:398:ILE:O	1:F:443:CYS:HB3	1.99	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
1:E:161:GLN:CD	1:E:322:LYS:HZ1	2.07	0.62
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:B:102:ILE:HD12	1:B:102:ILE:C	2.18	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:299:LEU:HD21	1:E:324:ILE:HG21	1.80	0.62
1:E:304:PHE:HB3	1:E:308:PHE:CD1	2.35	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:F:223:LYS:HD3	1:F:224:ASP:C	2.24	0.62
1:F:223:LYS:HE2	1:F:225:LEU:C	2.23	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:D:432:MET:HE2	1:D:446:ILE:HG12	1.80	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:153:ASN:ND2	1:E:276:GLU:OE2	2.19	0.61
1:E:220:LEU:H	1:E:249:TYR:HE1	1.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:340:SER:HA	1:F:314:ARG:CZ	2.30	0.61
1:F:223:LYS:HE3	1:F:226:GLU:O	2.01	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:E:79:LEU:C	1:E:80:LYS:HG2	2.24	0.61
1:A:102:ILE:HD11	1:A:430:VAL:HA	1.83	0.61
1:B:386:LYS:NZ	1:B:387:ILE:O	2.29	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:D:307:ALA:O	1:D:364:MET:HE1	1.99	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: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:135:ASN:HD22	1:E:135:ASN:C	2.08	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:F:384:GLY:HA3	1:F:403:TYR:CE1	2.36	0.60
1:A:411:PHE:HE2	1:A:423:TYR:HA	1.66	0.60
1:D:427:LYS:HD3	1:D:427:LYS:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:119:GLU:CD	1:F:123:ASN:ND2	2.60	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
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:74:PRO:O	1:F:76:VAL:N	2.32	0.59
1:F:356:ALA:H	1:F:357:GLY:CA	2.15	0.59
1:F:356:ALA:HA	1:F:361:VAL:CG1	2.33	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:283:ALA:HB2	1:F:391:GLN:HB3	1.85	0.59
1:F:370:GLU:CG	1:F:372:ARG:HH21	2.16	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:75:ARG:NH2	1:E:204:ASP:H	2.01	0.59
1:E:150:LYS:HG2	1:E:155:LEU:O	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:84:THR:C	1:D:88:THR:HG23	2.28	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:409:GLU:C	1:F:414:ILE:HG21	2.27	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
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:A:111:PHE:HB2	1:A:364:MET:HE1	1.86	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:369:ARG:O	1:F:372:ARG:HD3	2.03	0.57
1:F:371:ARG:N	1:F:372:ARG:NH2	2.48	0.57
1:B:450:THR:OG1	1:B:454:VAL:HG21	2.04	0.57
1:F:273:GLU:C	1:F:302:ASN:HD21	2.12	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: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: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:222:PRO:HD3	1:E:256:GLU:CD	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:148:LYS:NZ	1:E:276:GLU:OE1	2.31	0.57
1:F:372:ARG:CG	1:F:373:ASP:N	2.68	0.57
1:B:91:ALA:HA	1:B:95:VAL:HG21	1.87	0.57
1:F:143:GLU:C	1:F:147:ARG:NE	2.61	0.57
1:D:432:MET:HE1	1:D:462:ILE:HD11	1.86	0.57
1:E:125:ILE:HD13	1:F:122:ILE:HD11	1.86	0.57
1:F:119:GLU:CD	1:F:123:ASN:HD21	2.13	0.57
1:A:356:ALA:C	1:A:361:VAL:HG11	2.29	0.56
1:B:399:ASP:OD1	1:B:401:SER:OG	2.17	0.56
1:F:223:LYS:O	1:F:225:LEU:HD23	2.04	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:C:337:SER:HB2	1:D:169:LYS:HE3	1.85	0.56
1:E:230:THR:HG22	1:E:232:LYS:H	1.70	0.56
1:E:361:VAL:HA	1:E:364:MET:HE2	1.87	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: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
1:C:131:ARG:HB3	1:D:108:GLU:OE1	2.05	0.56
1:E:467:GLU:C	1:E:469:LEU:H	2.14	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: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:219:LEU:HG	1:F:249:TYR:HD2	1.71	0.56
1:F:243:ASN:OD1	1:F:244:PRO:HA	2.06	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:223:LYS:CG	1:F:224:ASP:C	2.77	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:93:THR:HA	1:D:96:GLN:CB	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:ASP:OD2	1:D:322:LYS:HE3	2.05	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:F:353:LEU:HB3	1:F:357:GLY:O	2.05	0.55
1:F:467:GLU:C	1:F:469:LEU:H	2.14	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:O	1:F:448:TYR:CD1	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: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:HD12	1:F:396:LEU:O	2.06	0.55
1:B:81:PRO:O	1:B:82:SER:HB3	2.07	0.54
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:83:LYS:HD2	1:D:436:ASP:CG	2.32	0.54
1:F:381:ASP:CG	1:F:382:ILE:N	2.64	0.54
1:F:430:VAL:HG12	1:F:432:MET:HE2	1.89	0.54
1:E:249:TYR:C	1:E:253:LEU:HB3	2.33	0.54
1:D:75:ARG:HA	1:D:78:SER:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:PRO:O	1:E:76:VAL:N	2.36	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:78:SER:C	1:F:79:LEU:HD23	2.33	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: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:B:91:ALA:C	1:B:93:THR:H	2.17	0.53
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:229:LEU:HD21	1:F:267:LEU:CD2	2.38	0.53
1:B:90:LEU:O	1:B:95:VAL:HG21	2.08	0.53
1:B:463:ARG:HH11	1:B:464:LYS:HD2	1.73	0.53
1:C:306:LYS:HZ2	2:C:701:PLP:C4A	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:PRO:HG2	1:C:324:ILE:HD12	1.90	0.53
1:F:84:THR:HB	1:F:88:THR:HG21	1.91	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: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:111:PHE:HB2	1:C:364:MET:HE2	1.91	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: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:75:ARG:NH2	1:E:202:LEU:C	2.67	0.53
1:E:440:ASP:OD1	1:E:442:SER:OG	2.25	0.53
1:F:223:LYS:HE3	1:F:227:SER:N	2.21	0.53
1:D:82:SER:CB	1:D:85:MET:HE3	2.33	0.53
1:F:273:GLU:CA	1:F:302:ASN:HD21	2.21	0.53
1:B:102:ILE:CD1	1:B:102:ILE:C	2.79	0.52
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HG12	1:F:385:VAL:CG1	2.39	0.52
1:F:382:ILE:O	1:F:385:VAL:HG22	2.09	0.52
1:A:411:PHE:CD2	1:A:423:TYR:HD1	2.28	0.52
1:B:436:ASP:HA	1:F:413:LEU:HD21	1.92	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:F:417:SER:C	1:F:434:PRO:HB3	2.35	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:HD12	1:F:455:LEU:H	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:C	1:E:254:LEU:N	2.67	0.51
1:E:252:SER:HA	1:E:255:GLU:HB2	1.92	0.51
1:F:353:LEU:HB3	1:F:357:GLY:CA	2.39	0.51
1:A:337:SER:OG	1:A:338:GLY:N	2.41	0.51
1:C:404:TYR:CE1	1:C:420:LEU:HD12	2.44	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:F:370:GLU:C	1:F:372:ARG:HH21	2.04	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:91:ALA:O	1:F:103:ARG:NH2	2.44	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:B:413:LEU:C	1:B:414:ILE:HD12	2.36	0.51
1:D:401:SER:C	1:D:403:TYR:N	2.69	0.51
1:E:87:ILE:HG13	1:E:425:LEU:HD22	1.93	0.51
1:F:101:VAL:HG23	1:F:429:GLN:C	2.36	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: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:247:SER:OG	1:F:391:GLN:CD	2.54	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:223:LYS:C	1:F:225:LEU:HD23	2.36	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:OE2	1:E:255:GLU:HA	2.11	0.50
1:F:353:LEU:HB3	1:F:357:GLY:HA3	1.93	0.50
1:B:80:LYS:HD2	1:F:411:PHE:HD2	1.77	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: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: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:F:225:LEU:O	1:F:227:SER:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:131:ARG:O	1:E:341:SER:OG	2.29	0.50
1:F:187:ILE:HD11	1:F:229:LEU:HA	1.93	0.50
1:F:194:VAL:O	1:F:198:GLU:OE2	2.29	0.50
1:A:81:PRO:O	1:A:82:SER:HB3	2.12	0.50
1:B:409:GLU:CD	1:B:410:GLY:H	2.19	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:223:LYS:HE2	1:F:224:ASP:C	2.37	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:E:409:GLU:C	1:E:411:PHE:H	2.19	0.50
1:A:234:ARG:HH22	1:B:71:SER:HA	1.76	0.49
1:E:75:ARG:HH21	1:E:204:ASP:N	2.06	0.49
1:E:222:PRO:HG2	1:E:223:LYS:HD3	1.93	0.49
1:F:413:LEU:C	1:F:414:ILE:HG22	2.37	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:110:ASP:CG	1:F:371:ARG:HH22	2.20	0.49
1:F:457:ALA:N	1:F:460:GLU:OE1	2.45	0.49
1:A:432:MET:HE1	1:A:462:ILE:HD11	1.94	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: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
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:264:HIS:C	1:F:297:ARG:HH22	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:401:SER:C	1:F:403:TYR:N	2.70	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:90:LEU:O	1:F:94:LEU:HD23	2.12	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:D:401:SER:C	1:D:403:TYR:H	2.20	0.48
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:E:307:ALA:O	1:E:364:MET:HE1	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:93:THR:HG23	1:C:94:LEU:H	1.78	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:D:90:LEU:O	1:D:94:LEU:C	2.56	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:E:252:SER:C	1:E:254:LEU:H	2.20	0.48
1:F:188:ILE:HD12	1:F:188:ILE:O	2.14	0.48
1:F:280:TYR:CD1	1:F:369:ARG:HD3	2.48	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:254:LEU:CA	1:E:291:LEU:HD11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:401:SER:C	1:F:403:TYR:H	2.19	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:E:339:ALA:C	1:F:314:ARG:NH1	2.71	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:129:PHE:CE2	1:E:345:LYS:HE2	2.49	0.48
1:E:291:LEU:CD2	1:E:292:PRO:HD2	2.44	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:C:404:TYR:C	1:C:406:SER:H	2.17	0.47
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:F:223:LYS:CG	1:F:225:LEU:C	2.86	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:D:80:LYS:NZ	1:D:83:LYS:HZ1	2.11	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:F:457:ALA:C	1:F:460:GLU:OE1	2.56	0.47
1:C:299:LEU:HD21	1:C:324:ILE:HG21	1.97	0.47
1:D:102:ILE:CG1	1:D:430:VAL:HA	2.35	0.47
1:D:412:GLY:O	1:D:414:ILE:N	2.31	0.47
1:F:305:SER:HB3	1:F:311:THR:HA	1.95	0.47
1:F:315:LEU:HD12	1:F:315:LEU:HA	1.50	0.47
1:F:404:TYR:OH	1:F:417:SER:N	2.47	0.47
1:B:92:ALA:HA	1:B:103:ARG:NH2	2.29	0.47
1:B:434:PRO:HB2	1:B:436:ASP:HB3	1.96	0.47
1:F:164:VAL:HG23	1:F:317:TYR:CB	2.34	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:96:GLN:NE2	1:D:97:SER:OG	2.48	0.47
1:D:102:ILE:HG23	1:D:429:GLN:O	2.15	0.47
1:E:80:LYS:HE2	1:E:80:LYS:HB3	1.49	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:459:VAL:O	1:E:463:ARG:HG3	2.15	0.47
1:F:145:ILE:HD13	1:F:317:TYR:CD2	2.49	0.47
1:F:150:LYS:HA	1:F:155:LEU:N	2.29	0.47
1:F:158:ALA:HB3	1:F:160:ASP:OD1	2.14	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: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:86:VAL:HA	1:E:89:ASP:HB2	1.96	0.47
1:E:195:SER:HA	1:E:198:GLU:OE1	2.15	0.47
1:F:228:LYS:C	1:F:229:LEU:O	2.56	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:E:417:SER:HG	1:E:436:ASP:HB2	1.80	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:C:265:PRO:O	1:D:70:MET:HE3	2.15	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:C:416:ASP:HB2	1:C:419:SER:HG	1.79	0.46
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:95:VAL:O	1:D:99:VAL:O	2.33	0.46
1:D:281:ALA:HB1	1:D:282:PRO:HD3	1.96	0.46
1:E:194:VAL:HG22	1:E:198:GLU:CD	2.40	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:87:ILE:HG13	1:B:425:LEU:CD2	2.42	0.46
1:B:91:ALA:C	1:B:93:THR:N	2.74	0.46
1:B:240:SER:HB2	1:B:249:TYR:HD2	1.81	0.46
1:B:355:LYS:C	1:B:357:GLY:HA2	2.41	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:161:GLN:CD	1:E:322:LYS:NZ	2.74	0.46
1:E:365:VAL:O	1:E:365:VAL:HG12	2.16	0.46
1:F:106:ALA:O	1:F:447:SER:OG	2.17	0.46
1:A:165:SER:OG	1:A:332:GLN:OE1	2.32	0.46
1:A:383:LYS:HD2	1:A:383:LYS:N	2.31	0.46
1:B:411:PHE:O	1:B:414:ILE:HG13	2.15	0.46
1:E:132:TYR:OH	2:F:701:PLP:O1P	2.27	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:A:102:ILE:HG12	1:A:430:VAL:HG22	1.97	0.46
1:E:131:ARG:HG2	1:F:108:GLU:HG2	1.97	0.46
1:E:173:LEU:HB2	1:E:199:GLN:OE1	2.16	0.46
1:F:155:LEU:HD23	1:F:295:TYR:HD2	1.81	0.46
1:F:214:ILE:HG13	1:F:218:PHE:CZ	2.51	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: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: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:A:275:TYR:HE2	2:A:701:PLP:H2A3	1.81	0.45
1:D:107:GLY:O	1:D:306:LYS:HE3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:TYR:O	1:F:317:TYR:CD2	2.69	0.45
1:F:361:VAL:O	1:F:362:ALA:C	2.59	0.45
1:C:273:GLU:OE1	1:C:285:HIS:NE2	2.33	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: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: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:HD23	1:B:94:LEU:H	1.81	0.45
1:C:327:ALA:HB1	1:D:76:VAL:HG21	1.98	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:E:234:ARG:HD3	1:E:266:ARG:HB3	1.98	0.45
1:E:236:LEU:HD21	1:E:238:LEU:HG	1.99	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:356:ALA:HB3	1:F:358:GLY:C	2.42	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:F:239:CYS:HA	1:F:272:ASP:CB	2.46	0.45
1:D:417:SER:HB3	1:D:441:ASP:O	2.17	0.45
1:F:259:ARG:H	1:F:259:ARG:HG3	1.44	0.45
1:F:330:LYS:HB3	1:F:330:LYS:HE3	1.48	0.45
1:F:383:LYS:H	1:F:383:LYS:HG3	1.48	0.45
1:B:80:LYS:HG3	1:B:81:PRO:CD	2.43	0.45
1:C:404:TYR:C	1:C:406:SER:N	2.75	0.45
1:D:432:MET:CE	1:D:462:ILE:HD11	2.46	0.45
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:92:ALA:O	1:F:93:THR:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:273:GLU:C	1:F:302:ASN:ND2	2.75	0.45
1:A:79:LEU:O	1:A:80:LYS:HD2	2.17	0.44
1:A:102:ILE:H	1:A:102:ILE:HG13	1.51	0.44
1:B:403:TYR:OH	1:B:466:LEU:HD21	2.17	0.44
1:C:184:ASP:CG	1:C:266:ARG:HH22	2.25	0.44
1:D:428:PHE:O	1:D:430:VAL:HG23	2.17	0.44
1:E:291:LEU:HD23	1:E:291:LEU:HA	1.64	0.44
1:A:83:LYS:HZ1	1:A:418:SER:HA	1.82	0.44
1:D:85:MET:HE2	1:D:85:MET:HB3	1.66	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:356:ALA:CB	1:F:361:VAL:HG22	2.47	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:335:VAL:O	1:F:169:LYS:HB3	2.17	0.44
1:E:361:VAL:HA	1:E:364:MET:HB2	1.99	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:F:398:ILE:C	1:F:443:CYS:HB3	2.42	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:ASN:OD1	1:E:415:ASN:N	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:306:LYS:NZ	2:F:701:PLP:C4	2.79	0.44
1:F:450:THR:OG1	1:F:455:LEU:HD11	2.18	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:90:LEU:HD12	1:C:90:LEU:HA	1.83	0.44
1:C:102:ILE:HD11	1:C:431:ALA:H	1.83	0.44
1:C:411:PHE:CE2	1:C:427:LYS:NZ	2.86	0.44
1:D:94:LEU:HA	1:D:95:VAL:HA	1.84	0.44
1:D:404:TYR:OH	1:D:417:SER:HA	2.17	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:C:293:ASP:C	1:C:294:MET:HE2	2.43	0.43
1:E:95:VAL:HG13	1:E:99:VAL:HB	2.00	0.43
1:E:234:ARG:CD	1:E:266:ARG:HB3	2.48	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: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:90:LEU:HD23	1:F:90:LEU:N	2.33	0.43
1:F:110:ASP:N	1:F:449:ALA:HB1	2.34	0.43
1:F:408:ALA:N	1:F:409:GLU:HG2	2.33	0.43
1:A:150:LYS:NZ	1:A:156:SER:OG	2.50	0.43
1:C:79:LEU:HD23	1:C:79:LEU:HA	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: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
1:F:223:LYS:CG	1:F:226:GLU:H	2.23	0.43
1:F:225:LEU:HD23	1:F:225:LEU:H	1.83	0.43
1:F:278:ILE:CG2	1:F:368:TYR:HD2	2.30	0.43
1:F:303:GLY:HA2	1:F:317:TYR:CE1	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:75:ARG:CZ	1:E:202:LEU:C	2.91	0.43
1:E:251:LYS:HD3	1:E:252:SER:N	2.33	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:F:424:PHE:CD2	1:F:432:MET:HE1	2.53	0.43
1:A:80:LYS:N	1:A:81:PRO:CD	2.79	0.43
1:A:233:SER:HB3	1:A:267:LEU:HD13	2.00	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:D:411:PHE:O	1:D:412:GLY:C	2.62	0.43
1:E:234:ARG:CD	1:E:266:ARG:HE	2.32	0.43
1:E:254:LEU:HD13	1:E:291:LEU:CG	2.47	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:F:223:LYS:CE	1:F:224:ASP:C	2.92	0.43
1:E:225:LEU:O	1:E:229:LEU:HG	2.18	0.43
1:F:191:PRO:CB	1:F:244:PRO:HG2	2.44	0.43
1:F:235:LEU:HD23	1:F:236:LEU:N	2.33	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:E:79:LEU:HD21	1:E:198:GLU:HG2	2.01	0.43
1:F:243:ASN:CG	1:F:445:ARG:HH12	2.27	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:F:430:VAL:CG1	1:F:432:MET:HE2	2.49	0.43
1:A:90:LEU:HD13	1:A:90:LEU:HA	1.88	0.42
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:E:75:ARG:NE	1:E:201:ARG:O	2.52	0.42
1:E:135:ASN:HD21	1:E:332:GLN:HE21	1.67	0.42
1:E:252:SER:HA	1:E:255:GLU:CB	2.49	0.42
1:F:428:PHE:CG	1:F:465:ALA:HB2	2.54	0.42
1:F:452:LEU:HD23	1:F:452:LEU:C	2.44	0.42
1:A:87:ILE:HG23	1:A:88:THR:N	2.32	0.42
1:A:102:ILE:CD1	1:A:431:ALA:H	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:PHE:CE2	1:A:423:TYR:CD1	3.03	0.42
1:A:420:LEU:HA	1:A:420:LEU:HD12	1.77	0.42
1:B:441:ASP:CG	1:F:413:LEU:HD13	2.44	0.42
1:D:335:VAL:O	1:D:336:SER:OG	2.23	0.42
1:D:400:PHE:C	1:D:401:SER:O	2.62	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:333:GLY:C	1:C:334:GLN:NE2	2.75	0.42
1:C:420:LEU:O	1:C:424:PHE:CD1	2.70	0.42
1:D:396:LEU:HA	1:D:396:LEU:HD23	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:97:SER:HA	1:E:98:GLY:HA2	1.46	0.42
1:E:280:TYR:N	1:E:391:GLN:O	2.51	0.42
1:A:84:THR:O	1:A:88:THR:HG22	2.19	0.42
1:B:467:GLU:C	1:B:469:LEU:H	2.27	0.42
1:C:122:ILE:HG23	1:D:122:ILE:HD13	2.01	0.42
1:D:80:LYS:HE3	1:D:81:PRO:O	2.19	0.42
1:D:466:LEU:CD1	1:D:466:LEU:N	2.70	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:H	1:E:359:GLU:HG2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:PRO:C	1:E:76:VAL:N	2.78	0.42
1:F:102:ILE:HG21	1:F:458:ALA:HB2	2.02	0.42
1:F:143:GLU:C	1:F:147:ARG:CD	2.92	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:95:VAL:HB	1:D:99:VAL:CG1	2.49	0.42
1:D:190:ALA:HA	1:D:191:PRO:C	2.45	0.42
1:D:191:PRO:HA	1:D:438:PHE:O	2.20	0.42
1:F:301:VAL:C	1:F:302:ASN:ND2	2.68	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:83:LYS:NZ	1:F:412:GLY:HA3	2.35	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:177:LEU:HD23	1:B:203:ALA:HB2	2.02	0.42
1:E:102:ILE:HG12	1:E:430:VAL:HG22	2.02	0.42
1:E:105:ALA:HB1	1:E:433:VAL:CG2	2.50	0.42
1:E:409:GLU:C	1:E:411:PHE:N	2.78	0.42
1:E:468:PRO:C	1:E:469:LEU:HD12	2.44	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:HD12	1:F:214:ILE:N	2.33	0.41
1:F:381:ASP:OD1	1:F:382:ILE:N	2.53	0.41
1:F:414:ILE:HG13	1:F:414:ILE:O	2.20	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: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:221:ASP:CG	1:E:222:PRO:HD2	2.46	0.41
1:E:291:LEU:HD23	1:E:292:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:VAL:HG21	1:F:425:LEU:CD1	2.50	0.41
1:F:270:LEU:HD23	1:F:270:LEU:C	2.46	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: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:H	1:F:147:ARG:HE	1.68	0.41
1:F:168:ALA:C	1:F:172:LEU:HD12	2.45	0.41
1:D:453:ASP:OD1	1:D:454:VAL:HG23	2.20	0.41
1:E:250:PRO:C	1:E:252:SER:N	2.79	0.41
1:F:105:ALA:HB1	1:F:433:VAL:HG23	2.02	0.41
1:F:188:ILE:CD1	1:F:209:VAL:HA	2.49	0.41
1:F:318:LEU:HD13	1:F:318:LEU:HA	1.79	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:B:240:SER:HA	1:B:241:PRO:C	2.45	0.41
1:C:281:ALA:HB3	1:C:282:PRO:HD3	2.02	0.41
1:C:314:ARG:HH12	1:D:132:TYR:HE1	1.67	0.41
1:C:466:LEU:HA	1:C:469:LEU:HD13	2.02	0.41
1:D:421:ALA:HB3	1:D:434:PRO:HG3	2.02	0.41
1:F:317:TYR:O	1:F:317:TYR:CG	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:242:SER:C	1:F:246:GLY:HA3	2.46	0.41
1:F:244:PRO:HG3	1:F:438:PHE:CB	2.51	0.41
1:A:102:ILE:CG1	1:A:430:VAL:HA	2.51	0.41
1:A:467:GLU:HB2	1:A:468:PRO:HD3	2.02	0.41
1:D:87:ILE:O	1:D:88:THR:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:ILE:C	1:E:125:ILE:HD11	2.46	0.41
1:E:135:ASN:C	1:E:135:ASN:ND2	2.78	0.41
1:E:149:LEU:HD13	1:E:157:TYR:CD2	2.56	0.41
1:E:256:GLU:C	1:E:257:ILE:O	2.62	0.41
1:E:257:ILE:H	1:E:257:ILE:CD1	2.33	0.41
1:E:315:LEU:HA	1:E:315:LEU:HD12	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:F:310:MET:HB3	1:F:310:MET:HE2	1.73	0.41
1:A:466:LEU:HA	1:A:466:LEU:HD23	1.86	0.41
1:C:279:ILE:HD13	1:C:279:ILE:HG21	1.88	0.41
1:D:464:LYS:CA	1:D:467:GLU:HG3	2.47	0.41
1:E:240:SER:HA	1:E:241:PRO:C	2.46	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:86:VAL:O	1:F:90:LEU:CD2	2.67	0.41
1:F:90:LEU:HD11	1:F:425:LEU:HD23	2.03	0.41
1:B:102:ILE:HG13	1:B:430:VAL:HA	2.03	0.40
1:B:403:TYR:CE2	1:B:466:LEU:HG	2.56	0.40
1:D:102:ILE:HG12	1:D:429:GLN:O	2.21	0.40
1:D:240:SER:HA	1:D:241:PRO:C	2.45	0.40
1:D:463:ARG:HA	1:D:466:LEU:HD11	2.03	0.40
1:E:75:ARG:HA	1:E:78:SER:OG	2.21	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: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:190:ALA:HA	1:F:191:PRO:C	2.46	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:278:ILE:HB	1:F:393:ALA:HA	2.02	0.40
1:F:375:LEU:HD12	1:F:459:VAL:HG11	2.03	0.40
1:B:142:ARG:HH11	1:B:142:ARG:HD2	1.62	0.40
1:B:425:LEU:O	1:B:426:ASP:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:90:LEU:C	1:F:92:ALA:O	2.63	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:330:LYS:HZ2	1:F:330:LYS:HG2	1.70	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
1:F:378:SER:O	1:F:381:ASP:OD1	2.39	0.40
1:F:442:SER:OG	1:F:443:CYS:SG	2.53	0.40
1:F:445:ARG:HH11	1:F:445:ARG:HD3	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:178:ALA:HA	1:F:76:VAL:HG21	2.03	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

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%)	6	31
1	B	397/475 (84%)	374 (94%)	13 (3%)	10 (2%)	4	23
1	C	399/475 (84%)	378 (95%)	17 (4%)	4 (1%)	12	45
1	D	398/475 (84%)	371 (93%)	18 (4%)	9 (2%)	5	25
1	E	397/475 (84%)	368 (93%)	21 (5%)	8 (2%)	6	28
1	F	393/475 (83%)	353 (90%)	22 (6%)	18 (5%)	2	11
All	All	2382/2850 (84%)	2222 (93%)	104 (4%)	56 (2%)	4	24

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

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Mol	Chain	Res	Type
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
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%)	327 (100%)	0	100	100
1	B	326/390 (84%)	326 (100%)	0	100	100
1	C	326/390 (84%)	326 (100%)	0	100	100
1	D	327/390 (84%)	326 (100%)	1 (0%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	326/390 (84%)	323 (99%)	3 (1%)	70	85
1	F	322/390 (83%)	321 (100%)	1 (0%)	86	91
All	All	1954/2340 (84%)	1949 (100%)	5 (0%)	86	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	466	LEU
1	E	253	LEU
1	E	255	GLU
1	E	413	LEU
1	F	397	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	334	GLN
1	B	135	ASN
1	B	166	ASN
1	C	96	GLN
1	C	123	ASN
1	C	135	ASN
1	D	96	GLN
1	D	217	ASN
1	D	429	GLN
1	E	135	ASN
1	E	323	HIS
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 oligosaccharides 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	B	701	-	15,15,16	1.31	1 (6%)	21,22,23	1.48	4 (19%)
2	PLP	D	701	-	15,15,16	1.72	1 (6%)	21,22,23	1.42	4 (19%)
2	PLP	A	701	-	15,15,16	1.48	2 (13%)	21,22,23	1.74	8 (38%)
2	PLP	F	701	-	15,15,16	1.22	1 (6%)	21,22,23	1.21	2 (9%)
2	PLP	E	701	-	15,15,16	1.01	0	21,22,23	0.94	0
2	PLP	C	701	-	15,15,16	1.62	2 (13%)	21,22,23	1.32	3 (14%)

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	B	701	-	-	5/6/6/8	0/1/1/1
2	PLP	D	701	-	-	5/6/6/8	0/1/1/1
2	PLP	A	701	-	-	3/6/6/8	0/1/1/1
2	PLP	F	701	-	-	3/6/6/8	0/1/1/1
2	PLP	E	701	-	-	3/6/6/8	0/1/1/1
2	PLP	C	701	-	-	3/6/6/8	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	-4.58	1.36	1.41
2	A	701	PLP	C3-C2	-3.71	1.37	1.41
2	C	701	PLP	C3-C2	-3.18	1.37	1.41
2	B	701	PLP	C2A-C2	2.51	1.54	1.50
2	F	701	PLP	C3-C2	-2.29	1.38	1.41
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 (21) 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	3.48	115.89	109.36
2	B	701	PLP	O3P-P-O4P	3.34	115.36	106.67
2	C	701	PLP	C5-C6-N1	-2.67	119.49	123.83
2	B	701	PLP	C6-N1-C2	2.55	123.82	119.20
2	A	701	PLP	C2A-C2-C3	-2.53	117.83	120.80
2	A	701	PLP	O2P-P-O4P	2.43	113.00	106.67
2	A	701	PLP	O3-C3-C4	2.40	124.36	118.10
2	A	701	PLP	C5-C6-N1	-2.39	119.94	123.83
2	A	701	PLP	O4P-C5A-C5	2.28	113.64	109.36
2	F	701	PLP	C2A-C2-C3	-2.28	118.12	120.80
2	C	701	PLP	C6-C5-C4	2.25	119.94	118.10
2	D	701	PLP	C5-C6-N1	-2.25	120.18	123.83
2	D	701	PLP	O3-C3-C4	2.24	123.96	118.10
2	A	701	PLP	C2A-C2-N1	2.24	121.86	117.64
2	D	701	PLP	C6-N1-C2	2.19	123.18	119.20
2	C	701	PLP	C2A-C2-C3	-2.19	118.24	120.80
2	F	701	PLP	C5-C6-N1	-2.12	120.39	123.83
2	B	701	PLP	O3-C3-C2	2.05	121.83	117.58
2	A	701	PLP	C6-N1-C2	2.05	122.91	119.20
2	B	701	PLP	C4A-C4-C3	-2.02	117.16	120.52

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	PLP	C5A-O4P-P-O2P
2	A	701	PLP	C5A-O4P-P-O3P
2	B	701	PLP	C4-C5-C5A-O4P
2	B	701	PLP	C6-C5-C5A-O4P

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Mol	Chain	Res	Type	Atoms
2	B	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	D	701	PLP	C6-C5-C5A-O4P
2	D	701	PLP	C5A-O4P-P-O3P
2	E	701	PLP	C5A-O4P-P-O2P
2	E	701	PLP	C5A-O4P-P-O3P
2	F	701	PLP	C5A-O4P-P-O3P
2	A	701	PLP	C5A-O4P-P-O1P
2	B	701	PLP	C5A-O4P-P-O1P
2	E	701	PLP	C5A-O4P-P-O1P
2	F	701	PLP	C5A-O4P-P-O1P
2	B	701	PLP	C5A-O4P-P-O2P
2	D	701	PLP	C5A-O4P-P-O2P
2	F	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 13 short contacts:

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

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	399/475 (84%)	-0.34	5 (1%) 75 53	30, 50, 99, 172	1 (0%)
1	B	399/475 (84%)	-0.40	3 (0%) 82 64	37, 47, 98, 162	0
1	C	401/475 (84%)	-0.33	3 (0%) 84 66	38, 53, 96, 185	0
1	D	400/475 (84%)	-0.26	2 (0%) 87 72	37, 49, 107, 195	0
1	E	399/475 (84%)	0.23	9 (2%) 61 38	57, 88, 133, 173	0
1	F	397/475 (83%)	0.42	10 (2%) 58 35	60, 107, 167, 235	0
All	All	2395/2850 (84%)	-0.11	32 (1%) 75 53	30, 63, 134, 235	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	254	LEU	5.0
1	E	253	LEU	3.6
1	F	368	TYR	3.6
1	E	365	VAL	3.0
1	E	89	ASP	2.9
1	F	327	ALA	2.9
1	D	412	GLY	2.8
1	C	409	GLU	2.7
1	A	81	PRO	2.7
1	F	396	LEU	2.6
1	F	245	THR	2.6
1	F	411	PHE	2.5
1	F	90	LEU	2.5
1	A	415	ASN	2.5
1	F	448	TYR	2.4
1	E	364	MET	2.4
1	D	85	MET	2.4
1	F	408	ALA	2.3
1	A	416	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	388	SER	2.3
1	E	339	ALA	2.3
1	A	411	PHE	2.3
1	C	413	LEU	2.2
1	F	91	ALA	2.2
1	C	415	ASN	2.2
1	F	357	GLY	2.2
1	B	426	ASP	2.2
1	B	92	ALA	2.1
1	E	410	GLY	2.1
1	A	92	ALA	2.1
1	E	82	SER	2.1
1	E	83	LYS	2.1

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLP	F	701	15/16	0.90	0.15	97,115,123,125	0
2	PLP	E	701	15/16	0.92	0.12	80,86,96,101	0
2	PLP	C	701	15/16	0.94	0.11	41,48,59,65	0
2	PLP	D	701	15/16	0.94	0.09	39,40,66,69	0
2	PLP	A	701	15/16	0.95	0.10	37,50,56,62	0
2	PLP	B	701	15/16	0.96	0.07	38,47,56,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.