



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 16, 2018 – 10:00 am GMT

PDB ID : 6AP1  
EMDB ID: : EMD-8887  
Title : Vps4p-Vta1p complex with peptide binding to the central pore of Vps4p  
Authors : Han, H.; Monroe, N.; Shen, P.; Sundquist, W.I.; Hill, C.P.  
Deposited on : 2017-08-16  
Resolution : 3.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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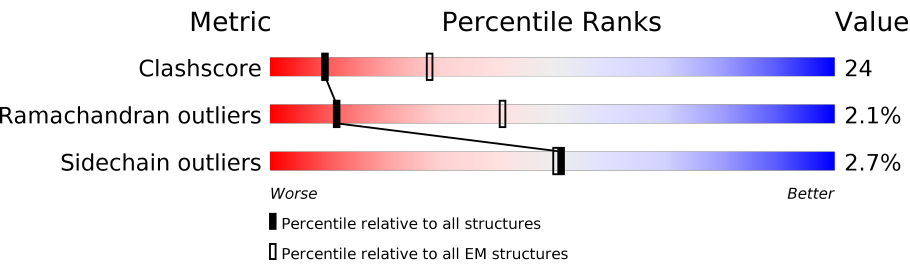
MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

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  $\geq 3$ , 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	519	49% 9% . 39%
1	B	519	50% 11% . 38%
1	C	519	50% 11% . 38%
1	D	519	51% 9% . 38%
1	E	519	45% 12% . 41%
1	F	519	35% 22% . 41%
2	G	10	90% 10%
3	H	330	5% 8% 87%
3	I	330	8% 5% 87%

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

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18838 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,Protein hcp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	314	Total	C	N	O	S	0	0
			2427	1530	414	474	9		
1	B	322	Total	C	N	O	S	0	0
			2491	1568	427	487	9		
1	C	322	Total	C	N	O	S	0	0
			2491	1568	427	487	9		
1	D	322	Total	C	N	O	S	0	0
			2491	1568	427	487	9		
1	E	304	Total	C	N	O	S	0	0
			2360	1489	401	461	9		
1	F	308	Total	C	N	O	S	0	0
			2387	1507	405	466	9		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	GLY	-	expression tag	UNP P52917
A	438	GLY	-	linker	UNP P52917
A	439	GLY	-	linker	UNP P52917
A	440	GLY	-	linker	UNP P52917
A	441	GLY	-	linker	UNP P52917
A	442	SER	-	linker	UNP P52917
A	443	GLY	-	linker	UNP P52917
A	444	GLY	-	linker	UNP P52917
A	445	GLY	-	linker	UNP P52917
A	446	GLY	-	linker	UNP P52917
A	447	SER	-	linker	UNP P52917
A	448	GLY	-	linker	UNP P52917
A	449	GLY	-	linker	UNP P52917
A	450	GLY	-	linker	UNP P52917
A	451	GLY	-	linker	UNP P52917
A	452	SER	-	linker	UNP P52917
A	453	GLY	-	linker	UNP P52917
A	454	GLY	-	linker	UNP P52917

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Chain	Residue	Modelled	Actual	Comment	Reference
A	455	GLY	-	linker	UNP P52917
A	618	GLY	-	expression tag	UNP Q9I747
B	100	GLY	-	expression tag	UNP P52917
B	438	GLY	-	linker	UNP P52917
B	439	GLY	-	linker	UNP P52917
B	440	GLY	-	linker	UNP P52917
B	441	GLY	-	linker	UNP P52917
B	442	SER	-	linker	UNP P52917
B	443	GLY	-	linker	UNP P52917
B	444	GLY	-	linker	UNP P52917
B	445	GLY	-	linker	UNP P52917
B	446	GLY	-	linker	UNP P52917
B	447	SER	-	linker	UNP P52917
B	448	GLY	-	linker	UNP P52917
B	449	GLY	-	linker	UNP P52917
B	450	GLY	-	linker	UNP P52917
B	451	GLY	-	linker	UNP P52917
B	452	SER	-	linker	UNP P52917
B	453	GLY	-	linker	UNP P52917
B	454	GLY	-	linker	UNP P52917
B	455	GLY	-	linker	UNP P52917
B	618	GLY	-	expression tag	UNP Q9I747
C	100	GLY	-	expression tag	UNP P52917
C	438	GLY	-	linker	UNP P52917
C	439	GLY	-	linker	UNP P52917
C	440	GLY	-	linker	UNP P52917
C	441	GLY	-	linker	UNP P52917
C	442	SER	-	linker	UNP P52917
C	443	GLY	-	linker	UNP P52917
C	444	GLY	-	linker	UNP P52917
C	445	GLY	-	linker	UNP P52917
C	446	GLY	-	linker	UNP P52917
C	447	SER	-	linker	UNP P52917
C	448	GLY	-	linker	UNP P52917
C	449	GLY	-	linker	UNP P52917
C	450	GLY	-	linker	UNP P52917
C	451	GLY	-	linker	UNP P52917
C	452	SER	-	linker	UNP P52917
C	453	GLY	-	linker	UNP P52917
C	454	GLY	-	linker	UNP P52917
C	455	GLY	-	linker	UNP P52917
C	618	GLY	-	expression tag	UNP Q9I747

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Chain	Residue	Modelled	Actual	Comment	Reference
D	100	GLY	-	expression tag	UNP P52917
D	438	GLY	-	linker	UNP P52917
D	439	GLY	-	linker	UNP P52917
D	440	GLY	-	linker	UNP P52917
D	441	GLY	-	linker	UNP P52917
D	442	SER	-	linker	UNP P52917
D	443	GLY	-	linker	UNP P52917
D	444	GLY	-	linker	UNP P52917
D	445	GLY	-	linker	UNP P52917
D	446	GLY	-	linker	UNP P52917
D	447	SER	-	linker	UNP P52917
D	448	GLY	-	linker	UNP P52917
D	449	GLY	-	linker	UNP P52917
D	450	GLY	-	linker	UNP P52917
D	451	GLY	-	linker	UNP P52917
D	452	SER	-	linker	UNP P52917
D	453	GLY	-	linker	UNP P52917
D	454	GLY	-	linker	UNP P52917
D	455	GLY	-	linker	UNP P52917
D	618	GLY	-	expression tag	UNP Q9I747
E	100	GLY	-	expression tag	UNP P52917
E	438	GLY	-	linker	UNP P52917
E	439	GLY	-	linker	UNP P52917
E	440	GLY	-	linker	UNP P52917
E	441	GLY	-	linker	UNP P52917
E	442	SER	-	linker	UNP P52917
E	443	GLY	-	linker	UNP P52917
E	444	GLY	-	linker	UNP P52917
E	445	GLY	-	linker	UNP P52917
E	446	GLY	-	linker	UNP P52917
E	447	SER	-	linker	UNP P52917
E	448	GLY	-	linker	UNP P52917
E	449	GLY	-	linker	UNP P52917
E	450	GLY	-	linker	UNP P52917
E	451	GLY	-	linker	UNP P52917
E	452	SER	-	linker	UNP P52917
E	453	GLY	-	linker	UNP P52917
E	454	GLY	-	linker	UNP P52917
E	455	GLY	-	linker	UNP P52917
E	618	GLY	-	expression tag	UNP Q9I747
F	100	GLY	-	expression tag	UNP P52917
F	438	GLY	-	linker	UNP P52917

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Chain	Residue	Modelled	Actual	Comment	Reference
F	439	GLY	-	linker	UNP P52917
F	440	GLY	-	linker	UNP P52917
F	441	GLY	-	linker	UNP P52917
F	442	SER	-	linker	UNP P52917
F	443	GLY	-	linker	UNP P52917
F	444	GLY	-	linker	UNP P52917
F	445	GLY	-	linker	UNP P52917
F	446	GLY	-	linker	UNP P52917
F	447	SER	-	linker	UNP P52917
F	448	GLY	-	linker	UNP P52917
F	449	GLY	-	linker	UNP P52917
F	450	GLY	-	linker	UNP P52917
F	451	GLY	-	linker	UNP P52917
F	452	SER	-	linker	UNP P52917
F	453	GLY	-	linker	UNP P52917
F	454	GLY	-	linker	UNP P52917
F	455	GLY	-	linker	UNP P52917
F	618	GLY	-	expression tag	UNP Q9I747

- Molecule 2 is a protein called ACE-ASP-GLU-ILE-VAL-ASN-LYS-VAL-LEU-NH2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	10	Total	C	N	O	1	1
			68	43	11	14		

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

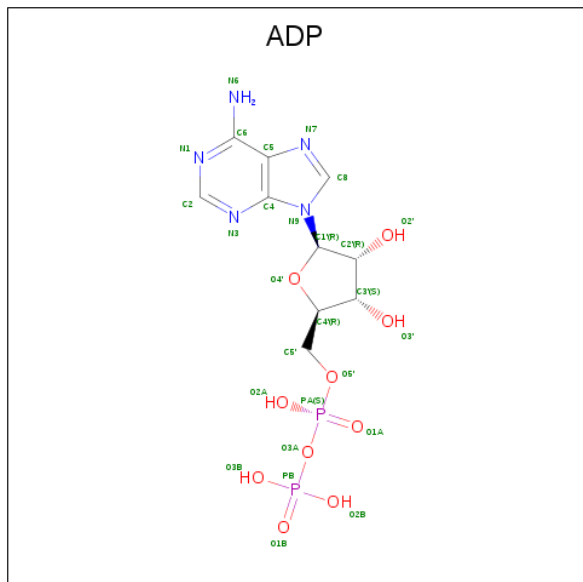
Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	42	Total	C	N	O	0	0
			331	209	54	68		
3	I	42	Total	C	N	O	0	0
			331	209	54	68		
3	J	42	Total	C	N	O	0	0
			331	209	54	68		
3	K	42	Total	C	N	O	0	0
			331	209	54	68		
3	L	42	Total	C	N	O	0	0
			331	209	54	68		
3	M	42	Total	C	N	O	0	0
			331	209	54	68		
3	N	42	Total	C	N	O	0	0
			331	209	54	68		

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Mol	Chain	Residues	Atoms				AltConf	Trace
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		

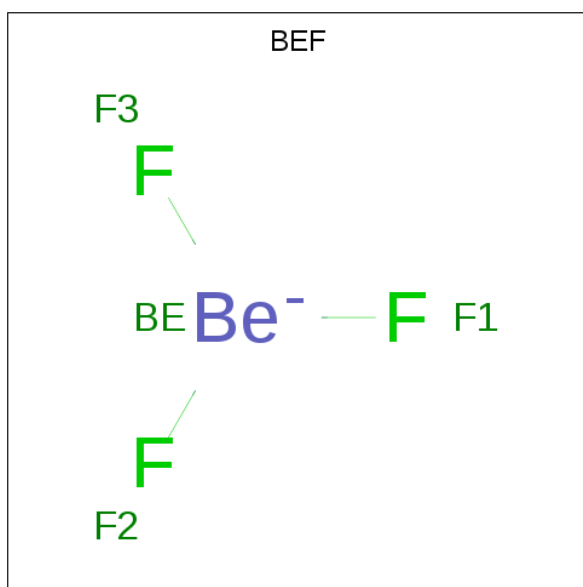
- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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	B	1	Total	Be	F	0
			4	1	3	
5	C	1	Total	Be	F	0
			4	1	3	

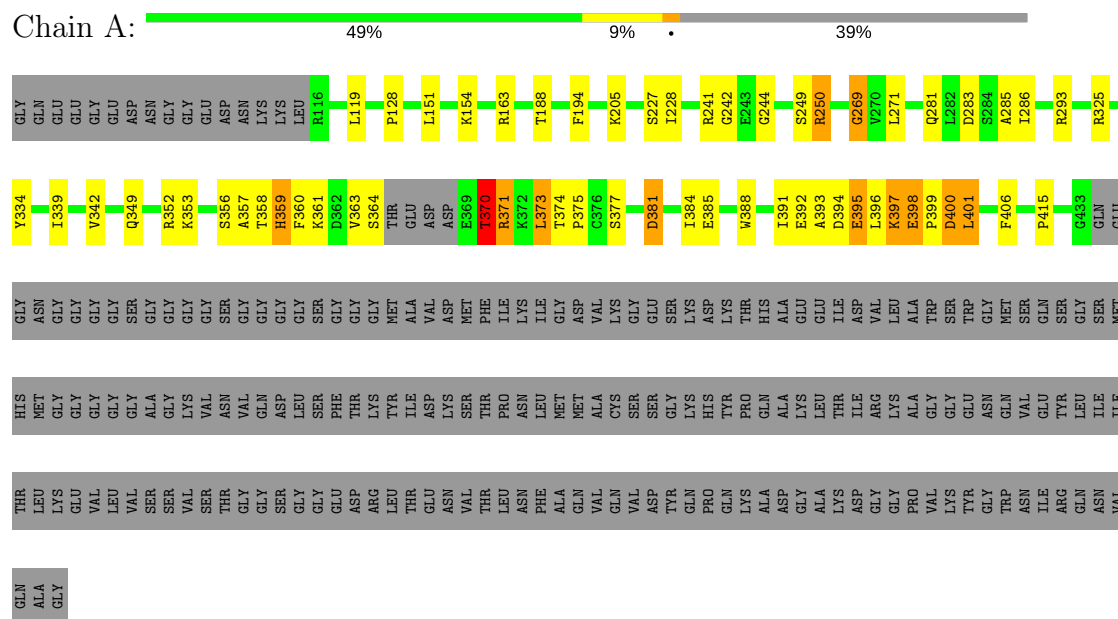
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

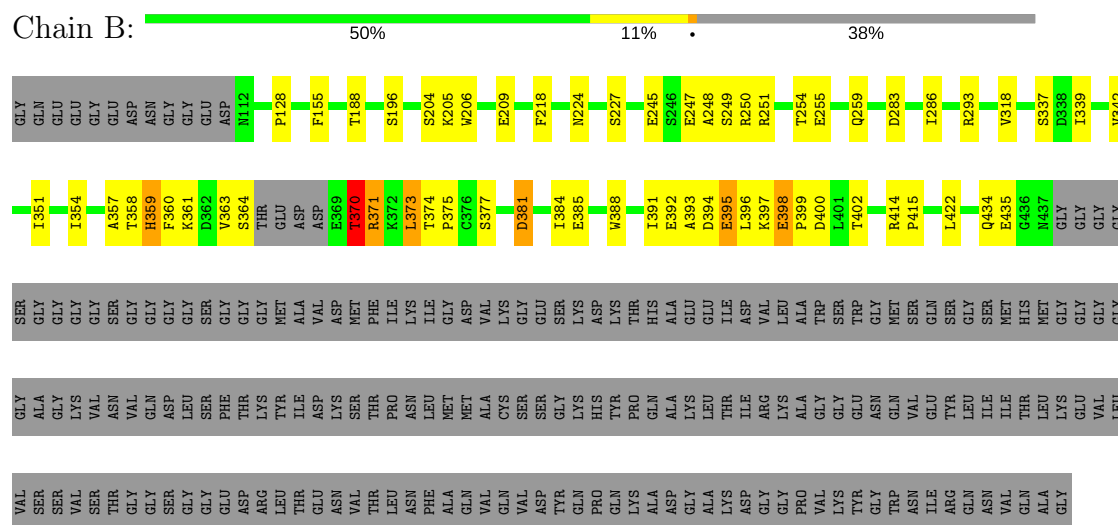
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Vacuolar protein sorting-associated protein 4, Protein hcp1

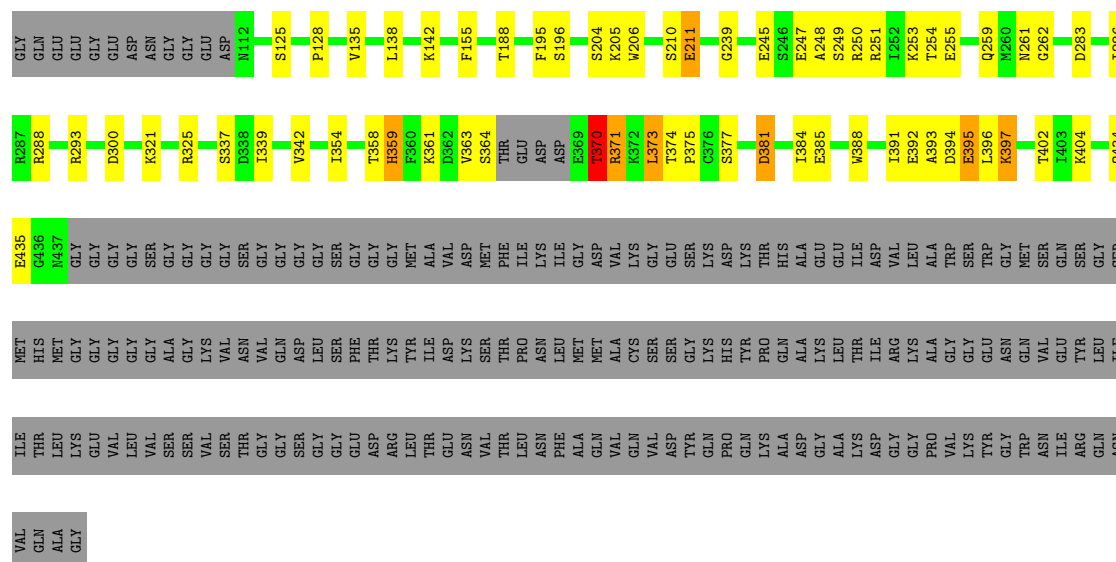


- Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1



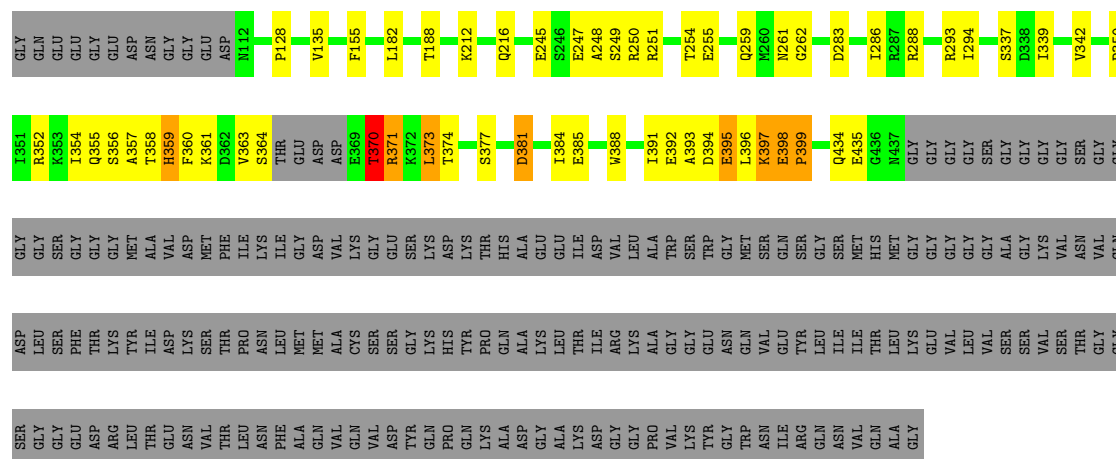
- Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1

Chain C:



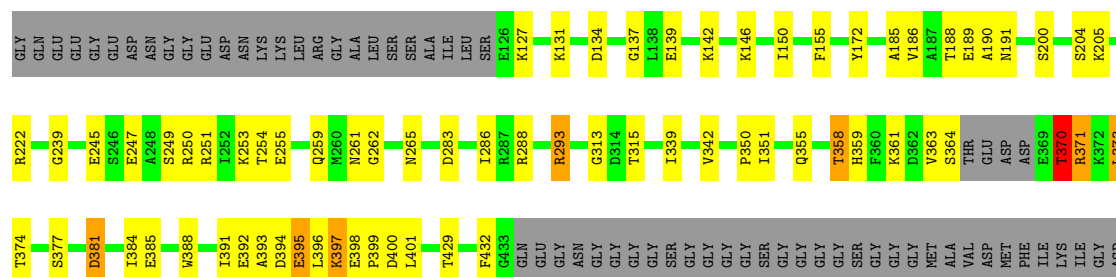
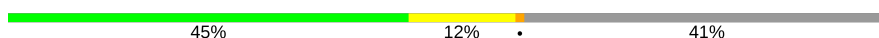
- Molecule 1: Vacuolar protein sorting-associated protein 4,Protein hcp1

Chain D:



- Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1

Chain E:



VAL	GLN	VAL	ASP	TYR	GLN	PRO	GLN	LYS	ALA	ASP	GLY	ALA	LYS	ASP	GLY	GLY	PRO	VAL	LYS	TYR	GLY	TRP	ASN	ILE	ARG	GLN	ASN	VAL	GLN	ALA	GLY
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- Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1

Chain F:  35% 22% 0% 41%

[illegible]

PHE	THR	THR	THR	TYR	ILE	ASP	LYS	SER	PRO	PRO	ASN	LEU	MET	MET	ALA	CYS	SER	SER	GLY	LYS	LYS	THR	THR	ILE	ARG	LYS	ALA	GLY	GLY	GLU	ASN	GLN	GLN	VAL	GLU	GLU	TYR	THR	LEU	ILE	ILE	THR	LYS	LEU	GLU	VAL	SER	SER	SER	VAL	SER	THR	GLY	GLY	SER	GLY	...
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GLU	ASP	ARG	LEU	THR	GLU	ASN	VAL	THR	LEU	ASN	PHE	ALA	GLN	VAL	GLN	VAL	ASP	TYR	GLN	PRO	GLN	LYS	ALA	ASP	GLY	ALA	LYS	ASP	GLY	GLY	GLY	PRO	VAL	LYS	TYR	GLY	TRP	ASN	ILE	ARG	GLN	ASN	VAL	GLN	ALA	GLY
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- Molecule 2: ACE-ASP-GLU-ILE-VAL-ASN-LYS-VAL-LEU-NH2

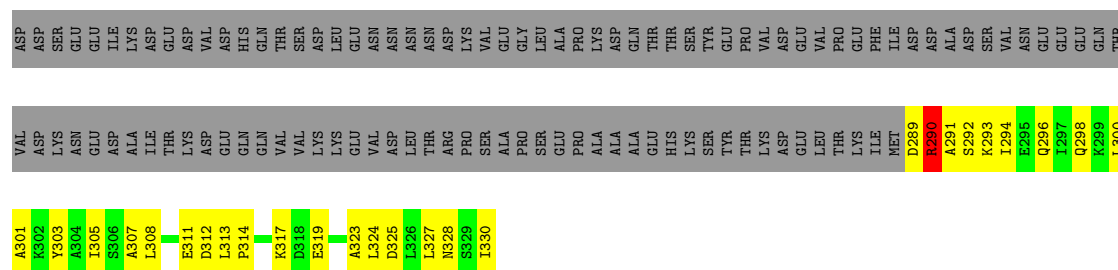
Chain G:  90% 10%

- Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain H:  5% 8% 87%

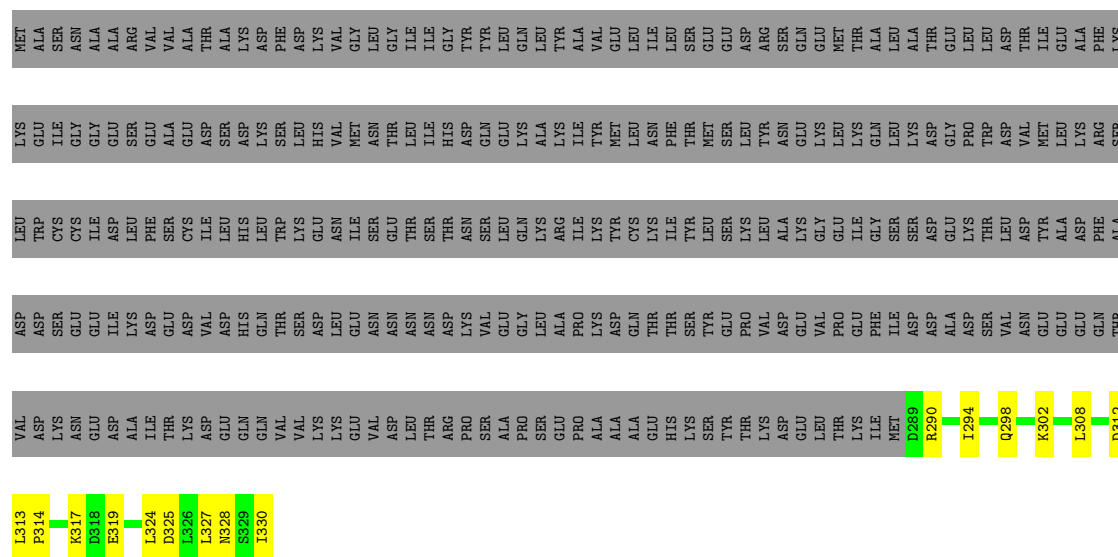
LYS GLU GLU ILE GLY GLY GLU SER GLU GLU ALA GLU ASP ASP LYS SER SER LEU LEU HIS VAL MET MET ASN ASN THR LEU ILE ILE HIS ASP GLN GLU LYS LYS LYS LYS ASN THR THR PHE MET MET SER SER LEU LEU TYR TYR ASN GLU LYS LEU LEU GLN LEU LYS ASP ASP VAL ASP ASP ARG

[illegible]



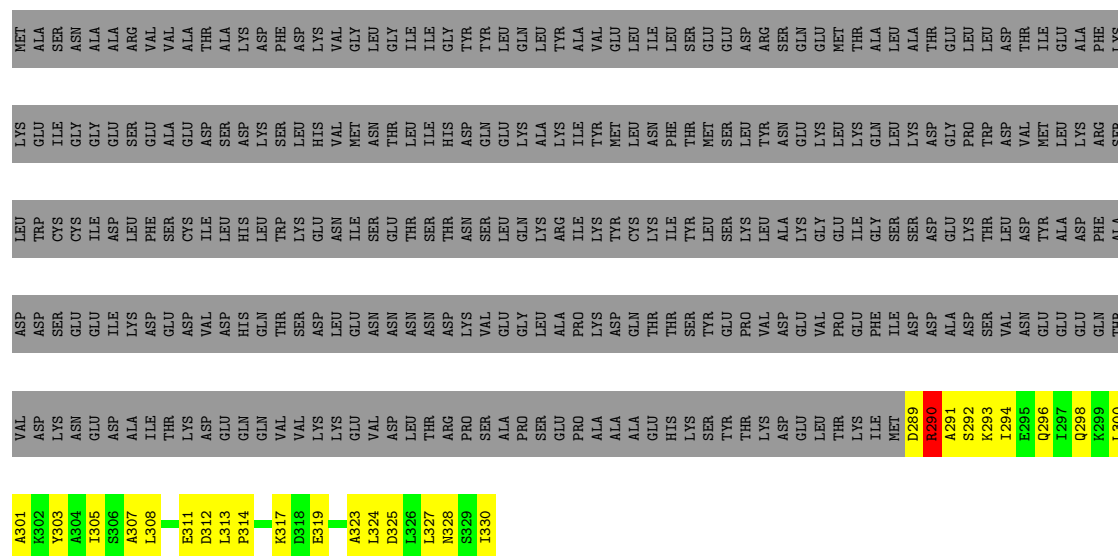
• Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain I: 8% 5% 87%



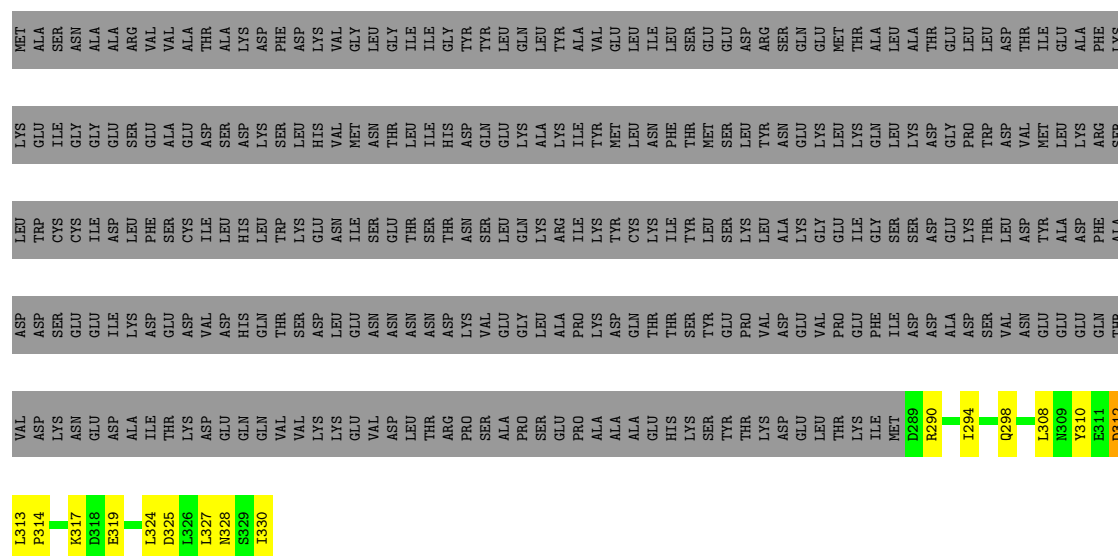
• Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain J: 5% 8% 87%



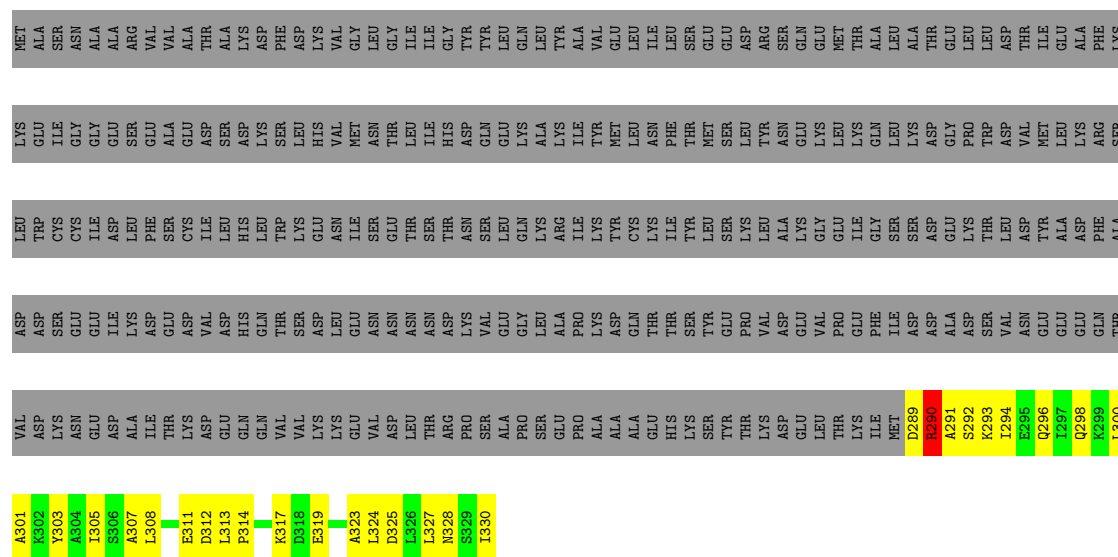
• Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain K:  8% . 87%



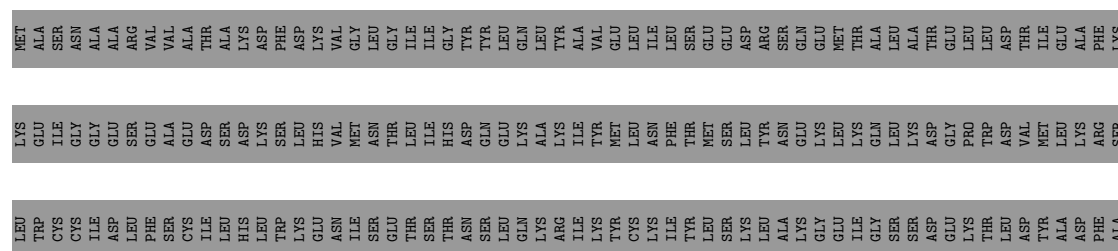
- Molecule 3: Vacuolar protein sorting-associated protein VTA1

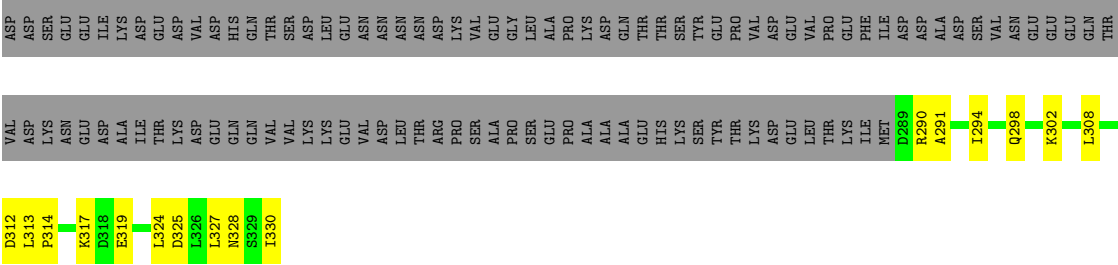
Chain L:  5% 8% 87%



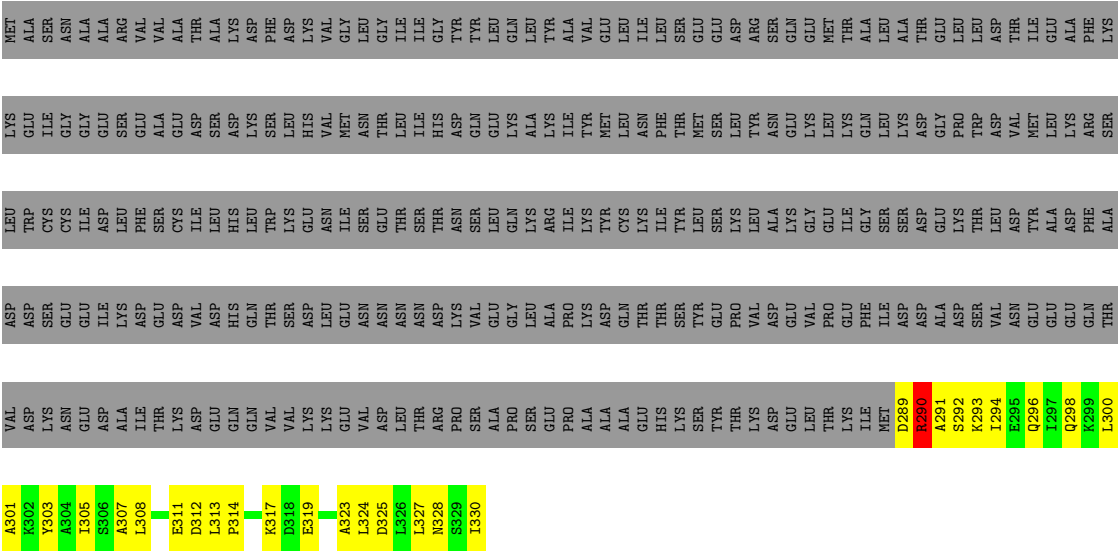
- Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain M:  8% 5% 87%

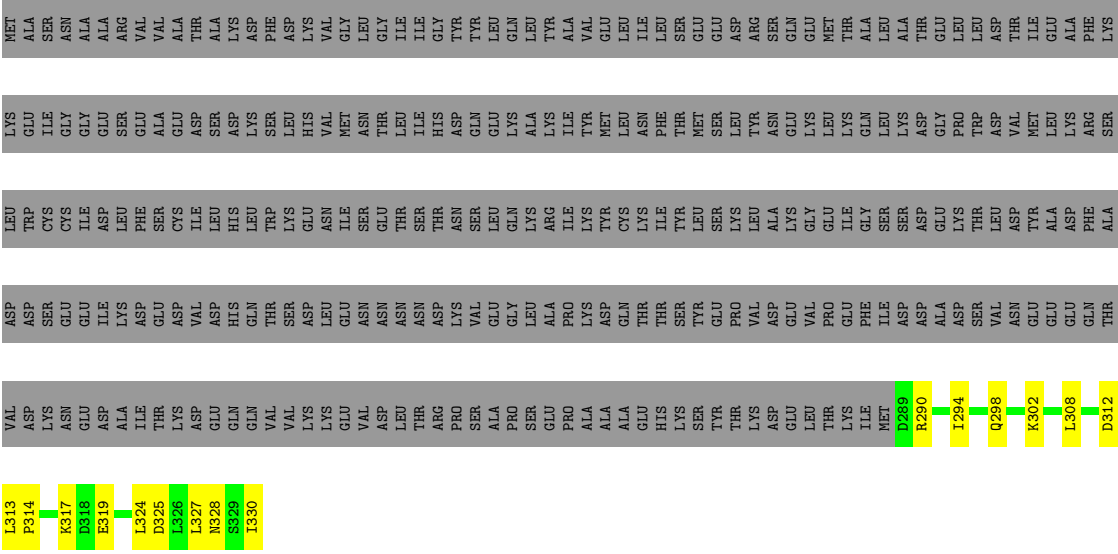




● Molecule 3: Vacuolar protein sorting-associated protein VTA1



● Molecule 3: Vacuolar protein sorting-associated protein VTA1



● Molecule 3: Vacuolar protein sorting-associated protein VTA1





ASP  
ASP  
SER  
GLU  
GLU  
ILE  
LYS  
ASP  
GLU  
ASP  
VAL  
ASP  
HIS  
GLN  
THR  
SER  
ASP  
LEU  
GLU  
ASN  
ASN  
ASN  
ASN  
ASP  
LYS  
VAL  
GLU  
GLY  
LEU  
ALA  
PRO  
LYS  
ASP  
GLN  
THR  
THR  
SER  
TYR  
GLU  
PRO  
VAL  
ASP  
GLU  
VAL  
PRO  
GLU  
PHE  
ILE  
MET  
ASP  
ASP  
ALA  
ASP  
SER  
VAL  
ASN  
GLU  
GLU  
GLN  
THR

VAL  
ASP  
LYS  
ASN  
GLU  
ASP  
ALA  
ILE  
THR  
LYS  
ASP  
GLU  
GLN  
VAL  
VAL  
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● Molecule 3: Vacuolar protein sorting-associated protein VTA1

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Q298  
L308  
K309  
Y310  
E311  
D312

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P314  
K317  
D318  
E319  
L324  
D325  
L326  
L327  
N328  
S329  
I330

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	82225	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.55	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, NH2

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	0.71	0/2468	0.81	2/3334 (0.1%)
1	B	0.78	0/2532	0.79	0/3418
1	C	0.79	1/2532 (0.0%)	0.83	2/3418 (0.1%)
1	D	0.75	0/2532	0.78	0/3418
1	E	0.70	0/2401	0.79	0/3244
1	F	0.59	0/2428	0.70	2/3281 (0.1%)
2	G	1.02	0/64	1.07	0/86
3	H	0.53	0/333	0.75	0/447
3	I	0.54	0/333	0.69	0/447
3	J	0.53	0/333	0.75	0/447
3	K	0.54	0/333	0.69	0/447
3	L	0.52	0/333	0.75	0/447
3	M	0.54	0/333	0.70	0/447
3	N	0.53	0/333	0.75	0/447
3	O	0.54	0/333	0.70	0/447
3	P	0.52	0/333	0.74	0/447
3	Q	0.54	0/333	0.69	0/447
3	R	0.53	0/333	0.75	0/447
3	S	0.54	0/333	0.69	0/447
All	All	0.69	1/18953 (0.0%)	0.77	6/25563 (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	1
1	B	0	1
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	211	GLU	CG-CD	-5.85	1.43	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ARG	NE-CZ-NH1	-6.81	116.89	120.30
1	C	138	LEU	CB-CG-CD2	-6.21	100.45	111.00
1	A	119	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	F	269	GLY	N-CA-C	5.18	126.06	113.10
1	F	287	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	195	PHE	CB-CG-CD1	5.11	124.38	120.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	GLY	Peptide
1	B	205	LYS	Peptide
1	C	125	SER	Mainchain

## 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	2427	0	2449	107	0
1	B	2491	0	2516	71	0
1	C	2491	0	2516	86	0
1	D	2491	0	2516	78	0
1	E	2360	0	2377	124	0
1	F	2387	0	2409	340	0
2	G	68	0	71	1	0
3	H	331	0	344	33	0
3	I	331	0	344	17	0
3	J	331	0	344	33	0
3	K	331	0	344	22	0
3	L	331	0	344	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	331	0	344	22	0
3	N	331	0	344	34	0
3	O	331	0	344	19	0
3	P	331	0	344	33	0
3	Q	331	0	344	18	0
3	R	331	0	344	36	0
3	S	331	0	344	29	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	0	0
4	E	27	0	12	0	0
5	A	4	0	0	1	0
5	B	4	0	0	1	0
5	C	4	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
6	D	1	0	0	0	0
All	All	18838	0	19042	904	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 24.

All (904) 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:172:TYR:CZ	1:F:428:PHE:CD2	1.78	1.63
1:F:172:TYR:CZ	1:F:428:PHE:HD2	0.93	1.57
1:F:295:TYR:CE1	1:F:425:GLN:HB3	1.37	1.54
1:F:199:SER:HB3	1:F:237:LEU:CG	1.39	1.53
1:E:388:TRP:CZ3	1:F:151:LEU:CD1	1.90	1.52
1:A:325:ARG:CZ	3:S:310:TYR:HB3	1.37	1.51
1:F:172:TYR:CE1	1:F:428:PHE:CD2	2.01	1.48
1:E:388:TRP:CE3	1:F:151:LEU:HD13	1.46	1.46
1:E:355:GLN:CG	1:F:151:LEU:HD22	1.45	1.43
1:F:295:TYR:CE1	1:F:425:GLN:CB	2.00	1.43
1:F:323:ASP:CB	1:F:403:ILE:HD12	1.46	1.42
1:E:355:GLN:NE2	1:F:151:LEU:HD21	1.29	1.41
1:F:172:TYR:CE1	1:F:428:PHE:CE2	2.13	1.35
1:B:354:ILE:CD1	1:B:396:LEU:HD11	1.54	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:TRP:CZ3	1:F:151:LEU:HD12	1.52	1.34
1:A:151:LEU:HD21	1:F:355:GLN:NE2	1.41	1.33
1:E:388:TRP:CE3	1:F:151:LEU:CD1	2.06	1.33
1:E:355:GLN:HG2	1:F:151:LEU:CD2	1.59	1.33
1:A:241:ARG:NE	1:F:205:LYS:CA	1.87	1.32
1:B:354:ILE:HD11	1:B:396:LEU:CD1	1.60	1.31
1:F:317:CYS:CB	1:F:401:LEU:HD23	1.60	1.31
1:E:388:TRP:CH2	1:F:151:LEU:HB2	1.66	1.30
1:A:163:ARG:CZ	1:F:351:ILE:HD11	1.60	1.29
1:F:350:PRO:O	1:F:399:PRO:HD2	1.20	1.29
1:A:151:LEU:HD21	1:F:355:GLN:CD	1.52	1.29
1:F:173:GLY:HA2	1:F:425:GLN:CD	1.59	1.23
1:F:199:SER:CB	1:F:237:LEU:HG	1.68	1.22
1:F:350:PRO:HB3	1:F:399:PRO:O	1.31	1.22
1:E:388:TRP:CZ2	1:F:151:LEU:HB2	1.76	1.20
1:E:388:TRP:CZ3	1:F:151:LEU:HD13	1.60	1.20
1:F:295:TYR:CD1	1:F:425:GLN:HB3	1.75	1.20
1:F:173:GLY:HA2	1:F:425:GLN:NE2	1.57	1.19
1:A:151:LEU:CD2	1:F:355:GLN:CD	2.10	1.19
1:D:358:THR:O	1:D:359:HIS:CD2	1.95	1.19
1:E:355:GLN:HA	1:E:388:TRP:CD1	1.78	1.18
1:F:358:THR:HA	1:F:386:MET:O	1.39	1.18
1:A:241:ARG:HE	1:F:205:LYS:CA	1.47	1.18
1:E:355:GLN:NE2	1:F:151:LEU:CD2	2.07	1.18
1:E:388:TRP:CD2	1:F:151:LEU:HD13	1.79	1.18
1:F:353:LYS:HB2	1:F:399:PRO:CG	1.74	1.17
1:F:317:CYS:HB3	1:F:401:LEU:CD2	1.73	1.17
1:A:325:ARG:CZ	3:S:310:TYR:CB	2.23	1.17
1:F:323:ASP:HB3	1:F:403:ILE:HD12	1.16	1.16
1:E:351:ILE:HD11	1:F:163:ARG:HD3	1.28	1.14
1:F:319:LEU:HD21	1:F:403:ILE:HA	1.30	1.13
1:E:351:ILE:HD11	1:F:163:ARG:CD	1.77	1.13
1:A:151:LEU:CD2	1:F:355:GLN:NE2	2.10	1.13
1:F:354:ILE:HG22	1:F:396:LEU:CD2	1.80	1.11
1:F:358:THR:HG23	1:F:359:HIS:N	1.63	1.11
1:E:355:GLN:CG	1:F:151:LEU:CD2	2.21	1.11
1:F:358:THR:O	1:F:360:PHE:CD1	2.04	1.11
1:F:350:PRO:O	1:F:399:PRO:CD	1.99	1.10
1:C:374:THR:HB	1:C:397:LYS:HG3	1.30	1.09
1:F:173:GLY:CA	1:F:425:GLN:NE2	2.15	1.09
1:F:354:ILE:HG13	1:F:399:PRO:HD3	1.10	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:293:ARG:HG2	1:F:428:PHE:HZ	1.11	1.08
1:E:355:GLN:HE21	1:F:151:LEU:CD2	1.64	1.08
1:E:388:TRP:CH2	1:F:151:LEU:CB	2.37	1.07
1:F:293:ARG:HG2	1:F:428:PHE:CZ	1.89	1.07
1:F:354:ILE:HG13	1:F:399:PRO:CD	1.85	1.07
1:F:319:LEU:CD2	1:F:403:ILE:HB	1.84	1.06
1:A:373:LEU:HD12	1:A:391:ILE:HD13	1.38	1.06
1:F:203:VAL:HG23	1:F:237:LEU:HD23	1.38	1.06
1:F:293:ARG:HB3	1:F:428:PHE:CE2	1.91	1.05
1:F:293:ARG:HB3	1:F:428:PHE:HE2	1.18	1.05
1:F:354:ILE:CG2	1:F:396:LEU:HG	1.86	1.05
1:A:241:ARG:HG3	1:F:204:SER:O	1.54	1.05
1:F:358:THR:HG23	1:F:359:HIS:H	0.97	1.05
1:F:373:LEU:HD12	1:F:391:ILE:HD13	1.38	1.05
1:F:358:THR:CA	1:F:386:MET:O	2.05	1.05
1:F:354:ILE:CG1	1:F:399:PRO:HD3	1.88	1.03
1:A:325:ARG:NH1	3:S:310:TYR:O	1.90	1.03
1:B:373:LEU:HD12	1:B:391:ILE:HD13	1.38	1.03
1:F:354:ILE:HG22	1:F:396:LEU:HD21	1.05	1.03
1:C:373:LEU:HD12	1:C:391:ILE:HD13	1.38	1.02
1:D:373:LEU:HD12	1:D:391:ILE:CD1	1.89	1.02
1:C:373:LEU:HD12	1:C:391:ILE:CD1	1.89	1.02
1:F:354:ILE:CG2	1:F:396:LEU:CG	2.37	1.02
1:D:358:THR:O	1:D:359:HIS:CG	2.13	1.02
1:F:373:LEU:HD12	1:F:391:ILE:CD1	1.89	1.02
1:A:373:LEU:HD12	1:A:391:ILE:CD1	1.89	1.02
1:D:373:LEU:HD12	1:D:391:ILE:HD13	1.38	1.02
1:A:163:ARG:CZ	1:F:351:ILE:CD1	2.37	1.01
1:E:373:LEU:HD12	1:E:391:ILE:CD1	1.89	1.01
1:F:172:TYR:CE2	1:F:428:PHE:CD2	2.47	1.01
1:F:295:TYR:HE1	1:F:425:GLN:CG	1.73	1.01
1:E:373:LEU:HD12	1:E:391:ILE:HD13	1.38	1.01
1:F:172:TYR:CE2	1:F:428:PHE:HB3	1.95	1.01
1:A:361:LYS:HD2	1:A:381:ASP:O	1.61	1.00
1:B:373:LEU:HD12	1:B:391:ILE:CD1	1.89	1.00
1:F:323:ASP:CA	1:F:403:ILE:HD12	1.91	1.00
1:F:361:LYS:HD2	1:F:381:ASP:O	1.61	1.00
1:B:361:LYS:HD2	1:B:381:ASP:O	1.61	1.00
1:A:325:ARG:NE	3:S:310:TYR:HB3	1.76	1.00
1:A:241:ARG:NE	1:F:205:LYS:HA	0.99	0.99
1:D:361:LYS:HD2	1:D:381:ASP:O	1.61	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:VAL:HG23	1:F:237:LEU:CD2	1.92	0.99
1:C:361:LYS:HD2	1:C:381:ASP:O	1.61	0.99
1:E:361:LYS:HD2	1:E:381:ASP:O	1.61	0.99
1:F:353:LYS:HB2	1:F:399:PRO:HG2	1.03	0.99
1:F:358:THR:O	1:F:360:PHE:HD1	1.39	0.98
1:F:354:ILE:CG2	1:F:396:LEU:CD2	2.41	0.98
1:F:354:ILE:CG2	1:F:396:LEU:HD21	1.92	0.97
1:F:293:ARG:HD3	1:F:432:PHE:HB3	1.44	0.97
1:C:377:SER:OG	3:L:307:ALA:HA	1.65	0.97
1:B:377:SER:OG	3:J:307:ALA:HA	1.64	0.97
1:F:377:SER:OG	3:R:307:ALA:HA	1.64	0.97
1:F:203:VAL:CG2	1:F:237:LEU:HD23	1.95	0.97
1:A:377:SER:OG	3:H:307:ALA:HA	1.64	0.96
1:F:323:ASP:CB	1:F:403:ILE:CD1	2.41	0.96
1:F:172:TYR:OH	1:F:428:PHE:HD2	1.47	0.96
1:E:377:SER:OG	3:P:307:ALA:HA	1.64	0.96
1:D:377:SER:OG	3:N:307:ALA:HA	1.64	0.96
1:F:199:SER:CB	1:F:237:LEU:CG	2.33	0.96
1:F:295:TYR:CE1	1:F:425:GLN:CG	2.48	0.95
1:F:173:GLY:C	1:F:425:GLN:NE2	2.20	0.95
1:F:199:SER:HB3	1:F:237:LEU:CD1	1.96	0.94
1:F:353:LYS:CB	1:F:399:PRO:HG2	1.94	0.94
1:F:350:PRO:C	1:F:399:PRO:HD2	1.87	0.94
1:E:388:TRP:CH2	1:F:151:LEU:CD1	2.50	0.94
1:F:319:LEU:HD23	1:F:403:ILE:HB	1.47	0.94
1:F:174:PRO:HB2	1:F:417:VAL:HG11	1.50	0.94
1:F:238:THR:HA	1:F:253:LYS:HD3	1.49	0.93
1:F:323:ASP:HB3	1:F:403:ILE:CD1	1.98	0.93
1:F:172:TYR:CE1	1:F:428:PHE:HE2	1.83	0.93
1:E:355:GLN:CD	1:F:151:LEU:CD2	2.37	0.93
1:E:351:ILE:O	1:E:355:GLN:OE1	1.87	0.92
1:A:163:ARG:NH2	1:F:351:ILE:HD11	1.83	0.92
1:F:247:GLU:O	1:F:251:ARG:HB2	1.69	0.92
1:E:398:GLU:OE1	1:F:163:ARG:NH1	2.03	0.92
1:F:174:PRO:HD3	1:F:421:ASP:OD2	1.70	0.92
1:B:245:GLU:O	1:B:249:SER:HB3	1.69	0.91
1:F:357:ALA:O	1:F:360:PHE:HE1	1.54	0.90
1:A:325:ARG:NH1	3:S:310:TYR:HB3	1.84	0.90
1:F:245:GLU:O	1:F:249:SER:HB3	1.69	0.90
1:F:354:ILE:HG23	1:F:396:LEU:HG	1.53	0.90
1:A:154:LYS:NZ	1:F:388:TRP:CZ3	2.39	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:TRP:CH2	1:F:151:LEU:HD13	2.06	0.89
1:F:173:GLY:CA	1:F:425:GLN:HE22	1.85	0.89
1:F:350:PRO:CB	1:F:399:PRO:O	2.20	0.88
1:F:319:LEU:CD2	1:F:403:ILE:CA	2.51	0.88
1:F:354:ILE:HG23	1:F:396:LEU:CG	2.04	0.88
1:E:355:GLN:CA	1:E:388:TRP:CD1	2.56	0.88
1:F:199:SER:CB	1:F:237:LEU:CD1	2.51	0.88
1:F:319:LEU:CD2	1:F:403:ILE:HA	2.03	0.88
1:F:319:LEU:CD2	1:F:403:ILE:CB	2.51	0.88
1:C:245:GLU:O	1:C:249:SER:HB3	1.74	0.87
1:C:374:THR:HB	1:C:397:LYS:CG	2.03	0.87
1:F:173:GLY:C	1:F:425:GLN:HE22	1.77	0.87
1:F:319:LEU:HD21	1:F:403:ILE:CA	2.04	0.87
1:D:358:THR:HG22	1:D:359:HIS:CD2	2.10	0.86
1:A:163:ARG:NH1	1:F:351:ILE:HD11	1.89	0.86
1:E:186:VAL:O	1:E:190:ALA:HB2	1.75	0.86
1:C:374:THR:CB	1:C:397:LYS:HG3	2.06	0.86
1:F:323:ASP:CG	1:F:403:ILE:HD12	1.96	0.86
1:E:355:GLN:HA	1:E:388:TRP:HD1	1.35	0.85
1:F:172:TYR:CD1	1:F:428:PHE:CE2	2.63	0.85
1:A:154:LYS:HD3	1:F:388:TRP:HZ3	1.39	0.85
1:E:351:ILE:HD11	1:F:163:ARG:CG	2.07	0.85
1:F:295:TYR:CZ	1:F:425:GLN:CB	2.60	0.84
1:E:351:ILE:CD1	1:F:163:ARG:HD3	2.05	0.84
1:F:355:GLN:O	1:F:388:TRP:CD1	2.29	0.84
1:F:295:TYR:CE1	1:F:425:GLN:HB2	2.13	0.83
1:F:250:ARG:O	1:F:254:THR:OG1	1.95	0.83
1:E:358:THR:HG23	1:E:359:HIS:CD2	2.14	0.83
1:F:357:ALA:HB3	1:F:360:PHE:CZ	2.14	0.83
1:D:245:GLU:O	1:D:249:SER:HB3	1.80	0.81
1:B:358:THR:O	1:B:359:HIS:HB2	1.79	0.81
1:F:374:THR:HB	1:F:397:LYS:HB3	1.62	0.81
1:E:313:GLY:HA3	1:F:162:ASN:HD21	1.45	0.81
3:L:311:GLU:CD	3:M:290:ARG:HH12	1.84	0.81
1:F:295:TYR:CZ	1:F:425:GLN:HB2	2.14	0.81
1:F:358:THR:CG2	1:F:359:HIS:N	2.39	0.80
3:P:311:GLU:CD	3:Q:290:ARG:HH12	1.84	0.80
3:H:311:GLU:CD	3:I:290:ARG:HH12	1.85	0.80
3:J:311:GLU:CD	3:K:290:ARG:HH12	1.85	0.80
1:F:317:CYS:HB3	1:F:401:LEU:HD23	0.83	0.80
3:N:311:GLU:CD	3:O:290:ARG:HH12	1.85	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:TRP:HZ3	1:F:151:LEU:HD12	1.45	0.79
1:F:199:SER:HB3	1:F:237:LEU:HG	0.81	0.79
1:E:398:GLU:OE1	1:F:163:ARG:CZ	2.30	0.79
3:R:311:GLU:CD	3:S:290:ARG:HH12	1.84	0.79
1:D:358:THR:O	1:D:359:HIS:CB	2.29	0.79
1:F:199:SER:HB3	1:F:237:LEU:CD2	2.13	0.79
1:F:199:SER:CB	1:F:237:LEU:HD11	2.13	0.78
1:F:357:ALA:O	1:F:360:PHE:CE1	2.36	0.78
1:F:238:THR:O	1:F:283:ASP:HB2	1.83	0.78
1:C:354:ILE:HD13	1:C:375:PRO:CG	2.13	0.78
1:F:319:LEU:HD22	1:F:403:ILE:HB	1.65	0.78
1:F:172:TYR:HE2	1:F:428:PHE:HB3	1.49	0.78
1:E:388:TRP:CE2	1:F:151:LEU:HD13	2.18	0.77
3:J:291:ALA:HA	3:J:294:ILE:HD11	1.66	0.77
1:F:173:GLY:HA2	1:F:425:GLN:OE1	1.84	0.77
1:A:358:THR:HG22	1:A:359:HIS:CD2	2.18	0.77
3:J:289:ASP:O	3:J:290:ARG:HB3	1.84	0.77
3:P:289:ASP:O	3:P:290:ARG:HB3	1.84	0.77
3:R:291:ALA:HA	3:R:294:ILE:HD11	1.67	0.77
3:L:291:ALA:HA	3:L:294:ILE:HD11	1.67	0.77
1:E:361:LYS:CD	1:E:381:ASP:O	2.33	0.77
3:N:308:LEU:HD12	3:O:298:GLN:HG3	1.67	0.77
3:P:308:LEU:HD12	3:Q:298:GLN:HG3	1.67	0.77
1:C:361:LYS:CD	1:C:381:ASP:O	2.33	0.77
3:L:308:LEU:HD12	3:M:298:GLN:HG3	1.67	0.77
3:P:291:ALA:HA	3:P:294:ILE:HD11	1.66	0.77
3:H:289:ASP:O	3:H:290:ARG:HB3	1.84	0.76
3:R:289:ASP:O	3:R:290:ARG:HB3	1.84	0.76
1:F:319:LEU:HD23	1:F:403:ILE:CB	2.14	0.76
3:N:289:ASP:O	3:N:290:ARG:HB3	1.84	0.76
3:N:291:ALA:HA	3:N:294:ILE:HD11	1.66	0.76
1:A:361:LYS:CD	1:A:381:ASP:O	2.33	0.76
1:D:361:LYS:CD	1:D:381:ASP:O	2.33	0.76
1:F:361:LYS:CD	1:F:381:ASP:O	2.33	0.76
1:A:154:LYS:HD3	1:F:388:TRP:CZ3	2.20	0.76
3:L:289:ASP:O	3:L:290:ARG:HB3	1.84	0.75
3:H:308:LEU:HD12	3:I:298:GLN:HG3	1.68	0.75
3:J:308:LEU:HD12	3:K:298:GLN:HG3	1.67	0.75
1:F:353:LYS:CB	1:F:399:PRO:CG	2.59	0.75
3:R:308:LEU:HD12	3:S:298:GLN:HG3	1.67	0.75
1:D:358:THR:O	1:D:359:HIS:HD2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:TRP:CH2	1:D:155:PHE:CE2	2.74	0.75
1:F:317:CYS:CB	1:F:401:LEU:CD2	2.45	0.74
3:H:291:ALA:HA	3:H:294:ILE:HD11	1.67	0.74
1:B:354:ILE:HD11	1:B:396:LEU:HD11	0.78	0.74
1:A:241:ARG:CZ	1:F:205:LYS:C	2.54	0.74
1:C:321:LYS:HD3	3:K:310:TYR:HD1	1.52	0.74
1:F:323:ASP:CG	1:F:403:ILE:CD1	2.55	0.74
1:F:354:ILE:HG23	1:F:396:LEU:CD1	2.17	0.74
1:F:354:ILE:HG21	1:F:396:LEU:HG	1.69	0.73
1:B:361:LYS:CD	1:B:381:ASP:O	2.33	0.73
1:F:174:PRO:HB2	1:F:417:VAL:CG1	2.19	0.72
1:F:172:TYR:OH	1:F:428:PHE:CD2	2.29	0.72
1:B:388:TRP:HH2	1:C:155:PHE:CE2	2.08	0.72
1:B:388:TRP:CH2	1:C:155:PHE:CE2	2.78	0.72
1:E:355:GLN:HB3	1:E:388:TRP:NE1	2.05	0.72
1:C:388:TRP:HH2	1:D:155:PHE:CE2	2.08	0.71
1:F:323:ASP:OD1	1:F:403:ILE:HD13	1.89	0.71
1:B:358:THR:O	1:B:359:HIS:CB	2.37	0.71
1:F:172:TYR:CZ	1:F:428:PHE:CG	2.73	0.71
1:E:394:ASP:O	1:E:396:LEU:N	2.23	0.71
1:F:172:TYR:CE2	1:F:428:PHE:CB	2.71	0.71
1:A:358:THR:O	1:A:359:HIS:CD2	2.44	0.71
1:F:317:CYS:HA	1:F:401:LEU:HB3	1.72	0.71
1:A:242:GLY:HA2	1:F:207:MET:HE3	1.73	0.71
1:F:346:ALA:CB	1:F:406:PHE:CD1	2.74	0.71
1:B:394:ASP:O	1:B:396:LEU:N	2.24	0.71
1:F:240:THR:HA	1:F:283:ASP:OD1	1.90	0.71
1:F:394:ASP:O	1:F:396:LEU:N	2.24	0.70
1:C:394:ASP:O	1:C:396:LEU:N	2.24	0.70
1:F:349:GLN:OE1	1:F:352:ARG:HD2	1.92	0.70
1:F:358:THR:O	1:F:360:PHE:CE1	2.44	0.70
1:A:394:ASP:O	1:A:396:LEU:N	2.23	0.70
1:D:358:THR:HG21	3:N:303:TYR:CE1	2.25	0.70
1:F:373:LEU:CD1	1:F:391:ILE:HD13	2.20	0.70
1:E:388:TRP:CH2	1:F:151:LEU:CA	2.73	0.70
1:F:174:PRO:CD	1:F:421:ASP:OD2	2.39	0.70
1:C:404:LYS:NZ	3:M:291:ALA:HB1	2.06	0.70
1:D:388:TRP:HZ3	1:E:155:PHE:CZ	2.08	0.70
1:A:163:ARG:NH2	1:F:351:ILE:CD1	2.54	0.70
1:B:373:LEU:CD1	1:B:391:ILE:CD1	2.69	0.70
1:A:241:ARG:CZ	1:F:205:LYS:O	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ARG:NE	1:F:205:LYS:C	2.44	0.70
1:A:373:LEU:CD1	1:A:391:ILE:CD1	2.69	0.70
1:F:199:SER:OG	1:F:237:LEU:CD1	2.41	0.69
1:B:373:LEU:CD1	1:B:391:ILE:HD13	2.20	0.69
1:A:325:ARG:NH2	3:S:310:TYR:CB	2.55	0.69
1:D:394:ASP:O	1:D:396:LEU:N	2.24	0.69
1:A:154:LYS:CD	1:F:388:TRP:HZ3	2.05	0.69
1:A:373:LEU:CD1	1:A:391:ILE:HD13	2.20	0.69
1:F:346:ALA:HB3	1:F:406:PHE:CE1	2.28	0.69
1:A:358:THR:O	1:A:359:HIS:CB	2.41	0.69
1:C:373:LEU:CD1	1:C:391:ILE:HD13	2.20	0.68
1:F:247:GLU:OE1	1:F:251:ARG:NH1	2.26	0.68
1:F:263:VAL:HG12	1:F:267:SER:CB	2.23	0.68
1:A:151:LEU:CD2	1:F:355:GLN:OE1	2.40	0.68
1:C:358:THR:O	1:C:359:HIS:CB	2.42	0.68
1:F:354:ILE:HG12	1:F:397:LYS:O	1.93	0.68
1:F:172:TYR:CD1	1:F:428:PHE:CD2	2.79	0.67
1:E:373:LEU:CD1	1:E:391:ILE:HD13	2.20	0.67
1:B:354:ILE:CG1	1:B:396:LEU:HD11	2.22	0.67
1:F:263:VAL:HG12	1:F:267:SER:HB2	1.76	0.67
3:N:308:LEU:HD12	3:O:298:GLN:CG	2.25	0.67
1:A:374:THR:HB	1:A:397:LYS:HB3	1.76	0.67
1:A:151:LEU:HD22	1:F:355:GLN:CD	2.09	0.67
1:C:373:LEU:CD1	1:C:391:ILE:CD1	2.70	0.67
1:F:373:LEU:CD1	1:F:391:ILE:CD1	2.69	0.67
1:F:298:LEU:HD21	1:F:417:VAL:HG21	1.77	0.67
3:J:308:LEU:HD13	3:K:294:ILE:HG23	1.77	0.67
1:E:373:LEU:CD1	1:E:391:ILE:CD1	2.69	0.67
3:R:308:LEU:HD13	3:S:294:ILE:HG23	1.77	0.67
1:C:358:THR:O	1:C:359:HIS:CD2	2.48	0.66
1:F:293:ARG:CG	1:F:428:PHE:CZ	2.73	0.66
3:L:308:LEU:HD12	3:M:298:GLN:CG	2.25	0.66
3:P:308:LEU:HD12	3:Q:298:GLN:CG	2.25	0.66
1:D:373:LEU:CD1	1:D:391:ILE:HD13	2.20	0.66
3:H:308:LEU:HD12	3:I:298:GLN:CG	2.25	0.66
1:A:358:THR:O	1:A:359:HIS:HB2	1.96	0.66
1:F:172:TYR:CE2	1:F:428:PHE:CG	2.83	0.66
3:J:308:LEU:HD12	3:K:298:GLN:CG	2.25	0.66
1:F:317:CYS:CB	1:F:401:LEU:HB3	2.25	0.66
1:F:355:GLN:O	1:F:388:TRP:CG	2.49	0.66
1:C:358:THR:O	1:C:359:HIS:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:291:ALA:HA	3:L:294:ILE:CD1	2.26	0.66
3:N:308:LEU:HD13	3:O:294:ILE:HG23	1.78	0.66
1:E:388:TRP:CH2	1:F:151:LEU:HA	2.31	0.66
1:A:151:LEU:HD23	1:F:355:GLN:NE2	2.10	0.66
1:D:373:LEU:CD1	1:D:391:ILE:CD1	2.70	0.66
1:F:358:THR:CG2	1:F:359:HIS:H	1.83	0.66
1:F:359:HIS:CE1	1:F:385:GLU:HB2	2.31	0.66
3:N:291:ALA:HA	3:N:294:ILE:CD1	2.26	0.66
1:A:151:LEU:HD21	1:F:355:GLN:CG	2.26	0.65
3:R:308:LEU:HD12	3:S:298:GLN:CG	2.25	0.65
1:F:323:ASP:OD1	1:F:403:ILE:CD1	2.44	0.65
1:F:174:PRO:N	1:F:425:GLN:NE2	2.44	0.65
1:B:245:GLU:O	1:B:249:SER:CB	2.44	0.65
1:C:359:HIS:CE1	1:C:385:GLU:HB2	2.31	0.65
1:D:337:SER:OG	1:E:288:ARG:NH1	2.30	0.65
3:L:308:LEU:HD13	3:M:294:ILE:HG23	1.77	0.65
1:A:359:HIS:CE1	1:A:385:GLU:HB2	2.32	0.65
1:B:359:HIS:CE1	1:B:385:GLU:HB2	2.31	0.65
1:E:359:HIS:CE1	1:E:385:GLU:HB2	2.32	0.65
1:F:293:ARG:CB	1:F:428:PHE:CE2	2.73	0.65
1:D:359:HIS:CE1	1:D:385:GLU:HB2	2.31	0.65
3:P:291:ALA:HA	3:P:294:ILE:CD1	2.26	0.65
1:F:199:SER:O	1:F:237:LEU:HD21	1.96	0.65
1:F:238:THR:C	1:F:283:ASP:HB2	2.17	0.65
1:F:405:ASP:O	1:F:408:LYS:HB3	1.97	0.65
3:H:291:ALA:HA	3:H:294:ILE:CD1	2.26	0.65
3:P:308:LEU:HD13	3:Q:294:ILE:HG23	1.77	0.65
3:R:291:ALA:HA	3:R:294:ILE:CD1	2.26	0.65
1:B:248:ALA:HB1	1:C:251:ARG:HH22	1.62	0.64
1:E:396:LEU:CD2	1:F:158:LEU:HD11	2.27	0.64
1:F:250:ARG:O	1:F:254:THR:CB	2.45	0.64
3:H:308:LEU:HD13	3:I:294:ILE:HG23	1.78	0.64
1:F:354:ILE:HG23	1:F:396:LEU:HD11	1.79	0.64
1:F:357:ALA:C	1:F:360:PHE:HE1	2.00	0.64
1:F:323:ASP:HA	1:F:403:ILE:HD12	1.74	0.64
3:J:291:ALA:HA	3:J:294:ILE:CD1	2.26	0.64
1:A:388:TRP:CH2	1:B:155:PHE:CE2	2.86	0.64
1:F:358:THR:C	1:F:386:MET:O	2.36	0.64
1:F:397:LYS:HZ2	1:F:397:LYS:HA	1.62	0.64
1:E:245:GLU:O	1:E:249:SER:HB3	1.98	0.64
1:F:167:SER:OG	1:F:263:VAL:HG21	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:404:LYS:HE2	3:R:311:GLU:CD	2.18	0.64
1:A:242:GLY:HA2	1:F:207:MET:CE	2.28	0.63
1:D:354:ILE:HD13	1:D:396:LEU:HD11	1.80	0.63
1:E:127:LYS:NZ	1:E:188:THR:O	2.29	0.63
1:F:323:ASP:HA	1:F:403:ILE:CD1	2.28	0.63
1:A:281:GLN:OE1	1:B:250:ARG:NH2	2.31	0.63
1:A:151:LEU:HD22	1:F:355:GLN:OE1	1.98	0.63
1:F:404:LYS:NZ	3:R:311:GLU:OE1	2.31	0.63
1:A:357:ALA:HB1	1:A:360:PHE:CE1	2.34	0.63
1:D:388:TRP:CZ3	1:E:155:PHE:CE2	2.87	0.62
1:A:325:ARG:NH2	3:S:310:TYR:HB2	2.13	0.62
1:E:247:GLU:HG2	1:E:251:ARG:HD2	1.79	0.62
1:A:400:ASP:OD1	1:A:400:ASP:N	2.25	0.62
1:F:169:ILE:HB	1:F:273:LEU:HD23	1.80	0.62
1:A:242:GLY:CA	1:F:207:MET:HE3	2.30	0.62
1:E:388:TRP:CZ2	1:F:151:LEU:HD13	2.35	0.62
1:E:377:SER:OG	3:P:307:ALA:CA	2.46	0.62
1:C:354:ILE:HD13	1:C:375:PRO:HG3	1.80	0.62
1:A:154:LYS:NZ	1:F:389:THR:HG22	2.15	0.62
1:A:377:SER:OG	3:H:307:ALA:CA	2.46	0.61
1:D:377:SER:OG	3:N:307:ALA:CA	2.46	0.61
1:E:355:GLN:CD	1:F:151:LEU:HD21	2.02	0.61
1:F:319:LEU:HD23	1:F:403:ILE:CA	2.30	0.61
1:C:321:LYS:HD3	3:K:310:TYR:CD1	2.36	0.61
1:E:398:GLU:OE1	1:F:163:ARG:NH2	2.32	0.61
1:F:317:CYS:HB2	1:F:401:LEU:CG	2.30	0.61
1:E:247:GLU:O	1:E:251:ARG:HB2	2.01	0.61
1:C:388:TRP:HH2	1:D:155:PHE:HE2	1.47	0.60
1:A:358:THR:O	1:A:358:THR:HG22	2.00	0.60
1:A:358:THR:O	1:A:359:HIS:CG	2.55	0.60
1:A:241:ARG:NE	1:F:205:LYS:O	2.34	0.60
3:N:290:ARG:O	3:N:294:ILE:HG12	2.02	0.60
1:F:323:ASP:CA	1:F:403:ILE:CD1	2.74	0.60
1:E:355:GLN:HG2	1:F:151:LEU:HD22	0.65	0.60
1:A:388:TRP:CZ3	1:B:155:PHE:CZ	2.89	0.60
1:C:388:TRP:HZ3	1:D:155:PHE:CZ	2.20	0.60
3:R:290:ARG:O	3:R:294:ILE:HG12	2.02	0.60
1:D:358:THR:O	1:D:358:THR:HG22	2.01	0.59
3:J:290:ARG:O	3:J:294:ILE:HG12	2.02	0.59
1:F:346:ALA:HB3	1:F:406:PHE:CD1	2.37	0.59
1:F:317:CYS:CA	1:F:401:LEU:HB3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:418:ASN:OD1	1:F:419:GLU:N	2.35	0.59
3:L:290:ARG:O	3:L:294:ILE:HG12	2.02	0.59
1:C:388:TRP:CZ3	1:D:155:PHE:CZ	2.89	0.59
1:F:199:SER:OG	1:F:237:LEU:HD11	2.00	0.59
1:F:295:TYR:HE1	1:F:425:GLN:CD	2.05	0.59
1:A:388:TRP:HZ3	1:B:155:PHE:CZ	2.20	0.59
1:F:357:ALA:C	1:F:360:PHE:CE1	2.75	0.59
3:H:290:ARG:O	3:H:294:ILE:HG12	2.01	0.59
1:A:373:LEU:HD12	1:A:391:ILE:HD11	1.84	0.59
3:P:290:ARG:O	3:P:294:ILE:HG12	2.02	0.59
1:E:355:GLN:CB	1:E:388:TRP:NE1	2.66	0.59
1:F:203:VAL:CG2	1:F:237:LEU:CD2	2.68	0.58
1:C:358:THR:O	1:C:358:THR:HG23	2.02	0.58
1:D:128:PRO:O	1:D:188:THR:OG1	2.20	0.58
1:F:350:PRO:CA	1:F:399:PRO:HD2	2.32	0.58
1:F:377:SER:OG	3:R:307:ALA:CA	2.46	0.58
1:F:394:ASP:C	1:F:396:LEU:H	2.07	0.58
1:B:358:THR:O	1:B:358:THR:HG23	2.03	0.58
1:E:204:SER:OG	1:E:205:LYS:N	2.37	0.58
1:D:358:THR:O	1:D:359:HIS:HB2	2.03	0.58
3:R:298:GLN:HG3	3:S:308:LEU:HD12	1.86	0.58
1:F:373:LEU:HD12	1:F:391:ILE:HD11	1.84	0.58
3:N:298:GLN:HG3	3:O:308:LEU:HD12	1.86	0.58
1:E:351:ILE:CD1	1:F:163:ARG:CG	2.79	0.58
3:J:298:GLN:HG3	3:K:308:LEU:HD12	1.86	0.58
1:D:388:TRP:CH2	1:E:155:PHE:HE2	2.22	0.58
1:C:128:PRO:O	1:C:188:THR:OG1	2.22	0.58
1:E:396:LEU:HD23	1:F:158:LEU:HD11	1.86	0.58
1:A:241:ARG:HD2	1:F:205:LYS:O	2.04	0.58
1:F:358:THR:O	1:F:359:HIS:C	2.41	0.58
1:E:222:ARG:NE	1:E:265:ASN:O	2.37	0.57
1:F:317:CYS:CB	1:F:401:LEU:CG	2.82	0.57
3:N:300:LEU:HD12	3:N:323:ALA:CA	2.34	0.57
1:B:373:LEU:HD12	1:B:391:ILE:HD11	1.84	0.57
1:D:388:TRP:CZ3	1:E:155:PHE:CZ	2.91	0.57
3:H:298:GLN:HG3	3:I:308:LEU:HD12	1.86	0.57
3:H:300:LEU:HD12	3:H:323:ALA:CA	2.35	0.57
1:C:247:GLU:O	1:C:251:ARG:HB2	2.03	0.57
1:C:354:ILE:HD13	1:C:375:PRO:HG2	1.87	0.57
1:C:404:LYS:HZ2	3:M:291:ALA:HB1	1.67	0.57
1:E:398:GLU:CD	1:F:163:ARG:HH22	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:PHE:O	1:F:312:VAL:HG13	2.05	0.57
1:F:300:ASP:OD1	1:F:303:ALA:HB3	2.05	0.57
1:E:355:GLN:CB	1:E:388:TRP:CD1	2.88	0.57
1:F:404:LYS:HA	1:F:407:LEU:HD12	1.86	0.57
3:P:300:LEU:HD12	3:P:323:ALA:CA	2.34	0.57
3:R:300:LEU:HD12	3:R:323:ALA:CA	2.35	0.57
1:D:352:ARG:O	1:D:356:SER:HB3	2.05	0.57
3:L:298:GLN:HG3	3:M:308:LEU:HD12	1.86	0.57
1:E:373:LEU:HD11	1:E:391:ILE:HG12	1.87	0.57
3:P:298:GLN:HG3	3:Q:308:LEU:HD12	1.86	0.57
1:C:358:THR:O	1:C:359:HIS:CG	2.58	0.57
1:E:185:ALA:O	1:E:189:GLU:HB2	2.04	0.57
1:F:350:PRO:HB3	1:F:399:PRO:C	2.18	0.57
1:B:373:LEU:HD11	1:B:391:ILE:HG12	1.87	0.56
1:C:394:ASP:C	1:C:396:LEU:H	2.08	0.56
1:E:351:ILE:HG23	1:E:355:GLN:HE22	1.69	0.56
4:C:701:ADP:O3B	5:C:702:BEF:F2	2.13	0.56
1:E:388:TRP:HH2	1:F:151:LEU:CA	2.18	0.56
1:B:394:ASP:C	1:B:396:LEU:H	2.08	0.56
1:F:373:LEU:HD11	1:F:391:ILE:HG12	1.87	0.56
3:J:300:LEU:HD12	3:J:323:ALA:CA	2.35	0.56
1:A:154:LYS:CE	1:F:388:TRP:HZ3	2.18	0.56
1:A:394:ASP:C	1:A:396:LEU:H	2.08	0.56
1:C:373:LEU:HD11	1:C:391:ILE:HG12	1.87	0.56
1:F:203:VAL:HG21	1:F:237:LEU:HD23	1.87	0.56
3:L:300:LEU:HD12	3:L:323:ALA:CA	2.34	0.56
1:A:227:SER:H	1:A:269:GLY:HA2	1.71	0.56
1:A:285:ALA:HB2	1:F:205:LYS:CE	2.36	0.56
1:A:373:LEU:HD11	1:A:391:ILE:HG12	1.87	0.55
1:E:358:THR:HG23	1:E:359:HIS:HD2	1.66	0.55
1:E:373:LEU:HD12	1:E:391:ILE:HD11	1.84	0.55
1:A:154:LYS:CE	1:F:388:TRP:CZ3	2.89	0.55
1:C:377:SER:OG	3:L:307:ALA:CA	2.46	0.55
1:E:394:ASP:C	1:E:396:LEU:H	2.07	0.55
1:D:373:LEU:HD11	1:D:391:ILE:HG12	1.87	0.55
1:E:313:GLY:HA3	1:F:162:ASN:ND2	2.19	0.55
1:B:377:SER:OG	3:J:307:ALA:CA	2.46	0.55
1:C:373:LEU:HD12	1:C:391:ILE:HD11	1.84	0.55
1:E:255:GLU:OE2	1:E:259:GLN:NE2	2.40	0.55
1:D:394:ASP:C	1:D:396:LEU:H	2.08	0.55
1:F:295:TYR:CE1	1:F:425:GLN:HG3	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:LEU:HD12	1:D:391:ILE:HD11	1.84	0.54
1:E:131:LYS:N	1:E:134:ASP:OD2	2.41	0.54
1:F:280:TRP:CH2	1:F:424:LYS:HD3	2.43	0.54
1:A:128:PRO:O	1:A:188:THR:OG1	2.25	0.54
1:D:245:GLU:O	1:D:249:SER:CB	2.53	0.54
1:F:349:GLN:OE1	1:F:352:ARG:NH1	2.39	0.54
3:J:290:ARG:HG3	3:J:291:ALA:N	2.22	0.54
1:B:255:GLU:O	1:B:259:GLN:HB2	2.08	0.54
1:B:388:TRP:CZ3	1:C:155:PHE:CZ	2.95	0.54
1:C:248:ALA:HB1	1:D:251:ARG:HH22	1.72	0.54
1:D:377:SER:HG	3:N:307:ALA:HA	1.71	0.54
3:H:290:ARG:HG3	3:H:291:ALA:N	2.22	0.54
1:C:255:GLU:O	1:C:259:GLN:HB2	2.08	0.54
1:C:325:ARG:HH22	3:K:312:ASP:HB2	1.72	0.54
1:D:255:GLU:O	1:D:259:GLN:HB2	2.08	0.54
1:E:388:TRP:CE3	1:F:151:LEU:HD11	2.32	0.54
1:F:304:ARG:NH1	1:F:328:GLY:O	2.40	0.54
1:E:255:GLU:O	1:E:259:GLN:HB2	2.08	0.54
3:P:290:ARG:HG3	3:P:291:ALA:N	2.22	0.54
3:L:290:ARG:HG3	3:L:291:ALA:N	2.22	0.54
1:B:255:GLU:OE2	1:B:259:GLN:NE2	2.40	0.54
1:F:174:PRO:CG	1:F:421:ASP:OD2	2.56	0.54
3:R:290:ARG:HG3	3:R:291:ALA:N	2.22	0.54
1:F:353:LYS:HB2	1:F:399:PRO:HG3	1.82	0.53
1:D:255:GLU:OE2	1:D:259:GLN:NE2	2.40	0.53
1:F:300:ASP:OD1	1:F:303:ALA:CB	2.56	0.53
1:E:388:TRP:HH2	1:F:151:LEU:HA	1.72	0.53
1:E:293:ARG:NH2	1:E:432:PHE:O	2.41	0.53
1:C:354:ILE:HD12	1:C:396:LEU:HD11	1.91	0.53
1:F:295:TYR:HE1	1:F:425:GLN:HG3	1.65	0.53
1:E:355:GLN:HE21	1:F:151:LEU:HD21	0.67	0.53
1:F:323:ASP:HB3	1:F:403:ILE:CG1	2.39	0.53
1:A:353:LYS:O	1:A:375:PRO:HG2	2.08	0.53
1:D:135:VAL:HG11	1:D:182:LEU:HD13	1.90	0.53
3:N:290:ARG:HG3	3:N:291:ALA:N	2.22	0.53
1:B:393:ALA:O	1:B:394:ASP:OD1	2.27	0.52
1:B:337:SER:OG	1:C:288:ARG:NH1	2.42	0.52
1:C:393:ALA:O	1:C:394:ASP:OD1	2.27	0.52
1:E:397:LYS:HG3	1:E:397:LYS:O	2.09	0.52
1:F:393:ALA:O	1:F:394:ASP:OD1	2.27	0.52
1:F:342:VAL:HG12	1:F:413:THR:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:TRP:HH2	1:C:155:PHE:HE2	1.54	0.52
1:A:241:ARG:CD	1:F:205:LYS:O	2.57	0.52
3:K:330:ILE:OXT	3:K:330:ILE:HG22	2.09	0.52
1:A:388:TRP:HH2	1:B:155:PHE:CE2	2.26	0.52
1:F:245:GLU:O	1:F:249:SER:CB	2.51	0.52
1:F:339:ILE:HA	1:F:342:VAL:HG22	1.91	0.52
1:F:293:ARG:HD3	1:F:432:PHE:CB	2.29	0.52
3:N:330:ILE:HG22	3:N:330:ILE:OXT	2.09	0.52
3:Q:330:ILE:OXT	3:Q:330:ILE:HG22	2.10	0.52
1:E:146:LYS:O	1:E:150:ILE:HB	2.09	0.52
1:C:255:GLU:OE2	1:C:259:GLN:NE2	2.40	0.52
1:E:393:ALA:O	1:E:394:ASP:OD1	2.27	0.52
3:R:330:ILE:HG22	3:R:330:ILE:OXT	2.09	0.52
4:B:701:ADP:O3B	5:B:702:BEF:F2	2.17	0.52
1:D:393:ALA:O	1:D:394:ASP:OD1	2.27	0.52
1:F:350:PRO:HA	1:F:399:PRO:CG	2.39	0.52
3:H:330:ILE:OXT	3:H:330:ILE:HG22	2.10	0.52
1:F:238:THR:HB	1:F:283:ASP:HB3	1.91	0.51
3:M:325:ASP:HA	3:M:328:ASN:HD22	1.76	0.51
1:E:351:ILE:CG1	1:F:163:ARG:HD3	2.40	0.51
1:E:200:SER:OG	1:F:250:ARG:HD2	2.11	0.51
1:F:317:CYS:HB2	1:F:401:LEU:HG	1.91	0.51
3:J:325:ASP:HA	3:J:328:ASN:HD22	1.75	0.51
3:Q:325:ASP:HA	3:Q:328:ASN:HD22	1.75	0.51
1:B:204:SER:HB3	1:B:209:GLU:HB2	1.92	0.51
3:J:330:ILE:HG22	3:J:330:ILE:OXT	2.10	0.51
1:A:325:ARG:HH22	3:S:312:ASP:HB2	1.75	0.51
3:H:325:ASP:HA	3:H:328:ASN:HD22	1.75	0.51
3:P:330:ILE:HG22	3:P:330:ILE:OXT	2.10	0.51
1:A:393:ALA:O	1:A:394:ASP:OD1	2.27	0.51
1:E:351:ILE:HD11	1:F:163:ARG:HG3	1.87	0.51
1:A:154:LYS:CD	1:F:388:TRP:CZ3	2.89	0.51
3:P:325:ASP:HA	3:P:328:ASN:HD22	1.75	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:B:354:ILE:HD13	1:B:396:LEU:HD21	1.93	0.51
3:I:325:ASP:HA	3:I:328:ASN:HD22	1.75	0.51
3:I:330:ILE:OXT	3:I:330:ILE:HG22	2.10	0.51
1:A:325:ARG:NE	3:S:310:TYR:CB	2.59	0.51
3:P:289:ASP:HA	3:P:292:SER:OG	2.11	0.51
3:L:325:ASP:HA	3:L:328:ASN:HD22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:293:LYS:HZ2	3:L:330:ILE:HD13	1.76	0.51
1:F:350:PRO:HA	1:F:399:PRO:HB2	1.92	0.50
3:M:330:ILE:OXT	3:M:330:ILE:HG22	2.10	0.50
3:O:325:ASP:HA	3:O:328:ASN:HD22	1.75	0.50
3:L:330:ILE:HG22	3:L:330:ILE:OXT	2.10	0.50
1:C:211:GLU:OE1	1:C:251:ARG:HB3	2.12	0.50
1:D:250:ARG:O	1:D:254:THR:CB	2.60	0.50
3:N:325:ASP:HA	3:N:328:ASN:HD22	1.75	0.50
3:K:325:ASP:HA	3:K:328:ASN:HD22	1.75	0.50
3:O:330:ILE:OXT	3:O:330:ILE:HG22	2.10	0.50
1:A:325:ARG:NH2	3:S:312:ASP:HB2	2.26	0.50
1:B:128:PRO:O	1:B:188:THR:OG1	2.28	0.50
1:A:285:ALA:HB2	1:F:205:LYS:HE3	1.93	0.50
1:F:207:MET:SD	1:F:248:ALA:HB2	2.52	0.50
3:R:289:ASP:HA	3:R:292:SER:OG	2.12	0.50
1:B:250:ARG:O	1:B:254:THR:CB	2.60	0.50
1:E:250:ARG:O	1:E:254:THR:CB	2.60	0.50
3:H:293:LYS:HZ2	3:H:330:ILE:HD13	1.77	0.50
3:S:330:ILE:HG22	3:S:330:ILE:OXT	2.10	0.50
3:H:289:ASP:HA	3:H:292:SER:OG	2.12	0.50
1:C:393:ALA:O	1:C:394:ASP:CG	2.51	0.49
1:D:354:ILE:HG22	1:D:388:TRP:HB3	1.94	0.49
3:N:289:ASP:HA	3:N:292:SER:OG	2.11	0.49
3:L:289:ASP:HA	3:L:292:SER:OG	2.12	0.49
3:N:293:LYS:HZ2	3:N:330:ILE:HD13	1.77	0.49
1:B:250:ARG:O	1:B:254:THR:HB	2.13	0.49
1:B:400:ASP:OD1	1:B:400:ASP:N	2.42	0.49
1:B:388:TRP:HZ3	1:C:155:PHE:CZ	2.30	0.49
1:C:250:ARG:O	1:C:254:THR:HB	2.13	0.49
1:E:388:TRP:CH2	1:F:151:LEU:CG	2.95	0.49
1:F:350:PRO:O	1:F:354:ILE:HG13	2.11	0.49
1:D:250:ARG:O	1:D:254:THR:HB	2.12	0.49
1:F:392:GLU:HB2	1:F:395:GLU:CD	2.33	0.49
3:R:293:LYS:HZ2	3:R:330:ILE:HD13	1.78	0.49
1:A:393:ALA:O	1:A:394:ASP:CG	2.51	0.49
1:B:247:GLU:O	1:B:251:ARG:HB2	2.13	0.49
1:B:393:ALA:O	1:B:394:ASP:CG	2.50	0.49
1:B:392:GLU:HB2	1:B:395:GLU:CD	2.33	0.49
1:C:250:ARG:O	1:C:254:THR:CB	2.60	0.49
1:D:393:ALA:O	1:D:394:ASP:CG	2.50	0.49
1:D:294:ILE:HA	1:D:434:GLN:HB3	1.95	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:E:393:ALA:O	1:E:394:ASP:CG	2.51	0.49
1:F:393:ALA:O	1:F:394:ASP:CG	2.50	0.49
3:J:327:LEU:O	3:J:327:LEU:HD12	2.13	0.49
1:D:358:THR:C	1:D:359:HIS:CG	2.84	0.49
1:E:239:GLY:H	1:E:253:LYS:HE2	1.77	0.49
3:K:327:LEU:O	3:K:327:LEU:HD12	2.13	0.49
3:P:293:LYS:HZ2	3:P:330:ILE:HD13	1.78	0.49
1:C:321:LYS:HD3	3:K:310:TYR:HA	1.95	0.49
1:C:392:GLU:HB2	1:C:395:GLU:CD	2.33	0.49
1:A:244:GLY:C	1:A:250:ARG:HH12	2.16	0.48
1:F:404:LYS:O	1:F:407:LEU:HB2	2.12	0.48
3:H:313:LEU:N	3:H:314:PRO:CD	2.76	0.48
3:J:313:LEU:N	3:J:314:PRO:CD	2.76	0.48
3:P:313:LEU:N	3:P:314:PRO:CD	2.76	0.48
3:S:313:LEU:N	3:S:314:PRO:CD	2.76	0.48
1:D:388:TRP:CH2	1:E:155:PHE:CE2	3.01	0.48
1:E:250:ARG:O	1:E:254:THR:HB	2.12	0.48
1:F:395:GLU:HG3	1:F:395:GLU:O	2.13	0.48
3:I:327:LEU:HD12	3:I:327:LEU:O	2.13	0.48
1:A:392:GLU:HB2	1:A:395:GLU:CD	2.33	0.48
3:Q:327:LEU:O	3:Q:327:LEU:HD12	2.13	0.48
1:F:293:ARG:NH1	1:F:432:PHE:CD1	2.81	0.48
3:L:327:LEU:HD12	3:L:327:LEU:O	2.13	0.48
1:C:404:LYS:HZ3	3:M:291:ALA:HB1	1.78	0.48
3:O:313:LEU:N	3:O:314:PRO:CD	2.76	0.48
3:P:327:LEU:O	3:P:327:LEU:HD12	2.13	0.48
1:A:357:ALA:CB	1:A:360:PHE:CE1	2.96	0.48
1:D:392:GLU:HB2	1:D:395:GLU:CD	2.33	0.48
3:R:313:LEU:N	3:R:314:PRO:CD	2.76	0.48
1:E:355:GLN:HB3	1:E:388:TRP:HE1	1.75	0.48
3:S:327:LEU:O	3:S:327:LEU:HD12	2.13	0.48
3:I:313:LEU:N	3:I:314:PRO:CD	2.76	0.48
3:K:313:LEU:N	3:K:314:PRO:CD	2.76	0.48
1:A:401:LEU:HD13	1:A:406:PHE:CE2	2.49	0.48
1:C:397:LYS:HG3	1:C:397:LYS:O	2.14	0.48
1:C:395:GLU:HG3	1:C:395:GLU:O	2.14	0.48
1:E:395:GLU:HG3	1:E:395:GLU:O	2.14	0.48
3:J:289:ASP:HA	3:J:292:SER:OG	2.12	0.48
3:N:313:LEU:N	3:N:314:PRO:CD	2.76	0.48
3:N:327:LEU:O	3:N:327:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:ARG:NH2	3:K:312:ASP:HB2	2.28	0.48
3:M:327:LEU:O	3:M:327:LEU:HD12	2.13	0.48
1:F:257:LEU:HD23	1:F:289:ARG:HG3	1.95	0.47
3:N:296:GLN:HE21	3:N:300:LEU:HG	1.79	0.47
3:O:327:LEU:HD12	3:O:327:LEU:O	2.13	0.47
1:C:300:ASP:N	1:C:300:ASP:OD1	2.43	0.47
1:F:206:TRP:O	1:F:209:GLU:HG2	2.14	0.47
1:F:166:THR:HG23	1:F:291:GLU:OE1	2.13	0.47
3:L:313:LEU:N	3:L:314:PRO:CD	2.76	0.47
1:A:395:GLU:HG3	1:A:395:GLU:O	2.14	0.47
1:B:395:GLU:HG3	1:B:395:GLU:O	2.14	0.47
1:C:261:ASN:ND2	1:C:288:ARG:HH22	2.11	0.47
1:D:395:GLU:HG3	1:D:395:GLU:O	2.14	0.47
1:F:166:THR:HG23	1:F:291:GLU:CD	2.34	0.47
1:F:351:ILE:O	1:F:355:GLN:HG3	2.14	0.47
3:M:313:LEU:N	3:M:314:PRO:CD	2.76	0.47
3:Q:313:LEU:N	3:Q:314:PRO:CD	2.76	0.47
3:H:327:LEU:O	3:H:327:LEU:HD12	2.13	0.47
1:D:248:ALA:HB1	1:E:251:ARG:HH22	1.78	0.47
3:R:327:LEU:HD12	3:R:327:LEU:O	2.13	0.47
1:D:394:ASP:OD1	1:D:395:GLU:N	2.48	0.47
3:H:296:GLN:HE21	3:H:300:LEU:HG	1.79	0.47
1:F:311:ASN:HB3	1:F:343:VAL:HG11	1.97	0.47
3:P:296:GLN:HE21	3:P:300:LEU:HG	1.79	0.47
1:A:349:GLN:OE1	1:A:352:ARG:NH1	2.46	0.47
1:E:139:GLU:HA	1:E:142:LYS:HD2	1.96	0.47
1:F:394:ASP:OD1	1:F:395:GLU:N	2.48	0.47
3:J:296:GLN:HE21	3:J:300:LEU:HG	1.79	0.47
1:C:394:ASP:OD1	1:C:395:GLU:N	2.48	0.47
1:D:397:LYS:HA	1:D:397:LYS:HD2	1.31	0.47
1:E:186:VAL:O	1:E:190:ALA:CB	2.55	0.47
3:R:296:GLN:HE21	3:R:300:LEU:HG	1.79	0.47
4:A:701:ADP:O1B	5:A:702:BEF:F2	2.22	0.47
1:B:394:ASP:OD1	1:B:395:GLU:N	2.48	0.47
1:C:397:LYS:C	1:C:397:LYS:HD2	2.35	0.47
1:D:357:ALA:HB3	1:D:360:PHE:CE1	2.50	0.46
3:K:324:LEU:O	3:K:328:ASN:ND2	2.49	0.46
1:F:249:SER:HA	1:F:253:LYS:HE3	1.97	0.46
3:P:328:ASN:OD1	3:Q:317:LYS:HE3	2.16	0.46
1:A:394:ASP:OD1	1:A:395:GLU:N	2.48	0.46
1:F:317:CYS:CB	1:F:401:LEU:CB	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:324:LEU:O	3:O:328:ASN:ND2	2.49	0.46
3:R:311:GLU:OE1	3:S:290:ARG:NH1	2.49	0.46
3:R:317:LYS:HE3	3:S:328:ASN:OD1	2.16	0.46
1:E:394:ASP:HA	1:F:157:HIS:CE1	2.49	0.46
3:N:328:ASN:OD1	3:O:317:LYS:HE3	2.16	0.46
3:P:324:LEU:O	3:P:328:ASN:ND2	2.49	0.46
1:A:285:ALA:CB	1:F:205:LYS:CE	2.94	0.46
1:D:212:LYS:O	1:D:216:GLN:HB2	2.16	0.46
1:F:139:GLU:HG2	1:F:139:GLU:H	1.45	0.46
3:N:324:LEU:O	3:N:328:ASN:ND2	2.49	0.46
3:P:311:GLU:OE1	3:Q:290:ARG:NH1	2.49	0.46
1:D:374:THR:CB	1:D:397:LYS:O	2.64	0.46
3:J:317:LYS:HE3	3:K:328:ASN:OD1	2.16	0.46
3:L:317:LYS:HE3	3:M:328:ASN:OD1	2.16	0.46
3:N:311:GLU:OE1	3:O:290:ARG:NH1	2.49	0.46
3:N:317:LYS:HE3	3:O:328:ASN:OD1	2.16	0.46
3:P:317:LYS:HE3	3:Q:328:ASN:OD1	2.16	0.46
1:F:225:LYS:HD3	1:F:269:GLY:HA3	1.98	0.46
3:H:328:ASN:OD1	3:I:317:LYS:HE3	2.16	0.46
3:J:324:LEU:O	3:J:328:ASN:ND2	2.48	0.46
3:L:296:GLN:HE21	3:L:300:LEU:HG	1.80	0.46
3:R:324:LEU:O	3:R:328:ASN:ND2	2.49	0.46
1:E:351:ILE:CD1	1:F:163:ARG:HG3	2.45	0.46
1:E:358:THR:O	1:E:359:HIS:HB2	2.16	0.46
1:E:394:ASP:OD1	1:E:395:GLU:N	2.48	0.46
1:F:174:PRO:N	1:F:425:GLN:HE21	2.14	0.46
3:L:311:GLU:OE1	3:M:290:ARG:NH1	2.49	0.46
3:L:324:LEU:O	3:L:328:ASN:ND2	2.48	0.46
1:E:350:PRO:HB3	1:E:399:PRO:HB2	1.98	0.46
3:H:317:LYS:HE3	3:I:328:ASN:OD1	2.16	0.46
3:H:311:GLU:OE1	3:I:290:ARG:NH1	2.49	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	2.16	0.46
1:E:127:LYS:HZ3	1:E:191:ASN:H	1.64	0.45
1:F:298:LEU:CD2	1:F:417:VAL:HG21	2.45	0.45
1:E:172:TYR:HH	1:E:429:THR:HG1	1.63	0.45
1:F:136:ALA:HB1	1:F:303:ALA:HB1	1.98	0.45
1:F:315:THR:HG21	1:F:347:LEU:HD22	1.98	0.45
3:P:301:ALA:O	3:P:305:ILE:HG13	2.16	0.45
1:F:212:LYS:HE3	1:F:216:GLN:HE21	1.81	0.45
3:L:328:ASN:OD1	3:M:317:LYS:HE3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ARG:HD3	1:B:415:PRO:HD2	1.99	0.45
1:E:127:LYS:HG2	1:E:188:THR:HA	1.98	0.45
1:E:398:GLU:CD	1:F:163:ARG:NH2	2.69	0.45
1:F:250:ARG:O	1:F:254:THR:HB	2.15	0.45
3:H:324:LEU:O	3:H:328:ASN:ND2	2.49	0.45
3:L:301:ALA:O	3:L:305:ILE:HG13	2.16	0.45
3:N:301:ALA:O	3:N:305:ILE:HG13	2.16	0.45
3:R:328:ASN:OD1	3:S:317:LYS:HE3	2.16	0.45
3:S:324:LEU:O	3:S:328:ASN:ND2	2.49	0.45
1:A:370:THR:O	1:A:371:ARG:O	2.35	0.45
1:F:323:ASP:CG	1:F:403:ILE:HG21	2.36	0.45
3:J:311:GLU:OE1	3:K:290:ARG:NH1	2.49	0.45
3:M:324:LEU:O	3:M:328:ASN:ND2	2.49	0.45
3:Q:324:LEU:O	3:Q:328:ASN:ND2	2.49	0.45
3:R:301:ALA:O	3:R:305:ILE:HG13	2.16	0.45
1:E:374:THR:HB	1:E:397:LYS:HG2	1.97	0.45
1:F:263:VAL:CG1	1:F:267:SER:HB2	2.46	0.45
1:F:290:PHE:O	1:F:291:GLU:C	2.55	0.45
3:P:311:GLU:CD	3:Q:290:ARG:NH1	2.64	0.45
1:F:199:SER:CA	1:F:237:LEU:HD21	2.47	0.45
1:F:172:TYR:HE1	1:F:428:PHE:CE2	2.14	0.45
1:A:163:ARG:HD3	1:F:351:ILE:HG12	1.99	0.45
1:F:357:ALA:HB3	1:F:360:PHE:CE1	2.51	0.45
1:C:239:GLY:H	1:C:253:LYS:CE	2.30	0.45
1:D:247:GLU:O	1:D:251:ARG:HB2	2.17	0.45
1:F:385:GLU:OE2	3:R:303:TYR:OH	2.31	0.45
3:J:301:ALA:O	3:J:305:ILE:HG13	2.16	0.45
1:C:135:VAL:HB	1:C:142:LYS:HE2	1.99	0.44
1:C:245:GLU:O	1:C:249:SER:CB	2.57	0.44
1:C:370:THR:O	1:C:371:ARG:O	2.35	0.44
1:C:397:LYS:C	1:C:397:LYS:CD	2.85	0.44
1:D:355:GLN:HA	1:D:388:TRP:CD1	2.51	0.44
1:E:370:THR:O	1:E:371:ARG:O	2.35	0.44
1:C:206:TRP:HZ3	2:G:167:ILE:HB	1.82	0.44
3:J:300:LEU:HD12	3:J:323:ALA:HA	1.99	0.44
1:C:388:TRP:CZ3	1:D:155:PHE:CE2	3.04	0.44
1:D:388:TRP:HZ3	1:E:155:PHE:HZ	1.60	0.44
3:H:301:ALA:O	3:H:305:ILE:HG13	2.16	0.44
3:J:293:LYS:HZ2	3:J:330:ILE:HD13	1.81	0.44
1:A:334:TYR:CE1	1:A:415:PRO:HG3	2.52	0.44
1:B:370:THR:O	1:B:371:ARG:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:300:LEU:HD12	3:P:323:ALA:HA	1.99	0.44
3:P:308:LEU:CD1	3:Q:298:GLN:HG3	2.44	0.44
3:R:300:LEU:HD12	3:R:323:ALA:HA	1.99	0.44
1:E:400:ASP:CG	1:E:401:LEU:H	2.21	0.44
1:F:353:LYS:CB	1:F:399:PRO:HG3	2.41	0.44
1:A:194:PHE:HD1	1:A:228:ILE:HG23	1.83	0.44
1:A:385:GLU:OE2	3:H:303:TYR:OH	2.30	0.44
1:B:388:TRP:CH2	1:C:155:PHE:CZ	3.05	0.44
1:C:337:SER:OG	1:D:288:ARG:NH1	2.50	0.44
1:D:370:THR:O	1:D:371:ARG:O	2.35	0.44
1:F:354:ILE:CG2	1:F:396:LEU:HD11	2.46	0.44
1:F:363:VAL:O	1:F:364:SER:HB3	2.18	0.44
1:D:350:PRO:HB3	1:D:399:PRO:HB2	2.00	0.44
1:F:370:THR:O	1:F:371:ARG:O	2.35	0.43
1:A:363:VAL:O	1:A:364:SER:HB3	2.18	0.43
1:B:351:ILE:HA	1:B:354:ILE:HG22	2.00	0.43
1:B:363:VAL:O	1:B:364:SER:HB3	2.18	0.43
1:F:354:ILE:CG2	1:F:396:LEU:CD1	2.87	0.43
1:A:375:PRO:HD2	1:A:399:PRO:HG3	2.01	0.43
1:A:388:TRP:HH2	1:B:155:PHE:HE2	1.63	0.43
1:C:261:ASN:OD1	1:C:262:GLY:N	2.51	0.43
1:D:363:VAL:O	1:D:364:SER:HB3	2.18	0.43
1:F:351:ILE:CD1	1:F:398:GLU:OE1	2.66	0.43
1:A:358:THR:HG22	1:A:359:HIS:HD2	1.75	0.43
1:D:373:LEU:CD1	1:D:391:ILE:HG12	2.48	0.43
1:D:434:GLN:HG3	1:D:435:GLU:H	1.84	0.43
1:E:373:LEU:CD1	1:E:391:ILE:HG12	2.49	0.43
1:B:373:LEU:CD1	1:B:391:ILE:HG12	2.49	0.43
1:C:239:GLY:H	1:C:253:LYS:HE2	1.83	0.43
1:D:355:GLN:HA	1:D:388:TRP:HD1	1.84	0.43
3:N:311:GLU:CD	3:O:290:ARG:NH1	2.64	0.43
1:B:357:ALA:CB	1:B:375:PRO:HB3	2.49	0.43
1:B:434:GLN:HG3	1:B:435:GLU:H	1.84	0.43
1:C:385:GLU:OE2	3:L:303:TYR:OH	2.31	0.43
1:E:247:GLU:HG2	1:E:251:ARG:NH1	2.34	0.43
1:F:351:ILE:HD11	1:F:398:GLU:OE1	2.18	0.43
1:F:373:LEU:CD1	1:F:391:ILE:HG12	2.49	0.43
1:F:346:ALA:CB	1:F:406:PHE:CE1	2.96	0.43
3:H:300:LEU:HD12	3:H:323:ALA:HA	1.99	0.43
3:N:300:LEU:HD12	3:N:323:ALA:HA	1.99	0.43
1:C:210:SER:OG	1:C:247:GLU:OE2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:VAL:O	1:C:364:SER:HB3	2.18	0.43
1:D:374:THR:OG1	1:D:397:LYS:O	2.33	0.43
1:E:363:VAL:O	1:E:364:SER:HB3	2.18	0.43
1:F:132:TRP:CE2	1:F:189:GLU:HG3	2.53	0.43
1:A:358:THR:HG21	3:H:303:TYR:CE1	2.53	0.43
3:R:311:GLU:CD	3:S:290:ARG:NH1	2.64	0.43
1:A:398:GLU:H	1:A:398:GLU:HG3	1.59	0.43
3:L:300:LEU:HD12	3:L:323:ALA:HA	1.99	0.43
1:C:196:SER:O	1:C:196:SER:OG	2.35	0.43
1:C:283:ASP:HB3	1:C:286:ILE:HD12	2.01	0.43
1:C:434:GLN:HG3	1:C:435:GLU:H	1.84	0.42
1:F:354:ILE:CG1	1:F:399:PRO:CD	2.69	0.42
1:D:283:ASP:HB3	1:D:286:ILE:HD12	2.01	0.42
1:F:238:THR:O	1:F:283:ASP:CB	2.63	0.42
3:L:317:LYS:N	3:M:327:LEU:HD21	2.35	0.42
3:R:317:LYS:N	3:S:327:LEU:HD21	2.35	0.42
1:A:283:ASP:HB3	1:A:286:ILE:HD12	2.01	0.42
1:B:385:GLU:OE2	3:J:303:TYR:OH	2.31	0.42
1:D:398:GLU:HA	1:D:399:PRO:HD3	1.79	0.42
1:F:265:ASN:HD22	1:F:265:ASN:N	2.17	0.42
1:F:350:PRO:HA	1:F:399:PRO:CB	2.49	0.42
1:F:422:LEU:O	1:F:426:GLU:HG3	2.19	0.42
3:R:327:LEU:HD21	3:S:317:LYS:N	2.35	0.42
3:J:317:LYS:N	3:K:327:LEU:HD21	2.35	0.42
1:B:224:ASN:O	1:B:227:SER:OG	2.37	0.42
1:B:283:ASP:HB3	1:B:286:ILE:HD12	2.01	0.42
1:B:374:THR:HB	1:B:397:LYS:HB3	2.00	0.42
1:F:238:THR:HB	1:F:283:ASP:CB	2.50	0.42
3:H:327:LEU:HD21	3:I:317:LYS:N	2.35	0.42
3:N:300:LEU:HD12	3:N:323:ALA:N	2.35	0.42
3:P:300:LEU:HD12	3:P:323:ALA:N	2.35	0.42
1:A:249:SER:HB3	1:A:250:ARG:NH1	2.34	0.42
1:B:357:ALA:HB2	1:B:375:PRO:HB3	2.02	0.42
1:B:318:VAL:HG11	1:B:402:THR:HG23	2.00	0.42
1:F:174:PRO:HD3	1:F:425:GLN:HG3	2.02	0.42
1:F:173:GLY:CA	1:F:425:GLN:OE1	2.62	0.42
3:N:317:LYS:N	3:O:327:LEU:HD21	2.35	0.42
3:N:327:LEU:HD21	3:O:317:LYS:N	2.35	0.42
3:R:300:LEU:HD12	3:R:323:ALA:N	2.35	0.42
1:A:397:LYS:CD	1:A:397:LYS:C	2.88	0.42
1:B:218:PHE:CD2	1:B:259:GLN:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:ILE:CD1	1:D:396:LEU:HD11	2.49	0.42
1:E:359:HIS:HA	1:E:384:ILE:O	2.20	0.42
1:E:396:LEU:HD21	1:F:158:LEU:HD11	1.99	0.42
3:J:308:LEU:CD1	3:K:298:GLN:HG3	2.44	0.42
3:N:308:LEU:CD1	3:O:298:GLN:HG3	2.44	0.42
1:B:398:GLU:HA	1:B:399:PRO:HD3	1.96	0.42
3:H:317:LYS:N	3:I:327:LEU:HD21	2.35	0.42
3:L:327:LEU:HD21	3:M:317:LYS:N	2.35	0.42
3:P:317:LYS:N	3:Q:327:LEU:HD21	2.35	0.42
1:E:315:THR:OG1	1:F:162:ASN:HB2	2.20	0.42
1:B:359:HIS:HA	1:B:384:ILE:O	2.20	0.41
1:D:261:ASN:OD1	1:D:262:GLY:N	2.51	0.41
1:E:283:ASP:HB3	1:E:286:ILE:HD12	2.01	0.41
1:E:374:THR:HB	1:E:397:LYS:HB3	2.02	0.41
3:H:300:LEU:HD12	3:H:323:ALA:N	2.35	0.41
3:J:330:ILE:CG2	3:J:330:ILE:OXT	2.68	0.41
3:R:330:ILE:CG2	3:R:330:ILE:OXT	2.68	0.41
1:C:204:SER:OG	1:C:205:LYS:N	2.52	0.41
3:S:330:ILE:OXT	3:S:330:ILE:CG2	2.69	0.41
1:F:317:CYS:HB2	1:F:401:LEU:HB3	2.01	0.41
1:C:339:ILE:HA	1:C:342:VAL:HG22	2.03	0.41
1:D:250:ARG:O	1:D:254:THR:OG1	2.34	0.41
1:E:339:ILE:HA	1:E:342:VAL:HG22	2.03	0.41
3:J:327:LEU:HD21	3:K:317:LYS:N	2.35	0.41
1:A:373:LEU:CD1	1:A:391:ILE:HG12	2.49	0.41
1:B:196:SER:OG	1:B:196:SER:O	2.37	0.41
1:C:402:THR:HG22	1:C:404:LYS:H	1.84	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:L:305:ILE:HD13	3:M:302:LYS:HG3	2.03	0.41
3:L:311:GLU:CD	3:M:290:ARG:NH1	2.64	0.41
1:F:350:PRO:HA	1:F:399:PRO:HG2	2.01	0.41
3:H:330:ILE:OXT	3:H:330:ILE:CG2	2.68	0.41
3:J:311:GLU:CD	3:K:290:ARG:NH1	2.64	0.41
3:P:330:ILE:CG2	3:P:330:ILE:OXT	2.68	0.41
1:B:422:LEU:HA	1:B:422:LEU:HD23	1.89	0.41
1:D:339:ILE:HA	1:D:342:VAL:HG22	2.03	0.41
3:M:330:ILE:CG2	3:M:330:ILE:OXT	2.68	0.41
3:R:295:GLU:HG2	3:R:295:GLU:O	2.21	0.41
1:A:228:ILE:HD12	1:A:271:LEU:HD23	2.02	0.41
1:F:225:LYS:NZ	1:F:268:GLN:O	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:ARG:HG2	1:F:293:ARG:NH2	2.36	0.41
1:F:172:TYR:CZ	1:F:428:PHE:HB3	2.50	0.41
3:I:330:ILE:OXT	3:I:330:ILE:CG2	2.68	0.41
3:P:327:LEU:HD21	3:Q:317:LYS:N	2.35	0.41
1:A:205:LYS:HD3	1:B:206:TRP:HB3	2.02	0.41
1:B:339:ILE:HA	1:B:342:VAL:HG22	2.03	0.41
1:E:261:ASN:OD1	1:E:262:GLY:N	2.51	0.41
1:F:155:PHE:HB3	1:F:158:LEU:HD23	2.02	0.41
3:O:330:ILE:OXT	3:O:330:ILE:CG2	2.69	0.41
3:Q:330:ILE:OXT	3:Q:330:ILE:CG2	2.68	0.41
1:C:373:LEU:CD1	1:C:391:ILE:HG12	2.49	0.41
1:F:200:SER:HB3	1:F:233:GLU:OE1	2.21	0.41
3:L:300:LEU:HD12	3:L:323:ALA:N	2.35	0.41
1:B:357:ALA:HB3	1:B:360:PHE:CZ	2.55	0.40
1:C:359:HIS:HA	1:C:384:ILE:O	2.20	0.40
1:F:359:HIS:HA	1:F:384:ILE:O	2.20	0.40
1:F:295:TYR:CE1	1:F:425:GLN:CD	2.89	0.40
3:J:300:LEU:HD12	3:J:323:ALA:N	2.35	0.40
1:D:398:GLU:HG2	1:D:398:GLU:H	1.73	0.40
3:N:305:ILE:HD13	3:O:302:LYS:HG3	2.03	0.40
3:R:308:LEU:CD1	3:S:298:GLN:HG3	2.44	0.40
1:A:359:HIS:HA	1:A:384:ILE:O	2.20	0.40
3:P:295:GLU:HG2	3:P:295:GLU:O	2.21	0.40
1:A:339:ILE:HA	1:A:342:VAL:HG22	2.03	0.40
1:C:388:TRP:CH2	1:D:155:PHE:CZ	3.08	0.40
1:E:137:GLY:O	1:E:142:LYS:HE3	2.21	0.40
3:L:330:ILE:CG2	3:L:330:ILE:OXT	2.69	0.40
1:A:325:ARG:NH1	3:S:310:TYR:CB	2.64	0.40
3:L:308:LEU:CD1	3:M:298:GLN:HG3	2.44	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	310/519 (60%)	274 (88%)	31 (10%)	5 (2%)	11	47
1	B	318/519 (61%)	284 (89%)	29 (9%)	5 (2%)	11	47
1	C	318/519 (61%)	280 (88%)	33 (10%)	5 (2%)	11	47
1	D	318/519 (61%)	279 (88%)	33 (10%)	6 (2%)	9	43
1	E	300/519 (58%)	260 (87%)	36 (12%)	4 (1%)	13	52
1	F	304/519 (59%)	277 (91%)	20 (7%)	7 (2%)	7	38
2	G	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
3	H	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	18
3	I	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	36
3	J	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	18
3	K	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	36
3	L	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	18
3	M	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	36
3	N	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	18
3	O	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	36
3	P	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	18
3	Q	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	36
3	R	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	18
3	S	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	6	36
All	All	2356/7084 (33%)	2050 (87%)	256 (11%)	50 (2%)	12	40

All (50) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	F	299	PRO
1	F	371	ARG
1	F	395	GLU
1	C	359	HIS
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	359	HIS
1	B	381	ASP
1	C	381	ASP
1	D	381	ASP
1	E	381	ASP
1	F	381	ASP
3	H	290	ARG
3	J	290	ARG
3	L	290	ARG
3	N	290	ARG
3	P	290	ARG
3	R	290	ARG
1	F	359	HIS
1	A	370	THR
1	B	370	THR
1	C	370	THR
1	D	370	THR
1	E	370	THR
1	F	370	THR
1	D	399	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 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	266/418 (64%)	258 (97%)	8 (3%)	44	76
1	B	273/418 (65%)	269 (98%)	4 (2%)	67	88
1	C	273/418 (65%)	269 (98%)	4 (2%)	67	88
1	D	273/418 (65%)	268 (98%)	5 (2%)	62	85
1	E	259/418 (62%)	254 (98%)	5 (2%)	60	84
1	F	262/418 (63%)	251 (96%)	11 (4%)	32	69
2	G	8/8 (100%)	8 (100%)	0	100	100
3	H	36/294 (12%)	34 (94%)	2 (6%)	23	61
3	I	36/294 (12%)	35 (97%)	1 (3%)	47	77
3	J	36/294 (12%)	34 (94%)	2 (6%)	23	61
3	K	36/294 (12%)	35 (97%)	1 (3%)	47	77
3	L	36/294 (12%)	34 (94%)	2 (6%)	23	61
3	M	36/294 (12%)	35 (97%)	1 (3%)	47	77
3	N	36/294 (12%)	34 (94%)	2 (6%)	23	61
3	O	36/294 (12%)	35 (97%)	1 (3%)	47	77
3	P	36/294 (12%)	34 (94%)	2 (6%)	23	61
3	Q	36/294 (12%)	35 (97%)	1 (3%)	47	77
3	R	36/294 (12%)	34 (94%)	2 (6%)	23	61
3	S	36/294 (12%)	35 (97%)	1 (3%)	47	77
All	All	2046/6044 (34%)	1991 (97%)	55 (3%)	51	78

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	ARG
1	A	356	SER
1	A	370	THR
1	A	373	LEU

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Mol	Chain	Res	Type
1	A	397	LYS
1	A	398	GLU
1	A	400	ASP
1	A	401	LEU
1	B	293	ARG
1	B	370	THR
1	B	373	LEU
1	B	398	GLU
1	C	293	ARG
1	C	370	THR
1	C	373	LEU
1	C	397	LYS
1	D	293	ARG
1	D	370	THR
1	D	373	LEU
1	D	397	LYS
1	D	398	GLU
1	E	293	ARG
1	E	358	THR
1	E	370	THR
1	E	373	LEU
1	E	397	LYS
1	F	127	LYS
1	F	139	GLU
1	F	200	SER
1	F	209	GLU
1	F	278	ILE
1	F	291	GLU
1	F	370	THR
1	F	373	LEU
1	F	397	LYS
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

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	GLN
1	A	359	HIS
1	C	359	HIS
1	D	216	GLN
1	D	359	HIS
1	E	359	HIS
1	F	157	HIS
1	F	162	ASN
1	F	216	GLN
1	F	265	ASN
1	F	355	GLN
1	F	425	GLN
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	298	GLN
3	P	296	GLN
3	Q	298	GLN
3	R	296	GLN
3	S	298	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 12 ligands modelled in this entry, 4 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	701	5,6	25,29,29	1.42	3 (12%)	25,45,45	1.76	7 (28%)
5	BEF	A	702	4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	B	701	5,6	25,29,29	1.64	4 (16%)	25,45,45	1.62	5 (20%)
5	BEF	B	702	4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	C	701	5,6	25,29,29	1.68	6 (24%)	25,45,45	1.89	9 (36%)
5	BEF	C	702	4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	D	701	6	25,29,29	1.23	2 (8%)	25,45,45	2.06	7 (28%)
4	ADP	E	701	-	25,29,29	1.04	2 (8%)	25,45,45	1.88	3 (12%)

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	701	5,6	-	0/12/32/32	0/3/3/3
5	BEF	A	702	4	-	0/0/0/0	0/0/0/0
4	ADP	B	701	5,6	-	0/12/32/32	0/3/3/3
5	BEF	B	702	4	-	0/0/0/0	0/0/0/0
4	ADP	C	701	5,6	-	0/12/32/32	0/3/3/3
5	BEF	C	702	4	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	D	701	6	-	0/12/32/32	0/3/3/3
4	ADP	E	701	-	-	0/12/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	ADP	PB-O3A	-4.59	1.53	1.60
4	C	701	ADP	PB-O3A	-4.32	1.53	1.60
4	A	701	ADP	PB-O3A	-3.74	1.54	1.60
4	E	701	ADP	C8-N9	-3.24	1.33	1.36
4	D	701	ADP	C8-N9	-3.13	1.33	1.36
4	C	701	ADP	C8-N7	-3.09	1.29	1.34
4	B	701	ADP	C8-N7	-2.78	1.29	1.34
4	C	701	ADP	C8-N9	-2.59	1.33	1.36
4	A	701	ADP	C8-N7	-2.57	1.30	1.34
4	B	701	ADP	PA-O2A	-2.43	1.43	1.55
4	C	701	ADP	C5-C4	-2.17	1.35	1.40
4	A	701	ADP	PB-O2B	-2.17	1.46	1.54
4	C	701	ADP	PA-O2A	-2.16	1.44	1.55
4	B	701	ADP	PB-O2B	-2.12	1.46	1.54
4	C	701	ADP	PB-O2B	-2.10	1.46	1.54
4	E	701	ADP	C5-C4	2.14	1.45	1.40
4	D	701	ADP	C5-C4	2.22	1.45	1.40

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	701	ADP	N3-C2-N1	-6.77	123.07	128.86
4	D	701	ADP	N3-C2-N1	-6.08	123.66	128.86
4	C	701	ADP	C4'-O4'-C1'	-4.21	105.44	109.83
4	B	701	ADP	O3B-PB-O1B	-4.16	94.35	110.60
4	D	701	ADP	PA-O3A-PB	-4.15	118.69	132.63
4	A	701	ADP	C2'-C3'-C4'	-4.05	94.84	102.62
4	A	701	ADP	O3B-PB-O1B	-3.51	96.89	110.60
4	E	701	ADP	C4-C5-N7	-3.25	106.27	109.41
4	C	701	ADP	O3B-PB-O1B	-3.20	98.10	110.60
4	E	701	ADP	PA-O3A-PB	-3.09	122.24	132.63
4	C	701	ADP	PA-O3A-PB	-3.07	122.29	132.63
4	A	701	ADP	C4'-O4'-C1'	-2.87	106.83	109.83
4	D	701	ADP	O3'-C3'-C4'	-2.71	103.20	111.06
4	A	701	ADP	N3-C2-N1	-2.71	126.54	128.86
4	D	701	ADP	O3'-C3'-C2'	-2.68	103.23	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	ADP	PA-O3A-PB	-2.68	123.61	132.63
4	C	701	ADP	O4'-C4'-C3'	-2.47	100.27	105.15
4	B	701	ADP	O2'-C2'-C3'	-2.39	104.18	111.83
4	B	701	ADP	PA-O3A-PB	-2.35	124.72	132.63
4	B	701	ADP	O3'-C3'-C2'	-2.24	104.64	111.83
4	D	701	ADP	C4-C5-N7	-2.22	107.27	109.41
4	C	701	ADP	C2'-C3'-C4'	-2.14	98.51	102.62
4	C	701	ADP	N3-C2-N1	-2.13	127.04	128.86
4	C	701	ADP	O2'-C2'-C3'	-2.13	105.01	111.83
4	A	701	ADP	O4'-C4'-C3'	-2.04	101.12	105.15
4	C	701	ADP	O2A-PA-O5'	2.10	117.50	107.75
4	A	701	ADP	O5'-PA-O1A	2.25	117.85	109.07
4	D	701	ADP	O3B-PB-O2B	2.43	117.18	107.59
4	D	701	ADP	C4'-O4'-C1'	2.94	112.90	109.83
4	B	701	ADP	C4-C5-N7	3.12	112.42	109.41
4	C	701	ADP	C4-C5-N7	3.64	112.93	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	ADP	1	0
5	A	702	BEF	1	0
4	B	701	ADP	1	0
5	B	702	BEF	1	0
4	C	701	ADP	1	0
5	C	702	BEF	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.