



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 3, 2017 – 04:12 PM EDT

PDB ID : 5UIE
EMDB ID: : EMD-8549
Title : Vps4-Vta1 complex
Authors : Monroe, N.; Shen, P.; Han, H.; Sundquist, W.I.; Hill, C.P.
Deposited on : unknown
Resolution : 5.70 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

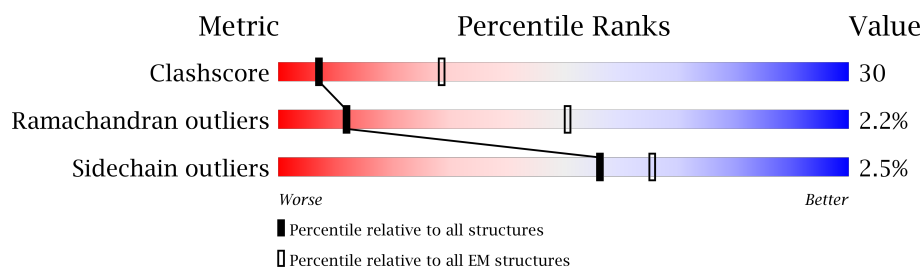
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	437	
1	B	437	
1	C	437	
1	D	437	
1	E	437	
1	F	437	
2	G	9	
3	H	330	
3	I	330	

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Mol	Chain	Length	Quality of chain
3	J	330	<div><div></div><div></div><div></div></div> 8% 87%
3	K	330	<div><div></div><div></div><div></div></div> 9% 5% 86%
3	L	330	<div><div></div><div></div><div></div></div> 5% 8% 87%
3	M	330	<div><div></div><div></div><div></div></div> 9% 5% 86%
3	N	330	<div><div></div><div></div><div></div></div> 5% 8% 87%
3	O	330	<div><div></div><div></div><div></div></div> 5% 8% 87%
3	P	330	<div><div></div><div></div><div></div></div> 5% 8% 87%
3	Q	330	<div><div></div><div></div><div></div></div> 5% 7% 87%
3	R	330	<div><div></div><div></div><div></div></div> 5% 7% 87%
3	S	330	<div><div></div><div></div><div></div></div> 5% 8% 87%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18682 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Vacuolar protein sorting-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	312	Total	C	N	O	S	0	0
			2412	1522	409	472	9		
1	B	311	Total	C	N	O	S	0	0
			2407	1519	408	471	9		
1	C	311	Total	C	N	O	S	0	0
			2407	1519	408	471	9		
1	D	311	Total	C	N	O	S	0	0
			2407	1519	408	471	9		
1	E	308	Total	C	N	O	S	0	0
			2387	1507	405	466	9		
1	F	302	Total	C	N	O	S	0	0
			2344	1484	396	455	9		

- Molecule 2 is a protein called DOA4-independent degradation protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	9	Total	C	N	O	0	0
			43	26	8	9		

- Molecule 3 is a protein called Vacuolar protein sorting-associated protein VTA1.

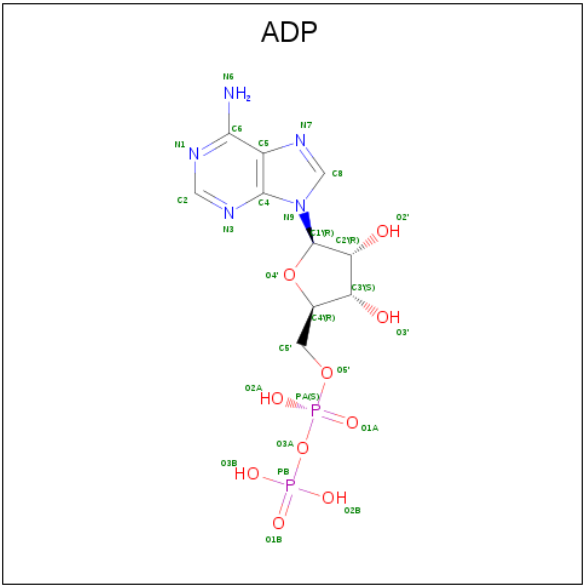
Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	42	Total	C	N	O		0	0
			331	209	54	68			
3	I	51	Total	C	N	O	S	0	0
			404	255	65	83	1		
3	J	42	Total	C	N	O		0	0
			331	209	54	68			
3	K	47	Total	C	N	O	S	0	0
			371	236	60	74	1		
3	L	42	Total	C	N	O		0	0
			331	209	54	68			
3	M	47	Total	C	N	O	S	0	0
			371	236	60	74	1		

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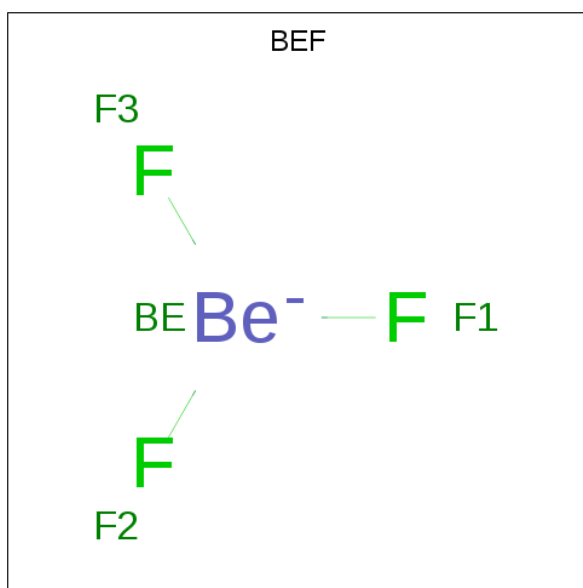
Mol	Chain	Residues	Atoms				AltConf	Trace
3	N	42	Total	C	N	O	0	0
			331	209	54	68		
3	O	42	Total	C	N	O	0	0
			331	209	54	68		
3	P	42	Total	C	N	O	0	0
			331	209	54	68		
3	Q	42	Total	C	N	O	0	0
			331	209	54	68		
3	R	42	Total	C	N	O	0	0
			331	209	54	68		
3	S	42	Total	C	N	O	0	0
			331	209	54	68		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

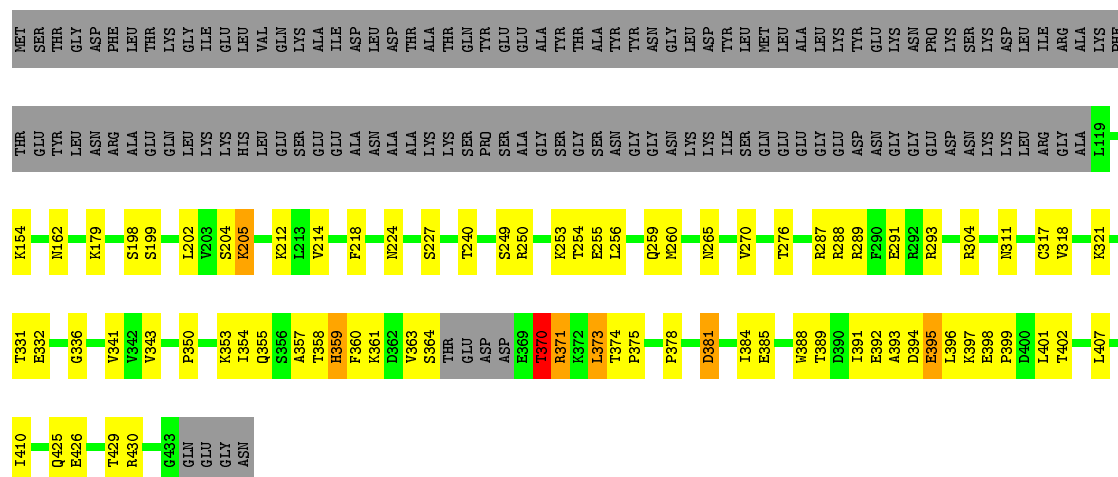
- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



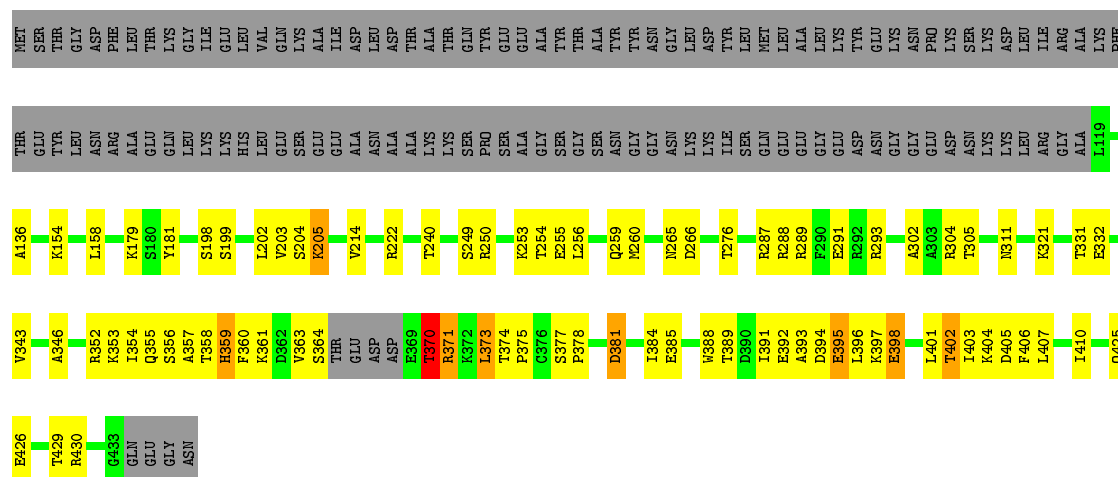
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Be	F	0
			4	1	3	
5	C	1	Total	Be	F	0
			8	2	6	
5	C	1	Total	Be	F	0
			8	2	6	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

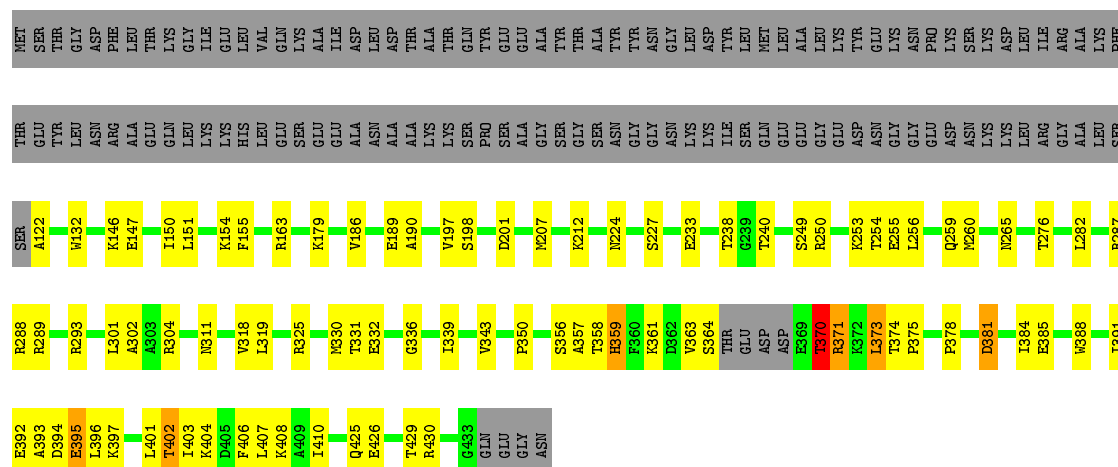
Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Mg	0
			1	1	
6	A	1	Total	Mg	0
			1	1	
6	C	1	Total	Mg	0
			1	1	



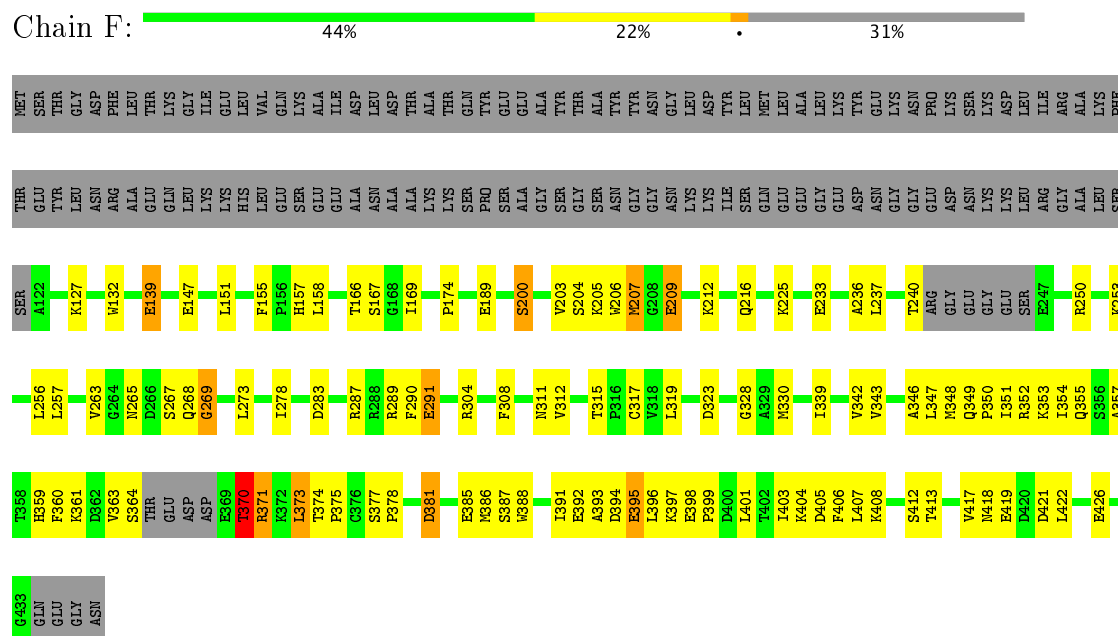
Chain D: 52% 17% 29%



Chain E: 50% 19% 30%



- Molecule 1: Vacuolar protein sorting-associated protein 4

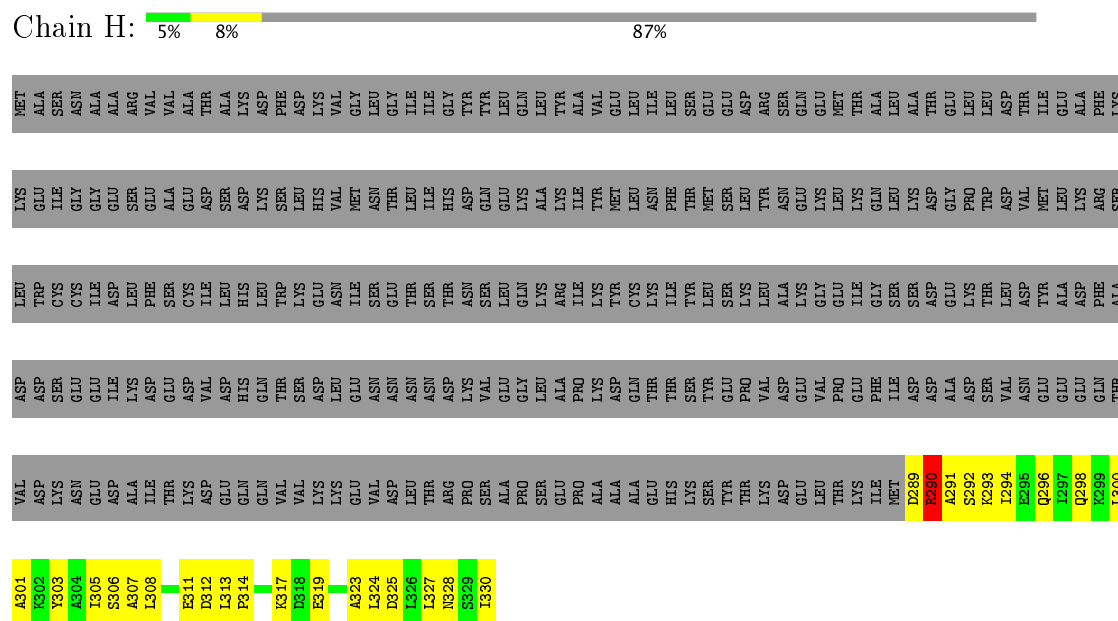


- Molecule 2: DOA4-independent degradation protein 4



There are no outlier residues recorded for this chain.

- Molecule 3: Vacuolar protein sorting-associated protein VTA1



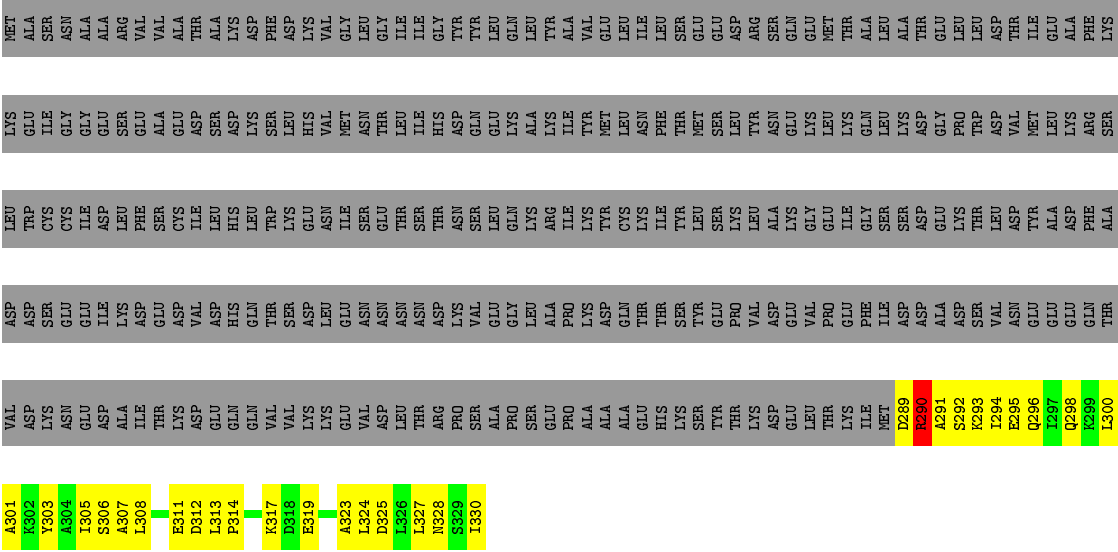
- Molecule 3: Vacuolar protein sorting-associated protein VTA1





● Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain J: 8% 87%

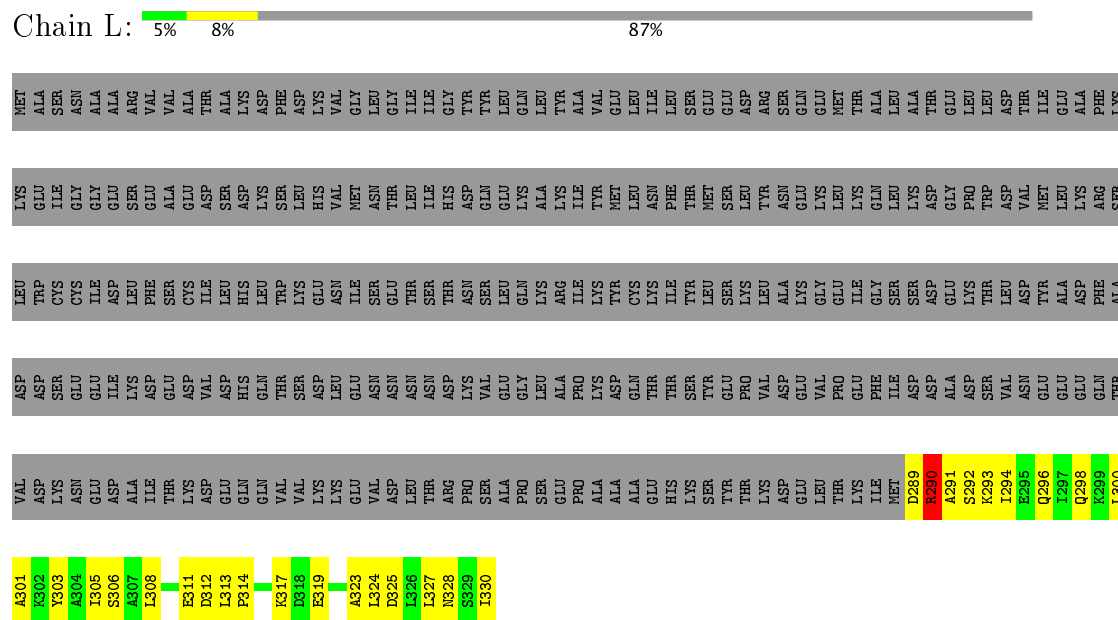


● Molecule 3: Vacuolar protein sorting-associated protein VTA1

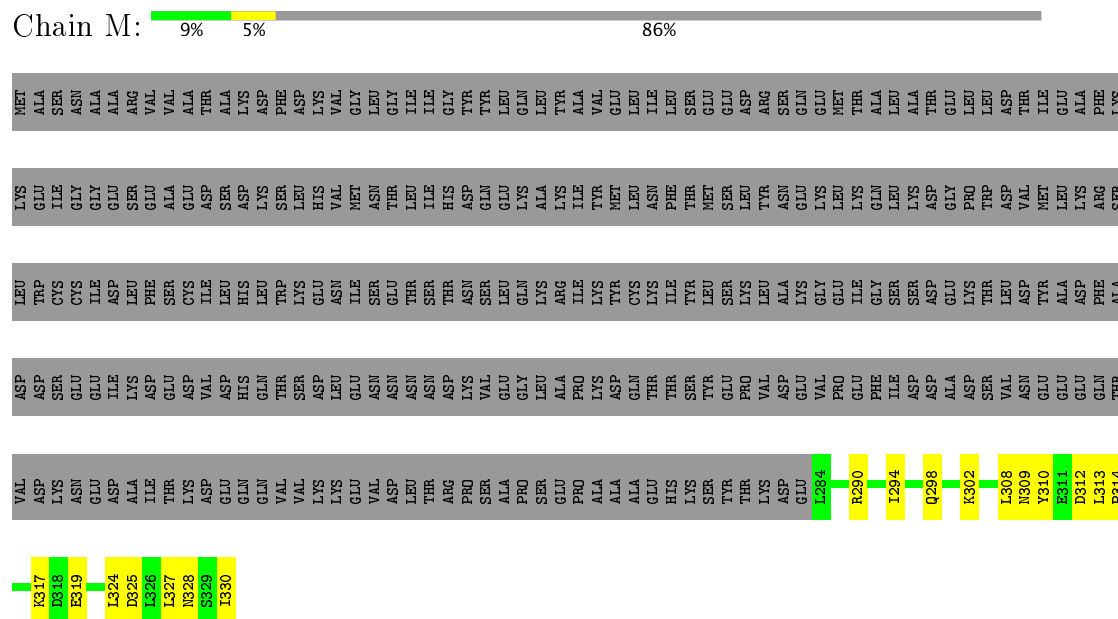
Chain K: 9% 5% 86%



- Molecule 3: Vacuolar protein sorting-associated protein VTA1



- Molecule 3: Vacuolar protein sorting-associated protein VTA1



- Molecule 3: Vacuolar protein sorting-associated protein VTA1

- Molecule 3: Vacuolar protein sorting-associated protein VTA1

- Molecule 3: Vacuolar protein sorting-associated protein VTA1

[illegible]

Chain S:  5% 8% 87%

A301	VAL	ASP	LEU	LVS	MET
I305	ASP	ASP	TPR	GLU	ALA
	LVS	SER	CYS	ILE	SER
	ASN	GLU	CYS	GLY	ASN
L308	GLU	GLU	ILE	GLY	ALA
	ASP	ILE	ASP	GLU	ALA
N309	ALA	LVS	LEU	SER	ARG
Y310	ILE	ASP	PHE	GLU	VAL
E311	THR	GLU	SER	ALA	VAL
D312	LVS	ASP	CYS	GLU	ALA
L313	ASP	VAL	ILE	ASP	THR
P314	GLU	ASP	LEU	SER	ALA
K317	GLN	HIS	LEU	ASP	LVS
	GLN	HIS	LEU	ASP	LVS
D318	VAL	GLN	TPR	SER	PHE
E319	VAL	SER	TPR	SER	ASP
A323	LVS	ASP	LVS	LEU	LVS
	LVS	ASP	GLU	HIS	VAL
L324	GLU	LEU	ASN	VAL	GLY
D325	GLU	GLU	ILE	MET	LEU
L326	VAL	ASN	SER	THR	GLY
L327	ASP	ASN	GLU	THR	ILE
N328	LEU	ASN	THR	LEU	ILE
S329	THR	ASN	SER	ILE	ILE
I330	ANG	ASP	THR	HIS	GLY
	PRO	LVS	ASN	ASP	TYR
S331	SER	VAL	SER	GLN	TYR
	ALA	GLU	LEU	GLU	LEU
D332	PRO	GLY	GLN	LVS	GLN
	SER	LEU	LVS	ALA	LEU
L333	GLU	ALA	ARG	LVS	TYR
	PRO	PRO	ILE	ILE	ALA
S334	ALA	LVS	LVS	TYR	VAL
	ALA	ASP	TPR	MET	GLU
D335	GLU	GLN	CYS	LEU	LEU
	GLU	THR	THR	ASN	ILE
L336	HIS	THR	ILE	PHE	LEU
	LVS	SER	TPR	SER	GLU
Q337	SER	TYR	LEU	SER	GLU
	THR	GLU	SER	GLU	ASP
Q338	THR	PRO	LVS	TYR	ARG
	LVS	VAL	LEU	TYR	SER
S339	ASP	ASP	ALA	ASN	SER
	GLU	GLU	LVS	GLU	GLN
D340	LEU	VAL	GLY	LVS	GLU
	THR	PRO	GLU	LEU	GLU
L341	LVS	GLU	ILE	LVS	THR
	ILE	PHE	GLY	GLN	ALA
Q342	ILE	ILE	SER	LEU	LEU
	D289	ASP	SER	LVS	ALA
K343	MET	ASP	ASP	ASP	THR
	ASP	ASP	GLU	GLY	GLU
Q344	D290	ALA	GLU	PRO	LEU
	S292	ASP	LVS	TPR	LEU
L345	K293	SER	THR	ASP	ASP
	L294	VAL	LEU	VAL	THR
Q346	E295	ASN	ASP	THR	ILE
	Q296	GLU	TPR	MET	GLU
S347	D297	GLU	ALA	LEU	ALA
	Q298	GLU	ASP	LVS	GLU
K348	Q299	GLN	PHE	ARG	PHE
	Q300	GLN	THR	THR	THR

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.3	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BEF, ACE, ADP

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 >2	RMSZ	# Z >2
1	A	0.35	0/2453	0.55	0/3315
1	B	0.36	0/2448	0.55	0/3308
1	C	0.36	0/2448	0.55	0/3308
1	D	0.36	0/2448	0.56	0/3308
1	E	0.35	0/2428	0.57	0/3281
1	F	0.60	0/2384	0.69	2/3222 (0.1%)
3	H	0.52	0/333	0.75	0/447
3	I	0.54	0/406	0.66	0/544
3	J	0.52	0/333	0.75	0/447
3	K	0.52	0/373	0.68	0/500
3	L	0.52	0/333	0.75	0/447
3	M	0.52	0/373	0.68	0/500
3	N	0.52	0/333	0.75	0/447
3	O	0.52	0/333	0.75	0/447
3	P	0.52	0/333	0.75	0/447
3	Q	0.52	0/333	0.75	0/447
3	R	0.53	0/333	0.75	0/447
3	S	0.53	0/333	0.75	0/447
All	All	0.43	0/18758	0.61	2/25309 (0.0%)

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	2
1	B	0	3
1	C	0	2
1	D	0	1
1	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	9

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	269	GLY	N-CA-C	5.16	126.00	113.10
1	F	287	ARG	NE-CZ-NH1	5.15	122.88	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	LYS	Peptide
1	A	250	ARG	Sidechain
1	B	205	LYS	Peptide
1	B	270	VAL	Mainchain
1	B	414	ARG	Peptide
1	C	205	LYS	Peptide
1	C	270	VAL	Mainchain
1	D	205	LYS	Peptide
1	E	356	SER	Peptide

5.2 Too-close contacts [i](#)

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	2412	0	2435	178	0
1	B	2407	0	2430	179	0
1	C	2407	0	2430	124	0
1	D	2407	0	2430	147	0
1	E	2387	0	2407	154	0
1	F	2344	0	2371	208	0
2	G	43	0	12	0	0
3	H	331	0	344	36	0
3	I	404	0	425	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	331	0	344	37	0
3	K	371	0	395	24	0
3	L	331	0	344	39	0
3	M	371	0	395	34	0
3	N	331	0	344	36	0
3	O	331	0	344	38	0
3	P	331	0	344	39	0
3	Q	331	0	344	29	0
3	R	331	0	344	27	0
3	S	331	0	344	59	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	2	0
4	E	27	0	12	1	0
5	A	4	0	0	0	0
5	C	8	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
All	All	18682	0	18886	1118	0

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 30.

All (1118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:ILE:HD13	1:C:375:PRO:CG	1.31	1.61
1:F:354:ILE:CG2	1:F:396:LEU:HD21	1.20	1.59
1:B:354:ILE:HA	1:B:375:PRO:CG	1.14	1.59
1:C:354:ILE:HD13	1:C:375:PRO:CD	1.31	1.55
1:D:389:THR:CG2	1:E:154:LYS:HZ1	1.16	1.54
1:A:254:THR:CB	1:F:205:LYS:HD3	1.12	1.54
1:C:354:ILE:CD1	1:C:375:PRO:HD3	1.39	1.50
1:A:325:ARG:HH12	3:S:312:ASP:CB	1.24	1.49
1:F:323:ASP:CB	1:F:403:ILE:HD12	1.46	1.46
1:A:254:THR:CB	1:F:205:LYS:CD	1.95	1.45
1:A:305:THR:HG21	3:S:310:TYR:CE1	1.48	1.44
1:B:354:ILE:O	1:B:360:PHE:CZ	1.72	1.42
1:C:354:ILE:CD1	1:C:375:PRO:CD	1.90	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LYS:CD	3:S:309:ASN:O	1.65	1.41
1:E:318:VAL:CG1	1:E:402:THR:HA	1.51	1.40
1:D:389:THR:CG2	1:E:154:LYS:NZ	1.87	1.36
1:B:321:LYS:HG2	3:I:310:TYR:CD1	1.59	1.36
1:A:325:ARG:NH1	3:S:312:ASP:HB2	1.36	1.36
1:B:321:LYS:CG	3:I:310:TYR:HD1	1.38	1.35
1:E:301:LEU:HD13	3:O:310:TYR:CD1	1.62	1.35
1:E:318:VAL:HB	1:E:401:LEU:O	1.26	1.34
1:B:354:ILE:CA	1:B:375:PRO:CG	2.02	1.33
1:A:325:ARG:NH1	3:S:312:ASP:CB	1.89	1.32
1:F:317:CYS:CB	1:F:401:LEU:HD23	1.60	1.31
1:B:321:LYS:CG	3:I:310:TYR:CD1	2.14	1.30
1:E:318:VAL:HG11	1:E:402:THR:CA	1.61	1.30
1:E:201:ASP:CG	1:F:250:ARG:NH2	1.83	1.29
1:E:404:LYS:HE2	3:P:311:GLU:CG	1.45	1.29
1:C:354:ILE:HA	1:C:375:PRO:CG	1.64	1.28
1:A:254:THR:HB	1:F:205:LYS:CD	1.61	1.27
1:A:254:THR:OG1	1:F:205:LYS:HD3	1.24	1.27
1:B:321:LYS:HD3	3:I:310:TYR:CD1	1.69	1.26
1:B:321:LYS:CD	3:I:310:TYR:CD1	2.19	1.26
1:F:354:ILE:CG2	1:F:396:LEU:CD2	2.14	1.25
1:A:250:ARG:NH1	1:F:204:SER:HB3	1.49	1.25
1:B:354:ILE:CA	1:B:375:PRO:HG2	1.64	1.25
1:F:360:PHE:CG	1:F:391:ILE:HD11	1.72	1.25
1:D:321:LYS:CD	3:M:310:TYR:HA	1.67	1.24
1:C:358:THR:O	1:C:359:HIS:CD2	1.90	1.24
1:A:388:TRP:CZ3	1:B:155:PHE:CZ	2.25	1.23
1:E:201:ASP:OD1	1:F:250:ARG:NH2	1.72	1.22
1:B:354:ILE:CA	1:B:375:PRO:HG3	1.65	1.22
1:B:355:GLN:NE2	1:B:388:TRP:CD2	2.08	1.22
1:B:355:GLN:CG	1:B:388:TRP:CD1	2.23	1.21
1:B:354:ILE:HG13	1:B:375:PRO:CD	1.72	1.19
1:D:389:THR:HG22	1:E:154:LYS:NZ	1.51	1.19
1:F:354:ILE:HG21	1:F:396:LEU:CD2	1.69	1.19
1:A:388:TRP:HZ3	1:B:155:PHE:CZ	1.60	1.19
1:A:322:GLU:CG	3:S:310:TYR:O	1.90	1.19
1:F:317:CYS:HB3	1:F:401:LEU:CD2	1.73	1.19
1:A:388:TRP:CZ3	1:B:155:PHE:CE2	2.31	1.18
1:A:254:THR:HG21	1:F:205:LYS:CG	1.74	1.18
1:E:404:LYS:CE	3:P:311:GLU:HG3	1.74	1.17
1:E:201:ASP:OD2	1:F:250:ARG:NH2	1.71	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:ASP:OD1	1:F:250:ARG:CZ	1.93	1.16
1:B:358:THR:O	1:B:359:HIS:CD2	1.96	1.16
1:B:355:GLN:CD	1:B:388:TRP:CD1	2.18	1.16
1:B:355:GLN:HG2	1:B:388:TRP:CG	1.80	1.16
1:B:355:GLN:HG2	1:B:388:TRP:CB	1.76	1.16
1:A:254:THR:HB	1:F:205:LYS:CE	1.74	1.16
1:E:404:LYS:CE	3:P:311:GLU:CG	2.23	1.16
1:F:323:ASP:HB3	1:F:403:ILE:HD12	1.16	1.15
1:E:301:LEU:HD13	3:O:310:TYR:CE1	1.82	1.15
1:A:305:THR:HG21	3:S:310:TYR:CZ	1.83	1.12
1:F:319:LEU:HD21	1:F:403:ILE:HA	1.30	1.12
1:E:393:ALA:HB1	1:F:157:HIS:CE1	1.81	1.12
1:C:354:ILE:HA	1:C:375:PRO:HG3	1.14	1.11
1:A:251:ARG:O	1:F:205:LYS:NZ	1.82	1.11
1:F:253:LYS:HE3	1:F:283:ASP:OD2	1.47	1.11
1:A:240:THR:HG21	1:A:250:ARG:HH21	1.07	1.11
1:B:354:ILE:HA	1:B:375:PRO:HG2	1.12	1.11
1:D:321:LYS:CG	3:M:310:TYR:HA	1.79	1.11
1:A:254:THR:CG2	1:F:205:LYS:CD	2.29	1.10
1:C:354:ILE:HD13	1:C:375:PRO:HG2	1.31	1.10
1:D:389:THR:HG23	1:E:154:LYS:NZ	1.67	1.10
1:B:358:THR:OG1	1:B:385:GLU:HG3	1.52	1.10
1:A:254:THR:HG21	1:F:205:LYS:HG2	1.19	1.09
1:B:355:GLN:CD	1:B:388:TRP:CG	2.26	1.09
1:C:354:ILE:HD12	1:C:375:PRO:HD3	1.26	1.09
1:A:250:ARG:NH1	1:F:204:SER:CB	2.16	1.08
1:D:321:LYS:HD3	3:M:310:TYR:HA	1.36	1.08
1:D:302:ALA:O	3:M:310:TYR:OH	1.72	1.08
1:B:355:GLN:HG2	1:B:388:TRP:HB3	1.24	1.07
1:F:319:LEU:CD2	1:F:403:ILE:HB	1.84	1.07
1:B:354:ILE:HG13	1:B:375:PRO:HD3	1.12	1.06
1:D:373:LEU:HD12	1:D:391:ILE:HD13	1.38	1.05
1:F:373:LEU:HD12	1:F:391:ILE:HD13	1.38	1.05
1:A:373:LEU:HD12	1:A:391:ILE:HD13	1.38	1.05
1:C:358:THR:O	1:C:359:HIS:CG	2.09	1.05
1:A:325:ARG:HH12	3:S:312:ASP:CG	1.57	1.04
1:B:355:GLN:CG	1:B:388:TRP:CG	2.38	1.04
1:D:389:THR:HG22	1:E:154:LYS:HZ1	0.99	1.04
1:A:353:LYS:HD2	1:A:399:PRO:HG2	1.36	1.03
1:D:321:LYS:HD3	3:M:310:TYR:CA	1.88	1.03
1:A:163:ARG:HD3	1:F:351:ILE:HG12	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:THR:CG2	3:S:310:TYR:CE1	2.41	1.03
1:C:354:ILE:CD1	1:C:375:PRO:CG	2.24	1.03
1:C:373:LEU:HD12	1:C:391:ILE:HD13	1.38	1.03
1:E:301:LEU:CD1	3:O:310:TYR:CD1	2.40	1.03
1:A:321:LYS:HD3	3:S:309:ASN:O	0.87	1.03
1:E:373:LEU:HD12	1:E:391:ILE:CD1	1.89	1.03
1:C:373:LEU:HD12	1:C:391:ILE:CD1	1.89	1.02
1:B:325:ARG:NH1	3:I:312:ASP:OD2	1.91	1.02
1:D:354:ILE:HA	1:D:375:PRO:CG	1.89	1.02
1:A:373:LEU:HD12	1:A:391:ILE:CD1	1.89	1.02
1:A:254:THR:HG21	1:F:205:LYS:CD	1.88	1.02
1:F:373:LEU:HD12	1:F:391:ILE:CD1	1.89	1.02
1:B:355:GLN:NE2	1:B:388:TRP:CG	2.26	1.02
1:B:373:LEU:HD12	1:B:391:ILE:HD13	1.38	1.02
1:D:321:LYS:HG2	3:M:310:TYR:HA	1.39	1.02
1:B:321:LYS:HG2	3:I:310:TYR:HD1	0.85	1.02
1:B:373:LEU:HD12	1:B:391:ILE:CD1	1.89	1.02
1:B:354:ILE:CG1	1:B:375:PRO:HD3	1.90	1.02
1:D:352:ARG:O	1:D:356:SER:HB3	1.59	1.01
1:F:360:PHE:CG	1:F:391:ILE:CD1	2.41	1.01
1:E:201:ASP:CG	1:F:250:ARG:HH22	1.52	1.01
1:F:354:ILE:HG23	1:F:396:LEU:HD11	1.39	1.01
1:D:373:LEU:HD12	1:D:391:ILE:CD1	1.89	1.01
1:A:322:GLU:HG2	3:S:310:TYR:O	1.54	1.01
1:A:250:ARG:HH11	1:F:204:SER:CB	1.71	1.01
1:F:323:ASP:CA	1:F:403:ILE:HD12	1.91	1.01
1:D:361:LYS:HD2	1:D:381:ASP:O	1.61	1.00
1:E:318:VAL:CB	1:E:401:LEU:O	2.07	1.00
1:E:361:LYS:HD2	1:E:381:ASP:O	1.61	1.00
1:D:358:THR:HG21	3:N:303:TYR:CE1	1.97	1.00
1:A:254:THR:CG2	1:F:205:LYS:HD3	1.90	1.00
1:F:361:LYS:HD2	1:F:381:ASP:O	1.61	1.00
1:C:354:ILE:HG23	1:C:360:PHE:HE2	1.27	0.99
1:C:361:LYS:HD2	1:C:381:ASP:O	1.61	0.99
1:E:325:ARG:NH2	3:O:310:TYR:O	1.94	0.99
1:B:361:LYS:HD2	1:B:381:ASP:O	1.61	0.99
1:F:357:ALA:HB1	1:F:375:PRO:HG3	1.45	0.99
1:E:373:LEU:HD12	1:E:391:ILE:HD13	1.38	0.99
1:B:358:THR:O	1:B:359:HIS:CG	2.15	0.99
1:A:251:ARG:CZ	1:F:205:LYS:O	2.10	0.98
1:A:361:LYS:HD2	1:A:381:ASP:O	1.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:ILE:HA	1:D:375:PRO:HG3	1.41	0.98
1:D:377:SER:OG	3:N:307:ALA:HA	1.62	0.98
1:F:323:ASP:CB	1:F:403:ILE:CD1	2.41	0.98
1:C:358:THR:OG1	1:C:385:GLU:HG3	1.62	0.98
1:D:358:THR:OG1	1:D:385:GLU:HG3	1.62	0.98
1:A:322:GLU:OE2	3:S:310:TYR:O	1.81	0.98
1:A:254:THR:CG2	1:F:205:LYS:HE2	1.94	0.97
1:F:360:PHE:HD1	1:F:386:MET:HG3	1.30	0.97
1:A:377:SER:OG	3:H:307:ALA:HA	1.64	0.97
1:B:354:ILE:HG12	1:B:360:PHE:HE2	1.28	0.97
1:F:354:ILE:HG23	1:F:396:LEU:HD21	1.46	0.97
1:B:354:ILE:CD1	1:B:396:LEU:CD1	2.43	0.96
1:B:354:ILE:HD11	1:B:396:LEU:HD12	1.47	0.96
1:D:389:THR:CB	1:E:154:LYS:HZ1	1.77	0.96
1:A:254:THR:HB	1:F:205:LYS:NZ	1.80	0.96
1:F:319:LEU:HD23	1:F:403:ILE:HB	1.47	0.96
1:D:321:LYS:CD	3:M:310:TYR:CA	2.41	0.96
1:D:321:LYS:HD3	3:M:309:ASN:O	1.65	0.96
1:D:354:ILE:HD11	1:D:398:GLU:HA	1.45	0.96
1:C:357:ALA:HB2	3:L:306:SER:HB2	1.48	0.95
1:D:388:TRP:CE3	1:E:155:PHE:HE2	1.82	0.95
1:A:254:THR:HB	1:F:205:LYS:HD3	1.15	0.95
1:B:354:ILE:HD13	1:B:396:LEU:HD11	1.45	0.95
1:A:321:LYS:HG2	3:S:310:TYR:CD1	2.01	0.95
1:F:323:ASP:HB3	1:F:403:ILE:CD1	1.98	0.94
1:A:388:TRP:CZ3	1:B:155:PHE:HZ	1.73	0.94
1:A:254:THR:CG2	1:F:205:LYS:CE	2.46	0.94
1:A:388:TRP:HZ3	1:B:155:PHE:HZ	1.03	0.94
1:B:346:ALA:O	1:B:401:LEU:CD2	2.15	0.94
1:E:357:ALA:HB1	3:P:306:SER:HB2	1.50	0.93
1:F:360:PHE:CD1	1:F:391:ILE:HD11	2.04	0.93
1:A:240:THR:CG2	1:A:250:ARG:HH21	1.81	0.93
1:D:321:LYS:HD3	3:M:309:ASN:C	1.89	0.93
1:B:355:GLN:HG2	1:B:388:TRP:CD1	1.97	0.92
1:B:354:ILE:HG13	1:B:375:PRO:CG	1.97	0.92
1:E:388:TRP:HZ2	1:F:147:GLU:OE1	1.50	0.92
1:C:354:ILE:HA	1:C:375:PRO:HG2	1.52	0.92
1:D:358:THR:O	1:D:359:HIS:CD2	2.22	0.92
1:A:305:THR:HG21	3:S:310:TYR:HE1	1.16	0.92
1:A:388:TRP:CZ3	1:B:155:PHE:HE2	1.87	0.91
1:E:393:ALA:HB1	1:F:157:HIS:HE1	1.29	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ILE:CD1	1:B:396:LEU:HD11	2.01	0.91
1:F:354:ILE:HG22	1:F:396:LEU:HD21	1.48	0.91
1:A:325:ARG:HH11	3:S:312:ASP:HB2	1.21	0.91
1:A:254:THR:CB	1:F:205:LYS:CE	2.42	0.90
1:A:325:ARG:NH1	3:S:312:ASP:OD2	2.04	0.90
1:C:318:VAL:HG11	1:C:402:THR:HA	1.52	0.90
1:D:305:THR:HB	3:M:310:TYR:OH	1.68	0.89
1:A:358:THR:O	1:A:359:HIS:CD2	2.26	0.89
1:B:355:GLN:HB3	1:B:388:TRP:CD1	2.08	0.89
1:A:353:LYS:CD	1:A:399:PRO:HG2	2.02	0.89
1:B:358:THR:OG1	1:B:385:GLU:CG	2.21	0.89
1:E:388:TRP:CZ2	1:F:147:GLU:OE1	2.26	0.89
1:B:354:ILE:HA	1:B:375:PRO:HG3	0.89	0.89
1:C:355:GLN:HG2	1:C:388:TRP:CD2	2.08	0.89
1:A:163:ARG:CD	1:F:351:ILE:HG12	2.03	0.89
1:A:322:GLU:CD	3:S:310:TYR:O	2.11	0.89
1:F:360:PHE:CD2	1:F:391:ILE:CD1	2.56	0.88
1:F:319:LEU:CD2	1:F:403:ILE:HA	2.03	0.88
1:A:240:THR:HG21	1:A:250:ARG:NH2	1.87	0.88
1:F:319:LEU:CD2	1:F:403:ILE:CB	2.51	0.88
1:D:354:ILE:CG2	1:D:396:LEU:HD11	2.02	0.88
1:B:321:LYS:CD	3:I:310:TYR:HD1	1.71	0.88
1:B:354:ILE:O	1:B:360:PHE:HZ	1.26	0.88
1:E:301:LEU:CD1	3:O:310:TYR:CG	2.56	0.88
1:F:319:LEU:HD21	1:F:403:ILE:CA	2.04	0.88
1:F:319:LEU:CD2	1:F:403:ILE:CA	2.51	0.88
1:B:355:GLN:CB	1:B:388:TRP:CD1	2.57	0.87
1:C:354:ILE:HG23	1:C:360:PHE:CE2	2.09	0.87
1:A:354:ILE:HD13	1:A:396:LEU:HD21	1.57	0.87
1:A:325:ARG:HH12	3:S:312:ASP:HB3	1.37	0.86
1:F:323:ASP:CG	1:F:403:ILE:HD12	1.96	0.86
1:A:388:TRP:CH2	1:B:155:PHE:HE2	1.92	0.86
1:F:354:ILE:HG23	1:F:396:LEU:CD1	2.06	0.85
1:A:254:THR:HB	1:F:205:LYS:HZ3	1.39	0.85
1:D:354:ILE:HD11	1:D:398:GLU:CA	2.06	0.85
1:A:163:ARG:HG3	1:F:348:MET:SD	2.16	0.85
1:D:388:TRP:HE3	1:E:155:PHE:HE2	1.20	0.85
1:D:388:TRP:CD2	1:E:154:LYS:NZ	2.36	0.85
1:A:250:ARG:HD2	1:F:204:SER:HB2	1.59	0.85
1:B:354:ILE:CB	1:B:375:PRO:CG	2.54	0.84
1:B:321:LYS:HD2	3:I:310:TYR:HA	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:SER:OG	3:J:307:ALA:HA	1.75	0.84
1:E:385:GLU:OE2	3:P:303:TYR:OH	1.95	0.84
1:E:357:ALA:CB	3:P:306:SER:HB2	2.08	0.84
1:F:355:GLN:O	1:F:388:TRP:CD1	2.31	0.83
1:A:325:ARG:CZ	3:S:312:ASP:OD2	2.26	0.83
1:F:354:ILE:HG21	1:F:396:LEU:HD21	0.85	0.83
1:E:318:VAL:HG11	1:E:402:THR:HA	0.84	0.83
1:A:254:THR:OG1	1:F:205:LYS:CD	2.12	0.83
1:E:301:LEU:HD13	3:O:310:TYR:CG	2.13	0.83
1:C:358:THR:OG1	1:C:385:GLU:CG	2.27	0.83
1:B:321:LYS:NZ	3:I:309:ASN:O	2.11	0.82
1:E:408:LYS:CE	3:Q:295:GLU:HB2	2.09	0.82
1:B:321:LYS:CG	3:I:310:TYR:CE1	2.61	0.82
1:A:251:ARG:NH1	1:F:205:LYS:O	2.11	0.82
1:D:389:THR:CA	1:E:154:LYS:HZ1	1.92	0.82
1:E:302:ALA:HB2	3:O:309:ASN:O	1.79	0.82
1:A:305:THR:HB	3:S:310:TYR:OH	1.80	0.82
1:D:385:GLU:OE2	3:N:303:TYR:OH	1.97	0.82
1:C:358:THR:HG23	1:C:359:HIS:CD2	2.14	0.81
1:D:354:ILE:HD11	1:D:398:GLU:HB3	1.61	0.81
1:C:354:ILE:CA	1:C:375:PRO:CG	2.53	0.81
1:F:350:PRO:HB3	1:F:399:PRO:O	1.80	0.81
1:B:354:ILE:HA	1:B:375:PRO:CB	2.11	0.81
1:D:389:THR:CA	1:E:154:LYS:NZ	2.44	0.81
1:B:354:ILE:O	1:B:360:PHE:CE2	2.33	0.81
3:J:311:GLU:CD	3:K:290:ARG:HH12	1.84	0.81
3:H:311:GLU:CD	3:I:290:ARG:HH12	1.84	0.80
3:L:311:GLU:CD	3:M:290:ARG:HH12	1.85	0.80
1:C:357:ALA:HB2	3:L:306:SER:CB	2.11	0.80
1:D:354:ILE:HG21	1:D:396:LEU:HD11	1.62	0.80
1:B:354:ILE:HD13	1:B:396:LEU:CD1	2.10	0.80
1:B:355:GLN:HB3	1:B:388:TRP:HD1	1.42	0.80
1:E:186:VAL:O	1:E:190:ALA:HB2	1.82	0.80
1:A:321:LYS:HG2	3:S:310:TYR:HD1	1.42	0.80
1:B:321:LYS:HD3	3:I:310:TYR:CE1	2.17	0.80
1:F:317:CYS:HB3	1:F:401:LEU:HD23	0.83	0.80
1:D:352:ARG:O	1:D:356:SER:CB	2.30	0.80
1:D:388:TRP:CE3	1:E:155:PHE:CE2	2.70	0.80
1:F:385:GLU:OE2	3:R:303:TYR:OH	1.99	0.80
1:E:249:SER:O	1:E:253:LYS:HB3	1.82	0.79
1:A:358:THR:OG1	1:A:385:GLU:HG3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:ALA:HB1	3:P:306:SER:CB	2.12	0.79
1:C:249:SER:O	1:C:253:LYS:HB3	1.82	0.79
1:B:321:LYS:CD	3:I:309:ASN:O	2.31	0.79
1:A:305:THR:CG2	3:S:310:TYR:HE1	1.86	0.79
1:A:358:THR:HG23	1:A:359:HIS:CD2	2.18	0.79
1:B:249:SER:O	1:B:253:LYS:HB3	1.82	0.79
1:A:254:THR:HG22	1:F:205:LYS:HE2	1.64	0.79
1:D:249:SER:O	1:D:253:LYS:HB3	1.82	0.79
1:E:408:LYS:HE3	3:Q:295:GLU:HB2	1.65	0.79
1:C:354:ILE:CD1	1:C:375:PRO:HD2	2.12	0.79
1:C:354:ILE:HD11	1:C:375:PRO:HD3	1.61	0.79
1:C:358:THR:O	1:C:359:HIS:CB	2.30	0.78
1:D:354:ILE:O	1:D:360:PHE:HZ	1.65	0.78
1:F:317:CYS:CB	1:F:401:LEU:CD2	2.45	0.78
1:D:321:LYS:HD3	3:M:310:TYR:N	1.97	0.78
1:E:146:LYS:O	1:E:150:ILE:HB	1.82	0.78
1:E:301:LEU:HD12	3:O:310:TYR:CG	2.18	0.78
1:A:321:LYS:HD2	3:S:309:ASN:O	1.81	0.78
1:E:201:ASP:OD1	1:F:250:ARG:NH1	2.14	0.78
1:B:354:ILE:CG1	1:B:375:PRO:CG	2.62	0.78
1:D:354:ILE:HA	1:D:375:PRO:HG2	1.65	0.78
1:E:358:THR:HG21	3:P:303:TYR:CE1	2.19	0.78
1:F:204:SER:O	1:F:207:MET:SD	2.41	0.78
1:B:321:LYS:HD3	3:I:309:ASN:O	1.82	0.78
1:C:396:LEU:HD23	1:D:158:LEU:HD21	1.65	0.78
3:P:289:ASP:O	3:P:290:ARG:HB3	1.84	0.78
3:S:289:ASP:O	3:S:290:ARG:HB3	1.84	0.78
1:A:246:SER:HA	1:A:250:ARG:HG2	1.64	0.78
1:C:354:ILE:CA	1:C:375:PRO:HG2	2.14	0.78
3:N:291:ALA:HA	3:N:294:ILE:HD11	1.66	0.77
1:B:354:ILE:HG12	1:B:360:PHE:CE2	2.18	0.77
1:D:354:ILE:CD1	1:D:398:GLU:HB3	2.14	0.77
3:O:291:ALA:HA	3:O:294:ILE:HD11	1.66	0.77
3:Q:291:ALA:HA	3:Q:294:ILE:HD11	1.66	0.77
3:J:291:ALA:HA	3:J:294:ILE:HD11	1.66	0.77
1:D:358:THR:O	1:D:359:HIS:CG	2.37	0.77
3:J:289:ASP:O	3:J:290:ARG:HB3	1.84	0.77
3:S:291:ALA:HA	3:S:294:ILE:HD11	1.66	0.77
1:B:358:THR:HG23	1:B:359:HIS:CD2	2.20	0.77
3:H:291:ALA:HA	3:H:294:ILE:HD11	1.66	0.77
3:L:291:ALA:HA	3:L:294:ILE:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:291:ALA:HA	3:P:294:ILE:HD11	1.66	0.77
1:C:361:LYS:CD	1:C:381:ASP:O	2.33	0.77
1:F:319:LEU:HD22	1:F:403:ILE:HB	1.65	0.77
3:L:289:ASP:O	3:L:290:ARG:HB3	1.84	0.77
3:Q:289:ASP:O	3:Q:290:ARG:HB3	1.84	0.77
1:B:358:THR:O	1:B:359:HIS:CB	2.32	0.76
1:E:361:LYS:CD	1:E:381:ASP:O	2.33	0.76
1:D:354:ILE:O	1:D:360:PHE:CZ	2.39	0.76
3:H:308:LEU:HD12	3:I:298:GLN:HG3	1.67	0.76
3:J:308:LEU:HD12	3:K:298:GLN:HG3	1.67	0.76
1:C:358:THR:O	1:C:359:HIS:HD2	1.67	0.76
3:O:289:ASP:O	3:O:290:ARG:HB3	1.84	0.76
1:B:361:LYS:CD	1:B:381:ASP:O	2.33	0.76
1:D:361:LYS:CD	1:D:381:ASP:O	2.33	0.76
3:H:289:ASP:O	3:H:290:ARG:HB3	1.84	0.75
3:N:289:ASP:O	3:N:290:ARG:HB3	1.84	0.75
1:D:354:ILE:HD11	1:D:398:GLU:CB	2.16	0.75
3:L:308:LEU:HD12	3:M:298:GLN:HG3	1.67	0.75
3:R:289:ASP:O	3:R:290:ARG:HB3	1.84	0.75
3:R:291:ALA:HA	3:R:294:ILE:HD11	1.66	0.75
1:D:346:ALA:O	1:D:401:LEU:HD13	1.86	0.75
1:D:389:THR:CG2	1:E:154:LYS:HZ2	1.94	0.75
1:F:323:ASP:CG	1:F:403:ILE:CD1	2.55	0.75
1:B:355:GLN:CD	1:B:388:TRP:CD2	2.57	0.75
1:A:358:THR:O	1:A:359:HIS:CB	2.34	0.75
1:C:354:ILE:HD11	1:C:375:PRO:CD	2.09	0.75
1:A:353:LYS:HD2	1:A:399:PRO:CG	2.16	0.75
1:A:358:THR:O	1:A:359:HIS:CG	2.39	0.75
1:A:361:LYS:CD	1:A:381:ASP:O	2.33	0.75
1:B:346:ALA:O	1:B:401:LEU:HD21	1.85	0.74
1:E:404:LYS:HE2	3:P:311:GLU:HG3	0.78	0.74
1:E:375:PRO:HB2	3:P:310:TYR:OH	1.86	0.74
1:F:361:LYS:CD	1:F:381:ASP:O	2.33	0.74
1:D:346:ALA:O	1:D:401:LEU:CD1	2.36	0.74
1:E:318:VAL:HG11	1:E:402:THR:CB	2.17	0.74
1:F:319:LEU:HD23	1:F:403:ILE:CB	2.14	0.74
1:D:389:THR:HG22	1:E:154:LYS:CE	2.16	0.74
1:B:354:ILE:CB	1:B:375:PRO:HG2	2.16	0.73
1:B:354:ILE:CG1	1:B:375:PRO:CD	2.58	0.73
1:A:305:THR:CG2	3:S:310:TYR:CZ	2.68	0.73
1:A:325:ARG:NH1	3:S:312:ASP:CG	2.25	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:GLU:O	1:E:151:LEU:HB3	1.88	0.73
1:A:250:ARG:HH11	1:F:204:SER:HB2	1.53	0.72
1:C:321:LYS:HG2	3:K:310:TYR:HD1	1.53	0.72
1:D:358:THR:O	1:D:359:HIS:CB	2.37	0.72
1:B:355:GLN:CB	1:B:388:TRP:HD1	2.00	0.72
1:F:323:ASP:OD1	1:F:403:ILE:HD13	1.89	0.72
1:C:318:VAL:HB	1:C:401:LEU:O	1.90	0.72
1:D:394:ASP:O	1:D:396:LEU:N	2.24	0.71
1:C:394:ASP:O	1:C:396:LEU:N	2.24	0.71
1:D:389:THR:HA	1:E:154:LYS:NZ	2.05	0.71
1:E:408:LYS:NZ	3:Q:295:GLU:HB2	2.06	0.71
1:F:394:ASP:O	1:F:396:LEU:N	2.24	0.71
1:C:321:LYS:HD3	3:K:309:ASN:O	1.90	0.71
1:E:394:ASP:O	1:E:396:LEU:N	2.24	0.71
1:F:360:PHE:CD1	1:F:391:ILE:CD1	2.71	0.71
1:D:358:THR:HG23	1:D:359:HIS:CD2	2.25	0.71
1:A:305:THR:CB	3:S:310:TYR:OH	2.39	0.71
1:B:355:GLN:OE1	1:B:388:TRP:NE1	2.24	0.71
1:B:354:ILE:HD11	1:B:396:LEU:CD1	2.12	0.70
1:D:358:THR:OG1	1:D:385:GLU:CG	2.37	0.70
1:E:318:VAL:CG1	1:E:401:LEU:O	2.39	0.70
1:F:355:GLN:O	1:F:388:TRP:NE1	2.24	0.70
1:F:373:LEU:CD1	1:F:391:ILE:CD1	2.69	0.70
1:B:398:GLU:N	1:B:398:GLU:OE1	2.21	0.70
1:D:402:THR:O	1:D:405:ASP:HB2	1.90	0.70
1:E:403:ILE:O	1:E:406:PHE:N	2.24	0.70
1:F:360:PHE:CE2	1:F:391:ILE:HD12	2.26	0.70
1:A:388:TRP:CH2	1:B:154:LYS:NZ	2.59	0.70
1:D:354:ILE:HG23	1:D:396:LEU:HD11	1.72	0.70
1:F:346:ALA:CB	1:F:406:PHE:CD2	2.74	0.70
1:F:349:GLN:OE1	1:F:352:ARG:HD2	1.92	0.70
1:B:354:ILE:HG13	1:B:375:PRO:HG3	1.69	0.70
1:C:318:VAL:CG1	1:C:402:THR:HA	2.22	0.70
1:A:251:ARG:HH12	1:F:206:TRP:HA	1.57	0.70
1:A:250:ARG:HH12	1:F:204:SER:HB3	1.55	0.70
1:A:305:THR:CG2	3:S:310:TYR:OH	2.39	0.69
1:B:354:ILE:CG1	1:B:375:PRO:HG3	2.19	0.69
1:F:346:ALA:HB3	1:F:406:PHE:CE2	2.27	0.69
1:B:352:ARG:O	1:B:356:SER:HB2	1.92	0.69
1:F:317:CYS:HA	1:F:401:LEU:HB3	1.72	0.69
1:A:325:ARG:NH2	3:S:312:ASP:OD2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:LEU:CD1	1:E:391:ILE:HD13	2.20	0.69
1:A:373:LEU:CD1	1:A:391:ILE:HD13	2.20	0.69
1:A:373:LEU:CD1	1:A:391:ILE:CD1	2.69	0.69
1:B:354:ILE:N	1:B:375:PRO:HG2	2.07	0.69
1:A:394:ASP:O	1:A:396:LEU:N	2.24	0.69
1:B:373:LEU:CD1	1:B:391:ILE:CD1	2.69	0.69
1:E:373:LEU:CD1	1:E:391:ILE:CD1	2.69	0.69
1:B:355:GLN:CG	1:B:388:TRP:HB3	2.15	0.68
1:B:398:GLU:HB2	1:B:399:PRO:HD2	1.74	0.68
1:B:346:ALA:O	1:B:401:LEU:HD22	1.93	0.68
1:A:254:THR:CG2	1:F:205:LYS:CG	2.59	0.68
1:C:350:PRO:HB3	1:C:399:PRO:HD2	1.74	0.68
1:D:373:LEU:CD1	1:D:391:ILE:CD1	2.69	0.68
1:F:323:ASP:HA	1:F:403:ILE:HD12	1.74	0.68
1:D:373:LEU:CD1	1:D:391:ILE:HD13	2.20	0.68
1:F:263:VAL:HG12	1:F:267:SER:CB	2.23	0.68
1:B:394:ASP:O	1:B:396:LEU:N	2.24	0.68
1:F:373:LEU:CD1	1:F:391:ILE:HD13	2.20	0.68
1:B:354:ILE:CD1	1:B:396:LEU:HD12	2.11	0.68
3:R:290:ARG:H	3:R:293:LYS:HG2	1.58	0.68
1:B:358:THR:O	1:B:359:HIS:HD2	1.70	0.67
1:A:155:PHE:HE2	1:F:388:TRP:CZ3	2.12	0.67
1:A:251:ARG:NH1	1:F:206:TRP:HA	2.09	0.67
1:A:322:GLU:OE2	3:S:311:GLU:HB2	1.94	0.67
1:A:250:ARG:CD	1:F:204:SER:HB2	2.22	0.67
3:J:308:LEU:HD12	3:K:298:GLN:CG	2.25	0.67
1:E:318:VAL:HG12	1:E:402:THR:HA	1.66	0.67
1:B:373:LEU:CD1	1:B:391:ILE:HD13	2.20	0.67
1:F:263:VAL:HG12	1:F:267:SER:HB2	1.77	0.67
1:C:374:THR:HB	1:C:397:LYS:HB3	1.76	0.67
1:F:253:LYS:CE	1:F:283:ASP:OD2	2.34	0.67
3:J:308:LEU:HD13	3:K:294:ILE:HG23	1.77	0.66
1:D:389:THR:HG23	1:E:154:LYS:HZ2	1.52	0.66
1:B:355:GLN:NE2	1:B:388:TRP:CE3	2.62	0.66
1:F:360:PHE:CD2	1:F:391:ILE:HD12	2.30	0.66
3:N:291:ALA:HA	3:N:294:ILE:CD1	2.26	0.66
3:R:291:ALA:HA	3:R:294:ILE:CD1	2.26	0.66
3:S:291:ALA:HA	3:S:294:ILE:CD1	2.26	0.66
1:A:358:THR:O	1:A:359:HIS:HB2	1.95	0.66
3:H:291:ALA:HA	3:H:294:ILE:CD1	2.26	0.66
3:H:308:LEU:HD13	3:I:294:ILE:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:LEU:CD1	1:C:391:ILE:CD1	2.69	0.66
3:Q:291:ALA:HA	3:Q:294:ILE:CD1	2.26	0.66
1:D:389:THR:N	1:E:154:LYS:HZ3	1.94	0.66
1:E:393:ALA:CB	1:F:157:HIS:CE1	2.69	0.66
1:F:323:ASP:OD1	1:F:403:ILE:CD1	2.44	0.66
3:H:308:LEU:HD12	3:I:298:GLN:CG	2.25	0.66
1:B:355:GLN:CG	1:B:388:TRP:CB	2.64	0.65
3:L:308:LEU:HD13	3:M:294:ILE:HG23	1.77	0.65
3:O:291:ALA:HA	3:O:294:ILE:CD1	2.26	0.65
3:P:291:ALA:HA	3:P:294:ILE:CD1	2.26	0.65
1:B:203:VAL:O	1:C:212:LYS:NZ	2.30	0.65
1:F:405:ASP:O	1:F:408:LYS:HB3	1.97	0.65
3:L:291:ALA:HA	3:L:294:ILE:CD1	2.26	0.65
3:L:308:LEU:HD12	3:M:298:GLN:CG	2.25	0.65
1:E:359:HIS:CE1	1:E:385:GLU:HB2	2.31	0.65
3:J:291:ALA:HA	3:J:294:ILE:CD1	2.26	0.65
1:F:317:CYS:CB	1:F:401:LEU:HB3	2.25	0.65
1:B:388:TRP:HH2	1:C:154:LYS:HD3	1.60	0.65
1:D:359:HIS:CE1	1:D:385:GLU:HB2	2.31	0.65
1:B:359:HIS:CE1	1:B:385:GLU:HB2	2.31	0.65
1:A:359:HIS:CE1	1:A:385:GLU:HB2	2.31	0.65
1:C:354:ILE:O	1:C:360:PHE:CZ	2.50	0.65
1:C:359:HIS:CE1	1:C:385:GLU:HB2	2.31	0.65
1:F:253:LYS:HE3	1:F:283:ASP:CG	2.16	0.65
1:C:373:LEU:CD1	1:C:391:ILE:HD13	2.20	0.64
1:E:179:LYS:NZ	1:E:276:THR:O	2.29	0.64
1:A:346:ALA:O	1:A:401:LEU:CD2	2.45	0.64
1:B:355:GLN:CD	1:B:388:TRP:NE1	2.50	0.64
1:A:358:THR:HG21	3:H:303:TYR:CE1	2.32	0.64
1:D:377:SER:OG	3:N:307:ALA:CA	2.41	0.64
1:F:323:ASP:HA	1:F:403:ILE:CD1	2.28	0.64
1:B:357:ALA:HB2	3:J:306:SER:HB2	1.79	0.64
1:A:346:ALA:O	1:A:401:LEU:HD21	1.98	0.64
1:C:354:ILE:CA	1:C:375:PRO:HG3	2.08	0.63
1:B:355:GLN:CD	1:B:388:TRP:CE2	2.72	0.63
1:B:347:LEU:CD2	1:B:401:LEU:HD11	2.29	0.63
1:D:321:LYS:CD	3:M:309:ASN:O	2.46	0.63
1:B:355:GLN:OE1	1:B:388:TRP:CD1	2.51	0.62
1:F:354:ILE:HG23	1:F:396:LEU:CD2	2.13	0.62
1:E:388:TRP:HZ3	1:F:151:LEU:HD13	1.64	0.62
1:F:167:SER:OG	1:F:263:VAL:HG21	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:169:ILE:HB	1:F:273:LEU:HD23	1.80	0.62
1:A:318:VAL:HG11	1:A:402:THR:HA	1.81	0.62
1:B:354:ILE:CG1	1:B:360:PHE:HE2	2.07	0.62
1:F:353:LYS:O	1:F:357:ALA:HB2	2.00	0.62
1:A:388:TRP:CE3	1:B:155:PHE:CZ	2.85	0.62
1:C:389:THR:HG22	1:D:154:LYS:NZ	2.14	0.62
1:A:251:ARG:HA	1:F:205:LYS:HD2	1.80	0.62
1:C:378:PRO:HG2	3:L:303:TYR:HB3	1.82	0.62
1:D:321:LYS:HG2	3:M:310:TYR:CA	2.23	0.62
1:D:358:THR:O	1:D:359:HIS:HB2	2.00	0.61
1:F:357:ALA:CB	1:F:375:PRO:HG3	2.26	0.61
1:B:259:GLN:O	1:B:265:ASN:ND2	2.33	0.61
1:D:259:GLN:O	1:D:265:ASN:ND2	2.33	0.61
1:E:304:ARG:HH12	1:E:332:GLU:HA	1.65	0.61
1:E:318:VAL:CG1	1:E:402:THR:CA	2.44	0.61
1:A:426:GLU:O	1:A:430:ARG:HB2	2.01	0.61
1:D:403:ILE:O	1:D:406:PHE:N	2.32	0.61
1:E:256:LEU:O	1:E:260:MET:HB2	2.00	0.61
1:A:305:THR:HG21	3:S:310:TYR:OH	2.00	0.61
1:B:256:LEU:O	1:B:260:MET:HB2	2.00	0.61
1:F:323:ASP:CA	1:F:403:ILE:CD1	2.74	0.61
1:A:350:PRO:HB3	1:A:399:PRO:HD2	1.81	0.61
1:C:426:GLU:O	1:C:430:ARG:HB2	2.01	0.61
1:C:304:ARG:HH12	1:C:332:GLU:HA	1.66	0.60
1:D:304:ARG:HH12	1:D:332:GLU:HA	1.65	0.60
1:D:357:ALA:HB1	3:N:306:SER:HB2	1.83	0.60
1:E:318:VAL:HG11	1:E:402:THR:CG2	2.30	0.60
1:D:256:LEU:O	1:D:260:MET:HB2	2.00	0.60
1:E:259:GLN:O	1:E:265:ASN:ND2	2.33	0.60
1:F:319:LEU:HD23	1:F:403:ILE:CA	2.30	0.60
1:A:377:SER:OG	3:H:307:ALA:CA	2.46	0.60
1:C:259:GLN:O	1:C:265:ASN:ND2	2.33	0.60
1:A:357:ALA:HB2	3:H:306:SER:HB2	1.83	0.60
3:J:290:ARG:O	3:J:294:ILE:HG12	2.02	0.60
1:A:136:ALA:H	4:A:501:ADP:HN62	1.49	0.60
1:A:304:ARG:HH12	1:A:332:GLU:HA	1.65	0.60
1:C:256:LEU:O	1:C:260:MET:HB2	2.00	0.60
1:F:317:CYS:HB2	1:F:401:LEU:CG	2.30	0.60
1:E:378:PRO:HG2	3:P:303:TYR:HB3	1.82	0.60
1:D:398:GLU:OE1	1:E:163:ARG:NH1	2.28	0.60
1:D:426:GLU:O	1:D:430:ARG:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:290:ARG:O	3:H:294:ILE:HG12	2.02	0.60
3:R:290:ARG:O	3:R:294:ILE:HG12	2.02	0.60
1:E:358:THR:OG1	1:E:385:GLU:HG3	2.01	0.60
3:S:290:ARG:O	3:S:294:ILE:HG12	2.02	0.60
1:A:246:SER:OG	1:A:250:ARG:CZ	2.49	0.60
3:L:290:ARG:O	3:L:294:ILE:HG12	2.02	0.60
3:Q:290:ARG:O	3:Q:294:ILE:HG12	2.02	0.59
1:B:304:ARG:HH12	1:B:332:GLU:HA	1.65	0.59
1:B:426:GLU:O	1:B:430:ARG:HB2	2.01	0.59
1:E:426:GLU:O	1:E:430:ARG:HB2	2.01	0.59
1:F:317:CYS:CA	1:F:401:LEU:HB3	2.32	0.59
1:D:346:ALA:HB1	1:D:401:LEU:HD11	1.83	0.59
3:N:290:ARG:O	3:N:294:ILE:HG12	2.02	0.59
3:P:290:ARG:O	3:P:294:ILE:HG12	2.02	0.59
1:B:347:LEU:HD23	1:B:401:LEU:HD11	1.85	0.59
1:F:418:ASN:OD1	1:F:419:GLU:N	2.35	0.59
3:O:290:ARG:O	3:O:294:ILE:HG12	2.02	0.59
1:A:246:SER:HA	1:A:250:ARG:CG	2.30	0.59
1:E:358:THR:O	1:E:359:HIS:HB2	2.02	0.59
1:F:360:PHE:CZ	1:F:388:TRP:HA	2.38	0.59
1:C:354:ILE:HD13	1:C:375:PRO:HG3	1.66	0.58
1:F:360:PHE:CB	1:F:391:ILE:HD11	2.29	0.58
1:F:346:ALA:HB3	1:F:406:PHE:CD2	2.37	0.58
1:F:404:LYS:HA	1:F:407:LEU:HD12	1.85	0.58
1:C:355:GLN:HG2	1:C:388:TRP:CE3	2.38	0.58
1:F:360:PHE:CZ	1:F:391:ILE:HD12	2.39	0.58
1:C:321:LYS:HG2	3:K:310:TYR:CD1	2.36	0.58
1:A:155:PHE:CE2	1:F:388:TRP:CZ3	2.91	0.58
1:C:394:ASP:C	1:C:396:LEU:H	2.07	0.58
1:D:388:TRP:HE3	1:E:155:PHE:CE2	2.12	0.58
1:E:388:TRP:CZ2	1:F:147:GLU:HB3	2.39	0.58
1:E:350:PRO:CG	1:E:401:LEU:HD13	2.32	0.58
3:H:298:GLN:HG3	3:I:308:LEU:HD12	1.86	0.58
1:C:358:THR:HG21	3:L:303:TYR:CZ	2.37	0.58
3:N:298:GLN:HG3	3:O:308:LEU:HD12	1.86	0.58
1:D:136:ALA:H	4:D:501:ADP:HN62	1.50	0.57
1:E:408:LYS:HZ2	3:Q:295:GLU:HB2	1.67	0.57
1:B:350:PRO:HB2	1:B:398:GLU:CG	2.34	0.57
1:F:308:PHE:O	1:F:312:VAL:HG13	2.04	0.57
3:H:300:LEU:HD12	3:H:323:ALA:CA	2.34	0.57
3:J:298:GLN:HG3	3:K:308:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:300:LEU:HD12	3:L:323:ALA:CA	2.34	0.57
1:D:255:GLU:O	1:D:259:GLN:HB3	2.04	0.57
1:E:224:ASN:O	1:E:227:SER:OG	2.23	0.57
1:B:357:ALA:CB	3:J:306:SER:HB2	2.35	0.57
3:N:300:LEU:HD12	3:N:323:ALA:CA	2.34	0.57
1:D:358:THR:CG2	3:N:303:TYR:CE1	2.81	0.57
1:E:255:GLU:O	1:E:259:GLN:HB3	2.04	0.57
1:E:394:ASP:C	1:E:396:LEU:H	2.07	0.57
3:P:300:LEU:HD12	3:P:323:ALA:CA	2.35	0.57
1:B:354:ILE:CB	1:B:375:PRO:HG3	2.26	0.57
1:C:255:GLU:O	1:C:259:GLN:HB3	2.04	0.57
3:Q:300:LEU:HD12	3:Q:323:ALA:CA	2.34	0.57
3:R:298:GLN:HG3	3:S:308:LEU:HD12	1.86	0.57
1:A:128:PRO:O	1:A:188:THR:OG1	2.23	0.57
1:F:204:SER:O	1:F:207:MET:HG3	2.03	0.57
1:D:389:THR:HA	1:E:154:LYS:CE	2.34	0.57
1:E:122:ALA:O	1:F:250:ARG:NH2	2.37	0.57
3:R:300:LEU:HD12	3:R:323:ALA:CA	2.35	0.57
3:S:300:LEU:HD12	3:S:323:ALA:CA	2.34	0.57
1:D:373:LEU:HD11	1:D:391:ILE:HG12	1.87	0.57
1:E:318:VAL:HG11	1:E:402:THR:HG23	1.87	0.57
1:F:373:LEU:HD11	1:F:391:ILE:HG12	1.87	0.57
3:P:308:LEU:HD12	3:Q:298:GLN:HG3	1.86	0.57
1:A:254:THR:HG21	1:F:205:LYS:CE	2.22	0.57
1:B:355:GLN:NE2	1:B:388:TRP:CE2	2.69	0.57
3:J:300:LEU:HD12	3:J:323:ALA:CA	2.34	0.57
3:P:298:GLN:HG3	3:Q:308:LEU:HD12	1.86	0.57
1:D:354:ILE:CA	1:D:375:PRO:HG2	2.33	0.57
1:E:373:LEU:HD12	1:E:391:ILE:HD11	1.84	0.57
1:B:255:GLU:O	1:B:259:GLN:HB3	2.04	0.56
1:F:394:ASP:C	1:F:396:LEU:H	2.07	0.56
1:A:373:LEU:HD12	1:A:391:ILE:HD11	1.84	0.56
1:E:373:LEU:HD11	1:E:391:ILE:HG12	1.87	0.56
1:A:357:ALA:CB	3:H:306:SER:HB2	2.35	0.56
3:O:300:LEU:HD12	3:O:323:ALA:CA	2.34	0.56
3:N:308:LEU:HD12	3:O:298:GLN:HG3	1.86	0.56
1:E:358:THR:HG23	1:E:359:HIS:CD2	2.40	0.56
1:F:317:CYS:CB	1:F:401:LEU:CG	2.82	0.56
3:L:298:GLN:HG3	3:M:308:LEU:HD12	1.86	0.56
1:B:398:GLU:CD	1:B:398:GLU:H	2.08	0.56
1:E:408:LYS:HE3	3:Q:295:GLU:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:360:PHE:CD1	1:F:386:MET:HG3	2.23	0.56
1:B:358:THR:O	1:B:359:HIS:HB2	2.06	0.56
1:D:304:ARG:NH1	1:D:331:THR:O	2.39	0.56
1:F:204:SER:O	1:F:207:MET:CG	2.53	0.56
3:R:308:LEU:HD12	3:S:298:GLN:HG3	1.86	0.56
1:A:394:ASP:C	1:A:396:LEU:H	2.07	0.56
1:A:341:VAL:HG11	1:B:291:GLU:HB2	1.88	0.56
1:C:304:ARG:NH1	1:C:331:THR:O	2.39	0.56
1:C:321:LYS:HD3	3:K:310:TYR:CD1	2.40	0.56
1:B:353:LYS:O	1:B:375:PRO:HB3	2.06	0.56
1:A:304:ARG:NH1	1:A:331:THR:O	2.39	0.55
1:B:373:LEU:HD11	1:B:391:ILE:HG12	1.87	0.55
1:B:304:ARG:NH1	1:B:331:THR:O	2.39	0.55
1:B:354:ILE:CD1	1:B:375:PRO:HD3	2.35	0.55
1:C:373:LEU:HD12	1:C:391:ILE:HD11	1.84	0.55
1:C:373:LEU:HD11	1:C:391:ILE:HG12	1.87	0.55
1:A:250:ARG:NH1	1:F:204:SER:HB2	2.11	0.55
1:F:349:GLN:OE1	1:F:352:ARG:NH1	2.39	0.55
1:A:373:LEU:HD11	1:A:391:ILE:HG12	1.87	0.55
1:E:304:ARG:NH1	1:E:331:THR:O	2.39	0.55
3:J:290:ARG:HG3	3:J:291:ALA:N	2.22	0.55
1:D:373:LEU:HD12	1:D:391:ILE:HD11	1.84	0.55
1:E:319:LEU:HD11	1:E:403:ILE:HB	1.88	0.55
3:S:290:ARG:HG3	3:S:291:ALA:N	2.22	0.55
1:A:358:THR:OG1	1:A:385:GLU:CG	2.55	0.55
3:N:290:ARG:HG3	3:N:291:ALA:N	2.22	0.55
1:D:287:ARG:O	1:D:293:ARG:NH2	2.38	0.54
1:C:358:THR:C	1:C:359:HIS:CG	2.80	0.54
1:B:287:ARG:O	1:B:293:ARG:NH2	2.38	0.54
1:D:357:ALA:CB	3:N:306:SER:HB2	2.37	0.54
1:F:304:ARG:NH1	1:F:328:GLY:O	2.40	0.54
3:L:290:ARG:HG3	3:L:291:ALA:N	2.22	0.54
1:D:353:LYS:O	1:D:375:PRO:CB	2.55	0.54
1:D:353:LYS:O	1:D:375:PRO:CG	2.56	0.54
1:F:360:PHE:HB3	1:F:373:LEU:HB2	1.90	0.54
1:F:354:ILE:HG23	1:F:396:LEU:CG	2.37	0.54
1:A:210:SER:HB2	1:A:252:ILE:HD11	1.89	0.54
1:D:249:SER:O	1:D:253:LYS:CB	2.55	0.54
1:D:394:ASP:C	1:D:396:LEU:H	2.07	0.54
3:H:290:ARG:HG3	3:H:291:ALA:N	2.22	0.54
1:F:253:LYS:NZ	1:F:283:ASP:OD1	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLU:HG3	3:S:310:TYR:O	1.97	0.54
1:A:174:PRO:HG3	1:A:425:GLN:HG3	1.90	0.53
3:R:290:ARG:HG3	3:R:291:ALA:N	2.22	0.53
1:A:240:THR:CB	1:A:250:ARG:HH21	2.21	0.53
1:F:323:ASP:HB3	1:F:403:ILE:CG1	2.39	0.53
3:O:290:ARG:HG3	3:O:291:ALA:N	2.22	0.53
1:E:388:TRP:CH2	1:F:147:GLU:HB3	2.43	0.53
1:F:342:VAL:HG12	1:F:413:THR:HB	1.91	0.53
3:Q:290:ARG:HG3	3:Q:291:ALA:N	2.22	0.53
1:B:354:ILE:CG1	1:B:360:PHE:CE2	2.87	0.53
1:E:393:ALA:HB1	1:F:157:HIS:NE2	2.18	0.53
1:E:336:GLY:HA3	4:E:501:ADP:C8	2.43	0.53
1:B:394:ASP:C	1:B:396:LEU:H	2.09	0.53
1:D:222:ARG:HD2	1:D:266:ASP:HB2	1.91	0.53
3:P:290:ARG:HG3	3:P:291:ALA:N	2.22	0.53
1:A:254:THR:CG2	1:F:205:LYS:HG2	2.13	0.53
1:B:321:LYS:HG3	3:I:310:TYR:CE1	2.44	0.53
3:O:310:TYR:O	3:O:310:TYR:CD2	2.62	0.53
1:D:393:ALA:O	1:D:394:ASP:OD1	2.27	0.53
1:B:393:ALA:O	1:B:394:ASP:OD1	2.27	0.53
1:C:318:VAL:CG1	1:C:401:LEU:O	2.56	0.53
1:D:353:LYS:C	1:D:375:PRO:HG2	2.30	0.53
1:F:317:CYS:HB2	1:F:401:LEU:HG	1.91	0.53
1:C:249:SER:O	1:C:253:LYS:CB	2.55	0.53
1:E:207:MET:HG2	1:E:207:MET:O	2.09	0.53
1:B:426:GLU:O	1:B:430:ARG:CB	2.57	0.52
1:F:357:ALA:HB1	1:F:375:PRO:CG	2.30	0.52
3:P:330:ILE:HG22	3:P:330:ILE:OXT	2.10	0.52
1:D:426:GLU:O	1:D:430:ARG:CB	2.57	0.52
1:A:426:GLU:O	1:A:430:ARG:CB	2.57	0.52
1:C:426:GLU:O	1:C:430:ARG:CB	2.57	0.52
1:E:249:SER:O	1:E:253:LYS:CB	2.55	0.52
1:E:426:GLU:O	1:E:430:ARG:CB	2.57	0.52
1:D:388:TRP:CZ3	1:E:155:PHE:CE2	2.97	0.52
3:M:330:ILE:HG22	3:M:330:ILE:OXT	2.10	0.52
3:S:330:ILE:HG22	3:S:330:ILE:OXT	2.10	0.52
1:A:287:ARG:O	1:A:293:ARG:NH2	2.38	0.52
1:E:393:ALA:O	1:E:394:ASP:OD1	2.27	0.52
3:H:330:ILE:HG22	3:H:330:ILE:OXT	2.09	0.52
1:A:349:GLN:OE1	1:A:352:ARG:NH1	2.43	0.52
1:D:389:THR:N	1:E:154:LYS:NZ	2.54	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ARG:NE	1:F:205:LYS:O	2.42	0.52
3:I:330:ILE:HG22	3:I:330:ILE:OXT	2.10	0.52
3:K:325:ASP:HA	3:K:328:ASN:HD22	1.75	0.52
3:L:325:ASP:HA	3:L:328:ASN:HD22	1.75	0.52
3:P:325:ASP:HA	3:P:328:ASN:HD22	1.75	0.52
1:C:354:ILE:N	1:C:375:PRO:HG2	2.25	0.52
1:C:358:THR:O	1:C:359:HIS:HB2	2.08	0.52
1:D:403:ILE:HG23	1:D:404:LYS:N	2.25	0.52
1:F:339:ILE:HA	1:F:342:VAL:HG22	1.91	0.52
3:L:330:ILE:HG22	3:L:330:ILE:OXT	2.10	0.52
1:B:358:THR:C	1:B:359:HIS:CG	2.82	0.52
1:C:355:GLN:HG2	1:C:388:TRP:CE2	2.45	0.52
1:F:354:ILE:CG2	1:F:396:LEU:CG	2.86	0.52
1:A:246:SER:CA	1:A:250:ARG:HG2	2.37	0.51
1:C:393:ALA:O	1:C:394:ASP:OD1	2.27	0.51
1:D:181:TYR:HB2	4:D:501:ADP:H5'2	1.92	0.51
3:M:325:ASP:HA	3:M:328:ASN:HD22	1.75	0.51
3:O:330:ILE:OXT	3:O:330:ILE:HG22	2.10	0.51
1:B:249:SER:O	1:B:253:LYS:CB	2.55	0.51
1:C:354:ILE:O	1:C:360:PHE:HZ	1.93	0.51
3:K:330:ILE:OXT	3:K:330:ILE:HG22	2.10	0.51
3:J:330:ILE:OXT	3:J:330:ILE:HG22	2.10	0.51
1:A:179:LYS:NZ	1:A:276:THR:O	2.39	0.51
1:A:393:ALA:O	1:A:394:ASP:OD1	2.27	0.51
1:C:288:ARG:NH2	5:C:501:BEF:F3	2.33	0.51
1:F:377:SER:OG	3:R:307:ALA:HA	2.10	0.51
3:R:330:ILE:OXT	3:R:330:ILE:HG22	2.10	0.51
3:O:325:ASP:HA	3:O:328:ASN:HD22	1.75	0.51
3:Q:325:ASP:HA	3:Q:328:ASN:HD22	1.75	0.51
1:E:238:THR:HG21	1:E:282:LEU:HA	1.91	0.51
3:J:325:ASP:HA	3:J:328:ASN:HD22	1.75	0.51
1:F:378:PRO:HD2	3:R:307:ALA:HB2	1.92	0.51
1:C:354:ILE:HG21	1:C:396:LEU:HD11	1.92	0.51
1:F:393:ALA:O	1:F:394:ASP:OD1	2.27	0.51
3:H:325:ASP:HA	3:H:328:ASN:HD22	1.75	0.51
3:N:330:ILE:HG22	3:N:330:ILE:OXT	2.10	0.51
3:R:325:ASP:HA	3:R:328:ASN:HD22	1.75	0.51
3:S:325:ASP:HA	3:S:328:ASN:HD22	1.75	0.51
1:E:318:VAL:CG1	1:E:402:THR:HG23	2.41	0.51
3:I:325:ASP:HA	3:I:328:ASN:HD22	1.75	0.51
1:E:350:PRO:HG2	1:E:401:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:373:LEU:HD12	1:F:391:ILE:HD11	1.84	0.50
3:H:289:ASP:HA	3:H:292:SER:OG	2.12	0.50
3:N:289:ASP:HA	3:N:292:SER:OG	2.12	0.50
3:O:293:LYS:HZ2	3:O:330:ILE:HD13	1.76	0.50
1:E:403:ILE:O	1:E:404:LYS:C	2.48	0.50
3:J:289:ASP:HA	3:J:292:SER:OG	2.12	0.50
1:D:378:PRO:HG2	3:N:303:TYR:O	2.11	0.50
3:P:293:LYS:HZ2	3:P:330:ILE:HD13	1.76	0.50
1:A:155:PHE:CE2	1:F:388:TRP:HZ3	2.30	0.50
3:O:289:ASP:HA	3:O:292:SER:OG	2.12	0.50
3:S:289:ASP:HA	3:S:292:SER:OG	2.12	0.50
1:C:311:ASN:HB3	1:C:343:VAL:HG11	1.94	0.50
1:E:301:LEU:HD13	3:O:310:TYR:CZ	2.41	0.50
3:P:289:ASP:HA	3:P:292:SER:OG	2.12	0.50
3:Q:289:ASP:HA	3:Q:292:SER:OG	2.12	0.50
3:H:293:LYS:HZ2	3:H:330:ILE:HD13	1.77	0.50
1:A:311:ASN:HB3	1:A:343:VAL:HG11	1.94	0.50
1:E:357:ALA:HB1	3:P:306:SER:OG	2.12	0.50
1:F:350:PRO:O	1:F:354:ILE:HG13	2.11	0.50
3:Q:330:ILE:OXT	3:Q:330:ILE:HG22	2.10	0.50
3:R:289:ASP:HA	3:R:292:SER:OG	2.12	0.50
1:C:393:ALA:O	1:C:394:ASP:CG	2.50	0.50
1:E:147:GLU:O	1:E:151:LEU:CB	2.58	0.50
1:E:311:ASN:HB3	1:E:343:VAL:HG11	1.94	0.50
1:F:393:ALA:O	1:F:394:ASP:CG	2.50	0.50
3:N:325:ASP:HA	3:N:328:ASN:HD22	1.75	0.50
1:D:392:GLU:HB2	1:D:395:GLU:CD	2.33	0.49
1:F:404:LYS:O	1:F:407:LEU:HB2	2.12	0.49
1:A:392:GLU:HB2	1:A:395:GLU:CD	2.33	0.49
1:B:311:ASN:HB3	1:B:343:VAL:HG11	1.94	0.49
1:E:375:PRO:CB	3:P:310:TYR:OH	2.58	0.49
1:A:388:TRP:CH2	1:B:155:PHE:CE2	2.76	0.49
1:C:392:GLU:HB2	1:C:395:GLU:CD	2.33	0.49
1:D:302:ALA:HA	3:M:310:TYR:CE2	2.48	0.49
1:E:393:ALA:O	1:E:394:ASP:CG	2.50	0.49
3:L:289:ASP:HA	3:L:292:SER:OG	2.11	0.49
1:A:155:PHE:HE2	1:F:388:TRP:HZ3	1.60	0.49
1:B:355:GLN:OE1	1:B:388:TRP:CE2	2.66	0.49
1:A:393:ALA:O	1:A:394:ASP:CG	2.50	0.49
1:B:377:SER:OG	3:J:307:ALA:CA	2.55	0.49
1:C:218:PHE:HD2	1:C:259:GLN:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:GLU:HB2	1:E:395:GLU:CD	2.33	0.49
1:F:392:GLU:HB2	1:F:395:GLU:CD	2.33	0.49
3:J:313:LEU:N	3:J:314:PRO:CD	2.76	0.49
1:C:354:ILE:CD1	1:C:375:PRO:HG3	2.33	0.49
1:B:373:LEU:HD12	1:B:391:ILE:HD11	1.84	0.49
1:D:250:ARG:O	1:D:254:THR:OG1	2.28	0.49
1:F:360:PHE:HE1	1:F:387:SER:C	2.16	0.49
1:B:321:LYS:CD	3:I:310:TYR:HA	2.39	0.49
3:O:327:LEU:O	3:O:327:LEU:HD12	2.13	0.49
3:P:327:LEU:O	3:P:327:LEU:HD12	2.13	0.49
3:R:313:LEU:N	3:R:314:PRO:CD	2.76	0.49
3:S:327:LEU:HD12	3:S:327:LEU:O	2.13	0.49
1:C:318:VAL:CB	1:C:401:LEU:O	2.60	0.49
1:E:357:ALA:CB	3:P:306:SER:CB	2.80	0.49
3:L:313:LEU:N	3:L:314:PRO:CD	2.76	0.49
3:M:313:LEU:N	3:M:314:PRO:CD	2.76	0.49
3:M:327:LEU:O	3:M:327:LEU:HD12	2.13	0.49
1:D:393:ALA:O	1:D:394:ASP:CG	2.50	0.48
1:A:254:THR:HG21	1:F:205:LYS:HE2	1.81	0.48
1:F:203:VAL:HG21	1:F:236:ALA:O	2.13	0.48
1:A:246:SER:HB3	1:A:250:ARG:HG3	1.93	0.48
1:A:246:SER:CA	1:A:250:ARG:CG	2.92	0.48
1:A:318:VAL:CG1	1:A:401:LEU:O	2.61	0.48
1:D:311:ASN:HB3	1:D:343:VAL:HG11	1.94	0.48
1:E:287:ARG:O	1:E:293:ARG:NH2	2.38	0.48
3:H:327:LEU:O	3:H:327:LEU:HD12	2.13	0.48
3:I:313:LEU:N	3:I:314:PRO:CD	2.76	0.48
3:O:313:LEU:N	3:O:314:PRO:CD	2.76	0.48
1:A:388:TRP:CE3	1:B:155:PHE:HZ	2.26	0.48
1:B:392:GLU:HB2	1:B:395:GLU:CD	2.33	0.48
1:D:250:ARG:O	1:D:254:THR:CB	2.62	0.48
3:J:327:LEU:O	3:J:327:LEU:HD12	2.13	0.48
3:N:327:LEU:HD12	3:N:327:LEU:O	2.13	0.48
3:Q:293:LYS:HZ2	3:Q:330:ILE:HD13	1.78	0.48
1:B:393:ALA:O	1:B:394:ASP:CG	2.50	0.48
1:C:202:LEU:HD22	1:C:214:VAL:HG22	1.95	0.48
1:E:250:ARG:O	1:E:254:THR:CB	2.62	0.48
3:L:327:LEU:HD12	3:L:327:LEU:O	2.13	0.48
1:C:287:ARG:O	1:C:293:ARG:NH2	2.38	0.48
1:A:202:LEU:HD22	1:A:214:VAL:HG22	1.95	0.48
1:C:250:ARG:O	1:C:254:THR:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:257:LEU:HD23	1:F:289:ARG:HG3	1.95	0.48
3:H:313:LEU:N	3:H:314:PRO:CD	2.76	0.48
1:E:357:ALA:HB2	3:P:306:SER:HB2	1.94	0.48
3:Q:313:LEU:N	3:Q:314:PRO:CD	2.76	0.48
1:F:253:LYS:HZ1	1:F:283:ASP:CG	2.16	0.48
1:D:179:LYS:NZ	1:D:276:THR:O	2.44	0.48
3:I:327:LEU:HD12	3:I:327:LEU:O	2.13	0.48
3:K:327:LEU:O	3:K:327:LEU:HD12	2.13	0.48
3:N:296:GLN:HE21	3:N:300:LEU:HG	1.79	0.48
3:N:313:LEU:N	3:N:314:PRO:CD	2.76	0.48
1:A:395:GLU:O	1:A:395:GLU:HG3	2.14	0.48
1:B:202:LEU:HD22	1:B:214:VAL:HG22	1.95	0.48
3:O:296:GLN:HE21	3:O:300:LEU:HG	1.79	0.48
3:P:313:LEU:N	3:P:314:PRO:CD	2.76	0.48
3:R:296:GLN:HE21	3:R:300:LEU:HG	1.79	0.48
1:B:250:ARG:O	1:B:254:THR:CB	2.62	0.48
1:C:354:ILE:HD13	1:C:375:PRO:HD2	1.64	0.48
1:C:395:GLU:O	1:C:395:GLU:HG3	2.14	0.48
1:F:166:THR:HG23	1:F:291:GLU:CD	2.34	0.48
1:F:351:ILE:O	1:F:355:GLN:HG3	2.14	0.48
3:L:296:GLN:HE21	3:L:300:LEU:HG	1.79	0.48
1:C:357:ALA:CB	3:L:306:SER:CB	2.88	0.48
3:P:296:GLN:HE21	3:P:300:LEU:HG	1.79	0.48
1:D:255:GLU:O	1:D:259:GLN:CB	2.63	0.47
3:J:296:GLN:HE21	3:J:300:LEU:HG	1.79	0.47
3:R:327:LEU:HD12	3:R:327:LEU:O	2.13	0.47
1:C:336:GLY:HA3	4:C:502:ADP:C8	2.49	0.47
1:F:166:THR:HG23	1:F:291:GLU:OE1	2.13	0.47
3:S:313:LEU:N	3:S:314:PRO:CD	2.76	0.47
1:C:179:LYS:NZ	1:C:276:THR:O	2.46	0.47
1:D:354:ILE:HG23	1:D:396:LEU:CD1	2.44	0.47
1:D:395:GLU:HG3	1:D:395:GLU:O	2.14	0.47
1:F:206:TRP:O	1:F:209:GLU:HG2	2.14	0.47
1:C:321:LYS:CG	3:K:310:TYR:HD1	2.26	0.47
1:B:395:GLU:O	1:B:395:GLU:HG3	2.14	0.47
1:B:341:VAL:HG11	1:C:291:GLU:HB2	1.96	0.47
1:C:396:LEU:CD2	1:D:158:LEU:HD21	2.38	0.47
3:K:313:LEU:N	3:K:314:PRO:CD	2.76	0.47
3:L:293:LYS:HZ2	3:L:330:ILE:HD13	1.78	0.47
3:Q:296:GLN:HE21	3:Q:300:LEU:HG	1.79	0.47
3:Q:327:LEU:HD12	3:Q:327:LEU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:296:GLN:HE21	3:S:300:LEU:HG	1.79	0.47
1:C:341:VAL:HG11	1:D:291:GLU:HB2	1.95	0.47
1:E:403:ILE:HG13	1:E:406:PHE:HB2	1.95	0.47
1:E:403:ILE:HG12	1:E:407:LEU:HG	1.97	0.47
1:A:254:THR:OG1	1:F:205:LYS:HB2	2.15	0.47
1:E:255:GLU:O	1:E:259:GLN:CB	2.62	0.47
1:F:311:ASN:HB3	1:F:343:VAL:HG11	1.97	0.47
1:C:394:ASP:OD1	1:C:395:GLU:N	2.48	0.47
1:D:202:LEU:HD22	1:D:214:VAL:HG22	1.95	0.47
1:E:395:GLU:HG3	1:E:395:GLU:O	2.14	0.47
1:C:389:THR:HG22	1:D:154:LYS:HZ1	1.76	0.47
1:D:321:LYS:HD2	3:M:310:TYR:CA	2.41	0.47
1:C:255:GLU:O	1:C:259:GLN:CB	2.62	0.47
1:C:358:THR:O	1:C:358:THR:HG23	2.13	0.47
1:F:395:GLU:HG3	1:F:395:GLU:O	2.14	0.47
1:B:358:THR:HG21	3:J:303:TYR:CZ	2.50	0.47
1:F:394:ASP:OD1	1:F:395:GLU:N	2.48	0.47
3:P:328:ASN:OD1	3:Q:317:LYS:HE3	2.15	0.47
1:D:394:ASP:OD1	1:D:395:GLU:N	2.48	0.46
1:E:358:THR:O	1:E:359:HIS:CB	2.63	0.46
1:E:394:ASP:OD1	1:E:395:GLU:N	2.48	0.46
3:H:328:ASN:OD1	3:I:317:LYS:HE3	2.16	0.46
3:L:317:LYS:HE3	3:M:328:ASN:OD1	2.16	0.46
1:B:336:GLY:HA3	4:B:501:ADP:C8	2.50	0.46
3:H:324:LEU:O	3:H:328:ASN:ND2	2.49	0.46
3:L:324:LEU:O	3:L:328:ASN:ND2	2.49	0.46
3:L:328:ASN:OD1	3:M:317:LYS:HE3	2.16	0.46
3:P:324:LEU:O	3:P:328:ASN:ND2	2.49	0.46
3:R:324:LEU:O	3:R:328:ASN:ND2	2.49	0.46
1:B:255:GLU:O	1:B:259:GLN:CB	2.62	0.46
3:I:324:LEU:O	3:I:328:ASN:ND2	2.49	0.46
3:J:328:ASN:OD1	3:K:317:LYS:HE3	2.15	0.46
3:N:324:LEU:O	3:N:328:ASN:ND2	2.49	0.46
3:N:328:ASN:OD1	3:O:317:LYS:HE3	2.16	0.46
3:N:317:LYS:HE3	3:O:328:ASN:OD1	2.16	0.46
3:Q:324:LEU:O	3:Q:328:ASN:ND2	2.49	0.46
1:A:394:ASP:OD1	1:A:395:GLU:N	2.48	0.46
1:B:224:ASN:O	1:B:227:SER:OG	2.33	0.46
1:B:394:ASP:OD1	1:B:395:GLU:N	2.48	0.46
1:E:393:ALA:CB	1:F:157:HIS:NE2	2.78	0.46
3:H:296:GLN:HE21	3:H:300:LEU:HG	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:311:GLU:OE1	3:I:290:ARG:NH1	2.49	0.46
3:O:301:ALA:O	3:O:305:ILE:HG13	2.16	0.46
1:D:403:ILE:HG23	1:D:404:LYS:H	1.81	0.46
3:J:301:ALA:O	3:J:305:ILE:HG13	2.16	0.46
3:M:324:LEU:O	3:M:328:ASN:ND2	2.49	0.46
3:O:324:LEU:O	3:O:328:ASN:ND2	2.49	0.46
3:R:328:ASN:OD1	3:S:317:LYS:HE3	2.16	0.46
3:H:301:ALA:O	3:H:305:ILE:HG13	2.16	0.46
3:J:293:LYS:HZ2	3:J:330:ILE:HD13	1.80	0.46
3:L:311:GLU:OE1	3:M:290:ARG:NH1	2.49	0.46
1:A:177:THR:HG22	1:A:298:LEU:HD23	1.97	0.46
1:E:132:TRP:CD1	1:E:189:GLU:HG3	2.51	0.46
1:F:225:LYS:HD3	1:F:269:GLY:HA3	1.98	0.46
1:C:198:SER:OG	1:C:199:SER:N	2.49	0.46
1:F:212:LYS:HE3	1:F:216:GLN:HE21	1.81	0.46
3:H:317:LYS:HE3	3:I:328:ASN:OD1	2.16	0.46
1:D:377:SER:HG	3:N:307:ALA:HA	1.73	0.46
3:R:317:LYS:HE3	3:S:328:ASN:OD1	2.16	0.46
1:A:322:GLU:OE2	3:S:311:GLU:CB	2.61	0.45
1:D:353:LYS:O	1:D:375:PRO:HB3	2.15	0.45
1:C:407:LEU:HD23	1:C:410:ILE:HD12	1.99	0.45
1:D:204:SER:HA	1:E:212:LYS:HZ3	1.80	0.45
1:F:317:CYS:CB	1:F:401:LEU:CB	2.93	0.45
1:B:378:PRO:HG2	3:J:303:TYR:HB3	1.98	0.45
3:N:301:ALA:O	3:N:305:ILE:HG13	2.16	0.45
3:N:293:LYS:HZ2	3:N:330:ILE:HD13	1.81	0.45
3:P:317:LYS:HE3	3:Q:328:ASN:OD1	2.16	0.45
1:A:325:ARG:NH1	3:S:312:ASP:HB3	2.06	0.45
1:A:407:LEU:HD23	1:A:410:ILE:HD12	1.98	0.45
1:F:139:GLU:H	1:F:139:GLU:HG2	1.45	0.45
1:F:315:THR:HG21	1:F:347:LEU:HD22	1.98	0.45
3:K:324:LEU:O	3:K:328:ASN:ND2	2.49	0.45
1:C:358:THR:CG2	3:L:303:TYR:CZ	3.00	0.45
1:F:354:ILE:HG12	1:F:398:GLU:HA	1.76	0.45
3:S:324:LEU:O	3:S:328:ASN:ND2	2.49	0.45
1:A:388:TRP:HH2	1:B:154:LYS:NZ	2.10	0.45
1:B:170:LEU:HB2	1:B:290:PHE:HB3	1.98	0.45
1:B:288:ARG:NH2	1:B:289:ARG:HH12	2.15	0.45
1:B:347:LEU:HA	1:B:401:LEU:HD21	1.99	0.45
3:J:324:LEU:O	3:J:328:ASN:ND2	2.49	0.45
3:J:317:LYS:HE3	3:K:328:ASN:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:301:ALA:O	3:L:305:ILE:HG13	2.16	0.45
3:R:301:ALA:O	3:R:305:ILE:HG13	2.16	0.45
1:A:198:SER:OG	1:A:199:SER:N	2.49	0.45
1:B:407:LEU:HD23	1:B:410:ILE:HD12	1.99	0.45
1:C:317:CYS:HA	1:C:401:LEU:HB2	1.98	0.45
1:D:204:SER:HA	1:E:212:LYS:NZ	2.32	0.45
1:F:323:ASP:CG	1:F:403:ILE:HG21	2.36	0.45
1:D:378:PRO:HD2	3:N:307:ALA:HB2	1.98	0.45
1:A:279:PRO:HB2	1:A:428:PHE:CE2	2.52	0.45
1:B:321:LYS:CE	3:I:309:ASN:O	2.65	0.45
3:P:301:ALA:O	3:P:305:ILE:HG13	2.16	0.45
3:S:301:ALA:O	3:S:305:ILE:HG13	2.16	0.45
1:B:370:THR:O	1:B:371:ARG:O	2.35	0.45
1:E:288:ARG:NH2	1:E:289:ARG:HH12	2.15	0.45
1:E:407:LEU:HD23	1:E:410:ILE:HD12	1.99	0.45
3:N:300:LEU:HD12	3:N:323:ALA:HA	1.99	0.45
3:P:300:LEU:HD12	3:P:323:ALA:HA	1.99	0.45
1:D:288:ARG:NH2	1:D:289:ARG:HH12	2.15	0.45
1:D:355:GLN:HE22	1:E:147:GLU:HG3	1.81	0.45
3:J:311:GLU:OE1	3:K:290:ARG:NH1	2.49	0.45
3:L:311:GLU:CD	3:M:290:ARG:NH1	2.64	0.45
1:B:250:ARG:O	1:B:254:THR:OG1	2.28	0.45
1:C:250:ARG:O	1:C:254:THR:OG1	2.28	0.45
1:D:370:THR:O	1:D:371:ARG:O	2.35	0.45
3:Q:301:ALA:O	3:Q:305:ILE:HG13	2.16	0.45
1:A:358:THR:O	1:A:359:HIS:HD2	1.91	0.44
1:D:198:SER:OG	1:D:199:SER:N	2.49	0.44
1:D:355:GLN:HA	1:D:388:TRP:CD1	2.52	0.44
1:F:370:THR:O	1:F:371:ARG:O	2.35	0.44
3:J:311:GLU:CD	3:K:290:ARG:NH1	2.64	0.44
3:R:300:LEU:HD12	3:R:323:ALA:HA	1.99	0.44
1:E:256:LEU:O	1:E:260:MET:CB	2.65	0.44
1:A:370:THR:O	1:A:371:ARG:O	2.35	0.44
1:B:352:ARG:O	1:B:356:SER:CB	2.63	0.44
1:C:355:GLN:HA	1:C:388:TRP:CE3	2.52	0.44
1:D:204:SER:OG	1:D:205:LYS:N	2.50	0.44
1:D:353:LYS:O	1:D:375:PRO:HG2	2.18	0.44
1:B:321:LYS:CD	3:I:310:TYR:CE1	2.77	0.44
3:L:300:LEU:HD12	3:L:323:ALA:HA	1.99	0.44
1:C:354:ILE:HD11	1:C:375:PRO:HD2	1.91	0.44
1:C:370:THR:O	1:C:371:ARG:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:370:THR:O	1:E:371:ARG:O	2.35	0.44
3:O:300:LEU:HD12	3:O:323:ALA:HA	1.99	0.44
1:A:288:ARG:NH2	1:A:289:ARG:HH12	2.15	0.44
1:A:363:VAL:O	1:A:364:SER:HB3	2.18	0.44
1:B:353:LYS:O	1:B:375:PRO:CB	2.65	0.44
1:E:330:MET:HG3	1:E:410:ILE:HG21	1.99	0.44
1:B:204:SER:OG	1:B:205:LYS:N	2.50	0.44
1:D:407:LEU:HD23	1:D:410:ILE:HD12	1.99	0.44
1:A:204:SER:OG	1:A:205:LYS:N	2.50	0.44
1:A:374:THR:HB	1:A:397:LYS:HB3	2.00	0.44
1:B:198:SER:OG	1:B:199:SER:N	2.49	0.44
1:C:218:PHE:CD2	1:C:259:GLN:HG3	2.52	0.44
1:C:363:VAL:O	1:C:364:SER:HB3	2.18	0.44
1:E:250:ARG:O	1:E:254:THR:OG1	2.28	0.44
1:A:388:TRP:CH2	1:B:154:LYS:CE	3.01	0.44
3:O:310:TYR:O	3:O:310:TYR:CG	2.71	0.44
1:C:256:LEU:O	1:C:260:MET:CB	2.65	0.43
1:B:179:LYS:NZ	1:B:276:THR:O	2.50	0.43
1:C:204:SER:OG	1:C:205:LYS:N	2.50	0.43
1:D:363:VAL:O	1:D:364:SER:HB3	2.18	0.43
1:F:346:ALA:CB	1:F:406:PHE:CE2	2.96	0.43
1:F:360:PHE:HD1	1:F:386:MET:CG	2.14	0.43
3:J:300:LEU:HD12	3:J:323:ALA:HA	1.99	0.43
3:S:300:LEU:HD12	3:S:323:ALA:HA	1.99	0.43
1:B:363:VAL:O	1:B:364:SER:HB3	2.18	0.43
1:C:288:ARG:NH2	1:C:289:ARG:HH12	2.15	0.43
1:F:132:TRP:CE2	1:F:189:GLU:HG3	2.53	0.43
1:F:363:VAL:O	1:F:364:SER:HB3	2.18	0.43
1:D:374:THR:HB	1:D:397:LYS:HB3	2.01	0.43
3:Q:300:LEU:HD12	3:Q:323:ALA:HA	1.99	0.43
1:B:177:THR:HG22	1:B:298:LEU:HD23	2.00	0.43
1:F:317:CYS:HB2	1:F:401:LEU:HB3	2.01	0.43
1:D:373:LEU:CD1	1:D:391:ILE:HG12	2.49	0.43
1:E:363:VAL:O	1:E:364:SER:HB3	2.18	0.43
1:E:374:THR:HB	1:E:397:LYS:HB3	2.01	0.43
1:F:290:PHE:O	1:F:291:GLU:C	2.55	0.43
1:A:322:GLU:HG2	3:S:310:TYR:HB3	2.00	0.43
1:A:350:PRO:HB3	1:A:399:PRO:CD	2.45	0.43
1:C:373:LEU:CD1	1:C:391:ILE:HG12	2.49	0.43
1:E:373:LEU:CD1	1:E:391:ILE:HG12	2.49	0.43
1:B:256:LEU:O	1:B:260:MET:CB	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ILE:HA	1:B:354:ILE:HG22	2.00	0.43
3:L:308:LEU:CD1	3:M:298:GLN:HG3	2.44	0.43
1:B:358:THR:HG23	1:B:358:THR:O	2.19	0.43
3:H:300:LEU:HD12	3:H:323:ALA:HA	1.99	0.43
1:A:373:LEU:CD1	1:A:391:ILE:HG12	2.49	0.43
1:A:425:GLN:O	1:A:429:THR:CB	2.67	0.43
1:B:373:LEU:CD1	1:B:391:ILE:HG12	2.49	0.43
1:D:358:THR:O	1:D:359:HIS:HD2	1.88	0.43
1:E:301:LEU:CD1	3:O:310:TYR:CD2	3.02	0.43
3:H:311:GLU:CD	3:I:290:ARG:NH1	2.64	0.43
1:F:360:PHE:CE1	1:F:391:ILE:HD12	2.54	0.42
1:F:373:LEU:CD1	1:F:391:ILE:HG12	2.49	0.42
3:L:317:LYS:N	3:M:327:LEU:HD21	2.35	0.42
1:A:318:VAL:HG12	1:A:401:LEU:O	2.19	0.42
1:D:425:GLN:O	1:D:429:THR:CB	2.67	0.42
1:F:174:PRO:HB3	1:F:421:ASP:OD2	2.19	0.42
3:H:327:LEU:HD21	3:I:317:LYS:N	2.35	0.42
3:N:327:LEU:HD21	3:O:317:LYS:N	2.35	0.42
1:C:353:LYS:O	1:C:375:PRO:HB3	2.19	0.42
1:F:155:PHE:HB3	1:F:158:LEU:HD23	2.01	0.42
3:O:300:LEU:HD12	3:O:323:ALA:N	2.35	0.42
3:P:327:LEU:HD21	3:Q:317:LYS:N	2.35	0.42
1:D:358:THR:C	1:D:359:HIS:CG	2.92	0.42
1:E:403:ILE:CG1	1:E:407:LEU:HG	2.50	0.42
1:F:355:GLN:O	1:F:388:TRP:CE2	2.73	0.42
3:J:317:LYS:N	3:K:327:LEU:HD21	2.35	0.42
1:C:358:THR:HG21	3:L:303:TYR:OH	2.20	0.42
3:R:317:LYS:N	3:S:327:LEU:HD21	2.35	0.42
1:A:138:LEU:HD13	1:A:182:LEU:HD13	2.02	0.42
1:C:240:THR:HB	1:C:253:LYS:HE2	2.02	0.42
1:D:354:ILE:CG2	1:D:396:LEU:CD1	2.86	0.42
1:F:374:THR:HB	1:F:397:LYS:HB3	2.01	0.42
3:J:300:LEU:HD12	3:J:323:ALA:N	2.35	0.42
3:P:300:LEU:HD12	3:P:323:ALA:N	2.35	0.42
3:P:317:LYS:N	3:Q:327:LEU:HD21	2.35	0.42
1:E:425:GLN:O	1:E:429:THR:CB	2.67	0.42
3:H:300:LEU:HD12	3:H:323:ALA:N	2.35	0.42
1:C:357:ALA:CB	3:L:306:SER:OG	2.68	0.42
1:D:250:ARG:O	1:D:254:THR:HB	2.20	0.42
1:D:256:LEU:O	1:D:260:MET:CB	2.65	0.42
3:J:327:LEU:HD21	3:K:317:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:327:LEU:HD21	3:S:317:LYS:N	2.35	0.42
1:A:358:THR:C	1:A:359:HIS:CG	2.93	0.42
1:B:359:HIS:HA	1:B:384:ILE:O	2.20	0.42
3:H:317:LYS:N	3:I:327:LEU:HD21	2.35	0.42
1:C:353:LYS:O	1:C:375:PRO:CB	2.68	0.41
1:E:359:HIS:HA	1:E:384:ILE:O	2.20	0.41
1:F:422:LEU:O	1:F:426:GLU:HG3	2.19	0.41
3:J:308:LEU:CD1	3:K:298:GLN:HG3	2.44	0.41
3:L:327:LEU:HD21	3:M:317:LYS:N	2.35	0.41
3:R:300:LEU:HD12	3:R:323:ALA:N	2.35	0.41
1:A:238:THR:HG21	1:A:282:LEU:HD12	2.02	0.41
1:E:253:LYS:HB3	1:E:253:LYS:HE3	1.88	0.41
1:F:263:VAL:HA	1:F:267:SER:HA	1.85	0.41
3:L:300:LEU:HD12	3:L:323:ALA:N	2.35	0.41
3:N:317:LYS:N	3:O:327:LEU:HD21	2.35	0.41
3:Q:300:LEU:HD12	3:Q:323:ALA:N	2.35	0.41
3:R:330:ILE:OXT	3:R:330:ILE:CG2	2.68	0.41
1:C:425:GLN:O	1:C:429:THR:CB	2.67	0.41
1:D:203:VAL:O	1:E:212:LYS:NZ	2.45	0.41
1:D:240:THR:HB	1:D:253:LYS:HE2	2.02	0.41
1:D:377:SER:OG	3:N:307:ALA:CB	2.69	0.41
1:B:250:ARG:O	1:B:254:THR:HB	2.20	0.41
1:E:250:ARG:O	1:E:254:THR:HB	2.20	0.41
1:F:237:LEU:CD1	1:F:256:LEU:HD22	2.50	0.41
3:N:300:LEU:HD12	3:N:323:ALA:N	2.35	0.41
3:O:330:ILE:CG2	3:O:330:ILE:OXT	2.68	0.41
3:S:293:LYS:HZ2	3:S:330:ILE:HD13	1.84	0.41
1:A:151:LEU:CD1	1:F:355:GLN:HG2	2.51	0.41
1:A:334:TYR:CD1	1:A:415:PRO:HG3	2.54	0.41
1:B:425:GLN:O	1:B:429:THR:CB	2.67	0.41
1:B:313:GLY:HA3	1:C:162:ASN:ND2	2.36	0.41
1:C:354:ILE:CD1	1:C:375:PRO:HG2	2.17	0.41
1:F:265:ASN:HD22	1:F:265:ASN:N	2.17	0.41
3:P:330:ILE:OXT	3:P:330:ILE:CG2	2.68	0.41
3:Q:330:ILE:OXT	3:Q:330:ILE:CG2	2.68	0.41
1:D:358:THR:HG23	1:D:358:THR:O	2.21	0.41
1:D:359:HIS:HA	1:D:384:ILE:O	2.20	0.41
3:H:305:ILE:HD13	3:I:302:LYS:HG3	2.03	0.41
3:S:300:LEU:HD12	3:S:323:ALA:N	2.35	0.41
1:C:250:ARG:O	1:C:254:THR:HB	2.20	0.41
1:E:240:THR:HB	1:E:253:LYS:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:305:ILE:HD13	3:M:302:LYS:HG3	2.03	0.41
3:S:295:GLU:O	3:S:295:GLU:HG2	2.21	0.41
1:F:263:VAL:CG1	1:F:267:SER:HB2	2.46	0.41
3:S:330:ILE:CG2	3:S:330:ILE:OXT	2.68	0.41
1:B:240:THR:HB	1:B:253:LYS:HE2	2.02	0.41
1:C:260:MET:SD	1:C:289:ARG:HB3	2.61	0.41
1:F:209:GLU:HG2	1:F:209:GLU:H	1.45	0.41
1:A:145:LEU:HA	1:A:145:LEU:HD23	1.92	0.41
1:A:353:LYS:HD2	1:A:399:PRO:CB	2.51	0.41
3:I:330:ILE:CG2	3:I:330:ILE:OXT	2.68	0.41
1:A:358:THR:HG23	1:A:358:THR:O	2.21	0.41
1:B:358:THR:OG1	1:B:385:GLU:HG2	2.17	0.41
1:D:358:THR:HG21	3:N:303:TYR:CZ	2.49	0.41
1:E:301:LEU:HB3	3:O:310:TYR:CD1	2.56	0.41
1:F:225:LYS:NZ	1:F:268:GLN:O	2.43	0.41
3:J:295:GLU:O	3:J:295:GLU:HG2	2.21	0.41
1:C:321:LYS:CD	3:K:310:TYR:CD1	3.03	0.41
1:B:145:LEU:HD13	1:B:186:VAL:HG21	2.03	0.40
1:B:350:PRO:HB2	1:B:398:GLU:HG3	2.04	0.40
1:C:224:ASN:O	1:C:227:SER:OG	2.40	0.40
3:J:330:ILE:CG2	3:J:330:ILE:OXT	2.68	0.40
3:K:330:ILE:OXT	3:K:330:ILE:CG2	2.68	0.40
3:L:330:ILE:CG2	3:L:330:ILE:OXT	2.68	0.40
3:M:330:ILE:CG2	3:M:330:ILE:OXT	2.68	0.40
3:O:295:GLU:O	3:O:295:GLU:HG2	2.21	0.40
1:B:347:LEU:HD21	1:B:401:LEU:HD11	2.03	0.40
1:E:304:ARG:HG2	1:E:339:ILE:HD11	2.03	0.40
1:F:200:SER:HB3	1:F:233:GLU:OE1	2.21	0.40
1:A:357:ALA:CB	3:H:306:SER:CB	3.00	0.40
1:A:359:HIS:HA	1:A:384:ILE:O	2.20	0.40
1:C:359:HIS:HA	1:C:384:ILE:O	2.20	0.40
1:E:197:VAL:HG22	1:E:198:SER:O	2.22	0.40
1:E:233:GLU:HA	1:E:276:THR:HA	2.02	0.40
1:F:330:MET:HE2	1:F:330:MET:HB2	1.76	0.40
1:B:304:ARG:HG2	1:B:339:ILE:HD11	2.03	0.40
1:B:350:PRO:HB3	1:B:399:PRO:HD2	2.03	0.40
3:N:330:ILE:OXT	3:N:330:ILE:CG2	2.68	0.40
1:A:304:ARG:HG2	1:A:339:ILE:HD11	2.03	0.40
3:H:330:ILE:OXT	3:H:330:ILE:CG2	2.68	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	308/437 (70%)	280 (91%)	23 (8%)	5 (2%)	11	51
1	B	307/437 (70%)	271 (88%)	31 (10%)	5 (2%)	11	51
1	C	307/437 (70%)	275 (90%)	27 (9%)	5 (2%)	11	51
1	D	307/437 (70%)	272 (89%)	30 (10%)	5 (2%)	11	51
1	E	304/437 (70%)	268 (88%)	31 (10%)	5 (2%)	11	51
1	F	296/437 (68%)	275 (93%)	15 (5%)	6 (2%)	9	47
3	H	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	I	49/330 (15%)	43 (88%)	5 (10%)	1 (2%)	9	47
3	J	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	K	45/330 (14%)	39 (87%)	5 (11%)	1 (2%)	8	44
3	L	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	M	45/330 (14%)	39 (87%)	5 (11%)	1 (2%)	8	44
3	N	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	O	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	P	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	Q	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	R	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	S	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
All	All	2328/6582 (35%)	2041 (88%)	235 (10%)	52 (2%)	12	44

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	HIS
1	A	371	ARG
1	A	395	GLU
1	B	359	HIS

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Mol	Chain	Res	Type
1	B	371	ARG
1	B	395	GLU
1	C	359	HIS
1	C	371	ARG
1	C	395	GLU
1	D	359	HIS
1	D	371	ARG
1	D	395	GLU
1	E	371	ARG
1	E	395	GLU
1	F	371	ARG
1	F	395	GLU
1	F	207	MET
3	H	312	ASP
3	I	312	ASP
3	J	312	ASP
3	K	312	ASP
3	L	312	ASP
3	M	312	ASP
3	N	312	ASP
3	O	312	ASP
3	P	312	ASP
3	Q	312	ASP
3	R	312	ASP
3	S	312	ASP
1	A	381	ASP
1	B	381	ASP
1	C	381	ASP
1	D	381	ASP
1	E	381	ASP
1	F	359	HIS
1	F	381	ASP
1	E	359	HIS
3	H	290	ARG
3	J	290	ARG
3	L	290	ARG
3	N	290	ARG
3	O	290	ARG
3	P	290	ARG
3	Q	290	ARG
3	R	290	ARG
3	S	290	ARG

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Mol	Chain	Res	Type
1	A	370	THR
1	B	370	THR
1	C	370	THR
1	D	370	THR
1	E	370	THR
1	F	370	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	265/367 (72%)	262 (99%)	3 (1%)	78	89
1	B	265/367 (72%)	259 (98%)	6 (2%)	56	78
1	C	265/367 (72%)	262 (99%)	3 (1%)	78	89
1	D	265/367 (72%)	261 (98%)	4 (2%)	70	85
1	E	262/367 (71%)	259 (99%)	3 (1%)	78	89
1	F	258/367 (70%)	247 (96%)	11 (4%)	33	64
3	H	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	I	45/294 (15%)	44 (98%)	1 (2%)	57	79
3	J	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	K	41/294 (14%)	40 (98%)	1 (2%)	54	77
3	L	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	M	41/294 (14%)	40 (98%)	1 (2%)	54	77
3	N	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	O	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	P	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	Q	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	R	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	S	36/294 (12%)	34 (94%)	2 (6%)	25	57
All	All	2031/5730 (35%)	1980 (98%)	51 (2%)	56	77

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	370	THR
1	A	373	LEU
1	A	400	ASP
1	B	370	THR
1	B	373	LEU
1	B	396	LEU
1	B	397	LYS
1	B	398	GLU
1	B	402	THR
1	C	370	THR
1	C	373	LEU
1	C	398	GLU
1	D	370	THR
1	D	373	LEU
1	D	398	GLU
1	D	402	THR
1	E	370	THR
1	E	373	LEU
1	E	402	THR
1	F	127	LYS
1	F	139	GLU
1	F	200	SER
1	F	209	GLU
1	F	240	THR
1	F	278	ILE
1	F	291	GLU
1	F	370	THR
1	F	373	LEU
1	F	412	SER
1	F	417	VAL
3	H	290	ARG
3	H	319	GLU
3	I	319	GLU
3	J	290	ARG
3	J	319	GLU
3	K	319	GLU
3	L	290	ARG
3	L	319	GLU
3	M	319	GLU
3	N	290	ARG
3	N	319	GLU
3	O	290	ARG

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Mol	Chain	Res	Type
3	O	319	GLU
3	P	290	ARG
3	P	319	GLU
3	Q	290	ARG
3	Q	319	GLU
3	R	290	ARG
3	R	319	GLU
3	S	290	ARG
3	S	319	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	HIS
1	B	359	HIS
1	C	359	HIS
1	D	355	GLN
1	D	359	HIS
1	E	359	HIS
1	E	425	GLN
1	F	216	GLN
1	F	265	ASN
3	H	296	GLN
3	I	298	GLN
3	J	296	GLN
3	K	298	GLN
3	L	296	GLN
3	M	298	GLN
3	N	296	GLN
3	O	296	GLN
3	P	296	GLN
3	Q	296	GLN
3	R	296	GLN
3	S	296	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 ⓘ

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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
4	ADP	A	501	5	25,29,29	0.93	1 (4%)	24,45,45	0.97	1 (4%)
5	BEF	A	502	4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	B	501	5	25,29,29	0.95	1 (4%)	24,45,45	0.90	1 (4%)
5	BEF	C	501	4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	C	502	5	25,29,29	0.82	0	24,45,45	0.98	1 (4%)
5	BEF	C	503	4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	D	501	-	25,29,29	0.95	1 (4%)	24,45,45	1.61	2 (8%)
4	ADP	E	501	-	25,29,29	0.99	1 (4%)	24,45,45	1.58	2 (8%)

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
4	ADP	A	501	5	-	0/12/32/32	0/3/3/3
5	BEF	A	502	4	-	0/0/0/0	0/0/0/0
4	ADP	B	501	5	-	0/12/32/32	0/3/3/3
5	BEF	C	501	4	-	0/0/0/0	0/0/0/0
4	ADP	C	502	5	-	0/12/32/32	0/3/3/3
5	BEF	C	503	4	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	D	501	-	-	0/12/32/32	0/3/3/3
4	ADP	E	501	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	ADP	PB-O3A	-2.06	1.56	1.60
4	A	501	ADP	PB-O1B	2.10	1.57	1.50
4	D	501	ADP	C5-C4	3.05	1.47	1.40
4	E	501	ADP	C5-C4	3.15	1.47	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	501	ADP	N3-C2-N1	-5.68	123.91	128.86
4	D	501	ADP	N3-C2-N1	-5.45	124.11	128.86
4	D	501	ADP	C4-C5-N7	-2.94	106.57	109.41
4	E	501	ADP	C4-C5-N7	-2.81	106.70	109.41
4	B	501	ADP	O2A-PA-O5'	2.33	119.14	108.14
4	A	501	ADP	O5'-PA-O1A	2.33	118.67	109.25
4	C	502	ADP	O2A-PA-O5'	2.55	120.19	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	ADP	1	0
4	B	501	ADP	1	0
5	C	501	BEF	1	0
4	C	502	ADP	1	0
4	D	501	ADP	2	0
4	E	501	ADP	1	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.