



Full wwPDB EM Validation Report ⓘ

Apr 1, 2026 – 12:29 AM UTC

PDB ID : 5VF3 / pdb_00005vf3
EMDB ID : EMD-8661
Title : Bacteriophage T4 isometric capsid
Authors : Chen, Z.; Sun, L.; Zhang, Z.; Fokine, A.; Padilla-Sanchez, V.; Hanein, D.;
Jiang, W.; Rossmann, M.G.; Rao, V.B.
Deposited on : 2017-04-06
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

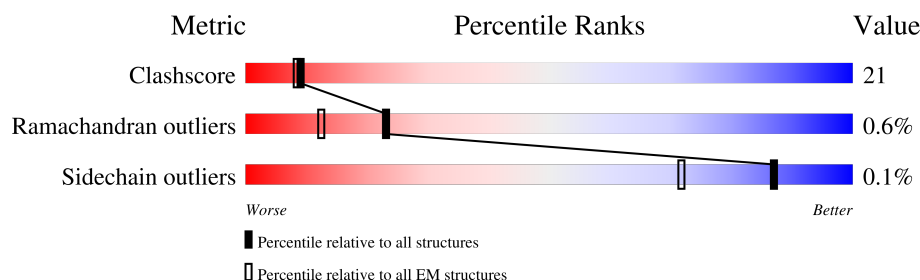
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



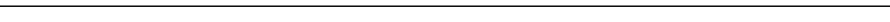
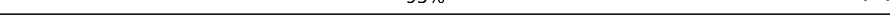
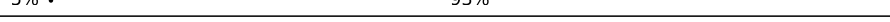
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	a	417	57% 41% .
2	A	456	58% 42%
2	B	456	52% 48%
2	C	456	56% 44%
2	D	456	55% 43% .
2	E	456	52% 48% .
2	F	456	53% 46% .
2	G	456	59% 40% .
2	H	456	57% 42%

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Mol	Chain	Length	Quality of chain
2	I	456	 55% 45%
2	J	456	 58% 41% .
2	K	456	 58% 41% .
2	L	456	 56% 43%
3	O	80	 69% 30% .
3	P	80	 60% 39% .
3	Q	80	 91% 8% .
3	R	80	 95% . .
3	S	80	 95% . .
3	T	80	 89% 10% .
3	U	80	 95% . .
3	V	80	 92% 6% .
3	W	80	 55% 44% .
3	X	80	 92% 6% .
3	Y	80	 95% . .
4	Z	376	 5% . 93%
5	z	15	 93% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 51584 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 Capsid vertex protein gp24.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	415	Total	C	N	O	S	0	0
			3208	2039	521	640	8		

- Molecule 2 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	B	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	C	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	D	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	E	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	F	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	G	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	H	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	I	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	J	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	K	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	L	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	THR	ALA	conflict	UNP P04535
B	275	THR	ALA	conflict	UNP P04535
C	275	THR	ALA	conflict	UNP P04535
D	275	THR	ALA	conflict	UNP P04535
E	275	THR	ALA	conflict	UNP P04535
F	275	THR	ALA	conflict	UNP P04535
G	275	THR	ALA	conflict	UNP P04535
H	275	THR	ALA	conflict	UNP P04535
I	275	THR	ALA	conflict	UNP P04535
J	275	THR	ALA	conflict	UNP P04535
K	275	THR	ALA	conflict	UNP P04535
L	275	THR	ALA	conflict	UNP P04535

- Molecule 3 is a protein called Small outer capsid protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	79	Total 633	C 403	N 106	O 124	0	0
3	P	79	Total 633	C 403	N 106	O 124	0	0
3	Q	79	Total 633	C 403	N 106	O 124	0	0
3	R	79	Total 633	C 403	N 106	O 124	0	0
3	S	79	Total 633	C 403	N 106	O 124	0	0
3	T	79	Total 633	C 403	N 106	O 124	0	0
3	U	79	Total 633	C 403	N 106	O 124	0	0
3	V	79	Total 633	C 403	N 106	O 124	0	0
3	W	79	Total 633	C 403	N 106	O 124	0	0
3	X	79	Total 633	C 403	N 106	O 124	0	0
3	Y	79	Total 633	C 403	N 106	O 124	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	4	ALA	THR	conflict	UNP P03715

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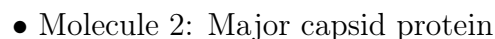
Chain	Residue	Modelled	Actual	Comment	Reference
O	28	VAL	ILE	conflict	UNP P03715
P	4	ALA	THR	conflict	UNP P03715
P	28	VAL	ILE	conflict	UNP P03715
Q	4	ALA	THR	conflict	UNP P03715
Q	28	VAL	ILE	conflict	UNP P03715
R	4	ALA	THR	conflict	UNP P03715
R	28	VAL	ILE	conflict	UNP P03715
S	4	ALA	THR	conflict	UNP P03715
S	28	VAL	ILE	conflict	UNP P03715
T	4	ALA	THR	conflict	UNP P03715
T	28	VAL	ILE	conflict	UNP P03715
U	4	ALA	THR	conflict	UNP P03715
U	28	VAL	ILE	conflict	UNP P03715
V	4	ALA	THR	conflict	UNP P03715
V	28	VAL	ILE	conflict	UNP P03715
W	4	ALA	THR	conflict	UNP P03715
W	28	VAL	ILE	conflict	UNP P03715
X	4	ALA	THR	conflict	UNP P03715
X	28	VAL	ILE	conflict	UNP P03715
Y	4	ALA	THR	conflict	UNP P03715
Y	28	VAL	ILE	conflict	UNP P03715

- Molecule 4 is a protein called Highly immunogenic outer capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	25	Total	C	N	O	S	0	0
			214	140	32	39	3		

- Molecule 5 is a protein called Highly immunogenic outer capsid protein.

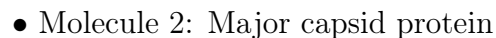
Mol	Chain	Residues	Atoms				AltConf	Trace
5	z	15	Total	C	N	O	0	0
			75	45	15	15		



Opinion	Percentage
Doing a good job	55%
Doing a bad job	43%

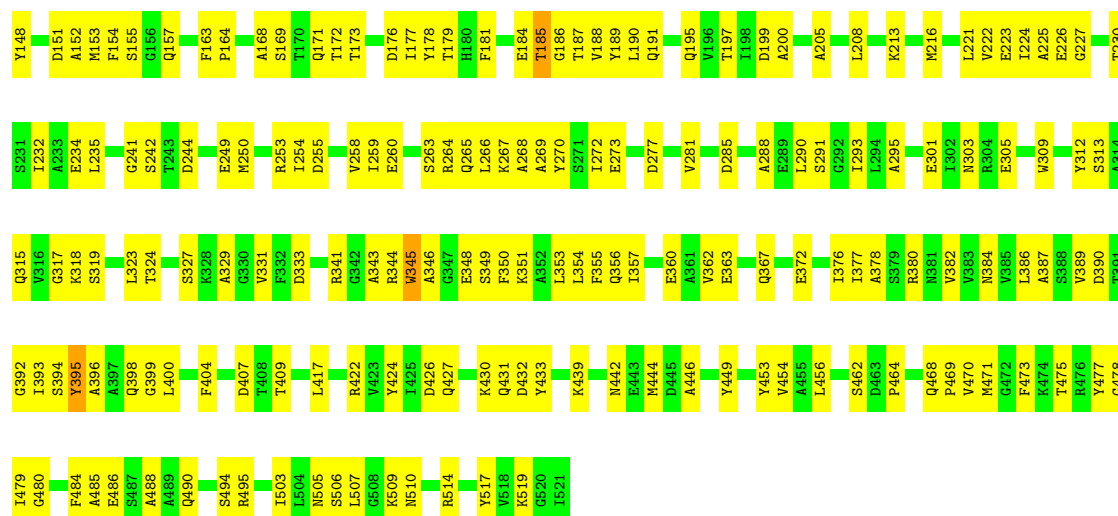


Category	Percentage
Satisfied	52%
Dissatisfied	48%



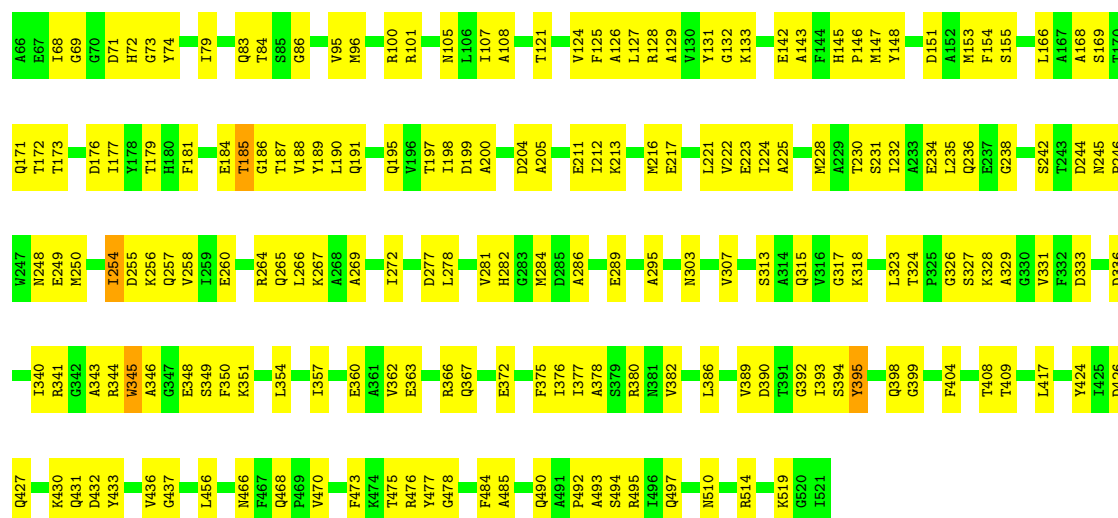
Opinion	Percentage
Doing a good job	53%
Doing a bad job	46%





• Molecule 2: Major capsid protein

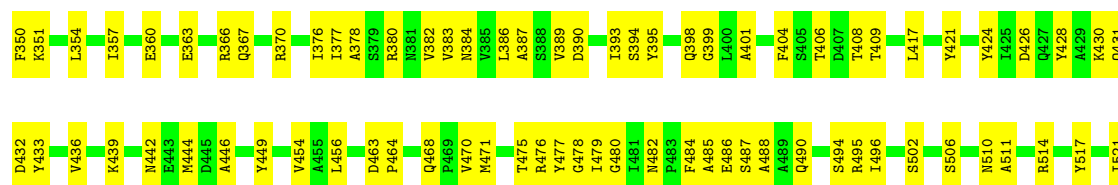
Chain G: 59% 40%



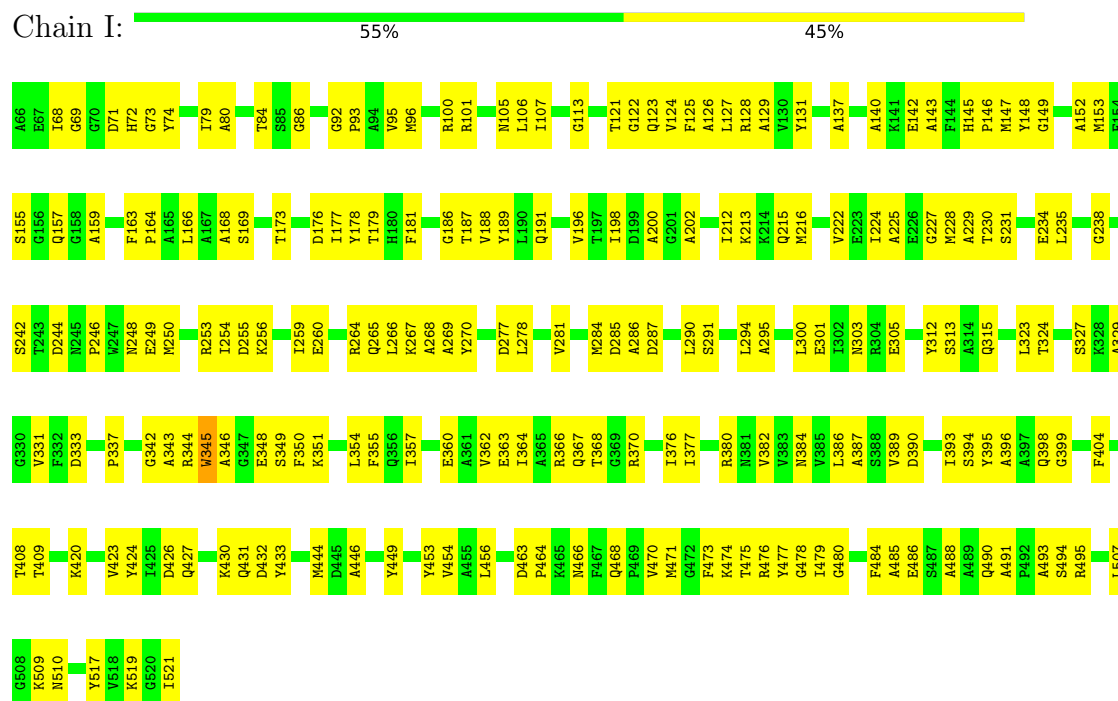
• Molecule 2: Major capsid protein

Chain H: 57% 42%

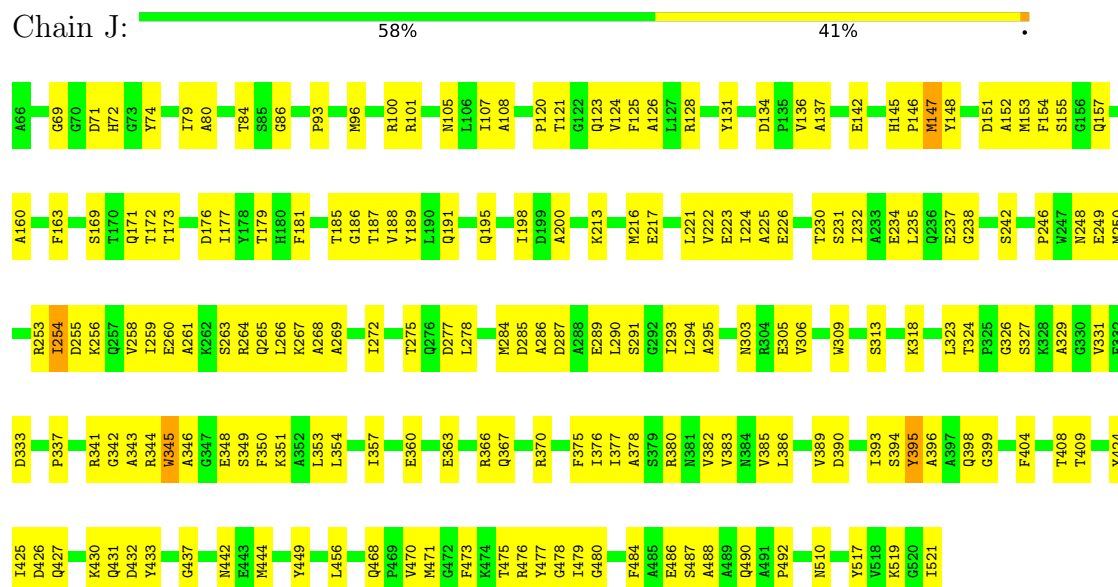




• Molecule 2: Major capsid protein

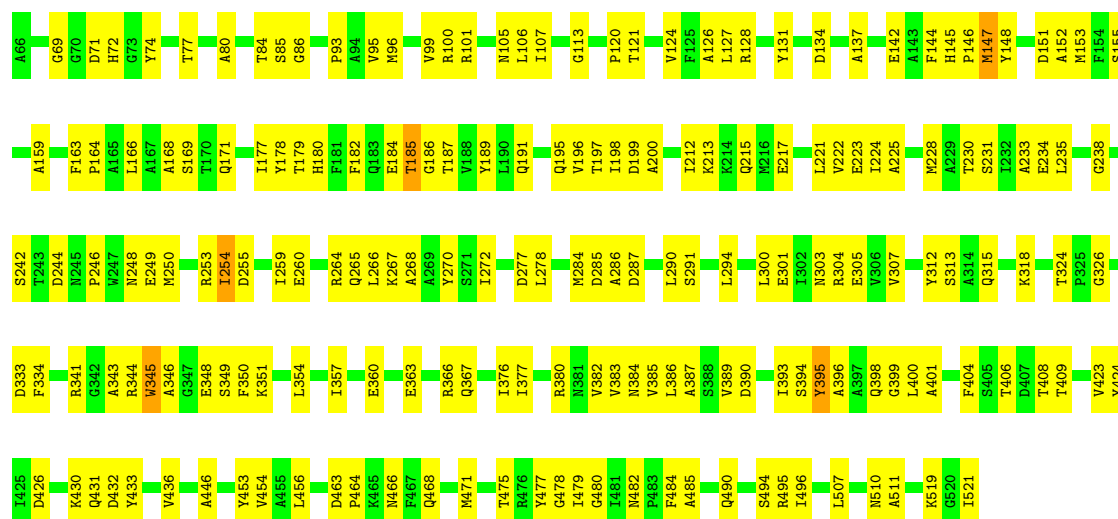


• Molecule 2: Major capsid protein



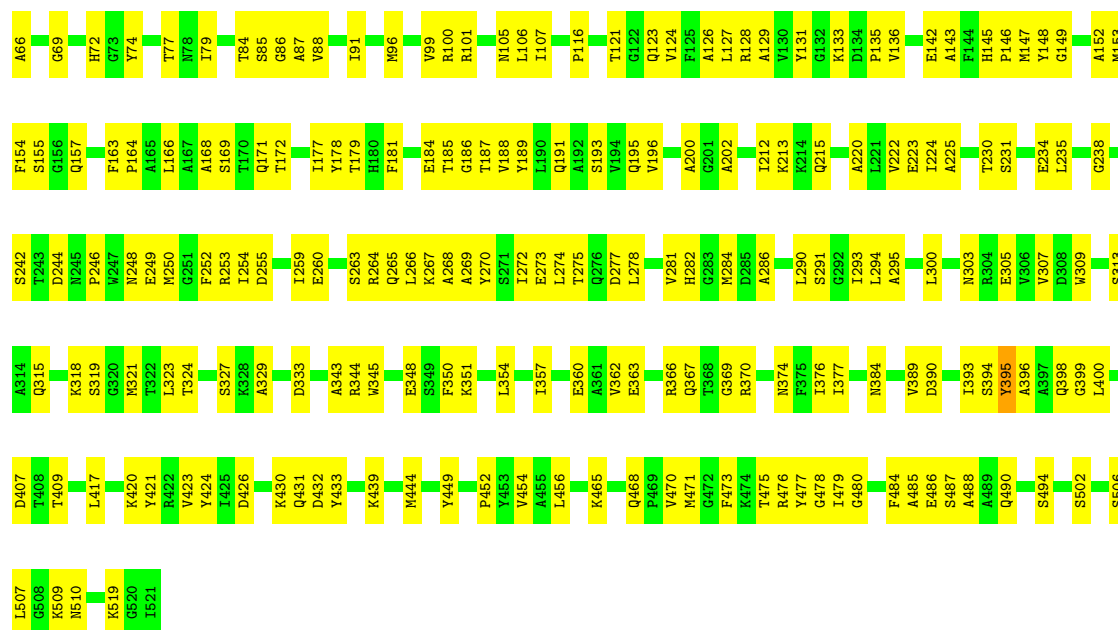
• Molecule 2: Major capsid protein

Chain K:  58% 41% .



• Molecule 2: Major capsid protein

Chain L:  56% 43% .



• Molecule 3: Small outer capsid protein

Chain O:  69% 30% .



• Molecule 3: Small outer capsid protein

Chain P:  60% 39%

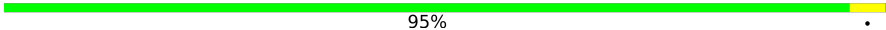


- Molecule 3: Small outer capsid protein

Chain Q:  91% 8%

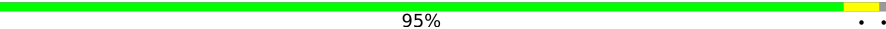


- Molecule 3: Small outer capsid protein

Chain R:  95%



- Molecule 3: Small outer capsid protein

Chain S:  95%

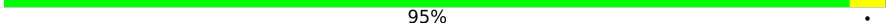


- Molecule 3: Small outer capsid protein

Chain T:  89% 10%



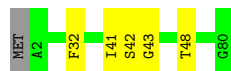
- Molecule 3: Small outer capsid protein

Chain U:  95%



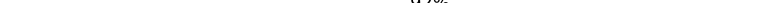
- Molecule 3: Small outer capsid protein

Chain V:  92% 6%



- Molecule 3: Small outer capsid protein

MET
A2
R5
G6
V7
V8
N9
I10
K11
T12
F13
E14
D18
K21
K22
K26
E27
F32
P33
L34
X35
S86
D37
V38
H39
K40
I41
S42
Y46
S51
A54
A55
Y56
Q64
R65
T66
E67
W68
I69
A70
A71
N72
T73
D74
L75

- Chain X:  92% 6%

A schematic diagram of a protein structure represented as a horizontal bar. Several residues are highlighted in yellow: MET (at the N-terminus), A2, F13, F32, Y46, F49, P50, and G80 (at the C-terminus). The residues are connected by a continuous line representing the protein backbone.

- Chain Y:  95%

- Chain Z: 5% 93%

THR	TYR	PRO	SER	ASN	GLU	LEU	ALA	MET
			S302	VAL	VAL	ALA	GLY	
				TYR	SER	SER	GLN	PHE
			I305	THR	THR	LEU	LYS	THR
			W306	VAL	THR	PRO	THR	VAL
				ASP	VAL	ASP	ILE	ASP
			W309	THR	ASN	GLY	LYS	THR
				SER	LYS	SER	ALA	THR
			D313	VAL	THR	ALA	VAL	PRO
				GLY	MET	THR	THR	LYS
			E321	SER	ASN	TYR	THR	THR
					PRO	GLN	ASN	PRO
			R326	THR	THR	TRP	LEU	GLY
				ASP	ILE	TYR	SER	ILE
				GLU	THR	VAL	GLY	ASP
				VAL	THR	ASP	GLY	GLU
				THR	THR	PRO	GLY	ASP
				SER	ALA	GLN	PRO	LYS
				TYR	THR	VAL	THR	GLN
				THR	THR	VAL	ALA	PHE
				LEU	ASN	GLY	GLU	THR
				ALA	VAL	GLU	ALA	ALA
				ARG	ASP	GLN	THR	THR
				TYR	GLN	ASN	THR	PRO
				ASN	ASP	SER	THR	SER
				PRO	ALA	THR	ILE	GLY
				VAL	SER	PHE	THR	GLN
				THR	ALA	SER	VAL	THR
				VAL	THR	TYR	LYS	GLY
				THR	PHE	THR	ASN	GLY
				LYS	THR	PRO	LYS	GLY
				ASP	THR	ALA	THR	THR
				TYR	GLY	ASN	THR	ILE
				PRO	ASN	VAL	THR	THR
				GLU	VAL	GLY	THR	TYR
				VAL	THR	VAL	THR	ALA
				ASP	VAL	LYS	LEU	TRP
				VAL	THR	ARG	ALA	SER
				GLN	ALA	ILE	VAL	VAL
				GLU	GLU	ILE	THR	ASP
				LYS	ALA	CYS	THR	ASN
				SER	VAL	VAL	ALA	ASN
				ARG	ALA	VAL	VAL	PRO
				ASN	PRO	ILE	SER	PRO
				GLY	GLU	GLN	PRO	GLN
				TYR	PRO	VAL	ALA	ASP
				ILE	THR	THR	ALA	GLY
				GLY	GLY	THR	GLY	ALA
				HIS	LYS	ASP	ILE	ALA
				THR	PRO	TYR	GLY	THR
				ALA	TYR	SER	THR	PHE
				LEU	VAL	ALA	PRO	SER
				GLU	HIS	LEU	VAL	TYR
				THR	PRO	VAL	GLN	VAL
				THR	PRO	SER	PHE	THR
				GLY	LEU	VAL	THR	LYS
				ILE	PRO	GLY	ALA	GLY

- Chain z: 93% 7%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	18000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF amplitude correction was performed during 3D reconstruction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-3500	Depositor
Magnification	18000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.49	0/3263	0.66	0/4430
2	A	0.54	0/3495	0.65	2/4734 (0.0%)
2	B	0.53	0/3495	0.64	1/4734 (0.0%)
2	C	0.54	0/3495	0.64	1/4734 (0.0%)
2	D	0.53	0/3495	0.63	2/4734 (0.0%)
2	E	0.55	0/3495	0.65	1/4734 (0.0%)
2	F	0.54	0/3495	0.64	2/4734 (0.0%)
2	G	0.53	0/3495	0.65	1/4734 (0.0%)
2	H	0.53	0/3495	0.64	1/4734 (0.0%)
2	I	0.52	0/3495	0.64	1/4734 (0.0%)
2	J	0.53	0/3495	0.64	1/4734 (0.0%)
2	K	0.53	0/3495	0.65	1/4734 (0.0%)
2	L	0.53	0/3495	0.64	0/4734
3	O	0.28	0/648	0.43	0/876
3	P	0.30	0/648	0.48	0/876
3	Q	0.25	0/648	0.45	0/876
3	R	0.25	0/648	0.45	0/876
3	S	0.24	0/648	0.43	0/876
3	T	0.21	0/648	0.40	0/876
3	U	0.23	0/648	0.46	0/876
3	V	0.18	0/648	0.41	0/876
3	W	0.26	0/648	0.46	0/876
3	X	0.20	0/648	0.44	0/876
3	Y	0.22	0/648	0.44	0/876
4	Z	0.18	0/222	0.43	0/301
All	All	0.50	0/52553	0.62	14/71175 (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.

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Mol	Chain	#Chirality outliers	#Planarity outliers
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Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	3
2	E	0	1
2	F	0	1
2	G	0	1
2	K	0	1
3	Q	0	1
All	All	0	8

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	186	GLY	N-CA-C	6.11	118.27	112.04
2	K	345	TRP	CA-CB-CG	5.90	124.81	113.60
2	H	345	TRP	CA-CB-CG	5.85	124.71	113.60
2	C	345	TRP	CA-CB-CG	5.72	124.48	113.60
2	D	345	TRP	CA-CB-CG	5.64	124.32	113.60
2	I	345	TRP	CA-CB-CG	5.63	124.31	113.60
2	F	345	TRP	CA-CB-CG	5.63	124.30	113.60
2	B	345	TRP	CA-CB-CG	5.62	124.27	113.60
2	J	345	TRP	CA-CB-CG	5.54	124.13	113.60
2	A	345	TRP	CA-CB-CG	5.40	123.87	113.60
2	F	107	ILE	N-CA-C	-5.22	107.66	112.83
2	G	345	TRP	CA-CB-CG	5.14	123.37	113.60
2	D	186	GLY	N-CA-C	5.08	117.22	112.04
2	E	345	TRP	CA-CB-CG	5.02	123.14	113.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	185	THR	Peptide
2	F	185	THR	Peptide
2	G	185	THR	Peptide
2	K	185	THR	Peptide
3	Q	63	ASN	Peptide
1	a	242	SER	Peptide
1	a	320	LEU	Peptide
1	a	35	ILE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3208	0	3205	147	0
2	A	3427	0	3373	182	0
2	B	3427	0	3373	204	0
2	C	3427	0	3373	207	0
2	D	3427	0	3373	192	0
2	E	3427	0	3373	213	0
2	F	3427	0	3373	207	0
2	G	3427	0	3373	184	0
2	H	3427	0	3373	172	0
2	I	3427	0	3373	192	0
2	J	3427	0	3373	178	0
2	K	3427	0	3373	184	0
2	L	3427	0	3373	194	0
3	O	633	0	608	21	0
3	P	633	0	608	25	0
3	Q	633	0	608	9	0
3	R	633	0	608	3	0
3	S	633	0	608	4	0
3	T	633	0	608	13	0
3	U	633	0	608	3	0
3	V	633	0	608	5	0
3	W	633	0	608	25	0
3	X	633	0	608	6	0
3	Y	633	0	608	3	0
4	Z	214	0	187	3	0
5	z	75	0	19	1	0
All	All	51584	0	50575	2109	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 21.

All (2109) 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)
2:A:152:ALA:HB1	2:A:225:ALA:HB2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:431:GLN:HE22	2:K:217:GLU:HB2	1.35	0.92
2:J:152:ALA:HB1	2:J:225:ALA:HB2	1.51	0.91
1:a:378:ARG:HH21	2:F:273:GLU:HB3	1.35	0.90
2:H:152:ALA:HB1	2:H:225:ALA:HB2	1.54	0.89
2:F:152:ALA:HB1	2:F:225:ALA:HB2	1.55	0.89
2:E:350:PHE:HB2	2:E:389:VAL:HG21	1.54	0.89
2:D:152:ALA:HB1	2:D:225:ALA:HB2	1.54	0.88
2:B:350:PHE:HB2	2:B:389:VAL:HG21	1.55	0.87
2:C:152:ALA:HB1	2:C:225:ALA:HB2	1.54	0.87
2:H:401:ALA:O	2:I:420:LYS:NZ	2.09	0.85
2:K:431:GLN:HE21	2:L:213:LYS:HB3	1.41	0.85
2:J:278:LEU:HD22	2:J:286:ALA:HB2	1.58	0.84
2:K:350:PHE:HB2	2:K:389:VAL:HG21	1.59	0.84
1:a:238:LEU:HD22	1:a:281:ILE:HD12	1.58	0.84
2:A:278:LEU:HD22	2:A:286:ALA:HB2	1.58	0.84
2:L:145:HIS:HD2	2:L:146:PRO:HD2	1.43	0.83
2:I:278:LEU:HD22	2:I:286:ALA:HB2	1.61	0.83
2:B:357:ILE:HD11	2:B:376:ILE:HG21	1.60	0.82
2:B:456:LEU:H	2:B:475:THR:HG22	1.43	0.82
2:D:350:PHE:HB2	2:D:389:VAL:HG21	1.61	0.82
2:G:278:LEU:HD22	2:G:286:ALA:HB2	1.62	0.82
2:C:357:ILE:HD11	2:C:376:ILE:HG21	1.60	0.82
2:C:456:LEU:H	2:C:475:THR:HG22	1.46	0.81
2:E:278:LEU:HD22	2:E:286:ALA:HB2	1.61	0.81
2:G:278:LEU:HD21	2:G:284:MET:HB2	1.60	0.81
2:F:145:HIS:HD2	2:F:146:PRO:HD2	1.43	0.81
2:F:350:PHE:HB2	2:F:389:VAL:HG21	1.61	0.81
2:I:350:PHE:HB2	2:I:389:VAL:HG21	1.63	0.81
2:I:107:ILE:H	2:I:303:ASN:HD21	1.29	0.81
2:J:264:ARG:NH1	2:K:155:SER:OG	2.14	0.81
2:A:372:GLU:HB2	2:F:407:ASP:HB3	1.61	0.80
2:J:107:ILE:H	2:J:303:ASN:HD21	1.29	0.80
1:a:44:ARG:NH2	1:a:346:THR:OG1	2.12	0.80
2:H:456:LEU:H	2:H:475:THR:HG22	1.46	0.80
1:a:206:MET:HG3	1:a:375:LEU:HD11	1.63	0.80
2:A:155:SER:HB3	2:F:266:LEU:HD11	1.64	0.80
2:G:105:ASN:ND2	2:G:409:THR:O	2.14	0.80
2:G:107:ILE:H	2:G:303:ASN:HD21	1.25	0.79
2:G:350:PHE:HB2	2:G:389:VAL:HG21	1.65	0.79
2:A:267:LYS:HB3	2:B:249:GLU:HG2	1.64	0.79
2:K:278:LEU:HD22	2:K:286:ALA:HB2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:128:ARG:HE	2:J:484:PHE:HE1	1.31	0.79
2:J:351:LYS:NZ	2:J:390:ASP:O	2.15	0.79
2:L:357:ILE:HD11	2:L:376:ILE:HD13	1.63	0.79
2:K:278:LEU:HD21	2:K:284:MET:HB2	1.63	0.79
2:B:264:ARG:NH1	2:C:155:SER:OG	2.16	0.79
2:F:84:THR:HG22	2:F:86:GLY:H	1.48	0.78
2:F:426:ASP:OD2	2:F:433:TYR:OH	2.02	0.78
2:H:145:HIS:HD2	2:H:146:PRO:HD2	1.48	0.78
2:L:152:ALA:HB1	2:L:225:ALA:HB2	1.65	0.78
2:B:105:ASN:ND2	2:B:409:THR:O	2.15	0.78
2:D:357:ILE:HD11	2:D:376:ILE:HD13	1.64	0.78
2:E:145:HIS:HD2	2:E:146:PRO:HD2	1.49	0.78
2:A:278:LEU:HD21	2:A:284:MET:HB2	1.63	0.78
2:C:87:ALA:O	2:G:495:ARG:NH2	2.17	0.78
2:A:431:GLN:HE21	2:B:213:LYS:HB3	1.47	0.78
2:E:107:ILE:H	2:E:303:ASN:HD21	1.31	0.78
2:H:380:ARG:NH2	2:H:408:THR:OG1	2.15	0.78
2:G:264:ARG:NH1	2:H:155:SER:OG	2.17	0.78
2:J:431:GLN:HE21	2:K:213:LYS:HB3	1.49	0.78
2:A:264:ARG:NH1	2:B:155:SER:OG	2.17	0.77
2:E:267:LYS:HB3	2:F:249:GLU:HG2	1.65	0.77
2:K:267:LYS:HB3	2:L:249:GLU:HG2	1.66	0.77
1:a:173:ARG:NH1	1:a:379:TYR:OH	2.18	0.77
2:D:495:ARG:NH2	2:L:87:ALA:O	2.17	0.77
2:H:107:ILE:H	2:H:303:ASN:HD21	1.31	0.77
2:B:278:LEU:HD21	2:B:284:MET:HB2	1.67	0.77
2:D:431:GLN:HE22	2:E:217:GLU:HB2	1.48	0.77
2:H:264:ARG:NH1	2:I:155:SER:OG	2.17	0.77
2:B:351:LYS:NZ	2:B:390:ASP:O	2.18	0.77
2:J:456:LEU:H	2:J:475:THR:HG22	1.50	0.76
2:J:147:MET:HE3	2:J:367:GLN:HG2	1.67	0.76
2:G:84:THR:HG22	2:G:86:GLY:H	1.50	0.76
2:C:88:VAL:HG21	2:L:278:LEU:HD12	1.68	0.76
2:K:105:ASN:ND2	2:K:409:THR:O	2.19	0.76
2:C:278:LEU:HD22	2:C:286:ALA:HB2	1.68	0.76
2:E:168:ALA:HB1	2:E:200:ALA:HA	1.67	0.76
2:B:96:MET:HE3	2:C:124:VAL:HG23	1.68	0.76
2:G:142:GLU:H	2:G:490:GLN:HG2	1.49	0.75
2:I:357:ILE:HD11	2:I:376:ILE:HD13	1.68	0.75
2:G:266:LEU:HD11	2:H:155:SER:HB3	1.68	0.75
2:B:128:ARG:HE	2:B:484:PHE:HE1	1.32	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:213:LYS:HB3	2:L:431:GLN:HE21	1.50	0.75
2:D:105:ASN:ND2	2:D:409:THR:O	2.19	0.75
2:H:426:ASP:OD2	2:H:433:TYR:OH	2.04	0.75
2:I:128:ARG:HE	2:I:484:PHE:HE1	1.33	0.75
2:I:266:LEU:HD11	2:J:155:SER:HB3	1.68	0.75
2:I:431:GLN:HE21	2:J:213:LYS:HB3	1.49	0.75
2:B:313:SER:OG	2:B:510:ASN:ND2	2.19	0.75
2:C:431:GLN:HE21	2:D:213:LYS:HB3	1.50	0.75
2:I:152:ALA:HB1	2:I:225:ALA:HB2	1.67	0.74
2:B:234:GLU:OE2	2:F:69:GLY:N	2.17	0.74
2:B:380:ARG:NH2	2:B:408:THR:OG1	2.20	0.74
2:E:266:LEU:HD11	2:F:155:SER:HB3	1.69	0.74
2:C:431:GLN:HE22	2:D:217:GLU:HB2	1.52	0.74
2:D:151:ASP:HB2	2:D:189:TYR:HE1	1.52	0.74
2:A:426:ASP:OD2	2:A:433:TYR:OH	2.04	0.74
2:D:145:HIS:HD2	2:D:146:PRO:HD2	1.53	0.74
2:E:456:LEU:H	2:E:475:THR:HG22	1.52	0.74
2:G:277:ASP:OD1	2:G:278:LEU:N	2.20	0.74
2:D:398:GLN:HG2	2:D:399:GLY:H	1.52	0.74
2:F:333:ASP:HB3	2:F:519:LYS:HB2	1.70	0.74
2:G:155:SER:OG	2:L:264:ARG:NH1	2.21	0.74
2:L:177:ILE:HG12	2:L:224:ILE:HD11	1.70	0.74
2:C:268:ALA:HB2	2:C:294:LEU:HD11	1.69	0.73
2:G:398:GLN:HG2	2:G:399:GLY:H	1.52	0.73
2:L:456:LEU:H	2:L:475:THR:HG22	1.53	0.73
2:D:267:LYS:HB3	2:E:249:GLU:HG2	1.68	0.73
2:K:344:ARG:HH11	2:L:344:ARG:HH12	1.37	0.73
2:A:107:ILE:H	2:A:303:ASN:HD21	1.35	0.73
2:B:278:LEU:HD22	2:B:286:ALA:HB2	1.69	0.73
2:E:351:LYS:NZ	2:E:390:ASP:O	2.21	0.73
2:K:142:GLU:H	2:K:490:GLN:HG2	1.53	0.73
2:A:234:GLU:OE2	2:E:69:GLY:N	2.21	0.72
2:K:147:MET:HE3	2:K:367:GLN:HG2	1.72	0.72
2:K:426:ASP:OD2	2:K:433:TYR:OH	2.07	0.72
2:B:145:HIS:HD2	2:B:146:PRO:HD2	1.53	0.72
2:H:278:LEU:HD21	2:H:284:MET:HB2	1.70	0.72
2:J:426:ASP:OD2	2:J:433:TYR:OH	2.07	0.72
2:I:313:SER:OG	2:I:510:ASN:ND2	2.22	0.72
2:G:456:LEU:H	2:G:475:THR:HG22	1.55	0.72
2:A:390:ASP:OD2	2:A:394:SER:OG	2.07	0.72
2:C:291:SER:HB2	2:C:471:MET:HE1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:145:HIS:HD2	2:I:146:PRO:HD2	1.55	0.72
2:C:274:LEU:HD12	2:L:69:GLY:HA2	1.70	0.71
2:B:107:ILE:H	2:B:303:ASN:HD21	1.39	0.71
2:D:426:ASP:OD2	2:D:433:TYR:OH	2.08	0.71
2:G:431:GLN:HE22	2:H:217:GLU:HB2	1.54	0.71
2:L:390:ASP:OD2	2:L:394:SER:OG	2.07	0.71
2:C:145:HIS:HD2	2:C:146:PRO:HD2	1.54	0.71
2:F:128:ARG:HE	2:F:484:PHE:HE1	1.35	0.71
2:G:145:HIS:HD2	2:G:146:PRO:HD2	1.54	0.71
2:A:171:GLN:HE21	2:A:195:GLN:NE2	1.88	0.71
2:A:313:SER:OG	2:A:510:ASN:ND2	2.24	0.71
2:G:357:ILE:HD11	2:G:376:ILE:HD13	1.71	0.71
2:H:313:SER:OG	2:H:510:ASN:ND2	2.23	0.71
2:K:313:SER:OG	2:K:510:ASN:ND2	2.22	0.71
2:L:313:SER:OG	2:L:510:ASN:ND2	2.23	0.71
2:A:456:LEU:H	2:A:475:THR:HG22	1.55	0.71
2:A:128:ARG:HE	2:A:484:PHE:HE1	1.39	0.70
2:D:313:SER:OG	2:D:510:ASN:ND2	2.24	0.70
2:E:426:ASP:OD2	2:E:433:TYR:OH	2.08	0.70
2:I:398:GLN:HG2	2:I:399:GLY:H	1.56	0.70
2:K:145:HIS:HD2	2:K:146:PRO:HD2	1.55	0.70
2:C:264:ARG:NH1	2:D:155:SER:OG	2.24	0.70
2:D:107:ILE:H	2:D:303:ASN:HD21	1.37	0.70
2:J:267:LYS:HB3	2:K:249:GLU:HG2	1.74	0.70
2:K:253:ARG:NE	2:K:255:ASP:OD2	2.23	0.70
3:P:15:GLN:HE21	3:P:23:ILE:HD12	1.54	0.70
2:H:279:ARG:NH2	2:H:285:ASP:OD1	2.25	0.70
2:L:278:LEU:HD22	2:L:286:ALA:HB2	1.72	0.70
2:A:431:GLN:HE22	2:B:217:GLU:HB2	1.55	0.70
2:A:124:VAL:HG23	2:F:96:MET:HE3	1.73	0.70
2:J:145:HIS:HD2	2:J:146:PRO:HD2	1.57	0.70
2:J:277:ASP:OD1	2:J:278:LEU:N	2.25	0.70
2:C:426:ASP:OD2	2:C:433:TYR:OH	2.10	0.70
2:E:277:ASP:OD1	2:E:278:LEU:N	2.25	0.69
2:A:151:ASP:HB2	2:A:189:TYR:HE1	1.57	0.69
2:B:152:ALA:HB1	2:B:225:ALA:HB2	1.74	0.69
2:C:398:GLN:HG2	2:C:399:GLY:H	1.55	0.69
2:A:145:HIS:HD2	2:A:146:PRO:HD2	1.57	0.69
2:L:268:ALA:HB2	2:L:294:LEU:HD11	1.74	0.69
2:B:426:ASP:OD2	2:B:433:TYR:OH	2.10	0.69
2:I:84:THR:HG22	2:I:86:GLY:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:363:GLU:OE2	2:K:366:ARG:NH2	2.25	0.69
2:D:351:LYS:NZ	2:D:390:ASP:O	2.25	0.69
2:J:398:GLN:HG2	2:J:399:GLY:H	1.57	0.69
2:E:151:ASP:HB2	2:E:189:TYR:HE1	1.56	0.69
1:a:298:LEU:HB2	1:a:302:ALA:HB3	1.75	0.69
2:C:333:ASP:HB3	2:C:519:LYS:HB2	1.74	0.69
2:F:456:LEU:H	2:F:475:THR:HG22	1.58	0.69
2:L:398:GLN:HG2	2:L:399:GLY:H	1.58	0.69
2:E:357:ILE:HD11	2:E:376:ILE:HG21	1.72	0.69
2:A:177:ILE:HG12	2:A:224:ILE:HD11	1.74	0.68
2:L:426:ASP:OD2	2:L:433:TYR:OH	2.10	0.68
1:a:177:THR:HG23	1:a:178:GLY:H	1.57	0.68
2:C:84:THR:HG22	2:C:86:GLY:H	1.58	0.68
2:G:426:ASP:OD2	2:G:433:TYR:OH	2.12	0.68
2:E:398:GLN:HG2	2:E:399:GLY:H	1.58	0.68
2:H:390:ASP:OD2	2:H:394:SER:OG	2.12	0.68
2:C:380:ARG:NH2	2:C:408:THR:OG1	2.26	0.68
2:G:431:GLN:HE21	2:H:213:LYS:HB3	1.58	0.68
1:a:276:ALA:HB2	1:a:316:THR:HG22	1.76	0.68
2:B:267:LYS:HB3	2:C:249:GLU:HG2	1.74	0.68
2:L:351:LYS:NZ	2:L:390:ASP:O	2.26	0.68
2:F:253:ARG:NE	2:F:255:ASP:OD2	2.26	0.68
2:A:69:GLY:N	2:C:234:GLU:OE2	2.27	0.68
2:G:166:LEU:HD22	2:G:212:ILE:HD11	1.76	0.68
2:E:431:GLN:HE21	2:F:213:LYS:HB3	1.58	0.68
2:A:351:LYS:NZ	2:A:390:ASP:O	2.23	0.68
2:I:278:LEU:HD21	2:I:284:MET:HB2	1.76	0.68
2:H:351:LYS:NZ	2:H:390:ASP:O	2.25	0.67
2:C:105:ASN:ND2	2:C:409:THR:O	2.27	0.67
2:D:431:GLN:NE2	2:E:213:LYS:O	2.27	0.67
2:H:267:LYS:HB3	2:I:249:GLU:HG2	1.76	0.67
2:G:476:ARG:HH21	2:H:230:THR:HG21	1.59	0.67
2:H:345:TRP:HB3	2:I:343:ALA:HA	1.75	0.67
2:L:107:ILE:H	2:L:303:ASN:HD21	1.41	0.67
2:F:268:ALA:HB1	2:F:290:LEU:HD13	1.75	0.67
2:I:277:ASP:OD1	2:I:278:LEU:N	2.27	0.67
2:J:84:THR:HG22	2:J:86:GLY:H	1.59	0.67
2:J:278:LEU:HD21	2:J:284:MET:HB2	1.75	0.67
2:G:177:ILE:HG12	2:G:224:ILE:HD11	1.77	0.67
2:C:351:LYS:NZ	2:C:390:ASP:O	2.27	0.67
2:J:142:GLU:H	2:J:490:GLN:HG2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:357:ILE:HD11	2:F:376:ILE:HD13	1.77	0.67
2:L:323:LEU:HD21	2:L:329:ALA:HA	1.77	0.67
2:C:107:ILE:H	2:C:303:ASN:HD21	1.41	0.67
2:F:357:ILE:HD11	2:F:376:ILE:HG21	1.76	0.67
2:G:362:VAL:HG21	2:L:384:ASN:HD21	1.59	0.67
2:F:323:LEU:HD21	2:F:329:ALA:HA	1.77	0.66
2:F:398:GLN:HG2	2:F:399:GLY:H	1.60	0.66
2:I:177:ILE:HG12	2:I:224:ILE:HD11	1.78	0.66
1:a:298:LEU:HD12	1:a:300:GLN:H	1.60	0.66
2:A:268:ALA:HB2	2:A:294:LEU:HD11	1.76	0.66
2:C:278:LEU:HD12	2:L:88:VAL:HG21	1.76	0.66
2:B:384:ASN:HD21	2:C:362:VAL:HG21	1.59	0.66
2:G:213:LYS:O	2:L:431:GLN:NE2	2.28	0.66
2:K:266:LEU:HD11	2:L:155:SER:HB3	1.77	0.66
2:E:142:GLU:H	2:E:490:GLN:HG2	1.61	0.66
2:D:69:GLY:N	2:F:234:GLU:OE2	2.21	0.66
2:D:77:THR:OG1	3:R:5:ARG:NH2	2.28	0.66
2:K:168:ALA:HB1	2:K:200:ALA:HA	1.77	0.66
2:C:431:GLN:NE2	2:D:213:LYS:O	2.29	0.66
2:F:295:ALA:HB2	2:F:473:PHE:HE2	1.60	0.66
3:O:26:LYS:NZ	3:O:74:ASP:OD2	2.29	0.66
2:B:398:GLN:HG2	2:B:399:GLY:H	1.61	0.66
2:E:278:LEU:HD21	2:E:284:MET:HB2	1.76	0.66
2:G:234:GLU:OE2	2:K:69:GLY:N	2.24	0.66
2:A:398:GLN:HG2	2:A:399:GLY:H	1.60	0.66
2:B:333:ASP:HB3	2:B:519:LYS:HB2	1.78	0.66
2:F:331:VAL:HG12	2:F:517:TYR:HB2	1.78	0.66
1:a:275:SER:HA	1:a:315:ASP:HB3	1.77	0.65
2:G:380:ARG:NH2	2:G:408:THR:OG1	2.29	0.65
2:K:96:MET:HE3	2:L:124:VAL:HG23	1.76	0.65
2:K:398:GLN:HG2	2:K:399:GLY:H	1.61	0.65
1:a:222:SER:O	1:a:224:ARG:NH1	2.29	0.65
2:F:222:VAL:HG22	2:F:223:GLU:H	1.61	0.65
2:I:74:TYR:CE2	2:J:260:GLU:HG2	2.32	0.65
2:I:269:ALA:HA	2:I:470:VAL:HA	1.78	0.65
2:I:426:ASP:OD2	2:I:433:TYR:OH	2.15	0.65
1:a:205:GLU:O	1:a:209:GLU:N	2.27	0.65
1:a:320:LEU:HB2	1:a:322:TYR:HD1	1.62	0.65
2:A:430:LYS:HE2	2:B:188:VAL:HG12	1.77	0.65
2:B:142:GLU:H	2:B:490:GLN:HG2	1.60	0.65
2:G:390:ASP:OD2	2:G:394:SER:OG	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:268:ALA:HB2	2:H:294:LEU:HD11	1.77	0.65
2:H:142:GLU:H	2:H:490:GLN:HG2	1.60	0.65
2:C:153:MET:HG2	2:C:189:TYR:CD2	2.32	0.65
2:D:222:VAL:HG22	2:D:223:GLU:H	1.62	0.65
2:H:128:ARG:HE	2:H:484:PHE:HE1	1.42	0.65
2:J:177:ILE:HG12	2:J:224:ILE:HD11	1.78	0.65
2:B:318:LYS:N	2:B:360:GLU:OE2	2.28	0.65
2:B:344:ARG:CZ	2:C:344:ARG:HH22	2.09	0.65
2:I:95:VAL:HG12	2:J:123:GLN:HE21	1.62	0.65
1:a:240:TYR:OH	1:a:277:ARG:NH2	2.29	0.65
2:K:482:ASN:HB3	2:K:485:ALA:HB2	1.79	0.65
3:P:33:PRO:HG2	3:P:62:GLU:OE1	1.96	0.65
2:G:69:GLY:N	2:I:234:GLU:OE2	2.28	0.64
2:H:95:VAL:HG12	2:I:123:GLN:HE21	1.62	0.64
2:B:390:ASP:OD2	2:B:394:SER:OG	2.12	0.64
2:I:431:GLN:HE22	2:J:217:GLU:HB2	1.62	0.64
2:K:222:VAL:HG22	2:K:223:GLU:H	1.61	0.64
2:A:249:GLU:HG2	2:F:267:LYS:HB3	1.80	0.64
2:C:153:MET:HE2	2:C:225:ALA:HA	1.79	0.64
2:F:318:LYS:N	2:F:360:GLU:OE2	2.30	0.64
2:A:105:ASN:ND2	2:A:409:THR:O	2.19	0.64
2:G:333:ASP:HB3	2:G:519:LYS:HB2	1.78	0.64
2:K:351:LYS:NZ	2:K:390:ASP:O	2.29	0.64
2:K:401:ALA:O	2:L:420:LYS:NZ	2.29	0.64
2:D:266:LEU:HD11	2:E:155:SER:HB3	1.78	0.64
2:D:400:LEU:HD11	2:E:417:LEU:HB3	1.80	0.64
2:D:431:GLN:HE21	2:E:213:LYS:HB3	1.62	0.64
2:I:268:ALA:HB1	2:I:290:LEU:HD13	1.78	0.64
1:a:29:ARG:NH1	1:a:200:ASP:OD2	2.31	0.64
2:H:277:ASP:OD1	2:H:278:LEU:N	2.30	0.64
2:K:456:LEU:H	2:K:475:THR:HG22	1.61	0.64
1:a:243:ALA:HB1	1:a:244:PRO:HD2	1.79	0.64
2:G:351:LYS:NZ	2:G:390:ASP:O	2.30	0.64
2:B:294:LEU:HD12	2:B:471:MET:HE2	1.80	0.63
2:E:398:GLN:HG2	2:E:399:GLY:N	2.14	0.63
1:a:165:LYS:NZ	2:F:91:ILE:O	2.31	0.63
2:B:268:ALA:HB1	2:B:290:LEU:HD13	1.80	0.63
2:K:101:ARG:HD2	2:L:146:PRO:HD3	1.80	0.63
2:L:166:LEU:HD22	2:L:212:ILE:HD11	1.80	0.63
2:B:345:TRP:HB3	2:C:343:ALA:HA	1.80	0.63
2:K:177:ILE:HG12	2:K:224:ILE:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:56:LYS:HD3	1:a:64:PHE:HE1	1.63	0.63
2:F:110:ASP:OD2	2:F:422:ARG:NH1	2.31	0.63
2:J:222:VAL:HG22	2:J:223:GLU:H	1.63	0.63
2:B:337:PRO:HB3	4:Z:306:TRP:HB3	1.81	0.63
2:A:131:TYR:HB3	2:A:250:MET:HG2	1.80	0.63
2:A:166:LEU:HD22	2:A:212:ILE:HD11	1.81	0.63
2:K:386:LEU:HB3	2:K:404:PHE:HE2	1.64	0.63
2:L:278:LEU:HD21	2:L:284:MET:HB2	1.79	0.63
2:G:222:VAL:HG22	2:G:223:GLU:H	1.64	0.63
2:I:142:GLU:H	2:I:490:GLN:HB3	1.63	0.63
2:J:121:THR:HA	2:J:259:ILE:O	1.99	0.63
2:A:357:ILE:HD11	2:A:376:ILE:HG21	1.81	0.63
1:a:363:VAL:HG11	2:F:464:PRO:HA	1.80	0.62
2:B:235:LEU:HD23	2:F:68:ILE:HD13	1.80	0.62
2:H:266:LEU:HD11	2:I:155:SER:HB3	1.81	0.62
2:E:269:ALA:HA	2:E:470:VAL:HA	1.80	0.62
2:J:363:GLU:OE2	2:J:366:ARG:NH2	2.32	0.62
2:F:378:ALA:O	2:F:426:ASP:N	2.29	0.62
2:B:163:PHE:HB2	2:B:179:THR:HG23	1.80	0.62
2:G:350:PHE:CB	2:G:389:VAL:HG21	2.29	0.62
2:A:333:ASP:HB3	2:A:519:LYS:HB2	1.82	0.62
2:E:84:THR:HG22	2:E:86:GLY:H	1.63	0.62
2:H:153:MET:HG2	2:H:189:TYR:CD2	2.34	0.62
2:K:264:ARG:NH1	2:L:155:SER:OG	2.33	0.62
3:W:11:LYS:HG3	3:W:27:GLU:HG2	1.81	0.62
1:a:339:SER:HG	1:a:413:SER:HG	1.46	0.62
2:E:121:THR:HA	2:E:259:ILE:O	1.99	0.62
2:E:345:TRP:HB3	2:F:343:ALA:HA	1.80	0.62
2:J:100:ARG:HG2	2:J:101:ARG:H	1.63	0.62
2:J:377:ILE:HG22	2:J:424:TYR:HB2	1.80	0.62
2:K:357:ILE:HD11	2:K:376:ILE:HG21	1.80	0.62
2:L:432:ASP:OD1	2:L:433:TYR:N	2.33	0.62
3:O:9:ASN:HB3	3:O:56:TYR:HE2	1.65	0.62
2:B:131:TYR:HB3	2:B:250:MET:HG2	1.82	0.62
2:C:343:ALA:HB1	2:C:348:GLU:HB3	1.82	0.62
2:I:80:ALA:HA	2:I:93:PRO:HG2	1.81	0.62
2:I:191:GLN:N	2:I:222:VAL:O	2.31	0.62
1:a:212:LYS:HG2	1:a:317:ASN:HD21	1.65	0.62
2:A:350:PHE:CB	2:A:389:VAL:HG21	2.29	0.62
2:C:350:PHE:CB	2:C:389:VAL:HG21	2.30	0.62
2:F:191:GLN:N	2:F:222:VAL:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:131:TYR:HD2	2:K:250:MET:HE3	1.65	0.62
2:A:498:SER:HB3	2:F:76:ALA:HB2	1.82	0.62
2:B:84:THR:HG22	2:B:86:GLY:H	1.65	0.62
2:D:128:ARG:HE	2:D:484:PHE:HE1	1.47	0.62
2:F:291:SER:HB2	2:F:471:MET:HE1	1.80	0.62
2:C:266:LEU:HD11	2:D:155:SER:HB3	1.82	0.62
2:C:468:GLN:NE2	2:H:234:GLU:O	2.32	0.62
2:D:333:ASP:HB3	2:D:519:LYS:HB2	1.81	0.62
2:J:313:SER:OG	2:J:510:ASN:ND2	2.33	0.62
2:L:105:ASN:ND2	2:L:409:THR:O	2.33	0.62
2:B:266:LEU:HD11	2:C:155:SER:HB3	1.81	0.61
2:C:222:VAL:HG22	2:C:223:GLU:H	1.63	0.61
2:C:277:ASP:OD1	2:C:278:LEU:N	2.33	0.61
2:D:353:LEU:HD13	2:D:385:VAL:HG11	1.82	0.61
2:F:351:LYS:NZ	2:F:390:ASP:O	2.31	0.61
2:H:181:PHE:HD1	2:H:187:THR:HB	1.64	0.61
2:I:267:LYS:HB3	2:J:249:GLU:HG2	1.81	0.61
2:K:121:THR:HG22	2:K:260:GLU:OE1	2.01	0.61
3:P:26:LYS:NZ	3:P:74:ASP:OD2	2.32	0.61
2:E:95:VAL:HG12	2:F:123:GLN:HE21	1.65	0.61
2:K:277:ASP:OD1	2:K:278:LEU:N	2.33	0.61
2:L:222:VAL:HG22	2:L:223:GLU:H	1.64	0.61
2:A:266:LEU:HD11	2:B:155:SER:HB3	1.82	0.61
2:G:100:ARG:HG2	2:G:101:ARG:H	1.65	0.61
2:G:131:TYR:HD2	2:G:250:MET:HE3	1.66	0.61
2:H:241:GLY:HA3	3:V:43:GLY:H	1.65	0.61
2:J:390:ASP:OD2	2:J:394:SER:OG	2.16	0.61
2:E:133:LYS:HE2	3:R:42:SER:HB2	1.83	0.61
2:G:155:SER:HB3	2:L:266:LEU:HD11	1.82	0.61
2:L:277:ASP:OD1	2:L:278:LEU:N	2.32	0.61
1:a:267:TYR:HB3	1:a:327:VAL:HG21	1.83	0.61
2:K:318:LYS:N	2:K:360:GLU:OE2	2.34	0.61
2:E:154:PHE:O	2:E:248:ASN:ND2	2.34	0.61
2:E:383:VAL:HG12	2:E:406:THR:HG22	1.81	0.61
2:F:244:ASP:HB2	3:Q:13:PHE:HE2	1.66	0.61
2:K:346:ALA:O	2:K:349:SER:N	2.34	0.61
1:a:35:ILE:HD12	1:a:39:ILE:HD11	1.83	0.61
1:a:258:VAL:HG21	1:a:310:LEU:HD11	1.83	0.61
2:A:222:VAL:HG22	2:A:223:GLU:H	1.66	0.61
2:D:430:LYS:HE2	2:E:188:VAL:CG1	2.30	0.61
2:I:350:PHE:CB	2:I:389:VAL:HG21	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:398:GLN:HG2	2:C:399:GLY:N	2.16	0.60
2:J:431:GLN:NE2	2:K:217:GLU:HB2	2.11	0.60
2:B:222:VAL:HG22	2:B:223:GLU:H	1.66	0.60
2:B:253:ARG:NE	2:B:255:ASP:OD2	2.33	0.60
2:D:145:HIS:NE2	2:D:487:SER:O	2.31	0.60
2:G:173:THR:OG1	2:G:176:ASP:OD2	2.18	0.60
2:H:147:MET:HE3	2:H:367:GLN:HG2	1.83	0.60
2:J:269:ALA:HA	2:J:470:VAL:HA	1.82	0.60
1:a:338:GLY:C	1:a:384:ASN:HD21	2.08	0.60
2:A:400:LEU:HD11	2:B:417:LEU:HB3	1.82	0.60
2:B:69:GLY:N	2:D:234:GLU:OE2	2.23	0.60
2:J:380:ARG:NH1	2:J:427:GLN:O	2.32	0.60
1:a:119:ILE:HG23	1:a:130:ILE:HD11	1.82	0.60
2:B:331:VAL:HG12	2:B:517:TYR:HB2	1.82	0.60
2:D:431:GLN:NE2	2:E:217:GLU:HB2	2.16	0.60
2:E:222:VAL:HG22	2:E:223:GLU:H	1.66	0.60
2:H:105:ASN:HD21	2:H:409:THR:C	2.09	0.60
2:I:253:ARG:NE	2:I:255:ASP:OD2	2.34	0.60
2:J:263:SER:HB2	2:K:230:THR:HG22	1.83	0.60
2:J:345:TRP:HB3	2:K:343:ALA:HA	1.82	0.60
2:K:166:LEU:HD11	2:K:221:LEU:HD21	1.83	0.60
2:J:131:TYR:HD2	2:J:250:MET:HE3	1.67	0.60
1:a:179:ILE:HD12	1:a:198:LEU:HD12	1.83	0.60
2:D:344:ARG:HD2	2:E:344:ARG:HH12	1.66	0.60
2:D:390:ASP:OD2	2:D:394:SER:OG	2.19	0.60
2:J:268:ALA:HB2	2:J:294:LEU:HD11	1.83	0.60
2:J:357:ILE:HD11	2:J:376:ILE:HD13	1.83	0.60
2:K:131:TYR:HB3	2:K:250:MET:HG2	1.82	0.60
2:C:344:ARG:HD3	5:z:1012:UNK:O	2.01	0.60
2:D:173:THR:OG1	2:D:176:ASP:OD2	2.18	0.60
2:D:377:ILE:HG22	2:D:424:TYR:HB2	1.82	0.60
2:E:367:GLN:HB3	2:E:511:ALA:HB1	1.83	0.60
2:H:222:VAL:HG22	2:H:223:GLU:H	1.66	0.60
2:I:96:MET:HB2	2:J:124:VAL:HG22	1.84	0.60
2:J:268:ALA:HB1	2:J:290:LEU:HD13	1.82	0.60
1:a:298:LEU:HB3	1:a:305:PHE:CE2	2.36	0.60
2:C:66:ALA:N	2:G:249:GLU:OE1	2.35	0.60
2:C:148:TYR:HD1	2:C:186:GLY:H	1.50	0.60
2:D:80:ALA:HA	2:D:93:PRO:HG2	1.83	0.60
2:D:456:LEU:H	2:D:475:THR:HG22	1.65	0.60
2:F:107:ILE:H	2:F:303:ASN:HD21	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:GLU:H	2:F:490:GLN:HG2	1.66	0.60
2:H:398:GLN:HG2	2:H:399:GLY:H	1.65	0.60
2:L:128:ARG:HE	2:L:484:PHE:HE1	1.49	0.60
1:a:384:ASN:ND2	1:a:412:LEU:HD22	2.17	0.59
2:A:409:THR:HG21	2:B:370:ARG:O	2.02	0.59
2:B:363:GLU:OE2	2:B:366:ARG:NH2	2.35	0.59
2:C:177:ILE:HG12	2:C:224:ILE:HD11	1.84	0.59
2:D:268:ALA:HB1	2:D:290:LEU:HD13	1.83	0.59
2:I:333:ASP:HB3	2:I:519:LYS:HB2	1.84	0.59
2:L:145:HIS:NE2	2:L:487:SER:O	2.29	0.59
2:H:357:ILE:HD11	2:H:376:ILE:HD13	1.83	0.59
3:P:65:ARG:O	3:P:68:TRP:N	2.35	0.59
2:E:105:ASN:ND2	2:E:409:THR:O	2.35	0.59
2:E:151:ASP:HB3	2:E:187:THR:HG23	1.85	0.59
2:E:313:SER:OG	2:E:510:ASN:ND2	2.36	0.59
2:E:291:SER:HB2	2:E:471:MET:HE1	1.84	0.59
2:H:164:PRO:HG2	2:H:178:TYR:HD1	1.68	0.59
2:J:145:HIS:CD2	2:J:146:PRO:HD2	2.36	0.59
1:a:108:TYR:HE2	1:a:132:ILE:HD11	1.68	0.59
2:D:169:SER:OG	2:D:200:ALA:HB2	2.02	0.59
2:F:105:ASN:ND2	2:F:409:THR:O	2.23	0.59
2:I:105:ASN:ND2	2:I:409:THR:O	2.27	0.59
3:P:11:LYS:HG3	3:P:27:GLU:HG2	1.84	0.59
2:C:345:TRP:HB3	2:D:343:ALA:HA	1.84	0.59
2:C:357:ILE:HD11	2:C:376:ILE:HD13	1.84	0.59
2:E:430:LYS:HE2	2:F:188:VAL:HG11	1.84	0.59
2:H:357:ILE:HD11	2:H:376:ILE:HG21	1.83	0.59
2:H:398:GLN:HE21	2:I:355:PHE:HB2	1.67	0.59
2:L:318:LYS:N	2:L:360:GLU:OE2	2.35	0.59
2:E:390:ASP:OD2	2:E:394:SER:OG	2.20	0.59
1:a:221:VAL:HG23	1:a:403:MET:HE1	1.84	0.59
2:D:264:ARG:NH1	2:E:155:SER:OG	2.34	0.59
2:G:147:MET:HE3	2:G:367:GLN:HG2	1.85	0.59
2:E:432:ASP:OD1	2:E:433:TYR:N	2.36	0.59
2:G:431:GLN:NE2	2:H:217:GLU:HB2	2.18	0.59
2:I:147:MET:HE3	2:I:367:GLN:HG2	1.84	0.59
2:K:377:ILE:HG22	2:K:424:TYR:HB2	1.84	0.59
1:a:49:VAL:HG11	1:a:167:GLN:HE21	1.68	0.58
1:a:235:PHE:HE2	1:a:419:LYS:HG3	1.67	0.58
2:A:147:MET:HE3	2:A:367:GLN:HG2	1.84	0.58
2:B:110:ASP:OD2	2:B:422:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:GLN:N	2:B:227:GLY:O	2.34	0.58
2:K:100:ARG:HG2	2:K:101:ARG:H	1.68	0.58
2:C:269:ALA:HA	2:C:470:VAL:HA	1.84	0.58
2:D:177:ILE:HG12	2:D:224:ILE:HD11	1.85	0.58
2:E:494:SER:HA	3:R:37:ASP:CG	2.28	0.58
2:H:145:HIS:CD2	2:H:146:PRO:HD2	2.35	0.58
2:A:376:ILE:HG12	2:A:423:VAL:HG22	1.85	0.58
2:D:85:SER:HB3	3:Q:32:PHE:HE1	1.68	0.58
2:J:151:ASP:HB2	2:J:189:TYR:HE1	1.68	0.58
2:J:153:MET:HE2	2:J:226:GLU:H	1.69	0.58
1:a:41:ALA:HB1	1:a:336:ILE:HG22	1.83	0.58
2:B:153:MET:HG2	2:B:189:TYR:CD2	2.39	0.58
2:B:482:ASN:ND2	2:B:512:TYR:OH	2.35	0.58
2:D:272:ILE:HG22	2:D:468:GLN:HE21	1.69	0.58
2:D:380:ARG:NH2	2:D:408:THR:OG1	2.34	0.58
2:E:323:LEU:HD21	2:E:329:ALA:HA	1.84	0.58
2:H:485:ALA:HB1	2:H:510:ASN:OD1	2.03	0.58
2:J:266:LEU:HD11	2:K:155:SER:HB3	1.85	0.58
2:K:343:ALA:HB1	2:K:348:GLU:HB3	1.86	0.58
3:O:62:GLU:HG2	3:P:4:ALA:HB2	1.85	0.58
2:A:191:GLN:N	2:A:222:VAL:O	2.31	0.58
2:A:344:ARG:HH12	2:F:344:ARG:NH1	2.01	0.58
2:A:432:ASP:OD1	2:A:433:TYR:N	2.35	0.58
2:D:383:VAL:HG12	2:D:406:THR:HG22	1.86	0.58
3:W:9:ASN:HB3	3:W:56:TYR:HE2	1.69	0.58
2:G:377:ILE:HG22	2:G:424:TYR:HB2	1.84	0.58
2:I:323:LEU:HD21	2:I:329:ALA:HA	1.85	0.58
2:J:476:ARG:HH21	2:K:230:THR:HG21	1.68	0.58
2:L:253:ARG:NE	2:L:255:ASP:OD2	2.32	0.58
2:D:249:GLU:OE1	2:L:66:ALA:N	2.36	0.58
2:E:268:ALA:HB1	2:E:290:LEU:HD13	1.86	0.58
2:G:131:TYR:HB3	2:G:250:MET:HG2	1.85	0.58
2:I:331:VAL:HG12	2:I:517:TYR:HB2	1.85	0.58
2:I:386:LEU:HB3	2:I:404:PHE:HE2	1.68	0.58
2:K:398:GLN:HG2	2:K:399:GLY:N	2.18	0.58
2:B:375:PHE:CZ	2:B:437:GLY:HA3	2.39	0.58
2:G:249:GLU:HG2	2:L:267:LYS:HB3	1.85	0.58
2:H:177:ILE:HG12	2:H:224:ILE:HD11	1.84	0.58
2:A:168:ALA:HB1	2:A:200:ALA:HA	1.85	0.58
2:G:72:HIS:CD2	2:H:121:THR:HG21	2.38	0.58
2:H:278:LEU:HD22	2:H:286:ALA:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:346:ALA:O	2:I:349:SER:N	2.37	0.58
2:I:456:LEU:H	2:I:475:THR:HG22	1.69	0.58
1:a:213:ASP:OD2	1:a:379:TYR:OH	2.14	0.58
2:B:431:GLN:HE21	2:C:213:LYS:HB3	1.67	0.58
2:E:232:ILE:HD11	3:T:49:PHE:HB3	1.86	0.58
2:J:80:ALA:HA	2:J:93:PRO:HG2	1.86	0.58
3:O:18:ASP:HB3	3:O:21:LYS:HD3	1.85	0.58
2:G:244:ASP:HB2	3:S:13:PHE:HE2	1.68	0.57
2:G:344:ARG:HH12	2:L:344:ARG:NH1	2.01	0.57
2:G:378:ALA:HB1	2:G:382:VAL:HG21	1.86	0.57
2:K:84:THR:HG22	2:K:86:GLY:H	1.68	0.57
2:K:264:ARG:HE	2:K:477:TYR:HE1	1.51	0.57
2:B:277:ASP:OD1	2:B:278:LEU:N	2.37	0.57
2:I:152:ALA:HB1	2:I:225:ALA:CB	2.34	0.57
2:L:121:THR:HA	2:L:259:ILE:O	2.03	0.57
2:D:407:ASP:HB3	2:E:372:GLU:HB2	1.86	0.57
2:E:101:ARG:HD2	2:F:146:PRO:HD3	1.86	0.57
2:G:100:ARG:NH2	2:G:289:GLU:OE1	2.37	0.57
2:L:363:GLU:OE2	2:L:366:ARG:NH2	2.37	0.57
2:B:269:ALA:HA	2:B:470:VAL:HA	1.87	0.57
2:G:191:GLN:N	2:G:222:VAL:O	2.37	0.57
2:C:398:GLN:HE21	2:D:355:PHE:HB2	1.69	0.57
2:D:323:LEU:HD21	2:D:329:ALA:HA	1.86	0.57
2:C:390:ASP:OD2	2:C:394:SER:OG	2.18	0.57
2:D:344:ARG:HD2	2:E:344:ARG:NH1	2.20	0.57
2:H:145:HIS:NE2	2:H:487:SER:O	2.36	0.57
2:K:432:ASP:OD1	2:K:433:TYR:N	2.38	0.57
3:O:64:GLN:HB3	3:O:67:GLU:HB2	1.86	0.57
2:F:390:ASP:OD2	2:F:394:SER:OG	2.17	0.57
2:A:121:THR:HG21	2:F:72:HIS:NE2	2.20	0.57
2:A:305:GLU:HA	2:B:225:ALA:HB3	1.86	0.57
2:B:268:ALA:HB2	2:B:294:LEU:HD11	1.87	0.57
2:C:181:PHE:HD1	2:C:187:THR:HB	1.69	0.57
2:G:430:LYS:HE2	2:H:188:VAL:CG1	2.34	0.57
2:I:153:MET:HG2	2:I:189:TYR:CD2	2.39	0.57
2:L:398:GLN:HG2	2:L:399:GLY:N	2.18	0.57
1:a:283:ALA:HB2	1:a:288:LEU:HD23	1.87	0.57
2:E:147:MET:HE3	2:E:367:GLN:HG2	1.87	0.57
2:I:291:SER:HB2	2:I:471:MET:HE1	1.86	0.57
2:C:396:ALA:O	2:D:395:TYR:HA	2.05	0.57
2:E:100:ARG:HG2	2:E:101:ARG:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:147:MET:HE1	2:I:366:ARG:NH1	2.19	0.57
2:I:456:LEU:HD12	2:I:475:THR:HG21	1.86	0.57
2:L:133:LYS:HE2	3:U:42:SER:HB2	1.86	0.57
2:L:313:SER:O	2:L:510:ASN:HB2	2.05	0.57
2:A:357:ILE:HD11	2:A:376:ILE:HD13	1.86	0.56
2:C:267:LYS:HB3	2:D:249:GLU:HG2	1.86	0.56
2:G:343:ALA:HB1	2:G:348:GLU:HB3	1.85	0.56
2:L:374:ASN:ND2	2:L:439:LYS:O	2.39	0.56
1:a:151:SER:OG	1:a:153:ASP:O	2.23	0.56
2:A:145:HIS:CD2	2:A:146:PRO:HD2	2.39	0.56
2:C:136:VAL:HG11	2:C:495:ARG:NH2	2.20	0.56
2:D:232:ILE:HD11	3:X:49:PHE:HB3	1.87	0.56
2:G:168:ALA:HB1	2:G:200:ALA:HA	1.87	0.56
2:J:131:TYR:HB3	2:J:250:MET:HG2	1.87	0.56
2:J:148:TYR:HD1	2:J:186:GLY:H	1.54	0.56
2:K:121:THR:HA	2:K:259:ILE:O	2.06	0.56
2:A:315:GLN:HG3	2:A:510:ASN:O	2.05	0.56
2:D:142:GLU:H	2:D:490:GLN:HG2	1.70	0.56
2:D:149:GLY:H	2:D:186:GLY:HA2	1.70	0.56
2:H:430:LYS:HG2	2:I:216:MET:HE1	1.86	0.56
2:K:153:MET:HG2	2:K:189:TYR:CD2	2.41	0.56
2:K:357:ILE:HD11	2:K:376:ILE:HD13	1.88	0.56
2:L:354:LEU:HA	2:L:357:ILE:HG22	1.88	0.56
3:P:14:GLU:HB3	3:P:25:GLY:N	2.21	0.56
2:A:269:ALA:HA	2:A:470:VAL:HA	1.88	0.56
2:C:69:GLY:HA2	2:L:274:LEU:HD13	1.87	0.56
2:C:238:GLY:HA2	2:C:242:SER:O	2.05	0.56
2:E:153:MET:HE2	2:E:226:GLU:H	1.70	0.56
2:G:188:VAL:CG1	2:L:430:LYS:HE2	2.35	0.56
2:H:171:GLN:NE2	2:H:195:GLN:HE21	2.03	0.56
2:H:432:ASP:OD1	2:H:433:TYR:N	2.37	0.56
2:K:164:PRO:HG2	2:K:178:TYR:HD1	1.70	0.56
1:a:40:VAL:HB	1:a:340:ILE:O	2.05	0.56
1:a:290:HIS:O	1:a:294:ASP:HB3	2.06	0.56
2:C:380:ARG:NH1	2:C:427:GLN:O	2.35	0.56
2:D:168:ALA:HB1	2:D:200:ALA:HA	1.88	0.56
2:J:191:GLN:N	2:J:222:VAL:O	2.38	0.56
2:K:354:LEU:HA	2:K:357:ILE:HG22	1.86	0.56
3:O:9:ASN:HB3	3:O:56:TYR:CE2	2.40	0.56
2:A:268:ALA:HB1	2:A:290:LEU:HD13	1.87	0.56
2:F:179:THR:HG22	2:F:189:TYR:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:301:GLU:OE1	2:J:155:SER:OG	2.21	0.56
2:A:96:MET:HE3	2:B:124:VAL:HG23	1.87	0.56
2:A:129:ALA:O	2:A:143:ALA:N	2.31	0.56
2:E:235:LEU:HD12	2:E:235:LEU:O	2.05	0.56
2:I:101:ARG:HH12	2:J:145:HIS:CD2	2.24	0.56
2:K:80:ALA:HA	2:K:93:PRO:HG2	1.88	0.56
2:L:152:ALA:HB1	2:L:225:ALA:CB	2.36	0.56
1:a:110:VAL:HA	1:a:137:VAL:HG12	1.88	0.56
1:a:235:PHE:CE2	1:a:419:LYS:HG3	2.41	0.56
2:A:74:TYR:CE2	2:B:260:GLU:HG2	2.41	0.56
2:B:430:LYS:HE2	2:C:188:VAL:HG11	1.86	0.56
2:G:393:ILE:HA	2:L:398:GLN:O	2.05	0.56
2:H:80:ALA:HA	2:H:93:PRO:HG2	1.87	0.56
2:A:155:SER:HB3	2:F:266:LEU:CD1	2.35	0.56
2:B:177:ILE:HG12	2:B:224:ILE:HD11	1.87	0.56
2:C:95:VAL:HG12	2:D:123:GLN:HE21	1.71	0.56
2:E:163:PHE:HB2	2:E:179:THR:HG23	1.87	0.56
2:I:100:ARG:HG2	2:I:101:ARG:H	1.71	0.56
2:L:269:ALA:HA	2:L:470:VAL:HA	1.86	0.56
1:a:362:VAL:HG22	1:a:373:ILE:HG12	1.87	0.55
2:A:185:THR:O	2:F:430:LYS:HE3	2.06	0.55
2:B:398:GLN:HG2	2:B:399:GLY:N	2.21	0.55
2:I:344:ARG:O	2:I:348:GLU:HB2	2.06	0.55
2:I:398:GLN:HG2	2:I:399:GLY:N	2.21	0.55
2:J:291:SER:HB2	2:J:471:MET:HE1	1.89	0.55
3:P:20:ASN:H	3:Q:16:LYS:HZ3	1.52	0.55
2:A:155:SER:OG	2:F:301:GLU:OE1	2.24	0.55
2:B:234:GLU:CD	2:F:69:GLY:H	2.13	0.55
2:C:384:ASN:HD21	2:D:362:VAL:HG21	1.72	0.55
2:E:234:GLU:O	2:L:468:GLN:NE2	2.40	0.55
2:E:380:ARG:NH2	2:E:408:THR:OG1	2.37	0.55
2:K:409:THR:HG21	2:L:370:ARG:O	2.06	0.55
3:W:65:ARG:O	3:W:68:TRP:N	2.39	0.55
2:A:323:LEU:HD21	2:A:329:ALA:HA	1.87	0.55
2:A:362:VAL:HG21	2:F:384:ASN:HD21	1.71	0.55
2:E:177:ILE:HG12	2:E:224:ILE:HD11	1.87	0.55
2:E:237:GLU:HG3	2:L:465:LYS:HB3	1.88	0.55
2:E:398:GLN:HE21	2:F:355:PHE:HB2	1.70	0.55
3:P:5:ARG:HD2	3:P:33:PRO:HG3	1.87	0.55
2:A:71:ASP:CG	2:C:231:SER:HB2	2.30	0.55
2:D:151:ASP:HB2	2:D:189:TYR:CE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:350:PHE:HB3	2:L:389:VAL:HG21	1.89	0.55
2:A:146:PRO:HB2	2:A:366:ARG:O	2.06	0.55
2:A:230:THR:HG22	2:F:263:SER:HB2	1.89	0.55
2:A:263:SER:HB2	2:B:230:THR:HG22	1.89	0.55
2:F:184:GLU:O	2:F:185:THR:OG1	2.22	0.55
2:G:313:SER:OG	2:G:510:ASN:ND2	2.40	0.55
2:K:291:SER:HB2	2:K:471:MET:HE1	1.87	0.55
2:H:121:THR:HA	2:H:259:ILE:O	2.06	0.55
2:H:291:SER:HB2	2:H:471:MET:HE1	1.88	0.55
2:K:147:MET:HE1	2:K:366:ARG:NH1	2.22	0.55
2:K:344:ARG:CZ	2:L:344:ARG:HH22	2.18	0.55
2:L:145:HIS:CD2	2:L:146:PRO:HD2	2.33	0.55
2:L:291:SER:HB2	2:L:471:MET:HE1	1.87	0.55
3:P:20:ASN:H	3:Q:16:LYS:NZ	2.04	0.55
2:A:135:PRO:HG3	2:A:251:GLY:HA3	1.89	0.55
2:B:263:SER:HB2	2:C:230:THR:HG22	1.89	0.55
2:G:344:ARG:O	2:G:348:GLU:HB2	2.07	0.55
2:H:323:LEU:HD21	2:H:329:ALA:HA	1.89	0.55
2:J:169:SER:OG	2:J:200:ALA:HB2	2.07	0.55
2:L:116:PRO:HA	2:L:452:PRO:HD2	1.88	0.55
2:G:432:ASP:OD1	2:G:433:TYR:N	2.39	0.55
2:G:456:LEU:HD12	2:G:475:THR:CG2	2.37	0.55
2:H:101:ARG:HH12	2:I:145:HIS:CD2	2.25	0.55
2:J:71:ASP:CG	2:L:231:SER:HB2	2.32	0.55
2:L:275:THR:HG22	2:L:286:ALA:HB3	1.88	0.55
2:A:386:LEU:HB3	2:A:404:PHE:HE2	1.72	0.55
2:C:191:GLN:N	2:C:222:VAL:O	2.35	0.55
2:D:197:THR:HG22	2:D:199:ASP:H	1.72	0.55
2:D:398:GLN:HG2	2:D:399:GLY:N	2.21	0.55
2:I:129:ALA:O	2:I:143:ALA:N	2.37	0.55
2:I:264:ARG:NH1	2:J:155:SER:OG	2.40	0.55
2:A:115:GLN:NE2	2:A:444:MET:SD	2.79	0.55
2:A:175:GLY:HA2	2:F:503:ILE:HD11	1.88	0.55
2:A:431:GLN:NE2	2:B:217:GLU:HB2	2.20	0.55
2:C:169:SER:OG	2:C:200:ALA:HB2	2.07	0.55
2:G:129:ALA:O	2:G:143:ALA:N	2.27	0.55
2:I:244:ASP:O	2:I:246:PRO:HD3	2.07	0.55
2:J:396:ALA:O	2:K:395:TYR:HA	2.07	0.55
2:K:333:ASP:HB3	2:K:519:LYS:HB2	1.88	0.55
1:a:378:ARG:NH2	2:F:273:GLU:HB3	2.15	0.54
2:B:430:LYS:HG2	2:C:216:MET:HE1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:74:TYR:CE2	2:F:260:GLU:HG2	2.42	0.54
2:G:188:VAL:HG11	2:L:430:LYS:HE2	1.89	0.54
2:K:106:LEU:HB3	2:K:303:ASN:ND2	2.22	0.54
2:K:430:LYS:HE2	2:L:188:VAL:CG1	2.37	0.54
2:D:346:ALA:O	2:D:349:SER:N	2.40	0.54
2:J:331:VAL:HG12	2:J:517:TYR:HB2	1.89	0.54
3:W:9:ASN:HB3	3:W:56:TYR:CE2	2.42	0.54
2:A:213:LYS:HB3	2:F:431:GLN:HE21	1.71	0.54
2:A:244:ASP:HB2	3:O:13:PHE:HE2	1.71	0.54
2:G:74:TYR:CE2	2:H:260:GLU:HG2	2.42	0.54
2:I:169:SER:OG	2:I:200:ALA:HB2	2.07	0.54
2:L:343:ALA:HB1	2:L:348:GLU:HB3	1.90	0.54
2:A:98:MET:SD	2:A:284:MET:HE3	2.46	0.54
2:K:166:LEU:HD22	2:K:212:ILE:HD11	1.89	0.54
1:a:274:ALA:HB3	1:a:279:ALA:HB2	1.89	0.54
2:C:502:SER:O	2:C:506:SER:OG	2.25	0.54
2:G:71:ASP:CG	2:I:231:SER:HB2	2.33	0.54
2:G:267:LYS:HB3	2:H:249:GLU:HG2	1.89	0.54
2:I:235:LEU:HD12	2:I:235:LEU:O	2.07	0.54
2:K:235:LEU:HD12	2:K:235:LEU:O	2.08	0.54
2:G:125:PHE:CE2	2:L:282:HIS:HE1	2.25	0.54
2:H:135:PRO:HB3	2:H:252:PHE:O	2.08	0.54
2:H:169:SER:OG	2:H:200:ALA:HB2	2.08	0.54
2:I:166:LEU:HD22	2:I:212:ILE:HD11	1.90	0.54
2:L:168:ALA:HB2	2:L:202:ALA:O	2.07	0.54
1:a:163:ILE:HD12	2:F:88:VAL:HG22	1.89	0.54
2:A:350:PHE:HB3	2:A:389:VAL:HG21	1.88	0.54
2:C:101:ARG:HH12	2:D:145:HIS:CD2	2.26	0.54
2:D:430:LYS:HE2	2:E:188:VAL:HG12	1.90	0.54
2:F:295:ALA:HB2	2:F:473:PHE:CE2	2.43	0.54
2:H:107:ILE:HG21	2:H:307:VAL:HG21	1.88	0.54
2:I:181:PHE:HD1	2:I:187:THR:HB	1.73	0.54
2:L:169:SER:OG	2:L:200:ALA:HB2	2.08	0.54
2:E:264:ARG:NH1	2:F:155:SER:OG	2.39	0.54
2:E:272:ILE:HG22	2:E:468:GLN:HE21	1.73	0.54
2:F:173:THR:OG1	2:F:176:ASP:OD2	2.25	0.54
2:F:177:ILE:HG12	2:F:224:ILE:HD11	1.88	0.54
2:F:235:LEU:HD12	2:F:235:LEU:O	2.08	0.54
2:F:353:LEU:O	2:F:356:GLN:N	2.41	0.54
2:I:444:MET:O	2:I:449:TYR:OH	2.26	0.54
1:a:275:SER:HB2	1:a:321:ASP:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:121:THR:O	2:F:93:PRO:HB3	2.08	0.54
2:A:142:GLU:H	2:A:490:GLN:HG2	1.72	0.54
2:C:398:GLN:NE2	2:D:355:PHE:HB2	2.23	0.54
2:D:179:THR:HG22	2:D:189:TYR:CE2	2.42	0.54
2:E:485:ALA:HB1	2:E:510:ASN:OD1	2.08	0.54
2:F:398:GLN:HG2	2:F:399:GLY:N	2.21	0.54
2:G:121:THR:HG21	2:L:72:HIS:CD2	2.42	0.54
2:H:383:VAL:HG12	2:H:406:THR:HG22	1.89	0.54
2:J:179:THR:HG22	2:J:189:TYR:CE2	2.43	0.54
2:H:96:MET:HE3	2:I:124:VAL:HG23	1.89	0.54
2:H:350:PHE:CB	2:H:389:VAL:HG21	2.37	0.54
2:H:377:ILE:HG22	2:H:424:TYR:HB2	1.90	0.54
2:K:153:MET:HE2	2:K:225:ALA:HA	1.90	0.54
3:O:65:ARG:O	3:O:68:TRP:N	2.41	0.54
2:A:378:ALA:HB1	2:A:382:VAL:CG2	2.39	0.53
2:C:268:ALA:HB1	2:C:290:LEU:HD13	1.89	0.53
2:F:277:ASP:O	2:F:281:VAL:HG12	2.08	0.53
2:H:133:LYS:HE2	3:W:42:SER:HB2	1.90	0.53
2:H:235:LEU:HD12	2:H:235:LEU:O	2.08	0.53
2:H:272:ILE:HG22	2:H:468:GLN:HG2	1.90	0.53
1:a:107:VAL:HG13	1:a:140:PHE:HB3	1.90	0.53
2:A:291:SER:HB2	2:A:471:MET:HE1	1.88	0.53
2:A:398:GLN:HG2	2:A:399:GLY:N	2.23	0.53
2:B:396:ALA:O	2:C:395:TYR:HA	2.08	0.53
2:C:493:ALA:O	2:C:494:SER:OG	2.25	0.53
2:E:128:ARG:HE	2:E:484:PHE:HE1	1.56	0.53
2:E:493:ALA:O	2:E:494:SER:OG	2.25	0.53
2:G:100:ARG:HG2	2:G:101:ARG:N	2.22	0.53
2:G:128:ARG:HE	2:G:484:PHE:HE1	1.56	0.53
2:G:238:GLY:HA2	2:G:242:SER:O	2.09	0.53
2:I:268:ALA:HB2	2:I:294:LEU:HD11	1.89	0.53
2:J:398:GLN:HG2	2:J:399:GLY:N	2.23	0.53
2:J:398:GLN:O	2:K:393:ILE:HA	2.08	0.53
2:K:128:ARG:HE	2:K:484:PHE:HE1	1.55	0.53
1:a:173:ARG:HH12	1:a:213:ASP:HB2	1.73	0.53
2:A:153:MET:HE2	2:A:225:ALA:HA	1.90	0.53
2:E:354:LEU:HA	2:E:357:ILE:HG22	1.90	0.53
2:G:181:PHE:HD1	2:G:187:THR:HB	1.73	0.53
2:K:184:GLU:HG3	2:K:366:ARG:HH12	1.73	0.53
3:W:68:TRP:CZ2	3:W:72:ASN:HB3	2.43	0.53
2:B:486:GLU:O	2:B:487:SER:OG	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:69:GLY:N	2:E:234:GLU:OE2	2.22	0.53
2:C:133:LYS:HE2	3:Y:42:SER:HB2	1.89	0.53
2:D:129:ALA:O	2:D:143:ALA:N	2.30	0.53
2:F:172:THR:O	2:F:195:GLN:HA	2.09	0.53
2:F:430:LYS:N	2:F:430:LYS:HD2	2.24	0.53
2:G:318:LYS:N	2:G:360:GLU:OE2	2.41	0.53
2:H:367:GLN:HB3	2:H:511:ALA:HB1	1.91	0.53
2:G:266:LEU:CD1	2:H:155:SER:HB3	2.38	0.53
2:I:164:PRO:HG2	2:I:178:TYR:HD1	1.72	0.53
2:L:106:LEU:HD21	2:L:300:LEU:HD23	1.90	0.53
2:B:344:ARG:HH11	2:C:344:ARG:HH12	1.57	0.53
2:C:80:ALA:HA	2:C:93:PRO:HG2	1.90	0.53
2:C:431:GLN:NE2	2:D:217:GLU:HB2	2.21	0.53
2:H:147:MET:HE1	2:H:366:ARG:CZ	2.39	0.53
2:H:494:SER:HA	3:W:37:ASP:CG	2.33	0.53
2:J:96:MET:HE3	2:K:124:VAL:HG23	1.90	0.53
2:J:442:ASN:HB3	2:J:444:MET:H	1.73	0.53
1:a:92:LYS:HB2	1:a:116:PHE:HD2	1.74	0.53
2:A:70:GLY:N	2:C:234:GLU:OE1	2.42	0.53
2:B:376:ILE:HG12	2:B:423:VAL:HG22	1.91	0.53
2:C:85:SER:HB3	3:T:32:PHE:CE1	2.43	0.53
2:D:486:GLU:C	2:D:488:ALA:H	2.17	0.53
2:H:163:PHE:HB2	2:H:179:THR:HG23	1.89	0.53
2:J:272:ILE:O	2:J:275:THR:HG22	2.09	0.53
2:L:85:SER:HB3	3:V:32:PHE:CE1	2.44	0.53
3:O:17:LEU:HD13	3:O:23:ILE:HD11	1.91	0.53
1:a:375:LEU:HD13	1:a:377:VAL:HG23	1.91	0.53
2:B:172:THR:O	2:B:195:GLN:HA	2.08	0.53
2:A:395:TYR:HA	2:F:396:ALA:O	2.08	0.53
2:B:374:ASN:ND2	2:B:439:LYS:O	2.42	0.53
2:D:238:GLY:HA2	2:D:242:SER:O	2.09	0.53
2:D:318:LYS:HE3	2:D:327:SER:HB3	1.90	0.53
2:E:244:ASP:HB2	3:T:13:PHE:HE2	1.74	0.53
2:G:431:GLN:NE2	2:H:213:LYS:O	2.41	0.53
2:J:444:MET:O	2:J:449:TYR:OH	2.17	0.53
2:J:476:ARG:NH2	2:K:230:THR:HG21	2.23	0.53
2:A:235:LEU:HD12	2:A:235:LEU:O	2.09	0.53
2:C:164:PRO:HG2	2:C:178:TYR:HD1	1.74	0.53
2:F:387:ALA:HB2	2:F:404:PHE:HB2	1.90	0.53
2:G:398:GLN:HG2	2:G:399:GLY:N	2.22	0.53
2:I:69:GLY:N	2:K:234:GLU:OE2	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:380:ARG:NH2	2:I:408:THR:OG1	2.42	0.53
2:K:184:GLU:O	2:K:185:THR:OG1	2.21	0.53
2:D:254:ILE:HD12	2:L:88:VAL:HG22	1.90	0.52
2:E:145:HIS:CD2	2:E:146:PRO:HD2	2.37	0.52
2:F:72:HIS:ND1	2:F:83:GLN:O	2.39	0.52
2:G:258:VAL:HG11	2:L:79:ILE:HB	1.91	0.52
2:H:363:GLU:OE2	2:H:366:ARG:NH2	2.41	0.52
2:I:71:ASP:CG	2:K:231:SER:HB2	2.33	0.52
2:I:164:PRO:HG2	2:I:178:TYR:CD1	2.44	0.52
2:L:153:MET:HG2	2:L:189:TYR:CD2	2.44	0.52
3:P:12:THR:HG21	3:P:75:LEU:HD13	1.91	0.52
2:A:417:LEU:HB3	2:F:400:LEU:HD11	1.91	0.52
2:B:95:VAL:HG12	2:C:123:GLN:HE21	1.74	0.52
2:B:386:LEU:HB3	2:B:404:PHE:HE2	1.74	0.52
2:E:268:ALA:HB2	2:E:294:LEU:HD11	1.90	0.52
2:G:153:MET:HE2	2:G:225:ALA:HA	1.92	0.52
2:H:331:VAL:HG12	2:H:517:TYR:HB2	1.91	0.52
2:L:244:ASP:O	2:L:246:PRO:HD3	2.10	0.52
3:P:10:ILE:HD11	3:P:35:TYR:CE1	2.44	0.52
2:A:237:GLU:HB2	2:A:246:PRO:HA	1.92	0.52
2:B:346:ALA:O	2:B:349:SER:N	2.43	0.52
2:C:100:ARG:HG2	2:C:101:ARG:H	1.74	0.52
2:D:181:PHE:HZ	2:D:490:GLN:HE22	1.56	0.52
2:D:350:PHE:CB	2:D:389:VAL:HG21	2.36	0.52
2:E:377:ILE:HG22	2:E:424:TYR:HB2	1.91	0.52
2:E:400:LEU:HD11	2:F:417:LEU:HB3	1.91	0.52
2:G:315:GLN:HG3	2:G:510:ASN:O	2.10	0.52
2:H:318:LYS:N	2:H:360:GLU:OE2	2.41	0.52
2:I:364:ILE:O	2:I:368:THR:OG1	2.25	0.52
2:J:318:LYS:N	2:J:360:GLU:OE2	2.40	0.52
2:K:272:ILE:HG22	2:K:468:GLN:HG2	1.90	0.52
2:C:135:PRO:HG3	2:C:251:GLY:HA3	1.91	0.52
2:F:113:GLY:HA2	2:F:439:LYS:HE2	1.92	0.52
2:I:305:GLU:HA	2:J:225:ALA:HB3	1.92	0.52
2:K:100:ARG:HG2	2:K:101:ARG:N	2.25	0.52
3:O:68:TRP:CZ2	3:O:72:ASN:HB3	2.45	0.52
2:I:96:MET:HE3	2:J:124:VAL:HG23	1.90	0.52
2:L:131:TYR:HB3	2:L:250:MET:HG2	1.92	0.52
2:B:100:ARG:HG2	2:B:101:ARG:N	2.25	0.52
2:G:95:VAL:HG12	2:H:123:GLN:HE21	1.75	0.52
2:I:337:PRO:O	2:I:342:GLY:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:463:ASP:OD1	2:I:464:PRO:HD2	2.10	0.52
2:A:354:LEU:HA	2:A:357:ILE:HG22	1.92	0.52
2:B:237:GLU:N	2:B:245:ASN:O	2.40	0.52
2:D:85:SER:HB3	3:Q:32:PHE:CE1	2.45	0.52
2:E:384:ASN:HD21	2:F:362:VAL:HG21	1.74	0.52
2:F:145:HIS:CD2	2:F:146:PRO:HD2	2.34	0.52
2:F:241:GLY:HA3	3:Q:43:GLY:HA2	1.90	0.52
2:F:313:SER:O	2:F:510:ASN:HB2	2.09	0.52
2:G:230:THR:HG22	2:L:263:SER:HB2	1.91	0.52
2:H:346:ALA:O	2:H:349:SER:N	2.42	0.52
3:O:11:LYS:HG3	3:O:27:GLU:HG2	1.92	0.52
2:C:266:LEU:CD1	2:D:155:SER:HB3	2.39	0.52
2:D:244:ASP:HB2	3:X:13:PHE:HE2	1.75	0.52
2:H:147:MET:HE1	2:H:366:ARG:NH1	2.25	0.52
2:K:376:ILE:HG12	2:K:423:VAL:HG22	1.92	0.52
2:L:344:ARG:O	2:L:348:GLU:HB2	2.10	0.52
2:A:179:THR:HG22	2:A:189:TYR:CE2	2.44	0.52
2:B:400:LEU:HD11	2:C:417:LEU:HB3	1.92	0.52
2:D:133:LYS:HE2	3:V:42:SER:HB2	1.92	0.52
2:D:244:ASP:O	2:D:246:PRO:HD3	2.10	0.52
2:F:100:ARG:HG2	2:F:101:ARG:N	2.25	0.52
2:G:357:ILE:HD11	2:G:376:ILE:HG21	1.91	0.52
2:J:101:ARG:HH12	2:K:145:HIS:CD2	2.28	0.52
2:L:181:PHE:HD1	2:L:187:THR:HB	1.75	0.52
2:D:279:ARG:HH21	2:D:285:ASP:HA	1.76	0.52
2:E:80:ALA:HA	2:E:93:PRO:HG2	1.91	0.52
2:H:72:HIS:CD2	2:I:121:THR:HG21	2.45	0.52
2:H:164:PRO:HG2	2:H:178:TYR:CD1	2.45	0.52
2:J:333:ASP:HB3	2:J:519:LYS:HB2	1.91	0.52
2:J:382:VAL:O	2:J:386:LEU:HD13	2.09	0.52
2:L:153:MET:HE2	2:L:225:ALA:HA	1.92	0.52
2:L:235:LEU:HD12	2:L:235:LEU:O	2.10	0.52
1:a:199:GLU:HB3	1:a:360:PHE:HE2	1.74	0.51
2:A:100:ARG:HG2	2:A:101:ARG:H	1.74	0.51
2:B:428:TYR:CZ	2:C:149:GLY:HA2	2.45	0.51
2:D:147:MET:SD	2:D:367:GLN:HG2	2.50	0.51
2:D:294:LEU:HD12	2:D:471:MET:HE2	1.90	0.51
2:E:164:PRO:HG2	2:E:178:TYR:CD1	2.46	0.51
2:I:266:LEU:CD1	2:J:155:SER:HB3	2.38	0.51
2:K:72:HIS:CD2	2:L:121:THR:HG21	2.45	0.51
3:W:40:LYS:H	3:W:72:ASN:ND2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:309:TRP:O	4:Z:313:ASP:N	2.40	0.51
2:A:277:ASP:O	2:A:281:VAL:HG12	2.10	0.51
2:A:396:ALA:O	2:B:395:TYR:HA	2.09	0.51
2:D:398:GLN:O	2:E:393:ILE:HA	2.09	0.51
2:F:380:ARG:NH1	2:F:427:GLN:O	2.44	0.51
2:G:147:MET:HE1	2:G:366:ARG:NH1	2.24	0.51
2:G:153:MET:HG2	2:G:189:TYR:CD2	2.45	0.51
2:J:100:ARG:HG2	2:J:101:ARG:N	2.25	0.51
2:K:164:PRO:HG2	2:K:178:TYR:CD1	2.45	0.51
2:A:100:ARG:HG2	2:A:101:ARG:N	2.25	0.51
2:A:155:SER:OG	2:F:264:ARG:NH1	2.40	0.51
2:B:235:LEU:HD12	2:B:235:LEU:O	2.10	0.51
2:B:305:GLU:HG2	2:B:309:TRP:CD1	2.45	0.51
2:C:235:LEU:HD12	2:C:235:LEU:O	2.10	0.51
2:C:344:ARG:O	2:C:348:GLU:HB2	2.10	0.51
2:F:113:GLY:H	2:F:446:ALA:HB1	1.75	0.51
2:G:197:THR:HG22	2:G:199:ASP:H	1.75	0.51
2:J:346:ALA:O	2:J:349:SER:N	2.43	0.51
1:a:265:SER:O	1:a:266:THR:HG22	2.10	0.51
2:B:153:MET:HE2	2:B:226:GLU:H	1.76	0.51
2:F:74:TYR:HA	2:F:79:ILE:HD11	1.93	0.51
2:I:377:ILE:HG22	2:I:424:TYR:HB2	1.93	0.51
2:J:380:ARG:NH2	2:J:408:THR:OG1	2.44	0.51
2:D:485:ALA:HB1	2:D:510:ASN:OD1	2.11	0.51
2:E:100:ARG:HG2	2:E:101:ARG:N	2.25	0.51
2:E:121:THR:HG22	2:E:260:GLU:OE1	2.11	0.51
2:F:131:TYR:CE2	2:F:143:ALA:HA	2.45	0.51
2:I:101:ARG:NH1	2:J:145:HIS:HD2	2.08	0.51
2:J:131:TYR:CB	2:J:250:MET:HG2	2.41	0.51
2:K:180:HIS:HD2	2:K:182:PHE:CE1	2.29	0.51
2:L:107:ILE:HG21	2:L:307:VAL:HG21	1.92	0.51
2:B:180:HIS:HD2	2:B:182:PHE:CD1	2.29	0.51
2:C:350:PHE:HB3	2:C:389:VAL:HG21	1.93	0.51
2:F:354:LEU:HA	2:F:357:ILE:HG22	1.93	0.51
2:H:263:SER:HB2	2:I:230:THR:HG22	1.92	0.51
2:L:148:TYR:HD1	2:L:186:GLY:H	1.57	0.51
2:L:333:ASP:HB3	2:L:519:LYS:HB2	1.93	0.51
3:P:72:ASN:OD1	3:P:73:GLU:N	2.43	0.51
1:a:418:VAL:HG12	1:a:420:LEU:HG	1.91	0.51
2:A:253:ARG:NE	2:A:255:ASP:OD2	2.44	0.51
2:B:493:ALA:O	2:B:494:SER:OG	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:197:THR:HG22	2:C:199:ASP:H	1.75	0.51
2:E:357:ILE:HD11	2:E:376:ILE:HD13	1.93	0.51
2:H:398:GLN:HG2	2:H:399:GLY:N	2.25	0.51
2:K:384:ASN:HD21	2:L:362:VAL:HG21	1.74	0.51
2:K:453:TYR:CD2	2:K:454:VAL:HG13	2.46	0.51
2:K:463:ASP:OD1	2:K:464:PRO:HD2	2.09	0.51
2:E:85:SER:HB3	3:O:32:PHE:CE1	2.46	0.51
2:E:96:MET:O	2:F:444:MET:HE1	2.11	0.51
2:K:238:GLY:HA2	2:K:242:SER:O	2.11	0.51
1:a:24:LEU:HD21	1:a:27:LEU:HD21	1.92	0.51
2:B:173:THR:OG1	2:B:176:ASP:OD2	2.28	0.51
2:C:502:SER:N	2:C:506:SER:OG	2.40	0.51
2:D:278:LEU:HD12	2:D:286:ALA:HB2	1.93	0.51
2:H:168:ALA:HB1	2:H:200:ALA:HA	1.93	0.51
1:a:258:VAL:HG22	1:a:325:VAL:HG11	1.92	0.51
1:a:378:ARG:NH1	2:F:277:ASP:OD1	2.34	0.51
2:B:383:VAL:HG21	2:B:425:ILE:HG12	1.93	0.51
2:C:126:ALA:N	2:C:255:ASP:O	2.44	0.51
2:C:494:SER:HA	3:Y:37:ASP:CG	2.36	0.51
2:G:96:MET:HE3	2:H:124:VAL:HG23	1.93	0.51
2:G:315:GLN:OE1	2:G:514:ARG:NH1	2.44	0.51
2:H:409:THR:HG21	2:I:370:ARG:O	2.11	0.51
2:K:131:TYR:CB	2:K:250:MET:HG2	2.41	0.51
2:K:344:ARG:HD2	2:L:344:ARG:NH1	2.26	0.51
3:O:10:ILE:HD11	3:O:35:TYR:CE1	2.46	0.51
2:A:188:VAL:CG1	2:F:430:LYS:HE2	2.41	0.50
2:B:323:LEU:HD21	2:B:329:ALA:HA	1.92	0.50
2:E:181:PHE:HD1	2:E:187:THR:HB	1.75	0.50
2:K:305:GLU:HA	2:L:225:ALA:HB3	1.93	0.50
1:a:411:ASP:HB2	1:a:412:LEU:HD12	1.92	0.50
2:A:120:PRO:HB2	2:A:121:THR:HG23	1.93	0.50
2:D:121:THR:HA	2:D:259:ILE:O	2.12	0.50
2:D:313:SER:O	2:D:510:ASN:HB2	2.11	0.50
2:G:363:GLU:OE2	2:G:366:ARG:NH2	2.44	0.50
2:H:179:THR:HG22	2:H:189:TYR:CD1	2.47	0.50
2:I:72:HIS:CD2	2:J:121:THR:HG21	2.46	0.50
2:K:265:GLN:C	2:K:266:LEU:HD12	2.36	0.50
2:L:131:TYR:CB	2:L:250:MET:HG2	2.41	0.50
1:a:357:VAL:HG12	1:a:377:VAL:HG13	1.94	0.50
2:B:79:ILE:HB	2:C:258:VAL:HG11	1.92	0.50
2:C:128:ARG:CZ	2:C:492:PRO:HD3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:235:LEU:HD12	2:D:235:LEU:O	2.11	0.50
2:D:344:ARG:CZ	2:E:344:ARG:HH22	2.23	0.50
2:E:134:ASP:HB3	2:E:137:ALA:HB2	1.93	0.50
2:E:442:ASN:HB3	2:E:444:MET:H	1.76	0.50
2:G:380:ARG:NH1	2:G:427:GLN:O	2.38	0.50
2:J:69:GLY:N	2:L:234:GLU:OE2	2.44	0.50
2:L:485:ALA:HB1	2:L:510:ASN:OD1	2.11	0.50
2:B:456:LEU:HD12	2:B:475:THR:HG21	1.94	0.50
2:C:430:LYS:HE2	2:D:188:VAL:CG1	2.41	0.50
2:F:244:ASP:HB2	3:Q:13:PHE:CE2	2.45	0.50
2:G:151:ASP:HB2	2:G:189:TYR:CE2	2.47	0.50
2:G:235:LEU:O	2:G:235:LEU:HD12	2.12	0.50
2:H:456:LEU:HD12	2:H:475:THR:HG21	1.93	0.50
3:W:64:GLN:HB3	3:W:67:GLU:HB2	1.93	0.50
1:a:132:ILE:HD13	1:a:139:LEU:HD11	1.93	0.50
2:A:151:ASP:HB2	2:A:189:TYR:CE1	2.43	0.50
2:B:100:ARG:HG2	2:B:101:ARG:H	1.74	0.50
2:C:164:PRO:HG2	2:C:178:TYR:CD1	2.47	0.50
2:D:164:PRO:HG2	2:D:178:TYR:HD1	1.77	0.50
2:E:120:PRO:O	2:E:121:THR:OG1	2.28	0.50
2:G:231:SER:HB2	2:K:71:ASP:CG	2.36	0.50
2:L:430:LYS:N	2:L:430:LYS:HD2	2.26	0.50
2:B:104:PRO:HB2	2:B:427:GLN:HE22	1.77	0.50
2:B:354:LEU:HA	2:B:357:ILE:HG22	1.93	0.50
2:C:345:TRP:HA	2:D:341:ARG:O	2.11	0.50
2:C:346:ALA:O	2:C:349:SER:N	2.45	0.50
2:D:153:MET:HE2	2:D:226:GLU:H	1.76	0.50
2:D:181:PHE:HD1	2:D:187:THR:HB	1.76	0.50
2:D:269:ALA:HA	2:D:470:VAL:HA	1.92	0.50
2:E:75:ASN:ND2	3:O:5:ARG:HA	2.27	0.50
2:J:353:LEU:HD13	2:J:385:VAL:HG11	1.93	0.50
2:J:386:LEU:HB3	2:J:404:PHE:HE2	1.77	0.50
2:C:96:MET:HB2	2:D:124:VAL:HG22	1.92	0.50
2:C:295:ALA:HB2	2:C:473:PHE:HE2	1.77	0.50
2:D:378:ALA:HB1	2:D:382:VAL:HG23	1.93	0.50
2:E:376:ILE:HG22	2:E:436:VAL:HG22	1.92	0.50
2:F:153:MET:HE2	2:F:226:GLU:H	1.77	0.50
2:G:362:VAL:HG21	2:L:384:ASN:ND2	2.25	0.50
2:H:344:ARG:NH1	2:I:344:ARG:HH12	2.08	0.50
2:I:344:ARG:CZ	2:J:344:ARG:HH12	2.25	0.50
2:L:444:MET:O	2:L:449:TYR:OH	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:310:ILE:HG23	2:A:513:PHE:CD2	2.46	0.50
2:B:164:PRO:HG2	2:B:178:TYR:CD1	2.46	0.50
2:C:270:TYR:HB3	2:C:290:LEU:HD12	1.93	0.50
2:F:153:MET:SD	2:F:157:GLN:HB3	2.52	0.50
2:G:260:GLU:HG2	2:L:74:TYR:CE2	2.47	0.50
2:H:148:TYR:HB3	2:H:186:GLY:HA2	1.94	0.50
2:H:444:MET:O	2:H:449:TYR:OH	2.30	0.50
2:J:134:ASP:HB3	2:J:137:ALA:HB2	1.93	0.50
2:J:350:PHE:HB3	2:J:389:VAL:HG21	1.94	0.50
2:A:481:ILE:HD11	2:A:510:ASN:HD21	1.77	0.50
2:B:360:GLU:O	2:B:363:GLU:N	2.45	0.50
2:D:331:VAL:HG12	2:D:517:TYR:HB2	1.94	0.50
2:H:343:ALA:HB1	2:H:348:GLU:HB3	1.94	0.50
2:J:323:LEU:HD21	2:J:329:ALA:HA	1.93	0.50
2:J:432:ASP:OD1	2:J:433:TYR:N	2.45	0.50
2:L:100:ARG:HG2	2:L:101:ARG:H	1.77	0.50
2:L:172:THR:O	2:L:195:GLN:HA	2.12	0.50
2:C:275:THR:HG22	2:C:286:ALA:HB3	1.94	0.49
2:C:324:THR:O	2:C:326:GLY:N	2.45	0.49
2:C:350:PHE:HB2	2:C:389:VAL:HG21	1.94	0.49
2:D:145:HIS:CD2	2:D:146:PRO:HD2	2.41	0.49
2:E:166:LEU:HD11	2:E:221:LEU:HD21	1.94	0.49
2:J:235:LEU:O	2:J:235:LEU:HD12	2.12	0.49
2:J:521:ILE:HA	2:K:341:ARG:NH2	2.27	0.49
3:W:38:VAL:HG11	3:W:69:ILE:HG12	1.94	0.49
1:a:396:ARG:HB3	2:F:89:THR:HG21	1.94	0.49
2:A:121:THR:HG22	2:A:260:GLU:OE1	2.12	0.49
2:D:476:ARG:HH21	2:E:230:THR:HG21	1.77	0.49
2:I:493:ALA:O	2:I:494:SER:OG	2.30	0.49
2:K:113:GLY:H	2:K:446:ALA:HB1	1.77	0.49
2:K:344:ARG:NH1	2:L:344:ARG:HH12	2.05	0.49
2:K:380:ARG:NH2	2:K:408:THR:OG1	2.44	0.49
2:A:173:THR:OG1	2:A:176:ASP:OD2	2.29	0.49
2:C:89:THR:HG23	2:G:495:ARG:NH2	2.27	0.49
2:E:129:ALA:O	2:E:143:ALA:N	2.34	0.49
2:F:285:ASP:HB3	2:F:288:ALA:HB3	1.93	0.49
2:K:171:GLN:HE21	2:K:195:GLN:HE21	1.60	0.49
1:a:84:ILE:O	1:a:102:LYS:NZ	2.45	0.49
2:A:430:LYS:HE2	2:B:188:VAL:CG1	2.42	0.49
2:B:77:THR:HG21	3:Y:5:ARG:NH2	2.27	0.49
2:H:486:GLU:C	2:H:488:ALA:H	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:179:THR:HG22	2:J:189:TYR:CD2	2.47	0.49
2:K:191:GLN:N	2:K:222:VAL:O	2.45	0.49
2:K:284:MET:HE1	2:L:127:LEU:HD12	1.95	0.49
1:a:281:ILE:HD13	1:a:420:LEU:HD11	1.93	0.49
2:B:113:GLY:H	2:B:446:ALA:HB1	1.77	0.49
2:B:121:THR:HG22	2:B:260:GLU:HA	1.93	0.49
2:C:100:ARG:HG2	2:C:101:ARG:N	2.28	0.49
2:D:268:ALA:HB2	2:D:294:LEU:HD11	1.93	0.49
2:D:277:ASP:O	2:D:281:VAL:HG12	2.13	0.49
2:F:100:ARG:HG2	2:F:101:ARG:H	1.77	0.49
2:G:336:ASP:O	2:G:340:ILE:HG12	2.13	0.49
1:a:162:GLN:HG3	1:a:396:ARG:HH22	1.78	0.49
2:A:80:ALA:HA	2:A:93:PRO:HG2	1.94	0.49
2:A:181:PHE:HD1	2:A:187:THR:HB	1.77	0.49
2:A:375:PHE:CZ	2:A:437:GLY:HA3	2.47	0.49
2:A:383:VAL:HG21	2:A:425:ILE:HG12	1.95	0.49
2:C:88:VAL:HG22	2:G:254:ILE:HD12	1.95	0.49
2:C:407:ASP:HB3	2:D:372:GLU:HB2	1.94	0.49
2:D:253:ARG:NE	2:D:255:ASP:OD2	2.43	0.49
2:G:101:ARG:HD2	2:H:146:PRO:HD3	1.94	0.49
2:H:269:ALA:HA	2:H:470:VAL:HA	1.95	0.49
2:J:383:VAL:HG21	2:J:425:ILE:HG12	1.95	0.49
2:K:344:ARG:HD2	2:L:344:ARG:CZ	2.42	0.49
1:a:108:TYR:CE1	1:a:128:LEU:HD21	2.47	0.49
1:a:396:ARG:HH12	2:F:87:ALA:C	2.20	0.49
2:B:169:SER:OG	2:B:200:ALA:HB2	2.12	0.49
2:B:398:GLN:O	2:C:393:ILE:HA	2.12	0.49
2:G:313:SER:O	2:G:510:ASN:HB2	2.12	0.49
2:I:430:LYS:HB3	2:J:216:MET:HE1	1.94	0.49
1:a:238:LEU:HD21	1:a:250:LEU:HB2	1.94	0.49
2:A:348:GLU:OE1	2:A:348:GLU:N	2.45	0.49
2:B:344:ARG:HD2	2:C:344:ARG:NH1	2.27	0.49
2:B:345:TRP:CD2	2:C:348:GLU:HG3	2.48	0.49
2:B:398:GLN:NE2	2:C:355:PHE:HB2	2.28	0.49
2:B:398:GLN:HE21	2:C:355:PHE:HB2	1.78	0.49
2:E:430:LYS:HG2	2:F:216:MET:HE1	1.95	0.49
2:H:171:GLN:HE21	2:H:195:GLN:HE21	1.58	0.49
1:a:280:ALA:O	1:a:284:ALA:N	2.40	0.49
2:C:145:HIS:CD2	2:C:146:PRO:HD2	2.42	0.49
2:E:396:ALA:O	2:F:395:TYR:HA	2.12	0.49
2:G:131:TYR:CB	2:G:250:MET:HG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:71:ASP:HB3	2:L:230:THR:HG23	1.95	0.49
2:J:345:TRP:HA	2:K:341:ARG:O	2.13	0.49
2:K:466:ASN:O	2:K:468:GLN:HG3	2.13	0.49
3:W:72:ASN:OD1	3:W:73:GLU:N	2.46	0.49
2:A:378:ALA:HB1	2:A:382:VAL:HG21	1.93	0.49
2:B:163:PHE:HB2	2:B:179:THR:CG2	2.43	0.49
2:C:74:TYR:CE2	2:D:260:GLU:HG2	2.48	0.49
2:C:147:MET:HE3	2:C:367:GLN:HG2	1.95	0.49
2:E:331:VAL:HG12	2:E:517:TYR:HB2	1.95	0.49
2:F:148:TYR:HB3	2:F:186:GLY:HA2	1.95	0.49
2:F:432:ASP:OD1	2:F:433:TYR:N	2.45	0.49
2:J:272:ILE:HG22	2:J:468:GLN:HE21	1.78	0.49
2:K:106:LEU:HD21	2:K:300:LEU:HD23	1.95	0.49
2:K:431:GLN:NE2	2:L:213:LYS:O	2.46	0.49
1:a:378:ARG:NH2	2:F:273:GLU:O	2.47	0.48
2:A:392:GLY:O	2:F:399:GLY:HA3	2.13	0.48
2:C:273:GLU:HG3	2:H:234:GLU:HA	1.94	0.48
2:D:396:ALA:O	2:E:395:TYR:HA	2.13	0.48
2:F:269:ALA:HA	2:F:470:VAL:HA	1.93	0.48
2:G:96:MET:HE2	2:H:122:GLY:HA3	1.94	0.48
2:G:395:TYR:HA	2:L:396:ALA:O	2.13	0.48
2:H:100:ARG:HG2	2:H:101:ARG:H	1.77	0.48
2:K:244:ASP:O	2:K:246:PRO:HD3	2.13	0.48
2:K:382:VAL:HG12	2:K:521:ILE:HD11	1.96	0.48
2:K:384:ASN:O	2:K:387:ALA:N	2.45	0.48
1:a:35:ILE:CD1	1:a:313:TYR:HB3	2.43	0.48
2:A:279:ARG:HD2	2:A:284:MET:O	2.12	0.48
2:A:398:GLN:O	2:B:393:ILE:HA	2.14	0.48
2:C:244:ASP:O	2:C:246:PRO:HD3	2.13	0.48
2:D:430:LYS:N	2:D:430:LYS:HD2	2.28	0.48
2:E:101:ARG:HG2	2:F:144:PHE:O	2.14	0.48
2:E:265:GLN:C	2:E:266:LEU:HD12	2.38	0.48
2:F:181:PHE:HD1	2:F:187:THR:HB	1.78	0.48
2:G:284:MET:HE1	2:H:127:LEU:HD12	1.93	0.48
2:G:345:TRP:NE1	2:G:348:GLU:OE1	2.47	0.48
2:G:375:PHE:CZ	2:G:437:GLY:HA3	2.48	0.48
2:H:313:SER:O	2:H:510:ASN:HB2	2.13	0.48
2:L:181:PHE:HZ	2:L:490:GLN:HE22	1.62	0.48
2:L:486:GLU:C	2:L:488:ALA:H	2.21	0.48
2:D:164:PRO:HG2	2:D:178:TYR:CD1	2.48	0.48
2:D:476:ARG:NH2	2:E:230:THR:HG21	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:313:SER:OG	2:F:510:ASN:ND2	2.45	0.48
2:G:147:MET:HE2	2:G:147:MET:HA	1.95	0.48
2:G:184:GLU:O	2:G:185:THR:OG1	2.32	0.48
2:G:341:ARG:O	2:L:345:TRP:HA	2.14	0.48
2:H:96:MET:HE2	2:I:122:GLY:HA3	1.95	0.48
2:B:128:ARG:NE	2:B:484:PHE:HE1	2.07	0.48
2:B:344:ARG:NH1	2:C:344:ARG:HH22	2.11	0.48
2:D:364:ILE:O	2:D:368:THR:OG1	2.21	0.48
2:E:148:TYR:HB3	2:E:186:GLY:HA2	1.94	0.48
2:A:80:ALA:HA	2:A:93:PRO:CG	2.44	0.48
2:C:121:THR:HA	2:C:259:ILE:O	2.13	0.48
2:D:377:ILE:HA	2:D:424:TYR:O	2.13	0.48
2:E:135:PRO:HB3	2:E:252:PHE:O	2.13	0.48
2:E:263:SER:HB2	2:F:230:THR:HG22	1.96	0.48
2:E:346:ALA:O	2:E:349:SER:N	2.46	0.48
2:E:456:LEU:HD12	2:E:475:THR:CG2	2.43	0.48
2:G:346:ALA:O	2:G:349:SER:N	2.47	0.48
2:H:428:TYR:CZ	2:I:149:GLY:HA2	2.49	0.48
2:K:285:ASP:C	2:K:287:ASP:H	2.22	0.48
2:L:142:GLU:H	2:L:490:GLN:HG2	1.78	0.48
2:L:238:GLY:HA2	2:L:242:SER:O	2.13	0.48
2:C:131:TYR:HB3	2:C:250:MET:HE3	1.95	0.48
2:F:157:GLN:N	2:F:227:GLY:O	2.46	0.48
2:F:360:GLU:O	2:F:363:GLU:N	2.46	0.48
2:G:79:ILE:CG2	2:H:121:THR:HB	2.43	0.48
2:H:152:ALA:HB1	2:H:225:ALA:CB	2.35	0.48
2:I:153:MET:HE2	2:I:225:ALA:HA	1.96	0.48
2:I:476:ARG:NH2	2:J:230:THR:HG21	2.29	0.48
3:W:9:ASN:ND2	3:W:51:SER:OG	2.45	0.48
2:B:184:GLU:O	2:B:185:THR:OG1	2.27	0.48
2:E:345:TRP:NE1	2:E:348:GLU:OE1	2.46	0.48
2:G:477:TYR:CD2	2:G:478:GLY:N	2.81	0.48
2:I:101:ARG:NH1	2:J:145:HIS:CD2	2.81	0.48
2:I:101:ARG:HD2	2:J:146:PRO:HD3	1.96	0.48
1:a:108:TYR:CE2	1:a:132:ILE:HD11	2.48	0.48
2:B:71:ASP:OD2	3:X:50:PRO:HG3	2.14	0.48
2:C:313:SER:OG	2:C:510:ASN:HB2	2.14	0.48
2:D:179:THR:HG22	2:D:189:TYR:CD2	2.48	0.48
2:F:377:ILE:HG22	2:F:424:TYR:HB2	1.96	0.48
2:F:494:SER:HA	3:P:37:ASP:CG	2.39	0.48
2:G:272:ILE:HG22	2:G:468:GLN:HE21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:153:MET:SD	2:H:157:GLN:HB3	2.53	0.48
2:K:313:SER:O	2:K:510:ASN:HB2	2.13	0.48
2:L:295:ALA:HB2	2:L:473:PHE:HE2	1.78	0.48
2:B:159:ALA:HB3	2:B:228:MET:CE	2.43	0.48
2:B:265:GLN:C	2:B:266:LEU:HD12	2.39	0.48
2:C:196:VAL:HG21	2:C:215:GLN:OE1	2.14	0.48
2:C:376:ILE:HG12	2:C:423:VAL:HG22	1.95	0.48
2:E:295:ALA:HB2	2:E:473:PHE:CE2	2.49	0.48
2:E:482:ASN:O	2:E:485:ALA:HB2	2.14	0.48
2:H:305:GLU:HA	2:I:225:ALA:HB3	1.95	0.48
2:H:378:ALA:O	2:H:426:ASP:N	2.46	0.48
2:I:131:TYR:HB3	2:I:250:MET:HE3	1.95	0.48
2:K:120:PRO:O	2:K:121:THR:OG1	2.31	0.48
3:W:26:LYS:HD2	3:W:75:LEU:HD23	1.95	0.48
3:W:68:TRP:O	3:W:71:ALA:N	2.47	0.48
1:a:387:THR:O	1:a:406:MET:HE1	2.14	0.48
2:A:260:GLU:HG2	2:F:74:TYR:CE2	2.49	0.48
2:D:172:THR:O	2:D:195:GLN:HA	2.14	0.48
2:D:348:GLU:OE1	2:D:348:GLU:N	2.45	0.48
2:F:171:GLN:NE2	2:F:195:GLN:HE21	2.11	0.48
2:F:505:ASN:OD1	2:F:506:SER:N	2.46	0.48
2:I:295:ALA:HB2	2:I:473:PHE:HE2	1.77	0.48
2:K:74:TYR:CE2	2:L:260:GLU:HG2	2.49	0.48
1:a:180:THR:HA	1:a:370:GLN:HB3	1.96	0.47
2:B:313:SER:O	2:B:510:ASN:HB2	2.14	0.47
2:C:147:MET:HE1	2:C:366:ARG:NH1	2.29	0.47
2:C:193:SER:OG	2:C:220:ALA:O	2.23	0.47
2:E:72:HIS:CD2	2:F:121:THR:HG21	2.48	0.47
2:E:407:ASP:HB3	2:F:372:GLU:HB2	1.95	0.47
2:G:345:TRP:HB3	2:H:343:ALA:HA	1.96	0.47
1:a:384:ASN:HD22	1:a:412:LEU:HD22	1.79	0.47
2:A:160:ALA:HB1	2:A:232:ILE:HG21	1.95	0.47
2:A:204:ASP:OD1	2:A:205:ALA:N	2.47	0.47
2:B:407:ASP:HB3	2:C:372:GLU:HB2	1.95	0.47
2:C:304:ARG:NH1	2:C:426:ASP:OD1	2.46	0.47
2:E:105:ASN:HB2	2:E:412:VAL:HG23	1.96	0.47
2:E:323:LEU:HD22	2:E:327:SER:HB2	1.95	0.47
2:I:270:TYR:HB3	2:I:290:LEU:HD12	1.95	0.47
2:A:266:LEU:CD1	2:B:155:SER:HB3	2.44	0.47
2:C:331:VAL:HG11	2:C:519:LYS:HE3	1.96	0.47
2:H:134:ASP:HB3	2:H:137:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:234:GLU:OE2	2:L:69:GLY:N	2.31	0.47
2:H:324:THR:O	2:H:326:GLY:N	2.47	0.47
2:I:396:ALA:O	2:J:395:TYR:HA	2.15	0.47
1:a:42:THR:HG22	1:a:342:TYR:HB3	1.97	0.47
1:a:179:ILE:HG23	1:a:183:LEU:HB3	1.96	0.47
2:B:120:PRO:O	2:B:121:THR:OG1	2.28	0.47
2:C:432:ASP:OD1	2:C:433:TYR:N	2.47	0.47
2:D:240:ASN:ND2	3:X:46:TYR:OH	2.48	0.47
2:E:318:LYS:N	2:E:360:GLU:OE2	2.47	0.47
2:E:386:LEU:HB3	2:E:404:PHE:HE2	1.79	0.47
2:F:152:ALA:HB1	2:F:225:ALA:CB	2.36	0.47
2:H:348:GLU:OE1	2:H:348:GLU:N	2.43	0.47
2:H:350:PHE:HB2	2:H:389:VAL:HG21	1.95	0.47
2:I:354:LEU:HA	2:I:357:ILE:HG22	1.97	0.47
2:J:125:PHE:HA	2:J:256:LYS:HA	1.96	0.47
2:J:348:GLU:OE1	2:J:348:GLU:N	2.47	0.47
2:J:389:VAL:HG12	2:J:390:ASP:N	2.29	0.47
2:K:196:VAL:HG21	2:K:215:GLN:OE1	2.13	0.47
2:K:398:GLN:O	2:L:393:ILE:HA	2.14	0.47
3:W:26:LYS:NZ	3:W:74:ASP:OD2	2.47	0.47
2:B:131:TYR:HD2	2:B:250:MET:HE3	1.80	0.47
2:B:384:ASN:ND2	2:C:362:VAL:HG21	2.28	0.47
2:I:128:ARG:NH1	2:I:490:GLN:O	2.44	0.47
2:I:345:TRP:HA	2:J:341:ARG:O	2.14	0.47
2:I:376:ILE:HG12	2:I:423:VAL:HG22	1.95	0.47
2:I:431:GLN:NE2	2:J:213:LYS:O	2.47	0.47
2:I:477:TYR:CD2	2:I:478:GLY:N	2.82	0.47
2:J:105:ASN:HD21	2:J:409:THR:C	2.16	0.47
2:L:377:ILE:HG22	2:L:424:TYR:HB2	1.95	0.47
2:C:71:ASP:CG	2:E:231:SER:HB2	2.39	0.47
2:C:295:ALA:HB2	2:C:473:PHE:CE2	2.49	0.47
2:D:96:MET:HE3	2:E:124:VAL:HG23	1.95	0.47
2:D:134:ASP:HB3	2:D:137:ALA:HB2	1.97	0.47
2:D:432:ASP:OD1	2:D:433:TYR:N	2.47	0.47
2:F:290:LEU:HD23	2:F:293:ILE:HD11	1.95	0.47
2:L:272:ILE:HG22	2:L:468:GLN:HG2	1.97	0.47
3:O:72:ASN:OD1	3:O:73:GLU:N	2.48	0.47
1:a:364:VAL:HG13	1:a:369:LEU:O	2.14	0.47
2:A:84:THR:HG22	2:A:86:GLY:H	1.78	0.47
2:B:152:ALA:HB1	2:B:225:ALA:CB	2.44	0.47
2:E:158:GLY:HA2	2:E:163:PHE:HE2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:147:MET:SD	2:F:367:GLN:HG2	2.55	0.47
2:F:357:ILE:CD1	2:F:376:ILE:HD13	2.43	0.47
2:G:190:LEU:HB3	2:G:221:LEU:HG	1.96	0.47
2:I:168:ALA:HB1	2:I:200:ALA:HA	1.97	0.47
2:I:430:LYS:O	2:J:213:LYS:HE2	2.15	0.47
2:K:344:ARG:O	2:K:348:GLU:HB2	2.13	0.47
2:K:477:TYR:CD2	2:K:478:GLY:N	2.83	0.47
3:P:9:ASN:HB3	3:P:56:TYR:CE2	2.50	0.47
1:a:221:VAL:CG2	1:a:403:MET:HE1	2.43	0.47
1:a:339:SER:N	1:a:384:ASN:HD21	2.13	0.47
2:C:277:ASP:O	2:C:281:VAL:HG12	2.15	0.47
2:E:151:ASP:HB3	2:E:187:THR:CG2	2.44	0.47
2:I:79:ILE:HB	2:J:258:VAL:HG11	1.96	0.47
2:I:432:ASP:OD1	2:I:433:TYR:N	2.48	0.47
2:J:146:PRO:HB2	2:J:366:ARG:O	2.15	0.47
2:J:378:ALA:HB1	2:J:382:VAL:CG2	2.45	0.47
2:K:163:PHE:HB2	2:K:179:THR:HG23	1.95	0.47
2:L:129:ALA:O	2:L:143:ALA:N	2.36	0.47
2:B:380:ARG:HH22	2:B:427:GLN:HB2	1.79	0.47
2:B:430:LYS:N	2:B:430:LYS:HD2	2.30	0.47
2:D:101:ARG:HH12	2:E:145:HIS:CD2	2.33	0.47
2:F:169:SER:OG	2:F:200:ALA:HB2	2.15	0.47
2:G:378:ALA:HB1	2:G:382:VAL:CG2	2.44	0.47
2:I:384:ASN:O	2:I:387:ALA:N	2.48	0.47
2:A:444:MET:O	2:A:449:TYR:OH	2.33	0.47
2:E:179:THR:HG22	2:E:189:TYR:CD2	2.50	0.47
2:E:521:ILE:HA	2:F:341:ARG:HH22	1.80	0.47
2:F:134:ASP:HB3	2:F:137:ALA:HB2	1.97	0.47
2:H:151:ASP:CG	2:H:154:PHE:HB2	2.40	0.47
2:H:163:PHE:HB2	2:H:179:THR:CG2	2.45	0.47
2:H:384:ASN:HD21	2:I:362:VAL:HG21	1.80	0.47
2:J:318:LYS:HE3	2:J:327:SER:HB3	1.97	0.47
2:J:477:TYR:CD2	2:J:478:GLY:N	2.83	0.47
3:P:40:LYS:H	3:P:72:ASN:HD22	1.62	0.47
1:a:244:PRO:O	1:a:247:GLY:N	2.47	0.46
1:a:265:SER:OG	1:a:412:LEU:HG	2.15	0.46
2:C:137:ALA:HB3	2:C:140:ALA:HB2	1.97	0.46
2:E:272:ILE:HG22	2:E:468:GLN:NE2	2.30	0.46
2:G:257:GLN:HG2	2:G:497:GLN:HG3	1.97	0.46
2:A:164:PRO:HG2	2:A:178:TYR:HD1	1.80	0.46
2:B:466:ASN:O	2:B:468:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:ALA:N	2:D:255:ASP:O	2.46	0.46
2:D:263:SER:HB2	2:E:230:THR:HG22	1.97	0.46
2:D:375:PHE:CE1	2:D:437:GLY:HA3	2.49	0.46
2:J:337:PRO:O	2:J:342:GLY:N	2.36	0.46
2:L:136:VAL:HG12	2:L:253:ARG:NE	2.30	0.46
2:L:265:GLN:C	2:L:266:LEU:HD12	2.40	0.46
1:a:179:ILE:CD1	1:a:198:LEU:HD12	2.46	0.46
2:A:79:ILE:HB	2:B:258:VAL:HG11	1.97	0.46
2:A:238:GLY:HA2	2:A:242:SER:O	2.15	0.46
2:A:458:PRO:HA	2:A:473:PHE:HD1	1.79	0.46
2:B:84:THR:HB	2:B:88:VAL:O	2.15	0.46
2:D:120:PRO:O	2:D:121:THR:OG1	2.33	0.46
2:E:131:TYR:CB	2:E:250:MET:HG2	2.45	0.46
2:G:386:LEU:HB3	2:G:404:PHE:HE2	1.79	0.46
2:G:409:THR:HG21	2:H:370:ARG:O	2.16	0.46
2:G:417:LEU:HB3	2:L:400:LEU:HD11	1.95	0.46
2:H:398:GLN:O	2:I:393:ILE:HA	2.16	0.46
2:I:147:MET:HE2	2:I:147:MET:HA	1.96	0.46
2:I:345:TRP:HB3	2:J:343:ALA:HA	1.98	0.46
2:I:398:GLN:O	2:J:393:ILE:HA	2.15	0.46
2:K:107:ILE:HG21	2:K:307:VAL:HG21	1.98	0.46
2:A:179:THR:HG22	2:A:189:TYR:CD2	2.51	0.46
2:B:153:MET:HE2	2:B:225:ALA:HA	1.98	0.46
2:E:164:PRO:HG2	2:E:178:TYR:HD1	1.78	0.46
2:E:241:GLY:HA3	3:T:43:GLY:HA2	1.97	0.46
2:E:431:GLN:NE2	2:F:213:LYS:HB3	2.28	0.46
2:F:121:THR:HA	2:F:259:ILE:O	2.14	0.46
2:G:216:MET:HA	2:G:221:LEU:O	2.15	0.46
2:G:348:GLU:HG3	2:L:345:TRP:CD2	2.50	0.46
2:I:343:ALA:HB1	2:I:348:GLU:HB3	1.97	0.46
2:K:390:ASP:OD2	2:K:394:SER:OG	2.30	0.46
2:L:149:GLY:H	2:L:186:GLY:HA2	1.81	0.46
2:B:397:ALA:HB1	2:C:393:ILE:HG22	1.97	0.46
2:C:145:HIS:HD2	2:C:146:PRO:CD	2.27	0.46
2:C:331:VAL:HG12	2:C:517:TYR:HB2	1.97	0.46
2:E:179:THR:HG22	2:E:189:TYR:CE2	2.51	0.46
2:F:106:LEU:HA	2:F:303:ASN:ND2	2.30	0.46
2:G:328:LYS:HD3	2:G:331:VAL:HG21	1.96	0.46
2:G:430:LYS:N	2:G:430:LYS:HD2	2.30	0.46
2:I:453:TYR:HB3	2:I:476:ARG:O	2.16	0.46
2:K:179:THR:HG22	2:K:189:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:10:ILE:HD11	3:O:35:TYR:HE1	1.80	0.46
3:W:5:ARG:NH1	3:W:33:PRO:HB3	2.29	0.46
1:a:56:LYS:HB3	1:a:386:TYR:HE1	1.79	0.46
1:a:215:LEU:HD13	1:a:315:ASP:OD1	2.15	0.46
2:A:231:SER:HB2	2:E:71:ASP:CG	2.41	0.46
2:C:78:ASN:OD1	3:T:5:ARG:HD3	2.15	0.46
2:D:100:ARG:HG2	2:D:101:ARG:H	1.80	0.46
2:E:334:PHE:CZ	2:E:353:LEU:HD12	2.50	0.46
2:G:79:ILE:HB	2:H:258:VAL:HG11	1.97	0.46
2:G:145:HIS:CD2	2:G:146:PRO:HD2	2.43	0.46
2:G:244:ASP:O	2:G:246:PRO:HD3	2.15	0.46
2:G:372:GLU:HB2	2:L:407:ASP:HB3	1.96	0.46
2:H:131:TYR:HB3	2:H:250:MET:HG2	1.97	0.46
2:H:502:SER:N	2:H:506:SER:OG	2.48	0.46
2:J:136:VAL:HG12	2:J:253:ARG:NE	2.30	0.46
2:L:309:TRP:O	2:L:313:SER:N	2.44	0.46
2:E:344:ARG:O	2:E:348:GLU:HB2	2.16	0.46
2:E:360:GLU:O	2:E:363:GLU:N	2.46	0.46
2:H:147:MET:HA	2:H:147:MET:HE2	1.98	0.46
2:L:100:ARG:HG2	2:L:101:ARG:N	2.31	0.46
3:O:27:GLU:HB3	3:O:56:TYR:CD1	2.50	0.46
1:a:111:LEU:HD21	1:a:138:ARG:HD3	1.98	0.46
1:a:217:SER:HA	1:a:220:THR:HG22	1.97	0.46
2:A:272:ILE:HG22	2:A:468:GLN:HG2	1.97	0.46
2:C:147:MET:HE1	2:C:366:ARG:CZ	2.46	0.46
2:C:171:GLN:HE21	2:C:195:GLN:NE2	2.13	0.46
2:C:432:ASP:O	2:C:433:TYR:HB3	2.16	0.46
2:C:465:LYS:HB3	2:H:237:GLU:HG3	1.98	0.46
2:D:337:PRO:O	2:D:342:GLY:N	2.33	0.46
2:F:377:ILE:HA	2:F:424:TYR:O	2.15	0.46
2:I:265:GLN:C	2:I:266:LEU:HD12	2.40	0.46
2:I:431:GLN:NE2	2:J:217:GLU:HB2	2.30	0.46
2:K:169:SER:OG	2:K:200:ALA:HB2	2.16	0.46
1:a:120:GLU:OE1	1:a:120:GLU:N	2.44	0.46
2:C:281:VAL:HG21	2:L:91:ILE:H	1.81	0.46
2:E:147:MET:HE2	2:E:366:ARG:HG2	1.98	0.46
2:H:265:GLN:C	2:H:266:LEU:HD12	2.41	0.46
2:H:354:LEU:HA	2:H:357:ILE:HG22	1.98	0.46
2:I:126:ALA:N	2:I:255:ASP:O	2.46	0.46
2:K:270:TYR:HB3	2:K:290:LEU:HD12	1.98	0.46
2:L:348:GLU:OE1	2:L:348:GLU:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:9:ASN:HB3	3:P:56:TYR:HE2	1.81	0.46
2:A:101:ARG:HD2	2:B:146:PRO:HD3	1.98	0.46
2:A:124:VAL:CG2	2:F:96:MET:HE3	2.44	0.46
2:B:131:TYR:CB	2:B:250:MET:HG2	2.46	0.46
2:B:193:SER:OG	2:B:220:ALA:O	2.26	0.46
2:D:107:ILE:HG22	2:D:303:ASN:HD21	1.81	0.46
2:E:106:LEU:HD21	2:E:300:LEU:HD23	1.98	0.46
2:F:163:PHE:HB2	2:F:179:THR:HG23	1.97	0.46
2:F:190:LEU:HB3	2:F:221:LEU:HG	1.97	0.46
2:G:244:ASP:HB2	3:S:13:PHE:CE2	2.49	0.46
2:H:69:GLY:N	2:J:234:GLU:OE2	2.46	0.46
2:H:241:GLY:HA3	3:V:43:GLY:N	2.31	0.46
2:I:137:ALA:HB3	2:I:140:ALA:HB2	1.97	0.46
2:L:184:GLU:O	2:L:185:THR:OG1	2.30	0.46
1:a:364:VAL:HA	1:a:371:PRO:HA	1.97	0.45
2:A:196:VAL:HG21	2:A:215:GLN:OE1	2.16	0.45
2:B:334:PHE:CZ	2:B:353:LEU:HD12	2.51	0.45
2:E:477:TYR:CD2	2:E:478:GLY:N	2.83	0.45
2:I:100:ARG:HG2	2:I:101:ARG:N	2.30	0.45
2:I:486:GLU:C	2:I:488:ALA:H	2.24	0.45
2:K:77:THR:HG21	3:U:5:ARG:NH2	2.31	0.45
2:K:131:TYR:CD2	2:K:250:MET:HE3	2.48	0.45
2:L:389:VAL:HG12	2:L:390:ASP:N	2.31	0.45
1:a:198:LEU:HD23	1:a:198:LEU:C	2.41	0.45
1:a:357:VAL:O	1:a:377:VAL:HG22	2.16	0.45
1:a:360:PHE:CD1	1:a:375:LEU:HB3	2.52	0.45
2:C:454:VAL:HG22	2:C:476:ARG:HB2	1.99	0.45
2:D:265:GLN:C	2:D:266:LEU:HD12	2.42	0.45
2:D:265:GLN:OE1	2:D:474:LYS:HE2	2.16	0.45
2:F:147:MET:HE1	2:F:184:GLU:HG2	1.98	0.45
2:F:324:THR:HB	2:F:327:SER:OG	2.17	0.45
2:F:343:ALA:HB1	2:F:348:GLU:HB3	1.98	0.45
2:G:169:SER:OG	2:G:200:ALA:HB2	2.16	0.45
2:G:269:ALA:HA	2:G:470:VAL:HA	1.97	0.45
2:G:380:ARG:HH21	2:G:408:THR:HG1	1.60	0.45
2:H:173:THR:OG1	2:H:176:ASP:OD2	2.32	0.45
2:K:396:ALA:O	2:L:395:TYR:HA	2.16	0.45
2:L:270:TYR:HB3	2:L:290:LEU:CD1	2.46	0.45
3:W:10:ILE:HD11	3:W:35:TYR:HE1	1.80	0.45
1:a:353:ASP:HB2	1:a:356:HIS:CD2	2.51	0.45
2:A:270:TYR:HB3	2:A:290:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:HIS:CD2	2:C:121:THR:HG21	2.51	0.45
2:B:270:TYR:HB3	2:B:290:LEU:CD1	2.47	0.45
2:B:432:ASP:O	2:B:433:TYR:HB3	2.17	0.45
2:C:171:GLN:HE21	2:C:195:GLN:HE21	1.63	0.45
2:D:284:MET:HE1	2:E:127:LEU:HD12	1.98	0.45
2:E:305:GLU:OE1	2:E:477:TYR:OH	2.25	0.45
2:F:312:TYR:CE1	2:F:507:LEU:HD12	2.51	0.45
2:F:453:TYR:CD2	2:F:454:VAL:HG13	2.52	0.45
2:H:74:TYR:CE2	2:I:260:GLU:HG2	2.51	0.45
2:H:100:ARG:NH1	2:H:289:GLU:OE1	2.48	0.45
2:H:107:ILE:HG21	2:H:307:VAL:CG2	2.46	0.45
2:J:430:LYS:N	2:J:430:LYS:HD2	2.32	0.45
2:J:486:GLU:C	2:J:488:ALA:H	2.24	0.45
2:K:152:ALA:HB1	2:K:225:ALA:HB2	1.98	0.45
2:K:430:LYS:HE2	2:L:188:VAL:HG11	1.98	0.45
1:a:58:LEU:HD22	1:a:62:ASN:O	2.16	0.45
2:B:244:ASP:O	2:B:246:PRO:HD3	2.16	0.45
2:D:285:ASP:C	2:D:287:ASP:H	2.24	0.45
2:D:336:ASP:O	2:D:340:ILE:HG12	2.16	0.45
2:E:131:TYR:HD2	2:E:250:MET:HE3	1.81	0.45
2:F:168:ALA:HB1	2:F:200:ALA:HA	1.97	0.45
2:J:354:LEU:HA	2:J:357:ILE:HG22	1.97	0.45
2:K:244:ASP:C	2:K:246:PRO:HD3	2.42	0.45
3:W:18:ASP:HB3	3:W:21:LYS:HD3	1.97	0.45
1:a:395:ALA:HB3	1:a:398:ILE:HD11	1.99	0.45
2:A:265:GLN:O	2:A:266:LEU:HD12	2.17	0.45
2:A:431:GLN:NE2	2:B:213:LYS:O	2.49	0.45
2:B:277:ASP:O	2:B:281:VAL:HG12	2.17	0.45
2:B:334:PHE:HZ	2:B:353:LEU:HD12	1.80	0.45
2:C:268:ALA:HB3	2:C:471:MET:CG	2.46	0.45
2:E:399:GLY:HA3	2:F:392:GLY:O	2.16	0.45
2:I:507:LEU:O	2:I:509:LYS:HG3	2.16	0.45
2:J:96:MET:HB2	2:K:124:VAL:HG22	1.98	0.45
2:J:181:PHE:HD1	2:J:187:THR:HB	1.82	0.45
2:J:216:MET:HA	2:J:221:LEU:O	2.16	0.45
2:J:284:MET:HE1	2:K:127:LEU:HD12	1.97	0.45
2:K:131:TYR:HB3	2:K:250:MET:HE3	1.99	0.45
2:L:196:VAL:HG21	2:L:215:GLN:OE1	2.16	0.45
1:a:167:GLN:O	1:a:399:ASP:HA	2.17	0.45
1:a:177:THR:HG23	1:a:178:GLY:N	2.29	0.45
2:A:109:PHE:HD1	2:A:112:CYS:SG	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:144:PHE:O	2:F:101:ARG:HG2	2.15	0.45
2:B:146:PRO:HB2	2:B:366:ARG:O	2.15	0.45
2:B:353:LEU:O	2:B:356:GLN:N	2.49	0.45
2:B:485:ALA:HB1	2:B:510:ASN:OD1	2.16	0.45
2:D:376:ILE:HG12	2:D:423:VAL:HG22	1.99	0.45
2:E:244:ASP:HB2	3:T:13:PHE:CE2	2.51	0.45
2:E:375:PHE:CZ	2:E:437:GLY:HA3	2.52	0.45
2:G:217:GLU:HB2	2:L:431:GLN:HE22	1.81	0.45
2:J:305:GLU:HG2	2:J:309:TRP:CD1	2.52	0.45
2:K:334:PHE:CZ	2:K:385:VAL:HG11	2.51	0.45
2:L:477:TYR:CD2	2:L:478:GLY:N	2.85	0.45
2:B:324:THR:O	2:B:326:GLY:N	2.49	0.45
2:E:131:TYR:HB3	2:E:250:MET:HG2	1.99	0.45
2:E:456:LEU:HD12	2:E:475:THR:HG21	1.98	0.45
2:F:378:ALA:HB1	2:F:382:VAL:CG2	2.46	0.45
2:G:146:PRO:HB2	2:G:366:ARG:O	2.17	0.45
2:G:272:ILE:HG22	2:G:468:GLN:HG2	1.99	0.45
2:G:456:LEU:HD12	2:G:475:THR:HG21	1.96	0.45
2:I:148:TYR:HD1	2:I:186:GLY:H	1.65	0.45
2:I:168:ALA:HB2	2:I:202:ALA:O	2.17	0.45
2:J:105:ASN:ND2	2:J:409:THR:O	2.24	0.45
3:W:41:ILE:HD13	3:W:46:TYR:CZ	2.52	0.45
1:a:36:TYR:O	1:a:40:VAL:HG22	2.16	0.45
1:a:261:ILE:HD11	1:a:414:VAL:HG22	1.98	0.45
1:a:290:HIS:O	1:a:291:LYS:HG2	2.17	0.45
2:C:72:HIS:CD2	2:D:121:THR:HG21	2.52	0.45
2:D:100:ARG:HG2	2:D:101:ARG:N	2.32	0.45
2:D:477:TYR:CD2	2:D:478:GLY:N	2.84	0.45
2:E:194:VAL:HG12	2:E:220:ALA:HA	1.99	0.45
2:F:477:TYR:CD2	2:F:478:GLY:N	2.85	0.45
2:G:124:VAL:HG22	2:L:96:MET:HB2	1.99	0.45
2:H:482:ASN:O	2:H:485:ALA:HB2	2.15	0.45
3:O:5:ARG:NH1	3:O:33:PRO:HB3	2.31	0.45
1:a:34:LEU:HD13	1:a:36:TYR:CE2	2.51	0.45
2:B:121:THR:HA	2:B:259:ILE:O	2.17	0.45
2:C:131:TYR:CB	2:C:250:MET:HG2	2.47	0.45
2:E:158:GLY:HA2	2:E:163:PHE:CE2	2.52	0.45
2:G:127:LEU:HD12	2:L:284:MET:HE1	1.98	0.45
2:G:344:ARG:NH1	2:L:344:ARG:HD2	2.31	0.45
2:H:383:VAL:O	2:H:387:ALA:N	2.47	0.45
2:L:164:PRO:HG2	2:L:178:TYR:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:140:PHE:CG	1:a:140:PHE:O	2.69	0.45
2:A:393:ILE:HA	2:F:398:GLN:O	2.17	0.45
2:C:69:GLY:H	2:E:234:GLU:CD	2.19	0.45
2:C:476:ARG:HH21	2:D:230:THR:HG21	1.81	0.45
2:E:301:GLU:OE1	2:F:155:SER:OG	2.29	0.45
2:E:333:ASP:HB3	2:E:519:LYS:HB2	1.98	0.45
2:F:131:TYR:CB	2:F:250:MET:HG2	2.47	0.45
2:F:270:TYR:HB3	2:F:290:LEU:CD1	2.47	0.45
2:I:121:THR:HA	2:I:259:ILE:O	2.17	0.45
2:I:479:ILE:HG22	2:I:480:GLY:N	2.32	0.45
2:J:145:HIS:NE2	2:J:487:SER:O	2.48	0.45
2:J:255:ASP:OD2	2:J:492:PRO:HG3	2.17	0.45
1:a:235:PHE:HB2	1:a:417:GLY:C	2.42	0.44
2:B:228:MET:SD	2:B:233:ALA:HB2	2.57	0.44
2:B:237:GLU:HB2	2:B:246:PRO:HA	1.98	0.44
2:B:503:ILE:HD11	2:C:175:GLY:HA2	1.99	0.44
2:D:344:ARG:O	2:D:348:GLU:HB2	2.17	0.44
2:E:72:HIS:C	2:E:74:TYR:H	2.25	0.44
2:G:245:ASN:OD1	2:G:245:ASN:N	2.50	0.44
2:G:255:ASP:OD2	2:G:492:PRO:HG2	2.17	0.44
2:J:278:LEU:CD2	2:J:284:MET:HB2	2.45	0.44
2:L:191:GLN:N	2:L:222:VAL:O	2.47	0.44
1:a:134:LEU:O	1:a:135:LEU:HG	2.17	0.44
2:A:105:ASN:HB2	2:A:412:VAL:HG23	1.98	0.44
2:A:344:ARG:O	2:A:348:GLU:HB2	2.17	0.44
2:A:377:ILE:HA	2:A:424:TYR:O	2.16	0.44
2:B:179:THR:HG22	2:B:189:TYR:CE1	2.52	0.44
2:C:190:LEU:HB3	2:C:221:LEU:HG	1.99	0.44
2:C:456:LEU:N	2:C:475:THR:HG22	2.23	0.44
2:D:456:LEU:HD12	2:D:475:THR:HG21	1.99	0.44
2:E:285:ASP:C	2:E:287:ASP:H	2.25	0.44
2:E:398:GLN:NE2	2:F:355:PHE:HB2	2.32	0.44
2:F:350:PHE:CB	2:F:389:VAL:HG21	2.40	0.44
2:F:479:ILE:HG22	2:F:480:GLY:N	2.31	0.44
2:H:232:ILE:HG12	3:V:48:THR:O	2.17	0.44
2:H:454:VAL:HG22	2:H:476:ARG:HB2	1.97	0.44
2:I:253:ARG:NH1	2:I:491:ALA:HB1	2.33	0.44
2:K:350:PHE:CB	2:K:389:VAL:HG21	2.40	0.44
2:A:345:TRP:NE1	2:A:348:GLU:OE1	2.50	0.44
2:D:157:GLN:N	2:D:227:GLY:O	2.49	0.44
2:E:345:TRP:CD2	2:F:348:GLU:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:458:PRO:HA	2:E:473:PHE:CD1	2.52	0.44
2:J:126:ALA:O	2:J:254:ILE:HA	2.17	0.44
2:L:290:LEU:HD23	2:L:293:ILE:HD11	1.99	0.44
2:L:345:TRP:NE1	2:L:348:GLU:OE1	2.50	0.44
2:C:272:ILE:HG22	2:C:468:GLN:HG2	1.99	0.44
2:C:282:HIS:HE1	2:D:125:PHE:CE2	2.35	0.44
2:D:444:MET:O	2:D:449:TYR:OH	2.12	0.44
2:F:153:MET:HE2	2:F:225:ALA:HA	1.99	0.44
2:G:148:TYR:HB3	2:G:186:GLY:HA2	2.00	0.44
2:G:171:GLN:NE2	2:G:195:GLN:HE21	2.15	0.44
2:G:217:GLU:HB2	2:L:431:GLN:NE2	2.33	0.44
2:H:456:LEU:HD12	2:H:475:THR:CG2	2.47	0.44
2:J:345:TRP:CD2	2:K:348:GLU:HG3	2.52	0.44
1:a:48:PRO:O	1:a:170:VAL:HG22	2.17	0.44
2:B:80:ALA:HA	2:B:93:PRO:CG	2.47	0.44
2:B:282:HIS:HE1	2:C:125:PHE:CE2	2.36	0.44
2:C:78:ASN:HD21	3:T:5:ARG:HB3	1.82	0.44
2:E:151:ASP:HB2	2:E:189:TYR:CE1	2.45	0.44
2:G:125:PHE:HA	2:G:256:LYS:HA	1.99	0.44
2:G:204:ASP:OD1	2:G:205:ALA:N	2.50	0.44
2:G:323:LEU:HD21	2:G:329:ALA:HA	2.00	0.44
2:G:324:THR:O	2:G:326:GLY:N	2.51	0.44
2:G:493:ALA:O	2:G:494:SER:OG	2.33	0.44
2:H:345:TRP:CD2	2:I:348:GLU:HG3	2.53	0.44
2:I:264:ARG:NH2	2:J:226:GLU:O	2.51	0.44
2:I:285:ASP:C	2:I:287:ASP:H	2.25	0.44
2:K:348:GLU:OE1	2:K:348:GLU:N	2.51	0.44
2:A:145:HIS:CD2	2:F:101:ARG:HH12	2.35	0.44
2:B:336:ASP:O	2:B:340:ILE:HG12	2.18	0.44
2:C:494:SER:O	2:C:495:ARG:HB2	2.16	0.44
2:D:474:LYS:HD3	2:L:273:GLU:OE2	2.18	0.44
2:F:232:ILE:HD11	3:Q:49:PHE:CB	2.48	0.44
2:G:295:ALA:HB2	2:G:473:PHE:HE2	1.83	0.44
2:J:100:ARG:NH1	2:J:289:GLU:OE1	2.51	0.44
2:K:376:ILE:HG22	2:K:436:VAL:HG22	2.00	0.44
2:L:477:TYR:CG	2:L:478:GLY:N	2.86	0.44
3:W:14:GLU:OE1	3:W:22:LYS:HD2	2.17	0.44
1:a:74:GLY:C	1:a:144:ALA:HB2	2.42	0.44
1:a:230:ILE:HG23	1:a:231:THR:N	2.33	0.44
2:A:265:GLN:C	2:A:266:LEU:HD12	2.42	0.44
2:B:332:PHE:HE2	2:B:334:PHE:CE1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:77:THR:HG21	3:P:5:ARG:NH2	2.33	0.44
2:G:494:SER:HA	3:T:37:ASP:CG	2.42	0.44
2:I:345:TRP:NE1	2:I:348:GLU:OE1	2.50	0.44
2:J:306:VAL:O	2:J:309:TRP:N	2.51	0.44
2:J:456:LEU:HD12	2:J:475:THR:CG2	2.48	0.44
2:J:479:ILE:HG22	2:J:480:GLY:N	2.33	0.44
2:K:367:GLN:HB3	2:K:511:ALA:HB1	2.00	0.44
2:L:305:GLU:HG2	2:L:309:TRP:CD1	2.52	0.44
1:a:212:LYS:HG2	1:a:317:ASN:ND2	2.32	0.44
1:a:336:ILE:O	1:a:341:PHE:HE2	2.01	0.44
2:A:164:PRO:HG2	2:A:178:TYR:CD1	2.52	0.44
2:B:151:ASP:HB3	2:B:187:THR:CG2	2.48	0.44
2:B:179:THR:HG22	2:B:189:TYR:CD1	2.52	0.44
2:D:72:HIS:HD2	2:E:260:GLU:OE2	2.01	0.44
2:E:171:GLN:HE21	2:E:195:GLN:HE21	1.65	0.44
2:E:171:GLN:NE2	2:E:195:GLN:HE21	2.16	0.44
2:E:196:VAL:HG21	2:E:215:GLN:OE1	2.18	0.44
2:F:266:LEU:HB3	2:F:267:LYS:H	1.65	0.44
2:F:305:GLU:HG2	2:F:309:TRP:CD1	2.52	0.44
2:G:73:GLY:O	2:G:74:TYR:HB2	2.17	0.44
2:G:133:LYS:HE2	3:T:42:SER:HB2	2.00	0.44
2:G:232:ILE:HG12	3:S:48:THR:O	2.18	0.44
2:H:100:ARG:HG2	2:H:101:ARG:N	2.32	0.44
2:J:145:HIS:ND1	2:J:148:TYR:CD2	2.86	0.44
2:J:238:GLY:HA2	2:J:242:SER:O	2.17	0.44
2:J:272:ILE:HG22	2:J:468:GLN:HG2	2.00	0.44
2:K:180:HIS:HD2	2:K:182:PHE:CD1	2.35	0.44
2:K:430:LYS:HD2	2:K:430:LYS:N	2.33	0.44
2:L:315:GLN:HG3	2:L:510:ASN:O	2.18	0.44
1:a:35:ILE:HG22	1:a:301:ASN:HB3	1.99	0.44
1:a:59:ASN:ND2	1:a:68:THR:HG21	2.32	0.44
1:a:271:PHE:CE1	1:a:273:VAL:HG23	2.53	0.44
2:A:309:TRP:O	2:A:313:SER:N	2.47	0.44
2:A:493:ALA:O	2:A:494:SER:OG	2.34	0.44
2:E:71:ASP:OD2	3:O:50:PRO:HG3	2.18	0.44
2:E:163:PHE:HB2	2:E:179:THR:CG2	2.48	0.44
2:E:313:SER:O	2:E:510:ASN:HB2	2.17	0.44
2:F:164:PRO:HG2	2:F:178:TYR:CD1	2.53	0.44
2:I:73:GLY:O	2:I:74:TYR:HB2	2.18	0.44
2:I:456:LEU:HD12	2:I:475:THR:CG2	2.48	0.44
2:L:324:THR:HB	2:L:327:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:7:TYR:CD1	3:W:54:ALA:HB2	2.53	0.44
1:a:199:GLU:HB3	1:a:360:PHE:CE2	2.52	0.43
2:A:147:MET:HE1	2:A:366:ARG:CZ	2.48	0.43
2:A:453:TYR:CD2	2:A:454:VAL:HG13	2.53	0.43
2:B:432:ASP:OD1	2:B:433:TYR:N	2.51	0.43
2:C:153:MET:HG2	2:C:189:TYR:HD2	1.80	0.43
2:E:142:GLU:H	2:E:490:GLN:CG	2.31	0.43
2:F:319:SER:HA	2:F:323:LEU:HG	1.99	0.43
2:F:432:ASP:O	2:F:433:TYR:HB3	2.17	0.43
2:G:376:ILE:HG22	2:G:436:VAL:HA	1.99	0.43
2:G:398:GLN:O	2:H:393:ILE:HA	2.18	0.43
2:I:485:ALA:HB1	2:I:510:ASN:OD1	2.18	0.43
2:J:173:THR:OG1	2:J:176:ASP:OD2	2.35	0.43
2:K:197:THR:HG22	2:K:199:ASP:H	1.83	0.43
2:L:193:SER:OG	2:L:220:ALA:O	2.34	0.43
1:a:389:ALA:HB2	1:a:405:LYS:HB3	1.99	0.43
2:A:377:ILE:HG22	2:A:424:TYR:HB2	2.00	0.43
2:B:479:ILE:HG22	2:B:480:GLY:N	2.33	0.43
2:D:382:VAL:O	2:D:386:LEU:HD13	2.17	0.43
2:E:238:GLY:HA2	2:E:242:SER:O	2.18	0.43
2:F:317:GLY:HA2	2:F:514:ARG:NH2	2.34	0.43
2:F:346:ALA:O	2:F:349:SER:N	2.51	0.43
2:F:444:MET:O	2:F:449:TYR:OH	2.34	0.43
2:G:72:HIS:ND1	2:G:83:GLN:O	2.51	0.43
2:H:431:GLN:NE2	2:I:213:LYS:O	2.51	0.43
2:I:68:ILE:HD11	2:K:235:LEU:HD23	2.00	0.43
2:I:409:THR:HG21	2:J:370:ARG:O	2.17	0.43
2:K:377:ILE:HA	2:K:424:TYR:O	2.17	0.43
2:L:171:GLN:NE2	2:L:195:GLN:HE21	2.16	0.43
2:L:350:PHE:CB	2:L:389:VAL:HG21	2.48	0.43
1:a:25:VAL:HG12	1:a:26:ALA:N	2.33	0.43
2:A:344:ARG:NH1	2:B:344:ARG:HH12	2.17	0.43
2:B:350:PHE:CB	2:B:389:VAL:HG21	2.36	0.43
2:E:159:ALA:HB2	2:E:248:ASN:ND2	2.33	0.43
2:I:131:TYR:CB	2:I:250:MET:HG2	2.48	0.43
2:I:145:HIS:CD2	2:I:146:PRO:HD2	2.45	0.43
2:J:305:GLU:HA	2:K:225:ALA:HB3	2.00	0.43
2:K:126:ALA:N	2:K:255:ASP:O	2.51	0.43
2:B:295:ALA:HB2	2:B:473:PHE:CE2	2.53	0.43
2:D:125:PHE:HA	2:D:256:LYS:HA	1.99	0.43
2:E:334:PHE:HZ	2:E:353:LEU:HD12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:432:ASP:O	2:E:433:TYR:HB3	2.18	0.43
2:H:110:ASP:O	2:H:439:LYS:HG2	2.18	0.43
2:J:264:ARG:NH1	2:K:155:SER:HG	2.15	0.43
2:L:146:PRO:HB3	2:L:369:GLY:HA3	2.00	0.43
2:A:126:ALA:N	2:A:255:ASP:O	2.51	0.43
2:A:350:PHE:HB2	2:A:389:VAL:HG21	2.00	0.43
2:D:121:THR:HG22	2:D:260:GLU:OE1	2.18	0.43
2:F:255:ASP:OD2	2:F:495:ARG:HG2	2.19	0.43
2:L:360:GLU:O	2:L:363:GLU:N	2.51	0.43
2:L:376:ILE:HG12	2:L:423:VAL:HG22	2.01	0.43
2:B:159:ALA:HB3	2:B:228:MET:HE1	2.00	0.43
2:F:133:LYS:HE2	3:P:42:SER:HB2	2.01	0.43
2:F:442:ASN:HB3	2:F:444:MET:H	1.83	0.43
2:I:323:LEU:HD21	2:I:329:ALA:CA	2.48	0.43
2:J:265:GLN:C	2:J:266:LEU:HD12	2.43	0.43
2:K:128:ARG:NE	2:K:484:PHE:HE1	2.15	0.43
2:L:479:ILE:HG22	2:L:480:GLY:N	2.34	0.43
1:a:76:ALA:O	1:a:80:ASP:HB3	2.19	0.43
2:B:164:PRO:HG2	2:B:178:TYR:HD1	1.82	0.43
2:B:430:LYS:HE2	2:C:188:VAL:CG1	2.49	0.43
2:C:351:LYS:HE3	2:C:394:SER:O	2.19	0.43
2:C:479:ILE:HG22	2:C:480:GLY:N	2.34	0.43
2:D:74:TYR:CE2	2:E:260:GLU:HG2	2.53	0.43
2:D:305:GLU:HG2	2:D:309:TRP:CD1	2.54	0.43
2:E:96:MET:HE3	2:F:124:VAL:HG23	1.99	0.43
2:E:378:ALA:HB1	2:E:382:VAL:HG21	2.00	0.43
2:G:145:HIS:HD2	2:G:146:PRO:CD	2.29	0.43
2:H:71:ASP:CG	2:J:231:SER:HB2	2.44	0.43
2:H:131:TYR:CB	2:H:250:MET:HG2	2.49	0.43
2:H:317:GLY:HA2	2:H:514:ARG:NH2	2.33	0.43
2:H:430:LYS:HE2	2:I:188:VAL:HG11	2.01	0.43
2:I:313:SER:O	2:I:510:ASN:HB2	2.18	0.43
3:O:33:PRO:HG2	3:O:62:GLU:OE1	2.18	0.43
2:A:351:LYS:HE3	2:A:394:SER:O	2.18	0.43
2:B:93:PRO:HB2	2:C:123:GLN:HB3	2.01	0.43
2:B:281:VAL:HG13	2:B:282:HIS:N	2.34	0.43
2:C:147:MET:HE2	2:C:147:MET:HA	2.00	0.43
2:C:456:LEU:HD12	2:C:475:THR:HG21	2.01	0.43
2:D:79:ILE:HB	2:E:258:VAL:HG11	2.00	0.43
2:D:131:TYR:CB	2:D:250:MET:HG2	2.48	0.43
2:D:290:LEU:HD23	2:D:293:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:375:PHE:CZ	2:D:437:GLY:HA3	2.54	0.43
2:D:380:ARG:NH1	2:D:427:GLN:O	2.42	0.43
2:E:146:PRO:HB2	2:E:366:ARG:O	2.18	0.43
2:E:398:GLN:O	2:F:393:ILE:HA	2.18	0.43
2:G:333:ASP:OD1	2:G:333:ASP:N	2.52	0.43
2:G:354:LEU:HA	2:G:357:ILE:HG22	2.01	0.43
2:H:153:MET:HE2	2:H:226:GLU:H	1.83	0.43
2:K:383:VAL:HG12	2:K:406:THR:HG22	2.01	0.43
2:L:454:VAL:HG22	2:L:476:ARG:HB2	2.01	0.43
3:P:14:GLU:HB3	3:P:25:GLY:H	1.82	0.43
1:a:35:ILE:O	1:a:35:ILE:HG13	2.19	0.43
2:B:99:VAL:HG12	2:C:484:PHE:CE2	2.54	0.43
2:C:354:LEU:HA	2:C:357:ILE:HG22	2.01	0.43
2:D:172:THR:HA	2:D:178:TYR:OH	2.19	0.43
2:D:305:GLU:OE1	2:D:477:TYR:OH	2.30	0.43
2:D:363:GLU:OE2	2:D:366:ARG:NH2	2.51	0.43
2:E:244:ASP:O	2:E:246:PRO:HD3	2.18	0.43
2:F:107:ILE:HG22	2:F:303:ASN:OD1	2.18	0.43
2:F:128:ARG:NE	2:F:484:PHE:HE1	2.11	0.43
2:K:134:ASP:HB3	2:K:137:ALA:HB2	2.01	0.43
2:K:268:ALA:HB2	2:K:294:LEU:HD11	2.01	0.43
3:W:12:THR:OG1	3:W:26:LYS:O	2.30	0.43
1:a:232:ASP:O	1:a:233:SER:OG	2.24	0.43
1:a:375:LEU:C	1:a:375:LEU:HD12	2.44	0.43
2:B:151:ASP:OD1	2:B:151:ASP:N	2.51	0.43
2:B:463:ASP:OD1	2:B:464:PRO:HD2	2.18	0.43
2:C:398:GLN:O	2:D:393:ILE:HA	2.18	0.43
2:C:444:MET:O	2:C:449:TYR:OH	2.23	0.43
2:F:345:TRP:NE1	2:F:348:GLU:OE1	2.51	0.43
2:J:153:MET:HE2	2:J:226:GLU:N	2.33	0.43
2:J:172:THR:O	2:J:195:GLN:HA	2.19	0.43
1:a:79:VAL:HB	1:a:155:GLU:HG3	2.01	0.42
2:A:331:VAL:HG12	2:A:517:TYR:HB2	2.00	0.42
2:B:296:THR:O	2:B:300:LEU:HG	2.19	0.42
2:D:493:ALA:O	2:D:494:SER:OG	2.25	0.42
2:E:113:GLY:H	2:E:446:ALA:HB1	1.83	0.42
2:F:131:TYR:HB3	2:F:250:MET:HE3	2.01	0.42
2:F:179:THR:HG22	2:F:189:TYR:CE2	2.54	0.42
2:H:430:LYS:HD2	2:H:430:LYS:N	2.33	0.42
2:I:157:GLN:N	2:I:227:GLY:O	2.52	0.42
2:I:196:VAL:HG21	2:I:215:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:430:LYS:HE2	2:J:188:VAL:CG1	2.49	0.42
2:I:521:ILE:HA	2:J:341:ARG:NH2	2.34	0.42
2:L:154:PHE:CZ	2:L:248:ASN:HB3	2.54	0.42
3:W:10:ILE:HD11	3:W:35:TYR:CE1	2.54	0.42
1:a:230:ILE:HG23	1:a:231:THR:H	1.84	0.42
2:A:169:SER:OG	2:A:200:ALA:HB2	2.19	0.42
2:E:482:ASN:ND2	2:E:512:TYR:OH	2.52	0.42
2:G:74:TYR:OH	2:I:229:ALA:HA	2.19	0.42
2:H:479:ILE:HG22	2:H:480:GLY:N	2.33	0.42
2:I:290:LEU:HA	2:I:290:LEU:HD23	1.80	0.42
2:L:107:ILE:HG21	2:L:307:VAL:CG2	2.49	0.42
3:P:40:LYS:O	3:P:40:LYS:HG3	2.19	0.42
1:a:126:LEU:O	1:a:130:ILE:HG23	2.19	0.42
2:B:80:ALA:HA	2:B:93:PRO:HG2	2.00	0.42
2:B:129:ALA:O	2:B:143:ALA:N	2.47	0.42
2:D:310:ILE:HG12	2:D:513:PHE:CE2	2.54	0.42
2:D:324:THR:HB	2:D:327:SER:OG	2.19	0.42
2:D:432:ASP:O	2:D:433:TYR:HB3	2.19	0.42
2:I:324:THR:HB	2:I:327:SER:OG	2.19	0.42
2:J:154:PHE:CZ	2:J:248:ASN:HB3	2.55	0.42
2:K:324:THR:O	2:K:326:GLY:N	2.52	0.42
3:W:8:VAL:HG23	3:W:32:PHE:HD1	1.85	0.42
1:a:177:THR:HG22	1:a:202:LEU:HD11	2.01	0.42
2:A:73:GLY:O	2:A:74:TYR:HB2	2.19	0.42
2:B:107:ILE:HG21	2:B:307:VAL:CG2	2.48	0.42
2:D:107:ILE:H	2:D:303:ASN:ND2	2.11	0.42
2:D:131:TYR:HB2	2:D:250:MET:HG2	2.01	0.42
2:D:315:GLN:HG3	2:D:510:ASN:O	2.18	0.42
2:E:305:GLU:HG2	2:E:309:TRP:CD1	2.54	0.42
2:E:453:TYR:CD2	2:E:454:VAL:HG13	2.55	0.42
2:H:386:LEU:HB3	2:H:404:PHE:HE2	1.83	0.42
2:J:151:ASP:CG	2:J:154:PHE:HB2	2.45	0.42
2:K:270:TYR:HB3	2:K:290:LEU:CD1	2.49	0.42
2:L:268:ALA:HB3	2:L:471:MET:HG3	2.02	0.42
1:a:220:THR:O	1:a:407:ALA:HA	2.19	0.42
2:A:295:ALA:HB2	2:A:473:PHE:CE2	2.54	0.42
2:A:346:ALA:O	2:A:349:SER:N	2.53	0.42
2:A:486:GLU:C	2:A:488:ALA:H	2.27	0.42
2:B:180:HIS:HD2	2:B:182:PHE:CE1	2.38	0.42
2:C:107:ILE:HG22	2:C:303:ASN:OD1	2.19	0.42
2:E:119:SER:HA	2:E:453:TYR:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:PRO:O	2:F:121:THR:OG1	2.37	0.42
2:F:315:GLN:HG3	2:F:510:ASN:O	2.20	0.42
2:H:136:VAL:HG12	2:H:253:ARG:NE	2.35	0.42
2:I:113:GLY:H	2:I:446:ALA:HB1	1.84	0.42
2:I:159:ALA:HB2	2:I:248:ASN:ND2	2.34	0.42
2:I:198:ILE:HD12	2:I:198:ILE:HG23	1.81	0.42
2:J:171:GLN:HG2	2:J:195:GLN:HE21	1.84	0.42
2:J:324:THR:O	2:J:326:GLY:N	2.52	0.42
2:A:128:ARG:NE	2:A:484:PHE:HE1	2.13	0.42
2:A:229:ALA:HA	2:E:74:TYR:OH	2.19	0.42
2:A:456:LEU:HD12	2:A:475:THR:CG2	2.50	0.42
2:C:101:ARG:NH1	2:D:145:HIS:CD2	2.87	0.42
2:D:236:GLN:HG3	2:D:247:TRP:CD1	2.55	0.42
2:F:197:THR:HG22	2:F:199:ASP:H	1.85	0.42
2:G:126:ALA:HB1	2:G:484:PHE:CE1	2.55	0.42
2:J:293:ILE:HG22	2:K:144:PHE:HE2	1.85	0.42
2:J:456:LEU:N	2:J:475:THR:HG22	2.27	0.42
2:K:315:GLN:HG3	2:K:510:ASN:O	2.20	0.42
2:A:123:GLN:HE21	2:F:95:VAL:HG12	1.85	0.42
2:C:91:ILE:H	2:L:281:VAL:HG21	1.85	0.42
2:C:278:LEU:HD21	2:C:284:MET:HB2	2.02	0.42
2:C:345:TRP:NE1	2:C:348:GLU:OE1	2.52	0.42
2:D:166:LEU:HD22	2:D:212:ILE:HD11	2.02	0.42
2:E:295:ALA:HB2	2:E:473:PHE:HE2	1.84	0.42
2:F:486:GLU:C	2:F:488:ALA:H	2.28	0.42
2:G:485:ALA:HB1	2:G:510:ASN:OD1	2.19	0.42
2:H:477:TYR:CD2	2:H:478:GLY:N	2.87	0.42
2:I:348:GLU:OE1	2:I:348:GLU:N	2.52	0.42
2:I:390:ASP:OD2	2:I:394:SER:OG	2.38	0.42
2:J:295:ALA:HB2	2:J:473:PHE:HE2	1.85	0.42
2:K:479:ILE:HG22	2:K:480:GLY:N	2.34	0.42
2:L:270:TYR:HB3	2:L:290:LEU:HD12	2.01	0.42
2:L:295:ALA:HB2	2:L:473:PHE:CE2	2.54	0.42
2:L:494:SER:HA	3:U:37:ASP:CG	2.45	0.42
3:P:61:GLU:N	3:P:64:GLN:OE1	2.52	0.42
1:a:17:ASN:OD1	1:a:18:SER:N	2.53	0.42
1:a:34:LEU:HD12	1:a:34:LEU:O	2.19	0.42
2:D:278:LEU:HD23	2:D:278:LEU:HA	1.79	0.42
2:E:117:MET:HE1	2:E:261:ALA:HB2	2.01	0.42
2:F:235:LEU:HD13	2:F:242:SER:HB3	2.01	0.42
2:F:341:ARG:HD3	2:F:341:ARG:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:106:LEU:HD21	2:I:300:LEU:HD23	2.01	0.42
2:I:270:TYR:HB3	2:I:290:LEU:CD1	2.49	0.42
2:J:237:GLU:OE1	2:J:246:PRO:HA	2.19	0.42
2:L:84:THR:HG22	2:L:86:GLY:H	1.84	0.42
2:L:135:PRO:HB3	2:L:252:PHE:O	2.19	0.42
3:W:65:ARG:O	3:W:69:ILE:N	2.41	0.42
1:a:198:LEU:HD13	1:a:373:ILE:HD12	2.01	0.42
2:A:121:THR:HA	2:A:259:ILE:O	2.19	0.42
2:A:228:MET:SD	2:A:233:ALA:HB2	2.59	0.42
2:A:234:GLU:OE1	2:E:70:GLY:N	2.43	0.42
2:B:255:ASP:HB2	2:B:492:PRO:HG3	2.00	0.42
2:B:364:ILE:O	2:B:368:THR:OG1	2.32	0.42
2:B:456:LEU:HD12	2:B:475:THR:CG2	2.50	0.42
2:C:85:SER:HB3	3:T:32:PHE:HE1	1.85	0.42
2:E:232:ILE:HD11	3:T:49:PHE:CB	2.49	0.42
2:F:164:PRO:HG2	2:F:178:TYR:HD1	1.85	0.42
2:F:386:LEU:HB3	2:F:404:PHE:HE2	1.84	0.42
2:I:253:ARG:HH21	2:I:495:ARG:CG	2.33	0.42
2:I:382:VAL:HG12	2:I:521:ILE:HD11	2.01	0.42
2:J:198:ILE:HD12	2:J:198:ILE:HG23	1.86	0.42
2:J:344:ARG:O	2:J:348:GLU:HB2	2.20	0.42
2:K:163:PHE:HB2	2:K:179:THR:CG2	2.49	0.42
2:L:77:THR:HG21	3:T:5:ARG:NH2	2.35	0.42
1:a:257:MET:O	1:a:261:ILE:HG12	2.20	0.42
1:a:324:ILE:HD11	1:a:415:LEU:HD12	2.02	0.42
2:A:101:ARG:HG2	2:B:144:PHE:O	2.20	0.42
2:A:101:ARG:HH12	2:B:145:HIS:CD2	2.38	0.42
2:B:85:SER:HB3	3:X:32:PHE:CE1	2.54	0.42
2:B:198:ILE:O	2:B:198:ILE:HG22	2.20	0.42
2:B:255:ASP:OD2	2:B:495:ARG:HG2	2.19	0.42
2:C:131:TYR:HB3	2:C:250:MET:HG2	2.01	0.42
2:C:167:ALA:H	2:C:170:THR:HG21	1.85	0.42
2:D:409:THR:HG21	2:E:370:ARG:O	2.19	0.42
2:F:131:TYR:HB3	2:F:250:MET:HG2	2.00	0.42
2:I:173:THR:OG1	2:I:176:ASP:OD2	2.38	0.42
2:J:131:TYR:CD2	2:J:250:MET:HE3	2.50	0.42
2:B:345:TRP:NE1	2:B:348:GLU:OE1	2.53	0.41
2:B:409:THR:HG21	2:C:370:ARG:O	2.20	0.41
2:B:442:ASN:HB3	2:B:444:MET:H	1.84	0.41
2:D:268:ALA:HB3	2:D:471:MET:CG	2.50	0.41
2:D:333:ASP:OD1	2:D:333:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:345:TRP:CD2	2:E:348:GLU:HG3	2.54	0.41
2:E:107:ILE:H	2:E:303:ASN:ND2	2.08	0.41
2:E:117:MET:HB2	2:E:451:ALA:HB1	2.02	0.41
2:F:205:ALA:O	2:F:208:LEU:N	2.53	0.41
2:H:157:GLN:N	2:H:227:GLY:O	2.53	0.41
2:J:153:MET:SD	2:J:157:GLN:HB3	2.60	0.41
2:J:324:THR:O	2:J:327:SER:N	2.47	0.41
2:K:80:ALA:HA	2:K:93:PRO:CG	2.50	0.41
2:L:106:LEU:HD22	2:L:303:ASN:HD22	1.85	0.41
2:L:153:MET:SD	2:L:157:GLN:HB3	2.59	0.41
1:a:237:ASP:OD1	1:a:237:ASP:N	2.53	0.41
2:A:244:ASP:HB2	3:O:13:PHE:CE2	2.54	0.41
2:A:275:THR:HG22	2:A:286:ALA:HB3	2.01	0.41
2:B:234:GLU:CD	2:F:68:ILE:HD12	2.45	0.41
2:B:386:LEU:HB3	2:B:404:PHE:CE2	2.55	0.41
2:C:67:GLU:OE1	2:L:290:LEU:HD11	2.20	0.41
2:C:166:LEU:HB2	2:C:178:TYR:HB3	2.02	0.41
2:C:306:VAL:HG11	2:C:450:TYR:HB2	2.02	0.41
2:D:482:ASN:O	2:D:485:ALA:HB2	2.20	0.41
2:F:153:MET:HE2	2:F:226:GLU:N	2.34	0.41
2:G:172:THR:O	2:G:195:GLN:HA	2.20	0.41
2:H:284:MET:HE1	2:I:127:LEU:HD12	2.01	0.41
2:H:442:ASN:HB3	2:H:444:MET:H	1.84	0.41
2:I:454:VAL:HG22	2:I:476:ARG:HB2	2.02	0.41
2:K:171:GLN:NE2	2:K:195:GLN:HE21	2.18	0.41
2:K:432:ASP:O	2:K:433:TYR:HB3	2.20	0.41
1:a:34:LEU:HB2	1:a:211:ASN:OD1	2.19	0.41
1:a:214:ILE:HD11	1:a:342:TYR:CD1	2.55	0.41
1:a:223:LYS:O	1:a:414:VAL:HA	2.20	0.41
1:a:299:SER:C	1:a:301:ASN:H	2.28	0.41
2:A:244:ASP:C	2:A:246:PRO:HD3	2.45	0.41
2:A:458:PRO:HA	2:A:473:PHE:CD1	2.55	0.41
2:B:331:VAL:HG11	2:B:519:LYS:HE3	2.02	0.41
2:B:502:SER:N	2:B:506:SER:OG	2.53	0.41
2:C:110:ASP:O	2:C:439:LYS:HG2	2.19	0.41
2:C:270:TYR:HB3	2:C:290:LEU:CD1	2.50	0.41
2:E:344:ARG:NH1	2:F:344:ARG:HH12	2.17	0.41
2:H:417:LEU:HD12	2:H:421:TYR:HD2	1.85	0.41
2:H:463:ASP:OD1	2:H:464:PRO:HD2	2.20	0.41
2:I:148:TYR:HB3	2:I:186:GLY:HA2	2.03	0.41
2:I:315:GLN:HG3	2:I:510:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:380:ARG:NH1	2:I:427:GLN:O	2.48	0.41
2:J:377:ILE:HA	2:J:424:TYR:O	2.19	0.41
2:K:301:GLU:OE1	2:L:155:SER:OG	2.31	0.41
2:K:305:GLU:HG3	2:L:225:ALA:O	2.19	0.41
3:P:40:LYS:H	3:P:72:ASN:ND2	2.18	0.41
1:a:257:MET:HB3	1:a:414:VAL:HG23	2.01	0.41
2:C:146:PRO:HB2	2:C:366:ARG:O	2.21	0.41
2:C:232:ILE:HG22	2:C:236:GLN:HE22	1.85	0.41
2:D:232:ILE:HD11	3:X:49:PHE:CB	2.50	0.41
2:D:332:PHE:O	2:D:518:VAL:HA	2.21	0.41
2:E:268:ALA:HB3	2:E:471:MET:CG	2.51	0.41
2:F:133:LYS:HG3	2:F:249:GLU:OE1	2.20	0.41
2:F:272:ILE:HG22	2:F:468:GLN:HG2	2.02	0.41
2:G:68:ILE:HD11	2:I:235:LEU:HD23	2.03	0.41
2:G:147:MET:HE1	2:G:366:ARG:CZ	2.51	0.41
2:G:198:ILE:O	2:G:211:GLU:HG2	2.20	0.41
2:G:344:ARG:HH12	2:L:344:ARG:HH11	1.67	0.41
2:G:431:GLN:OE1	2:H:217:GLU:HB2	2.21	0.41
2:H:154:PHE:CZ	2:H:248:ASN:HB3	2.56	0.41
2:H:476:ARG:HH21	2:I:230:THR:HG21	1.85	0.41
2:I:179:THR:HG22	2:I:189:TYR:CD1	2.54	0.41
2:J:79:ILE:CG2	2:K:121:THR:HB	2.51	0.41
1:a:39:ILE:HG21	1:a:39:ILE:HD13	1.85	0.41
2:B:348:GLU:OE1	2:B:348:GLU:N	2.50	0.41
2:C:96:MET:HE3	2:D:124:VAL:HG23	2.02	0.41
2:C:269:ALA:O	2:L:66:ALA:HA	2.20	0.41
2:C:365:ALA:HB2	2:C:372:GLU:HA	2.03	0.41
2:D:382:VAL:HG21	2:D:433:TYR:O	2.20	0.41
2:D:456:LEU:N	2:D:475:THR:HG22	2.34	0.41
2:E:110:ASP:O	2:E:439:LYS:HG2	2.21	0.41
2:E:376:ILE:HG12	2:E:423:VAL:HG22	2.01	0.41
2:H:282:HIS:HE1	2:I:125:PHE:CE2	2.38	0.41
2:H:495:ARG:O	2:H:496:ILE:HD13	2.21	0.41
2:I:125:PHE:HA	2:I:256:LYS:HA	2.02	0.41
2:I:312:TYR:CE1	2:I:507:LEU:HD12	2.55	0.41
2:I:360:GLU:O	2:I:363:GLU:N	2.53	0.41
2:J:260:GLU:HG3	2:J:261:ALA:N	2.35	0.41
2:J:324:THR:HB	2:J:327:SER:OG	2.21	0.41
2:K:95:VAL:HG12	2:L:123:GLN:HE21	1.85	0.41
2:K:386:LEU:HB3	2:K:404:PHE:CE2	2.50	0.41
2:K:400:LEU:HD11	2:L:417:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:507:LEU:O	2:L:509:LYS:HG3	2.20	0.41
2:A:74:TYR:OH	2:C:229:ALA:HA	2.19	0.41
2:A:386:LEU:HB3	2:A:404:PHE:CE2	2.53	0.41
2:A:432:ASP:O	2:A:433:TYR:HB3	2.21	0.41
2:B:453:TYR:HB3	2:B:476:ARG:O	2.20	0.41
2:C:113:GLY:H	2:C:446:ALA:HB1	1.86	0.41
2:D:463:ASP:OD1	2:D:464:PRO:HD2	2.20	0.41
2:E:131:TYR:HB3	2:E:250:MET:HE3	2.02	0.41
2:F:290:LEU:HD23	2:F:290:LEU:HA	1.91	0.41
2:G:244:ASP:C	2:G:246:PRO:HD3	2.45	0.41
2:G:494:SER:HA	3:T:37:ASP:OD2	2.21	0.41
2:I:238:GLY:HA2	2:I:242:SER:O	2.21	0.41
2:J:163:PHE:HB2	2:J:179:THR:HG23	2.03	0.41
2:J:360:GLU:O	2:J:363:GLU:N	2.53	0.41
2:K:145:HIS:CD2	2:K:146:PRO:HD2	2.43	0.41
2:K:228:MET:SD	2:K:233:ALA:HB2	2.60	0.41
1:a:35:ILE:HD13	1:a:313:TYR:HB3	2.03	0.41
1:a:92:LYS:HB2	1:a:116:PHE:CD2	2.53	0.41
2:A:255:ASP:OD2	2:A:495:ARG:HG2	2.21	0.41
2:A:355:PHE:HB2	2:F:398:GLN:HE21	1.84	0.41
2:B:262:LYS:HE3	2:B:500:MET:HE2	2.02	0.41
2:B:337:PRO:CB	4:Z:306:TRP:HB3	2.50	0.41
2:C:70:GLY:HA3	2:C:86:GLY:HA3	2.02	0.41
2:C:128:ARG:HE	2:C:484:PHE:HE1	1.69	0.41
2:D:106:LEU:HD21	2:D:300:LEU:HD23	2.02	0.41
2:D:268:ALA:HB3	2:D:471:MET:HG2	2.02	0.41
2:E:126:ALA:HB1	2:E:484:PHE:CE1	2.55	0.41
2:F:290:LEU:HA	2:F:293:ILE:HG12	2.02	0.41
2:F:462:SER:HA	2:F:469:PRO:HA	2.02	0.41
2:G:265:GLN:C	2:G:266:LEU:HD12	2.45	0.41
2:H:153:MET:HE2	2:H:225:ALA:HA	2.03	0.41
2:I:179:THR:HG22	2:I:189:TYR:CE1	2.56	0.41
2:J:375:PHE:CZ	2:J:437:GLY:HA3	2.55	0.41
2:K:146:PRO:HB2	2:K:366:ARG:O	2.21	0.41
2:K:301:GLU:O	2:K:305:GLU:N	2.54	0.41
2:L:420:LYS:HD2	2:L:421:TYR:CE2	2.56	0.41
1:a:290:HIS:CD2	1:a:298:LEU:HD21	2.55	0.41
2:A:345:TRP:HB3	2:B:343:ALA:HA	2.01	0.41
2:A:456:LEU:N	2:A:475:THR:HG22	2.30	0.41
2:B:304:ARG:HA	2:B:304:ARG:HD2	1.91	0.41
2:B:456:LEU:N	2:B:475:THR:HG22	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:507:LEU:O	2:D:509:LYS:HG3	2.21	0.41
2:E:117:MET:CE	2:E:261:ALA:HB2	2.51	0.41
2:E:136:VAL:HG12	2:E:253:ARG:NE	2.36	0.41
2:F:232:ILE:HD11	3:Q:49:PHE:HB3	2.03	0.41
2:H:268:ALA:HB1	2:H:290:LEU:HD13	2.01	0.41
2:K:198:ILE:HG23	2:K:198:ILE:HD12	1.76	0.41
2:K:312:TYR:CE1	2:K:507:LEU:HD12	2.55	0.41
2:L:163:PHE:HB2	2:L:179:THR:CG2	2.51	0.41
2:L:319:SER:HA	2:L:323:LEU:HG	2.03	0.41
2:L:502:SER:N	2:L:506:SER:OG	2.48	0.41
1:a:175:LEU:HD12	1:a:206:MET:HG2	2.03	0.41
1:a:315:ASP:OD2	1:a:322:TYR:OH	2.36	0.41
2:A:343:ALA:HA	2:F:345:TRP:HB3	2.03	0.41
2:B:74:TYR:CE2	2:C:260:GLU:HG2	2.56	0.41
2:B:399:GLY:HA3	2:C:392:GLY:O	2.20	0.41
2:B:477:TYR:CD2	2:B:478:GLY:N	2.88	0.41
2:C:453:TYR:HB3	2:C:476:ARG:O	2.21	0.41
2:D:323:LEU:HD22	2:D:327:SER:HB2	2.01	0.41
2:D:378:ALA:HB1	2:D:382:VAL:CG2	2.51	0.41
2:D:482:ASN:O	2:D:485:ALA:N	2.50	0.41
2:E:80:ALA:HA	2:E:93:PRO:CG	2.51	0.41
2:E:181:PHE:HA	2:E:187:THR:HA	2.03	0.41
2:E:191:GLN:N	2:E:222:VAL:O	2.51	0.41
2:F:151:ASP:CG	2:F:154:PHE:HB2	2.46	0.41
2:F:333:ASP:OD1	2:F:333:ASP:N	2.54	0.41
2:F:348:GLU:OE1	2:F:348:GLU:N	2.51	0.41
2:G:125:PHE:HE1	2:G:256:LYS:HE3	1.85	0.41
2:G:281:VAL:HG13	2:G:282:HIS:N	2.36	0.41
2:G:456:LEU:HD12	2:G:475:THR:HG22	2.03	0.41
2:I:142:GLU:H	2:I:490:GLN:HG2	1.86	0.41
2:I:163:PHE:HB2	2:I:179:THR:CG2	2.50	0.41
2:I:265:GLN:OE1	2:I:474:LYS:HE2	2.21	0.41
2:I:268:ALA:HB3	2:I:471:MET:CG	2.51	0.41
2:I:345:TRP:NE1	2:J:344:ARG:HH21	2.18	0.41
2:J:71:ASP:OD1	2:L:231:SER:HB2	2.21	0.41
2:J:160:ALA:HB1	2:J:232:ILE:HG21	2.03	0.41
2:K:99:VAL:HG12	2:L:484:PHE:CE2	2.55	0.41
2:K:345:TRP:CD2	2:L:348:GLU:HG3	2.56	0.41
2:L:147:MET:SD	2:L:367:GLN:HG2	2.60	0.41
2:L:168:ALA:HB1	2:L:200:ALA:HA	2.02	0.41
3:P:18:ASP:HB3	3:P:21:LYS:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:39:HIS:ND1	3:P:39:HIS:O	2.54	0.41
1:a:174:LYS:HG3	1:a:375:LEU:O	2.21	0.41
2:A:113:GLY:H	2:A:446:ALA:HB1	1.86	0.41
2:A:166:LEU:HD11	2:A:221:LEU:HD21	2.03	0.41
2:B:239:PHE:CD2	2:B:240:ASN:HB2	2.56	0.41
2:E:157:GLN:HB2	2:E:227:GLY:O	2.20	0.41
2:F:72:HIS:C	2:F:74:TYR:H	2.29	0.41
2:G:132:GLY:O	2:G:133:LYS:HB3	2.20	0.41
2:G:476:ARG:NH2	2:H:230:THR:HG21	2.31	0.41
2:G:484:PHE:CE2	2:L:99:VAL:HG12	2.56	0.41
2:H:382:VAL:HG12	2:H:521:ILE:HD11	2.03	0.41
2:I:277:ASP:O	2:I:281:VAL:HG12	2.21	0.41
2:I:466:ASN:O	2:I:468:GLN:HG3	2.21	0.41
2:K:147:MET:HE2	2:K:147:MET:HA	2.02	0.41
2:K:159:ALA:HB2	2:K:248:ASN:ND2	2.35	0.41
1:a:223:LYS:HB2	1:a:410:SER:O	2.21	0.40
1:a:342:TYR:O	1:a:380:ALA:HB3	2.21	0.40
2:A:407:ASP:HB3	2:B:372:GLU:HB2	2.03	0.40
2:C:253:ARG:NE	2:C:255:ASP:OD2	2.55	0.40
2:C:304:ARG:HH12	2:C:426:ASP:CG	2.28	0.40
2:C:318:LYS:N	2:C:360:GLU:OE2	2.54	0.40
2:D:269:ALA:CB	2:D:470:VAL:HG12	2.51	0.40
2:E:169:SER:OG	2:E:200:ALA:HB2	2.21	0.40
2:E:315:GLN:HG3	2:E:510:ASN:O	2.21	0.40
2:E:336:ASP:O	2:E:340:ILE:HG12	2.21	0.40
2:E:479:ILE:HG22	2:E:480:GLY:N	2.37	0.40
2:G:128:ARG:NE	2:G:484:PHE:HE1	2.18	0.40
2:G:317:GLY:HA2	2:G:514:ARG:NH2	2.36	0.40
2:G:318:LYS:HE3	2:G:327:SER:HB3	2.03	0.40
2:G:392:GLY:O	2:L:399:GLY:HA3	2.21	0.40
2:I:430:LYS:HE3	2:J:185:THR:O	2.20	0.40
2:J:120:PRO:O	2:J:121:THR:OG1	2.36	0.40
2:K:85:SER:HB3	3:S:32:PHE:CE1	2.55	0.40
2:K:255:ASP:OD2	2:K:495:ARG:HG2	2.20	0.40
2:K:266:LEU:CD1	2:L:155:SER:HB3	2.49	0.40
2:K:272:ILE:HG22	2:K:468:GLN:HE21	1.86	0.40
2:K:290:LEU:HA	2:K:290:LEU:HD23	1.83	0.40
2:L:184:GLU:OE2	2:L:321:MET:HB2	2.20	0.40
2:A:188:VAL:HG11	2:F:430:LYS:HE2	2.03	0.40
2:C:291:SER:CB	2:C:471:MET:HE1	2.47	0.40
2:D:96:MET:HB2	2:E:124:VAL:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:232:ILE:HG22	2:D:236:GLN:HE22	1.86	0.40
2:D:386:LEU:HB3	2:D:404:PHE:CE2	2.56	0.40
2:E:72:HIS:HD2	2:F:260:GLU:OE2	2.04	0.40
2:E:79:ILE:HB	2:F:258:VAL:HG11	2.03	0.40
2:F:344:ARG:O	2:F:348:GLU:HB2	2.22	0.40
2:F:507:LEU:O	2:F:509:LYS:HG3	2.21	0.40
2:G:107:ILE:HG21	2:G:307:VAL:CG2	2.51	0.40
2:J:285:ASP:C	2:J:287:ASP:H	2.29	0.40
2:K:148:TYR:HB3	2:K:186:GLY:HA2	2.03	0.40
2:K:151:ASP:HB3	2:K:187:THR:HG21	2.03	0.40
2:K:304:ARG:HA	2:K:304:ARG:HD2	1.89	0.40
2:L:147:MET:HE3	2:L:147:MET:HB3	1.92	0.40
1:a:235:PHE:HB2	1:a:417:GLY:O	2.21	0.40
1:a:254:VAL:O	1:a:258:VAL:HG23	2.20	0.40
2:A:345:TRP:CD2	2:B:348:GLU:HG3	2.56	0.40
2:B:326:GLY:HA3	2:B:338:ILE:HD13	2.02	0.40
2:E:521:ILE:HA	2:F:341:ARG:NH2	2.35	0.40
2:H:79:ILE:CG2	2:I:121:THR:HB	2.51	0.40
2:H:145:HIS:ND1	2:H:148:TYR:CD2	2.89	0.40
2:I:92:GLY:HA2	2:I:93:PRO:HD3	1.90	0.40
2:I:446:ALA:HB3	2:I:449:TYR:CE1	2.56	0.40
2:L:456:LEU:N	2:L:475:THR:HG22	2.29	0.40
1:a:237:ASP:HB3	1:a:419:LYS:HD2	2.02	0.40
2:A:71:ASP:OD1	2:C:231:SER:HB2	2.20	0.40
2:A:266:LEU:HD23	2:B:250:MET:HG3	2.02	0.40
2:B:260:GLU:HG3	2:B:261:ALA:N	2.36	0.40
2:B:382:VAL:HG12	2:B:521:ILE:HD11	2.03	0.40
2:C:198:ILE:O	2:C:198:ILE:HG22	2.22	0.40
2:C:332:PHE:HE2	2:C:334:PHE:CE1	2.40	0.40
2:C:483:PRO:O	2:C:484:PHE:HB2	2.22	0.40
2:E:463:ASP:HB3	2:E:466:ASN:OD1	2.20	0.40
2:F:265:GLN:C	2:F:266:LEU:HD12	2.47	0.40
2:F:485:ALA:HB1	2:F:510:ASN:OD1	2.22	0.40
2:G:148:TYR:HD1	2:G:186:GLY:H	1.69	0.40
2:G:228:MET:SD	2:G:236:GLN:NE2	2.95	0.40
2:G:466:ASN:O	2:G:468:GLN:HG3	2.22	0.40
2:H:185:THR:HG21	2:H:321:MET:HE1	2.04	0.40
2:H:336:ASP:O	2:H:340:ILE:HG12	2.22	0.40
2:I:159:ALA:HB3	2:I:228:MET:HE2	2.03	0.40
2:I:345:TRP:HE1	2:J:344:ARG:HH21	1.69	0.40
2:I:351:LYS:NZ	2:I:390:ASP:O	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:357:ILE:HD11	2:I:376:ILE:HG21	2.04	0.40
2:K:126:ALA:O	2:K:254:ILE:HA	2.22	0.40
2:L:126:ALA:HB1	2:L:484:PHE:CE1	2.57	0.40
1:a:41:ALA:HB1	1:a:336:ILE:CG2	2.49	0.40
1:a:320:LEU:O	1:a:321:ASP:HB2	2.22	0.40
2:A:244:ASP:O	2:A:246:PRO:HD3	2.22	0.40
2:C:142:GLU:N	2:C:490:GLN:OE1	2.37	0.40
2:C:386:LEU:HB3	2:C:404:PHE:HE2	1.85	0.40
2:E:279:ARG:NH1	2:E:283:GLY:O	2.55	0.40
2:G:154:PHE:CZ	2:G:248:ASN:HB3	2.57	0.40
2:G:179:THR:HG22	2:G:189:TYR:CE1	2.56	0.40
2:H:113:GLY:H	2:H:446:ALA:HB1	1.86	0.40
2:H:376:ILE:HG22	2:H:436:VAL:HG22	2.04	0.40
2:H:477:TYR:CG	2:H:478:GLY:N	2.90	0.40
2:I:131:TYR:HB3	2:I:250:MET:HG2	2.03	0.40
2:J:72:HIS:C	2:J:74:TYR:H	2.29	0.40
2:K:494:SER:C	2:K:496:ILE:H	2.30	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	413/417 (99%)	374 (91%)	34 (8%)	5 (1%)	10	37
2	A	454/456 (100%)	411 (90%)	41 (9%)	2 (0%)	30	60
2	B	454/456 (100%)	407 (90%)	44 (10%)	3 (1%)	18	49
2	C	454/456 (100%)	408 (90%)	43 (10%)	3 (1%)	18	49
2	D	454/456 (100%)	410 (90%)	41 (9%)	3 (1%)	18	49
2	E	454/456 (100%)	406 (89%)	44 (10%)	4 (1%)	14	43
2	F	454/456 (100%)	413 (91%)	39 (9%)	2 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	454/456 (100%)	413 (91%)	38 (8%)	3 (1%)	18	49
2	H	454/456 (100%)	407 (90%)	44 (10%)	3 (1%)	18	49
2	I	454/456 (100%)	408 (90%)	44 (10%)	2 (0%)	30	60
2	J	454/456 (100%)	413 (91%)	37 (8%)	4 (1%)	14	43
2	K	454/456 (100%)	410 (90%)	41 (9%)	3 (1%)	18	49
2	L	454/456 (100%)	409 (90%)	43 (10%)	2 (0%)	30	60
3	O	77/80 (96%)	69 (90%)	8 (10%)	0	100	100
3	P	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	Q	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	R	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	S	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	T	77/80 (96%)	71 (92%)	6 (8%)	0	100	100
3	U	77/80 (96%)	72 (94%)	5 (6%)	0	100	100
3	V	77/80 (96%)	69 (90%)	8 (10%)	0	100	100
3	W	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	X	77/80 (96%)	69 (90%)	8 (10%)	0	100	100
3	Y	77/80 (96%)	71 (92%)	6 (8%)	0	100	100
4	Z	23/376 (6%)	23 (100%)	0	0	100	100
All	All	6731/7145 (94%)	6083 (90%)	609 (9%)	39 (1%)	23	52

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	395	TYR
2	H	395	TYR
2	I	395	TYR
2	J	395	TYR
2	L	395	TYR
1	a	25	VAL
2	A	395	TYR
2	B	395	TYR
2	E	395	TYR
2	F	395	TYR
2	G	395	TYR
2	H	108	ALA
2	K	395	TYR

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Mol	Chain	Res	Type
2	B	108	ALA
2	C	108	ALA
2	D	147	MET
2	D	395	TYR
2	E	108	ALA
2	G	108	ALA
2	J	108	ALA
2	J	147	MET
2	E	147	MET
2	K	147	MET
1	a	243	ALA
1	a	364	VAL
1	a	340	ILE
2	A	254	ILE
2	C	254	ILE
2	D	254	ILE
2	J	254	ILE
2	E	254	ILE
2	F	254	ILE
2	G	254	ILE
2	H	254	ILE
2	I	254	ILE
2	K	254	ILE
2	B	254	ILE
2	L	254	ILE
1	a	357	VAL

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	350/352 (99%)	350 (100%)	0	100	100
2	A	346/346 (100%)	346 (100%)	0	100	100
2	B	346/346 (100%)	346 (100%)	0	100	100
2	C	346/346 (100%)	346 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	346/346 (100%)	346 (100%)	0	100	100
2	E	346/346 (100%)	346 (100%)	0	100	100
2	F	346/346 (100%)	346 (100%)	0	100	100
2	G	346/346 (100%)	346 (100%)	0	100	100
2	H	346/346 (100%)	346 (100%)	0	100	100
2	I	346/346 (100%)	346 (100%)	0	100	100
2	J	346/346 (100%)	346 (100%)	0	100	100
2	K	346/346 (100%)	346 (100%)	0	100	100
2	L	346/346 (100%)	346 (100%)	0	100	100
3	O	66/67 (98%)	66 (100%)	0	100	100
3	P	66/67 (98%)	66 (100%)	0	100	100
3	Q	66/67 (98%)	66 (100%)	0	100	100
3	R	66/67 (98%)	66 (100%)	0	100	100
3	S	66/67 (98%)	66 (100%)	0	100	100
3	T	66/67 (98%)	65 (98%)	1 (2%)	57	72
3	U	66/67 (98%)	66 (100%)	0	100	100
3	V	66/67 (98%)	65 (98%)	1 (2%)	57	72
3	W	66/67 (98%)	66 (100%)	0	100	100
3	X	66/67 (98%)	66 (100%)	0	100	100
3	Y	66/67 (98%)	66 (100%)	0	100	100
4	Z	21/319 (7%)	19 (90%)	2 (10%)	8	29
All	All	5249/5560 (94%)	5245 (100%)	4 (0%)	87	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	T	41	ILE
3	V	41	ILE
4	Z	305	ILE
4	Z	321	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	59	ASN
1	a	290	HIS
1	a	317	ASN
1	a	356	HIS
1	a	384	ASN
2	A	72	HIS
2	A	195	GLN
2	A	282	HIS
2	A	367	GLN
2	A	431	GLN
2	A	468	GLN
2	A	510	ASN
2	B	145	HIS
2	B	180	HIS
2	B	282	HIS
2	B	303	ASN
2	B	356	GLN
2	B	468	GLN
2	B	482	ASN
2	C	72	HIS
2	C	123	GLN
2	C	145	HIS
2	C	171	GLN
2	C	282	HIS
2	C	356	GLN
2	C	384	ASN
2	C	431	GLN
2	D	171	GLN
2	D	240	ASN
2	D	282	HIS
2	D	303	ASN
2	D	356	GLN
2	D	384	ASN
2	D	427	GLN
2	D	431	GLN
2	D	468	GLN
2	D	510	ASN
2	E	83	GLN
2	E	145	HIS
2	E	171	GLN
2	E	236	GLN
2	E	240	ASN
2	E	282	HIS

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Mol	Chain	Res	Type
2	E	303	ASN
2	E	356	GLN
2	E	367	GLN
2	E	398	GLN
2	E	468	GLN
2	F	145	HIS
2	F	171	GLN
2	F	236	GLN
2	F	282	HIS
2	F	356	GLN
2	F	510	ASN
2	G	145	HIS
2	G	171	GLN
2	G	240	ASN
2	G	282	HIS
2	G	303	ASN
2	G	356	GLN
2	G	431	GLN
2	G	468	GLN
2	G	510	ASN
2	H	72	HIS
2	H	171	GLN
2	H	282	HIS
2	H	303	ASN
2	H	311	ASN
2	H	356	GLN
2	H	384	ASN
2	H	398	GLN
2	H	427	GLN
2	H	510	ASN
2	I	171	GLN
2	I	282	HIS
2	I	303	ASN
2	I	356	GLN
2	I	384	ASN
2	I	431	GLN
2	I	510	ASN
2	J	115	GLN
2	J	195	GLN
2	J	236	GLN
2	J	282	HIS
2	J	303	ASN

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Mol	Chain	Res	Type
2	J	356	GLN
2	J	384	ASN
2	J	431	GLN
2	J	468	GLN
2	J	510	ASN
2	K	83	GLN
2	K	171	GLN
2	K	180	HIS
2	K	236	GLN
2	K	282	HIS
2	K	356	GLN
2	K	367	GLN
2	K	384	ASN
2	K	468	GLN
2	K	510	ASN
2	L	72	HIS
2	L	115	GLN
2	L	171	GLN
2	L	282	HIS
2	L	303	ASN
2	L	311	ASN
2	L	356	GLN
2	L	384	ASN
2	L	510	ASN
3	P	15	GLN
3	P	45	HIS
3	Q	15	GLN
3	Q	45	HIS
3	S	15	GLN
3	S	45	HIS
3	T	45	HIS
3	W	45	HIS
3	X	15	GLN
3	X	45	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8661. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.