



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:05 PM UTC

PDB ID : 5FLZ / pdb_00005flz
EMDB ID : EMD-2799
Title : Cryo-EM structure of gamma-TuSC oligomers in a closed conformation
Authors : Greenberg, C.H.; Kollman, J.; Zelter, A.; Johnson, R.; MacCoss, M.J.; Davis, T.N.; Agard, D.A.; Sali, A.
Deposited on : 2015-10-29
Resolution : 6.90 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:

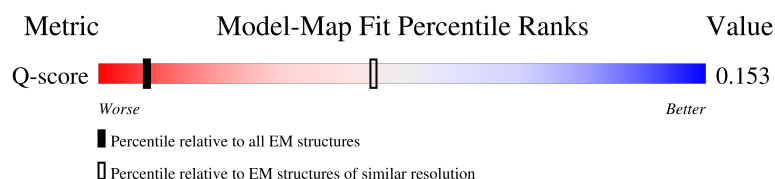
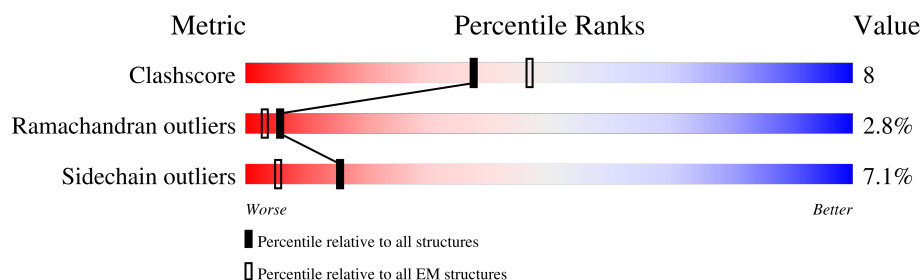
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 6.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	479 (6.40 - 7.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	823	
1	10-A	823	
1	2-A	823	
1	3-A	823	

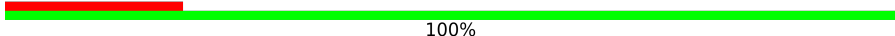
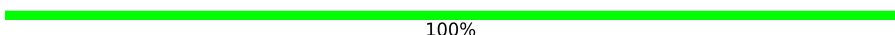
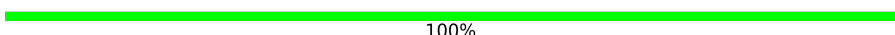
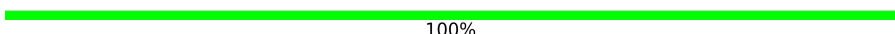
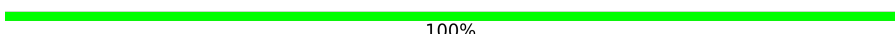
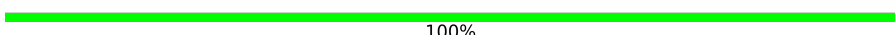
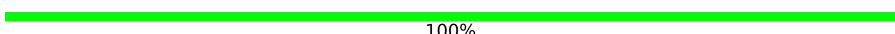
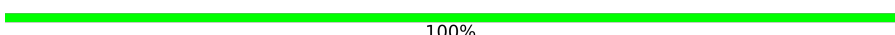
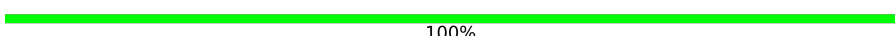
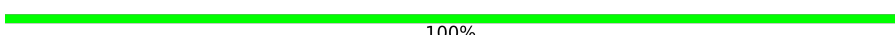
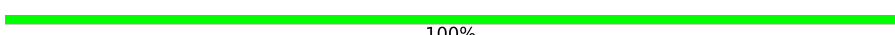
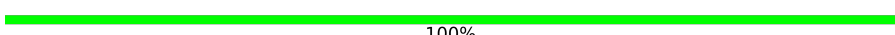
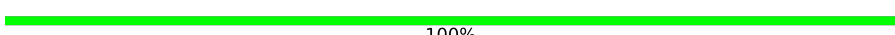
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Mol	Chain	Length	Quality of chain
1	4-A	823	
1	5-A	823	
1	6-A	823	
1	7-A	823	
1	8-A	823	
1	9-A	823	
2	1-B	846	
2	10-B	846	
2	2-B	846	
2	3-B	846	
2	4-B	846	
2	5-B	846	
2	6-B	846	
2	7-B	846	
2	8-B	846	
2	9-B	846	
3	1-C	473	
3	1-D	473	
3	10-C	473	
3	10-D	473	
3	2-C	473	
3	2-D	473	
3	3-C	473	
3	3-D	473	
3	4-C	473	

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Mol	Chain	Length	Quality of chain
3	4-D	473	 76%17% • 6%
3	5-C	473	 74%19% • 6%
3	5-D	473	 77%15% • 6%
3	6-C	473	 77%16% • 6%
3	6-D	473	 73%19% • 6%
3	7-C	473	 74%19% • 6%
3	7-D	473	 73%18% • 6%
3	8-C	473	 75%17% • 6%
3	8-D	473	 77%16% • 6%
3	9-C	473	 79%14% • 6%
3	9-D	473	 76%17% • 6%
4	1-E	44	 20%100%
4	1-F	44	 20%100%
4	10-E	44	 100%
4	10-F	44	 100%
4	2-E	44	 100%
4	2-F	44	 100%
4	3-E	44	 100%
4	3-F	44	 100%
4	4-E	44	 100%
4	4-F	44	 100%
4	5-E	44	 100%
4	5-F	44	 100%
4	6-E	44	 100%
4	6-F	44	 100%

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Mol	Chain	Length	Quality of chain
4	7-E	44	 100%
4	7-F	44	 100%
4	8-E	44	 100%
4	8-F	44	 95% 5%
4	9-E	44	 100%
4	9-F	44	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 169420 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 SPINDLE POLE BODY COMPONENT SPC97.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	2-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	3-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	4-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	5-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	6-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	7-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	8-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	9-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	10-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		

- Molecule 2 is a protein called SPINDLE POLE BODY COMPONENT SPC98.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	2-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	3-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	4-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	5-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	6-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	7-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	8-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	9-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	10-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		

- Molecule 3 is a protein called TUBULIN GAMMA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1-C	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	2-C	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	3-C	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	4-C	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	5-C	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	6-C	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	7-C	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	8-C	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	9-C	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	10-C	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	1-D	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	2-D	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	3-D	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	4-D	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	5-D	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	6-D	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	7-D	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	8-D	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	9-D	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		
3	10-D	445	Total	C	N	O	S	0	0
			3485	2180	591	695	19		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	58	CYS	SER	engineered mutation	UNP P53378
C	288	CYS	GLY	engineered mutation	UNP P53378
D	58	CYS	SER	engineered mutation	UNP P53378
D	288	CYS	GLY	engineered mutation	UNP P53378

- Molecule 4 is a protein called SPINDLE POLE BODY COMPONENT 110.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	1-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	2-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	3-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	4-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	5-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	6-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	7-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	8-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	9-E	44	Total	C	N	O	0	0
			220	132	44	44		

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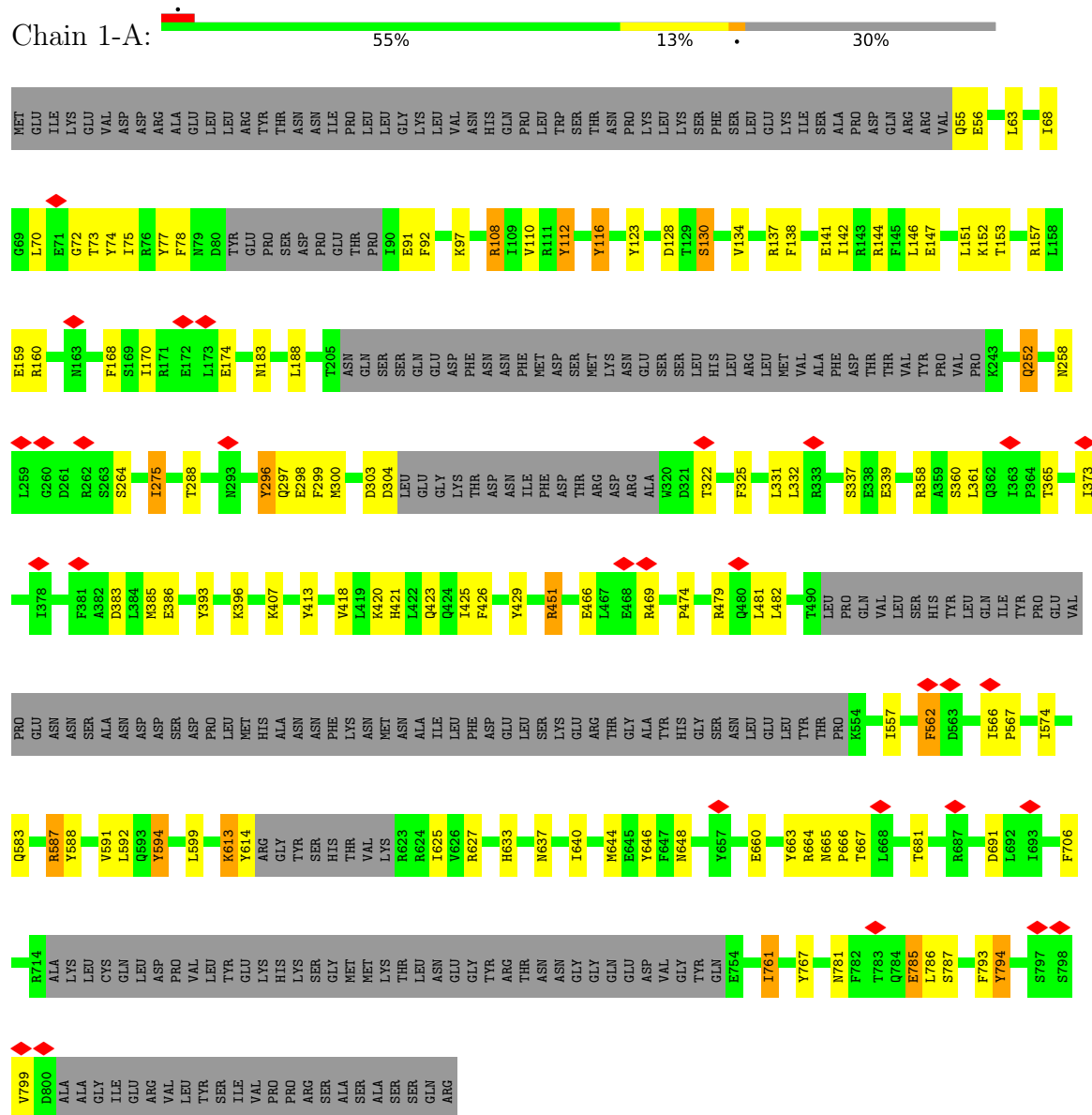
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Mol	Chain	Residues	Atoms				AltConf	Trace
4	10-E	44	Total 220	C 132	N 44	O 44	0	0
4	1-F	44	Total 220	C 132	N 44	O 44	0	0
4	2-F	44	Total 220	C 132	N 44	O 44	0	0
4	3-F	44	Total 220	C 132	N 44	O 44	0	0
4	4-F	44	Total 220	C 132	N 44	O 44	0	0
4	5-F	44	Total 220	C 132	N 44	O 44	0	0
4	6-F	44	Total 220	C 132	N 44	O 44	0	0
4	7-F	44	Total 220	C 132	N 44	O 44	0	0
4	8-F	44	Total 220	C 132	N 44	O 44	0	0
4	9-F	44	Total 220	C 132	N 44	O 44	0	0
4	10-F	44	Total 220	C 132	N 44	O 44	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: SPINDLE POLE BODY COMPONENT SPC97



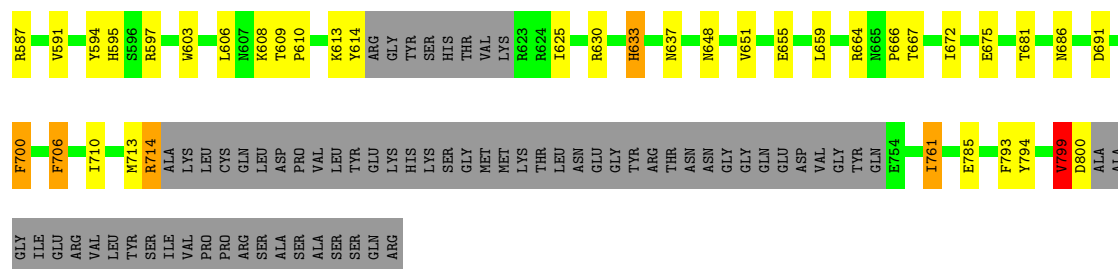
• Molecule 1: SPINDLE POLE BODY COMPONENT SPC97

Service	Percentage
Used	55%
Not used	13%
Don't know	30%



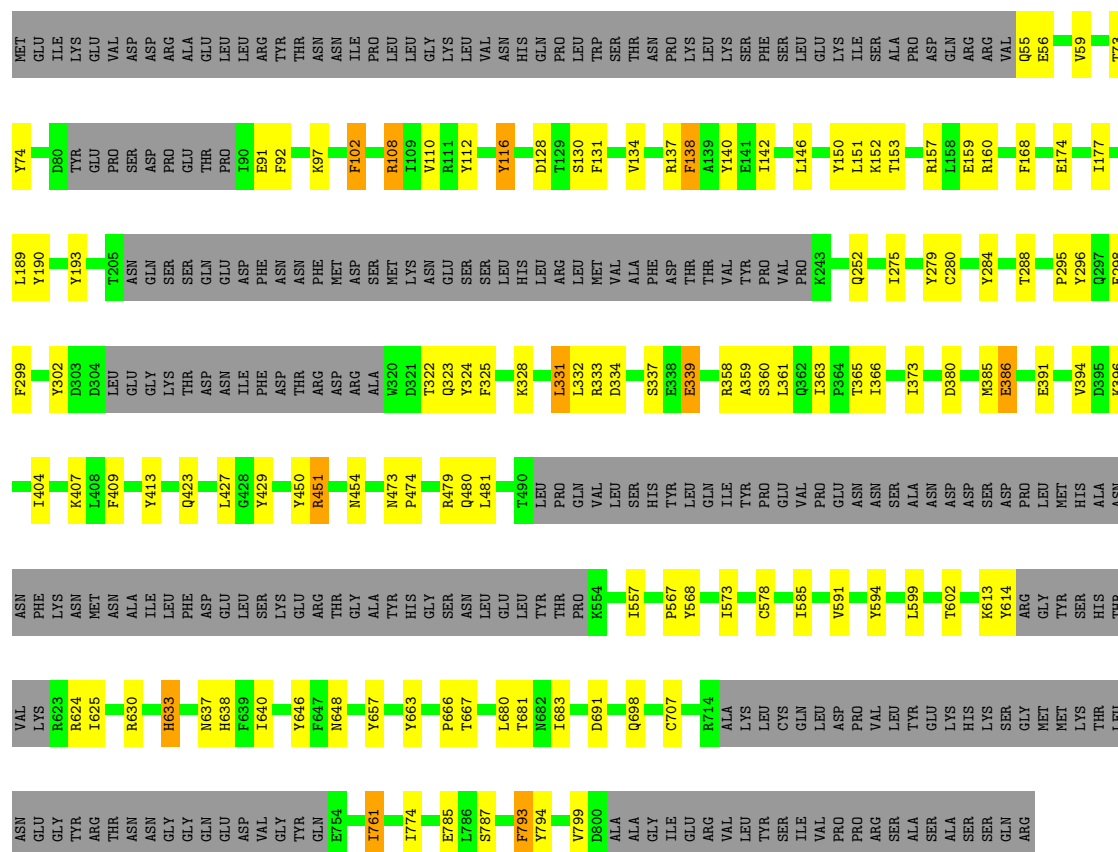
Frequency	Percentage
Daily	53%
Weekly	15%
Monthly	30%
Other	2%





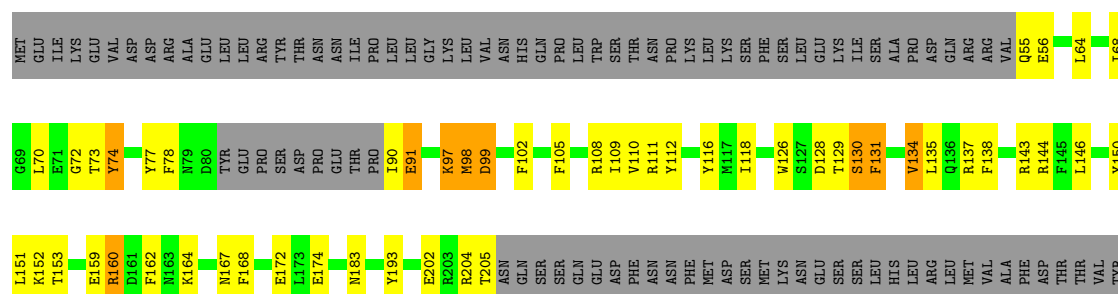
• Molecule 1: SPINDLE POLE BODY COMPONENT SPC97

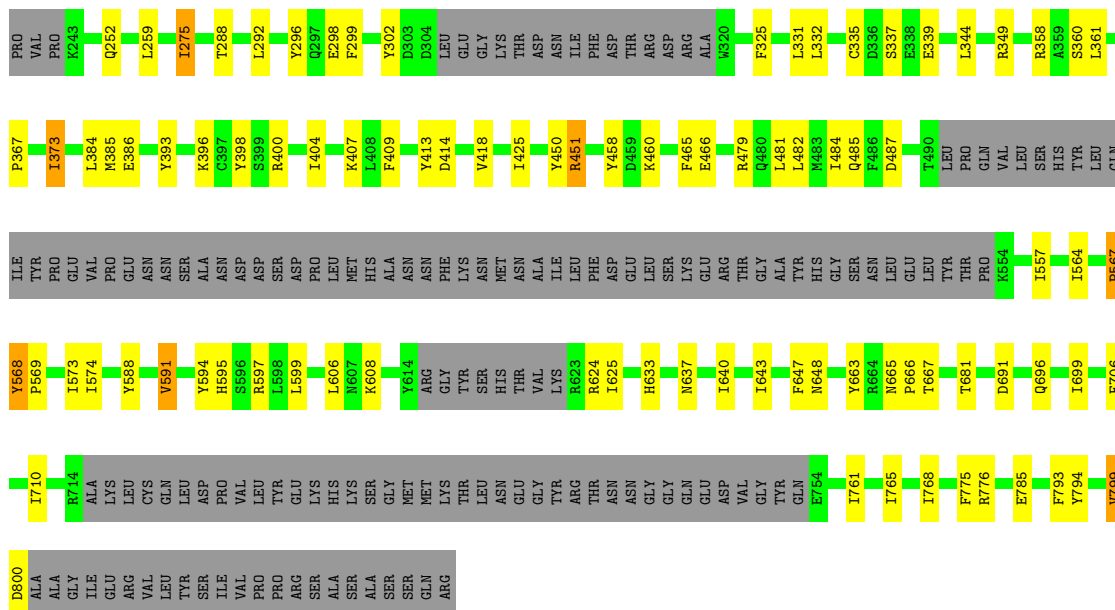
Chain 4-A: 55% 14% 30%



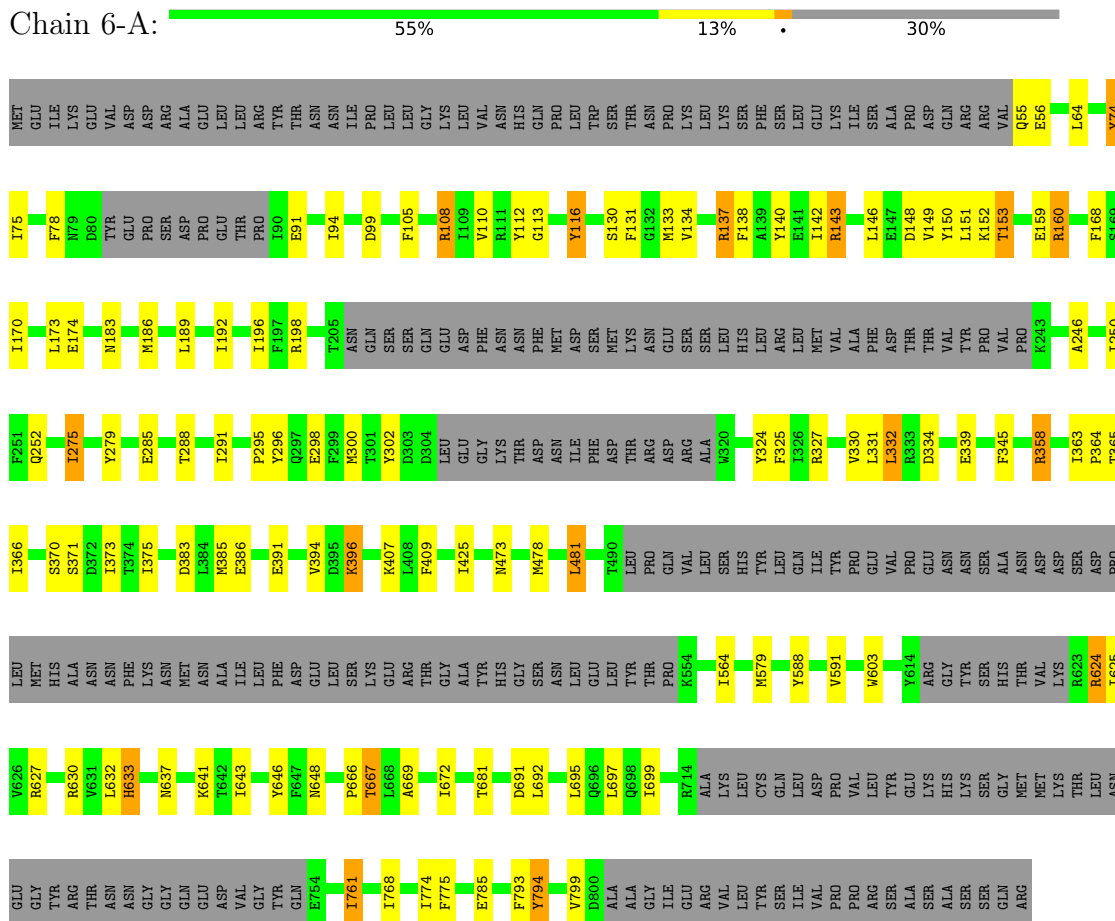
• Molecule 1: SPINDLE POLE BODY COMPONENT SPC97

Chain 5-A: 52% 16% 30%



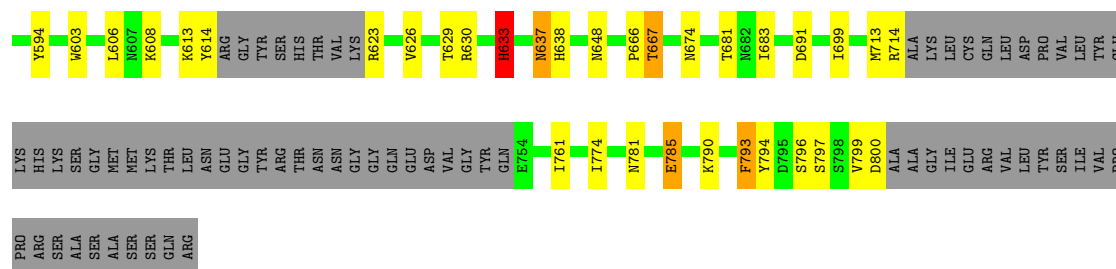


- Molecule 1: SPINDLE POLE BODY COMPONENT SPC97



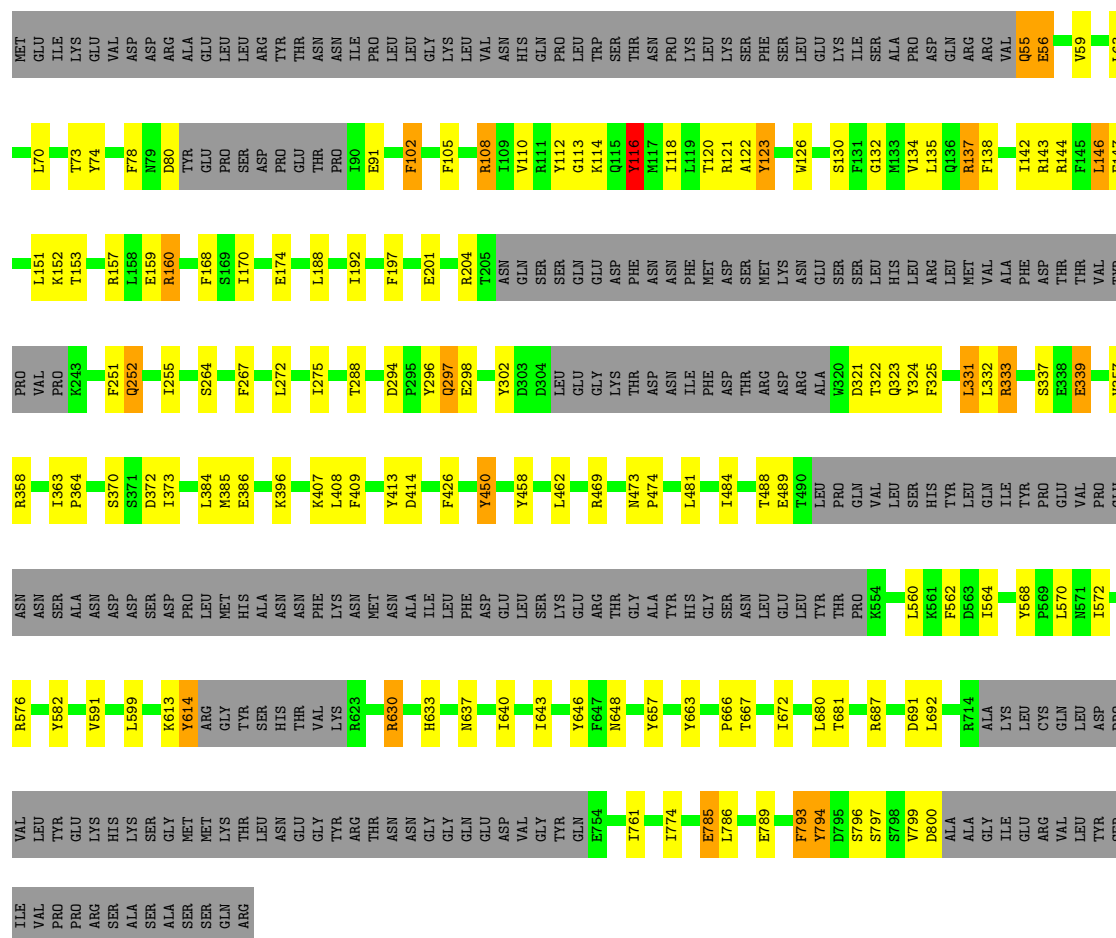
- Molecule 1: SPINDLE POLE BODY COMPONENT SPC97





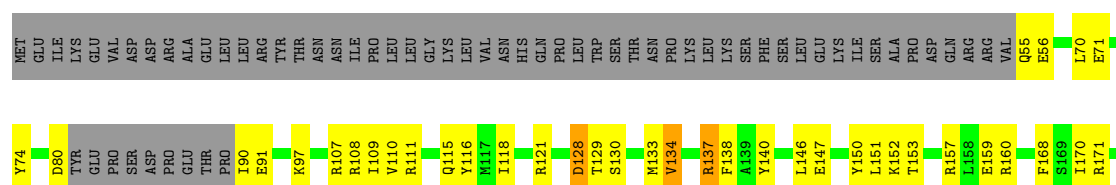
• Molecule 1: SPINDLE POLE BODY COMPONENT SPC97

Chain 9-A: 53% 14% 30%

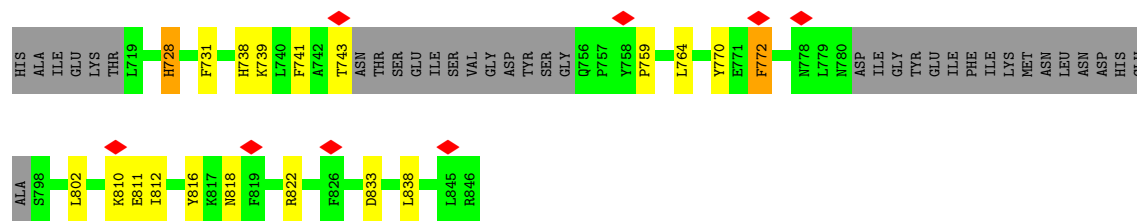


• Molecule 1: SPINDLE POLE BODY COMPONENT SPC97

Chain 10-A: 53% 15% 30%

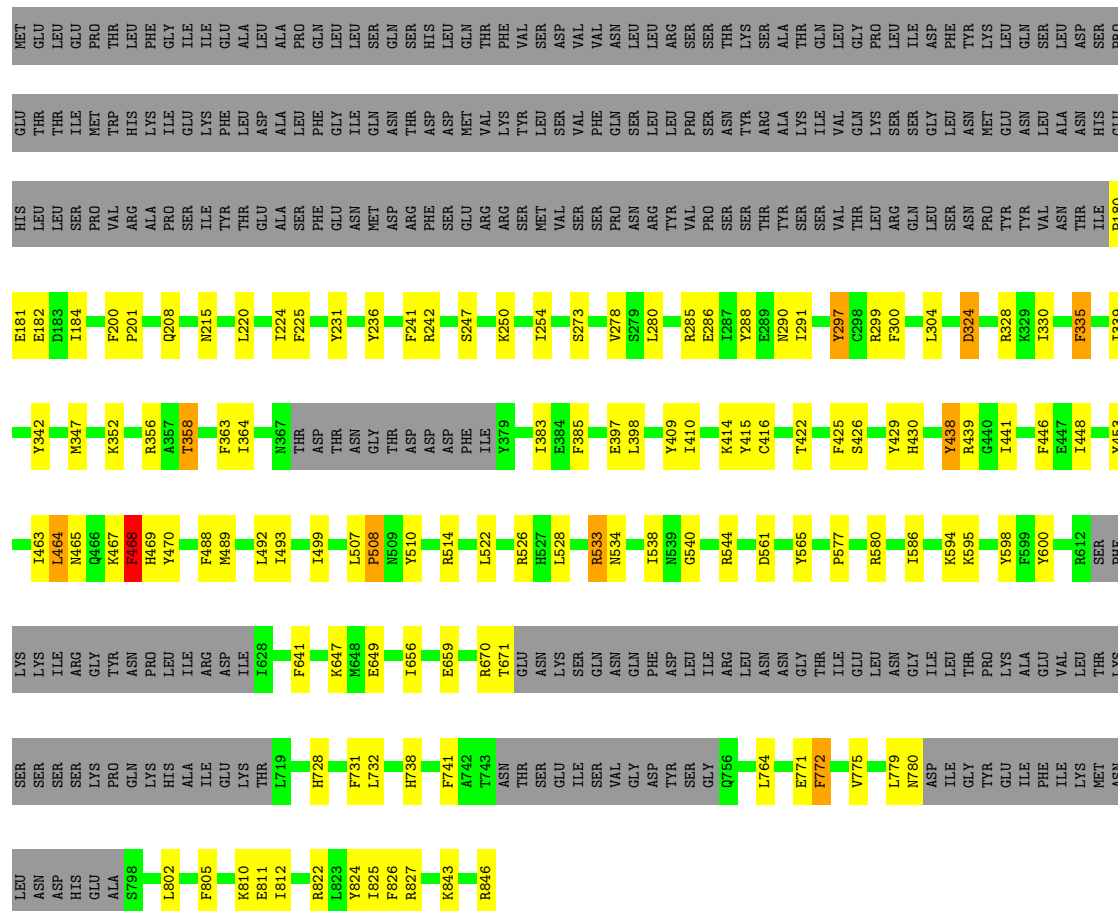






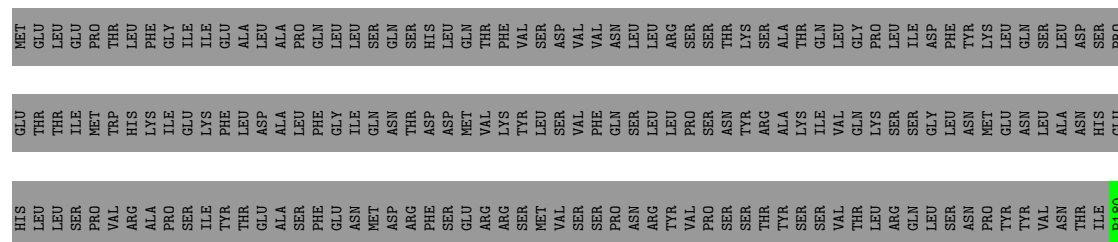
• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

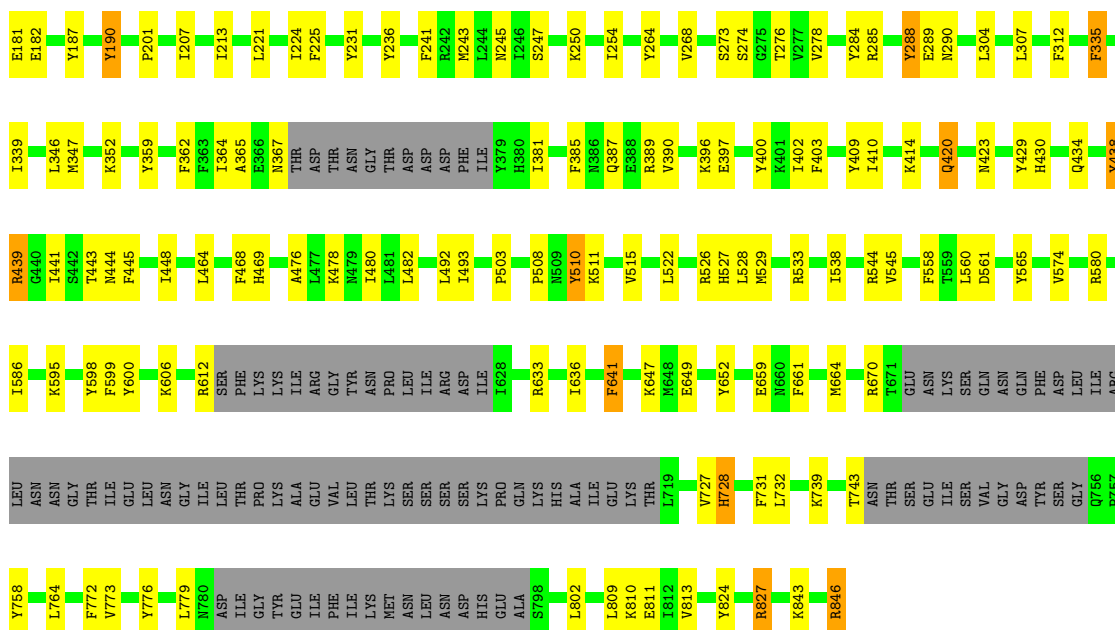
Chain 2-B: 52% 14% 33%



• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

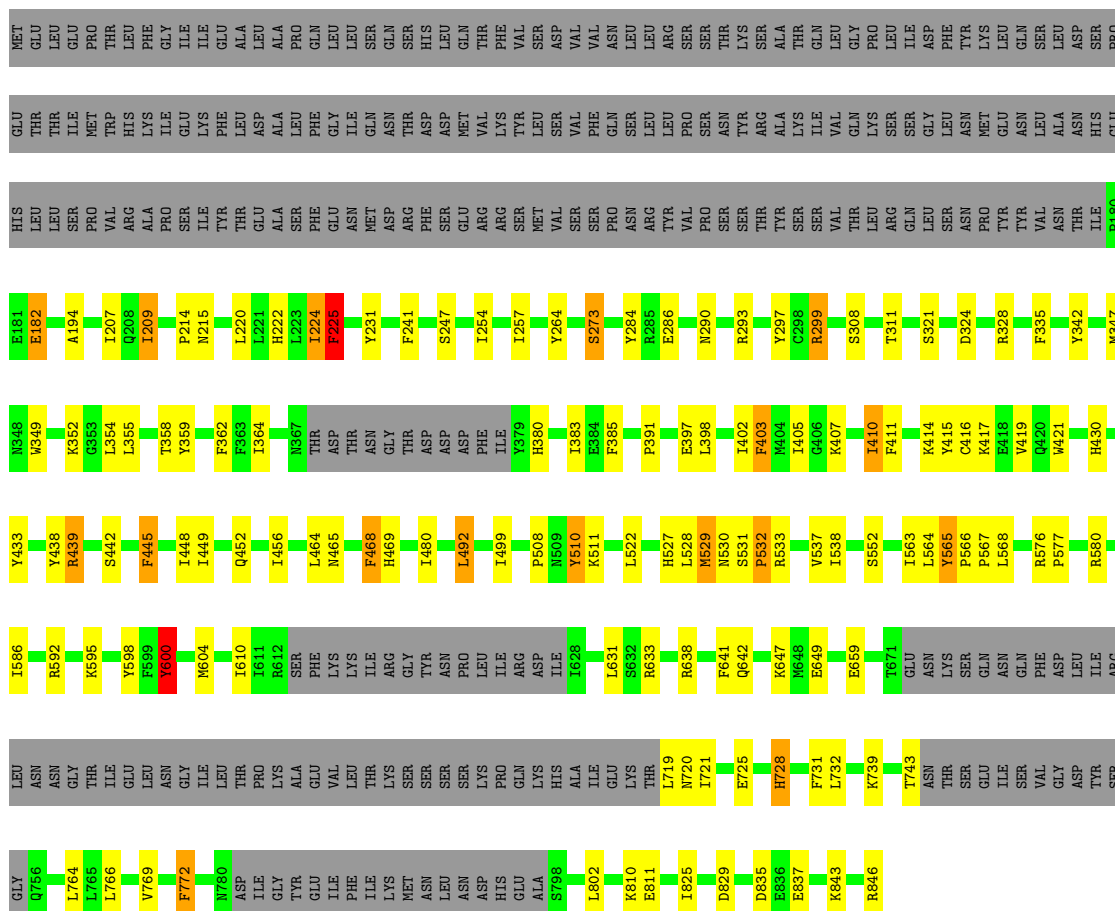
Chain 3-B: 51% 15% 33%





- Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

Chain 4-B:



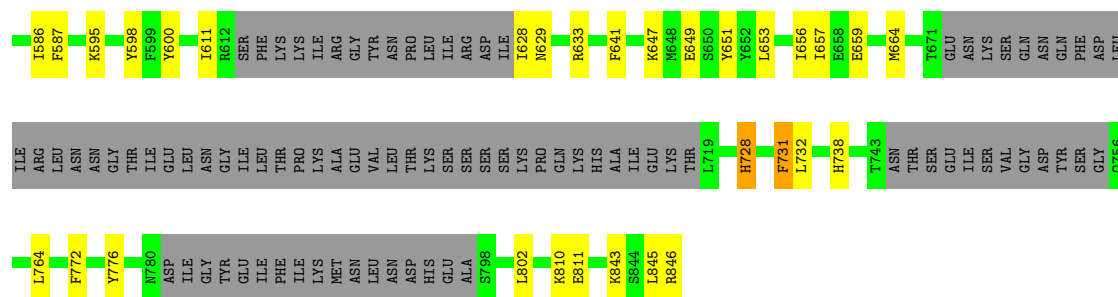
- Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

Frequency	Percentage
Daily	52%
Weekly	13%
Monthly	33%
Other	1%



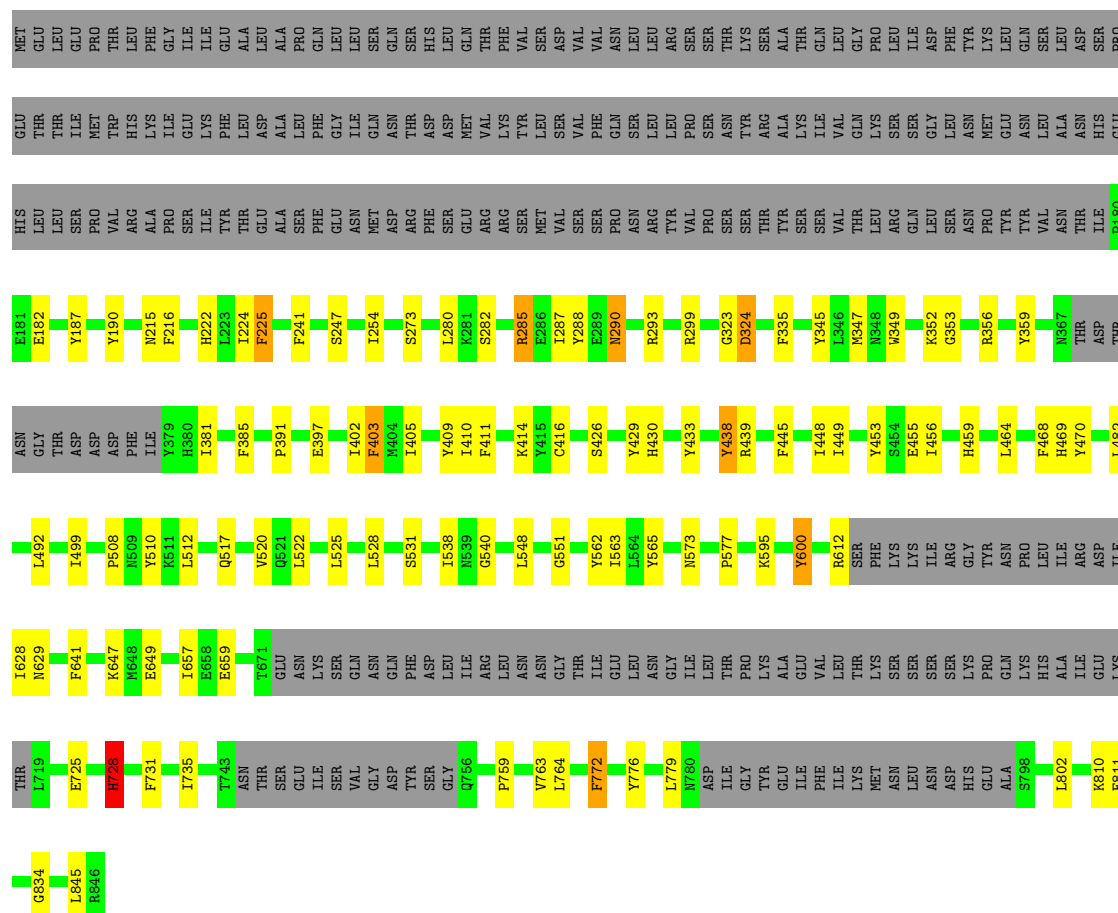
Service	Percentage
Used	52%
Not used	14%
Don't know	33%





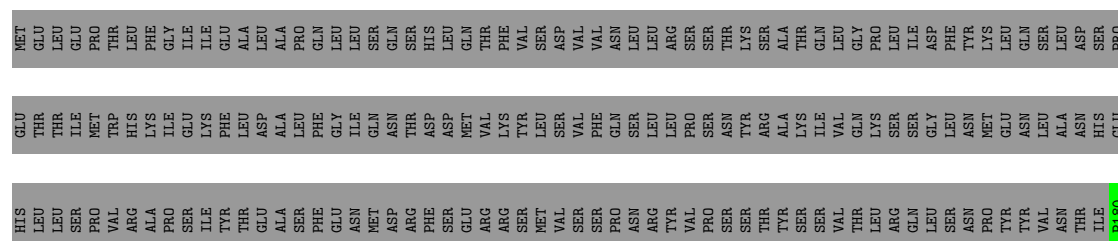
• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

Chain 7-B: 54% 11% 33%

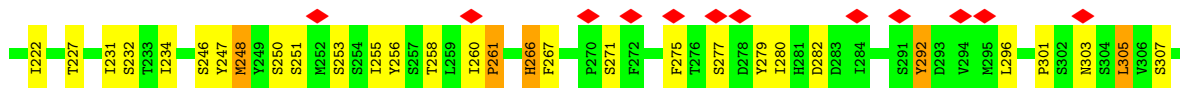


• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

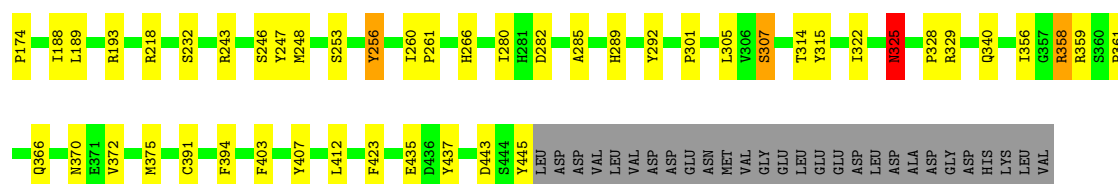
Chain 8-B: 52% 14% 33%





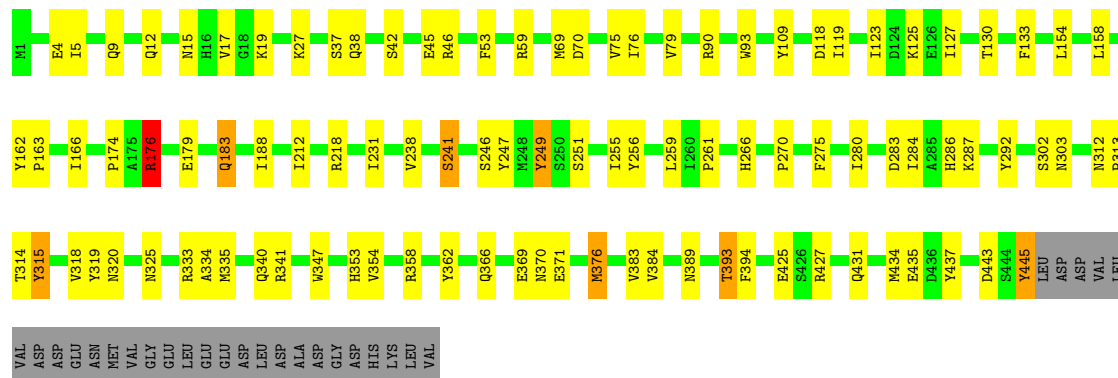






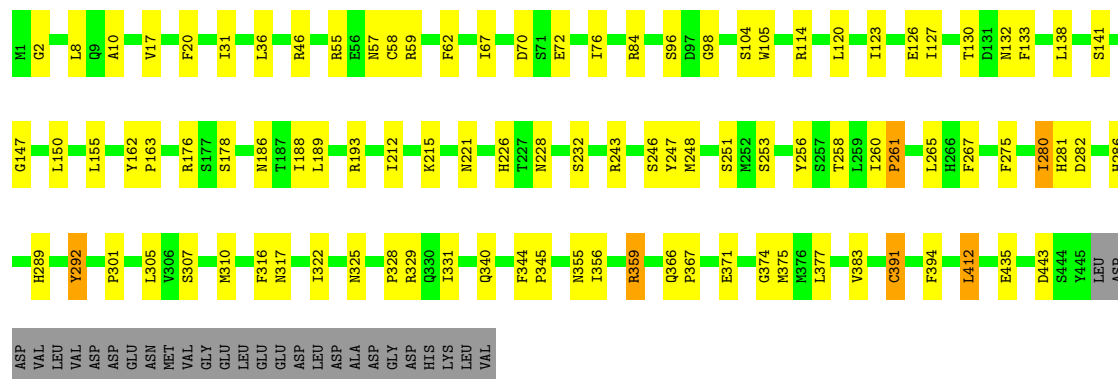
• Molecule 3: TUBULIN GAMMA CHAIN

Chain 6-D: 73% 19% 6%



• Molecule 3: TUBULIN GAMMA CHAIN

Chain 7-C: 74% 19% 6%



• Molecule 3: TUBULIN GAMMA CHAIN

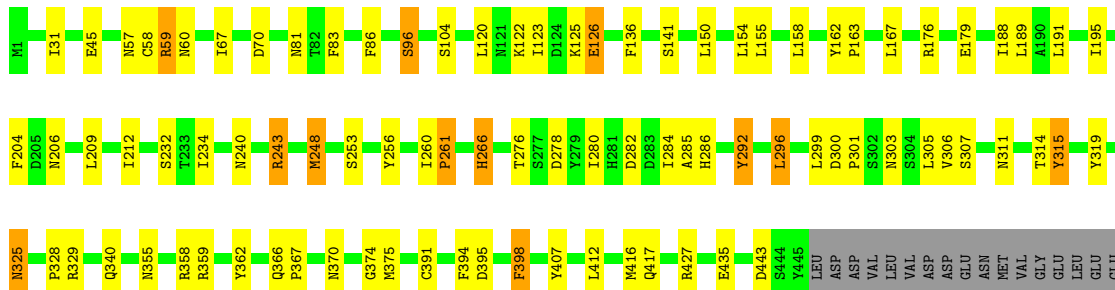
Chain 7-D: 73% 18% 6%



ASN
MET
VAL
GLY
GLU
LEU
GLU
GLU
ASP
LEU
ASP
ALA
ASP
GLY
ASP
HIS
LYS
LEU
VAL

• Molecule 3: TUBULIN GAMMA CHAIN

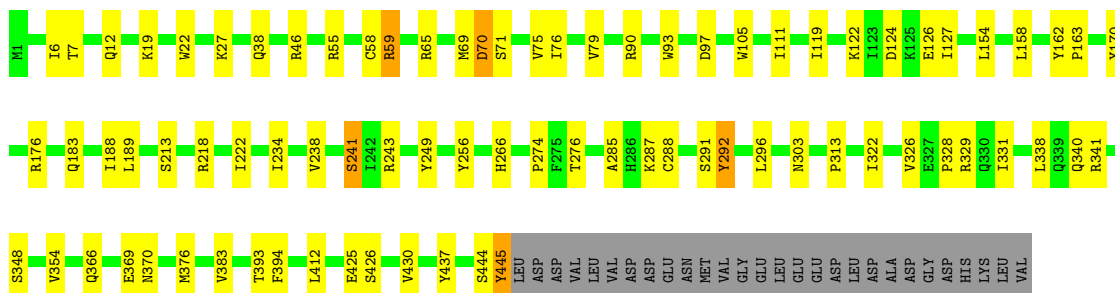
Chain 8-C: 75% 17% 6%



ASP
LEU
ASP
ALA
GLY
ASP
ASP
HIS
LYS
LEU
VAL

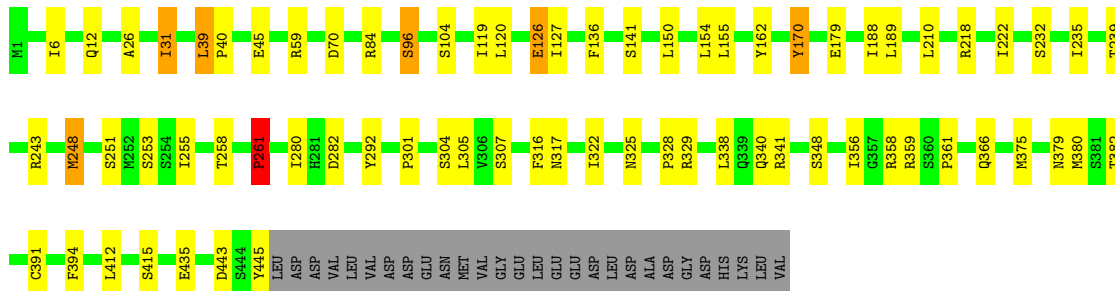
• Molecule 3: TUBULIN GAMMA CHAIN

Chain 8-D: 77% 16% 6%



• Molecule 3: TUBULIN GAMMA CHAIN

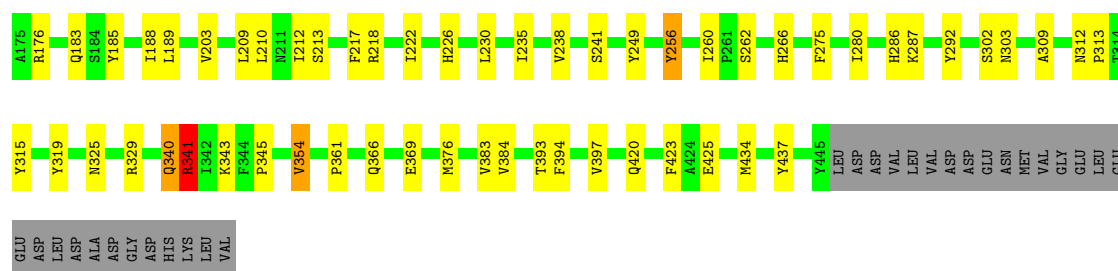
Chain 9-C: 79% 14% 6%



• Molecule 3: TUBULIN GAMMA CHAIN

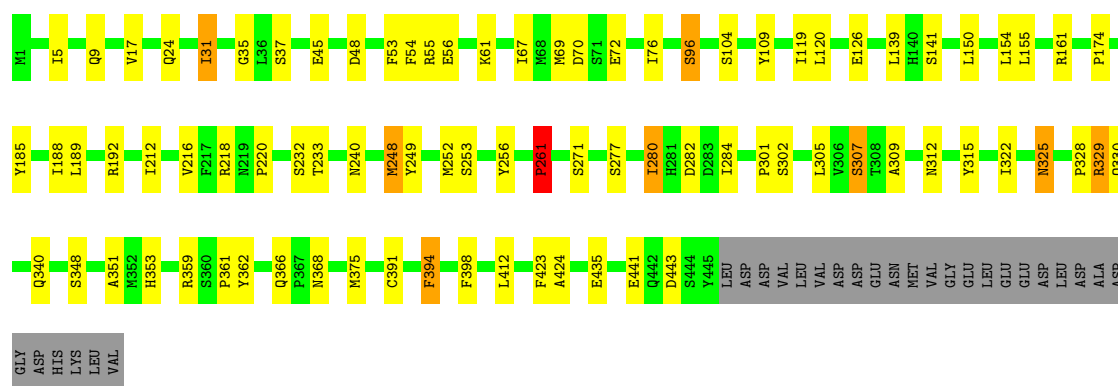
Chain 9-D: 76% 17% 6%





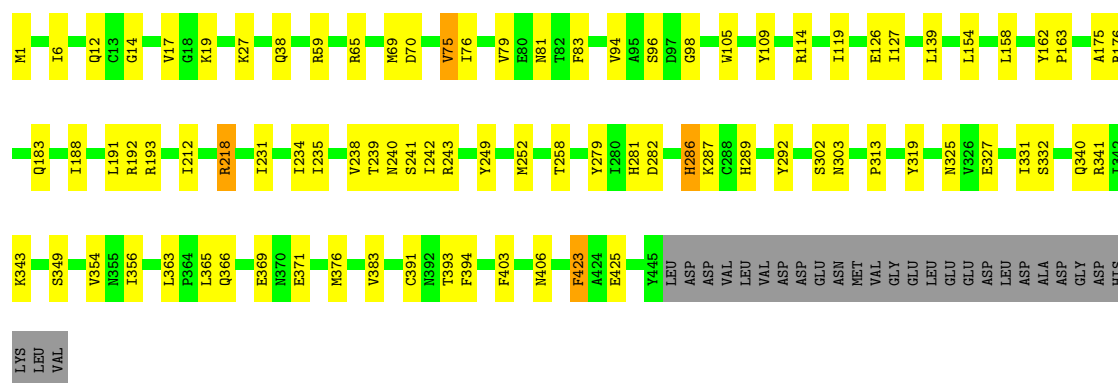
• Molecule 3: TUBULIN GAMMA CHAIN

Chain 10-C:

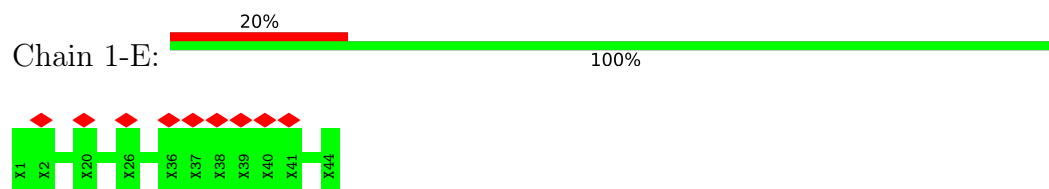


• Molecule 3: TUBULIN GAMMA CHAIN

Chain 10-D:

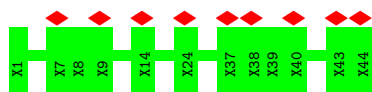


• Molecule 4: SPINDLE POLE BODY COMPONENT 110



• Molecule 4: SPINDLE POLE BODY COMPONENT 110





- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 2-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 2-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 3-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 3-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 4-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 4-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 5-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 5-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 6-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 6-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 7-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 7-F:  100%

There are no outlier residues recorded for this chain.

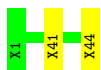
- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 8-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 8-F:  95% 5%



- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 9-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 9-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 10-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 10-F:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	Not provided	
CTF correction method	EACH MICROGRAPH	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	94000	Depositor
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	Depositor
Maximum map value	3.045	Depositor
Minimum map value	-1.944	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.314	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	398.56, 398.56, 398.56	wwPDB
Map dimensions	212, 212, 212	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.88, 1.88, 1.88	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	1-A	0.41	0/4917	0.47	0/6616
1	2-A	0.41	0/4917	0.47	0/6616
1	3-A	0.41	0/4917	0.47	0/6616
1	4-A	0.41	0/4917	0.47	0/6616
1	5-A	0.41	0/4917	0.47	0/6616
1	6-A	0.41	0/4917	0.47	0/6616
1	7-A	0.41	0/4917	0.47	0/6616
1	8-A	0.41	0/4917	0.47	0/6616
1	9-A	0.41	0/4917	0.47	0/6616
1	10-A	0.41	0/4917	0.47	0/6616
2	1-B	0.40	0/4803	0.48	0/6481
2	2-B	0.40	0/4803	0.48	0/6481
2	3-B	0.40	0/4803	0.48	0/6481
2	4-B	0.40	0/4803	0.48	0/6481
2	5-B	0.40	0/4803	0.48	0/6481
2	6-B	0.40	0/4803	0.48	0/6481
2	7-B	0.40	0/4803	0.48	0/6481
2	8-B	0.40	0/4803	0.48	0/6481
2	9-B	0.40	0/4803	0.48	0/6481
2	10-B	0.40	0/4803	0.48	0/6481
3	1-C	0.39	0/3560	0.46	0/4834
3	1-D	0.42	0/3560	0.45	0/4834
3	2-C	0.39	0/3560	0.46	0/4834
3	2-D	0.42	0/3560	0.45	0/4834
3	3-C	0.39	0/3560	0.46	0/4834
3	3-D	0.42	0/3560	0.45	0/4834
3	4-C	0.39	0/3560	0.46	0/4834
3	4-D	0.42	0/3560	0.45	0/4834
3	5-C	0.39	0/3560	0.46	0/4834
3	5-D	0.42	0/3560	0.45	0/4834
3	6-C	0.39	0/3560	0.46	0/4834
3	6-D	0.42	0/3560	0.45	0/4834
3	7-C	0.39	0/3560	0.46	0/4834
3	7-D	0.42	0/3560	0.45	0/4834

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	8-C	0.39	0/3560	0.46	0/4834
3	8-D	0.42	0/3560	0.45	0/4834
3	9-C	0.39	0/3560	0.46	0/4834
3	9-D	0.42	0/3560	0.45	0/4834
3	10-C	0.39	0/3560	0.46	0/4834
3	10-D	0.42	0/3560	0.45	0/4834
All	All	0.41	0/168400	0.47	0/227650

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	25
1	2-A	0	20
1	3-A	0	22
1	4-A	0	25
1	5-A	0	27
1	6-A	0	18
1	7-A	0	26
1	8-A	0	19
1	9-A	0	29
1	10-A	0	19
2	1-B	0	27
2	2-B	0	21
2	3-B	0	28
2	4-B	0	23
2	5-B	0	22
2	6-B	0	23
2	7-B	0	20
2	8-B	0	19
2	9-B	0	28
2	10-B	0	25
3	1-C	0	16
3	1-D	0	13
3	2-C	0	11
3	2-D	0	12
3	3-C	0	9
3	3-D	0	7
3	4-C	0	15
3	4-D	0	14

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	5-C	0	14
3	5-D	0	17
3	6-C	0	16
3	6-D	0	12
3	7-C	0	13
3	7-D	0	13
3	8-C	0	12
3	8-D	0	13
3	9-C	0	6
3	9-D	0	15
3	10-C	0	13
3	10-D	0	10
All	All	0	717

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (717) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	112	TYR	Sidechain
1	1-A	116	TYR	Sidechain
1	1-A	123	TYR	Sidechain
1	1-A	157	ARG	Sidechain
1	1-A	183	ASN	Mainchain
1	1-A	299	PHE	Sidechain
1	1-A	393	TYR	Sidechain
1	1-A	413	TYR	Sidechain
1	1-A	426	PHE	Sidechain
1	1-A	429	TYR	Sidechain
1	1-A	451	ARG	Sidechain
1	1-A	469	ARG	Sidechain
1	1-A	562	PHE	Sidechain
1	1-A	587	ARG	Sidechain
1	1-A	588	TYR	Sidechain
1	1-A	594	TYR	Sidechain
1	1-A	627	ARG	Sidechain
1	1-A	646	TYR	Sidechain
1	1-A	664	ARG	Sidechain
1	1-A	665	ASN	Mainchain
1	1-A	706	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	1-A	767	TYR	Sidechain
1	1-A	77	TYR	Sidechain
1	1-A	78	PHE	Sidechain
1	1-A	794	TYR	Sidechain
2	1-B	200	PHE	Sidechain
2	1-B	204	HIS	Sidechain
2	1-B	225	PHE	Sidechain
2	1-B	231	TYR	Sidechain
2	1-B	285	ARG	Sidechain
2	1-B	297	TYR	Sidechain
2	1-B	299	ARG	Sidechain
2	1-B	328	ARG	Sidechain
2	1-B	345	TYR	Sidechain
2	1-B	393	PHE	Sidechain
2	1-B	430	HIS	Sidechain
2	1-B	433	TYR	Sidechain
2	1-B	438	TYR	Sidechain
2	1-B	446	PHE	Sidechain
2	1-B	459	HIS	Sidechain
2	1-B	565	TYR	Sidechain
2	1-B	583	TYR	Sidechain
2	1-B	585	ARG	Sidechain
2	1-B	587	PHE	Sidechain
2	1-B	598	TYR	Sidechain
2	1-B	599	PHE	Sidechain
2	1-B	612	ARG	Sidechain
2	1-B	651	TYR	Sidechain
2	1-B	652	TYR	Sidechain
2	1-B	741	PHE	Sidechain
2	1-B	770	TYR	Sidechain
2	1-B	816	TYR	Sidechain
3	1-C	109	TYR	Sidechain
3	1-C	185	TYR	Sidechain
3	1-C	20	PHE	Sidechain
3	1-C	204	PHE	Sidechain
3	1-C	218	ARG	Sidechain
3	1-C	247	TYR	Sidechain
3	1-C	279	TYR	Sidechain
3	1-C	292	TYR	Sidechain
3	1-C	315	TYR	Sidechain
3	1-C	319	TYR	Sidechain
3	1-C	362	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	1-C	374	GLY	Mainchain
3	1-C	387	PHE	Sidechain
3	1-C	53	PHE	Sidechain
3	1-C	84	ARG	Sidechain
3	1-C	90	ARG	Sidechain
3	1-D	170	TYR	Sidechain
3	1-D	182	VAL	Mainchain
3	1-D	185	TYR	Sidechain
3	1-D	204	PHE	Sidechain
3	1-D	205	ASP	Mainchain
3	1-D	249	TYR	Sidechain
3	1-D	315	TYR	Sidechain
3	1-D	341	ARG	Sidechain
3	1-D	353	HIS	Sidechain
3	1-D	359	ARG	Sidechain
3	1-D	362	TYR	Sidechain
3	1-D	55	ARG	Sidechain
3	1-D	90	ARG	Sidechain
1	10-A	107	ARG	Sidechain
1	10-A	111	ARG	Sidechain
1	10-A	121	ARG	Sidechain
1	10-A	157	ARG	Sidechain
1	10-A	171	ARG	Sidechain
1	10-A	279	TYR	Sidechain
1	10-A	296	TYR	Sidechain
1	10-A	302	TYR	Sidechain
1	10-A	334	ASP	Mainchain
1	10-A	349	ARG	Sidechain
1	10-A	393	TYR	Sidechain
1	10-A	429	TYR	Sidechain
1	10-A	465	PHE	Sidechain
1	10-A	469	ARG	Sidechain
1	10-A	594	TYR	Sidechain
1	10-A	614	TYR	Sidechain
1	10-A	646	TYR	Sidechain
1	10-A	663	TYR	Sidechain
1	10-A	706	PHE	Sidechain
2	10-B	222	HIS	Sidechain
2	10-B	231	TYR	Sidechain
2	10-B	285	ARG	Sidechain
2	10-B	288	TYR	Sidechain
2	10-B	293	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	10-B	343	TYR	Sidechain
2	10-B	363	PHE	Sidechain
2	10-B	389	ARG	Sidechain
2	10-B	411	PHE	Sidechain
2	10-B	429	TYR	Sidechain
2	10-B	459	HIS	Sidechain
2	10-B	470	TYR	Sidechain
2	10-B	510	TYR	Sidechain
2	10-B	558	PHE	Mainchain
2	10-B	562	TYR	Sidechain
2	10-B	580	ARG	Sidechain
2	10-B	599	PHE	Sidechain
2	10-B	600	TYR	Sidechain
2	10-B	651	TYR	Sidechain
2	10-B	661	PHE	Sidechain
2	10-B	666	ARG	Sidechain
2	10-B	728	HIS	Sidechain
2	10-B	770	TYR	Sidechain
2	10-B	776	TYR	Sidechain
2	10-B	819	PHE	Sidechain
3	10-C	109	TYR	Sidechain
3	10-C	161	ARG	Sidechain
3	10-C	185	TYR	Sidechain
3	10-C	192	ARG	Sidechain
3	10-C	218	ARG	Sidechain
3	10-C	249	TYR	Sidechain
3	10-C	256	TYR	Sidechain
3	10-C	329	ARG	Sidechain
3	10-C	362	TYR	Sidechain
3	10-C	394	PHE	Sidechain
3	10-C	398	PHE	Sidechain
3	10-C	423	PHE	Sidechain
3	10-C	55	ARG	Sidechain
3	10-D	114	ARG	Sidechain
3	10-D	192	ARG	Sidechain
3	10-D	193	ARG	Sidechain
3	10-D	218	ARG	Sidechain
3	10-D	279	TYR	Sidechain
3	10-D	292	TYR	Sidechain
3	10-D	319	TYR	Sidechain
3	10-D	423	PHE	Sidechain
3	10-D	59	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	10-D	65	ARG	Sidechain
1	2-A	111	ARG	Sidechain
1	2-A	116	TYR	Sidechain
1	2-A	150	TYR	Sidechain
1	2-A	324	TYR	Sidechain
1	2-A	325	PHE	Sidechain
1	2-A	349	ARG	Sidechain
1	2-A	450	TYR	Sidechain
1	2-A	479	ARG	Sidechain
1	2-A	576	ARG	Sidechain
1	2-A	587	ARG	Sidechain
1	2-A	594	TYR	Sidechain
1	2-A	614	TYR	Sidechain
1	2-A	623	ARG	Sidechain
1	2-A	624	ARG	Sidechain
1	2-A	646	TYR	Sidechain
1	2-A	664	ARG	Sidechain
1	2-A	700	PHE	Sidechain
1	2-A	706	PHE	Sidechain
1	2-A	714	ARG	Sidechain
1	2-A	794	TYR	Sidechain
2	2-B	231	TYR	Sidechain
2	2-B	236	TYR	Sidechain
2	2-B	242	ARG	Sidechain
2	2-B	297	TYR	Sidechain
2	2-B	342	TYR	Sidechain
2	2-B	363	PHE	Sidechain
2	2-B	409	TYR	Sidechain
2	2-B	415	TYR	Sidechain
2	2-B	438	TYR	Sidechain
2	2-B	453	TYR	Sidechain
2	2-B	468	PHE	Sidechain
2	2-B	488	PHE	Sidechain
2	2-B	514	ARG	Sidechain
2	2-B	526	ARG	Sidechain
2	2-B	533	ARG	Sidechain
2	2-B	540	GLY	Mainchain
2	2-B	580	ARG	Sidechain
2	2-B	741	PHE	Sidechain
2	2-B	824	TYR	Sidechain
2	2-B	826	PHE	Sidechain
2	2-B	827	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	2-C	173	PHE	Sidechain
3	2-C	218	ARG	Sidechain
3	2-C	247	TYR	Sidechain
3	2-C	249	TYR	Sidechain
3	2-C	256	TYR	Sidechain
3	2-C	279	TYR	Sidechain
3	2-C	292	TYR	Sidechain
3	2-C	319	TYR	Sidechain
3	2-C	341	ARG	Sidechain
3	2-C	427	ARG	Sidechain
3	2-C	46	ARG	Sidechain
3	2-D	162	TYR	Sidechain
3	2-D	218	ARG	Sidechain
3	2-D	249	TYR	Sidechain
3	2-D	289	HIS	Sidechain
3	2-D	292	TYR	Sidechain
3	2-D	315	TYR	Sidechain
3	2-D	344	PHE	Sidechain
3	2-D	394	PHE	Sidechain
3	2-D	407	TYR	Sidechain
3	2-D	437	TYR	Sidechain
3	2-D	445	TYR	Sidechain
3	2-D	53	PHE	Sidechain
1	3-A	138	PHE	Sidechain
1	3-A	143	ARG	Sidechain
1	3-A	162	PHE	Sidechain
1	3-A	193	TYR	Sidechain
1	3-A	198	ARG	Sidechain
1	3-A	203	ARG	Sidechain
1	3-A	267	PHE	Sidechain
1	3-A	296	TYR	Sidechain
1	3-A	299	PHE	Sidechain
1	3-A	324	TYR	Sidechain
1	3-A	349	ARG	Sidechain
1	3-A	358	ARG	Sidechain
1	3-A	393	TYR	Sidechain
1	3-A	400	ARG	Sidechain
1	3-A	576	ARG	Sidechain
1	3-A	587	ARG	Sidechain
1	3-A	594	TYR	Sidechain
1	3-A	597	ARG	Sidechain
1	3-A	664	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	3-A	700	PHE	Sidechain
1	3-A	706	PHE	Sidechain
1	3-A	714	ARG	Sidechain
2	3-B	190	TYR	Sidechain
2	3-B	231	TYR	Sidechain
2	3-B	236	TYR	Sidechain
2	3-B	284	TYR	Sidechain
2	3-B	288	TYR	Sidechain
2	3-B	312	PHE	Sidechain
2	3-B	359	TYR	Sidechain
2	3-B	400	TYR	Sidechain
2	3-B	403	PHE	Sidechain
2	3-B	409	TYR	Sidechain
2	3-B	429	TYR	Sidechain
2	3-B	439	ARG	Sidechain
2	3-B	510	TYR	Sidechain
2	3-B	526	ARG	Sidechain
2	3-B	533	ARG	Sidechain
2	3-B	558	PHE	Sidechain
2	3-B	565	TYR	Sidechain
2	3-B	580	ARG	Sidechain
2	3-B	599	PHE	Sidechain
2	3-B	641	PHE	Sidechain
2	3-B	652	TYR	Sidechain
2	3-B	661	PHE	Sidechain
2	3-B	670	ARG	Sidechain
2	3-B	728	HIS	Sidechain
2	3-B	758	TYR	Sidechain
2	3-B	824	TYR	Sidechain
2	3-B	827	ARG	Sidechain
2	3-B	846	ARG	Sidechain
3	3-C	109	TYR	Sidechain
3	3-C	204	PHE	Sidechain
3	3-C	244	PHE	Sidechain
3	3-C	333	ARG	Sidechain
3	3-C	359	ARG	Sidechain
3	3-C	407	TYR	Sidechain
3	3-C	423	PHE	Sidechain
3	3-C	46	ARG	Sidechain
3	3-C	59	ARG	Sidechain
3	3-D	267	PHE	Sidechain
3	3-D	292	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	3-D	329	ARG	Sidechain
3	3-D	362	TYR	Sidechain
3	3-D	413	PHE	Sidechain
3	3-D	55	ARG	Sidechain
3	3-D	93	TRP	Mainchain
1	4-A	102	PHE	Sidechain
1	4-A	112	TYR	Sidechain
1	4-A	116	TYR	Sidechain
1	4-A	131	PHE	Sidechain
1	4-A	138	PHE	Sidechain
1	4-A	140	TYR	Sidechain
1	4-A	150	TYR	Sidechain
1	4-A	157	ARG	Sidechain
1	4-A	190	TYR	Sidechain
1	4-A	193	TYR	Sidechain
1	4-A	279	TYR	Sidechain
1	4-A	284	TYR	Sidechain
1	4-A	302	TYR	Sidechain
1	4-A	333	ARG	Sidechain
1	4-A	413	TYR	Sidechain
1	4-A	429	TYR	Sidechain
1	4-A	450	TYR	Sidechain
1	4-A	451	ARG	Sidechain
1	4-A	473	ASN	Peptide,Mainchain
1	4-A	568	TYR	Sidechain
1	4-A	646	TYR	Sidechain
1	4-A	657	TYR	Sidechain
1	4-A	663	TYR	Sidechain
1	4-A	92	PHE	Mainchain
2	4-B	225	PHE	Sidechain
2	4-B	231	TYR	Sidechain
2	4-B	264	TYR	Sidechain
2	4-B	284	TYR	Sidechain
2	4-B	293	ARG	Sidechain
2	4-B	299	ARG	Sidechain
2	4-B	328	ARG	Sidechain
2	4-B	342	TYR	Sidechain
2	4-B	359	TYR	Sidechain
2	4-B	403	PHE	Sidechain
2	4-B	411	PHE	Sidechain
2	4-B	415	TYR	Sidechain
2	4-B	433	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	4-B	439	ARG	Sidechain
2	4-B	445	PHE	Sidechain
2	4-B	468	PHE	Sidechain
2	4-B	510	TYR	Sidechain
2	4-B	565	TYR	Sidechain
2	4-B	580	ARG	Sidechain
2	4-B	592	ARG	Sidechain
2	4-B	598	TYR	Sidechain
2	4-B	600	TYR	Sidechain
2	4-B	772	PHE	Sidechain
3	4-C	109	TYR	Sidechain
3	4-C	136	PHE	Sidechain
3	4-C	170	TYR	Sidechain
3	4-C	185	TYR	Sidechain
3	4-C	192	ARG	Sidechain
3	4-C	218	ARG	Sidechain
3	4-C	243	ARG	Sidechain
3	4-C	249	TYR	Sidechain
3	4-C	279	TYR	Sidechain
3	4-C	319	TYR	Sidechain
3	4-C	358	ARG	Sidechain
3	4-C	407	TYR	Sidechain
3	4-C	423	PHE	Sidechain
3	4-C	427	ARG	Sidechain
3	4-C	46	ARG	Sidechain
3	4-D	176	ARG	Sidechain
3	4-D	192	ARG	Sidechain
3	4-D	193	ARG	Sidechain
3	4-D	218	ARG	Sidechain
3	4-D	267	PHE	Sidechain
3	4-D	341	ARG	Sidechain
3	4-D	344	PHE	Sidechain
3	4-D	362	TYR	Sidechain
3	4-D	413	PHE	Sidechain
3	4-D	423	PHE	Sidechain
3	4-D	445	TYR	Sidechain
3	4-D	54	PHE	Sidechain
3	4-D	65	ARG	Sidechain
3	4-D	90	ARG	Sidechain
1	5-A	105	PHE	Sidechain
1	5-A	111	ARG	Sidechain
1	5-A	112	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	5-A	131	PHE	Sidechain
1	5-A	144	ARG	Sidechain
1	5-A	150	TYR	Sidechain
1	5-A	162	PHE	Sidechain
1	5-A	183	ASN	Mainchain
1	5-A	204	ARG	Sidechain
1	5-A	302	TYR	Sidechain
1	5-A	349	ARG	Sidechain
1	5-A	393	TYR	Sidechain
1	5-A	398	TYR	Sidechain
1	5-A	413	TYR	Sidechain
1	5-A	450	TYR	Sidechain
1	5-A	451	ARG	Sidechain
1	5-A	465	PHE	Sidechain
1	5-A	568	TYR	Sidechain
1	5-A	588	TYR	Sidechain
1	5-A	597	ARG	Sidechain
1	5-A	624	ARG	Sidechain
1	5-A	647	PHE	Sidechain
1	5-A	663	TYR	Sidechain
1	5-A	665	ASN	Mainchain
1	5-A	74	TYR	Sidechain
1	5-A	77	TYR	Sidechain
1	5-A	776	ARG	Sidechain
2	5-B	288	TYR	Sidechain
2	5-B	328	ARG	Sidechain
2	5-B	359	TYR	Sidechain
2	5-B	379	TYR	Sidechain
2	5-B	385	PHE	Sidechain
2	5-B	389	ARG	Mainchain
2	5-B	409	TYR	Sidechain
2	5-B	415	TYR	Sidechain
2	5-B	510	TYR	Sidechain
2	5-B	562	TYR	Sidechain
2	5-B	565	TYR	Sidechain
2	5-B	576	ARG	Sidechain
2	5-B	580	ARG	Sidechain
2	5-B	583	TYR	Sidechain
2	5-B	598	TYR	Sidechain
2	5-B	600	TYR	Sidechain
2	5-B	612	ARG	Sidechain
2	5-B	651	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	5-B	742	ALA	Peptide
2	5-B	770	TYR	Sidechain
2	5-B	816	TYR	Sidechain
2	5-B	827	ARG	Sidechain
3	5-C	114	ARG	Sidechain
3	5-C	170	TYR	Sidechain
3	5-C	193	ARG	Sidechain
3	5-C	244	PHE	Sidechain
3	5-C	249	TYR	Sidechain
3	5-C	279	TYR	Sidechain
3	5-C	292	TYR	Sidechain
3	5-C	319	TYR	Sidechain
3	5-C	387	PHE	Sidechain
3	5-C	407	TYR	Sidechain
3	5-C	427	ARG	Sidechain
3	5-C	445	TYR	Sidechain
3	5-C	83	PHE	Sidechain
3	5-C	86	PHE	Sidechain
3	5-D	176	ARG	Sidechain
3	5-D	182	VAL	Mainchain
3	5-D	185	TYR	Sidechain
3	5-D	192	ARG	Sidechain
3	5-D	193	ARG	Sidechain
3	5-D	217	PHE	Sidechain
3	5-D	218	ARG	Sidechain
3	5-D	256	TYR	Sidechain
3	5-D	292	TYR	Sidechain
3	5-D	315	TYR	Sidechain
3	5-D	319	TYR	Sidechain
3	5-D	333	ARG	Sidechain
3	5-D	362	TYR	Sidechain
3	5-D	387	PHE	Sidechain
3	5-D	394	PHE	Sidechain
3	5-D	423	PHE	Sidechain
3	5-D	84	ARG	Sidechain
1	6-A	108	ARG	Sidechain
1	6-A	112	TYR	Sidechain
1	6-A	131	PHE	Sidechain
1	6-A	140	TYR	Sidechain
1	6-A	143	ARG	Sidechain
1	6-A	150	TYR	Sidechain
1	6-A	160	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	6-A	198	ARG	Sidechain
1	6-A	279	TYR	Sidechain
1	6-A	302	TYR	Sidechain
1	6-A	324	TYR	Sidechain
1	6-A	345	PHE	Sidechain
1	6-A	409	PHE	Sidechain
1	6-A	588	TYR	Sidechain
1	6-A	624	ARG	Sidechain
1	6-A	630	ARG	Sidechain
1	6-A	646	TYR	Sidechain
1	6-A	78	PHE	Sidechain
2	6-B	261	LEU	Mainchain
2	6-B	288	TYR	Sidechain
2	6-B	297	TYR	Sidechain
2	6-B	319	PHE	Sidechain
2	6-B	328	ARG	Sidechain
2	6-B	342	TYR	Sidechain
2	6-B	359	TYR	Sidechain
2	6-B	379	TYR	Sidechain
2	6-B	393	PHE	Sidechain
2	6-B	411	PHE	Sidechain
2	6-B	429	TYR	Sidechain
2	6-B	433	TYR	Sidechain
2	6-B	438	TYR	Sidechain
2	6-B	468	PHE	Sidechain
2	6-B	471	ARG	Sidechain
2	6-B	507	LEU	Mainchain
2	6-B	510	TYR	Sidechain
2	6-B	558	PHE	Sidechain
2	6-B	587	PHE	Sidechain
2	6-B	598	TYR	Sidechain
2	6-B	633	ARG	Sidechain
2	6-B	651	TYR	Sidechain
2	6-B	776	TYR	Sidechain
3	6-C	140	HIS	Mainchain
3	6-C	218	ARG	Sidechain
3	6-C	243	ARG	Sidechain
3	6-C	247	TYR	Sidechain
3	6-C	256	TYR	Sidechain
3	6-C	292	TYR	Sidechain
3	6-C	315	TYR	Sidechain
3	6-C	358	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	6-C	403	PHE	Sidechain
3	6-C	407	TYR	Sidechain
3	6-C	423	PHE	Sidechain
3	6-C	437	TYR	Sidechain
3	6-C	445	TYR	Sidechain
3	6-C	53	PHE	Sidechain
3	6-C	59	ARG	Sidechain
3	6-C	83	PHE	Sidechain
3	6-D	109	TYR	Sidechain
3	6-D	176	ARG	Sidechain
3	6-D	247	TYR	Sidechain
3	6-D	249	TYR	Sidechain
3	6-D	275	PHE	Sidechain
3	6-D	292	TYR	Sidechain
3	6-D	315	TYR	Sidechain
3	6-D	362	TYR	Sidechain
3	6-D	427	ARG	Sidechain
3	6-D	437	TYR	Sidechain
3	6-D	445	TYR	Sidechain
3	6-D	46	ARG	Sidechain
1	7-A	112	TYR	Sidechain
1	7-A	123	TYR	Sidechain
1	7-A	144	ARG	Sidechain
1	7-A	145	PHE	Sidechain
1	7-A	160	ARG	Sidechain
1	7-A	171	ARG	Sidechain
1	7-A	190	TYR	Sidechain
1	7-A	203	ARG	Sidechain
1	7-A	251	PHE	Sidechain
1	7-A	279	TYR	Sidechain
1	7-A	393	TYR	Sidechain
1	7-A	398	TYR	Sidechain
1	7-A	405	PHE	Sidechain
1	7-A	426	PHE	Sidechain
1	7-A	558	TYR	Sidechain
1	7-A	568	TYR	Sidechain
1	7-A	582	TYR	Sidechain
1	7-A	588	TYR	Sidechain
1	7-A	597	ARG	Sidechain
1	7-A	614	TYR	Sidechain
1	7-A	624	ARG	Sidechain
1	7-A	646	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	7-A	647	PHE	Sidechain
1	7-A	663	TYR	Sidechain
1	7-A	704	TYR	Sidechain
1	7-A	776	ARG	Sidechain
2	7-B	285	ARG	Sidechain
2	7-B	293	ARG	Mainchain,Sidechain
2	7-B	345	TYR	Sidechain
2	7-B	356	ARG	Sidechain
2	7-B	403	PHE	Sidechain
2	7-B	409	TYR	Sidechain
2	7-B	411	PHE	Sidechain
2	7-B	429	TYR	Sidechain
2	7-B	433	TYR	Sidechain
2	7-B	438	TYR	Sidechain
2	7-B	469	HIS	Sidechain
2	7-B	470	TYR	Sidechain
2	7-B	562	TYR	Sidechain
2	7-B	565	TYR	Sidechain
2	7-B	600	TYR	Sidechain
2	7-B	612	ARG	Sidechain
2	7-B	728	HIS	Sidechain
2	7-B	772	PHE	Sidechain
2	7-B	776	TYR	Sidechain
3	7-C	114	ARG	Sidechain
3	7-C	193	ARG	Sidechain
3	7-C	20	PHE	Sidechain
3	7-C	243	ARG	Sidechain
3	7-C	247	TYR	Sidechain
3	7-C	275	PHE	Sidechain
3	7-C	292	TYR	Sidechain
3	7-C	316	PHE	Mainchain
3	7-C	359	ARG	Sidechain
3	7-C	46	ARG	Sidechain
3	7-C	55	ARG	Sidechain
3	7-C	62	PHE	Sidechain
3	7-C	84	ARG	Sidechain
3	7-D	109	TYR	Sidechain
3	7-D	161	ARG	Sidechain
3	7-D	162	TYR	Sidechain
3	7-D	182	VAL	Mainchain
3	7-D	217	PHE	Sidechain
3	7-D	256	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	7-D	266	HIS	Sidechain
3	7-D	267	PHE	Sidechain
3	7-D	272	PHE	Sidechain
3	7-D	292	TYR	Sidechain
3	7-D	359	ARG	Sidechain
3	7-D	413	PHE	Sidechain
3	7-D	86	PHE	Sidechain
1	8-A	108	ARG	Sidechain
1	8-A	111	ARG	Sidechain
1	8-A	116	TYR	Sidechain
1	8-A	123	TYR	Sidechain
1	8-A	138	PHE	Sidechain
1	8-A	150	TYR	Sidechain
1	8-A	157	ARG	Sidechain
1	8-A	203	ARG	Sidechain
1	8-A	262	ARG	Sidechain
1	8-A	302	TYR	Sidechain
1	8-A	405	PHE	Sidechain
1	8-A	409	PHE	Sidechain
1	8-A	458	TYR	Sidechain
1	8-A	558	TYR	Sidechain
1	8-A	559	HIS	Sidechain
1	8-A	614	TYR	Sidechain
1	8-A	623	ARG	Sidechain
1	8-A	633	HIS	Sidechain
1	8-A	92	PHE	Sidechain
2	8-B	190	TYR	Sidechain
2	8-B	236	TYR	Sidechain
2	8-B	241	PHE	Sidechain
2	8-B	242	ARG	Sidechain
2	8-B	264	TYR	Sidechain
2	8-B	295	ARG	Sidechain
2	8-B	303	HIS	Sidechain
2	8-B	343	TYR	Sidechain
2	8-B	345	TYR	Sidechain
2	8-B	409	TYR	Sidechain
2	8-B	425	PHE	Sidechain
2	8-B	429	TYR	Sidechain
2	8-B	438	TYR	Sidechain
2	8-B	562	TYR	Sidechain
2	8-B	576	ARG	Sidechain
2	8-B	600	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	8-B	652	TYR	Sidechain
2	8-B	741	PHE	Sidechain
2	8-B	839	PHE	Sidechain
3	8-C	162	TYR	Sidechain
3	8-C	176	ARG	Sidechain
3	8-C	204	PHE	Sidechain
3	8-C	243	ARG	Sidechain
3	8-C	292	TYR	Sidechain
3	8-C	296	LEU	Mainchain
3	8-C	315	TYR	Sidechain
3	8-C	319	TYR	Sidechain
3	8-C	358	ARG	Sidechain
3	8-C	398	PHE	Sidechain
3	8-C	407	TYR	Sidechain
3	8-C	86	PHE	Sidechain
3	8-D	162	TYR	Sidechain
3	8-D	170	TYR	Sidechain
3	8-D	243	ARG	Sidechain
3	8-D	256	TYR	Sidechain
3	8-D	292	TYR	Sidechain
3	8-D	329	ARG	Sidechain
3	8-D	437	TYR	Sidechain
3	8-D	445	TYR	Sidechain
3	8-D	46	ARG	Sidechain
3	8-D	55	ARG	Sidechain
3	8-D	59	ARG	Sidechain
3	8-D	65	ARG	Sidechain
3	8-D	90	ARG	Sidechain
1	9-A	102	PHE	Sidechain
1	9-A	105	PHE	Sidechain
1	9-A	108	ARG	Sidechain
1	9-A	112	TYR	Sidechain
1	9-A	116	TYR	Sidechain
1	9-A	123	TYR	Sidechain
1	9-A	144	ARG	Sidechain
1	9-A	157	ARG	Sidechain
1	9-A	160	ARG	Sidechain
1	9-A	197	PHE	Sidechain
1	9-A	251	PHE	Sidechain
1	9-A	302	TYR	Sidechain
1	9-A	333	ARG	Sidechain
1	9-A	363	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	9-A	409	PHE	Sidechain
1	9-A	413	TYR	Sidechain
1	9-A	450	TYR	Sidechain
1	9-A	458	TYR	Sidechain
1	9-A	469	ARG	Sidechain
1	9-A	562	PHE	Sidechain
1	9-A	568	TYR	Sidechain
1	9-A	576	ARG	Sidechain
1	9-A	614	TYR	Sidechain
1	9-A	630	ARG	Sidechain
1	9-A	646	TYR	Sidechain
1	9-A	657	TYR	Sidechain
1	9-A	687	ARG	Sidechain
1	9-A	78	PHE	Mainchain
1	9-A	794	TYR	Sidechain
2	9-B	190	TYR	Sidechain
2	9-B	231	TYR	Sidechain
2	9-B	295	ARG	Sidechain
2	9-B	328	ARG	Sidechain
2	9-B	342	TYR	Sidechain
2	9-B	345	TYR	Sidechain
2	9-B	415	TYR	Sidechain
2	9-B	422	THR	Peptide
2	9-B	423	ASN	Peptide
2	9-B	424	GLU	Peptide
2	9-B	425	PHE	Peptide
2	9-B	426	SER	Peptide
2	9-B	433	TYR	Sidechain
2	9-B	470	TYR	Sidechain
2	9-B	471	ARG	Sidechain
2	9-B	488	PHE	Sidechain
2	9-B	510	TYR	Sidechain
2	9-B	526	ARG	Sidechain
2	9-B	558	PHE	Sidechain
2	9-B	578	PHE	Sidechain
2	9-B	585	ARG	Sidechain
2	9-B	599	PHE	Sidechain
2	9-B	644	PHE	Sidechain
2	9-B	651	TYR	Sidechain
2	9-B	670	ARG	Sidechain
2	9-B	758	TYR	Sidechain
2	9-B	770	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	9-B	778	ASN	Peptide
3	9-C	136	PHE	Sidechain
3	9-C	162	TYR	Sidechain
3	9-C	170	TYR	Sidechain
3	9-C	292	TYR	Sidechain
3	9-C	316	PHE	Sidechain
3	9-C	445	TYR	Sidechain
3	9-D	161	ARG	Sidechain
3	9-D	170	TYR	Sidechain
3	9-D	217	PHE	Sidechain
3	9-D	226	HIS	Sidechain
3	9-D	256	TYR	Sidechain
3	9-D	275	PHE	Sidechain
3	9-D	29	HIS	Sidechain
3	9-D	292	TYR	Sidechain
3	9-D	315	TYR	Sidechain
3	9-D	319	TYR	Sidechain
3	9-D	329	ARG	Sidechain
3	9-D	341	ARG	Sidechain
3	9-D	423	PHE	Sidechain
3	9-D	437	TYR	Sidechain
3	9-D	53	PHE	Sidechain

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	1-A	4831	0	4863	63	0
1	2-A	4831	0	4863	80	0
1	3-A	4831	0	4863	79	0
1	4-A	4831	0	4863	61	0
1	5-A	4831	0	4863	109	0
1	6-A	4831	0	4863	100	0
1	7-A	4831	0	4863	102	0
1	8-A	4831	0	4863	124	0
1	9-A	4831	0	4863	76	0
1	10-A	4831	0	4863	115	0
2	1-B	4701	0	4731	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2-B	4701	0	4731	94	0
2	3-B	4701	0	4731	63	0
2	4-B	4701	0	4731	104	0
2	5-B	4701	0	4731	86	0
2	6-B	4701	0	4731	90	0
2	7-B	4701	0	4731	82	0
2	8-B	4701	0	4730	107	0
2	9-B	4701	0	4731	131	0
2	10-B	4701	0	4731	101	0
3	1-C	3485	0	3342	63	0
3	1-D	3485	0	3342	45	0
3	2-C	3485	0	3340	37	0
3	2-D	3485	0	3342	43	0
3	3-C	3485	0	3341	69	0
3	3-D	3485	0	3342	77	0
3	4-C	3485	0	3342	38	0
3	4-D	3485	0	3342	44	0
3	5-C	3485	0	3342	62	0
3	5-D	3485	0	3342	36	0
3	6-C	3485	0	3342	33	0
3	6-D	3485	0	3342	68	0
3	7-C	3485	0	3340	62	0
3	7-D	3485	0	3341	60	0
3	8-C	3485	0	3340	32	0
3	8-D	3485	0	3341	29	0
3	9-C	3485	0	3342	32	0
3	9-D	3485	0	3342	37	0
3	10-C	3485	0	3342	50	0
3	10-D	3485	0	3342	60	0
4	1-E	220	0	46	0	0
4	1-F	220	0	46	0	0
4	2-E	220	0	46	0	0
4	2-F	220	0	46	0	0
4	3-E	220	0	46	0	0
4	3-F	220	0	46	0	0
4	4-E	220	0	46	0	0
4	4-F	220	0	46	0	0
4	5-E	220	0	46	0	0
4	5-F	220	0	46	0	0
4	6-E	220	0	46	0	0
4	6-F	220	0	46	0	0
4	7-E	220	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	7-F	220	0	46	0	0
4	8-E	220	0	46	0	0
4	8-F	220	0	46	1	0
4	9-E	220	0	46	0	0
4	9-F	220	0	46	0	0
4	10-E	220	0	46	0	0
4	10-F	220	0	46	0	0
All	All	169420	0	163690	2506	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 8.

All (2506) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ARG:HH22	2:B:292:ILE:CD1	1.12	1.60
1:A:585:ILE:CD1	1:A:683:ILE:HD13	1.26	1.56
1:A:70:LEU:CD2	2:B:216:PHE:CG	1.87	1.53
3:C:59:ARG:HG3	3:D:280:ILE:CD1	1.40	1.51
1:A:143:ARG:CZ	2:B:292:ILE:HD11	1.38	1.49
2:B:405:ILE:CD1	2:B:456:ILE:HD13	1.47	1.45
1:A:137:ARG:NH2	2:B:328:ARG:HH12	1.07	1.44
1:A:143:ARG:NH2	2:B:292:ILE:HD11	1.13	1.44
1:A:585:ILE:CD1	1:A:683:ILE:CD1	1.96	1.43
3:C:59:ARG:HH21	3:D:285:ALA:CB	1.28	1.43
1:A:143:ARG:NH2	2:B:288:TYR:HD2	1.08	1.42
1:A:137:ARG:NH2	2:B:328:ARG:HH22	1.14	1.40
1:A:143:ARG:NH2	2:B:292:ILE:HD11	1.09	1.39
3:C:188:ILE:HD13	3:C:394:PHE:CD1	1.59	1.38
3:C:58:CYS:SG	3:D:286:HIS:C	2.08	1.36
2:B:405:ILE:CD1	2:B:456:ILE:CD1	2.03	1.36
1:A:585:ILE:HD12	1:A:683:ILE:CD1	1.51	1.36
1:A:137:ARG:NH2	2:B:328:ARG:NH1	1.73	1.36
1:A:137:ARG:HH21	2:B:328:ARG:NH2	1.23	1.34
1:A:143:ARG:NH2	2:B:288:TYR:CD2	1.95	1.34
2:B:480:ILE:CD1	2:B:541:LEU:HD11	1.56	1.34
1:A:143:ARG:CZ	2:B:288:TYR:HE2	1.41	1.33
3:C:59:ARG:NH2	3:D:285:ALA:HB2	1.43	1.33
2:B:405:ILE:HG13	2:B:456:ILE:CD1	1.58	1.32
1:A:458:TYR:CD1	1:A:484:ILE:HD12	1.64	1.32
1:A:138:PHE:CE2	1:A:275:ILE:HD11	1.65	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:LEU:CD1	1:A:640:ILE:CD1	2.07	1.30
1:A:138:PHE:CZ	1:A:275:ILE:HD11	1.65	1.30
2:B:438:TYR:CD2	2:B:441:ILE:HD12	1.62	1.30
1:A:143:ARG:NE	2:B:288:TYR:CE2	1.99	1.30
3:C:59:ARG:CG	3:D:280:ILE:HD11	1.61	1.30
3:D:17:VAL:CB	3:D:231:ILE:HD11	1.62	1.29
1:A:118:ILE:HD12	1:A:190:TYR:CZ	1.66	1.28
1:A:70:LEU:HD22	2:B:216:PHE:CD1	1.24	1.27
3:D:188:ILE:CD1	3:D:394:PHE:HB2	1.62	1.27
3:C:188:ILE:CD1	3:C:394:PHE:CD1	2.17	1.27
1:A:296:TYR:CG	2:B:322:HIS:HE1	1.54	1.26
1:A:73:THR:HG22	2:B:215:ASN:ND2	1.48	1.25
2:B:213:ILE:HD11	2:B:221:LEU:CD1	1.64	1.25
1:A:72:GLY:O	2:B:215:ASN:CG	1.78	1.25
3:D:280:ILE:HD11	3:D:371:GLU:OE1	1.36	1.25
3:D:188:ILE:CD1	3:D:394:PHE:HB2	1.67	1.24
2:B:180:PRO:N	2:B:184:ILE:HD12	1.53	1.24
2:B:533:ARG:N	2:B:538:ILE:HD12	1.50	1.23
3:C:58:CYS:HB3	3:D:286:HIS:O	1.30	1.23
2:B:257:ILE:CD1	2:B:297:TYR:CD2	2.22	1.23
2:B:405:ILE:HG13	2:B:456:ILE:CD1	1.69	1.23
3:C:59:ARG:CG	3:D:280:ILE:CD1	2.15	1.23
3:C:188:ILE:HD13	3:C:394:PHE:CD2	1.73	1.22
2:B:257:ILE:HD12	2:B:297:TYR:CD2	1.73	1.22
1:A:140:TYR:CZ	2:B:324:ASP:OD1	1.91	1.22
3:D:188:ILE:CD1	3:D:394:PHE:HB2	1.68	1.22
1:A:426:PHE:CZ	1:A:564:ILE:CD1	2.23	1.21
2:B:445:PHE:CE1	2:B:449:ILE:HD11	1.75	1.21
1:A:143:ARG:CZ	2:B:288:TYR:CE2	2.24	1.21
3:D:5:ILE:HD12	3:D:53:PHE:CE2	1.76	1.21
3:D:5:ILE:HD12	3:D:53:PHE:CZ	1.76	1.21
3:D:188:ILE:HD12	3:D:394:PHE:CD1	1.75	1.21
3:C:258:THR:HG21	3:C:356:ILE:CD1	1.71	1.20
1:A:143:ARG:NH2	2:B:292:ILE:CD1	2.02	1.20
1:A:625:ILE:HD11	1:A:761:ILE:CD1	1.70	1.20
1:A:599:LEU:CD1	1:A:640:ILE:HD13	1.70	1.20
3:C:59:ARG:NH2	3:D:285:ALA:CB	1.97	1.20
3:C:59:ARG:NH2	3:D:279:TYR:HB3	1.55	1.20
3:D:188:ILE:HD11	3:D:394:PHE:CB	1.72	1.20
1:A:72:GLY:O	2:B:215:ASN:CB	1.89	1.20
1:A:625:ILE:CD1	1:A:761:ILE:HG21	1.70	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:ILE:CD1	2:B:439:ARG:HB2	1.69	1.19
2:B:296:ILE:HD13	2:B:319:PHE:CZ	1.76	1.19
1:A:140:TYR:CE2	2:B:324:ASP:OD1	1.94	1.19
1:A:72:GLY:CA	2:B:215:ASN:HB2	1.72	1.19
1:A:118:ILE:HD12	1:A:190:TYR:OH	1.41	1.18
2:B:355:LEU:HB2	2:B:364:ILE:CD1	1.72	1.18
2:B:405:ILE:CG1	2:B:456:ILE:CD1	2.21	1.18
2:B:296:ILE:CD1	2:B:327:ILE:HD12	1.72	1.18
3:C:188:ILE:HD12	3:C:394:PHE:CD1	1.77	1.18
1:A:151:LEU:HD12	2:B:285:ARG:HD3	1.26	1.17
3:C:59:ARG:NE	3:D:285:ALA:HB3	1.59	1.17
1:A:774:ILE:HD12	1:A:796:SER:CB	1.73	1.16
3:C:188:ILE:CD1	3:C:394:PHE:CD2	2.29	1.16
1:A:143:ARG:CZ	2:B:292:ILE:CD1	2.22	1.16
1:A:363:ILE:HD11	1:A:366:ILE:HB	1.21	1.16
1:A:137:ARG:CZ	2:B:325:LEU:HD22	1.76	1.16
2:B:533:ARG:HA	2:B:538:ILE:CD1	1.74	1.15
1:A:426:PHE:CE2	1:A:564:ILE:CD1	2.30	1.15
3:D:188:ILE:HD11	3:D:394:PHE:HB3	1.25	1.14
1:A:296:TYR:CG	2:B:322:HIS:CE1	2.35	1.14
2:B:296:ILE:CD1	2:B:319:PHE:CE1	2.28	1.14
2:B:405:ILE:HD13	2:B:456:ILE:CD1	1.78	1.14
1:A:625:ILE:CD1	1:A:761:ILE:HG23	1.77	1.14
1:A:143:ARG:NE	2:B:288:TYR:HE2	1.46	1.14
2:B:213:ILE:CD1	2:B:221:LEU:HD11	1.78	1.14
1:A:426:PHE:CZ	1:A:564:ILE:HD11	1.80	1.13
2:B:526:ARG:O	2:B:538:ILE:HD12	1.48	1.13
2:B:586:ILE:HD11	2:B:732:LEU:HD13	1.17	1.13
1:A:625:ILE:HD12	1:A:761:ILE:CG2	1.79	1.13
2:B:731:PHE:CE1	2:B:735:ILE:HD11	1.83	1.13
2:B:533:ARG:HA	2:B:538:ILE:HD12	1.17	1.13
1:A:70:LEU:HD22	2:B:216:PHE:CG	1.67	1.13
2:B:405:ILE:HG13	2:B:456:ILE:HD12	1.29	1.13
1:A:134:VAL:HG13	1:A:275:ILE:HD13	1.29	1.13
3:C:188:ILE:HD13	3:C:394:PHE:CE2	1.84	1.13
3:D:188:ILE:HD11	3:D:394:PHE:HA	1.18	1.12
1:A:357:VAL:HB	1:A:363:ILE:HD12	1.29	1.12
1:A:137:ARG:NH1	2:B:325:LEU:HD22	1.62	1.12
3:C:322:ILE:HD13	3:C:358:ARG:NH2	1.64	1.12
2:B:586:ILE:HD11	2:B:732:LEU:CD1	1.80	1.12
3:C:322:ILE:HD13	3:C:358:ARG:HH21	1.09	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HD13	2:B:286:GLU:OE2	1.49	1.11
3:C:188:ILE:CD1	3:C:394:PHE:CD2	2.33	1.11
1:A:458:TYR:CE1	1:A:484:ILE:HD12	1.84	1.11
1:A:151:LEU:HD12	2:B:285:ARG:CD	1.79	1.11
3:C:123:ILE:HD11	3:C:154:LEU:HD11	1.15	1.11
3:C:59:ARG:HE	3:D:285:ALA:HB3	1.07	1.11
1:A:625:ILE:CD1	1:A:761:ILE:CG2	2.28	1.11
1:A:143:ARG:NE	2:B:288:TYR:CE2	2.18	1.11
2:B:405:ILE:CG1	2:B:456:ILE:HD11	1.80	1.11
1:A:774:ILE:HD12	1:A:796:SER:OG	1.48	1.11
1:A:70:LEU:CD2	2:B:216:PHE:CD1	1.99	1.11
1:A:625:ILE:HD12	1:A:761:ILE:HG21	1.26	1.10
2:B:525:LEU:HD22	2:B:538:ILE:HD12	1.32	1.10
3:C:258:THR:OG1	3:C:356:ILE:HD11	1.48	1.10
2:B:355:LEU:CB	2:B:364:ILE:HD12	1.81	1.10
1:A:151:LEU:CD1	2:B:286:GLU:OE2	1.99	1.10
2:B:180:PRO:N	2:B:184:ILE:CD1	2.14	1.10
2:B:339:ILE:HD13	2:B:439:ARG:HB2	1.12	1.10
1:A:606:LEU:HD11	1:A:710:ILE:HD11	1.33	1.10
1:A:625:ILE:HD11	1:A:761:ILE:HD12	1.29	1.10
1:A:695:LEU:HD21	1:A:774:ILE:HD12	1.20	1.09
1:A:639:PHE:CZ	1:A:643:ILE:HD11	1.87	1.09
3:D:258:THR:HG21	3:D:356:ILE:HD12	1.20	1.09
1:A:706:PHE:HZ	1:A:710:ILE:HD12	1.12	1.09
2:B:405:ILE:HD12	2:B:453:TYR:CD1	1.86	1.09
1:A:72:GLY:HA2	2:B:215:ASN:CB	1.81	1.09
2:B:480:ILE:HD13	2:B:537:VAL:HG11	1.33	1.09
2:B:445:PHE:CE2	2:B:449:ILE:HD11	1.85	1.09
3:C:188:ILE:HD11	3:C:394:PHE:CE1	1.86	1.09
2:B:213:ILE:HD11	2:B:221:LEU:HD11	1.16	1.09
3:D:280:ILE:CD1	3:D:371:GLU:OE1	2.01	1.09
1:A:151:LEU:HD11	2:B:282:SER:CB	1.82	1.09
1:A:706:PHE:CZ	1:A:710:ILE:HD12	1.86	1.08
3:D:188:ILE:HD11	3:D:394:PHE:HB2	1.09	1.08
1:A:599:LEU:HD12	1:A:640:ILE:HD13	1.21	1.08
1:A:458:TYR:CD1	1:A:484:ILE:CD1	2.34	1.08
3:C:59:ARG:NH1	3:D:283:ASP:OD2	1.86	1.08
1:A:147:GLU:HG3	2:B:285:ARG:HG3	1.35	1.08
2:B:772:PHE:HE1	2:B:812:ILE:HD13	1.19	1.08
3:C:258:THR:HG21	3:C:356:ILE:HD11	1.09	1.08
2:B:355:LEU:HB2	2:B:364:ILE:HD12	1.21	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:NH2	2:B:328:ARG:NH2	1.83	1.08
2:B:586:ILE:HD11	2:B:732:LEU:CG	1.84	1.08
1:A:458:TYR:CE1	1:A:484:ILE:HD12	1.87	1.08
3:C:58:CYS:SG	3:D:286:HIS:N	2.25	1.07
2:B:405:ILE:CD1	2:B:452:GLN:OE1	2.03	1.07
3:C:242:ILE:HD11	3:C:252:MET:SD	1.94	1.07
3:D:119:ILE:CD1	3:D:154:LEU:HD13	1.85	1.07
3:C:123:ILE:HD11	3:C:154:LEU:HD11	1.35	1.07
1:A:72:GLY:HA2	2:B:215:ASN:HB2	1.20	1.07
1:A:557:ILE:CD1	1:A:594:TYR:OH	2.03	1.06
3:D:212:ILE:HD12	3:D:303:ASN:ND2	1.69	1.06
2:B:364:ILE:CD1	2:B:383:ILE:HD11	1.86	1.06
1:A:105:PHE:CZ	1:A:109:ILE:HD11	1.90	1.06
2:B:430:HIS:CG	2:B:448:ILE:HD13	1.89	1.06
1:A:68:ILE:CD1	2:B:281:LYS:HD3	1.85	1.06
1:A:585:ILE:HD11	1:A:683:ILE:HD13	1.26	1.06
1:A:625:ILE:HD11	1:A:761:ILE:HG23	1.11	1.06
3:D:188:ILE:HD11	3:D:394:PHE:HB2	1.13	1.06
3:C:188:ILE:HD13	3:C:394:PHE:CD2	1.88	1.06
1:A:698:GLN:OE1	1:A:774:ILE:CD1	2.04	1.05
3:D:17:VAL:HG22	3:D:231:ILE:HD12	1.35	1.05
2:B:405:ILE:HG23	2:B:456:ILE:HD12	1.37	1.05
1:A:128:ASP:OD1	2:B:299:ARG:NH2	1.87	1.05
2:B:209:ILE:HD13	2:B:213:ILE:HD12	1.37	1.05
1:A:143:ARG:NH1	2:B:292:ILE:CD1	2.19	1.05
1:A:151:LEU:HG	2:B:285:ARG:NE	1.63	1.05
3:C:59:ARG:HG3	3:D:280:ILE:HD13	1.39	1.05
2:B:209:ILE:CD1	2:B:213:ILE:HD12	1.86	1.05
1:A:409:PHE:CE1	1:A:573:ILE:CD1	2.40	1.05
3:D:188:ILE:HD11	3:D:394:PHE:HB2	1.09	1.04
2:B:364:ILE:HD11	2:B:383:ILE:CD1	1.88	1.04
3:C:188:ILE:CD1	3:C:394:PHE:CD2	2.39	1.04
3:C:59:ARG:HG3	3:D:280:ILE:HD11	1.06	1.04
3:C:166:ILE:HD13	3:C:256:TYR:CD2	1.92	1.04
1:A:695:LEU:CD2	1:A:774:ILE:HD12	1.86	1.04
2:B:480:ILE:HD13	2:B:537:VAL:CG1	1.86	1.04
3:C:255:ILE:HD11	3:C:358:ARG:HH11	1.16	1.04
1:A:138:PHE:CE2	1:A:275:ILE:CD1	2.40	1.04
3:C:204:PHE:CD2	3:C:231:ILE:HD11	1.91	1.04
1:A:108:ARG:HH21	1:A:177:ILE:HD12	1.22	1.04
3:C:188:ILE:HD11	3:C:394:PHE:CB	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:276:THR:OG1	3:C:284:ILE:CD1	2.05	1.04
2:B:257:ILE:CD1	2:B:297:TYR:CE2	2.41	1.03
1:A:567:PRO:HD2	1:A:574:ILE:HD11	1.35	1.03
2:B:533:ARG:CA	2:B:538:ILE:HD12	1.86	1.03
2:B:241:PHE:HB3	2:B:254:ILE:CD1	1.87	1.03
1:A:357:VAL:HB	1:A:363:ILE:CD1	1.89	1.03
3:C:258:THR:CG2	3:C:356:ILE:CD1	2.36	1.03
3:D:212:ILE:HD11	3:D:302:SER:O	1.56	1.03
1:A:409:PHE:CE1	1:A:573:ILE:HD11	1.94	1.03
2:B:405:ILE:HD11	2:B:456:ILE:HD13	1.04	1.02
1:A:699:ILE:CD1	1:A:775:PHE:CE1	2.42	1.02
2:B:241:PHE:HB3	2:B:254:ILE:HD11	1.39	1.02
1:A:566:ILE:HG13	1:A:574:ILE:CD1	1.89	1.02
2:B:296:ILE:HD11	2:B:319:PHE:CE1	1.93	1.02
1:A:73:THR:CG2	2:B:215:ASN:HD21	1.71	1.02
2:B:405:ILE:HD12	2:B:456:ILE:HD11	1.40	1.02
2:B:339:ILE:CD1	2:B:439:ARG:CB	2.37	1.02
2:B:586:ILE:HD11	2:B:732:LEU:HD22	1.37	1.02
2:B:405:ILE:CD1	2:B:456:ILE:HD11	1.90	1.02
1:A:774:ILE:CD1	1:A:796:SER:HB2	1.89	1.02
2:B:480:ILE:CD1	2:B:541:LEU:CD1	2.37	1.01
3:C:58:CYS:CB	3:D:286:HIS:O	2.08	1.01
1:A:143:ARG:HH12	2:B:292:ILE:HD12	1.23	1.01
2:B:296:ILE:HD11	2:B:327:ILE:CD1	1.88	1.01
3:D:213:SER:HB3	3:D:222:ILE:HD11	1.42	1.01
1:A:425:ILE:HD13	1:A:564:ILE:HD12	1.37	1.01
3:D:188:ILE:HD11	3:D:394:PHE:CB	1.89	1.01
3:C:188:ILE:HD11	3:C:394:PHE:CG	1.95	1.01
2:B:499:ILE:HD11	2:B:508:PRO:HG3	1.40	1.01
2:B:405:ILE:HD12	2:B:456:ILE:CD1	1.85	1.01
2:B:405:ILE:CD1	2:B:456:ILE:HD11	1.91	1.01
3:D:21:LEU:HD12	3:D:235:ILE:HD13	1.40	1.01
2:B:405:ILE:HG23	2:B:456:ILE:HD12	1.02	1.01
1:A:599:LEU:HD22	1:A:640:ILE:HD11	1.38	1.01
2:B:634:ILE:HD12	2:B:772:PHE:CE1	1.95	1.01
1:A:151:LEU:HD11	2:B:282:SER:OG	1.60	1.00
3:C:188:ILE:HD12	3:C:394:PHE:CG	1.96	1.00
1:A:698:GLN:OE1	1:A:774:ILE:HD13	1.61	1.00
3:D:256:TYR:CE1	3:D:260:ILE:HD12	1.95	1.00
3:C:258:THR:HG21	3:C:356:ILE:CD1	1.91	1.00
3:D:188:ILE:HD11	3:D:394:PHE:CA	1.91	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ILE:HG13	1:A:765:ILE:CD1	1.91	1.00
1:A:425:ILE:CD1	1:A:564:ILE:HD12	1.91	1.00
3:C:212:ILE:HD11	3:C:302:SER:O	1.61	1.00
2:B:405:ILE:HG13	2:B:456:ILE:HD11	1.02	1.00
2:B:586:ILE:HD11	2:B:732:LEU:HG	1.44	1.00
1:A:151:LEU:CD1	2:B:285:ARG:HD3	1.92	1.00
1:A:202:GLU:O	1:A:205:THR:O	1.80	1.00
3:C:199:ASP:O	3:C:260:ILE:CD1	2.10	1.00
2:B:405:ILE:HD11	2:B:456:ILE:HG13	1.41	1.00
1:A:585:ILE:HD11	1:A:683:ILE:CG2	1.91	0.99
1:A:357:VAL:CB	1:A:363:ILE:HD12	1.91	0.99
1:A:143:ARG:HH22	2:B:292:ILE:CD1	1.69	0.99
2:B:402:ILE:CG2	2:B:449:ILE:HD12	1.92	0.99
3:D:17:VAL:HB	3:D:231:ILE:CD1	1.91	0.99
3:C:59:ARG:NE	3:D:280:ILE:HD11	1.77	0.99
3:C:127:ILE:CD1	3:C:162:TYR:CZ	2.45	0.99
2:B:405:ILE:HD13	2:B:456:ILE:HD11	0.99	0.99
1:A:137:ARG:HH22	2:B:328:ARG:NH1	1.54	0.98
3:C:58:CYS:HB3	3:D:286:HIS:C	1.88	0.98
3:C:123:ILE:HD13	3:C:158:LEU:HD21	1.43	0.98
1:A:643:ILE:HD13	1:A:696:GLN:HE22	1.28	0.98
1:A:130:SER:OG	2:B:322:HIS:NE2	1.95	0.98
1:A:138:PHE:CZ	1:A:275:ILE:CD1	2.46	0.98
3:D:119:ILE:HD12	3:D:154:LEU:CD1	1.93	0.98
3:C:188:ILE:CD1	3:C:394:PHE:CG	2.46	0.98
2:B:405:ILE:CG2	2:B:456:ILE:HD12	1.94	0.97
1:A:426:PHE:CE2	1:A:564:ILE:HD13	1.98	0.97
1:A:695:LEU:CD2	1:A:774:ILE:CD1	2.42	0.97
1:A:458:TYR:CD1	1:A:484:ILE:CD1	2.46	0.97
1:A:625:ILE:CD1	1:A:761:ILE:HG21	1.95	0.97
1:A:625:ILE:CD1	1:A:761:ILE:CG2	2.42	0.97
1:A:118:ILE:CD1	1:A:190:TYR:CZ	2.46	0.97
2:B:731:PHE:CE1	2:B:735:ILE:CD1	2.48	0.97
3:D:258:THR:HG21	3:D:356:ILE:CD1	1.93	0.97
1:A:699:ILE:HD11	1:A:775:PHE:CE1	2.00	0.97
2:B:533:ARG:HA	2:B:538:ILE:CD1	1.95	0.97
1:A:606:LEU:CD1	1:A:710:ILE:HD11	1.94	0.96
3:C:166:ILE:CD1	3:C:256:TYR:CD2	2.46	0.96
1:A:143:ARG:NH1	2:B:292:ILE:HD12	1.78	0.96
1:A:138:PHE:HB3	1:A:275:ILE:HD11	1.44	0.96
3:C:58:CYS:SG	3:D:286:HIS:CA	1.13	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:ARG:NH1	3:D:283:ASP:OD1	1.97	0.96
1:A:606:LEU:CD1	1:A:710:ILE:CD1	2.44	0.96
2:B:241:PHE:HB3	2:B:254:ILE:CD1	1.95	0.96
1:A:625:ILE:HD13	1:A:761:ILE:HG12	1.44	0.96
3:C:59:ARG:HH21	3:D:285:ALA:HB2	0.96	0.96
3:C:255:ILE:CD1	3:C:358:ARG:HH11	1.78	0.96
3:D:188:ILE:HD11	3:D:394:PHE:HA	1.48	0.96
3:C:188:ILE:CD1	3:C:394:PHE:CE1	2.45	0.96
1:A:585:ILE:HD11	1:A:683:ILE:HG21	1.48	0.96
1:A:151:LEU:HD22	2:B:285:ARG:HG3	1.44	0.96
3:D:188:ILE:CD1	3:D:394:PHE:HA	1.96	0.96
1:A:585:ILE:HD13	1:A:683:ILE:HG12	1.45	0.95
3:C:188:ILE:CD1	3:C:394:PHE:CG	2.48	0.95
2:B:586:ILE:HD13	2:B:732:LEU:HB2	1.45	0.95
1:A:599:LEU:HD13	1:A:640:ILE:CD1	1.95	0.95
3:D:258:THR:CG2	3:D:356:ILE:HD12	1.95	0.95
1:A:138:PHE:CE1	1:A:275:ILE:HD11	2.01	0.95
3:C:59:ARG:CD	3:D:280:ILE:HD11	1.96	0.95
1:A:643:ILE:CD1	1:A:696:GLN:NE2	2.30	0.95
3:C:127:ILE:HD13	3:C:162:TYR:CZ	2.02	0.95
3:D:188:ILE:CD1	3:D:394:PHE:HB3	1.96	0.95
1:A:135:LEU:HD13	1:A:247:ILE:HD13	1.46	0.95
1:A:625:ILE:HD13	1:A:761:ILE:CG2	1.93	0.95
2:B:398:LEU:CG	2:B:449:ILE:HD12	1.96	0.95
3:D:255:ILE:HD12	3:D:358:ARG:CZ	1.97	0.94
2:B:346:LEU:HD11	2:B:402:ILE:HD13	1.48	0.94
2:B:656:ILE:HD11	2:B:738:HIS:CD2	2.02	0.94
1:A:72:GLY:O	2:B:215:ASN:HB3	1.67	0.94
3:D:212:ILE:CD1	3:D:303:ASN:CG	2.40	0.94
2:B:398:LEU:HG	2:B:449:ILE:CD1	1.97	0.94
1:A:151:LEU:CG	2:B:285:ARG:NE	2.12	0.94
1:A:138:PHE:CD2	1:A:275:ILE:HD11	2.00	0.94
2:B:493:ILE:HD12	2:B:598:TYR:CB	1.97	0.94
1:A:557:ILE:HD13	1:A:594:TYR:OH	1.67	0.94
1:A:147:GLU:CG	2:B:285:ARG:HG3	1.97	0.94
2:B:293:ARG:HE	2:B:330:ILE:HD11	1.30	0.94
1:A:151:LEU:HD22	2:B:285:ARG:HB3	1.45	0.94
1:A:585:ILE:CD1	1:A:683:ILE:CG1	2.44	0.94
3:C:123:ILE:CD1	3:C:154:LEU:HD11	1.96	0.94
2:B:480:ILE:HD11	2:B:541:LEU:CD1	1.98	0.94
3:C:188:ILE:CD1	3:C:394:PHE:CB	2.44	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:276:THR:CB	3:C:284:ILE:HD12	1.96	0.94
3:D:17:VAL:CG2	3:D:231:ILE:HD12	1.98	0.94
1:A:566:ILE:HG13	1:A:574:ILE:HD13	1.48	0.94
2:B:297:TYR:OH	2:B:330:ILE:HD13	1.68	0.94
2:B:430:HIS:CG	2:B:448:ILE:CD1	2.51	0.94
2:B:480:ILE:HD12	2:B:541:LEU:HD11	1.48	0.94
2:B:241:PHE:CB	2:B:254:ILE:CD1	2.46	0.94
2:B:241:PHE:HB3	2:B:254:ILE:HD11	1.47	0.94
1:A:138:PHE:HE2	1:A:275:ILE:CD1	1.80	0.94
1:A:625:ILE:HD11	1:A:761:ILE:CG2	1.98	0.93
3:C:204:PHE:CG	3:C:231:ILE:HD11	2.03	0.93
1:A:375:ILE:HD13	1:A:396:LYS:HE3	1.50	0.93
3:D:119:ILE:HD12	3:D:154:LEU:HD13	1.49	0.93
1:A:108:ARG:NH2	1:A:177:ILE:HD12	1.82	0.93
3:C:59:ARG:CG	3:D:280:ILE:HD13	1.96	0.93
3:C:199:ASP:O	3:C:260:ILE:HD13	1.68	0.93
2:B:525:LEU:HD22	2:B:538:ILE:CD1	1.98	0.93
2:B:526:ARG:O	2:B:538:ILE:CD1	2.16	0.93
3:D:213:SER:HB3	3:D:222:ILE:CD1	1.99	0.93
1:A:599:LEU:HD12	1:A:640:ILE:CD1	1.85	0.93
1:A:458:TYR:CE1	1:A:484:ILE:CD1	2.50	0.93
3:C:240:ASN:OD1	3:C:322:ILE:HD11	1.69	0.93
2:B:438:TYR:CD2	2:B:441:ILE:CD1	2.51	0.92
2:B:296:ILE:HD11	2:B:327:ILE:HD12	0.95	0.92
2:B:405:ILE:HG23	2:B:456:ILE:CD1	1.95	0.92
3:C:127:ILE:CD1	3:C:162:TYR:CE2	2.51	0.92
2:B:586:ILE:HD11	2:B:732:LEU:CD2	1.99	0.92
1:A:72:GLY:CA	2:B:215:ASN:CB	2.44	0.92
2:B:586:ILE:CD1	2:B:732:LEU:HD12	1.98	0.92
1:A:409:PHE:CZ	1:A:573:ILE:HD13	2.04	0.92
1:A:68:ILE:CD1	2:B:281:LYS:CD	2.46	0.92
3:C:258:THR:CG2	3:C:356:ILE:HD11	1.99	0.92
1:A:143:ARG:HH22	2:B:292:ILE:HD11	1.15	0.92
3:D:17:VAL:HB	3:D:231:ILE:HD11	0.94	0.92
3:C:188:ILE:CD1	3:C:394:PHE:HB2	2.00	0.92
1:A:143:ARG:HH22	2:B:292:ILE:CG1	1.83	0.92
2:B:499:ILE:HD11	2:B:508:PRO:HD3	1.49	0.92
2:B:209:ILE:CD1	2:B:213:ILE:CD1	2.47	0.92
1:A:625:ILE:HD13	1:A:761:ILE:CB	1.99	0.91
2:B:339:ILE:HD12	2:B:439:ARG:CB	2.00	0.91
2:B:296:ILE:CD1	2:B:319:PHE:CZ	2.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:TRP:O	1:A:572:ILE:HD12	1.70	0.91
1:A:585:ILE:HD13	1:A:683:ILE:CG1	2.00	0.91
3:D:242:ILE:HD11	3:D:252:MET:HB2	1.52	0.91
1:A:143:ARG:CZ	2:B:288:TYR:CE2	2.53	0.91
3:D:188:ILE:HD11	3:D:394:PHE:CB	1.99	0.91
2:B:480:ILE:HD11	2:B:541:LEU:HD11	1.53	0.91
3:C:258:THR:CG2	3:C:356:ILE:HD11	1.99	0.91
1:A:143:ARG:CZ	2:B:288:TYR:CD2	2.52	0.91
2:B:405:ILE:CG1	2:B:456:ILE:CD1	2.43	0.91
2:B:241:PHE:HB3	2:B:254:ILE:HD11	1.51	0.91
3:C:58:CYS:CB	3:D:286:HIS:C	2.30	0.91
1:A:699:ILE:CD1	1:A:775:PHE:CE2	2.54	0.91
1:A:606:LEU:HG	1:A:710:ILE:HD13	1.51	0.91
2:B:739:LYS:O	2:B:743:THR:O	1.89	0.91
3:C:59:ARG:CZ	3:D:285:ALA:HB3	2.00	0.91
3:C:188:ILE:HD12	3:C:394:PHE:CD2	2.02	0.91
3:D:213:SER:HB3	3:D:222:ILE:HD12	1.49	0.91
1:A:774:ILE:CD1	1:A:796:SER:CB	2.45	0.91
2:B:482:LEU:HD12	2:B:657:ILE:HD12	1.54	0.91
3:C:59:ARG:HH21	3:D:285:ALA:CA	1.84	0.91
3:C:280:ILE:HD13	3:C:284:ILE:HG12	1.53	0.91
1:A:699:ILE:HD13	1:A:775:PHE:CE1	2.05	0.90
1:A:147:GLU:HB3	2:B:285:ARG:HD3	1.52	0.90
2:B:257:ILE:HD13	2:B:297:TYR:CE2	2.06	0.90
2:B:634:ILE:HD12	2:B:772:PHE:HE1	1.33	0.90
3:D:258:THR:OG1	3:D:356:ILE:HD11	1.71	0.90
2:B:533:ARG:CA	2:B:538:ILE:HD12	2.02	0.90
3:D:188:ILE:CD1	3:D:394:PHE:HA	1.99	0.90
3:C:58:CYS:HB3	3:D:286:HIS:O	1.70	0.90
1:A:567:PRO:HD2	1:A:574:ILE:CD1	2.01	0.90
2:B:533:ARG:O	2:B:538:ILE:HD12	1.72	0.90
1:A:137:ARG:NH1	2:B:325:LEU:CD2	2.35	0.90
2:B:188:VAL:HG13	2:B:224:ILE:HD11	1.51	0.90
1:A:143:ARG:CZ	2:B:292:ILE:HD11	2.00	0.90
1:A:426:PHE:HZ	1:A:564:ILE:HD11	1.31	0.90
1:A:147:GLU:HG2	2:B:285:ARG:HG2	1.52	0.90
1:A:151:LEU:HG	2:B:285:ARG:HE	1.32	0.90
1:A:585:ILE:HD12	1:A:683:ILE:HD13	0.91	0.89
3:C:58:CYS:H	3:D:287:LYS:HG3	1.35	0.89
1:A:296:TYR:CD1	2:B:322:HIS:CE1	2.59	0.89
2:B:493:ILE:CD1	2:B:598:TYR:HB2	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:HH21	2:B:328:ARG:NH1	1.46	0.89
3:C:6:ILE:HD13	3:C:126:GLU:HB3	1.53	0.89
3:C:58:CYS:HG	3:D:286:HIS:HA	1.08	0.89
3:D:166:ILE:HD12	3:D:256:TYR:CG	2.07	0.89
1:A:625:ILE:HD12	1:A:761:ILE:HG23	1.53	0.89
2:B:209:ILE:HD11	2:B:213:ILE:CD1	2.02	0.89
1:A:320:TRP:O	1:A:572:ILE:CD1	2.21	0.88
1:A:639:PHE:CE1	1:A:643:ILE:HD11	2.07	0.88
3:C:58:CYS:O	3:D:285:ALA:HA	1.72	0.88
1:A:138:PHE:CE1	1:A:275:ILE:HD11	2.08	0.88
1:A:581:LYS:HB3	1:A:683:ILE:HD13	1.54	0.88
2:B:607:SER:HB3	2:B:634:ILE:HD13	1.56	0.88
1:A:557:ILE:CD1	1:A:594:TYR:CZ	2.57	0.88
2:B:405:ILE:HD11	2:B:452:GLN:OE1	1.73	0.88
2:B:586:ILE:CD1	2:B:732:LEU:HB2	2.04	0.88
3:D:256:TYR:HE1	3:D:260:ILE:HD12	1.34	0.88
2:B:445:PHE:HE1	2:B:449:ILE:HD11	1.25	0.88
1:A:375:ILE:HD11	1:A:396:LYS:HG2	1.54	0.88
1:A:409:PHE:CE1	1:A:573:ILE:HD13	2.09	0.88
1:A:366:ILE:HD11	1:A:371:SER:HB3	1.54	0.87
1:A:421:HIS:CE1	1:A:425:ILE:HD11	2.09	0.87
3:C:123:ILE:HD11	3:C:154:LEU:CD1	2.01	0.87
1:A:409:PHE:CZ	1:A:573:ILE:HD11	2.09	0.87
1:A:128:ASP:HB3	2:B:299:ARG:HH22	1.38	0.87
3:D:276:THR:OG1	3:D:284:ILE:HD13	1.73	0.87
3:C:58:CYS:SG	3:D:284:ILE:O	2.32	0.87
1:A:138:PHE:HE2	1:A:192:ILE:HD12	1.38	0.87
2:B:586:ILE:HD11	2:B:732:LEU:CD1	2.03	0.87
2:B:398:LEU:HG	2:B:449:ILE:HD12	1.55	0.87
3:C:123:ILE:CD1	3:C:154:LEU:HD11	2.03	0.87
3:D:212:ILE:CD1	3:D:303:ASN:ND2	2.37	0.87
2:B:364:ILE:HD13	2:B:403:PHE:HD1	1.38	0.87
2:B:586:ILE:HD11	2:B:732:LEU:HD12	1.54	0.87
1:A:585:ILE:HD13	1:A:683:ILE:HD13	1.57	0.87
1:A:566:ILE:CG1	1:A:574:ILE:HD12	2.04	0.87
3:C:59:ARG:NH2	3:D:278:ASP:O	2.07	0.87
3:C:255:ILE:HD11	3:C:358:ARG:NH1	1.88	0.87
2:B:241:PHE:HB2	2:B:254:ILE:HD13	1.57	0.86
3:C:241:SER:OG	3:C:322:ILE:CD1	2.23	0.86
2:B:445:PHE:CE2	2:B:449:ILE:CD1	2.58	0.86
2:B:181:GLU:OE1	2:B:184:ILE:HD11	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:ILE:HD12	2:B:439:ARG:HB3	1.56	0.86
2:B:296:ILE:HD13	2:B:319:PHE:CE1	2.05	0.86
2:B:533:ARG:CA	2:B:538:ILE:CD1	2.53	0.86
3:C:255:ILE:CD1	3:C:358:ARG:NH1	2.37	0.86
3:C:188:ILE:CD1	3:C:394:PHE:CG	2.59	0.86
2:B:402:ILE:HG12	2:B:449:ILE:HD13	1.57	0.86
3:C:280:ILE:CD1	3:C:284:ILE:HD11	2.05	0.86
3:D:212:ILE:HD11	3:D:302:SER:O	1.74	0.86
1:A:625:ILE:CG2	1:A:765:ILE:HD13	2.04	0.86
3:C:212:ILE:CD1	3:C:302:SER:O	2.24	0.86
1:A:71:GLU:HA	1:A:75:ILE:HD13	1.58	0.86
2:B:213:ILE:HD11	2:B:221:LEU:HD12	1.55	0.86
2:B:493:ILE:HD12	2:B:598:TYR:CG	2.11	0.86
1:A:371:SER:OG	1:A:404:ILE:HD11	1.76	0.86
2:B:398:LEU:CD1	2:B:449:ILE:HD12	2.06	0.86
1:A:426:PHE:HE2	1:A:564:ILE:HD13	1.41	0.86
1:A:147:GLU:CG	2:B:285:ARG:CG	2.53	0.86
2:B:405:ILE:HD13	2:B:452:GLN:OE1	1.74	0.85
2:B:398:LEU:CD2	2:B:449:ILE:HD12	2.07	0.85
3:C:256:TYR:CD1	3:C:260:ILE:HD12	2.10	0.85
1:A:72:GLY:C	2:B:215:ASN:CB	2.48	0.85
1:A:557:ILE:HD13	1:A:594:TYR:OH	1.75	0.85
3:C:56:GLU:OE1	3:D:286:HIS:CE1	2.29	0.85
2:B:355:LEU:HG	2:B:364:ILE:HD12	1.57	0.85
1:A:426:PHE:CE2	1:A:564:ILE:HD12	2.09	0.85
2:B:731:PHE:CZ	2:B:735:ILE:HD11	2.10	0.85
2:B:586:ILE:HD12	2:B:735:ILE:CD1	2.06	0.85
2:B:533:ARG:HD3	2:B:538:ILE:HD13	1.57	0.85
3:D:139:LEU:HD21	3:D:235:ILE:CD1	2.07	0.85
1:A:68:ILE:HD12	2:B:281:LYS:CD	2.07	0.85
3:D:17:VAL:CB	3:D:231:ILE:CD1	2.51	0.85
3:C:188:ILE:HD12	3:C:394:PHE:CD2	2.11	0.85
2:B:241:PHE:CB	2:B:254:ILE:CD1	2.54	0.84
1:A:118:ILE:CD1	1:A:190:TYR:CE1	2.60	0.84
2:B:293:ARG:NE	2:B:330:ILE:HD11	1.90	0.84
3:D:119:ILE:HD11	3:D:154:LEU:HD13	1.58	0.84
2:B:445:PHE:CE1	2:B:449:ILE:CD1	2.59	0.84
2:B:405:ILE:HD12	2:B:453:TYR:HD1	1.40	0.84
3:C:56:GLU:HB2	3:D:286:HIS:CD2	2.12	0.84
3:C:188:ILE:HD11	3:C:394:PHE:CD1	2.12	0.84
3:C:188:ILE:HD11	3:C:394:PHE:CB	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:276:THR:HB	3:C:284:ILE:HD12	1.58	0.84
1:A:663:TYR:HD1	1:A:672:ILE:HD13	1.43	0.84
2:B:772:PHE:CE1	2:B:812:ILE:HD13	2.11	0.84
3:C:57:ASN:HB2	3:D:285:ALA:HA	1.59	0.84
3:D:216:VAL:O	3:D:280:ILE:HD12	1.78	0.84
3:D:188:ILE:CD1	3:D:394:PHE:CB	2.53	0.84
3:C:188:ILE:CD1	3:C:394:PHE:CD1	2.60	0.84
1:A:118:ILE:HD13	1:A:190:TYR:CE1	2.12	0.84
1:A:74:TYR:HB3	2:B:215:ASN:HD22	1.41	0.84
1:A:425:ILE:HD13	1:A:482:LEU:HD13	1.58	0.84
2:B:526:ARG:NH2	2:B:538:ILE:HD11	1.93	0.84
3:D:127:ILE:CD1	3:D:162:TYR:CZ	2.61	0.84
3:D:242:ILE:HD11	3:D:252:MET:SD	2.17	0.84
3:D:280:ILE:HD13	3:D:371:GLU:CD	2.03	0.84
1:A:363:ILE:HD11	1:A:408:LEU:HD11	1.57	0.84
2:B:480:ILE:HD13	2:B:541:LEU:HD11	1.60	0.84
3:C:123:ILE:HD13	3:C:158:LEU:HD21	1.57	0.84
2:B:405:ILE:CD1	2:B:456:ILE:CD1	2.52	0.84
3:D:188:ILE:HD11	3:D:394:PHE:CB	2.08	0.84
1:A:643:ILE:HD13	1:A:692:LEU:HD21	1.58	0.84
1:A:366:ILE:HD12	1:A:404:ILE:HD11	1.60	0.83
3:D:242:ILE:CD1	3:D:252:MET:HE2	2.07	0.83
3:C:188:ILE:CD1	3:C:394:PHE:CD1	2.60	0.83
2:B:533:ARG:N	2:B:538:ILE:CD1	2.37	0.83
1:A:625:ILE:CD1	1:A:761:ILE:CB	2.56	0.83
3:C:188:ILE:CD1	3:C:394:PHE:HD2	1.85	0.83
2:B:493:ILE:CD1	2:B:598:TYR:CB	2.55	0.83
2:B:241:PHE:HB2	2:B:254:ILE:HD13	1.58	0.83
3:D:127:ILE:HD13	3:D:162:TYR:CZ	2.13	0.83
3:D:188:ILE:HD12	3:D:394:PHE:CB	2.09	0.83
2:B:438:TYR:CE2	2:B:441:ILE:HD12	2.14	0.83
2:B:533:ARG:HA	2:B:538:ILE:HD13	1.58	0.83
1:A:73:THR:H	2:B:215:ASN:ND2	1.75	0.83
2:B:257:ILE:HD12	2:B:297:TYR:CG	2.14	0.83
3:C:58:CYS:HB3	3:D:286:HIS:C	2.01	0.83
2:B:653:LEU:HD23	2:B:657:ILE:HD12	1.59	0.83
3:C:276:THR:OG1	3:C:284:ILE:HD11	1.76	0.83
1:A:128:ASP:HB3	2:B:299:ARG:NH2	1.94	0.83
1:A:557:ILE:CD1	1:A:594:TYR:OH	2.27	0.83
2:B:611:ILE:HD13	2:B:777:CYS:SG	2.18	0.83
1:A:625:ILE:HD12	1:A:761:ILE:HG21	1.53	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:139:LEU:HD21	3:D:235:ILE:HD13	1.61	0.83
1:A:143:ARG:HH12	2:B:292:ILE:CD1	1.89	0.82
2:B:430:HIS:ND1	2:B:448:ILE:HD11	1.92	0.82
2:B:398:LEU:HD11	2:B:449:ILE:HD12	1.60	0.82
1:A:70:LEU:HD22	2:B:220:LEU:HD21	1.60	0.82
3:D:216:VAL:O	3:D:280:ILE:CD1	2.27	0.82
3:C:166:ILE:HD13	3:C:256:TYR:CE2	2.13	0.82
2:B:241:PHE:CB	2:B:254:ILE:HD13	2.09	0.82
2:B:364:ILE:HD11	2:B:383:ILE:HD11	0.92	0.82
1:A:143:ARG:NH2	2:B:292:ILE:CD1	1.90	0.82
2:B:405:ILE:CG1	2:B:456:ILE:HD11	2.08	0.82
1:A:126:TRP:CZ2	1:A:192:ILE:HD13	2.14	0.82
3:C:188:ILE:HD11	3:C:394:PHE:CE1	2.15	0.82
3:C:58:CYS:SG	3:D:286:HIS:HA	0.24	0.82
2:B:489:MET:HE2	2:B:493:ILE:HD11	1.61	0.82
2:B:493:ILE:HD12	2:B:598:TYR:HB2	1.60	0.82
1:A:458:TYR:CD1	1:A:484:ILE:HD12	2.09	0.82
3:D:188:ILE:CD1	3:D:394:PHE:CD1	2.61	0.82
1:A:192:ILE:HD13	1:A:254:LYS:HG3	1.61	0.82
2:B:241:PHE:CB	2:B:254:ILE:HD11	2.08	0.82
1:A:425:ILE:HD13	1:A:564:ILE:CD1	2.10	0.82
3:C:188:ILE:HD13	3:C:394:PHE:CG	2.15	0.82
1:A:296:TYR:CB	2:B:322:HIS:HE1	1.92	0.82
1:A:134:VAL:HG13	1:A:275:ILE:HD13	1.62	0.82
1:A:599:LEU:CD1	1:A:640:ILE:HD12	2.09	0.81
3:D:127:ILE:HD13	3:D:162:TYR:CZ	2.15	0.81
1:A:625:ILE:HD13	1:A:761:ILE:HB	1.60	0.81
1:A:699:ILE:HD11	1:A:775:PHE:CE2	2.14	0.81
2:B:257:ILE:HD12	2:B:297:TYR:CD2	2.15	0.81
2:B:586:ILE:CD1	2:B:732:LEU:CD1	2.58	0.81
1:A:68:ILE:HD11	2:B:281:LYS:CD	2.10	0.81
1:A:557:ILE:HD13	1:A:594:TYR:CZ	2.15	0.81
1:A:366:ILE:HD12	1:A:404:ILE:CD1	2.11	0.81
3:C:59:ARG:HE	3:D:280:ILE:HD11	1.42	0.81
3:C:255:ILE:HD11	3:C:358:ARG:HH11	1.46	0.81
1:A:585:ILE:HD13	1:A:683:ILE:CD1	2.10	0.81
1:A:409:PHE:HE1	1:A:573:ILE:HD11	1.40	0.81
3:C:59:ARG:NH2	3:D:279:TYR:CB	2.41	0.81
1:A:585:ILE:CD1	1:A:683:ILE:HG21	2.11	0.81
3:D:166:ILE:HD12	3:D:252:MET:CE	2.10	0.81
1:A:74:TYR:HB3	2:B:215:ASN:ND2	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ILE:CD1	1:A:761:ILE:HD13	2.11	0.81
3:D:188:ILE:CD1	3:D:394:PHE:CB	2.41	0.81
3:D:188:ILE:HD11	3:D:394:PHE:CA	2.10	0.81
3:C:188:ILE:HD13	3:C:394:PHE:CD2	2.14	0.81
2:B:355:LEU:HB2	2:B:364:ILE:HD11	1.61	0.81
1:A:151:LEU:HD11	2:B:282:SER:HB2	1.60	0.81
2:B:335:PHE:CE2	2:B:339:ILE:HD11	2.16	0.80
2:B:480:ILE:CD1	2:B:537:VAL:HG13	2.11	0.80
1:A:566:ILE:CG1	1:A:574:ILE:CD1	2.57	0.80
3:D:241:SER:OG	3:D:322:ILE:HD12	1.81	0.80
1:A:585:ILE:HD12	1:A:683:ILE:HD11	1.58	0.80
2:B:241:PHE:CB	2:B:254:ILE:HD13	2.11	0.80
1:A:625:ILE:HD11	1:A:761:ILE:HD13	1.63	0.80
1:A:138:PHE:HD1	1:A:275:ILE:HD11	1.45	0.80
1:A:321:ASP:HB3	1:A:572:ILE:HD11	1.60	0.80
1:A:484:ILE:HD11	1:A:560:LEU:HD11	1.63	0.80
3:D:98:GLY:O	3:D:111:ILE:HD13	1.81	0.80
1:A:643:ILE:CD1	1:A:696:GLN:HE22	1.89	0.80
3:D:166:ILE:HD12	3:D:256:TYR:CD1	2.16	0.80
2:B:257:ILE:HD12	2:B:297:TYR:CE2	2.14	0.80
1:A:255:ILE:CD1	1:A:272:LEU:HD22	2.12	0.80
1:A:699:ILE:HD13	1:A:775:PHE:CE2	2.14	0.80
2:B:405:ILE:HD11	2:B:456:ILE:CG1	2.11	0.80
2:B:480:ILE:CD1	2:B:537:VAL:CG1	2.59	0.80
1:A:147:GLU:HG2	2:B:285:ARG:CG	2.10	0.80
1:A:699:ILE:HD13	1:A:775:PHE:HE2	1.47	0.80
1:A:613:LYS:HD3	1:A:614:TYR:O	1.81	0.80
3:C:123:ILE:HD11	3:C:154:LEU:HD11	1.64	0.80
1:A:147:GLU:HG3	2:B:285:ARG:CG	2.11	0.80
1:A:557:ILE:HD13	1:A:594:TYR:OH	1.80	0.80
1:A:375:ILE:CD1	1:A:396:LYS:HG2	2.11	0.80
1:A:138:PHE:CE2	1:A:192:ILE:HD12	2.16	0.80
3:C:58:CYS:CB	3:D:286:HIS:O	2.30	0.80
1:A:130:SER:CB	2:B:322:HIS:NE2	2.44	0.80
3:C:188:ILE:CD1	3:C:394:PHE:HB3	2.11	0.79
3:D:188:ILE:HD12	3:D:394:PHE:HB2	1.60	0.79
1:A:460:LYS:HZ2	2:B:833:ASP:CG	1.90	0.79
3:C:59:ARG:CZ	3:D:285:ALA:CB	2.57	0.79
3:C:188:ILE:HD11	3:C:394:PHE:HB2	1.56	0.79
2:B:533:ARG:O	2:B:538:ILE:CD1	2.31	0.79
3:C:188:ILE:HD12	3:C:394:PHE:CG	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:ARG:NH2	3:D:371:GLU:OE2	2.16	0.79
2:B:586:ILE:HD13	2:B:732:LEU:HD22	1.61	0.79
1:A:68:ILE:HD12	2:B:281:LYS:HD3	1.64	0.79
3:C:188:ILE:HD11	3:C:394:PHE:CD1	2.04	0.79
3:D:139:LEU:HD21	3:D:235:ILE:CD1	2.12	0.79
2:B:257:ILE:HD11	2:B:297:TYR:CD2	2.18	0.79
1:A:73:THR:HG22	2:B:215:ASN:HD21	1.46	0.79
3:C:241:SER:OG	3:C:322:ILE:HD11	1.82	0.79
1:A:74:TYR:H	2:B:215:ASN:HD21	1.31	0.79
1:A:425:ILE:HD13	1:A:482:LEU:HD11	1.65	0.78
3:C:60:ASN:H	3:D:286:HIS:CE1	2.01	0.78
2:B:257:ILE:HD12	2:B:297:TYR:CE2	2.17	0.78
3:C:127:ILE:HD12	3:C:162:TYR:CZ	2.18	0.78
3:D:119:ILE:HD13	3:D:154:LEU:HD22	1.66	0.78
3:D:255:ILE:HD13	3:D:358:ARG:NH2	1.98	0.78
3:C:242:ILE:CD1	3:C:252:MET:SD	2.71	0.78
2:B:250:LYS:HD3	2:B:254:ILE:HD11	1.64	0.78
1:A:774:ILE:CD1	1:A:796:SER:OG	2.30	0.78
1:A:625:ILE:CD1	1:A:761:ILE:HG23	2.12	0.78
1:A:68:ILE:HD11	2:B:281:LYS:HD3	1.64	0.78
1:A:566:ILE:HG13	1:A:574:ILE:HD12	1.63	0.78
3:C:258:THR:HG21	3:C:356:ILE:HD13	1.64	0.78
3:D:188:ILE:CD1	3:D:394:PHE:CB	2.61	0.78
1:A:70:LEU:HD11	2:B:216:PHE:O	1.83	0.78
2:B:493:ILE:CD1	2:B:598:TYR:CG	2.67	0.78
3:C:188:ILE:HD11	3:C:394:PHE:HB3	1.65	0.78
1:A:73:THR:CG2	2:B:215:ASN:ND2	2.47	0.78
3:D:127:ILE:HD13	3:D:162:TYR:HE2	1.49	0.78
1:A:143:ARG:NH1	2:B:292:ILE:HD11	1.86	0.78
3:D:139:LEU:HD21	3:D:235:ILE:HD11	1.66	0.78
1:A:599:LEU:HD11	1:A:640:ILE:CD1	2.12	0.78
3:D:5:ILE:CD1	3:D:53:PHE:CE2	2.64	0.78
2:B:499:ILE:HD12	2:B:511:LYS:HD3	1.66	0.78
1:A:599:LEU:HD13	1:A:640:ILE:HD12	1.64	0.77
3:D:280:ILE:HD13	3:D:371:GLU:HG3	1.65	0.77
2:B:634:ILE:CD1	2:B:772:PHE:CE1	2.67	0.77
3:C:127:ILE:CD1	3:C:162:TYR:CE2	2.68	0.77
2:B:772:PHE:HE1	2:B:812:ILE:CD1	1.96	0.77
2:B:402:ILE:CG2	2:B:449:ILE:HD13	2.14	0.77
1:A:663:TYR:CD1	1:A:672:ILE:HD13	2.18	0.77
1:A:118:ILE:CD1	1:A:190:TYR:OH	2.29	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:ARG:HH21	3:D:279:TYR:HB3	1.49	0.77
2:B:209:ILE:HD11	2:B:213:ILE:HD11	1.64	0.77
3:D:212:ILE:HD12	3:D:303:ASN:HD21	1.48	0.77
3:D:255:ILE:CD1	3:D:358:ARG:NH2	2.48	0.77
1:A:138:PHE:CD1	1:A:275:ILE:HD11	2.20	0.77
2:B:209:ILE:HD13	2:B:213:ILE:CD1	2.13	0.77
3:C:210:LEU:HG	3:C:222:ILE:HD11	1.64	0.77
2:B:296:ILE:CD1	2:B:319:PHE:HE1	1.90	0.77
1:A:643:ILE:HD13	1:A:696:GLN:NE2	1.97	0.77
3:D:188:ILE:HD11	3:D:427:ARG:NH2	1.99	0.77
1:A:421:HIS:CE1	1:A:425:ILE:CD1	2.68	0.77
2:B:213:ILE:HD11	2:B:221:LEU:HD22	1.66	0.77
2:B:367:ASN:O	2:B:384:GLU:OE2	2.03	0.77
3:D:212:ILE:HD12	3:D:303:ASN:ND2	1.99	0.77
1:A:296:TYR:CB	2:B:322:HIS:CE1	2.68	0.76
3:C:123:ILE:HD13	3:C:158:LEU:HD21	1.67	0.76
1:A:73:THR:HG22	2:B:215:ASN:ND2	1.99	0.76
3:C:188:ILE:CD1	3:C:394:PHE:CB	2.63	0.76
1:A:151:LEU:HD11	2:B:288:TYR:HE2	1.49	0.76
1:A:128:ASP:HB3	2:B:299:ARG:NH2	1.99	0.76
3:C:188:ILE:CD1	3:C:394:PHE:CB	2.63	0.76
3:D:188:ILE:HD11	3:D:394:PHE:N	2.00	0.76
2:B:405:ILE:HG23	2:B:456:ILE:CD1	2.16	0.76
1:A:797:SER:O	1:A:800:ASP:O	2.02	0.76
1:A:625:ILE:HD11	1:A:758:LEU:CD1	2.16	0.76
1:A:151:LEU:HD11	2:B:281:LYS:HE2	1.65	0.76
1:A:70:LEU:O	2:B:216:PHE:CE2	2.38	0.76
2:B:482:LEU:HB3	2:B:657:ILE:HD11	1.66	0.76
1:A:625:ILE:HD13	1:A:761:ILE:HD13	1.66	0.76
1:A:143:ARG:NH2	2:B:288:TYR:CE2	2.54	0.76
1:A:625:ILE:HD11	1:A:758:LEU:HD12	1.68	0.76
2:B:209:ILE:HD12	2:B:213:ILE:CD1	2.16	0.76
3:C:204:PHE:CB	3:C:231:ILE:HD11	2.16	0.76
1:A:195:GLU:HG3	1:A:250:ILE:HD13	1.67	0.76
3:C:322:ILE:CD1	3:C:358:ARG:NH2	2.46	0.75
2:B:586:ILE:CD1	2:B:732:LEU:CD2	2.64	0.75
2:B:631:LEU:HD12	2:B:631:LEU:H	1.50	0.75
1:A:625:ILE:CD1	1:A:761:ILE:CD1	2.60	0.75
3:D:280:ILE:HD13	3:D:371:GLU:CG	2.16	0.75
2:B:241:PHE:CB	2:B:254:ILE:HD11	2.16	0.75
1:A:557:ILE:HD11	1:A:594:TYR:CZ	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:612:ARG:O	2:B:776:TYR:CD2	2.38	0.75
3:C:58:CYS:HB2	3:D:284:ILE:HB	1.67	0.75
3:C:188:ILE:HD11	3:C:394:PHE:HB2	1.68	0.75
1:A:585:ILE:HD11	1:A:683:ILE:HG21	1.67	0.75
2:B:499:ILE:HD13	2:B:508:PRO:HA	1.69	0.75
2:B:743:THR:O	2:B:756:GLN:HA	1.85	0.75
2:B:525:LEU:HB2	2:B:538:ILE:HD12	1.69	0.75
2:B:656:ILE:HD13	2:B:738:HIS:CD2	2.22	0.74
2:B:772:PHE:HE1	2:B:812:ILE:CD1	1.99	0.74
2:B:493:ILE:HD13	2:B:598:TYR:CB	2.17	0.74
2:B:739:LYS:O	2:B:743:THR:O	2.05	0.74
3:D:188:ILE:HD13	3:D:394:PHE:HB2	1.69	0.74
2:B:843:LYS:O	2:B:846:ARG:O	2.04	0.74
1:A:151:LEU:HB3	2:B:285:ARG:CZ	2.17	0.74
2:B:250:LYS:HD2	2:B:254:ILE:HD12	1.66	0.74
3:D:123:ILE:HD11	3:D:154:LEU:HD11	1.69	0.74
1:A:625:ILE:CD1	1:A:761:ILE:CD1	2.65	0.74
3:D:212:ILE:HD13	3:D:275:PHE:CE2	2.22	0.74
1:A:409:PHE:HZ	1:A:573:ILE:HD11	1.52	0.74
2:B:445:PHE:CZ	2:B:449:ILE:HD11	2.21	0.74
3:C:188:ILE:CD1	3:C:394:PHE:HB2	2.17	0.74
3:D:127:ILE:CD1	3:D:162:TYR:CE2	2.71	0.74
3:C:188:ILE:HD12	3:C:394:PHE:CB	2.17	0.74
3:C:188:ILE:CD1	3:C:394:PHE:CD1	2.70	0.74
1:A:321:ASP:CB	1:A:572:ILE:HD11	2.17	0.74
1:A:625:ILE:HD13	1:A:761:ILE:CG1	2.18	0.74
2:B:405:ILE:CG2	2:B:456:ILE:HD12	2.17	0.74
1:A:625:ILE:CG2	1:A:765:ILE:CD1	2.65	0.74
3:D:212:ILE:HD11	3:D:302:SER:C	2.12	0.74
1:A:133:MET:SD	2:B:322:HIS:HA	2.28	0.74
1:A:118:ILE:HD12	1:A:189:LEU:HD11	1.68	0.74
3:D:127:ILE:CD1	3:D:162:TYR:CZ	2.70	0.74
1:A:371:SER:OG	1:A:404:ILE:CD1	2.36	0.73
1:A:143:ARG:HH21	2:B:288:TYR:HD2	0.75	0.73
2:B:402:ILE:HG22	2:B:449:ILE:HD12	1.70	0.73
3:D:212:ILE:CD1	3:D:302:SER:O	2.35	0.73
3:D:188:ILE:CD1	3:D:394:PHE:CB	2.65	0.73
3:C:188:ILE:HD12	3:C:394:PHE:CD1	2.23	0.73
2:B:586:ILE:CD1	2:B:735:ILE:CD1	2.66	0.73
1:A:375:ILE:CD1	1:A:396:LYS:CE	2.66	0.73
3:C:188:ILE:HD12	3:C:394:PHE:CG	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:212:ILE:HD13	3:D:303:ASN:ND2	2.03	0.73
1:A:108:ARG:HH21	1:A:177:ILE:CD1	1.97	0.73
3:C:258:THR:CG2	3:C:356:ILE:HD12	2.19	0.73
1:A:128:ASP:HB3	2:B:299:ARG:HH12	1.52	0.73
1:A:625:ILE:HG21	1:A:765:ILE:CD1	2.18	0.73
3:D:280:ILE:CD1	3:D:371:GLU:CD	2.59	0.73
2:B:526:ARG:NH2	2:B:538:ILE:CD1	2.50	0.73
3:C:188:ILE:CD1	3:C:394:PHE:CG	2.71	0.73
3:C:255:ILE:CD1	3:C:358:ARG:NH1	2.52	0.73
2:B:349:TRP:CZ3	2:B:364:ILE:HD11	2.23	0.73
2:B:493:ILE:HD13	2:B:598:TYR:HB3	1.69	0.73
3:D:188:ILE:HD12	3:D:394:PHE:HB3	1.70	0.73
3:D:166:ILE:HD12	3:D:252:MET:HE2	1.69	0.73
1:A:80:ASP:O	1:A:90:ILE:N	2.22	0.73
1:A:363:ILE:HD11	1:A:366:ILE:CB	2.12	0.73
1:A:108:ARG:HH11	1:A:177:ILE:HD12	1.54	0.73
1:A:142:ILE:HD13	1:A:189:LEU:CD1	2.19	0.73
2:B:739:LYS:O	2:B:743:THR:O	2.05	0.73
3:D:17:VAL:CG2	3:D:231:ILE:HD11	2.19	0.73
3:C:210:LEU:CD1	3:C:222:ILE:HD13	2.19	0.72
2:B:493:ILE:HD12	2:B:598:TYR:CB	2.18	0.72
1:A:134:VAL:HG13	1:A:275:ILE:CD1	2.15	0.72
3:C:5:ILE:HD11	3:C:252:MET:CE	2.18	0.72
1:A:599:LEU:CD1	1:A:640:ILE:HD11	2.15	0.72
2:B:525:LEU:O	2:B:538:ILE:CD1	2.37	0.72
1:A:138:PHE:HE2	1:A:192:ILE:CD1	2.02	0.72
1:A:147:GLU:OE2	2:B:288:TYR:CE2	2.42	0.72
3:C:212:ILE:HD11	3:C:300:ASP:O	1.87	0.72
1:A:143:ARG:HD2	2:B:288:TYR:OH	1.89	0.72
1:A:71:GLU:HA	2:B:216:PHE:CZ	2.24	0.72
3:D:284:ILE:HG22	3:D:370:ASN:H	1.54	0.72
1:A:72:GLY:O	2:B:215:ASN:OD1	2.06	0.72
1:A:133:MET:SD	2:B:323:GLY:HA3	2.28	0.72
3:C:280:ILE:HD11	3:C:284:ILE:HD11	1.72	0.72
2:B:533:ARG:CD	2:B:538:ILE:HD13	2.18	0.72
2:B:822:ARG:NH1	2:B:825:ILE:HD12	2.04	0.72
1:A:797:SER:O	1:A:800:ASP:O	2.06	0.72
2:B:405:ILE:HG13	2:B:456:ILE:HD11	1.69	0.72
3:D:222:ILE:HD11	3:D:227:THR:OG1	1.89	0.72
3:C:127:ILE:HD12	3:C:162:TYR:HE2	1.55	0.72
3:C:188:ILE:CD1	3:C:394:PHE:HD2	1.97	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD12	2:B:216:PHE:CE2	2.25	0.72
3:D:188:ILE:HD11	3:D:427:ARG:HH21	1.54	0.72
2:B:250:LYS:HD2	2:B:254:ILE:CD1	2.20	0.72
1:A:356:VAL:HG13	1:A:572:ILE:HD12	1.71	0.72
2:B:241:PHE:HB3	2:B:254:ILE:HD13	1.71	0.72
3:C:56:GLU:CB	3:D:286:HIS:CD2	2.73	0.71
2:B:499:ILE:HD11	2:B:508:PRO:CD	2.19	0.71
2:B:564:LEU:HD13	2:B:564:LEU:H	1.55	0.71
2:B:398:LEU:HD21	2:B:449:ILE:HD11	1.73	0.71
3:D:255:ILE:HD11	3:D:320:ASN:ND2	2.06	0.71
2:B:512:LEU:HA	2:B:515:VAL:HG22	1.73	0.71
2:B:441:ILE:HD12	2:B:443:THR:HG22	1.71	0.71
3:D:188:ILE:HD11	3:D:394:PHE:CD2	2.25	0.71
1:A:375:ILE:CD1	1:A:396:LYS:HE3	2.20	0.71
2:B:364:ILE:HD13	2:B:403:PHE:CD1	2.25	0.71
3:D:127:ILE:CD1	3:D:162:TYR:OH	2.39	0.71
3:D:195:ILE:HD11	3:D:423:PHE:HE1	1.56	0.71
2:B:405:ILE:CD1	2:B:456:ILE:CG1	2.68	0.71
3:D:213:SER:HB3	3:D:222:ILE:CD1	2.20	0.71
1:A:321:ASP:CG	1:A:572:ILE:HD11	2.16	0.71
1:A:599:LEU:CD2	1:A:640:ILE:HD11	2.17	0.71
1:A:625:ILE:HG13	1:A:765:ILE:HD11	1.71	0.71
1:A:143:ARG:NH2	2:B:288:TYR:CD2	2.59	0.71
1:A:695:LEU:HD23	1:A:774:ILE:HD11	1.73	0.71
1:A:557:ILE:HD11	1:A:594:TYR:OH	1.90	0.71
1:A:73:THR:HG22	2:B:215:ASN:ND2	2.06	0.70
2:B:250:LYS:CD	2:B:254:ILE:CD1	2.69	0.70
2:B:499:ILE:HD12	2:B:512:LEU:HD22	1.71	0.70
3:C:322:ILE:HD13	3:C:358:ARG:HH21	1.54	0.70
1:A:133:MET:SD	2:B:323:GLY:N	2.64	0.70
1:A:699:ILE:HD12	1:A:775:PHE:CZ	2.26	0.70
1:A:136:GLN:HE22	2:B:324:ASP:HB2	1.55	0.70
1:A:70:LEU:HD22	2:B:216:PHE:O	1.90	0.70
1:A:460:LYS:NZ	2:B:833:ASP:CG	2.49	0.70
3:D:5:ILE:CD1	3:D:53:PHE:CZ	2.67	0.70
1:A:151:LEU:HD22	2:B:285:ARG:CB	2.21	0.70
3:D:188:ILE:HD12	3:D:394:PHE:HB2	1.70	0.70
2:B:499:ILE:CD1	2:B:508:PRO:HA	2.20	0.70
1:A:661:LYS:HG2	1:A:664:ARG:HH21	1.57	0.70
2:B:628:ILE:HG12	2:B:629:ASN:H	1.57	0.70
3:D:188:ILE:HD12	3:D:394:PHE:CG	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ILE:HD13	1:A:393:TYR:HA	1.74	0.70
2:B:480:ILE:HD11	2:B:541:LEU:HD13	1.74	0.70
3:C:188:ILE:HD11	3:C:391:CYS:HA	1.74	0.70
1:A:557:ILE:HD13	1:A:594:TYR:CE2	2.27	0.70
2:B:586:ILE:HD12	2:B:732:LEU:HD12	1.73	0.70
1:A:625:ILE:HD12	1:A:761:ILE:CD1	2.21	0.70
2:B:567:PRO:HG2	2:B:721:ILE:HD12	1.72	0.70
3:D:188:ILE:HD12	3:D:394:PHE:HB2	1.74	0.70
1:A:585:ILE:HD11	1:A:683:ILE:HG23	1.74	0.70
3:C:59:ARG:HH22	3:D:279:TYR:HB3	1.53	0.70
1:A:148:ASP:OD1	2:B:288:TYR:OH	2.10	0.70
1:A:138:PHE:CE2	1:A:275:ILE:HD11	2.27	0.70
2:B:412:LEU:CD1	2:B:463:ILE:HD13	2.22	0.70
3:C:127:ILE:HD13	3:C:162:TYR:CE2	2.26	0.69
3:D:188:ILE:CD1	3:D:394:PHE:HB3	2.22	0.69
1:A:625:ILE:HD11	1:A:765:ILE:HG13	1.72	0.69
3:C:258:THR:HG23	3:C:356:ILE:HD11	1.74	0.69
3:C:188:ILE:HD11	3:C:394:PHE:HD2	1.56	0.69
1:A:72:GLY:C	2:B:215:ASN:HB2	2.12	0.69
1:A:567:PRO:CD	1:A:574:ILE:HD11	2.18	0.69
1:A:599:LEU:HD22	1:A:640:ILE:HD13	1.74	0.69
2:B:586:ILE:CD1	2:B:732:LEU:HD22	2.18	0.69
1:A:585:ILE:HD13	1:A:683:ILE:CD1	2.23	0.69
2:B:445:PHE:HE1	2:B:449:ILE:CD1	2.00	0.69
1:A:695:LEU:CD2	1:A:774:ILE:HD11	2.22	0.69
1:A:606:LEU:CG	1:A:710:ILE:HD13	2.21	0.69
3:C:280:ILE:CD1	3:C:284:ILE:CG1	2.70	0.69
2:B:349:TRP:CH2	2:B:383:ILE:HD13	2.27	0.69
3:D:139:LEU:HD21	3:D:235:ILE:HD11	1.74	0.69
3:D:188:ILE:HD13	3:D:394:PHE:CD1	2.27	0.69
1:A:421:HIS:HE1	1:A:425:ILE:HD11	1.55	0.69
3:D:188:ILE:CD1	3:D:394:PHE:CG	2.74	0.69
3:C:123:ILE:HD11	3:C:154:LEU:HD11	1.73	0.69
1:A:625:ILE:CG1	1:A:765:ILE:CD1	2.70	0.69
3:C:280:ILE:CD1	3:C:284:ILE:CD1	2.70	0.69
3:C:127:ILE:CD1	3:C:162:TYR:HE2	2.05	0.69
3:D:195:ILE:CD1	3:D:423:PHE:HE1	2.05	0.69
3:C:123:ILE:HD11	3:C:154:LEU:CD1	2.23	0.69
1:A:375:ILE:HD12	1:A:396:LYS:HE2	1.73	0.69
3:C:255:ILE:HD11	3:C:358:ARG:NH1	2.06	0.69
2:B:365:ALA:HB2	2:B:389:ARG:HH22	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ILE:HD11	1:A:478:MET:HA	1.75	0.69
2:B:405:ILE:CD1	2:B:456:ILE:HG13	2.21	0.69
3:C:280:ILE:HD13	3:C:284:ILE:CG1	2.22	0.69
3:C:188:ILE:HD13	3:C:394:PHE:CD1	2.28	0.69
1:A:136:GLN:NE2	2:B:324:ASP:HB2	2.07	0.69
1:A:774:ILE:HD13	1:A:796:SER:HB2	1.74	0.69
2:B:612:ARG:O	2:B:776:TYR:CE2	2.45	0.69
2:B:398:LEU:CD2	2:B:449:ILE:HD11	2.22	0.69
3:D:242:ILE:CD1	3:D:252:MET:HB2	2.23	0.69
3:D:258:THR:OG1	3:D:356:ILE:CD1	2.40	0.69
3:C:188:ILE:HD12	3:C:394:PHE:HB2	1.74	0.68
2:B:234:LEU:CD2	2:B:257:ILE:HD11	2.22	0.68
1:A:74:TYR:CB	2:B:215:ASN:ND2	2.56	0.68
1:A:128:ASP:CG	2:B:299:ARG:HH22	1.99	0.68
1:A:606:LEU:HD12	1:A:710:ILE:CD1	2.21	0.68
2:B:234:LEU:HD23	2:B:257:ILE:HD11	1.74	0.68
3:C:8:LEU:CD2	3:C:67:ILE:HD12	2.23	0.68
1:A:774:ILE:HD12	1:A:796:SER:HB2	1.51	0.68
2:B:430:HIS:ND1	2:B:448:ILE:CD1	2.56	0.68
3:C:127:ILE:HD12	3:C:162:TYR:OH	1.94	0.68
1:A:70:LEU:HD13	2:B:216:PHE:HA	1.74	0.68
3:D:119:ILE:CD1	3:D:154:LEU:HD22	2.23	0.68
3:D:127:ILE:HD12	3:D:162:TYR:OH	1.94	0.68
3:D:98:GLY:CA	3:D:111:ILE:HD12	2.23	0.68
2:B:656:ILE:CD1	2:B:738:HIS:CD2	2.76	0.68
1:A:375:ILE:HD13	1:A:396:LYS:CE	2.24	0.68
1:A:73:THR:HG22	2:B:215:ASN:HD21	0.75	0.68
1:A:73:THR:CG2	2:B:215:ASN:ND2	2.43	0.68
1:A:105:PHE:CZ	1:A:109:ILE:CD1	2.73	0.68
2:B:438:TYR:CG	2:B:441:ILE:HD12	2.28	0.68
2:B:257:ILE:HD12	2:B:297:TYR:CD2	2.29	0.68
1:A:625:ILE:HD12	1:A:761:ILE:CG2	2.07	0.68
1:A:357:VAL:CG2	1:A:363:ILE:HD12	2.23	0.68
2:B:213:ILE:CD1	2:B:221:LEU:HD22	2.23	0.68
1:A:138:PHE:CE1	1:A:275:ILE:CD1	2.74	0.68
3:C:59:ARG:HE	3:D:280:ILE:CD1	2.05	0.68
3:C:188:ILE:HD11	3:C:394:PHE:HB2	1.75	0.68
3:C:258:THR:HG21	3:C:356:ILE:HD13	1.77	0.68
1:A:366:ILE:CD1	1:A:404:ILE:HD13	2.24	0.68
3:C:58:CYS:N	3:D:287:LYS:HG3	2.09	0.67
1:A:643:ILE:HD11	1:A:696:GLN:NE2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HD21	2:B:282:SER:HB2	1.75	0.67
1:A:599:LEU:HD11	1:A:640:ILE:HD13	1.73	0.67
3:C:188:ILE:HD11	3:C:394:PHE:HB3	1.73	0.67
1:A:143:ARG:CZ	2:B:288:TYR:HE2	1.97	0.67
1:A:70:LEU:CD2	2:B:220:LEU:HD21	2.24	0.67
2:B:398:LEU:HD21	2:B:449:ILE:CD1	2.25	0.67
2:B:430:HIS:CG	2:B:448:ILE:HD12	2.29	0.67
1:A:426:PHE:CZ	1:A:564:ILE:HD12	2.24	0.67
3:C:123:ILE:HD11	3:C:154:LEU:CD1	2.21	0.67
2:B:402:ILE:CG2	2:B:449:ILE:CD1	2.70	0.67
1:A:105:PHE:CE1	1:A:109:ILE:HD11	2.28	0.67
1:A:641:LYS:HG2	3:C:356:ILE:HD13	1.77	0.67
1:A:151:LEU:CD2	2:B:285:ARG:HG3	2.23	0.67
1:A:68:ILE:CD1	2:B:281:LYS:HD2	2.24	0.67
2:B:739:LYS:O	2:B:743:THR:O	2.13	0.67
2:B:493:ILE:HD13	2:B:598:TYR:HB3	1.77	0.67
2:B:287:ILE:HG12	2:B:290:ASN:HD21	1.59	0.67
2:B:402:ILE:HD11	2:B:449:ILE:HD11	1.77	0.67
2:B:402:ILE:CG2	2:B:449:ILE:CD1	2.73	0.67
3:D:188:ILE:CD1	3:D:394:PHE:CG	2.78	0.67
2:B:296:ILE:HD13	2:B:319:PHE:HZ	1.54	0.67
2:B:772:PHE:CD2	2:B:812:ILE:HD13	2.30	0.67
3:C:59:ARG:NH2	3:D:285:ALA:HB3	1.95	0.67
1:A:133:MET:SD	2:B:323:GLY:CA	2.83	0.67
2:B:532:PRO:C	2:B:538:ILE:HD12	2.21	0.66
1:A:143:ARG:HH21	2:B:288:TYR:HD2	1.42	0.66
3:C:204:PHE:CD2	3:C:231:ILE:CD1	2.76	0.66
1:A:639:PHE:CZ	1:A:643:ILE:CD1	2.71	0.66
3:D:213:SER:HB3	3:D:222:ILE:HD11	1.76	0.66
3:C:258:THR:OG1	3:C:356:ILE:HD11	1.95	0.66
2:B:405:ILE:HD13	2:B:452:GLN:CD	2.20	0.66
1:A:557:ILE:CD1	1:A:594:TYR:CZ	2.78	0.66
2:B:779:LEU:HG	2:B:780:ASN:O	1.96	0.66
3:D:255:ILE:HD12	3:D:358:ARG:NE	2.10	0.66
1:A:557:ILE:HD11	1:A:594:TYR:CZ	2.31	0.66
2:B:293:ARG:HG3	2:B:330:ILE:CD1	2.26	0.66
1:A:202:GLU:HA	1:A:205:THR:O	1.95	0.66
1:A:625:ILE:HG22	1:A:765:ILE:HD13	1.76	0.66
2:B:349:TRP:CH2	2:B:383:ILE:CD1	2.79	0.66
3:C:59:ARG:HG2	3:D:280:ILE:CD1	2.23	0.66
2:B:586:ILE:CD1	2:B:732:LEU:HG	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:TRP:HH2	2:B:383:ILE:HD13	1.61	0.66
2:B:540:GLY:HA3	2:B:563:ILE:HD13	1.77	0.66
3:C:188:ILE:CD1	3:C:394:PHE:CE2	2.67	0.66
2:B:493:ILE:CD1	2:B:598:TYR:CB	2.73	0.66
3:D:242:ILE:HD12	3:D:252:MET:HE2	1.76	0.66
2:B:843:LYS:O	2:B:846:ARG:O	2.13	0.66
2:B:546:LEU:HB2	2:B:550:HIS:CE1	2.31	0.65
3:D:209:LEU:HD21	3:D:231:ILE:HD11	1.77	0.65
2:B:772:PHE:CE1	2:B:812:ILE:CD1	2.78	0.65
2:B:772:PHE:CE1	2:B:812:ILE:HD13	2.30	0.65
1:A:356:VAL:CG1	1:A:572:ILE:HD12	2.26	0.65
3:D:328:PRO:HB2	3:D:331:ILE:HD12	1.78	0.65
2:B:355:LEU:HB3	2:B:364:ILE:HD12	1.73	0.65
1:A:137:ARG:HH21	2:B:328:ARG:HH12	0.67	0.65
3:D:320:ASN:HD22	3:D:356:ILE:HB	1.62	0.65
1:A:134:VAL:HG13	1:A:275:ILE:HD13	1.79	0.65
2:B:586:ILE:HD12	2:B:735:ILE:HD12	1.75	0.65
2:B:402:ILE:HG12	2:B:449:ILE:CD1	2.27	0.65
2:B:527:HIS:CE1	2:B:538:ILE:HD11	2.31	0.65
2:B:628:ILE:HG12	2:B:629:ASN:H	1.62	0.65
1:A:112:TYR:CZ	1:A:177:ILE:HD13	2.32	0.65
1:A:137:ARG:HA	2:B:324:ASP:OD1	1.96	0.65
3:C:280:ILE:CD1	3:C:284:ILE:HG12	2.26	0.65
3:D:119:ILE:CD1	3:D:154:LEU:CD1	2.59	0.65
3:D:84:ARG:H	3:D:84:ARG:HE	1.45	0.65
1:A:296:TYR:HB2	2:B:322:HIS:CE1	2.31	0.65
3:D:213:SER:HB3	3:D:222:ILE:CD1	2.24	0.65
3:D:98:GLY:O	3:D:111:ILE:CD1	2.45	0.65
1:A:698:GLN:OE1	1:A:774:ILE:HD11	1.96	0.65
1:A:137:ARG:HH22	2:B:328:ARG:HH12	1.43	0.65
1:A:70:LEU:O	2:B:216:PHE:CD2	2.50	0.65
1:A:458:TYR:CD1	1:A:484:ILE:HD13	2.32	0.65
1:A:63:LEU:HG	1:A:170:ILE:HD11	1.79	0.65
2:B:499:ILE:HD11	2:B:508:PRO:CG	2.24	0.65
2:B:822:ARG:HH11	2:B:825:ILE:HD12	1.62	0.65
1:A:625:ILE:CG1	1:A:765:ILE:HD11	2.26	0.65
1:A:151:LEU:HD12	2:B:285:ARG:CG	2.27	0.64
3:D:255:ILE:CD1	3:D:358:ARG:CZ	2.71	0.64
2:B:220:LEU:HD13	2:B:224:ILE:HD12	1.79	0.64
3:C:258:THR:OG1	3:C:356:ILE:CD1	2.37	0.64
3:D:328:PRO:HB2	3:D:331:ILE:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:LEU:HD21	3:C:67:ILE:HD12	1.80	0.64
3:D:212:ILE:HD13	3:D:303:ASN:CG	2.21	0.64
1:A:142:ILE:HD13	1:A:189:LEU:HD13	1.79	0.64
3:C:276:THR:CB	3:C:284:ILE:CD1	2.67	0.64
3:D:98:GLY:N	3:D:111:ILE:HD12	2.13	0.64
3:D:188:ILE:HD11	3:D:393:THR:C	2.22	0.64
1:A:699:ILE:HD12	1:A:775:PHE:HZ	1.61	0.64
1:A:255:ILE:HD13	1:A:272:LEU:HD22	1.78	0.64
3:C:127:ILE:HD12	3:C:162:TYR:CE2	2.33	0.64
2:B:293:ARG:HD3	2:B:330:ILE:CD1	2.28	0.64
2:B:567:PRO:CG	2:B:721:ILE:HD12	2.27	0.64
1:A:372:ASP:HB3	1:A:375:ILE:HD12	1.80	0.64
1:A:73:THR:CG2	2:B:215:ASN:HD21	2.09	0.64
1:A:133:MET:HE3	2:B:323:GLY:CA	2.28	0.64
2:B:586:ILE:CD1	2:B:732:LEU:CG	2.72	0.64
3:D:97:ASP:HB2	3:D:111:ILE:HD11	1.80	0.63
1:A:128:ASP:CB	2:B:299:ARG:NH2	2.61	0.63
1:A:695:LEU:HD21	1:A:774:ILE:CD1	2.04	0.63
1:A:699:ILE:HD13	1:A:775:PHE:CZ	2.33	0.63
2:B:586:ILE:HD11	2:B:735:ILE:HD12	1.80	0.63
3:D:443:ASP:HB3	3:D:445:TYR:O	1.98	0.63
3:C:188:ILE:HD12	3:C:394:PHE:CB	2.28	0.63
2:B:772:PHE:CE2	2:B:812:ILE:HD13	2.34	0.63
1:A:625:ILE:HG21	1:A:765:ILE:HD12	1.80	0.63
2:B:202:PHE:CD1	2:B:207:ILE:HD11	2.33	0.63
1:A:137:ARG:HH12	2:B:325:LEU:CD2	2.09	0.63
1:A:643:ILE:HD13	1:A:692:LEU:HD13	1.81	0.63
2:B:250:LYS:CD	2:B:254:ILE:HD11	2.28	0.63
1:A:151:LEU:HG	2:B:282:SER:HA	1.80	0.63
2:B:405:ILE:CD1	2:B:456:ILE:HD13	2.28	0.63
2:B:493:ILE:HD12	2:B:598:TYR:HB2	1.80	0.63
2:B:493:ILE:HD11	2:B:598:TYR:CD1	2.33	0.63
1:A:643:ILE:HD11	1:A:696:GLN:HE21	1.62	0.63
1:A:133:MET:HE3	2:B:323:GLY:HA3	1.80	0.63
2:B:430:HIS:HB3	2:B:448:ILE:HD13	1.81	0.63
3:C:280:ILE:HD12	3:C:284:ILE:HD11	1.81	0.63
1:A:625:ILE:CD1	1:A:761:ILE:HG12	2.26	0.63
1:A:366:ILE:CD1	1:A:404:ILE:CD1	2.77	0.63
3:C:188:ILE:CD1	3:C:394:PHE:HB2	2.29	0.63
1:A:474:PRO:HB3	2:B:670:ARG:HH22	1.64	0.63
3:C:241:SER:OG	3:C:322:ILE:HD12	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:ILE:CD1	2:B:221:LEU:CD1	2.49	0.63
3:C:265:LEU:HD22	3:C:317:ASN:HD22	1.64	0.63
3:C:204:PHE:HB3	3:C:231:ILE:HD11	1.81	0.63
2:B:342:TYR:CE2	2:B:394:ILE:HD12	2.34	0.63
1:A:339:GLU:CD	1:A:339:GLU:H	2.07	0.63
2:B:296:ILE:CD1	2:B:327:ILE:CD1	2.63	0.62
3:C:59:ARG:NH2	3:D:284:ILE:C	2.57	0.62
3:D:412:LEU:H	3:D:412:LEU:HD22	1.62	0.62
1:A:71:GLU:HA	2:B:216:PHE:CE2	2.34	0.62
3:C:256:TYR:CD1	3:C:260:ILE:HD12	2.34	0.62
3:D:72:GLU:HG3	3:D:76:ILE:HD12	1.80	0.62
3:C:17:VAL:HG22	3:C:228:ASN:HB3	1.80	0.62
3:C:292:TYR:CE1	3:C:296:LEU:HD21	2.34	0.62
2:B:250:LYS:HD3	2:B:254:ILE:CD1	2.30	0.62
2:B:601:GLN:HE22	2:B:605:LEU:HD11	1.65	0.62
2:B:296:ILE:HD11	2:B:319:PHE:HE1	1.57	0.62
2:B:405:ILE:CD1	2:B:452:GLN:CD	2.72	0.62
3:C:188:ILE:HD13	3:C:394:PHE:HD1	1.54	0.62
2:B:405:ILE:CD1	2:B:456:ILE:CD1	2.76	0.62
2:B:207:ILE:HD13	2:B:221:LEU:HD22	1.81	0.62
1:A:73:THR:HG22	2:B:215:ASN:CG	2.24	0.62
3:D:212:ILE:HD12	3:D:303:ASN:ND2	2.14	0.62
3:D:139:LEU:HD21	3:D:235:ILE:HD11	1.82	0.62
1:A:366:ILE:HD11	1:A:371:SER:CB	2.27	0.62
1:A:128:ASP:CB	2:B:299:ARG:HH22	2.12	0.62
2:B:349:TRP:CZ3	2:B:383:ILE:CD1	2.82	0.62
3:D:241:SER:OG	3:D:255:ILE:HD11	1.97	0.62
3:D:6:ILE:HD13	3:D:126:GLU:HB3	1.82	0.62
1:A:484:ILE:CD1	1:A:560:LEU:HD11	2.30	0.62
3:C:5:ILE:HD11	3:C:252:MET:HE1	1.82	0.62
2:B:250:LYS:HE2	2:B:254:ILE:HD12	1.81	0.62
3:C:258:THR:HG21	3:C:356:ILE:HD12	1.71	0.62
1:A:285:GLU:HB3	1:A:291:ILE:HG23	1.82	0.62
1:A:68:ILE:HD12	2:B:281:LYS:HD2	1.82	0.62
2:B:250:LYS:CD	2:B:254:ILE:HD12	2.30	0.62
1:A:133:MET:HE3	2:B:323:GLY:HA3	1.82	0.62
1:A:599:LEU:HD13	1:A:640:ILE:HD11	1.80	0.61
2:B:181:GLU:HB3	2:B:184:ILE:HD12	1.82	0.61
1:A:585:ILE:CD1	1:A:683:ILE:CG2	2.73	0.61
1:A:375:ILE:HD11	1:A:396:LYS:CG	2.29	0.61
3:D:241:SER:OG	3:D:322:ILE:CD1	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:CD1	2:B:288:TYR:HE2	2.11	0.61
2:B:188:VAL:CG1	2:B:224:ILE:HD11	2.28	0.61
3:D:212:ILE:CD1	3:D:303:ASN:HA	2.30	0.61
2:B:493:ILE:HD12	2:B:598:TYR:CG	2.36	0.61
1:A:128:ASP:OD1	2:B:295:ARG:CZ	2.47	0.61
1:A:368:SER:HA	1:A:373:ILE:HD13	1.81	0.61
1:A:421:HIS:NE2	1:A:425:ILE:HD12	2.15	0.61
2:B:405:ILE:CG1	2:B:456:ILE:HD13	2.07	0.61
1:A:133:MET:HE1	2:B:323:GLY:H	1.66	0.61
1:A:581:LYS:HB3	1:A:683:ILE:CD1	2.27	0.61
1:A:625:ILE:HG13	1:A:765:ILE:HD13	1.77	0.61
1:A:606:LEU:HD11	1:A:710:ILE:CD1	2.30	0.61
2:B:241:PHE:HB3	2:B:254:ILE:CD1	2.30	0.61
1:A:141:GLU:HG3	1:A:144:ARG:HH21	1.66	0.61
3:C:322:ILE:HD13	3:C:358:ARG:CZ	2.30	0.61
1:A:425:ILE:CD1	1:A:482:LEU:HD13	2.31	0.61
2:B:634:ILE:HD11	2:B:772:PHE:CD1	2.35	0.61
3:D:98:GLY:HA2	3:D:111:ILE:HD12	1.82	0.61
1:A:367:PRO:HG3	1:A:373:ILE:HD13	1.82	0.61
3:C:322:ILE:HD13	3:C:358:ARG:NH2	2.16	0.61
2:B:349:TRP:CZ3	2:B:364:ILE:CD1	2.84	0.61
3:D:258:THR:CG2	3:D:356:ILE:CD1	2.68	0.61
1:A:122:ALA:HB1	1:A:126:TRP:CZ2	2.36	0.61
3:D:212:ILE:HD12	3:D:303:ASN:HA	1.82	0.61
2:B:612:ARG:O	2:B:776:TYR:CD2	2.53	0.61
2:B:402:ILE:HD11	2:B:449:ILE:HD13	1.83	0.61
3:D:127:ILE:CD1	3:D:162:TYR:OH	2.48	0.61
2:B:493:ILE:CD1	2:B:598:TYR:HB2	2.31	0.61
2:B:478:LYS:HA	2:B:482:LEU:HD23	1.80	0.61
2:B:607:SER:CB	2:B:634:ILE:HD13	2.28	0.61
2:B:207:ILE:HD11	2:B:225:PHE:HA	1.82	0.61
3:C:234:ILE:HD11	3:C:303:ASN:ND2	2.16	0.60
2:B:257:ILE:CD1	2:B:297:TYR:CD2	2.83	0.60
3:D:97:ASP:O	3:D:111:ILE:HD13	2.00	0.60
2:B:339:ILE:HD11	2:B:439:ARG:HD3	1.82	0.60
3:D:97:ASP:CB	3:D:111:ILE:HD11	2.31	0.60
3:C:4:GLU:HG3	3:C:131:ASP:H	1.67	0.60
3:D:17:VAL:CG2	3:D:231:ILE:CD1	2.79	0.60
3:C:57:ASN:O	3:D:286:HIS:ND1	2.24	0.60
3:C:188:ILE:CD1	3:C:394:PHE:HD2	2.11	0.60
3:C:296:LEU:HD13	3:C:376:MET:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:127:ILE:HD12	3:D:162:TYR:OH	2.02	0.60
1:A:126:TRP:HH2	1:A:192:ILE:HD13	1.66	0.60
3:C:210:LEU:CG	3:C:222:ILE:HD11	2.30	0.60
3:C:188:ILE:HD13	3:C:394:PHE:CG	2.34	0.60
2:B:297:TYR:OH	2:B:330:ILE:HD12	2.02	0.60
1:A:557:ILE:CD1	1:A:594:TYR:OH	2.49	0.60
3:C:93:TRP:CD1	3:C:122:LYS:HZ1	2.19	0.60
1:A:625:ILE:HD12	1:A:761:ILE:HD11	1.84	0.60
1:A:613:LYS:HG3	1:A:614:TYR:O	2.00	0.60
1:A:630:ARG:HA	1:A:633:HIS:CD2	2.36	0.60
1:A:606:LEU:CD1	1:A:710:ILE:HD13	2.31	0.60
2:B:402:ILE:HG23	2:B:449:ILE:HD13	1.82	0.60
2:B:525:LEU:CD2	2:B:538:ILE:HD12	2.21	0.60
1:A:375:ILE:CD1	1:A:396:LYS:HB3	2.31	0.60
3:D:166:ILE:HD12	3:D:252:MET:HE3	1.81	0.60
2:B:346:LEU:HD11	2:B:402:ILE:HD13	1.84	0.60
1:A:699:ILE:HD11	1:A:775:PHE:HE1	1.60	0.60
3:C:59:ARG:HG2	3:D:280:ILE:HD13	1.80	0.60
1:A:603:TRP:CD1	1:A:637:ASN:HD21	2.19	0.60
3:D:98:GLY:HA3	3:D:111:ILE:HD13	1.84	0.60
3:C:7:THR:HG23	3:C:139:LEU:HD13	1.84	0.59
2:B:430:HIS:CB	2:B:448:ILE:HD13	2.32	0.59
2:B:731:PHE:CE1	2:B:735:ILE:HD12	2.34	0.59
1:A:566:ILE:HD12	1:A:576:ARG:HG2	1.83	0.59
2:B:209:ILE:HD12	2:B:213:ILE:HD13	1.83	0.59
3:C:72:GLU:HB2	3:C:76:ILE:HD11	1.83	0.59
1:A:70:LEU:HD12	2:B:216:PHE:CD2	2.36	0.59
3:D:188:ILE:CD1	3:D:394:PHE:CD1	2.85	0.59
3:C:59:ARG:HH21	3:D:285:ALA:N	2.01	0.59
1:A:72:GLY:HA2	2:B:215:ASN:HB3	1.78	0.59
1:A:151:LEU:HD11	2:B:282:SER:OG	2.02	0.59
1:A:143:ARG:HH22	2:B:292:ILE:HD13	1.46	0.59
3:C:127:ILE:HD12	3:C:162:TYR:CE2	2.34	0.59
3:C:395:ASP:HA	3:C:398:PHE:CE2	2.37	0.59
3:C:59:ARG:HE	3:D:280:ILE:CG1	2.14	0.59
3:C:127:ILE:HD11	3:C:162:TYR:CE2	2.36	0.59
3:D:5:ILE:HD12	3:D:53:PHE:HE2	1.61	0.59
1:A:201:GLU:HA	1:A:204:ARG:HE	1.67	0.59
3:C:31:ILE:HD12	3:C:35:GLY:HA2	1.83	0.59
3:D:258:THR:OG1	3:D:356:ILE:HD11	2.03	0.59
1:A:409:PHE:CE1	1:A:573:ILE:HD11	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:LEU:HD11	2:B:463:ILE:HD13	1.83	0.59
1:A:625:ILE:CD1	1:A:761:ILE:HD13	2.33	0.59
3:C:412:LEU:HD22	3:C:412:LEU:H	1.68	0.59
2:B:607:SER:CB	2:B:634:ILE:CD1	2.81	0.59
1:A:56:GLU:CD	1:A:56:GLU:H	2.11	0.59
1:A:157:ARG:HH11	1:A:173:LEU:HD22	1.67	0.59
3:D:17:VAL:HG21	3:D:231:ILE:CD1	2.33	0.59
1:A:147:GLU:CB	2:B:285:ARG:HD3	2.29	0.59
3:D:119:ILE:HD13	3:D:154:LEU:HD11	1.84	0.59
3:D:127:ILE:HD11	3:D:162:TYR:CE2	2.38	0.59
1:A:606:LEU:HD21	1:A:710:ILE:HD13	1.84	0.58
3:C:58:CYS:HG	3:D:286:HIS:CA	1.77	0.58
1:A:414:ASP:O	1:A:418:VAL:HG23	2.02	0.58
1:A:625:ILE:CD1	1:A:758:LEU:HD12	2.32	0.58
1:A:699:ILE:CD1	1:A:775:PHE:CZ	2.86	0.58
3:C:258:THR:CG2	3:C:356:ILE:CD1	2.81	0.58
2:B:289:GLU:CD	2:B:289:GLU:H	2.10	0.58
1:A:699:ILE:HD11	1:A:775:PHE:CE2	2.38	0.58
1:A:128:ASP:OD1	2:B:299:ARG:NH2	2.35	0.58
2:B:246:ILE:HG12	2:B:247:SER:H	1.68	0.58
3:C:204:PHE:HB3	3:C:231:ILE:CD1	2.33	0.58
3:C:212:ILE:HD11	3:C:300:ASP:C	2.29	0.58
2:B:499:ILE:HD13	2:B:511:LYS:HZ3	1.67	0.58
3:D:130:THR:HG21	3:D:133:PHE:HB2	1.85	0.58
1:A:774:ILE:HD11	1:A:796:SER:CB	2.33	0.58
2:B:607:SER:HB3	2:B:634:ILE:CD1	2.32	0.58
2:B:402:ILE:HG22	2:B:449:ILE:HD13	1.85	0.58
2:B:290:ASN:HD22	2:B:290:ASN:H	1.52	0.58
1:A:409:PHE:CZ	1:A:573:ILE:CD1	2.84	0.58
1:A:458:TYR:CG	1:A:484:ILE:CD1	2.86	0.58
3:C:127:ILE:HD13	3:C:162:TYR:CZ	2.38	0.58
1:A:375:ILE:CD1	1:A:396:LYS:CG	2.81	0.58
2:B:297:TYR:OH	2:B:330:ILE:CD1	2.48	0.58
2:B:250:LYS:HE2	2:B:254:ILE:CD1	2.33	0.58
1:A:137:ARG:NH2	2:B:325:LEU:HD22	2.17	0.58
1:A:196:ILE:HD11	1:A:250:ILE:HD13	1.86	0.58
2:B:499:ILE:HD12	2:B:512:LEU:HD23	1.86	0.58
2:B:398:LEU:CD2	2:B:449:ILE:CD1	2.82	0.58
3:D:119:ILE:HD12	3:D:154:LEU:HD11	1.82	0.58
2:B:527:HIS:HB2	2:B:529:MET:HE1	1.84	0.58
1:A:695:LEU:CG	1:A:774:ILE:CD1	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:ARG:CD	2:B:330:ILE:HD11	2.33	0.58
2:B:586:ILE:CD1	2:B:732:LEU:HD23	2.33	0.58
2:B:771:GLU:OE1	2:B:812:ILE:HD11	2.04	0.58
2:B:207:ILE:CD1	2:B:221:LEU:HD22	2.34	0.58
2:B:339:ILE:HD13	2:B:343:TYR:OH	2.04	0.58
3:C:127:ILE:HD13	3:C:162:TYR:OH	2.03	0.58
3:C:250:SER:O	3:C:255:ILE:HD12	2.04	0.58
2:B:241:PHE:CB	2:B:254:ILE:HD11	2.25	0.58
1:A:126:TRP:CE2	1:A:192:ILE:HD13	2.39	0.58
3:D:412:LEU:H	3:D:412:LEU:HD22	1.69	0.57
3:D:139:LEU:HD21	3:D:235:ILE:HD13	1.85	0.57
2:B:480:ILE:HD11	2:B:537:VAL:HG13	1.83	0.57
1:A:151:LEU:HD12	2:B:286:GLU:OE2	1.99	0.57
1:A:151:LEU:HD11	2:B:282:SER:OG	2.04	0.57
2:B:319:PHE:CE1	2:B:327:ILE:HD11	2.39	0.57
1:A:151:LEU:HD22	2:B:285:ARG:CG	2.29	0.57
3:C:58:CYS:HB3	3:D:287:LYS:N	2.20	0.57
3:D:188:ILE:HD13	3:D:394:PHE:HA	1.86	0.57
3:D:188:ILE:CD1	3:D:394:PHE:CG	2.87	0.57
3:C:57:ASN:O	3:D:286:HIS:CG	2.58	0.57
3:C:58:CYS:O	3:D:286:HIS:CB	2.52	0.57
1:A:566:ILE:HG12	1:A:574:ILE:HD12	1.82	0.57
1:A:638:HIS:CE1	3:C:355:ASN:H	2.23	0.57
3:C:221:ASN:O	3:C:226:HIS:CE1	2.57	0.57
1:A:70:LEU:HG	2:B:216:PHE:CB	2.34	0.57
1:A:105:PHE:CD1	1:A:170:ILE:HD11	2.39	0.57
1:A:695:LEU:HG	1:A:774:ILE:CD1	2.35	0.57
2:B:489:MET:CE	2:B:493:ILE:HD11	2.34	0.57
1:A:375:ILE:CD1	1:A:396:LYS:HE2	2.34	0.57
1:A:699:ILE:HD11	1:A:775:PHE:CZ	2.38	0.57
1:A:699:ILE:HD13	1:A:793:PHE:HZ	1.69	0.57
3:C:119:ILE:HD11	3:C:154:LEU:HD22	1.86	0.57
3:D:222:ILE:CD1	3:D:227:THR:OG1	2.53	0.56
2:B:548:LEU:O	2:B:550:HIS:CD2	2.58	0.56
1:A:371:SER:HG	1:A:404:ILE:HD11	1.69	0.56
3:C:188:ILE:HD12	3:C:394:PHE:CB	2.31	0.56
2:B:812:ILE:HG23	2:B:816:TYR:CE2	2.39	0.56
3:D:283:ASP:HA	3:D:370:ASN:HB2	1.87	0.56
3:D:139:LEU:CD2	3:D:235:ILE:HD11	2.35	0.56
2:B:526:ARG:HH22	2:B:538:ILE:CD1	2.18	0.56
1:A:699:ILE:HD13	1:A:793:PHE:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:525:LEU:HD11	2:B:538:ILE:HG13	1.86	0.56
3:C:46:ARG:HH12	3:C:365:LEU:H	1.52	0.56
1:A:585:ILE:HD13	1:A:683:ILE:HG21	1.88	0.56
3:D:67:ILE:HD11	3:D:122:LYS:HB2	1.87	0.56
1:A:261:ASP:O	1:A:265:VAL:HG23	2.05	0.56
1:A:699:ILE:CD1	1:A:775:PHE:HE1	2.09	0.56
3:D:17:VAL:CG1	3:D:231:ILE:HD11	2.34	0.56
2:B:402:ILE:HD11	2:B:449:ILE:HD13	1.87	0.56
2:B:405:ILE:CG1	2:B:456:ILE:HD13	2.34	0.56
3:C:188:ILE:HD12	3:C:394:PHE:HD1	1.55	0.56
3:C:188:ILE:HD13	3:C:394:PHE:CG	2.41	0.56
3:D:70:ASP:CG	3:D:71:SER:H	2.12	0.56
2:B:364:ILE:CD1	2:B:403:PHE:HD1	2.14	0.56
2:B:527:HIS:CD2	2:B:538:ILE:HD11	2.40	0.56
2:B:532:PRO:C	2:B:538:ILE:CD1	2.78	0.56
2:B:825:ILE:HG22	2:B:837:GLU:HB2	1.88	0.56
1:A:625:ILE:CD1	1:A:758:LEU:CD1	2.83	0.56
3:C:130:THR:HG21	3:C:133:PHE:HB2	1.87	0.56
3:D:17:VAL:HG21	3:D:231:ILE:HD13	1.86	0.56
3:D:188:ILE:HD11	3:D:394:PHE:CG	2.41	0.56
1:A:73:THR:HG22	2:B:215:ASN:CG	2.30	0.56
1:A:138:PHE:CE2	1:A:275:ILE:CD1	2.86	0.56
1:A:599:LEU:HD12	1:A:640:ILE:CD1	2.36	0.55
1:A:78:PHE:HB2	1:A:91:GLU:H	1.71	0.55
3:D:326:VAL:HG21	3:D:370:ASN:HD22	1.70	0.55
3:C:56:GLU:HB2	3:D:286:HIS:NE2	2.22	0.55
3:C:188:ILE:HD12	3:C:394:PHE:HB2	1.87	0.55
3:C:240:ASN:OD1	3:C:322:ILE:CD1	2.49	0.55
1:A:592:LEU:HB3	1:A:644:MET:HE1	1.88	0.55
2:B:818:ASN:HB3	2:B:822:ARG:HH12	1.71	0.55
1:A:72:GLY:HA2	2:B:215:ASN:HB3	1.88	0.55
1:A:599:LEU:HD12	1:A:640:ILE:HD11	1.88	0.55
1:A:599:LEU:HD13	1:A:640:ILE:CD1	2.36	0.55
2:B:366:GLU:CD	2:B:367:ASN:O	2.49	0.55
1:A:151:LEU:HG	2:B:285:ARG:CD	2.34	0.55
2:B:430:HIS:CG	2:B:448:ILE:HD11	2.34	0.55
2:B:430:HIS:CB	2:B:448:ILE:CD1	2.84	0.55
1:A:420:LYS:HA	1:A:423:GLN:HE21	1.72	0.55
2:B:463:ILE:HA	2:B:467:LYS:HG2	1.89	0.55
3:D:166:ILE:CD1	3:D:252:MET:HE3	2.36	0.55
1:A:169:SER:HA	1:A:171:ARG:HH21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:546:LEU:H	2:B:550:HIS:CE1	2.24	0.55
1:A:284:TYR:O	1:A:288:THR:HG22	2.05	0.55
1:A:603:TRP:CE2	1:A:633:HIS:HB2	2.41	0.55
2:B:349:TRP:HE1	2:B:403:PHE:HA	1.71	0.55
2:B:430:HIS:CG	2:B:448:ILE:HD13	2.41	0.55
1:A:479:ARG:HG3	1:A:480:GLN:HE21	1.72	0.55
2:B:182:GLU:CD	2:B:182:GLU:H	2.14	0.55
3:D:391:CYS:HA	3:D:394:PHE:CD2	2.41	0.55
2:B:349:TRP:CZ3	2:B:383:ILE:HD11	2.41	0.55
3:D:391:CYS:HA	3:D:394:PHE:CD2	2.42	0.55
3:C:322:ILE:CD1	3:C:358:ARG:HH21	2.01	0.55
1:A:603:TRP:CE2	1:A:633:HIS:HB2	2.42	0.55
1:A:328:LYS:H	1:A:328:LYS:HD2	1.72	0.55
3:D:31:ILE:HG22	3:D:37:SER:HA	1.89	0.55
1:A:109:ILE:HD11	1:A:170:ILE:HD13	1.87	0.55
3:D:105:TRP:CH2	3:D:109:TYR:CD2	2.94	0.55
2:B:413:GLU:OE2	2:B:419:VAL:HG11	2.07	0.55
2:B:402:ILE:HD11	2:B:449:ILE:CD1	2.36	0.55
2:B:533:ARG:CA	2:B:538:ILE:HD12	2.36	0.55
1:A:557:ILE:HD11	1:A:594:TYR:OH	1.97	0.55
1:A:138:PHE:CE2	1:A:142:ILE:CD1	2.90	0.55
1:A:142:ILE:CD1	1:A:189:LEU:HD13	2.36	0.55
2:B:207:ILE:HG12	2:B:209:ILE:H	1.72	0.55
2:B:220:LEU:HD11	2:B:224:ILE:HD11	1.88	0.55
1:A:706:PHE:CD1	1:A:768:ILE:HD13	2.41	0.55
3:D:412:LEU:H	3:D:412:LEU:HD22	1.71	0.55
1:A:120:THR:HA	1:A:123:TYR:CZ	2.42	0.55
2:B:437:SER:HB2	2:B:441:ILE:HD11	1.87	0.55
2:B:412:LEU:HD13	2:B:463:ILE:HD13	1.88	0.55
3:D:127:ILE:HD13	3:D:162:TYR:CE2	2.41	0.55
3:D:173:PHE:CD1	3:D:203:VAL:HG13	2.41	0.55
3:D:123:ILE:HD13	3:D:158:LEU:HD21	1.88	0.55
3:D:188:ILE:HD12	3:D:394:PHE:CE1	2.39	0.55
1:A:151:LEU:HD12	2:B:285:ARG:HD3	1.88	0.55
3:C:276:THR:HG1	3:C:284:ILE:HD11	1.72	0.55
3:C:210:LEU:CD1	3:C:222:ILE:HD11	2.36	0.55
2:B:574:VAL:HG23	2:B:576:ARG:H	1.72	0.54
2:B:493:ILE:HD12	2:B:598:TYR:HB3	1.88	0.54
1:A:363:ILE:HD11	1:A:412:GLY:O	2.07	0.54
2:B:349:TRP:CE3	2:B:364:ILE:HD11	2.42	0.54
1:A:625:ILE:CD1	1:A:761:ILE:HB	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ILE:CD1	2:B:403:PHE:CD1	2.90	0.54
1:A:140:TYR:OH	2:B:324:ASP:OD1	2.24	0.54
1:A:606:LEU:HD11	1:A:710:ILE:HD12	1.89	0.54
3:D:97:ASP:O	3:D:111:ILE:CD1	2.55	0.54
1:A:462:LEU:HD22	1:A:484:ILE:HG22	1.89	0.54
3:D:258:THR:CG2	3:D:356:ILE:HD13	2.38	0.54
1:A:699:ILE:HD11	1:A:775:PHE:CD1	2.43	0.54
1:A:375:ILE:CD1	1:A:396:LYS:CB	2.85	0.54
3:D:292:TYR:CZ	3:D:296:LEU:HD11	2.42	0.54
3:D:67:ILE:HD11	3:D:122:LYS:CB	2.38	0.54
1:A:567:PRO:HD3	1:A:574:ILE:CD1	2.37	0.54
1:A:137:ARG:NH2	2:B:328:ARG:HH12	2.05	0.54
1:A:280:CYS:HB3	1:A:380:ASP:HA	1.89	0.54
1:A:585:ILE:HD11	1:A:683:ILE:HG23	1.83	0.54
3:D:17:VAL:CG2	3:D:231:ILE:CD1	2.82	0.54
2:B:346:LEU:HD23	2:B:445:PHE:CZ	2.43	0.54
1:A:357:VAL:CG2	1:A:363:ILE:CD1	2.86	0.54
3:C:6:ILE:HD13	3:C:126:GLU:HB3	1.88	0.54
3:D:243:ARG:HH12	3:D:363:LEU:HD21	1.71	0.54
1:A:564:ILE:HD13	1:A:579:MET:HG3	1.89	0.54
1:A:625:ILE:CD1	1:A:761:ILE:CG1	2.86	0.54
3:C:17:VAL:HG22	3:C:228:ASN:HB3	1.90	0.54
1:A:328:LYS:H	1:A:328:LYS:HD2	1.71	0.54
3:C:188:ILE:HD11	3:C:394:PHE:CD2	2.39	0.54
2:B:354:LEU:HD21	2:B:410:ILE:CD1	2.37	0.54
3:C:188:ILE:HD12	3:C:394:PHE:HD2	1.62	0.54
3:D:105:TRP:CZ2	3:D:109:TYR:CD2	2.96	0.54
2:B:354:LEU:CD2	2:B:410:ILE:HD12	2.38	0.54
3:D:124:ASP:HA	3:D:127:ILE:HG12	1.90	0.54
3:C:358:ARG:HE	3:C:358:ARG:HA	1.72	0.54
2:B:657:ILE:HG22	2:B:735:ILE:HD11	1.89	0.54
3:D:119:ILE:CD1	3:D:154:LEU:HD21	2.38	0.54
2:B:181:GLU:OE1	2:B:184:ILE:CD1	2.53	0.54
3:C:17:VAL:HG21	3:C:231:ILE:HG23	1.89	0.54
3:D:124:ASP:HA	3:D:127:ILE:HG12	1.90	0.54
1:A:114:LYS:HE3	1:A:118:ILE:HD11	1.90	0.54
1:A:138:PHE:HB2	1:A:275:ILE:HD11	1.89	0.54
2:B:527:HIS:CE1	2:B:538:ILE:HG23	2.42	0.54
2:B:653:LEU:CD2	2:B:657:ILE:HD12	2.35	0.54
1:A:625:ILE:CD1	1:A:765:ILE:HD11	2.37	0.54
3:C:119:ILE:HD13	3:C:154:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:GLU:CD	2:B:289:GLU:H	2.16	0.53
1:A:323:GLN:HG2	1:A:324:TYR:H	1.73	0.53
3:C:188:ILE:HD11	3:C:427:ARG:HH22	1.73	0.53
1:A:75:ILE:HG12	1:A:94:ILE:HG22	1.90	0.53
2:B:426:SER:O	2:B:430:HIS:CG	2.61	0.53
2:B:525:LEU:O	2:B:538:ILE:HD13	2.08	0.53
3:C:10:ALA:HB1	3:C:147:GLY:HA2	1.89	0.53
2:B:489:MET:O	2:B:493:ILE:HG13	2.08	0.53
2:B:282:SER:HA	2:B:285:ARG:HE	1.74	0.53
3:D:318:VAL:HG22	3:D:319:TYR:N	2.23	0.53
2:B:507:LEU:HB2	2:B:508:PRO:HD3	1.90	0.53
1:A:72:GLY:HA3	2:B:215:ASN:ND2	2.24	0.53
3:C:123:ILE:HG22	3:C:127:ILE:CD1	2.38	0.53
2:B:611:ILE:HD13	2:B:777:CYS:CB	2.38	0.53
1:A:138:PHE:HE2	1:A:275:ILE:HD12	1.70	0.53
2:B:555:TRP:CE3	2:B:595:LYS:HD2	2.43	0.53
3:C:258:THR:HG21	3:C:356:ILE:CD1	2.37	0.53
3:C:292:TYR:CZ	3:C:296:LEU:HD11	2.42	0.53
2:B:586:ILE:CD1	2:B:735:ILE:HD11	2.39	0.53
3:C:59:ARG:HA	3:D:281:HIS:CE1	2.43	0.53
1:A:126:TRP:CH2	1:A:192:ILE:HD13	2.44	0.53
3:C:78:ASP:HB3	3:C:87:PHE:CE2	2.44	0.53
3:C:188:ILE:HD12	3:C:394:PHE:HB2	1.91	0.53
1:A:129:THR:H	1:A:130:SER:HA	1.74	0.53
3:D:193:ARG:HH12	3:D:419:VAL:HG11	1.72	0.53
1:A:132:GLY:HA3	1:A:135:LEU:HD13	1.90	0.53
3:D:312:ASN:HA	3:D:380:MET:HE1	1.91	0.53
1:A:458:TYR:CE1	1:A:484:ILE:CD1	2.73	0.53
1:A:567:PRO:CD	1:A:574:ILE:CD1	2.86	0.53
3:C:59:ARG:HH12	3:D:283:ASP:CG	2.14	0.53
1:A:300:MET:HE2	1:A:300:MET:HA	1.90	0.53
1:A:151:LEU:CD1	2:B:285:ARG:CD	2.64	0.53
2:B:390:VAL:HG23	2:B:396:LYS:HD2	1.91	0.53
2:B:719:LEU:HD23	2:B:720:ASN:H	1.73	0.53
2:B:241:PHE:CB	2:B:254:ILE:CD1	2.86	0.53
2:B:405:ILE:HD11	2:B:456:ILE:HD13	1.90	0.53
1:A:63:LEU:HG	1:A:170:ILE:HD11	1.91	0.53
1:A:774:ILE:HD11	1:A:796:SER:HB2	1.90	0.53
1:A:137:ARG:HD2	2:B:324:ASP:HA	1.90	0.53
1:A:713:MET:HE2	1:A:714:ARG:O	2.08	0.53
2:B:355:LEU:CB	2:B:364:ILE:CD1	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ILE:CD1	1:A:761:ILE:HD11	2.36	0.53
1:A:359:ALA:C	1:A:361:LEU:H	2.16	0.53
1:A:372:ASP:HB3	1:A:375:ILE:CD1	2.38	0.53
2:B:480:ILE:HD11	2:B:537:VAL:HG22	1.91	0.53
2:B:563:ILE:HD13	2:B:565:TYR:OH	2.09	0.53
3:C:166:ILE:HD11	3:C:256:TYR:CD2	2.42	0.53
1:A:189:LEU:O	1:A:192:ILE:HG12	2.08	0.53
3:D:234:ILE:HD13	3:D:303:ASN:CG	2.34	0.53
3:D:212:ILE:HD11	3:D:302:SER:O	2.09	0.53
1:A:151:LEU:HD11	2:B:282:SER:HB2	1.91	0.53
1:A:142:ILE:HD13	1:A:188:LEU:HD13	1.89	0.52
1:A:361:LEU:HG	1:A:365:THR:H	1.74	0.52
3:D:213:SER:HB3	3:D:222:ILE:HD11	1.86	0.52
2:B:445:PHE:CE2	2:B:449:ILE:HD11	2.44	0.52
3:C:59:ARG:CZ	3:D:286:HIS:ND1	2.72	0.52
3:D:123:ILE:HD12	3:D:161:ARG:HH12	1.74	0.52
1:A:625:ILE:CB	1:A:765:ILE:HD13	2.39	0.52
3:D:21:LEU:HD12	3:D:235:ILE:CD1	2.26	0.52
1:A:624:ARG:H	1:A:624:ARG:HE	1.56	0.52
3:C:210:LEU:HD11	3:C:222:ILE:HD13	1.89	0.52
1:A:137:ARG:NH2	2:B:328:ARG:CZ	2.69	0.52
3:D:258:THR:HG21	3:D:356:ILE:HD13	1.91	0.52
1:A:126:TRP:CD2	1:A:135:LEU:HB3	2.45	0.52
3:C:8:LEU:HD22	3:C:67:ILE:HD11	1.91	0.52
3:D:127:ILE:HD13	3:D:162:TYR:CE2	2.38	0.52
1:A:151:LEU:CD1	2:B:282:SER:OG	2.46	0.52
2:B:586:ILE:HD11	2:B:735:ILE:HD11	1.91	0.52
2:B:335:PHE:CE2	2:B:339:ILE:HD11	2.44	0.52
3:D:188:ILE:HD13	3:D:394:PHE:CG	2.44	0.52
2:B:600:TYR:CD1	2:B:604:MET:HE2	2.44	0.52
1:A:695:LEU:HD23	1:A:774:ILE:CD1	2.27	0.52
1:A:133:MET:HE3	2:B:323:GLY:CA	2.38	0.52
1:A:599:LEU:HG	1:A:640:ILE:HD11	1.90	0.52
2:B:288:TYR:O	2:B:291:ILE:HG12	2.09	0.52
3:C:188:ILE:CD1	3:C:394:PHE:CG	2.92	0.52
1:A:133:MET:CE	2:B:323:GLY:H	2.22	0.52
2:B:402:ILE:HG22	2:B:449:ILE:CD1	2.40	0.52
3:C:22:TRP:CZ2	3:C:66:ALA:HB2	2.44	0.52
1:A:599:LEU:HG	1:A:640:ILE:CD1	2.40	0.52
2:B:546:LEU:H	2:B:550:HIS:HE1	1.55	0.52
1:A:625:ILE:HD13	1:A:761:ILE:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:568:LEU:HD23	2:B:721:ILE:HD11	1.91	0.52
1:A:183:ASN:HD22	1:A:183:ASN:H	1.58	0.52
1:A:624:ARG:HG2	1:A:627:ARG:HH21	1.74	0.52
3:C:258:THR:HG21	3:C:356:ILE:HD11	1.92	0.52
3:C:67:ILE:HD11	3:C:126:GLU:HG3	1.92	0.52
3:C:81:ASN:C	3:C:83:PHE:H	2.18	0.52
2:B:402:ILE:HG23	2:B:449:ILE:HD12	1.86	0.52
3:C:380:MET:HG3	3:C:382:THR:HG22	1.92	0.52
3:C:234:ILE:HD11	3:C:303:ASN:ND2	2.25	0.52
3:C:5:ILE:HD12	3:C:53:PHE:CZ	2.45	0.52
2:B:220:LEU:HD13	2:B:224:ILE:CD1	2.40	0.52
3:C:398:PHE:HA	3:C:404:LEU:HD21	1.92	0.52
3:C:111:ILE:HA	3:C:114:ARG:HE	1.75	0.52
3:C:21:LEU:HD13	3:C:235:ILE:HG23	1.92	0.52
2:B:247:SER:HA	2:B:359:TYR:CE2	2.45	0.52
2:B:455:GLU:O	2:B:459:HIS:CD2	2.63	0.52
4:F:41:UNK:O	4:F:44:UNK:O	2.27	0.52
1:A:466:GLU:HG3	1:A:479:ARG:HH21	1.75	0.52
2:B:533:ARG:HD3	2:B:538:ILE:CD1	2.37	0.52
3:C:59:ARG:NH2	3:D:284:ILE:HG21	2.24	0.52
3:C:234:ILE:HG12	3:C:272:PHE:CD2	2.45	0.52
1:A:138:PHE:CE2	1:A:142:ILE:HD12	2.45	0.52
2:B:206:GLN:HG2	2:B:207:ILE:H	1.75	0.52
3:D:4:GLU:HB2	3:D:130:THR:HG23	1.92	0.52
1:A:130:SER:HG	2:B:322:HIS:CE1	2.15	0.52
3:D:212:ILE:CD1	3:D:303:ASN:ND2	2.59	0.52
1:A:68:ILE:HD11	2:B:281:LYS:HD2	1.91	0.51
2:B:181:GLU:CD	2:B:181:GLU:H	2.18	0.51
2:B:222:HIS:HA	2:B:225:PHE:CE2	2.45	0.51
1:A:143:ARG:NE	2:B:288:TYR:CD2	2.70	0.51
1:A:625:ILE:HD11	1:A:765:ILE:HD11	1.92	0.51
1:A:72:GLY:HA3	2:B:215:ASN:HB3	1.92	0.51
3:C:195:ILE:HD12	3:C:423:PHE:HZ	1.75	0.51
1:A:421:HIS:NE2	1:A:425:ILE:CD1	2.74	0.51
2:B:220:LEU:CD1	2:B:224:ILE:CD1	2.88	0.51
2:B:532:PRO:HB2	2:B:538:ILE:HD11	1.92	0.51
3:D:320:ASN:ND2	3:D:356:ILE:HD12	2.25	0.51
3:D:17:VAL:HG21	3:D:231:ILE:HD12	1.92	0.51
3:D:188:ILE:HD13	3:D:394:PHE:HB2	1.91	0.51
1:A:202:GLU:C	1:A:205:THR:O	2.52	0.51
1:A:585:ILE:HD11	1:A:683:ILE:CG2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:231:ILE:O	3:D:235:ILE:HG13	2.11	0.51
1:A:285:GLU:HB3	1:A:291:ILE:HG23	1.92	0.51
1:A:105:PHE:O	1:A:109:ILE:HG13	2.11	0.51
2:B:493:ILE:HD13	2:B:598:TYR:CB	2.40	0.51
3:D:256:TYR:CZ	3:D:260:ILE:HD11	2.45	0.51
3:D:69:MET:HE1	3:D:119:ILE:HG22	1.93	0.51
1:A:425:ILE:CD1	1:A:478:MET:HA	2.40	0.51
3:C:188:ILE:HD12	3:C:394:PHE:CG	2.46	0.51
3:D:4:GLU:HB2	3:D:130:THR:HG23	1.92	0.51
2:B:405:ILE:HG13	2:B:456:ILE:CD1	2.41	0.51
3:C:59:ARG:NH2	3:D:285:ALA:N	2.58	0.51
1:A:294:ASP:HB3	1:A:297:GLN:HA	1.93	0.51
3:C:201:THR:HG22	3:C:266:HIS:CD2	2.45	0.51
2:B:181:GLU:H	2:B:184:ILE:HD12	1.76	0.51
1:A:606:LEU:CD1	1:A:710:ILE:HD12	2.40	0.51
3:C:338:LEU:HA	3:C:341:ARG:HE	1.75	0.51
1:A:155:VAL:HG21	2:B:278:VAL:CG2	2.41	0.51
1:A:630:ARG:HE	1:A:633:HIS:CE1	2.29	0.51
1:A:451:ARG:H	1:A:454:ASN:HB2	1.75	0.51
2:B:319:PHE:CE1	2:B:327:ILE:HG23	2.46	0.51
3:C:188:ILE:HD11	3:C:394:PHE:CB	2.33	0.51
3:D:212:ILE:HD11	3:D:303:ASN:CG	2.33	0.51
3:C:395:ASP:HA	3:C:398:PHE:CZ	2.46	0.51
1:A:566:ILE:HG22	1:A:574:ILE:HD11	1.93	0.51
1:A:109:ILE:HA	1:A:112:TYR:CD2	2.46	0.51
1:A:320:TRP:O	1:A:572:ILE:HD11	2.10	0.51
2:B:181:GLU:OE1	2:B:184:ILE:HD11	2.11	0.51
2:B:606:LYS:HE2	2:B:773:VAL:HG11	1.92	0.51
1:A:366:ILE:HD11	1:A:404:ILE:HD13	1.91	0.51
3:D:256:TYR:HE1	3:D:260:ILE:CD1	2.16	0.51
1:A:626:VAL:O	1:A:629:THR:HG22	2.11	0.51
1:A:606:LEU:CG	1:A:710:ILE:CD1	2.87	0.51
2:B:285:ARG:HH21	2:B:286:GLU:HB2	1.76	0.50
1:A:655:GLU:O	1:A:659:LEU:HD13	2.10	0.50
2:B:843:LYS:O	2:B:846:ARG:O	2.29	0.50
2:B:405:ILE:HD13	2:B:452:GLN:NE2	2.25	0.50
1:A:625:ILE:CD1	1:A:761:ILE:HD13	2.34	0.50
1:A:625:ILE:HD11	1:A:758:LEU:HD11	1.89	0.50
3:D:105:TRP:CE3	3:D:189:LEU:HD23	2.46	0.50
3:D:188:ILE:CD1	3:D:394:PHE:HB2	2.41	0.50
3:C:72:GLU:HB2	3:C:76:ILE:CD1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ASP:OD2	1:A:572:ILE:HD12	2.11	0.50
2:B:402:ILE:HG21	2:B:449:ILE:CD1	2.42	0.50
2:B:430:HIS:HB3	2:B:448:ILE:CD1	2.39	0.50
2:B:355:LEU:HD12	2:B:362:PHE:CD2	2.46	0.50
3:D:215:LYS:HG3	3:D:216:VAL:HG23	1.94	0.50
3:C:57:ASN:CG	3:C:58:CYS:H	2.19	0.50
1:A:151:LEU:CG	2:B:282:SER:HA	2.39	0.50
3:C:289:HIS:CE1	3:C:331:ILE:HG22	2.47	0.50
1:A:625:ILE:CD1	1:A:765:ILE:CD1	2.89	0.50
2:B:634:ILE:CD1	2:B:772:PHE:CD1	2.93	0.50
2:B:779:LEU:HG	2:B:780:ASN:H	1.76	0.50
3:D:17:VAL:HG21	3:D:231:ILE:HD12	1.91	0.50
2:B:293:ARG:HD3	2:B:330:ILE:HD12	1.93	0.50
3:D:17:VAL:CG1	3:D:231:ILE:CD1	2.89	0.50
2:B:419:VAL:C	2:B:421:TRP:H	2.19	0.50
1:A:142:ILE:CD1	1:A:188:LEU:HD13	2.42	0.50
3:D:403:PHE:CZ	3:D:406:ASN:HB2	2.46	0.50
3:D:16:HIS:CG	3:D:228:ASN:HD21	2.30	0.50
1:A:425:ILE:HD11	1:A:564:ILE:HD12	1.88	0.50
1:A:133:MET:CE	2:B:323:GLY:H	2.25	0.50
3:D:288:CYS:H	3:D:291:SER:HB2	1.75	0.50
2:B:603:GLU:OE1	2:B:770:TYR:HA	2.12	0.50
3:C:322:ILE:CD1	3:C:358:ARG:HH21	2.21	0.50
3:D:212:ILE:HD12	3:D:303:ASN:CG	2.33	0.50
1:A:335:CYS:HA	1:A:340:ASP:HB3	1.93	0.50
2:B:572:LEU:HG	2:B:580:ARG:HE	1.77	0.50
2:B:200:PHE:N	2:B:200:PHE:CD1	2.79	0.50
1:A:368:SER:OG	1:A:373:ILE:CD1	2.59	0.50
2:B:430:HIS:HB3	2:B:448:ILE:HD12	1.94	0.50
1:A:706:PHE:HD1	1:A:768:ILE:HD13	1.77	0.50
3:C:191:LEU:HD13	3:C:191:LEU:O	2.11	0.50
1:A:370:SER:C	1:A:372:ASP:H	2.19	0.50
2:B:421:TRP:O	2:B:424:GLU:HG2	2.12	0.50
2:B:280:LEU:C	2:B:280:LEU:HD23	2.37	0.50
3:C:72:GLU:HB2	3:C:76:ILE:HD12	1.94	0.50
2:B:422:THR:HA	2:B:425:PHE:CD2	2.47	0.50
2:B:515:VAL:HA	2:B:518:GLU:HG3	1.92	0.50
3:C:195:ILE:HD11	3:C:423:PHE:HE1	1.76	0.50
1:A:713:MET:SD	1:A:714:ARG:O	2.69	0.50
2:B:633:ARG:NH1	3:D:445:TYR:O	2.45	0.50
3:D:97:ASP:O	3:D:111:ILE:HD13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:TYR:H	2:B:215:ASN:ND2	2.04	0.50
1:A:72:GLY:C	2:B:215:ASN:HB3	2.28	0.50
2:B:405:ILE:HD11	2:B:453:TYR:HB2	1.93	0.50
1:A:450:TYR:HA	1:A:488:THR:HG21	1.92	0.50
1:A:73:THR:HG22	2:B:215:ASN:OD1	2.12	0.50
3:C:188:ILE:HD13	3:C:394:PHE:CE2	2.38	0.50
2:B:220:LEU:CD1	2:B:224:ILE:HD12	2.42	0.50
1:A:133:MET:CE	2:B:323:GLY:N	2.75	0.50
3:D:242:ILE:HD11	3:D:252:MET:HE2	1.94	0.50
1:A:151:LEU:HD11	2:B:282:SER:CB	2.41	0.50
3:D:6:ILE:HD13	3:D:126:GLU:HB2	1.92	0.50
1:A:466:GLU:CG	1:A:479:ARG:HH21	2.25	0.49
3:C:12:GLN:HE22	3:C:144:GLY:HA2	1.76	0.49
3:D:234:ILE:HD13	3:D:303:ASN:CG	2.37	0.49
3:C:97:ASP:O	3:C:111:ILE:HD13	2.11	0.49
1:A:72:GLY:HA3	2:B:215:ASN:HB3	1.94	0.49
1:A:246:ALA:O	1:A:250:ILE:HG13	2.12	0.49
2:B:434:GLN:HA	2:B:439:ARG:HH22	1.75	0.49
1:A:357:VAL:HG23	1:A:363:ILE:HD12	1.94	0.49
1:A:286:TRP:CZ2	1:A:351:GLY:HA3	2.46	0.49
3:D:56:GLU:HG2	3:D:62:PHE:CE1	2.46	0.49
2:B:398:LEU:HD23	2:B:449:ILE:HD12	1.92	0.49
1:A:564:ILE:CD1	1:A:579:MET:HG3	2.41	0.49
3:D:105:TRP:CH2	3:D:109:TYR:CD1	3.01	0.49
2:B:326:THR:O	2:B:330:ILE:HG13	2.12	0.49
1:A:173:LEU:HD12	1:A:173:LEU:H	1.76	0.49
3:C:56:GLU:OE1	3:D:286:HIS:HE1	1.88	0.49
2:B:430:HIS:HD1	2:B:448:ILE:HD11	1.76	0.49
3:C:7:THR:CG2	3:C:139:LEU:HD13	2.42	0.49
1:A:613:LYS:HG3	1:A:614:TYR:O	2.10	0.49
1:A:339:GLU:CD	1:A:339:GLU:H	2.20	0.49
2:B:567:PRO:HG2	2:B:721:ILE:CD1	2.42	0.49
3:C:256:TYR:CD2	3:C:260:ILE:HD12	2.47	0.49
1:A:146:LEU:HD22	1:A:150:TYR:OH	2.12	0.49
1:A:625:ILE:HD13	1:A:761:ILE:HG21	1.89	0.49
3:D:120:LEU:HD22	3:D:161:ARG:HH11	1.78	0.49
1:A:625:ILE:HB	1:A:765:ILE:HD13	1.95	0.49
3:C:256:TYR:CE1	3:C:260:ILE:HD11	2.47	0.49
2:B:346:LEU:HD11	2:B:402:ILE:HD13	1.95	0.49
2:B:493:ILE:HD11	2:B:598:TYR:CG	2.46	0.49
3:C:78:ASP:HB3	3:C:87:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:166:ILE:CD1	3:D:252:MET:CE	2.85	0.49
1:A:632:LEU:HD21	1:A:768:ILE:HG23	1.95	0.49
3:D:180:VAL:HG12	3:D:181:VAL:H	1.78	0.49
2:B:402:ILE:HD11	2:B:449:ILE:CD1	2.42	0.49
2:B:491:ALA:HB2	3:D:1:MET:HE1	1.95	0.49
3:D:255:ILE:CD1	3:D:320:ASN:ND2	2.74	0.49
3:C:258:THR:CG2	3:C:356:ILE:HD11	2.43	0.49
1:A:113:GLY:HA2	1:A:116:TYR:CD2	2.47	0.49
3:C:24:GLN:HE22	3:C:233:THR:HA	1.78	0.49
1:A:451:ARG:HE	1:A:451:ARG:HA	1.78	0.49
2:B:812:ILE:HB	2:B:816:TYR:CZ	2.48	0.49
2:B:465:ASN:O	2:B:469:HIS:HA	2.13	0.49
3:C:39:LEU:H	3:C:40:PRO:CD	2.25	0.49
3:D:213:SER:HB2	3:D:222:ILE:HD11	1.95	0.49
2:B:482:LEU:HA	2:B:590:LEU:CD1	2.43	0.48
3:D:188:ILE:CD1	3:D:427:ARG:HH21	2.23	0.48
3:D:258:THR:OG1	3:D:356:ILE:CD1	2.61	0.48
3:C:315:TYR:CG	3:C:438:VAL:HG13	2.48	0.48
2:B:283:LEU:O	2:B:287:ILE:HG12	2.13	0.48
1:A:570:LEU:HD22	1:A:570:LEU:H	1.77	0.48
3:D:384:VAL:HB	3:D:434:MET:HE1	1.95	0.48
2:B:527:HIS:NE2	2:B:538:ILE:HD11	2.28	0.48
2:B:765:LEU:O	2:B:769:VAL:HG23	2.12	0.48
3:C:56:GLU:HB3	3:D:286:HIS:CD2	2.48	0.48
2:B:207:ILE:HD12	2:B:221:LEU:HD11	1.95	0.48
3:D:124:ASP:HA	3:D:127:ILE:HG12	1.95	0.48
1:A:651:VAL:HG13	1:A:686:ASN:HD21	1.76	0.48
1:A:638:HIS:CG	3:C:354:VAL:HG13	2.48	0.48
3:C:363:LEU:HD12	3:C:366:GLN:HB3	1.94	0.48
1:A:138:PHE:CD1	1:A:275:ILE:HD11	2.45	0.48
2:B:499:ILE:HD12	2:B:507:LEU:CD2	2.43	0.48
3:C:212:ILE:HD13	3:C:275:PHE:CE1	2.48	0.48
3:D:238:VAL:HG22	3:D:375:MET:HE1	1.95	0.48
2:B:534:ASN:HD22	2:B:534:ASN:H	1.60	0.48
1:A:375:ILE:HD13	1:A:396:LYS:HG2	1.96	0.48
1:A:135:LEU:HB2	1:A:247:ILE:HD13	1.94	0.48
1:A:789:GLU:HB3	1:A:793:PHE:CZ	2.48	0.48
1:A:591:VAL:HA	1:A:594:TYR:CE2	2.48	0.48
3:D:205:ASP:HB3	3:D:305:LEU:H	1.78	0.48
3:C:59:ARG:HH22	3:D:279:TYR:CB	2.18	0.48
3:C:289:HIS:H	3:C:289:HIS:CD2	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:441:ILE:HG22	2:B:444:ASN:H	1.79	0.48
2:B:639:THR:HG21	3:D:261:PRO:HA	1.95	0.48
3:C:234:ILE:HD13	3:C:303:ASN:OD1	2.13	0.48
3:D:6:ILE:HD13	3:D:126:GLU:HB3	1.94	0.48
1:A:454:ASN:HD22	1:A:488:THR:HG21	1.78	0.48
1:A:73:THR:HG23	2:B:215:ASN:ND2	2.28	0.48
1:A:108:ARG:HH22	1:A:112:TYR:HB2	1.78	0.48
3:C:256:TYR:CE1	3:C:260:ILE:HD12	2.46	0.48
3:C:292:TYR:CE1	3:C:296:LEU:HD11	2.48	0.48
3:D:119:ILE:CD1	3:D:154:LEU:CD2	2.92	0.48
3:D:270:PRO:HB2	3:D:375:MET:HE1	1.96	0.48
3:C:255:ILE:HD13	3:C:358:ARG:NH1	2.27	0.48
2:B:657:ILE:HG22	2:B:735:ILE:CD1	2.44	0.48
2:B:499:ILE:HD11	2:B:508:PRO:HA	1.96	0.48
1:A:128:ASP:CG	2:B:295:ARG:CZ	2.87	0.48
1:A:108:ARG:HH12	1:A:112:TYR:HB2	1.78	0.48
2:B:204:HIS:CG	2:B:204:HIS:O	2.66	0.48
3:C:120:LEU:HA	3:C:161:ARG:HH12	1.79	0.48
1:A:390:LEU:O	1:A:394:VAL:HG23	2.14	0.48
3:C:123:ILE:HD13	3:C:158:LEU:CD2	2.29	0.48
1:A:138:PHE:CE2	1:A:142:ILE:HD11	2.49	0.48
1:A:97:LYS:HD2	1:A:98:MET:HE2	1.95	0.48
3:D:212:ILE:CD1	3:D:302:SER:O	2.46	0.48
1:A:115:GLN:NE2	1:A:118:ILE:HD11	2.29	0.48
3:D:75:VAL:HG21	3:D:94:VAL:HG12	1.96	0.48
1:A:72:GLY:CA	2:B:215:ASN:HB3	2.44	0.48
2:B:586:ILE:CD1	2:B:732:LEU:HD13	2.12	0.48
2:B:366:GLU:OE1	2:B:367:ASN:O	2.32	0.48
2:B:390:VAL:HB	2:B:391:PRO:HD2	1.96	0.48
2:B:201:PRO:HB2	2:B:208:GLN:H	1.79	0.48
1:A:602:THR:HG21	1:A:707:CYS:SG	2.54	0.48
3:D:98:GLY:N	3:D:111:ILE:CD1	2.76	0.48
2:B:241:PHE:HB3	2:B:254:ILE:CD1	2.34	0.48
2:B:571:VAL:HA	2:B:575:ASN:HD22	1.78	0.48
3:C:179:GLU:H	3:C:179:GLU:CD	2.21	0.48
2:B:592:ARG:HE	2:B:592:ARG:HA	1.79	0.48
2:B:469:HIS:O	2:B:473:VAL:HG23	2.14	0.48
2:B:335:PHE:CD2	2:B:339:ILE:HD11	2.48	0.48
1:A:672:ILE:O	1:A:675:GLU:HG2	2.14	0.48
3:C:60:ASN:N	3:D:286:HIS:CE1	2.78	0.48
3:D:188:ILE:HD11	3:D:394:PHE:HB3	1.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:441:ILE:HD12	2:B:443:THR:CG2	2.40	0.48
1:A:151:LEU:HD21	2:B:282:SER:CA	2.44	0.48
3:D:188:ILE:CD1	3:D:394:PHE:HB2	2.42	0.48
1:A:142:ILE:HD11	1:A:188:LEU:CD1	2.44	0.48
2:B:430:HIS:CD2	2:B:448:ILE:HD13	2.45	0.48
1:A:781:ASN:HD21	1:A:787:SER:HB2	1.77	0.47
3:C:322:ILE:HD13	3:C:358:ARG:CZ	2.40	0.47
3:D:209:LEU:HD21	3:D:231:ILE:HD11	1.95	0.47
1:A:410:PHE:O	1:A:414:ASP:HA	2.12	0.47
2:B:489:MET:HG2	2:B:594:LYS:HG2	1.95	0.47
1:A:280:CYS:HB2	1:A:380:ASP:CG	2.39	0.47
1:A:799:VAL:HG12	1:A:800:ASP:O	2.14	0.47
1:A:196:ILE:CD1	1:A:250:ILE:HD13	2.43	0.47
1:A:126:TRP:HH2	1:A:192:ILE:HD13	1.78	0.47
1:A:585:ILE:HD11	1:A:683:ILE:HG23	1.95	0.47
2:B:578:PHE:C	2:B:580:ARG:H	2.20	0.47
2:B:491:ALA:HB1	2:B:522:LEU:HD23	1.95	0.47
3:C:5:ILE:HD12	3:C:53:PHE:CZ	2.49	0.47
2:B:442:SER:HA	2:B:445:PHE:CD2	2.50	0.47
3:D:97:ASP:C	3:D:111:ILE:CD1	2.88	0.47
2:B:366:GLU:OE2	2:B:367:ASN:O	2.31	0.47
1:A:142:ILE:HD11	1:A:186:MET:HB3	1.96	0.47
1:A:781:ASN:HD22	1:A:790:LYS:HG3	1.79	0.47
3:D:242:ILE:CD1	3:D:252:MET:CE	2.87	0.47
3:D:6:ILE:HD13	3:D:126:GLU:CB	2.44	0.47
3:D:212:ILE:HD11	3:D:302:SER:N	2.29	0.47
3:D:212:ILE:HD12	3:D:303:ASN:CG	2.27	0.47
1:A:151:LEU:CD1	2:B:285:ARG:CG	2.93	0.47
1:A:433:HIS:CE1	3:C:242:ILE:O	2.67	0.47
3:D:188:ILE:HD11	3:D:394:PHE:CG	2.41	0.47
2:B:582:GLU:O	2:B:585:ARG:HG2	2.15	0.47
2:B:772:PHE:HE1	2:B:812:ILE:HD12	1.74	0.47
1:A:425:ILE:HD13	1:A:481:LEU:HD21	1.96	0.47
2:B:284:TYR:OH	2:B:291:ILE:CD1	2.62	0.47
3:C:234:ILE:HD11	3:C:303:ASN:CG	2.40	0.47
3:C:10:ALA:HB1	3:C:147:GLY:HA2	1.97	0.47
2:B:405:ILE:HG13	2:B:456:ILE:HD13	1.76	0.47
2:B:532:PRO:C	2:B:538:ILE:HD11	2.39	0.47
2:B:480:ILE:HD12	2:B:541:LEU:CD1	2.25	0.47
3:C:29:HIS:HE1	3:C:243:ARG:HH11	1.61	0.47
1:A:466:GLU:HA	1:A:479:ARG:HE	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:LYS:O	2:B:328:ARG:HG3	2.15	0.47
2:B:612:ARG:O	2:B:779:LEU:HD11	2.15	0.47
1:A:133:MET:CE	2:B:323:GLY:N	2.77	0.47
3:C:221:ASN:O	3:C:226:HIS:HE1	1.98	0.47
2:B:556:ASP:HA	2:B:592:ARG:HH22	1.78	0.47
3:D:93:TRP:HE1	3:D:118:ASP:HB3	1.79	0.47
1:A:562:PHE:H	1:A:583:GLN:HG3	1.79	0.47
3:D:323:ILE:HB	3:D:359:ARG:HA	1.95	0.47
3:D:240:ASN:HA	3:D:243:ARG:HE	1.79	0.47
3:C:250:SER:HA	3:C:255:ILE:HD11	1.96	0.47
3:C:292:TYR:CE1	3:C:374:GLY:HA3	2.50	0.47
2:B:202:PHE:CD1	2:B:207:ILE:CD1	2.97	0.47
2:B:759:PRO:O	2:B:763:VAL:HG23	2.14	0.47
3:D:124:ASP:HA	3:D:127:ILE:HG12	1.96	0.47
1:A:134:VAL:HA	1:A:137:ARG:HH11	1.79	0.47
1:A:774:ILE:HD11	1:A:796:SER:HB3	1.96	0.47
1:A:361:LEU:HD12	1:A:364:PRO:HA	1.97	0.47
2:B:412:LEU:HD13	2:B:463:ILE:CD1	2.45	0.47
2:B:480:ILE:HG23	2:B:481:LEU:N	2.30	0.47
3:D:212:ILE:HD12	3:D:303:ASN:OD1	2.15	0.47
2:B:405:ILE:HG12	2:B:453:TYR:CD1	2.49	0.47
2:B:526:ARG:HH21	2:B:538:ILE:HD11	1.75	0.47
3:C:204:PHE:CB	3:C:231:ILE:CD1	2.90	0.47
2:B:362:PHE:CE2	2:B:364:ILE:HD12	2.50	0.47
2:B:387:GLN:CD	2:B:387:GLN:H	2.22	0.47
2:B:827:ARG:HH22	3:D:353:HIS:CD2	2.33	0.47
3:D:213:SER:CB	3:D:222:ILE:CD1	2.84	0.47
2:B:365:ALA:HB2	2:B:386:ASN:HB2	1.96	0.47
1:A:183:ASN:H	1:A:183:ASN:ND2	2.12	0.47
1:A:183:ASN:HA	1:A:186:MET:SD	2.55	0.47
1:A:391:GLU:HA	1:A:394:VAL:HG22	1.95	0.47
2:B:664:MET:HG2	2:B:727:VAL:HG22	1.97	0.47
2:B:385:PHE:CZ	2:B:390:VAL:HG11	2.49	0.47
3:D:193:ARG:HH12	3:D:419:VAL:CG1	2.28	0.47
1:A:136:GLN:HE22	2:B:324:ASP:N	2.12	0.47
3:C:176:ARG:HG3	3:C:176:ARG:HH11	1.80	0.47
3:C:292:TYR:CZ	3:C:374:GLY:HA3	2.49	0.47
1:A:478:MET:HE2	1:A:478:MET:HA	1.97	0.47
1:A:557:ILE:HD13	1:A:594:TYR:CZ	2.45	0.47
2:B:629:ASN:H	2:B:629:ASN:HD22	1.63	0.47
2:B:319:PHE:HA	2:B:322:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LYS:HE2	3:C:2:GLY:H	1.80	0.47
3:D:139:LEU:CD2	3:D:235:ILE:CD1	2.85	0.47
2:B:355:LEU:HD13	2:B:356:ARG:N	2.30	0.47
1:A:609:THR:HG23	1:A:610:PRO:HD3	1.97	0.47
3:C:59:ARG:HH21	3:D:284:ILE:HG21	1.79	0.47
1:A:567:PRO:CD	1:A:574:ILE:HD12	2.44	0.47
1:A:67:LEU:HD21	1:A:113:GLY:HA3	1.96	0.47
3:C:36:LEU:HD12	3:C:36:LEU:H	1.80	0.47
3:C:322:ILE:HG12	3:C:358:ARG:HE	1.79	0.47
3:D:188:ILE:HD11	3:D:394:PHE:CB	2.42	0.47
2:B:526:ARG:NH2	2:B:538:ILE:HD13	2.30	0.46
1:A:128:ASP:OD1	2:B:299:ARG:NH2	2.47	0.46
3:D:89:PRO:HD2	3:D:90:ARG:HH11	1.80	0.46
1:A:774:ILE:HB	1:A:793:PHE:CD2	2.50	0.46
1:A:73:THR:HG22	2:B:215:ASN:ND2	2.29	0.46
2:B:499:ILE:CD1	2:B:511:LYS:HD3	2.40	0.46
3:D:244:PHE:CE1	3:D:363:LEU:HD21	2.50	0.46
2:B:464:LEU:HD23	2:B:468:PHE:CZ	2.49	0.46
2:B:349:TRP:CH2	2:B:383:ILE:HD11	2.49	0.46
2:B:772:PHE:CZ	2:B:812:ILE:HD13	2.50	0.46
2:B:802:LEU:HA	2:B:805:PHE:CD2	2.50	0.46
1:A:64:LEU:HD13	1:A:64:LEU:C	2.40	0.46
1:A:699:ILE:CD1	1:A:775:PHE:CE1	2.99	0.46
1:A:123:TYR:CD1	1:A:139:ALA:HB1	2.50	0.46
1:A:774:ILE:HD12	1:A:796:SER:HG	1.71	0.46
1:A:582:TYR:CZ	1:A:680:LEU:HD21	2.49	0.46
1:A:151:LEU:HB2	2:B:285:ARG:HH11	1.79	0.46
2:B:527:HIS:O	2:B:532:PRO:HA	2.16	0.46
3:D:412:LEU:H	3:D:412:LEU:HD22	1.79	0.46
1:A:105:PHE:CD1	1:A:170:ILE:CD1	2.98	0.46
3:C:6:ILE:HD13	3:C:126:GLU:HB3	1.98	0.46
2:B:424:GLU:HG2	2:B:425:PHE:CD1	2.51	0.46
3:C:152:SER:HB3	3:C:193:ARG:HG3	1.98	0.46
1:A:402:ASN:O	1:A:406:LEU:HD23	2.16	0.46
2:B:336:ASN:O	2:B:339:ILE:HG22	2.15	0.46
1:A:286:TRP:HB2	1:A:292:LEU:HD22	1.97	0.46
3:C:330:GLN:CD	3:C:330:GLN:H	2.23	0.46
3:D:289:HIS:CE1	3:D:331:ILE:HG22	2.50	0.46
2:B:349:TRP:CE2	2:B:364:ILE:CD1	2.99	0.46
3:C:105:TRP:CH2	3:C:109:TYR:CD2	3.03	0.46
2:B:633:ARG:HH12	3:D:444:SER:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:CYS:HB2	1:A:344:LEU:HD22	1.97	0.46
3:D:21:LEU:CD1	3:D:235:ILE:HD13	2.29	0.46
1:A:105:PHE:HD1	1:A:170:ILE:HD11	1.81	0.46
3:D:213:SER:HB3	3:D:222:ILE:HD13	1.95	0.46
2:B:533:ARG:N	2:B:538:ILE:HD12	2.31	0.46
3:D:4:GLU:HB2	3:D:130:THR:HG23	1.98	0.46
3:D:320:ASN:HD21	3:D:358:ARG:HE	1.64	0.46
2:B:586:ILE:CD1	2:B:732:LEU:CB	2.87	0.46
2:B:604:MET:HB3	2:B:638:ARG:HE	1.80	0.46
1:A:72:GLY:CA	2:B:215:ASN:HB3	2.46	0.46
3:D:119:ILE:O	3:D:123:ILE:HG13	2.15	0.46
1:A:151:LEU:HD21	2:B:282:SER:CB	2.43	0.46
2:B:314:ILE:O	2:B:318:ILE:HG13	2.15	0.46
2:B:533:ARG:HH21	2:B:534:ASN:HD21	1.62	0.46
2:B:349:TRP:CZ2	2:B:364:ILE:HD13	2.51	0.46
2:B:526:ARG:HH22	2:B:538:ILE:HD13	1.81	0.46
1:A:630:ARG:HA	1:A:633:HIS:CD2	2.51	0.46
3:D:213:SER:CB	3:D:222:ILE:HD11	2.45	0.46
1:A:557:ILE:HD13	1:A:594:TYR:CE1	2.51	0.46
2:B:526:ARG:HH21	2:B:538:ILE:CD1	2.29	0.46
1:A:109:ILE:HD11	1:A:170:ILE:HD11	1.97	0.46
1:A:297:GLN:HG2	1:A:327:ARG:HH21	1.80	0.46
2:B:181:GLU:N	2:B:184:ILE:HD12	2.30	0.46
3:C:57:ASN:O	3:D:286:HIS:ND1	2.47	0.46
3:D:16:HIS:HB3	3:D:228:ASN:HD21	1.81	0.46
3:D:256:TYR:CE2	3:D:260:ILE:HD11	2.51	0.46
2:B:293:ARG:CD	2:B:330:ILE:CD1	2.94	0.46
3:C:356:ILE:HG22	3:C:357:GLY:N	2.31	0.46
3:C:212:ILE:HD11	3:C:300:ASP:O	2.16	0.46
3:D:90:ARG:HB3	3:D:125:LYS:HE2	1.98	0.46
3:C:317:ASN:HB3	3:C:379:ASN:HB3	1.98	0.46
2:B:527:HIS:CG	2:B:538:ILE:HD11	2.51	0.46
3:C:68:MET:HB3	3:C:92:THR:HG23	1.98	0.46
3:C:205:ASP:CB	3:C:305:LEU:H	2.28	0.46
3:D:263:PRO:O	3:D:266:HIS:CD2	2.68	0.46
3:D:287:LYS:HB2	3:D:291:SER:CB	2.46	0.46
2:B:422:THR:HA	2:B:425:PHE:CD2	2.51	0.46
3:D:435:GLU:O	3:D:438:VAL:HG12	2.16	0.46
3:C:391:CYS:HA	3:C:394:PHE:CD2	2.51	0.46
1:A:423:GLN:O	1:A:427:LEU:HB3	2.15	0.46
2:B:308:SER:O	2:B:311:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PHE:CD2	1:A:90:ILE:HD12	2.51	0.46
2:B:656:ILE:CD1	2:B:738:HIS:CG	2.99	0.46
3:D:17:VAL:HG11	3:D:231:ILE:HD13	1.97	0.46
1:A:251:PHE:CE2	1:A:275:ILE:HD13	2.51	0.46
2:B:317:ASN:HB3	2:B:335:PHE:CE2	2.51	0.46
1:A:418:VAL:HA	1:A:421:HIS:CD2	2.51	0.45
1:A:451:ARG:HG3	1:A:451:ARG:HH11	1.81	0.45
1:A:288:THR:HG23	1:A:289:GLN:HG3	1.98	0.45
3:C:188:ILE:HD12	3:C:394:PHE:CB	2.28	0.45
1:A:799:VAL:HG22	1:A:800:ASP:O	2.16	0.45
2:B:809:LEU:O	2:B:813:VAL:HG23	2.16	0.45
1:A:557:ILE:CD1	1:A:594:TYR:OH	2.54	0.45
3:C:105:TRP:HB2	3:C:186:ASN:HD22	1.81	0.45
3:D:290:SER:HA	3:D:335:MET:HG3	1.98	0.45
3:D:74:SER:O	3:D:77:ALA:HB3	2.16	0.45
3:D:17:VAL:HG11	3:D:231:ILE:CD1	2.46	0.45
3:D:119:ILE:HD12	3:D:154:LEU:HD21	1.96	0.45
3:D:188:ILE:HD13	3:D:394:PHE:CB	2.44	0.45
2:B:353:GLY:HA3	2:B:410:ILE:HG23	1.98	0.45
1:A:387:GLY:H	1:A:390:LEU:HG	1.81	0.45
1:A:580:ILE:O	1:A:584:ILE:HG13	2.17	0.45
3:D:363:LEU:HD12	3:D:365:LEU:O	2.16	0.45
3:C:292:TYR:CZ	3:C:374:GLY:HA3	2.52	0.45
3:C:192:ARG:HH11	3:C:423:PHE:HB2	1.80	0.45
1:A:353:LEU:HD22	1:A:401:ALA:HB1	1.98	0.45
2:B:420:GLN:HB3	2:B:423:ASN:HD22	1.80	0.45
3:D:21:LEU:HD22	3:D:235:ILE:HG21	1.99	0.45
2:B:442:SER:HA	2:B:445:PHE:CE2	2.51	0.45
3:C:29:HIS:CE1	3:C:243:ARG:HH11	2.34	0.45
1:A:172:GLU:H	1:A:172:GLU:CD	2.24	0.45
2:B:445:PHE:CD2	2:B:449:ILE:CD1	2.99	0.45
3:D:369:GLU:HG3	3:D:371:GLU:H	1.81	0.45
3:D:437:TYR:HA	3:D:442:GLN:HB2	1.98	0.45
1:A:569:PRO:O	1:A:572:ILE:HG12	2.16	0.45
1:A:488:THR:HG21	1:A:559:HIS:CD2	2.51	0.45
3:D:184:SER:O	3:D:188:ILE:HG13	2.17	0.45
3:D:240:ASN:HB2	3:D:358:ARG:HH12	1.81	0.45
1:A:143:ARG:CD	2:B:288:TYR:CE2	2.95	0.45
3:D:347:TRP:CE2	3:D:353:HIS:HA	2.52	0.45
3:C:212:ILE:HD11	3:C:300:ASP:O	2.16	0.45
1:A:323:GLN:HG2	1:A:324:TYR:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ASN:HD22	1:A:264:SER:HB2	1.81	0.45
3:C:210:LEU:CD1	3:C:222:ILE:CD1	2.93	0.45
1:A:138:PHE:HD1	1:A:275:ILE:HD11	1.81	0.45
1:A:143:ARG:HH22	2:B:292:ILE:HG13	1.76	0.45
2:B:430:HIS:CG	2:B:448:ILE:HD12	2.51	0.45
2:B:499:ILE:HD12	2:B:512:LEU:CD2	2.47	0.45
2:B:349:TRP:CE2	2:B:406:GLY:HA3	2.52	0.45
2:B:364:ILE:HD11	2:B:403:PHE:HB2	1.98	0.45
3:D:339:GLN:HA	3:D:342:ILE:HG22	1.97	0.45
3:C:31:ILE:CG2	3:C:35:GLY:HA2	2.46	0.45
3:C:424:ALA:HA	3:C:427:ARG:HH21	1.81	0.45
1:A:143:ARG:NE	2:B:288:TYR:CD2	2.76	0.45
1:A:643:ILE:CD1	1:A:692:LEU:HD13	2.47	0.45
2:B:366:GLU:HA	2:B:383:ILE:HG22	1.97	0.45
2:B:653:LEU:HD12	2:B:657:ILE:HD12	1.98	0.45
1:A:557:ILE:CD1	1:A:594:TYR:CE2	2.98	0.45
3:D:93:TRP:HB2	3:D:122:LYS:HE2	1.99	0.45
2:B:533:ARG:CA	2:B:538:ILE:CD1	2.94	0.45
3:D:185:TYR:CZ	3:D:397:VAL:HG13	2.51	0.45
2:B:430:HIS:CB	2:B:448:ILE:HD13	2.44	0.45
3:D:258:THR:CB	3:D:356:ILE:CD1	2.94	0.45
3:D:212:ILE:HD11	3:D:303:ASN:CA	2.46	0.45
1:A:603:TRP:CE3	1:A:633:HIS:HB2	2.51	0.45
2:B:775:VAL:HG11	2:B:805:PHE:CD1	2.51	0.45
1:A:706:PHE:CZ	1:A:710:ILE:CD1	2.78	0.45
1:A:359:ALA:C	1:A:361:LEU:H	2.24	0.45
1:A:118:ILE:HD13	1:A:193:TYR:CE2	2.51	0.45
3:C:166:ILE:HD11	3:C:256:TYR:CG	2.52	0.45
1:A:113:GLY:HA2	1:A:116:TYR:CD2	2.51	0.45
2:B:628:ILE:HG23	2:B:630:LYS:H	1.82	0.45
3:C:213:SER:HB2	3:C:222:ILE:HD11	1.97	0.45
1:A:581:LYS:CB	1:A:683:ILE:CD1	2.95	0.45
2:B:405:ILE:CD1	2:B:456:ILE:HD11	2.41	0.45
1:A:150:TYR:CE2	2:B:281:LYS:HE2	2.52	0.45
1:A:779:LEU:C	1:A:779:LEU:HD13	2.42	0.45
3:D:191:LEU:HB3	3:D:423:PHE:CZ	2.52	0.45
2:B:511:LYS:O	2:B:515:VAL:HG13	2.17	0.45
1:A:624:ARG:H	1:A:624:ARG:HD3	1.82	0.45
3:C:188:ILE:HD12	3:C:394:PHE:CD1	2.52	0.45
1:A:196:ILE:HD13	1:A:250:ILE:CD1	2.47	0.45
1:A:375:ILE:HD13	1:A:396:LYS:CG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:LEU:HD13	1:A:794:TYR:HA	1.99	0.45
3:C:188:ILE:HD12	3:C:394:PHE:HB3	1.97	0.45
1:A:264:SER:HA	1:A:267:PHE:CE2	2.52	0.45
2:B:219:GLY:O	2:B:222:HIS:HB2	2.16	0.45
2:B:293:ARG:CG	2:B:330:ILE:CD1	2.93	0.45
1:A:71:GLU:HA	1:A:75:ILE:CD1	2.39	0.45
2:B:398:LEU:HG	2:B:449:ILE:HD13	1.92	0.45
2:B:398:LEU:CD2	2:B:449:ILE:HD12	2.47	0.45
1:A:425:ILE:HD11	1:A:478:MET:HA	1.99	0.45
3:C:12:GLN:CD	3:C:12:GLN:H	2.25	0.45
1:A:151:LEU:HD11	2:B:282:SER:CB	2.47	0.45
3:C:17:VAL:HG13	3:C:139:LEU:HD23	1.98	0.45
1:A:141:GLU:HG2	1:A:144:ARG:NH2	2.32	0.45
3:D:119:ILE:HD12	3:D:154:LEU:CD2	2.46	0.45
3:D:272:PHE:HB2	3:D:303:ASN:HD21	1.82	0.45
1:A:73:THR:HG22	2:B:215:ASN:CG	2.41	0.45
1:A:151:LEU:HB2	2:B:285:ARG:HB2	1.99	0.45
1:A:699:ILE:HD12	1:A:775:PHE:CE1	2.52	0.45
1:A:430:GLN:HA	3:C:246:SER:H	1.82	0.45
3:C:58:CYS:O	3:D:286:HIS:HB3	2.16	0.45
3:C:123:ILE:CD1	3:C:158:LEU:HD21	2.44	0.45
3:D:119:ILE:HD12	3:D:154:LEU:CD2	2.46	0.45
3:C:239:THR:HB	3:C:243:ARG:HE	1.82	0.45
1:A:134:VAL:CG1	1:A:275:ILE:HD13	2.42	0.45
3:D:212:ILE:HD11	3:D:302:SER:C	2.42	0.45
1:A:372:ASP:O	1:A:375:ILE:HG22	2.16	0.44
2:B:664:MET:HE3	2:B:727:VAL:HG13	1.99	0.44
3:D:289:HIS:CD2	3:D:289:HIS:H	2.34	0.44
2:B:222:HIS:HA	2:B:225:PHE:CD2	2.52	0.44
3:D:242:ILE:HD12	3:D:252:MET:CE	2.46	0.44
3:D:391:CYS:HA	3:D:394:PHE:CE2	2.52	0.44
3:D:338:LEU:HD13	3:D:338:LEU:C	2.42	0.44
2:B:493:ILE:CD1	2:B:598:TYR:HB3	2.44	0.44
2:B:807:THR:O	2:B:811:GLU:HG3	2.17	0.44
1:A:128:ASP:OD1	2:B:295:ARG:NE	2.50	0.44
1:A:140:TYR:OH	2:B:325:LEU:HD22	2.16	0.44
2:B:412:LEU:HD13	2:B:463:ILE:HD13	1.99	0.44
3:D:239:THR:O	3:D:242:ILE:HG12	2.17	0.44
3:D:240:ASN:HA	3:D:243:ARG:HE	1.82	0.44
2:B:482:LEU:HA	2:B:590:LEU:HD13	1.99	0.44
2:B:610:ILE:HG12	2:B:610:ILE:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:258:THR:CG2	3:D:356:ILE:CD1	2.94	0.44
1:A:112:TYR:CE2	1:A:177:ILE:HD11	2.52	0.44
3:C:58:CYS:SG	3:D:285:ALA:C	2.98	0.44
2:B:465:ASN:O	2:B:469:HIS:HA	2.17	0.44
2:B:533:ARG:O	2:B:538:ILE:HD13	2.15	0.44
1:A:567:PRO:HD3	1:A:574:ILE:HD12	1.98	0.44
1:A:567:PRO:CD	1:A:574:ILE:HD11	2.47	0.44
3:C:127:ILE:CD1	3:C:162:TYR:OH	2.65	0.44
3:D:381:SER:O	3:D:384:VAL:HG12	2.17	0.44
1:A:303:ASP:OD1	1:A:304:ASP:O	2.36	0.44
3:C:329:ARG:HH11	3:C:359:ARG:HH11	1.64	0.44
3:C:300:ASP:HB3	3:C:301:PRO:HD3	1.99	0.44
2:B:612:ARG:HB3	2:B:776:TYR:CE2	2.52	0.44
3:C:127:ILE:HD13	3:C:162:TYR:CE1	2.52	0.44
1:A:423:GLN:O	1:A:427:LEU:HB2	2.17	0.44
2:B:596:ASN:HA	2:B:599:PHE:CD2	2.53	0.44
3:C:210:LEU:HD12	3:C:222:ILE:CD1	2.48	0.44
3:D:212:ILE:CD1	3:D:303:ASN:CA	2.95	0.44
2:B:398:LEU:HD21	2:B:446:PHE:CD1	2.53	0.44
2:B:493:ILE:HG21	2:B:598:TYR:CD2	2.53	0.44
2:B:383:ILE:H	2:B:407:LYS:NZ	2.16	0.44
3:C:315:TYR:CD2	3:C:348:SER:HA	2.53	0.44
1:A:128:ASP:OD2	2:B:295:ARG:NH2	2.50	0.44
2:B:441:ILE:HG12	2:B:444:ASN:H	1.82	0.44
3:C:342:ILE:HD12	3:C:344:PHE:HE1	1.82	0.44
1:A:123:TYR:HD1	1:A:139:ALA:HB1	1.83	0.44
1:A:359:ALA:C	1:A:361:LEU:H	2.26	0.44
3:D:7:THR:HG21	3:D:22:TRP:CH2	2.52	0.44
1:A:134:VAL:HG13	1:A:275:ILE:HG21	2.00	0.44
1:A:435:VAL:O	1:A:439:LEU:HD23	2.18	0.44
3:D:234:ILE:HD11	3:D:303:ASN:CG	2.43	0.44
1:A:151:LEU:CD2	2:B:285:ARG:HB3	2.32	0.44
1:A:585:ILE:CD1	1:A:683:ILE:HG23	2.44	0.44
2:B:241:PHE:HB3	2:B:254:ILE:HD11	2.00	0.44
2:B:367:ASN:O	2:B:381:ILE:HD11	2.17	0.44
3:C:212:ILE:HA	3:C:215:LYS:HZ3	1.83	0.44
3:D:426:SER:O	3:D:430:VAL:HG23	2.17	0.44
3:D:9:GLN:HE21	3:D:15:ASN:HA	1.83	0.44
3:C:45:GLU:H	3:C:45:GLU:CD	2.25	0.44
3:D:14:GLY:HA2	3:D:139:LEU:HG	1.98	0.44
1:A:562:PHE:HB2	1:A:587:ARG:HH22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HG21	2:B:278:VAL:HG22	2.00	0.44
1:A:630:ARG:HE	1:A:633:HIS:HE1	1.64	0.44
1:A:74:TYR:CE1	2:B:216:PHE:CZ	3.05	0.44
2:B:656:ILE:HD13	2:B:738:HIS:CG	2.52	0.44
1:A:476:ASN:ND2	1:A:479:ARG:HE	2.16	0.44
3:C:26:ALA:HA	3:C:31:ILE:HD12	1.99	0.44
3:D:256:TYR:CE2	3:D:260:ILE:CD1	3.01	0.44
3:D:258:THR:HG1	3:D:356:ILE:HD11	1.78	0.44
3:D:289:HIS:CD2	3:D:332:SER:HA	2.53	0.44
1:A:112:TYR:CE2	1:A:177:ILE:CD1	3.01	0.44
1:A:151:LEU:CD1	2:B:285:ARG:HB2	2.47	0.44
2:B:438:TYR:CG	2:B:441:ILE:CD1	2.96	0.44
1:A:557:ILE:HD13	1:A:594:TYR:HH	1.78	0.44
1:A:625:ILE:HB	1:A:765:ILE:CD1	2.48	0.44
3:C:31:ILE:HD13	3:C:62:PHE:CD2	2.53	0.44
1:A:366:ILE:CD1	1:A:371:SER:CB	2.95	0.44
3:D:93:TRP:HE1	3:D:118:ASP:HB3	1.83	0.44
3:D:284:ILE:HG12	3:D:370:ASN:H	1.82	0.44
1:A:277:GLN:HE22	1:A:381:PHE:HA	1.82	0.44
1:A:300:MET:CE	1:A:327:ARG:HH21	2.31	0.44
2:B:202:PHE:CE1	2:B:206:GLN:HA	2.53	0.44
2:B:533:ARG:HA	2:B:538:ILE:CD1	2.48	0.44
3:D:212:ILE:HD11	3:D:302:SER:H	1.82	0.44
2:B:728:HIS:CD2	2:B:728:HIS:C	2.95	0.44
1:A:111:ARG:HE	1:A:111:ARG:C	2.26	0.44
3:C:212:ILE:HD11	3:C:301:PRO:HA	2.00	0.44
3:C:381:SER:O	3:C:384:VAL:HG22	2.18	0.44
1:A:567:PRO:HD2	1:A:574:ILE:CD1	2.47	0.44
2:B:349:TRP:CE3	2:B:353:GLY:HA2	2.52	0.44
2:B:499:ILE:CD1	2:B:507:LEU:CD2	2.96	0.44
2:B:499:ILE:CD1	2:B:508:PRO:HD3	2.35	0.44
3:C:56:GLU:CD	3:D:286:HIS:NE2	2.75	0.44
2:B:234:LEU:HD22	2:B:257:ILE:HD11	2.00	0.44
2:B:560:LEU:HD23	2:B:560:LEU:HA	1.88	0.44
2:B:499:ILE:HD13	2:B:508:PRO:HB3	2.00	0.44
1:A:295:PRO:HG3	2:B:321:SER:CB	2.48	0.44
3:C:306:VAL:HG13	3:C:386:VAL:HG23	1.98	0.44
1:A:363:ILE:HG12	1:A:365:THR:H	1.82	0.44
1:A:109:ILE:HD11	1:A:170:ILE:CD1	2.48	0.44
3:C:53:PHE:HB2	3:C:54:PHE:CD1	2.53	0.44
3:C:56:GLU:OE1	3:D:286:HIS:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:176:ARG:HE	3:D:176:ARG:HA	1.83	0.43
2:B:544:ARG:HE	2:B:545:VAL:H	1.65	0.43
2:B:586:ILE:HD11	2:B:732:LEU:HD13	1.99	0.43
2:B:419:VAL:HG23	2:B:421:TRP:NE1	2.32	0.43
3:C:93:TRP:CZ3	3:C:95:ALA:HB2	2.52	0.43
1:A:485:GLN:HE22	1:A:487:ASP:CG	2.26	0.43
2:B:426:SER:HA	2:B:429:TYR:CE2	2.53	0.43
2:B:405:ILE:CG2	2:B:456:ILE:CD1	2.89	0.43
1:A:473:ASN:HB2	1:A:474:PRO:HD2	1.99	0.43
2:B:339:ILE:CD1	2:B:439:ARG:HD3	2.48	0.43
3:D:29:HIS:HD1	3:D:47:ASP:HA	1.83	0.43
1:A:281:THR:HA	1:A:284:TYR:CD2	2.53	0.43
3:D:176:ARG:CD	3:D:386:VAL:HG22	2.48	0.43
1:A:585:ILE:HD11	1:A:683:ILE:CD1	2.05	0.43
1:A:386:GLU:H	1:A:386:GLU:CD	2.26	0.43
2:B:296:ILE:CD1	2:B:327:ILE:HD12	2.49	0.43
3:C:105:TRP:CZ2	3:C:109:TYR:CD1	3.06	0.43
1:A:375:ILE:HD13	1:A:396:LYS:HB3	1.99	0.43
1:A:142:ILE:HD11	1:A:188:LEU:HD13	1.99	0.43
1:A:138:PHE:CD2	1:A:275:ILE:CD1	2.85	0.43
3:C:234:ILE:CD1	3:C:303:ASN:CG	2.91	0.43
1:A:137:ARG:HD2	1:A:137:ARG:O	2.18	0.43
2:B:493:ILE:CD1	2:B:598:TYR:CG	3.01	0.43
1:A:142:ILE:HD13	1:A:189:LEU:HD11	1.96	0.43
3:D:255:ILE:HD13	3:D:255:ILE:HG21	1.87	0.43
1:A:186:MET:HA	1:A:189:LEU:HD12	1.99	0.43
1:A:625:ILE:HD11	1:A:761:ILE:CG1	2.43	0.43
2:B:316:LEU:HG	2:B:335:PHE:CE2	2.53	0.43
1:A:774:ILE:HG22	1:A:793:PHE:HB2	2.01	0.43
1:A:133:MET:HG2	2:B:322:HIS:CE1	2.54	0.43
1:A:386:GLU:HG3	1:A:389:ASN:H	1.83	0.43
1:A:613:LYS:HG2	1:A:614:TYR:H	1.83	0.43
2:B:284:TYR:OH	2:B:291:ILE:HD12	2.18	0.43
3:D:397:VAL:HG11	3:D:420:GLN:HE22	1.82	0.43
3:C:139:LEU:N	3:C:139:LEU:HD12	2.33	0.43
3:C:212:ILE:O	3:C:216:VAL:HG22	2.18	0.43
3:D:242:ILE:HD13	3:D:252:MET:HE3	2.00	0.43
3:D:258:THR:HG23	3:D:356:ILE:CD1	2.48	0.43
2:B:285:ARG:O	2:B:288:TYR:HB2	2.19	0.43
2:B:827:ARG:HH22	3:D:353:HIS:CG	2.36	0.43
3:C:212:ILE:CD1	3:C:300:ASP:O	2.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:TYR:CD1	1:A:484:ILE:HD13	2.40	0.43
2:B:628:ILE:HG23	2:B:629:ASN:N	2.34	0.43
1:A:370:SER:HB3	1:A:400:ARG:HG3	2.00	0.43
2:B:187:TYR:HA	2:B:190:TYR:CD2	2.53	0.43
3:D:279:TYR:CG	3:D:280:ILE:N	2.87	0.43
1:A:375:ILE:CD1	1:A:393:TYR:HA	2.45	0.43
2:B:251:LYS:O	2:B:255:ILE:HG13	2.18	0.43
3:D:354:VAL:O	3:D:354:VAL:HG22	2.19	0.43
2:B:843:LYS:O	2:B:846:ARG:O	2.36	0.43
3:C:188:ILE:HD11	3:C:394:PHE:HD2	1.80	0.43
1:A:64:LEU:HD22	1:A:167:ASN:HD22	1.84	0.43
3:D:166:ILE:CD1	3:D:256:TYR:CD1	2.96	0.43
3:D:255:ILE:O	3:D:259:LEU:HG	2.18	0.43
3:C:105:TRP:HB2	3:C:186:ASN:HD22	1.83	0.43
1:A:135:LEU:HB2	1:A:247:ILE:CD1	2.49	0.43
3:C:292:TYR:CZ	3:C:374:GLY:HA3	2.53	0.43
1:A:80:ASP:HA	1:A:121:ARG:HH12	1.82	0.43
1:A:323:GLN:HG2	1:A:324:TYR:H	1.83	0.43
3:C:119:ILE:HD12	3:C:154:LEU:HD23	2.00	0.43
2:B:731:PHE:HE1	2:B:735:ILE:CD1	2.17	0.43
3:C:230:LEU:O	3:C:234:ILE:HG13	2.18	0.43
3:D:195:ILE:HD11	3:D:430:VAL:HG21	2.01	0.43
3:C:123:ILE:HD12	3:C:161:ARG:HH12	1.83	0.43
3:C:292:TYR:CE1	3:C:374:GLY:HA3	2.53	0.43
1:A:296:TYR:CD2	2:B:322:HIS:HE1	2.25	0.43
1:A:485:GLN:HG3	1:A:561:LYS:HB2	2.01	0.43
3:C:416:MET:CG	3:C:417:GLN:H	2.32	0.43
1:A:137:ARG:HH22	2:B:328:ARG:HH11	1.53	0.43
1:A:458:TYR:CE1	1:A:484:ILE:HD11	2.49	0.43
3:D:52:PRO:O	3:D:65:ARG:HD2	2.18	0.43
1:A:425:ILE:HD11	1:A:482:LEU:HD13	2.01	0.43
3:D:366:GLN:CD	3:D:366:GLN:H	2.27	0.43
1:A:425:ILE:CD1	1:A:481:LEU:HD21	2.49	0.43
3:D:212:ILE:CD1	3:D:303:ASN:ND2	2.82	0.43
2:B:517:GLN:O	2:B:520:VAL:HG22	2.19	0.43
1:A:251:PHE:HE2	1:A:275:ILE:HD13	1.84	0.43
3:C:136:PHE:CD1	3:C:167:LEU:HD13	2.54	0.43
3:C:188:ILE:HD11	3:C:427:ARG:HE	1.84	0.43
1:A:587:ARG:O	1:A:591:VAL:HG23	2.18	0.43
2:B:365:ALA:HB2	2:B:389:ARG:HH22	1.84	0.43
3:C:141:SER:C	3:C:143:ALA:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:664:MET:HG3	2:B:727:VAL:HG13	2.00	0.43
3:C:394:PHE:CD2	3:C:394:PHE:C	2.97	0.43
3:C:10:ALA:HB1	3:C:147:GLY:HA2	2.01	0.43
3:D:333:ARG:HH21	3:D:334:ALA:HA	1.84	0.43
1:A:357:VAL:CB	1:A:363:ILE:CD1	2.69	0.43
1:A:294:ASP:HA	1:A:298:GLU:H	1.84	0.43
1:A:585:ILE:HD12	1:A:683:ILE:HG21	2.00	0.43
1:A:606:LEU:HD11	1:A:710:ILE:CD1	2.11	0.43
3:C:441:GLU:CD	3:C:441:GLU:H	2.26	0.43
3:D:234:ILE:HD13	3:D:303:ASN:OD1	2.19	0.43
1:A:109:ILE:HD13	1:A:109:ILE:HG21	1.82	0.43
3:C:364:PRO:HD2	3:C:365:LEU:HD22	2.01	0.43
2:B:196:THR:HA	2:B:202:PHE:HB2	2.01	0.43
2:B:325:LEU:CD2	2:B:325:LEU:H	2.32	0.43
1:A:67:LEU:CD2	1:A:113:GLY:HA3	2.49	0.43
1:A:384:LEU:N	1:A:384:LEU:HD22	2.33	0.43
2:B:556:ASP:HA	2:B:592:ARG:NH2	2.34	0.43
2:B:493:ILE:HD12	2:B:598:TYR:CB	2.49	0.43
3:D:81:ASN:C	3:D:83:PHE:H	2.26	0.43
1:A:252:GLN:HE21	1:A:252:GLN:HA	1.84	0.43
3:D:70:ASP:CG	3:D:71:SER:H	2.26	0.43
2:B:470:TYR:CE1	2:B:565:TYR:CE2	3.07	0.43
1:A:591:VAL:O	1:A:595:HIS:CD2	2.72	0.43
1:A:300:MET:HB3	1:A:332:LEU:H	1.84	0.43
1:A:697:LEU:HD22	1:A:697:LEU:HA	1.92	0.43
2:B:357:ALA:O	2:B:358:THR:HG22	2.19	0.43
3:C:256:TYR:CE2	3:C:260:ILE:HD12	2.54	0.43
1:A:571:ASN:HA	1:A:574:ILE:HD12	2.01	0.43
2:B:222:HIS:HA	2:B:225:PHE:CD2	2.53	0.43
2:B:284:TYR:CZ	2:B:291:ILE:CD1	3.02	0.43
2:B:493:ILE:HD13	2:B:493:ILE:HG21	1.91	0.43
2:B:499:ILE:HD11	2:B:508:PRO:CA	2.48	0.43
1:A:660:GLU:HA	1:A:663:TYR:CD2	2.54	0.42
3:C:280:ILE:HG23	3:C:282:ASP:H	1.83	0.42
3:C:306:VAL:HG11	3:C:383:VAL:HA	2.00	0.42
1:A:409:PHE:CZ	1:A:573:ILE:HD11	2.54	0.42
3:C:356:ILE:HG12	3:C:357:GLY:N	2.34	0.42
1:A:143:ARG:HD2	2:B:288:TYR:CZ	2.54	0.42
1:A:327:ARG:HD3	1:A:330:VAL:HG23	2.00	0.42
3:C:57:ASN:O	3:D:286:HIS:HB3	2.19	0.42
3:D:431:GLN:O	3:D:435:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:725:GLU:HA	2:B:728:HIS:CD2	2.53	0.42
3:D:13:CYS:O	3:D:17:VAL:HG23	2.19	0.42
2:B:601:GLN:HE22	2:B:605:LEU:CD1	2.31	0.42
3:C:195:ILE:HA	3:C:266:HIS:CE1	2.54	0.42
1:A:114:LYS:HG3	1:A:118:ILE:HD12	2.01	0.42
2:B:398:LEU:HD21	2:B:449:ILE:HD13	2.01	0.42
2:B:516:LEU:C	2:B:516:LEU:HD23	2.44	0.42
2:B:643:GLN:HE21	3:D:354:VAL:HG11	1.83	0.42
1:A:610:PRO:O	1:A:713:MET:HE3	2.19	0.42
3:D:281:HIS:CG	3:D:282:ASP:N	2.87	0.42
1:A:482:LEU:HA	1:A:564:ILE:HG22	2.02	0.42
1:A:564:ILE:HG12	1:A:579:MET:HE2	2.00	0.42
3:D:127:ILE:HD11	3:D:162:TYR:CE2	2.54	0.42
3:D:17:VAL:HG23	3:D:231:ILE:HG23	2.00	0.42
3:D:335:MET:HB3	3:D:335:MET:HE3	1.86	0.42
1:A:292:LEU:HD22	1:A:299:PHE:CE2	2.54	0.42
3:D:6:ILE:HD13	3:D:126:GLU:HB2	2.00	0.42
1:A:781:ASN:HD22	1:A:790:LYS:H	1.66	0.42
2:B:201:PRO:HG2	2:B:208:GLN:HE21	1.83	0.42
2:B:611:ILE:HG21	2:B:777:CYS:SG	2.60	0.42
3:C:251:SER:O	3:C:255:ILE:HG13	2.19	0.42
3:D:105:TRP:CD2	3:D:189:LEU:HB3	2.54	0.42
1:A:679:GLY:O	1:A:683:ILE:HG13	2.19	0.42
3:D:119:ILE:HD12	3:D:154:LEU:HD21	2.00	0.42
3:D:212:ILE:CD1	3:D:302:SER:O	2.67	0.42
1:A:285:GLU:HB3	1:A:291:ILE:HB	2.00	0.42
1:A:450:TYR:O	1:A:451:ARG:HG2	2.19	0.42
3:C:34:ASP:HB3	3:C:85:GLY:HA3	2.01	0.42
3:C:138:LEU:HB3	3:C:169:THR:HG22	2.01	0.42
3:D:9:GLN:HE21	3:D:15:ASN:HA	1.83	0.42
3:D:251:SER:O	3:D:255:ILE:HG13	2.18	0.42
2:B:240:LYS:HD3	2:B:240:LYS:C	2.45	0.42
1:A:357:VAL:HG22	1:A:408:LEU:HD22	2.00	0.42
2:B:220:LEU:O	2:B:224:ILE:HG13	2.19	0.42
2:B:453:TYR:O	2:B:456:ILE:HG22	2.19	0.42
2:B:743:THR:HA	2:B:759:PRO:HD3	2.02	0.42
3:C:131:ASP:O	3:C:132:ASN:HB2	2.19	0.42
3:D:123:ILE:HG22	3:D:127:ILE:HD12	2.01	0.42
2:B:430:HIS:CG	2:B:448:ILE:HD13	2.53	0.42
1:A:358:ARG:HH21	1:A:363:ILE:HG23	1.84	0.42
1:A:564:ILE:HD11	1:A:579:MET:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:MET:HE1	2:B:323:GLY:H	1.84	0.42
1:A:638:HIS:CE1	3:C:355:ASN:H	2.37	0.42
3:D:306:VAL:HG12	3:D:382:THR:HG21	2.01	0.42
1:A:296:TYR:HB2	2:B:322:HIS:ND1	2.35	0.42
1:A:557:ILE:HD12	1:A:594:TYR:OH	2.10	0.42
2:B:280:LEU:O	2:B:284:TYR:CD2	2.73	0.42
3:D:234:ILE:O	3:D:238:VAL:HG23	2.19	0.42
1:A:624:ARG:CZ	1:A:627:ARG:HH12	2.31	0.42
1:A:196:ILE:CD1	1:A:250:ILE:CD1	2.98	0.42
2:B:533:ARG:C	2:B:538:ILE:HD12	2.45	0.42
1:A:128:ASP:OD1	2:B:295:ARG:NH1	2.53	0.42
3:C:37:SER:H	3:C:61:LYS:HD2	1.84	0.42
2:B:207:ILE:CD1	2:B:221:LEU:HD11	2.49	0.42
3:D:212:ILE:CD1	3:D:303:ASN:OD1	2.65	0.42
1:A:609:THR:HB	1:A:610:PRO:HD3	2.01	0.42
2:B:300:PHE:O	2:B:304:LEU:HB2	2.19	0.42
2:B:307:LEU:HD23	2:B:307:LEU:HA	1.86	0.42
1:A:578:CYS:SG	1:A:680:LEU:HD21	2.60	0.42
2:B:566:PRO:HA	2:B:567:PRO:C	2.44	0.42
1:A:99:ASP:HB3	1:A:102:PHE:CD2	2.54	0.42
1:A:606:LEU:HD11	1:A:710:ILE:HD11	2.01	0.42
2:B:441:ILE:HD13	2:B:444:ASN:HB2	2.01	0.42
3:C:102:GLY:HA3	3:C:107:ASN:HD22	1.85	0.42
2:B:220:LEU:HD22	2:B:220:LEU:H	1.84	0.42
2:B:430:HIS:HB3	2:B:448:ILE:HD13	2.01	0.42
3:D:320:ASN:HB3	3:D:358:ARG:HH21	1.83	0.42
2:B:241:PHE:HB2	2:B:254:ILE:CD1	2.49	0.42
3:C:267:PHE:HB2	3:C:383:VAL:HG11	2.00	0.42
1:A:481:LEU:HA	1:A:565:ASN:HD22	1.84	0.42
2:B:207:ILE:HG22	2:B:225:PHE:CD1	2.54	0.42
3:C:240:ASN:HA	3:C:243:ARG:HE	1.84	0.42
1:A:630:ARG:HD2	3:C:261:PRO:O	2.19	0.42
3:D:340:GLN:HE22	3:D:341:ARG:HE	1.68	0.42
1:A:706:PHE:O	1:A:710:ILE:HG13	2.20	0.42
3:C:123:ILE:O	3:C:127:ILE:HG13	2.20	0.42
3:C:176:ARG:H	3:C:207:ALA:HB2	1.85	0.42
3:C:176:ARG:HE	3:C:210:LEU:HD23	1.84	0.42
1:A:595:HIS:HB3	1:A:700:PHE:CD1	2.55	0.42
2:B:405:ILE:CD1	2:B:452:GLN:NE2	2.83	0.42
2:B:533:ARG:NH1	2:B:538:ILE:HD11	2.35	0.42
2:B:766:LEU:O	2:B:769:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:829:ASP:HA	2:B:835:ASP:HB2	2.02	0.42
3:D:3:GLY:HA2	3:D:132:ASN:O	2.20	0.42
1:A:142:ILE:HG12	1:A:146:LEU:HD22	2.00	0.42
1:A:613:LYS:HD3	1:A:614:TYR:O	2.20	0.42
2:B:482:LEU:CB	2:B:657:ILE:HD11	2.42	0.42
3:D:363:LEU:H	3:D:363:LEU:HD23	1.85	0.42
2:B:363:PHE:HA	2:B:389:ARG:HE	1.84	0.42
2:B:636:ILE:HG22	3:D:261:PRO:HB2	2.02	0.42
3:C:140:HIS:CE1	3:C:142:VAL:HG12	2.55	0.42
3:D:435:GLU:O	3:D:438:VAL:HG22	2.20	0.42
1:A:68:ILE:HG22	1:A:70:LEU:HG	2.01	0.42
2:B:429:TYR:HB3	2:B:433:TYR:CZ	2.54	0.42
2:B:445:PHE:CD2	2:B:449:ILE:HD12	2.55	0.42
3:D:212:ILE:HD11	3:D:300:ASP:O	2.20	0.42
1:A:70:LEU:HD11	2:B:216:PHE:HA	2.02	0.42
1:A:151:LEU:CB	2:B:285:ARG:NE	2.76	0.42
2:B:366:GLU:OE2	2:B:381:ILE:HD11	2.19	0.42
1:A:557:ILE:CD1	1:A:595:HIS:HE1	2.33	0.42
1:A:577:THR:O	1:A:580:ILE:HG12	2.19	0.42
3:D:195:ILE:HD11	3:D:423:PHE:CE1	2.44	0.42
2:B:405:ILE:HD13	2:B:452:GLN:HE22	1.84	0.42
3:D:359:ARG:H	3:D:359:ARG:NE	2.17	0.42
1:A:149:VAL:O	1:A:153:THR:HG23	2.20	0.42
2:B:239:GLU:HA	2:B:242:ARG:HH21	1.84	0.42
3:D:154:LEU:O	3:D:158:LEU:HG	2.20	0.42
3:D:325:ASN:H	3:D:359:ARG:HH22	1.68	0.42
1:A:581:LYS:CB	1:A:683:ILE:HD13	2.38	0.42
3:D:328:PRO:HB2	3:D:331:ILE:CD1	2.48	0.42
3:C:188:ILE:CD1	3:C:394:PHE:CB	2.85	0.42
3:D:188:ILE:HD13	3:D:188:ILE:HG21	1.80	0.42
1:A:63:LEU:CG	1:A:170:ILE:HD11	2.48	0.42
3:C:205:ASP:HB3	3:C:305:LEU:H	1.84	0.42
3:D:212:ILE:HD11	3:D:302:SER:C	2.45	0.42
2:B:670:ARG:C	2:B:671:THR:O	2.62	0.42
1:A:187:GLU:HG2	1:A:190:TYR:CZ	2.55	0.42
2:B:304:LEU:HA	2:B:307:LEU:O	2.20	0.42
2:B:476:ALA:O	2:B:480:ILE:HG22	2.19	0.42
3:D:127:ILE:CD1	3:D:162:TYR:CE2	3.02	0.42
1:A:363:ILE:HD13	1:A:363:ILE:HG21	1.88	0.42
2:B:493:ILE:HG21	2:B:598:TYR:HB3	2.02	0.42
2:B:641:PHE:CZ	2:B:765:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:ILE:CD1	3:C:126:GLU:HB3	2.49	0.42
3:C:322:ILE:HA	3:C:358:ARG:HB3	2.01	0.42
3:D:183:GLN:HE22	3:D:393:THR:HG21	1.84	0.42
3:D:384:VAL:HB	3:D:434:MET:SD	2.60	0.42
1:A:449:HIS:H	1:A:449:HIS:CD2	2.37	0.42
1:A:697:LEU:HD22	1:A:697:LEU:HA	1.93	0.42
3:C:8:LEU:HD23	3:C:67:ILE:HB	2.02	0.42
3:C:59:ARG:NH1	3:C:60:ASN:HD22	2.18	0.42
3:C:206:ASN:HA	3:C:209:LEU:HB2	2.02	0.42
1:A:634:ALA:HB2	3:C:261:PRO:HB3	2.02	0.42
3:D:212:ILE:HD12	3:D:303:ASN:CG	2.45	0.42
2:B:604:MET:HG3	2:B:638:ARG:HG2	2.01	0.41
2:B:356:ARG:HE	2:B:358:THR:H	1.67	0.41
2:B:187:TYR:HA	2:B:190:TYR:CD2	2.55	0.41
2:B:586:ILE:HD12	2:B:732:LEU:HD22	2.02	0.41
3:C:284:ILE:HD13	3:C:284:ILE:HG21	1.85	0.41
3:D:212:ILE:HD13	3:D:275:PHE:CD2	2.55	0.41
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.79	0.41
3:C:299:LEU:HD13	3:C:299:LEU:HA	1.87	0.41
2:B:664:MET:HE1	2:B:731:PHE:CD2	2.54	0.41
3:C:325:ASN:HB3	3:C:372:VAL:HA	2.02	0.41
1:A:70:LEU:HG	2:B:216:PHE:HB3	2.02	0.41
1:A:143:ARG:HH11	1:A:147:GLU:HG3	1.84	0.41
2:B:180:PRO:HD2	2:B:185:LEU:HD21	2.02	0.41
2:B:446:PHE:HA	2:B:449:ILE:HG12	2.02	0.41
3:D:209:LEU:HD22	3:D:230:LEU:HD12	2.02	0.41
2:B:339:ILE:HD13	2:B:339:ILE:HG21	1.87	0.41
3:D:231:ILE:O	3:D:235:ILE:HG13	2.20	0.41
2:B:492:LEU:HD13	2:B:492:LEU:C	2.45	0.41
1:A:128:ASP:OD1	2:B:299:ARG:NH1	2.53	0.41
2:B:320:LYS:HA	2:B:328:ARG:HA	2.01	0.41
2:B:578:PHE:HA	2:B:581:LYS:HB2	2.01	0.41
3:C:123:ILE:CD1	3:C:161:ARG:HH12	2.33	0.41
3:D:270:PRO:HA	3:D:376:MET:O	2.20	0.41
2:B:813:VAL:HG11	3:D:445:TYR:HB2	2.01	0.41
3:D:173:PHE:CD1	3:D:203:VAL:HG13	2.54	0.41
2:B:538:ILE:HD13	2:B:538:ILE:HG21	1.85	0.41
1:A:146:LEU:CD2	1:A:183:ASN:HD22	2.33	0.41
1:A:151:LEU:CD1	2:B:285:ARG:CB	2.99	0.41
3:C:279:TYR:CE1	3:C:281:HIS:CE1	3.09	0.41
2:B:363:PHE:HA	2:B:389:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:499:ILE:HD13	2:B:499:ILE:HG21	1.89	0.41
3:C:344:PHE:HB3	3:C:345:PRO:HD3	2.01	0.41
3:D:433:LEU:HD12	3:D:433:LEU:HA	1.84	0.41
2:B:339:ILE:HD13	2:B:343:TYR:OH	2.20	0.41
2:B:346:LEU:CD1	2:B:402:ILE:HD13	2.51	0.41
3:C:59:ARG:HH22	3:D:371:GLU:HG3	1.85	0.41
3:C:20:PHE:O	3:C:24:GLN:HG3	2.20	0.41
1:A:151:LEU:HD12	2:B:285:ARG:CG	2.51	0.41
3:C:17:VAL:HG22	3:C:228:ASN:CB	2.49	0.41
2:B:607:SER:CB	2:B:634:ILE:HD11	2.50	0.41
3:C:93:TRP:CH2	3:C:95:ALA:HB2	2.56	0.41
3:C:188:ILE:HD12	3:C:394:PHE:CD1	2.55	0.41
3:C:322:ILE:HD11	3:C:377:LEU:HD12	2.03	0.41
3:D:217:PHE:CE1	3:D:226:HIS:CD2	3.09	0.41
1:A:375:ILE:HD12	1:A:396:LYS:HG2	1.96	0.41
1:A:360:SER:C	1:A:362:GLN:H	2.28	0.41
2:B:402:ILE:CG1	2:B:449:ILE:HD13	2.41	0.41
3:D:105:TRP:CZ2	3:D:109:TYR:CD2	3.09	0.41
3:D:70:ASP:HB2	3:D:71:SER:H	1.71	0.41
2:B:438:TYR:HB2	2:B:441:ILE:HD11	2.01	0.41
2:B:349:TRP:HE1	2:B:403:PHE:HA	1.85	0.41
3:C:46:ARG:HD2	3:C:365:LEU:HB2	2.02	0.41
1:A:567:PRO:HD2	1:A:574:ILE:HD11	2.02	0.41
3:C:64:PRO:HD3	3:C:86:PHE:CD1	2.55	0.41
3:D:444:SER:C	3:D:445:TYR:O	2.62	0.41
3:C:12:GLN:CD	3:C:12:GLN:H	2.27	0.41
2:B:427:LYS:HB2	2:B:448:ILE:HD12	2.02	0.41
1:A:693:ILE:HD13	1:A:693:ILE:HG21	1.81	0.41
3:D:188:ILE:HD11	3:D:394:PHE:HB3	1.99	0.41
3:C:188:ILE:HD13	3:C:188:ILE:HG21	1.84	0.41
3:D:67:ILE:HG23	3:D:122:LYS:HD3	2.03	0.41
1:A:142:ILE:HD11	1:A:271:LEU:HG	2.02	0.41
3:D:67:ILE:HD11	3:D:122:LYS:HB2	2.02	0.41
1:A:160:ARG:HH22	1:A:164:LYS:HD2	1.86	0.41
1:A:400:ARG:O	1:A:404:ILE:HG13	2.21	0.41
1:A:568:TYR:CD1	1:A:569:PRO:HA	2.55	0.41
2:B:381:ILE:HB	2:B:570:LEU:HD21	2.02	0.41
3:D:5:ILE:HD11	3:D:252:MET:HG2	2.01	0.41
1:A:79:ASN:O	1:A:80:ASP:O	2.39	0.41
2:B:427:LYS:CB	2:B:448:ILE:HD12	2.51	0.41
2:B:244:LEU:HD13	2:B:244:LEU:HA	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:532:PRO:HA	2:B:535:SER:HB3	2.03	0.41
3:C:68:MET:SD	3:C:75:VAL:HG22	2.61	0.41
3:D:318:VAL:CG2	3:D:319:TYR:N	2.84	0.41
1:A:421:HIS:HE2	1:A:425:ILE:HD12	1.82	0.41
2:B:213:ILE:HD11	2:B:221:LEU:HD12	2.01	0.41
2:B:434:GLN:HE22	2:B:444:ASN:HB3	1.86	0.41
2:B:560:LEU:HD13	2:B:561:ASP:N	2.35	0.41
3:C:31:ILE:HG21	3:C:35:GLY:HA2	2.03	0.41
3:C:188:ILE:HD12	3:C:394:PHE:HB3	1.86	0.41
3:D:234:ILE:HD13	3:D:303:ASN:OD1	2.21	0.41
3:C:212:ILE:HD12	3:C:302:SER:O	2.15	0.41
2:B:728:HIS:O	2:B:732:LEU:HG	2.20	0.41
2:B:402:ILE:HG21	2:B:402:ILE:HD13	1.75	0.41
1:A:674:ASN:HD22	1:A:674:ASN:HA	1.72	0.41
2:B:234:LEU:O	2:B:238:VAL:HG23	2.20	0.41
3:D:210:LEU:HD23	3:D:210:LEU:HA	1.95	0.41
1:A:409:PHE:CZ	1:A:573:ILE:CD1	2.80	0.41
1:A:693:ILE:HG23	1:A:694:PRO:HD3	2.03	0.41
2:B:451:ASP:O	2:B:455:GLU:HG3	2.20	0.41
2:B:339:ILE:HG12	2:B:343:TYR:CE1	2.56	0.41
3:C:266:HIS:CE1	3:C:267:PHE:CZ	3.08	0.41
3:C:271:SER:CB	3:C:296:LEU:HB3	2.50	0.41
1:A:560:LEU:HD12	1:A:560:LEU:HA	1.82	0.41
1:A:599:LEU:HD22	1:A:703:VAL:HG11	2.02	0.41
2:B:426:SER:HA	2:B:429:TYR:CD2	2.56	0.41
3:C:237:SER:HB2	3:C:375:MET:HE1	2.02	0.41
1:A:378:ILE:HD13	1:A:378:ILE:HG21	1.85	0.41
3:C:24:GLN:HE22	3:C:232:SER:HB2	1.85	0.41
2:B:529:MET:SD	2:B:531:SER:HB2	2.61	0.41
3:C:36:LEU:HD12	3:C:36:LEU:H	1.85	0.41
3:C:394:PHE:CD1	3:C:394:PHE:C	2.99	0.41
3:D:318:VAL:HG23	3:D:354:VAL:HG12	2.03	0.41
1:A:384:LEU:HD12	1:A:384:LEU:HA	1.90	0.41
2:B:238:VAL:O	2:B:242:ARG:HG3	2.20	0.41
2:B:412:LEU:HD13	2:B:463:ILE:CD1	2.50	0.41
1:A:59:VAL:HB	1:A:102:PHE:CE2	2.55	0.41
3:C:271:SER:HA	3:C:302:SER:HA	2.02	0.41
1:A:75:ILE:HD11	1:A:92:PHE:HB3	2.02	0.41
3:C:255:ILE:HD13	3:C:358:ARG:NH1	2.33	0.41
3:D:217:PHE:HA	3:D:280:ILE:HD12	2.02	0.41
2:B:220:LEU:HD21	2:B:280:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:544:ARG:HB2	2:B:561:ASP:HB2	2.02	0.41
1:A:609:THR:CG2	1:A:610:PRO:HD3	2.51	0.41
2:B:264:TYR:O	2:B:268:VAL:HG23	2.21	0.41
1:A:391:GLU:HA	1:A:394:VAL:HG22	2.03	0.41
3:D:271:SER:HB3	3:D:376:MET:HB3	2.01	0.41
2:B:202:PHE:CE1	2:B:207:ILE:HD11	2.56	0.41
2:B:296:ILE:HD12	2:B:327:ILE:HD12	2.03	0.41
2:B:489:MET:HE1	2:B:591:TRP:CD1	2.56	0.41
1:A:133:MET:HE3	2:B:323:GLY:N	2.36	0.41
3:D:318:VAL:HG22	3:D:319:TYR:N	2.35	0.41
1:A:189:LEU:HB3	1:A:193:TYR:CZ	2.56	0.41
1:A:357:VAL:HB	1:A:363:ILE:HD11	1.91	0.41
3:C:122:LYS:O	3:C:125:LYS:HG2	2.20	0.41
1:A:55:GLN:HB3	1:A:56:GLU:H	1.68	0.41
1:A:321:ASP:HB3	1:A:572:ILE:CD1	2.42	0.41
2:B:499:ILE:CD1	2:B:507:LEU:HD23	2.50	0.41
2:B:826:PHE:O	2:B:829:ASP:HB3	2.21	0.41
3:C:188:ILE:HD12	3:C:394:PHE:CD1	2.50	0.41
1:A:150:TYR:HE2	2:B:281:LYS:HE2	1.86	0.41
1:A:760:LEU:HD13	1:A:760:LEU:C	2.46	0.41
2:B:363:PHE:CD2	2:B:390:VAL:HG22	2.56	0.41
3:C:9:GLN:O	3:C:69:MET:HE2	2.21	0.41
3:C:394:PHE:CE2	3:C:424:ALA:HB2	2.56	0.41
2:B:838:LEU:HD13	2:B:838:LEU:C	2.45	0.41
3:C:256:TYR:CE1	3:C:260:ILE:HD12	2.56	0.41
2:B:464:LEU:HD23	2:B:468:PHE:CE2	2.56	0.41
2:B:480:ILE:HD13	2:B:480:ILE:HG21	1.93	0.41
1:A:669:ALA:O	1:A:672:ILE:HG12	2.21	0.41
3:C:286:HIS:CD2	3:C:371:GLU:HB3	2.56	0.41
3:D:105:TRP:CH2	3:D:109:TYR:CD2	3.09	0.41
1:A:643:ILE:CD1	1:A:692:LEU:HD21	2.38	0.41
3:C:170:TYR:CD2	3:C:235:ILE:HG22	2.55	0.41
3:D:266:HIS:CD2	3:D:266:HIS:C	2.98	0.41
1:A:637:ASN:HA	1:A:640:ILE:HG12	2.03	0.41
2:B:493:ILE:CD1	2:B:595:LYS:HA	2.51	0.41
2:B:544:ARG:HA	2:B:544:ARG:NE	2.36	0.41
3:C:280:ILE:HD11	3:C:284:ILE:CD1	2.41	0.41
2:B:738:HIS:CD2	2:B:738:HIS:N	2.84	0.40
3:C:206:ASN:HA	3:C:209:LEU:HD12	2.03	0.40
3:D:238:VAL:HG13	3:D:375:MET:HE2	2.03	0.40
1:A:484:ILE:HD13	1:A:484:ILE:HG21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:LEU:HB2	3:C:138:LEU:HD12	2.03	0.40
1:A:135:LEU:CD1	1:A:247:ILE:HD13	2.33	0.40
1:A:262:ARG:O	1:A:263:SER:HB2	2.20	0.40
1:A:268:LEU:O	1:A:268:LEU:HD23	2.21	0.40
1:A:280:CYS:HB3	1:A:380:ASP:HA	2.02	0.40
1:A:481:LEU:HB3	1:A:564:ILE:HG23	2.03	0.40
1:A:606:LEU:HD23	1:A:606:LEU:HA	1.82	0.40
1:A:781:ASN:ND2	1:A:790:LYS:H	2.19	0.40
2:B:330:ILE:HD13	2:B:330:ILE:HG21	1.88	0.40
2:B:478:LYS:C	2:B:478:LYS:HD3	2.46	0.40
2:B:508:PRO:O	2:B:512:LEU:HD23	2.20	0.40
3:C:127:ILE:HD13	3:C:127:ILE:HG21	1.91	0.40
2:B:363:PHE:CG	2:B:390:VAL:HG22	2.56	0.40
1:A:361:LEU:O	1:A:361:LEU:HD23	2.21	0.40
1:A:599:LEU:HD13	1:A:640:ILE:HD11	1.92	0.40
1:A:599:LEU:HD11	1:A:640:ILE:HD11	1.89	0.40
3:C:72:GLU:HA	3:C:75:VAL:HG12	2.03	0.40
2:B:642:GLN:HE22	3:D:257:SER:HB2	1.87	0.40
3:C:67:ILE:HD13	3:C:67:ILE:HG21	1.93	0.40
1:A:126:TRP:CG	1:A:135:LEU:HB3	2.57	0.40
3:C:75:VAL:HG13	3:C:92:THR:CG2	2.51	0.40
3:C:72:GLU:HB2	3:C:76:ILE:CD1	2.50	0.40
3:C:299:LEU:HD22	3:C:299:LEU:C	2.47	0.40
1:A:252:GLN:HE22	1:A:272:LEU:HD11	1.85	0.40
1:A:176:ILE:HD13	1:A:176:ILE:HG21	1.93	0.40
1:A:423:GLN:HA	1:A:427:LEU:HB2	2.03	0.40
3:C:67:ILE:HG21	3:C:67:ILE:HD13	1.87	0.40
3:C:195:ILE:HD11	3:C:423:PHE:CE1	2.56	0.40
3:C:210:LEU:HD12	3:C:227:THR:HG21	2.02	0.40
3:D:219:ASN:HB2	3:D:279:TYR:CE2	2.57	0.40
1:A:139:ALA:CB	1:A:143:ARG:HH21	2.34	0.40
3:D:105:TRP:CE2	3:D:189:LEU:HB3	2.56	0.40
1:A:606:LEU:HD21	1:A:710:ILE:CD1	2.50	0.40
2:B:276:THR:HG23	2:B:278:VAL:HG12	2.02	0.40
3:D:376:MET:HE3	3:D:378:SER:HB3	2.03	0.40
1:A:594:TYR:CZ	1:A:595:HIS:CE1	3.10	0.40
3:D:176:ARG:HE	3:D:389:ASN:HB2	1.86	0.40
2:B:505:ASP:H	2:B:508:PRO:HG2	1.86	0.40
3:D:247:TYR:CE1	3:D:361:PRO:HD2	2.57	0.40
1:A:331:LEU:HD12	1:A:332:LEU:H	1.87	0.40
1:A:425:ILE:HD13	1:A:478:MET:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:GLU:CD	2:B:289:GLU:H	2.27	0.40
1:A:59:VAL:HG11	1:A:102:PHE:CE1	2.57	0.40
2:B:725:GLU:HA	2:B:728:HIS:CD2	2.56	0.40
1:A:134:VAL:CG1	1:A:275:ILE:HD13	2.22	0.40
1:A:72:GLY:CA	2:B:215:ASN:HB3	2.37	0.40
2:B:207:ILE:HD13	2:B:221:LEU:HD21	2.02	0.40
2:B:660:ASN:HB3	2:B:731:PHE:CD1	2.56	0.40
2:B:349:TRP:CE2	2:B:364:ILE:HD11	2.57	0.40
3:C:250:SER:O	3:C:255:ILE:CD1	2.69	0.40
2:B:250:LYS:O	2:B:254:ILE:HG13	2.21	0.40
2:B:443:THR:C	2:B:445:PHE:H	2.29	0.40
1:A:59:VAL:HG11	1:A:102:PHE:CZ	2.56	0.40
3:D:164:LYS:O	3:D:164:LYS:HG2	2.21	0.40
2:B:843:LYS:HD2	2:B:846:ARG:HB2	2.03	0.40
1:A:363:ILE:HG22	1:A:365:THR:H	1.86	0.40
3:C:412:LEU:H	3:C:412:LEU:HD12	1.87	0.40
3:D:119:ILE:HD13	3:D:154:LEU:HD21	2.03	0.40
2:B:743:THR:O	2:B:756:GLN:CA	2.63	0.40
3:C:84:ARG:H	3:C:84:ARG:HG2	1.69	0.40
2:B:199:LEU:HD23	2:B:199:LEU:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	1-A	561/823 (68%)	526 (94%)	21 (4%)	14 (2%)	4	26
1	2-A	561/823 (68%)	524 (93%)	19 (3%)	18 (3%)	3	21
1	3-A	561/823 (68%)	521 (93%)	24 (4%)	16 (3%)	3	23
1	4-A	561/823 (68%)	523 (93%)	25 (4%)	13 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-A	561/823 (68%)	524 (93%)	23 (4%)	14 (2%)	4	26
1	6-A	561/823 (68%)	525 (94%)	26 (5%)	10 (2%)	6	34
1	7-A	561/823 (68%)	519 (92%)	27 (5%)	15 (3%)	4	25
1	8-A	561/823 (68%)	519 (92%)	26 (5%)	16 (3%)	3	23
1	9-A	561/823 (68%)	526 (94%)	23 (4%)	12 (2%)	5	30
1	10-A	561/823 (68%)	528 (94%)	19 (3%)	14 (2%)	4	26
2	1-B	553/846 (65%)	512 (93%)	26 (5%)	15 (3%)	4	25
2	2-B	553/846 (65%)	505 (91%)	41 (7%)	7 (1%)	9	42
2	3-B	553/846 (65%)	512 (93%)	30 (5%)	11 (2%)	6	31
2	4-B	553/846 (65%)	503 (91%)	32 (6%)	18 (3%)	3	21
2	5-B	553/846 (65%)	512 (93%)	30 (5%)	11 (2%)	6	31
2	6-B	553/846 (65%)	502 (91%)	36 (6%)	15 (3%)	4	25
2	7-B	553/846 (65%)	515 (93%)	24 (4%)	14 (2%)	4	26
2	8-B	553/846 (65%)	516 (93%)	29 (5%)	8 (1%)	9	40
2	9-B	553/846 (65%)	505 (91%)	24 (4%)	24 (4%)	2	17
2	10-B	553/846 (65%)	512 (93%)	30 (5%)	11 (2%)	6	31
3	1-C	443/473 (94%)	403 (91%)	29 (6%)	11 (2%)	4	26
3	1-D	443/473 (94%)	395 (89%)	37 (8%)	11 (2%)	4	26
3	2-C	443/473 (94%)	395 (89%)	29 (6%)	19 (4%)	2	17
3	2-D	443/473 (94%)	390 (88%)	33 (7%)	20 (4%)	2	17
3	3-C	443/473 (94%)	396 (89%)	33 (7%)	14 (3%)	3	21
3	3-D	443/473 (94%)	393 (89%)	33 (7%)	17 (4%)	2	19
3	4-C	443/473 (94%)	401 (90%)	29 (6%)	13 (3%)	3	23
3	4-D	443/473 (94%)	402 (91%)	29 (6%)	12 (3%)	4	25
3	5-C	443/473 (94%)	400 (90%)	27 (6%)	16 (4%)	2	20
3	5-D	443/473 (94%)	401 (90%)	28 (6%)	14 (3%)	3	21
3	6-C	443/473 (94%)	397 (90%)	34 (8%)	12 (3%)	4	25
3	6-D	443/473 (94%)	396 (89%)	32 (7%)	15 (3%)	3	21
3	7-C	443/473 (94%)	403 (91%)	29 (6%)	11 (2%)	4	26
3	7-D	443/473 (94%)	389 (88%)	33 (7%)	21 (5%)	2	16
3	8-C	443/473 (94%)	391 (88%)	29 (6%)	23 (5%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	8-D	443/473 (94%)	408 (92%)	26 (6%)	9 (2%)	6	31
3	9-C	443/473 (94%)	403 (91%)	29 (6%)	11 (2%)	4	26
3	9-D	443/473 (94%)	401 (90%)	29 (6%)	13 (3%)	3	23
3	10-C	443/473 (94%)	396 (89%)	29 (6%)	18 (4%)	2	18
3	10-D	443/473 (94%)	403 (91%)	29 (6%)	11 (2%)	4	26
All	All	20000/26150 (76%)	18292 (92%)	1141 (6%)	567 (3%)	6	24

All (567) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	91	GLU
1	1-A	97	LYS
1	1-A	130	SER
1	1-A	785	GLU
2	1-B	247	SER
2	1-B	533	ARG
2	1-B	564	LEU
2	1-B	610	ILE
3	1-C	246	SER
3	1-C	325	ASN
3	1-D	143	ALA
3	1-D	262	SER
3	1-D	274	PRO
3	1-D	354	VAL
1	2-A	91	GLU
1	2-A	97	LYS
1	2-A	337	SER
1	2-A	432	GLY
1	2-A	569	PRO
2	2-B	441	ILE
2	2-B	577	PRO
3	2-C	132	ASN
3	2-C	163	PRO
3	2-C	218	ARG
3	2-C	223	ASP
3	2-C	315	TYR
3	2-D	37	SER
3	2-D	43	SER
3	2-D	70	ASP
3	2-D	86	PHE

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Mol	Chain	Res	Type
3	2-D	266	HIS
3	2-D	288	CYS
1	3-A	91	GLU
1	3-A	331	LEU
2	3-B	245	ASN
2	3-B	469	HIS
3	3-C	44	THR
3	3-C	132	ASN
3	3-C	325	ASN
1	4-A	91	GLU
1	4-A	97	LYS
1	4-A	299	PHE
1	4-A	322	THR
1	4-A	365	THR
1	4-A	474	PRO
1	4-A	787	SER
2	4-B	380	HIS
2	4-B	416	CYS
2	4-B	530	ASN
3	4-C	132	ASN
3	4-C	261	PRO
3	4-C	278	ASP
3	4-C	325	ASN
3	4-C	416	MET
3	4-D	100	SER
3	4-D	328	PRO
1	5-A	91	GLU
1	5-A	337	SER
1	5-A	361	LEU
1	5-A	384	LEU
1	5-A	567	PRO
2	5-B	546	LEU
2	5-B	575	ASN
3	5-C	70	ASP
3	5-C	174	PRO
3	5-C	218	ARG
3	5-C	248	MET
3	5-D	45	GLU
3	5-D	131	ASP
3	5-D	163	PRO
3	5-D	325	ASN
1	6-A	91	GLU

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Mol	Chain	Res	Type
2	6-B	196	THR
2	6-B	210	PRO
2	6-B	244	LEU
2	6-B	419	VAL
2	6-B	531	SER
3	6-C	132	ASN
3	6-C	174	PRO
3	6-C	285	ALA
3	6-D	314	THR
3	6-D	325	ASN
1	7-A	91	GLU
1	7-A	129	THR
1	7-A	331	LEU
1	7-A	337	SER
2	7-B	573	ASN
3	7-C	132	ASN
3	7-C	280	ILE
3	7-D	49	ASP
3	7-D	163	PRO
3	7-D	179	GLU
3	7-D	261	PRO
3	7-D	266	HIS
3	7-D	287	LYS
3	7-D	328	PRO
3	7-D	416	MET
1	8-A	91	GLU
1	8-A	331	LEU
1	8-A	364	PRO
2	8-B	206	GLN
2	8-B	416	CYS
3	8-C	45	GLU
3	8-C	59	ARG
3	8-C	285	ALA
3	8-C	325	ASN
3	8-D	59	ARG
3	8-D	266	HIS
3	8-D	274	PRO
1	9-A	91	GLU
2	9-B	194	ALA
2	9-B	206	GLN
2	9-B	212	LYS
2	9-B	416	CYS

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Mol	Chain	Res	Type
2	9-B	417	LYS
2	9-B	427	LYS
2	9-B	572	LEU
2	9-B	610	ILE
3	9-C	304	SER
3	9-D	43	SER
3	9-D	163	PRO
3	9-D	325	ASN
1	10-A	91	GLU
1	10-A	97	LYS
1	10-A	331	LEU
1	10-A	337	SER
1	10-A	567	PRO
2	10-B	416	CYS
3	10-C	174	PRO
3	10-C	277	SER
3	10-C	307	SER
3	10-C	325	ASN
3	10-D	286	HIS
3	10-D	327	GLU
3	10-D	371	GLU
1	1-A	337	SER
1	1-A	360	SER
1	1-A	383	ASP
2	1-B	324	ASP
3	1-C	70	ASP
3	1-C	266	HIS
3	1-C	277	SER
3	1-C	361	PRO
3	1-D	70	ASP
3	1-D	174	PRO
3	1-D	307	SER
3	1-D	325	ASN
1	2-A	129	THR
1	2-A	263	SER
1	2-A	414	ASP
1	2-A	613	LYS
1	2-A	785	GLU
2	2-B	416	CYS
3	2-C	174	PRO
3	2-C	251	SER
3	2-D	163	PRO

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Mol	Chain	Res	Type
1	3-A	295	PRO
1	3-A	335	CYS
1	3-A	608	LYS
1	3-A	666	PRO
1	3-A	799	VAL
2	3-B	420	GLN
2	3-B	529	MET
3	3-C	248	MET
3	3-C	274	PRO
3	3-C	369	GLU
3	3-D	70	ASP
3	3-D	74	SER
3	3-D	277	SER
3	3-D	365	LEU
1	4-A	334	ASP
1	4-A	337	SER
1	4-A	360	SER
2	4-B	273	SER
2	4-B	552	SER
2	4-B	577	PRO
2	4-B	610	ILE
3	4-C	70	ASP
3	4-C	248	MET
3	4-D	70	ASP
3	4-D	163	PRO
3	4-D	282	ASP
3	4-D	325	ASN
1	5-A	131	PHE
1	5-A	299	PHE
1	5-A	608	LYS
1	5-A	666	PRO
2	5-B	198	ALA
3	5-C	132	ASN
3	5-C	266	HIS
3	5-D	70	ASP
1	6-A	666	PRO
2	6-B	570	LEU
2	6-B	611	ILE
3	6-C	70	ASP
3	6-C	314	THR
3	6-C	325	ASN
3	6-D	70	ASP

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Mol	Chain	Res	Type
3	6-D	266	HIS
1	7-A	364	PRO
1	7-A	365	THR
1	7-A	386	GLU
1	7-A	432	GLY
1	7-A	449	HIS
1	7-A	489	GLU
2	7-B	416	CYS
2	7-B	531	SER
2	7-B	834	GLY
2	7-B	845	LEU
3	7-C	70	ASP
3	7-C	178	SER
3	7-C	251	SER
3	7-C	281	HIS
3	7-C	310	MET
3	7-D	70	ASP
3	7-D	181	VAL
1	8-A	97	LYS
1	8-A	263	SER
1	8-A	432	GLY
1	8-A	450	TYR
3	8-C	96	SER
3	8-C	163	PRO
3	8-C	286	HIS
3	8-C	314	THR
3	8-C	362	TYR
3	8-D	70	ASP
1	9-A	297	GLN
1	9-A	414	ASP
1	9-A	489	GLU
1	9-A	786	LEU
2	9-B	424	GLU
2	9-B	574	VAL
3	9-C	70	ASP
3	9-C	248	MET
3	9-C	261	PRO
3	9-C	348	SER
3	9-C	361	PRO
3	9-D	280	ILE
3	9-D	361	PRO
1	10-A	470	GLN

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Mol	Chain	Res	Type
2	10-B	210	PRO
2	10-B	533	ARG
3	10-C	248	MET
3	10-C	348	SER
3	10-C	351	ALA
3	10-C	353	HIS
3	10-C	368	ASN
3	10-D	70	ASP
3	10-D	96	SER
3	10-D	343	LYS
3	10-D	349	SER
2	1-B	194	ALA
2	1-B	382	PRO
2	1-B	577	PRO
2	1-B	833	ASP
3	1-C	248	MET
3	1-C	251	SER
3	1-C	261	PRO
3	1-D	266	HIS
1	2-A	331	LEU
1	2-A	471	SER
2	2-B	324	ASP
3	2-C	45	GLU
3	2-C	59	ARG
3	2-C	70	ASP
3	2-C	261	PRO
3	2-C	328	PRO
3	2-C	353	HIS
3	2-C	361	PRO
3	2-C	416	MET
3	2-D	33	THR
3	2-D	57	ASN
3	2-D	103	ASN
3	2-D	261	PRO
3	2-D	278	ASP
3	2-D	311	ASN
1	3-A	96	LYS
1	3-A	322	THR
1	3-A	361	LEU
1	3-A	370	SER
1	3-A	482	LEU
2	3-B	779	LEU

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Mol	Chain	Res	Type
3	3-C	47	ASP
3	3-C	70	ASP
3	3-C	261	PRO
3	3-C	275	PHE
3	3-C	309	ALA
3	3-C	361	PRO
3	3-D	71	SER
3	3-D	84	ARG
3	3-D	221	ASN
3	3-D	288	CYS
1	4-A	331	LEU
1	4-A	666	PRO
2	4-B	194	ALA
3	4-C	96	SER
3	4-D	98	GLY
3	4-D	174	PRO
1	5-A	97	LYS
1	5-A	98	MET
1	5-A	259	LEU
2	5-B	278	VAL
2	5-B	324	ASP
2	5-B	382	PRO
2	5-B	577	PRO
3	5-C	57	ASN
3	5-C	99	ALA
3	5-C	280	ILE
3	5-C	307	SER
3	5-D	41	ASP
3	5-D	98	GLY
3	5-D	100	SER
3	5-D	164	LYS
1	6-A	334	ASP
1	6-A	370	SER
2	6-B	416	CYS
2	6-B	550	HIS
3	6-C	59	ARG
3	6-C	307	SER
3	6-C	370	ASN
3	6-D	174	PRO
3	6-D	246	SER
1	7-A	98	MET
2	7-B	381	ILE

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Mol	Chain	Res	Type
2	7-B	540	GLY
2	7-B	563	ILE
2	7-B	577	PRO
3	7-C	98	GLY
3	7-C	261	PRO
3	7-C	367	PRO
3	7-D	283	ASP
3	7-D	325	ASN
1	8-A	470	GLN
1	8-A	613	LYS
1	8-A	785	GLU
3	8-C	70	ASP
3	8-C	261	PRO
3	8-C	266	HIS
3	8-C	311	ASN
3	8-C	367	PRO
3	8-D	348	SER
1	9-A	322	THR
1	9-A	331	LEU
1	9-A	337	SER
2	9-B	197	SER
2	9-B	540	GLY
3	9-C	96	SER
3	9-D	70	ASP
3	9-D	132	ASN
1	10-A	128	ASP
1	10-A	129	THR
1	10-A	414	ASP
1	10-A	488	THR
1	10-A	785	GLU
3	10-C	70	ASP
3	10-C	315	TYR
3	10-D	98	GLY
3	10-D	325	ASN
1	1-A	296	TYR
2	1-B	201	PRO
2	1-B	206	GLN
2	1-B	358	THR
2	1-B	438	TYR
3	1-D	313	PRO
1	2-A	364	PRO
1	2-A	608	LYS

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Mol	Chain	Res	Type
1	2-A	786	LEU
2	2-B	278	VAL
2	2-B	358	THR
3	2-C	43	SER
1	3-A	128	ASP
1	3-A	337	SER
1	3-A	369	ASN
1	3-A	470	GLN
2	3-B	247	SER
2	3-B	574	VAL
3	3-D	42	SER
3	3-D	102	GLY
3	3-D	103	ASN
2	4-B	209	ILE
2	4-B	247	SER
2	4-B	417	LYS
2	4-B	529	MET
3	4-C	266	HIS
3	4-C	309	ALA
3	4-D	87	PHE
3	4-D	101	ALA
3	4-D	266	HIS
1	5-A	99	ASP
2	5-B	247	SER
2	5-B	527	HIS
3	5-C	251	SER
3	5-C	313	PRO
3	5-D	58	CYS
3	5-D	246	SER
1	6-A	99	ASP
1	6-A	295	PRO
1	6-A	667	THR
2	6-B	211	SER
2	6-B	547	ASP
2	6-B	845	LEU
3	6-C	246	SER
3	6-C	266	HIS
3	6-D	59	ARG
3	6-D	179	GLU
3	6-D	312	ASN
1	7-A	367	PRO
2	7-B	324	ASP

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Mol	Chain	Res	Type
3	7-D	45	GLU
3	7-D	285	ALA
3	7-D	311	ASN
3	7-D	312	ASN
1	8-A	300	MET
1	8-A	360	SER
1	8-A	608	LYS
1	8-A	666	PRO
2	8-B	247	SER
2	8-B	357	ALA
2	8-B	395	PRO
3	8-C	179	GLU
3	8-C	276	THR
3	8-D	163	PRO
1	9-A	785	GLU
2	9-B	247	SER
2	9-B	395	PRO
2	9-B	485	LYS
3	9-C	45	GLU
3	9-C	218	ARG
3	9-C	415	SER
3	9-D	174	PRO
3	9-D	309	ALA
3	9-D	312	ASN
3	9-D	343	LYS
3	9-D	345	PRO
2	10-B	381	ILE
2	10-B	395	PRO
3	10-C	96	SER
3	10-C	312	ASN
3	10-D	163	PRO
1	1-A	322	THR
1	1-A	567	PRO
1	1-A	666	PRO
1	1-A	786	LEU
2	1-B	531	SER
3	1-D	328	PRO
1	2-A	361	LEU
1	2-A	365	THR
3	2-D	218	ARG
3	2-D	274	PRO
3	2-D	277	SER

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Mol	Chain	Res	Type
3	2-D	361	PRO
3	2-D	415	SER
2	3-B	243	MET
2	3-B	274	SER
3	3-C	368	ASN
3	3-D	131	ASP
2	4-B	324	ASP
2	4-B	358	THR
3	4-C	348	SER
1	5-A	360	SER
3	5-C	278	ASP
2	6-B	548	LEU
3	6-D	42	SER
3	6-D	45	GLU
1	7-A	785	GLU
3	7-C	163	PRO
3	7-D	310	MET
3	7-D	345	PRO
2	8-B	274	SER
3	8-C	58	CYS
3	8-C	248	MET
3	8-C	278	ASP
3	8-C	315	TYR
3	8-D	58	CYS
3	8-D	444	SER
1	9-A	333	ARG
1	9-A	666	PRO
2	9-B	244	LEU
2	9-B	324	ASP
2	9-B	358	THR
2	9-B	381	ILE
2	9-B	426	SER
2	9-B	535	SER
2	9-B	564	LEU
3	9-D	262	SER
1	10-A	360	SER
2	10-B	215	ASN
2	10-B	552	SER
2	10-B	577	PRO
3	10-C	48	ASP
3	10-C	261	PRO
3	10-C	361	PRO

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Mol	Chain	Res	Type
3	10-D	175	ALA
1	1-A	297	GLN
1	1-A	613	LYS
2	1-B	213	ILE
3	2-C	97	ASP
2	3-B	201	PRO
3	3-C	218	ARG
3	3-D	39	LEU
3	3-D	40	PRO
3	3-D	176	ARG
1	4-A	567	PRO
2	4-B	576	ARG
3	4-C	282	ASP
3	4-C	443	ASP
3	4-D	58	CYS
2	5-B	205	GLU
3	5-C	361	PRO
3	5-D	221	ASN
1	6-A	383	ASP
2	6-B	382	PRO
3	6-D	37	SER
3	6-D	315	TYR
1	7-A	666	PRO
2	7-B	548	LEU
2	7-B	779	LEU
3	7-D	41	ASP
3	7-D	245	PRO
1	8-A	667	THR
2	8-B	524	SER
3	8-C	284	ILE
3	8-C	370	ASN
3	8-D	276	THR
3	9-C	39	LEU
1	10-A	372	ASP
1	10-A	489	GLU
2	10-B	247	SER
2	10-B	438	TYR
3	10-C	309	ALA
3	1-C	163	PRO
3	1-C	345	PRO
1	2-A	666	PRO
2	2-B	247	SER

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Mol	Chain	Res	Type
3	2-C	2	GLY
2	3-B	503	PRO
3	5-C	261	PRO
3	6-D	163	PRO
1	7-A	166	PRO
2	7-B	551	GLY
3	8-C	306	VAL
2	9-B	565	TYR
2	10-B	382	PRO
3	2-D	174	PRO
3	2-D	301	PRO
3	5-D	364	PRO
3	6-D	261	PRO
2	7-B	391	PRO
1	9-A	364	PRO
2	9-B	201	PRO
3	10-C	220	PRO
3	2-C	280	ILE
3	3-D	328	PRO
2	4-B	532	PRO
2	5-B	532	PRO
3	7-D	174	PRO
2	4-B	391	PRO
3	5-D	361	PRO
1	6-A	364	PRO
1	6-A	473	ASN
2	6-B	395	PRO
3	6-C	361	PRO
2	8-B	210	PRO
2	4-B	214	PRO
3	5-C	245	PRO
1	8-A	367	PRO
3	3-D	274	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	542/766 (71%)	498 (92%)	44 (8%)	11	31
1	2-A	542/766 (71%)	498 (92%)	44 (8%)	11	31
1	3-A	542/766 (71%)	498 (92%)	44 (8%)	11	31
1	4-A	542/766 (71%)	498 (92%)	44 (8%)	11	31
1	5-A	542/766 (71%)	498 (92%)	44 (8%)	11	31
1	6-A	542/766 (71%)	498 (92%)	44 (8%)	11	31
1	7-A	542/766 (71%)	498 (92%)	44 (8%)	11	31
1	8-A	542/766 (71%)	498 (92%)	44 (8%)	11	31
1	9-A	542/766 (71%)	498 (92%)	44 (8%)	11	31
1	10-A	542/766 (71%)	498 (92%)	44 (8%)	11	31
2	1-B	528/787 (67%)	494 (94%)	34 (6%)	16	37
2	2-B	528/787 (67%)	494 (94%)	34 (6%)	16	37
2	3-B	528/787 (67%)	494 (94%)	34 (6%)	16	37
2	4-B	528/787 (67%)	494 (94%)	34 (6%)	16	37
2	5-B	528/787 (67%)	494 (94%)	34 (6%)	16	37
2	6-B	528/787 (67%)	494 (94%)	34 (6%)	16	37
2	7-B	528/787 (67%)	494 (94%)	34 (6%)	16	37
2	8-B	528/787 (67%)	494 (94%)	34 (6%)	16	37
2	9-B	528/787 (67%)	494 (94%)	34 (6%)	16	37
2	10-B	528/787 (67%)	494 (94%)	34 (6%)	16	37
3	1-C	396/421 (94%)	367 (93%)	29 (7%)	13	34
3	1-D	396/421 (94%)	370 (93%)	26 (7%)	15	37
3	2-C	396/421 (94%)	367 (93%)	29 (7%)	13	34
3	2-D	396/421 (94%)	370 (93%)	26 (7%)	15	37
3	3-C	396/421 (94%)	367 (93%)	29 (7%)	13	34
3	3-D	396/421 (94%)	370 (93%)	26 (7%)	15	37
3	4-C	396/421 (94%)	367 (93%)	29 (7%)	13	34
3	4-D	396/421 (94%)	370 (93%)	26 (7%)	15	37
3	5-C	396/421 (94%)	367 (93%)	29 (7%)	13	34
3	5-D	396/421 (94%)	370 (93%)	26 (7%)	15	37
3	6-C	396/421 (94%)	367 (93%)	29 (7%)	13	34
3	6-D	396/421 (94%)	370 (93%)	26 (7%)	15	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	7-C	396/421 (94%)	367 (93%)	29 (7%)	13	34
3	7-D	396/421 (94%)	370 (93%)	26 (7%)	15	37
3	8-C	396/421 (94%)	367 (93%)	29 (7%)	13	34
3	8-D	396/421 (94%)	370 (93%)	26 (7%)	15	37
3	9-C	396/421 (94%)	367 (93%)	29 (7%)	13	34
3	9-D	396/421 (94%)	370 (93%)	26 (7%)	15	37
3	10-C	396/421 (94%)	367 (93%)	29 (7%)	13	34
3	10-D	396/421 (94%)	370 (93%)	26 (7%)	15	37
All	All	18620/23950 (78%)	17290 (93%)	1330 (7%)	15	35

All (1330) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	55	GLN
1	1-A	56	GLU
1	1-A	74	TYR
1	1-A	108	ARG
1	1-A	110	VAL
1	1-A	116	TYR
1	1-A	130	SER
1	1-A	134	VAL
1	1-A	137	ARG
1	1-A	146	LEU
1	1-A	152	LYS
1	1-A	153	THR
1	1-A	159	GLU
1	1-A	160	ARG
1	1-A	168	PHE
1	1-A	174	GLU
1	1-A	252	GLN
1	1-A	275	ILE
1	1-A	288	THR
1	1-A	296	TYR
1	1-A	298	GLU
1	1-A	325	PHE
1	1-A	331	LEU
1	1-A	332	LEU
1	1-A	339	GLU
1	1-A	358	ARG

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Mol	Chain	Res	Type
1	1-A	373	ILE
1	1-A	385	MET
1	1-A	386	GLU
1	1-A	396	LYS
1	1-A	407	LYS
1	1-A	481	LEU
1	1-A	591	VAL
1	1-A	633	HIS
1	1-A	637	ASN
1	1-A	648	ASN
1	1-A	667	THR
1	1-A	681	THR
1	1-A	691	ASP
1	1-A	761	ILE
1	1-A	785	GLU
1	1-A	793	PHE
1	1-A	794	TYR
1	1-A	799	VAL
2	1-B	182	GLU
2	1-B	224	ILE
2	1-B	225	PHE
2	1-B	273	SER
2	1-B	290	ASN
2	1-B	335	PHE
2	1-B	347	MET
2	1-B	352	LYS
2	1-B	385	PHE
2	1-B	397	GLU
2	1-B	410	ILE
2	1-B	414	LYS
2	1-B	438	TYR
2	1-B	439	ARG
2	1-B	464	LEU
2	1-B	468	PHE
2	1-B	492	LEU
2	1-B	508	PRO
2	1-B	510	TYR
2	1-B	522	LEU
2	1-B	528	LEU
2	1-B	595	LYS
2	1-B	600	TYR
2	1-B	641	PHE

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Mol	Chain	Res	Type
2	1-B	647	LYS
2	1-B	649	GLU
2	1-B	659	GLU
2	1-B	728	HIS
2	1-B	731	PHE
2	1-B	764	LEU
2	1-B	772	PHE
2	1-B	802	LEU
2	1-B	810	LYS
2	1-B	811	GLU
3	1-C	31	ILE
3	1-C	96	SER
3	1-C	104	SER
3	1-C	120	LEU
3	1-C	126	GLU
3	1-C	141	SER
3	1-C	150	LEU
3	1-C	155	LEU
3	1-C	189	LEU
3	1-C	232	SER
3	1-C	248	MET
3	1-C	253	SER
3	1-C	261	PRO
3	1-C	280	ILE
3	1-C	282	ASP
3	1-C	301	PRO
3	1-C	305	LEU
3	1-C	307	SER
3	1-C	325	ASN
3	1-C	328	PRO
3	1-C	329	ARG
3	1-C	340	GLN
3	1-C	359	ARG
3	1-C	366	GLN
3	1-C	375	MET
3	1-C	391	CYS
3	1-C	412	LEU
3	1-C	435	GLU
3	1-C	443	ASP
3	1-D	12	GLN
3	1-D	19	LYS
3	1-D	27	LYS

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Mol	Chain	Res	Type
3	1-D	38	GLN
3	1-D	69	MET
3	1-D	75	VAL
3	1-D	76	ILE
3	1-D	79	VAL
3	1-D	158	LEU
3	1-D	176	ARG
3	1-D	183	GLN
3	1-D	218	ARG
3	1-D	238	VAL
3	1-D	241	SER
3	1-D	249	TYR
3	1-D	287	LYS
3	1-D	313	PRO
3	1-D	340	GLN
3	1-D	341	ARG
3	1-D	354	VAL
3	1-D	366	GLN
3	1-D	369	GLU
3	1-D	376	MET
3	1-D	383	VAL
3	1-D	393	THR
3	1-D	425	GLU
1	2-A	55	GLN
1	2-A	56	GLU
1	2-A	74	TYR
1	2-A	108	ARG
1	2-A	110	VAL
1	2-A	116	TYR
1	2-A	130	SER
1	2-A	134	VAL
1	2-A	137	ARG
1	2-A	146	LEU
1	2-A	152	LYS
1	2-A	153	THR
1	2-A	159	GLU
1	2-A	160	ARG
1	2-A	168	PHE
1	2-A	174	GLU
1	2-A	252	GLN
1	2-A	275	ILE
1	2-A	288	THR

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Mol	Chain	Res	Type
1	2-A	296	TYR
1	2-A	298	GLU
1	2-A	325	PHE
1	2-A	331	LEU
1	2-A	332	LEU
1	2-A	339	GLU
1	2-A	358	ARG
1	2-A	373	ILE
1	2-A	385	MET
1	2-A	386	GLU
1	2-A	396	LYS
1	2-A	407	LYS
1	2-A	481	LEU
1	2-A	591	VAL
1	2-A	633	HIS
1	2-A	637	ASN
1	2-A	648	ASN
1	2-A	667	THR
1	2-A	681	THR
1	2-A	691	ASP
1	2-A	761	ILE
1	2-A	785	GLU
1	2-A	793	PHE
1	2-A	794	TYR
1	2-A	799	VAL
2	2-B	182	GLU
2	2-B	224	ILE
2	2-B	225	PHE
2	2-B	273	SER
2	2-B	290	ASN
2	2-B	335	PHE
2	2-B	347	MET
2	2-B	352	LYS
2	2-B	385	PHE
2	2-B	397	GLU
2	2-B	410	ILE
2	2-B	414	LYS
2	2-B	438	TYR
2	2-B	439	ARG
2	2-B	464	LEU
2	2-B	468	PHE
2	2-B	492	LEU

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Mol	Chain	Res	Type
2	2-B	508	PRO
2	2-B	510	TYR
2	2-B	522	LEU
2	2-B	528	LEU
2	2-B	595	LYS
2	2-B	600	TYR
2	2-B	641	PHE
2	2-B	647	LYS
2	2-B	649	GLU
2	2-B	659	GLU
2	2-B	728	HIS
2	2-B	731	PHE
2	2-B	764	LEU
2	2-B	772	PHE
2	2-B	802	LEU
2	2-B	810	LYS
2	2-B	811	GLU
3	2-C	31	ILE
3	2-C	96	SER
3	2-C	104	SER
3	2-C	120	LEU
3	2-C	126	GLU
3	2-C	141	SER
3	2-C	150	LEU
3	2-C	155	LEU
3	2-C	189	LEU
3	2-C	232	SER
3	2-C	248	MET
3	2-C	253	SER
3	2-C	261	PRO
3	2-C	280	ILE
3	2-C	282	ASP
3	2-C	301	PRO
3	2-C	305	LEU
3	2-C	307	SER
3	2-C	325	ASN
3	2-C	328	PRO
3	2-C	329	ARG
3	2-C	340	GLN
3	2-C	359	ARG
3	2-C	366	GLN
3	2-C	375	MET

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Mol	Chain	Res	Type
3	2-C	391	CYS
3	2-C	412	LEU
3	2-C	435	GLU
3	2-C	443	ASP
3	2-D	12	GLN
3	2-D	19	LYS
3	2-D	27	LYS
3	2-D	38	GLN
3	2-D	69	MET
3	2-D	75	VAL
3	2-D	76	ILE
3	2-D	79	VAL
3	2-D	158	LEU
3	2-D	176	ARG
3	2-D	183	GLN
3	2-D	218	ARG
3	2-D	238	VAL
3	2-D	241	SER
3	2-D	249	TYR
3	2-D	287	LYS
3	2-D	313	PRO
3	2-D	340	GLN
3	2-D	341	ARG
3	2-D	354	VAL
3	2-D	366	GLN
3	2-D	369	GLU
3	2-D	376	MET
3	2-D	383	VAL
3	2-D	393	THR
3	2-D	425	GLU
1	3-A	55	GLN
1	3-A	56	GLU
1	3-A	74	TYR
1	3-A	108	ARG
1	3-A	110	VAL
1	3-A	116	TYR
1	3-A	130	SER
1	3-A	134	VAL
1	3-A	137	ARG
1	3-A	146	LEU
1	3-A	152	LYS
1	3-A	153	THR

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Mol	Chain	Res	Type
1	3-A	159	GLU
1	3-A	160	ARG
1	3-A	168	PHE
1	3-A	174	GLU
1	3-A	252	GLN
1	3-A	275	ILE
1	3-A	288	THR
1	3-A	296	TYR
1	3-A	298	GLU
1	3-A	325	PHE
1	3-A	331	LEU
1	3-A	332	LEU
1	3-A	339	GLU
1	3-A	358	ARG
1	3-A	373	ILE
1	3-A	385	MET
1	3-A	386	GLU
1	3-A	396	LYS
1	3-A	407	LYS
1	3-A	481	LEU
1	3-A	591	VAL
1	3-A	633	HIS
1	3-A	637	ASN
1	3-A	648	ASN
1	3-A	667	THR
1	3-A	681	THR
1	3-A	691	ASP
1	3-A	761	ILE
1	3-A	785	GLU
1	3-A	793	PHE
1	3-A	794	TYR
1	3-A	799	VAL
2	3-B	182	GLU
2	3-B	224	ILE
2	3-B	225	PHE
2	3-B	273	SER
2	3-B	290	ASN
2	3-B	335	PHE
2	3-B	347	MET
2	3-B	352	LYS
2	3-B	385	PHE
2	3-B	397	GLU

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Mol	Chain	Res	Type
2	3-B	410	ILE
2	3-B	414	LYS
2	3-B	438	TYR
2	3-B	439	ARG
2	3-B	464	LEU
2	3-B	468	PHE
2	3-B	492	LEU
2	3-B	508	PRO
2	3-B	510	TYR
2	3-B	522	LEU
2	3-B	528	LEU
2	3-B	595	LYS
2	3-B	600	TYR
2	3-B	641	PHE
2	3-B	647	LYS
2	3-B	649	GLU
2	3-B	659	GLU
2	3-B	728	HIS
2	3-B	731	PHE
2	3-B	764	LEU
2	3-B	772	PHE
2	3-B	802	LEU
2	3-B	810	LYS
2	3-B	811	GLU
3	3-C	31	ILE
3	3-C	96	SER
3	3-C	104	SER
3	3-C	120	LEU
3	3-C	126	GLU
3	3-C	141	SER
3	3-C	150	LEU
3	3-C	155	LEU
3	3-C	189	LEU
3	3-C	232	SER
3	3-C	248	MET
3	3-C	253	SER
3	3-C	261	PRO
3	3-C	280	ILE
3	3-C	282	ASP
3	3-C	301	PRO
3	3-C	305	LEU
3	3-C	307	SER

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Mol	Chain	Res	Type
3	3-C	325	ASN
3	3-C	328	PRO
3	3-C	329	ARG
3	3-C	340	GLN
3	3-C	359	ARG
3	3-C	366	GLN
3	3-C	375	MET
3	3-C	391	CYS
3	3-C	412	LEU
3	3-C	435	GLU
3	3-C	443	ASP
3	3-D	12	GLN
3	3-D	19	LYS
3	3-D	27	LYS
3	3-D	38	GLN
3	3-D	69	MET
3	3-D	75	VAL
3	3-D	76	ILE
3	3-D	79	VAL
3	3-D	158	LEU
3	3-D	176	ARG
3	3-D	183	GLN
3	3-D	218	ARG
3	3-D	238	VAL
3	3-D	241	SER
3	3-D	249	TYR
3	3-D	287	LYS
3	3-D	313	PRO
3	3-D	340	GLN
3	3-D	341	ARG
3	3-D	354	VAL
3	3-D	366	GLN
3	3-D	369	GLU
3	3-D	376	MET
3	3-D	383	VAL
3	3-D	393	THR
3	3-D	425	GLU
1	4-A	55	GLN
1	4-A	56	GLU
1	4-A	74	TYR
1	4-A	108	ARG
1	4-A	110	VAL

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Mol	Chain	Res	Type
1	4-A	116	TYR
1	4-A	130	SER
1	4-A	134	VAL
1	4-A	137	ARG
1	4-A	146	LEU
1	4-A	152	LYS
1	4-A	153	THR
1	4-A	159	GLU
1	4-A	160	ARG
1	4-A	168	PHE
1	4-A	174	GLU
1	4-A	252	GLN
1	4-A	275	ILE
1	4-A	288	THR
1	4-A	296	TYR
1	4-A	298	GLU
1	4-A	325	PHE
1	4-A	331	LEU
1	4-A	332	LEU
1	4-A	339	GLU
1	4-A	358	ARG
1	4-A	373	ILE
1	4-A	385	MET
1	4-A	386	GLU
1	4-A	396	LYS
1	4-A	407	LYS
1	4-A	481	LEU
1	4-A	591	VAL
1	4-A	633	HIS
1	4-A	637	ASN
1	4-A	648	ASN
1	4-A	667	THR
1	4-A	681	THR
1	4-A	691	ASP
1	4-A	761	ILE
1	4-A	785	GLU
1	4-A	793	PHE
1	4-A	794	TYR
1	4-A	799	VAL
2	4-B	182	GLU
2	4-B	224	ILE
2	4-B	225	PHE

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Mol	Chain	Res	Type
2	4-B	273	SER
2	4-B	290	ASN
2	4-B	335	PHE
2	4-B	347	MET
2	4-B	352	LYS
2	4-B	385	PHE
2	4-B	397	GLU
2	4-B	410	ILE
2	4-B	414	LYS
2	4-B	438	TYR
2	4-B	439	ARG
2	4-B	464	LEU
2	4-B	468	PHE
2	4-B	492	LEU
2	4-B	508	PRO
2	4-B	510	TYR
2	4-B	522	LEU
2	4-B	528	LEU
2	4-B	595	LYS
2	4-B	600	TYR
2	4-B	641	PHE
2	4-B	647	LYS
2	4-B	649	GLU
2	4-B	659	GLU
2	4-B	728	HIS
2	4-B	731	PHE
2	4-B	764	LEU
2	4-B	772	PHE
2	4-B	802	LEU
2	4-B	810	LYS
2	4-B	811	GLU
3	4-C	31	ILE
3	4-C	96	SER
3	4-C	104	SER
3	4-C	120	LEU
3	4-C	126	GLU
3	4-C	141	SER
3	4-C	150	LEU
3	4-C	155	LEU
3	4-C	189	LEU
3	4-C	232	SER
3	4-C	248	MET

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Mol	Chain	Res	Type
3	4-C	253	SER
3	4-C	261	PRO
3	4-C	280	ILE
3	4-C	282	ASP
3	4-C	301	PRO
3	4-C	305	LEU
3	4-C	307	SER
3	4-C	325	ASN
3	4-C	328	PRO
3	4-C	329	ARG
3	4-C	340	GLN
3	4-C	359	ARG
3	4-C	366	GLN
3	4-C	375	MET
3	4-C	391	CYS
3	4-C	412	LEU
3	4-C	435	GLU
3	4-C	443	ASP
3	4-D	12	GLN
3	4-D	19	LYS
3	4-D	27	LYS
3	4-D	38	GLN
3	4-D	69	MET
3	4-D	75	VAL
3	4-D	76	ILE
3	4-D	79	VAL
3	4-D	158	LEU
3	4-D	176	ARG
3	4-D	183	GLN
3	4-D	218	ARG
3	4-D	238	VAL
3	4-D	241	SER
3	4-D	249	TYR
3	4-D	287	LYS
3	4-D	313	PRO
3	4-D	340	GLN
3	4-D	341	ARG
3	4-D	354	VAL
3	4-D	366	GLN
3	4-D	369	GLU
3	4-D	376	MET
3	4-D	383	VAL

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Mol	Chain	Res	Type
3	4-D	393	THR
3	4-D	425	GLU
1	5-A	55	GLN
1	5-A	56	GLU
1	5-A	74	TYR
1	5-A	108	ARG
1	5-A	110	VAL
1	5-A	116	TYR
1	5-A	130	SER
1	5-A	134	VAL
1	5-A	137	ARG
1	5-A	146	LEU
1	5-A	152	LYS
1	5-A	153	THR
1	5-A	159	GLU
1	5-A	160	ARG
1	5-A	168	PHE
1	5-A	174	GLU
1	5-A	252	GLN
1	5-A	275	ILE
1	5-A	288	THR
1	5-A	296	TYR
1	5-A	298	GLU
1	5-A	325	PHE
1	5-A	331	LEU
1	5-A	332	LEU
1	5-A	339	GLU
1	5-A	358	ARG
1	5-A	373	ILE
1	5-A	385	MET
1	5-A	386	GLU
1	5-A	396	LYS
1	5-A	407	LYS
1	5-A	481	LEU
1	5-A	591	VAL
1	5-A	633	HIS
1	5-A	637	ASN
1	5-A	648	ASN
1	5-A	667	THR
1	5-A	681	THR
1	5-A	691	ASP
1	5-A	761	ILE

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Mol	Chain	Res	Type
1	5-A	785	GLU
1	5-A	793	PHE
1	5-A	794	TYR
1	5-A	799	VAL
2	5-B	182	GLU
2	5-B	224	ILE
2	5-B	225	PHE
2	5-B	273	SER
2	5-B	290	ASN
2	5-B	335	PHE
2	5-B	347	MET
2	5-B	352	LYS
2	5-B	385	PHE
2	5-B	397	GLU
2	5-B	410	ILE
2	5-B	414	LYS
2	5-B	438	TYR
2	5-B	439	ARG
2	5-B	464	LEU
2	5-B	468	PHE
2	5-B	492	LEU
2	5-B	508	PRO
2	5-B	510	TYR
2	5-B	522	LEU
2	5-B	528	LEU
2	5-B	595	LYS
2	5-B	600	TYR
2	5-B	641	PHE
2	5-B	647	LYS
2	5-B	649	GLU
2	5-B	659	GLU
2	5-B	728	HIS
2	5-B	731	PHE
2	5-B	764	LEU
2	5-B	772	PHE
2	5-B	802	LEU
2	5-B	810	LYS
2	5-B	811	GLU
3	5-C	31	ILE
3	5-C	96	SER
3	5-C	104	SER
3	5-C	120	LEU

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Mol	Chain	Res	Type
3	5-C	126	GLU
3	5-C	141	SER
3	5-C	150	LEU
3	5-C	155	LEU
3	5-C	189	LEU
3	5-C	232	SER
3	5-C	248	MET
3	5-C	253	SER
3	5-C	261	PRO
3	5-C	280	ILE
3	5-C	282	ASP
3	5-C	301	PRO
3	5-C	305	LEU
3	5-C	307	SER
3	5-C	325	ASN
3	5-C	328	PRO
3	5-C	329	ARG
3	5-C	340	GLN
3	5-C	359	ARG
3	5-C	366	GLN
3	5-C	375	MET
3	5-C	391	CYS
3	5-C	412	LEU
3	5-C	435	GLU
3	5-C	443	ASP
3	5-D	12	GLN
3	5-D	19	LYS
3	5-D	27	LYS
3	5-D	38	GLN
3	5-D	69	MET
3	5-D	75	VAL
3	5-D	76	ILE
3	5-D	79	VAL
3	5-D	158	LEU
3	5-D	176	ARG
3	5-D	183	GLN
3	5-D	218	ARG
3	5-D	238	VAL
3	5-D	241	SER
3	5-D	249	TYR
3	5-D	287	LYS
3	5-D	313	PRO

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Mol	Chain	Res	Type
3	5-D	340	GLN
3	5-D	341	ARG
3	5-D	354	VAL
3	5-D	366	GLN
3	5-D	369	GLU
3	5-D	376	MET
3	5-D	383	VAL
3	5-D	393	THR
3	5-D	425	GLU
1	6-A	55	GLN
1	6-A	56	GLU
1	6-A	74	TYR
1	6-A	108	ARG
1	6-A	110	VAL
1	6-A	116	TYR
1	6-A	130	SER
1	6-A	134	VAL
1	6-A	137	ARG
1	6-A	146	LEU
1	6-A	152	LYS
1	6-A	153	THR
1	6-A	159	GLU
1	6-A	160	ARG
1	6-A	168	PHE
1	6-A	174	GLU
1	6-A	252	GLN
1	6-A	275	ILE
1	6-A	288	THR
1	6-A	296	TYR
1	6-A	298	GLU
1	6-A	325	PHE
1	6-A	331	LEU
1	6-A	332	LEU
1	6-A	339	GLU
1	6-A	358	ARG
1	6-A	373	ILE
1	6-A	385	MET
1	6-A	386	GLU
1	6-A	396	LYS
1	6-A	407	LYS
1	6-A	481	LEU
1	6-A	591	VAL

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Mol	Chain	Res	Type
1	6-A	633	HIS
1	6-A	637	ASN
1	6-A	648	ASN
1	6-A	667	THR
1	6-A	681	THR
1	6-A	691	ASP
1	6-A	761	ILE
1	6-A	785	GLU
1	6-A	793	PHE
1	6-A	794	TYR
1	6-A	799	VAL
2	6-B	182	GLU
2	6-B	224	ILE
2	6-B	225	PHE
2	6-B	273	SER
2	6-B	290	ASN
2	6-B	335	PHE
2	6-B	347	MET
2	6-B	352	LYS
2	6-B	385	PHE
2	6-B	397	GLU
2	6-B	410	ILE
2	6-B	414	LYS
2	6-B	438	TYR
2	6-B	439	ARG
2	6-B	464	LEU
2	6-B	468	PHE
2	6-B	492	LEU
2	6-B	508	PRO
2	6-B	510	TYR
2	6-B	522	LEU
2	6-B	528	LEU
2	6-B	595	LYS
2	6-B	600	TYR
2	6-B	641	PHE
2	6-B	647	LYS
2	6-B	649	GLU
2	6-B	659	GLU
2	6-B	728	HIS
2	6-B	731	PHE
2	6-B	764	LEU
2	6-B	772	PHE

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Mol	Chain	Res	Type
2	6-B	802	LEU
2	6-B	810	LYS
2	6-B	811	GLU
3	6-C	31	ILE
3	6-C	96	SER
3	6-C	104	SER
3	6-C	120	LEU
3	6-C	126	GLU
3	6-C	141	SER
3	6-C	150	LEU
3	6-C	155	LEU
3	6-C	189	LEU
3	6-C	232	SER
3	6-C	248	MET
3	6-C	253	SER
3	6-C	261	PRO
3	6-C	280	ILE
3	6-C	282	ASP
3	6-C	301	PRO
3	6-C	305	LEU
3	6-C	307	SER
3	6-C	325	ASN
3	6-C	328	PRO
3	6-C	329	ARG
3	6-C	340	GLN
3	6-C	359	ARG
3	6-C	366	GLN
3	6-C	375	MET
3	6-C	391	CYS
3	6-C	412	LEU
3	6-C	435	GLU
3	6-C	443	ASP
3	6-D	12	GLN
3	6-D	19	LYS
3	6-D	27	LYS
3	6-D	38	GLN
3	6-D	69	MET
3	6-D	75	VAL
3	6-D	76	ILE
3	6-D	79	VAL
3	6-D	158	LEU
3	6-D	176	ARG

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Mol	Chain	Res	Type
3	6-D	183	GLN
3	6-D	218	ARG
3	6-D	238	VAL
3	6-D	241	SER
3	6-D	249	TYR
3	6-D	287	LYS
3	6-D	313	PRO
3	6-D	340	GLN
3	6-D	341	ARG
3	6-D	354	VAL
3	6-D	366	GLN
3	6-D	369	GLU
3	6-D	376	MET
3	6-D	383	VAL
3	6-D	393	THR
3	6-D	425	GLU
1	7-A	55	GLN
1	7-A	56	GLU
1	7-A	74	TYR
1	7-A	108	ARG
1	7-A	110	VAL
1	7-A	116	TYR
1	7-A	130	SER
1	7-A	134	VAL
1	7-A	137	ARG
1	7-A	146	LEU
1	7-A	152	LYS
1	7-A	153	THR
1	7-A	159	GLU
1	7-A	160	ARG
1	7-A	168	PHE
1	7-A	174	GLU
1	7-A	252	GLN
1	7-A	275	ILE
1	7-A	288	THR
1	7-A	296	TYR
1	7-A	298	GLU
1	7-A	325	PHE
1	7-A	331	LEU
1	7-A	332	LEU
1	7-A	339	GLU
1	7-A	358	ARG

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Mol	Chain	Res	Type
1	7-A	373	ILE
1	7-A	385	MET
1	7-A	386	GLU
1	7-A	396	LYS
1	7-A	407	LYS
1	7-A	481	LEU
1	7-A	591	VAL
1	7-A	633	HIS
1	7-A	637	ASN
1	7-A	648	ASN
1	7-A	667	THR
1	7-A	681	THR
1	7-A	691	ASP
1	7-A	761	ILE
1	7-A	785	GLU
1	7-A	793	PHE
1	7-A	794	TYR
1	7-A	799	VAL
2	7-B	182	GLU
2	7-B	224	ILE
2	7-B	225	PHE
2	7-B	273	SER
2	7-B	290	ASN
2	7-B	335	PHE
2	7-B	347	MET
2	7-B	352	LYS
2	7-B	385	PHE
2	7-B	397	GLU
2	7-B	410	ILE
2	7-B	414	LYS
2	7-B	438	TYR
2	7-B	439	ARG
2	7-B	464	LEU
2	7-B	468	PHE
2	7-B	492	LEU
2	7-B	508	PRO
2	7-B	510	TYR
2	7-B	522	LEU
2	7-B	528	LEU
2	7-B	595	LYS
2	7-B	600	TYR
2	7-B	641	PHE

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Mol	Chain	Res	Type
2	7-B	647	LYS
2	7-B	649	GLU
2	7-B	659	GLU
2	7-B	728	HIS
2	7-B	731	PHE
2	7-B	764	LEU
2	7-B	772	PHE
2	7-B	802	LEU
2	7-B	810	LYS
2	7-B	811	GLU
3	7-C	31	ILE
3	7-C	96	SER
3	7-C	104	SER
3	7-C	120	LEU
3	7-C	126	GLU
3	7-C	141	SER
3	7-C	150	LEU
3	7-C	155	LEU
3	7-C	189	LEU
3	7-C	232	SER
3	7-C	248	MET
3	7-C	253	SER
3	7-C	261	PRO
3	7-C	280	ILE
3	7-C	282	ASP
3	7-C	301	PRO
3	7-C	305	LEU
3	7-C	307	SER
3	7-C	325	ASN
3	7-C	328	PRO
3	7-C	329	ARG
3	7-C	340	GLN
3	7-C	359	ARG
3	7-C	366	GLN
3	7-C	375	MET
3	7-C	391	CYS
3	7-C	412	LEU
3	7-C	435	GLU
3	7-C	443	ASP
3	7-D	12	GLN
3	7-D	19	LYS
3	7-D	27	LYS

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Mol	Chain	Res	Type
3	7-D	38	GLN
3	7-D	69	MET
3	7-D	75	VAL
3	7-D	76	ILE
3	7-D	79	VAL
3	7-D	158	LEU
3	7-D	176	ARG
3	7-D	183	GLN
3	7-D	218	ARG
3	7-D	238	VAL
3	7-D	241	SER
3	7-D	249	TYR
3	7-D	287	LYS
3	7-D	313	PRO
3	7-D	340	GLN
3	7-D	341	ARG
3	7-D	354	VAL
3	7-D	366	GLN
3	7-D	369	GLU
3	7-D	376	MET
3	7-D	383	VAL
3	7-D	393	THR
3	7-D	425	GLU
1	8-A	55	GLN
1	8-A	56	GLU
1	8-A	74	TYR
1	8-A	108	ARG
1	8-A	110	VAL
1	8-A	116	TYR
1	8-A	130	SER
1	8-A	134	VAL
1	8-A	137	ARG
1	8-A	146	LEU
1	8-A	152	LYS
1	8-A	153	THR
1	8-A	159	GLU
1	8-A	160	ARG
1	8-A	168	PHE
1	8-A	174	GLU
1	8-A	252	GLN
1	8-A	275	ILE
1	8-A	288	THR

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Mol	Chain	Res	Type
1	8-A	296	TYR
1	8-A	298	GLU
1	8-A	325	PHE
1	8-A	331	LEU
1	8-A	332	LEU
1	8-A	339	GLU
1	8-A	358	ARG
1	8-A	373	ILE
1	8-A	385	MET
1	8-A	386	GLU
1	8-A	396	LYS
1	8-A	407	LYS
1	8-A	481	LEU
1	8-A	591	VAL
1	8-A	633	HIS
1	8-A	637	ASN
1	8-A	648	ASN
1	8-A	667	THR
1	8-A	681	THR
1	8-A	691	ASP
1	8-A	761	ILE
1	8-A	785	GLU
1	8-A	793	PHE
1	8-A	794	TYR
1	8-A	799	VAL
2	8-B	182	GLU
2	8-B	224	ILE
2	8-B	225	PHE
2	8-B	273	SER
2	8-B	290	ASN
2	8-B	335	PHE
2	8-B	347	MET
2	8-B	352	LYS
2	8-B	385	PHE
2	8-B	397	GLU
2	8-B	410	ILE
2	8-B	414	LYS
2	8-B	438	TYR
2	8-B	439	ARG
2	8-B	464	LEU
2	8-B	468	PHE
2	8-B	492	LEU

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Mol	Chain	Res	Type
2	8-B	508	PRO
2	8-B	510	TYR
2	8-B	522	LEU
2	8-B	528	LEU
2	8-B	595	LYS
2	8-B	600	TYR
2	8-B	641	PHE
2	8-B	647	LYS
2	8-B	649	GLU
2	8-B	659	GLU
2	8-B	728	HIS
2	8-B	731	PHE
2	8-B	764	LEU
2	8-B	772	PHE
2	8-B	802	LEU
2	8-B	810	LYS
2	8-B	811	GLU
3	8-C	31	ILE
3	8-C	96	SER
3	8-C	104	SER
3	8-C	120	LEU
3	8-C	126	GLU
3	8-C	141	SER
3	8-C	150	LEU
3	8-C	155	LEU
3	8-C	189	LEU
3	8-C	232	SER
3	8-C	248	MET
3	8-C	253	SER
3	8-C	261	PRO
3	8-C	280	ILE
3	8-C	282	ASP
3	8-C	301	PRO
3	8-C	305	LEU
3	8-C	307	SER
3	8-C	325	ASN
3	8-C	328	PRO
3	8-C	329	ARG
3	8-C	340	GLN
3	8-C	359	ARG
3	8-C	366	GLN
3	8-C	375	MET

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Mol	Chain	Res	Type
3	8-C	391	CYS
3	8-C	412	LEU
3	8-C	435	GLU
3	8-C	443	ASP
3	8-D	12	GLN
3	8-D	19	LYS
3	8-D	27	LYS
3	8-D	38	GLN
3	8-D	69	MET
3	8-D	75	VAL
3	8-D	76	ILE
3	8-D	79	VAL
3	8-D	158	LEU
3	8-D	176	ARG
3	8-D	183	GLN
3	8-D	218	ARG
3	8-D	238	VAL
3	8-D	241	SER
3	8-D	249	TYR
3	8-D	287	LYS
3	8-D	313	PRO
3	8-D	340	GLN
3	8-D	341	ARG
3	8-D	354	VAL
3	8-D	366	GLN
3	8-D	369	GLU
3	8-D	376	MET
3	8-D	383	VAL
3	8-D	393	THR
3	8-D	425	GLU
1	9-A	55	GLN
1	9-A	56	GLU
1	9-A	74	TYR
1	9-A	108	ARG
1	9-A	110	VAL
1	9-A	116	TYR
1	9-A	130	SER
1	9-A	134	VAL
1	9-A	137	ARG
1	9-A	146	LEU
1	9-A	152	LYS
1	9-A	153	THR

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Mol	Chain	Res	Type
1	9-A	159	GLU
1	9-A	160	ARG
1	9-A	168	PHE
1	9-A	174	GLU
1	9-A	252	GLN
1	9-A	275	ILE
1	9-A	288	THR
1	9-A	296	TYR
1	9-A	298	GLU
1	9-A	325	PHE
1	9-A	331	LEU
1	9-A	332	LEU
1	9-A	339	GLU
1	9-A	358	ARG
1	9-A	373	ILE
1	9-A	385	MET
1	9-A	386	GLU
1	9-A	396	LYS
1	9-A	407	LYS
1	9-A	481	LEU
1	9-A	591	VAL
1	9-A	633	HIS
1	9-A	637	ASN
1	9-A	648	ASN
1	9-A	667	THR
1	9-A	681	THR
1	9-A	691	ASP
1	9-A	761	ILE
1	9-A	785	GLU
1	9-A	793	PHE
1	9-A	794	TYR
1	9-A	799	VAL
2	9-B	182	GLU
2	9-B	224	ILE
2	9-B	225	PHE
2	9-B	273	SER
2	9-B	290	ASN
2	9-B	335	PHE
2	9-B	347	MET
2	9-B	352	LYS
2	9-B	385	PHE
2	9-B	397	GLU

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Mol	Chain	Res	Type
2	9-B	410	ILE
2	9-B	414	LYS
2	9-B	438	TYR
2	9-B	439	ARG
2	9-B	464	LEU
2	9-B	468	PHE
2	9-B	492	LEU
2	9-B	508	PRO
2	9-B	510	TYR
2	9-B	522	LEU
2	9-B	528	LEU
2	9-B	595	LYS
2	9-B	600	TYR
2	9-B	641	PHE
2	9-B	647	LYS
2	9-B	649	GLU
2	9-B	659	GLU
2	9-B	728	HIS
2	9-B	731	PHE
2	9-B	764	LEU
2	9-B	772	PHE
2	9-B	802	LEU
2	9-B	810	LYS
2	9-B	811	GLU
3	9-C	31	ILE
3	9-C	96	SER
3	9-C	104	SER
3	9-C	120	LEU
3	9-C	126	GLU
3	9-C	141	SER
3	9-C	150	LEU
3	9-C	155	LEU
3	9-C	189	LEU
3	9-C	232	SER
3	9-C	248	MET
3	9-C	253	SER
3	9-C	261	PRO
3	9-C	280	ILE
3	9-C	282	ASP
3	9-C	301	PRO
3	9-C	305	LEU
3	9-C	307	SER

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Mol	Chain	Res	Type
3	9-C	325	ASN
3	9-C	328	PRO
3	9-C	329	ARG
3	9-C	340	GLN
3	9-C	359	ARG
3	9-C	366	GLN
3	9-C	375	MET
3	9-C	391	CYS
3	9-C	412	LEU
3	9-C	435	GLU
3	9-C	443	ASP
3	9-D	12	GLN
3	9-D	19	LYS
3	9-D	27	LYS
3	9-D	38	GLN
3	9-D	69	MET
3	9-D	75	VAL
3	9-D	76	ILE
3	9-D	79	VAL
3	9-D	158	LEU
3	9-D	176	ARG
3	9-D	183	GLN
3	9-D	218	ARG
3	9-D	238	VAL
3	9-D	241	SER
3	9-D	249	TYR
3	9-D	287	LYS
3	9-D	313	PRO
3	9-D	340	GLN
3	9-D	341	ARG
3	9-D	354	VAL
3	9-D	366	GLN
3	9-D	369	GLU
3	9-D	376	MET
3	9-D	383	VAL
3	9-D	393	THR
3	9-D	425	GLU
1	10-A	55	GLN
1	10-A	56	GLU
1	10-A	74	TYR
1	10-A	108	ARG
1	10-A	110	VAL

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Mol	Chain	Res	Type
1	10-A	116	TYR
1	10-A	130	SER
1	10-A	134	VAL
1	10-A	137	ARG
1	10-A	146	LEU
1	10-A	152	LYS
1	10-A	153	THR
1	10-A	159	GLU
1	10-A	160	ARG
1	10-A	168	PHE
1	10-A	174	GLU
1	10-A	252	GLN
1	10-A	275	ILE
1	10-A	288	THR
1	10-A	296	TYR
1	10-A	298	GLU
1	10-A	325	PHE
1	10-A	331	LEU
1	10-A	332	LEU
1	10-A	339	GLU
1	10-A	358	ARG
1	10-A	373	ILE
1	10-A	385	MET
1	10-A	386	GLU
1	10-A	396	LYS
1	10-A	407	LYS
1	10-A	481	LEU
1	10-A	591	VAL
1	10-A	633	HIS
1	10-A	637	ASN
1	10-A	648	ASN
1	10-A	667	THR
1	10-A	681	THR
1	10-A	691	ASP
1	10-A	761	ILE
1	10-A	785	GLU
1	10-A	793	PHE
1	10-A	794	TYR
1	10-A	799	VAL
2	10-B	182	GLU
2	10-B	224	ILE
2	10-B	225	PHE

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Mol	Chain	Res	Type
2	10-B	273	SER
2	10-B	290	ASN
2	10-B	335	PHE
2	10-B	347	MET
2	10-B	352	LYS
2	10-B	385	PHE
2	10-B	397	GLU
2	10-B	410	ILE
2	10-B	414	LYS
2	10-B	438	TYR
2	10-B	439	ARG
2	10-B	464	LEU
2	10-B	468	PHE
2	10-B	492	LEU
2	10-B	508	PRO
2	10-B	510	TYR
2	10-B	522	LEU
2	10-B	528	LEU
2	10-B	595	LYS
2	10-B	600	TYR
2	10-B	641	PHE
2	10-B	647	LYS
2	10-B	649	GLU
2	10-B	659	GLU
2	10-B	728	HIS
2	10-B	731	PHE
2	10-B	764	LEU
2	10-B	772	PHE
2	10-B	802	LEU
2	10-B	810	LYS
2	10-B	811	GLU
3	10-C	31	ILE
3	10-C	96	SER
3	10-C	104	SER
3	10-C	120	LEU
3	10-C	126	GLU
3	10-C	141	SER
3	10-C	150	LEU
3	10-C	155	LEU
3	10-C	189	LEU
3	10-C	232	SER
3	10-C	248	MET

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Mol	Chain	Res	Type
3	10-C	253	SER
3	10-C	261	PRO
3	10-C	280	ILE
3	10-C	282	ASP
3	10-C	301	PRO
3	10-C	305	LEU
3	10-C	307	SER
3	10-C	325	ASN
3	10-C	328	PRO
3	10-C	329	ARG
3	10-C	340	GLN
3	10-C	359	ARG
3	10-C	366	GLN
3	10-C	375	MET
3	10-C	391	CYS
3	10-C	412	LEU
3	10-C	435	GLU
3	10-C	443	ASP
3	10-D	12	GLN
3	10-D	19	LYS
3	10-D	27	LYS
3	10-D	38	GLN
3	10-D	69	MET
3	10-D	75	VAL
3	10-D	76	ILE
3	10-D	79	VAL
3	10-D	158	LEU
3	10-D	176	ARG
3	10-D	183	GLN
3	10-D	218	ARG
3	10-D	238	VAL
3	10-D	241	SER
3	10-D	249	TYR
3	10-D	287	LYS
3	10-D	313	PRO
3	10-D	340	GLN
3	10-D	341	ARG
3	10-D	354	VAL
3	10-D	366	GLN
3	10-D	369	GLU
3	10-D	376	MET
3	10-D	383	VAL

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Mol	Chain	Res	Type
3	10-D	393	THR
3	10-D	425	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (652) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	55	GLN
1	1-A	65	ASN
1	1-A	115	GLN
1	1-A	183	ASN
1	1-A	252	GLN
1	1-A	253	GLN
1	1-A	258	ASN
1	1-A	421	HIS
1	1-A	423	GLN
1	1-A	434	ASN
1	1-A	442	ASN
1	1-A	454	ASN
1	1-A	457	ASN
1	1-A	473	ASN
1	1-A	476	ASN
1	1-A	480	GLN
1	1-A	559	HIS
1	1-A	583	GLN
1	1-A	589	GLN
1	1-A	607	ASN
1	1-A	665	ASN
1	1-A	673	GLN
1	1-A	770	ASN
1	1-A	781	ASN
2	1-B	208	GLN
2	1-B	222	HIS
2	1-B	290	ASN
2	1-B	322	HIS
2	1-B	336	ASN
2	1-B	367	ASN
2	1-B	386	ASN
2	1-B	450	ASN
2	1-B	462	GLN
2	1-B	466	GLN
2	1-B	479	ASN
2	1-B	521	GLN

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Mol	Chain	Res	Type
2	1-B	527	HIS
2	1-B	534	ASN
2	1-B	539	ASN
2	1-B	654	ASN
2	1-B	818	ASN
2	1-B	832	ASN
3	1-C	12	GLN
3	1-C	15	ASN
3	1-C	29	HIS
3	1-C	60	ASN
3	1-C	107	ASN
3	1-C	153	ASN
3	1-C	219	ASN
3	1-C	240	ASN
3	1-C	266	HIS
3	1-C	320	ASN
3	1-C	339	GLN
3	1-C	340	GLN
3	1-C	366	GLN
3	1-C	368	ASN
3	1-C	389	ASN
3	1-C	392	ASN
3	1-C	408	ASN
3	1-C	442	GLN
3	1-D	29	HIS
3	1-D	38	GLN
3	1-D	115	ASN
3	1-D	116	GLN
3	1-D	137	GLN
3	1-D	219	ASN
3	1-D	266	HIS
3	1-D	312	ASN
3	1-D	320	ASN
3	1-D	379	ASN
3	1-D	418	ASN
3	1-D	442	GLN
1	2-A	65	ASN
1	2-A	136	GLN
1	2-A	191	ASN
1	2-A	252	GLN
1	2-A	273	ASN
1	2-A	274	ASN

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Mol	Chain	Res	Type
1	2-A	297	GLN
1	2-A	379	ASN
1	2-A	452	ASN
1	2-A	455	ASN
1	2-A	475	ASN
1	2-A	476	ASN
1	2-A	559	HIS
1	2-A	593	GLN
1	2-A	595	HIS
1	2-A	673	GLN
2	2-B	206	GLN
2	2-B	208	GLN
2	2-B	215	ASN
2	2-B	262	GLN
2	2-B	263	ASN
2	2-B	270	ASN
2	2-B	380	HIS
2	2-B	387	GLN
2	2-B	420	GLN
2	2-B	423	ASN
2	2-B	452	GLN
2	2-B	534	ASN
2	2-B	539	ASN
2	2-B	642	GLN
2	2-B	738	HIS
2	2-B	756	GLN
2	2-B	767	ASN
3	2-C	24	GLN
3	2-C	29	HIS
3	2-C	57	ASN
3	2-C	81	ASN
3	2-C	91	ASN
3	2-C	219	ASN
3	2-C	221	ASN
3	2-C	289	HIS
3	2-C	303	ASN
3	2-C	353	HIS
3	2-C	366	GLN
3	2-C	389	ASN
3	2-C	408	ASN
3	2-C	414	GLN
3	2-C	417	GLN

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Mol	Chain	Res	Type
3	2-C	418	ASN
3	2-D	24	GLN
3	2-D	57	ASN
3	2-D	107	ASN
3	2-D	153	ASN
3	2-D	219	ASN
3	2-D	229	GLN
3	2-D	312	ASN
3	2-D	320	ASN
3	2-D	340	GLN
3	2-D	355	ASN
3	2-D	418	ASN
3	2-D	431	GLN
1	3-A	163	ASN
1	3-A	175	GLN
1	3-A	258	ASN
1	3-A	362	GLN
1	3-A	389	ASN
1	3-A	421	HIS
1	3-A	454	ASN
1	3-A	455	ASN
1	3-A	476	ASN
1	3-A	583	GLN
1	3-A	589	GLN
1	3-A	633	HIS
1	3-A	649	GLN
1	3-A	650	ASN
1	3-A	665	ASN
1	3-A	686	ASN
1	3-A	770	ASN
2	3-B	222	HIS
2	3-B	262	GLN
2	3-B	420	GLN
2	3-B	423	ASN
2	3-B	434	GLN
2	3-B	450	ASN
2	3-B	465	ASN
2	3-B	469	HIS
2	3-B	527	HIS
2	3-B	534	ASN
2	3-B	550	HIS
2	3-B	601	GLN

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Mol	Chain	Res	Type
2	3-B	608	ASN
2	3-B	669	GLN
2	3-B	729	ASN
2	3-B	738	HIS
2	3-B	808	ASN
3	3-C	16	HIS
3	3-C	24	GLN
3	3-C	103	ASN
3	3-C	116	GLN
3	3-C	140	HIS
3	3-C	266	HIS
3	3-C	289	HIS
3	3-C	312	ASN
3	3-C	317	ASN
3	3-C	325	ASN
3	3-C	339	GLN
3	3-C	355	ASN
3	3-C	368	ASN
3	3-C	392	ASN
3	3-C	414	GLN
3	3-C	420	GLN
3	3-D	38	GLN
3	3-D	60	ASN
3	3-D	103	ASN
3	3-D	228	ASN
3	3-D	229	GLN
3	3-D	320	ASN
3	3-D	339	GLN
3	3-D	353	HIS
3	3-D	355	ASN
3	3-D	389	ASN
3	3-D	414	GLN
1	4-A	79	ASN
1	4-A	421	HIS
1	4-A	434	ASN
1	4-A	449	HIS
1	4-A	452	ASN
1	4-A	470	GLN
1	4-A	473	ASN
1	4-A	480	GLN
1	4-A	595	HIS
1	4-A	633	HIS

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Mol	Chain	Res	Type
1	4-A	637	ASN
1	4-A	638	HIS
1	4-A	648	ASN
1	4-A	665	ASN
1	4-A	674	ASN
1	4-A	762	GLN
2	4-B	204	HIS
2	4-B	206	GLN
2	4-B	208	GLN
2	4-B	215	ASN
2	4-B	222	HIS
2	4-B	269	ASN
2	4-B	380	HIS
2	4-B	450	ASN
2	4-B	509	ASN
2	4-B	521	GLN
2	4-B	534	ASN
2	4-B	550	HIS
2	4-B	643	GLN
2	4-B	669	GLN
2	4-B	780	ASN
2	4-B	818	ASN
2	4-B	832	ASN
3	4-C	12	GLN
3	4-C	16	HIS
3	4-C	29	HIS
3	4-C	103	ASN
3	4-C	137	GLN
3	4-C	153	ASN
3	4-C	183	GLN
3	4-C	186	ASN
3	4-C	281	HIS
3	4-C	311	ASN
3	4-C	312	ASN
3	4-C	339	GLN
3	4-C	355	ASN
3	4-C	366	GLN
3	4-C	379	ASN
3	4-C	414	GLN
3	4-D	103	ASN
3	4-D	137	GLN
3	4-D	206	ASN

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Mol	Chain	Res	Type
3	4-D	219	ASN
3	4-D	281	HIS
3	4-D	312	ASN
3	4-D	317	ASN
3	4-D	325	ASN
3	4-D	355	ASN
3	4-D	370	ASN
1	5-A	55	GLN
1	5-A	65	ASN
1	5-A	163	ASN
1	5-A	167	ASN
1	5-A	175	GLN
1	5-A	252	GLN
1	5-A	297	GLN
1	5-A	433	HIS
1	5-A	449	HIS
1	5-A	452	ASN
1	5-A	455	ASN
1	5-A	475	ASN
1	5-A	485	GLN
1	5-A	559	HIS
1	5-A	595	HIS
1	5-A	665	ASN
1	5-A	696	GLN
1	5-A	762	GLN
1	5-A	781	ASN
2	5-B	430	HIS
2	5-B	450	ASN
2	5-B	466	GLN
2	5-B	517	GLN
2	5-B	550	HIS
2	5-B	629	ASN
2	5-B	642	GLN
2	5-B	669	GLN
2	5-B	728	HIS
2	5-B	734	ASN
2	5-B	738	HIS
2	5-B	756	GLN
2	5-B	806	ASN
3	5-C	15	ASN
3	5-C	29	HIS
3	5-C	60	ASN

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Mol	Chain	Res	Type
3	5-C	107	ASN
3	5-C	140	HIS
3	5-C	186	ASN
3	5-C	219	ASN
3	5-C	312	ASN
3	5-C	317	ASN
3	5-C	325	ASN
3	5-C	339	GLN
3	5-C	355	ASN
3	5-C	366	GLN
3	5-C	406	ASN
3	5-D	29	HIS
3	5-D	38	GLN
3	5-D	60	ASN
3	5-D	91	ASN
3	5-D	107	ASN
3	5-D	206	ASN
3	5-D	289	HIS
3	5-D	320	ASN
3	5-D	325	ASN
3	5-D	339	GLN
3	5-D	355	ASN
3	5-D	370	ASN
3	5-D	385	ASN
1	6-A	55	GLN
1	6-A	175	GLN
1	6-A	183	ASN
1	6-A	252	GLN
1	6-A	273	ASN
1	6-A	297	GLN
1	6-A	362	GLN
1	6-A	379	ASN
1	6-A	421	HIS
1	6-A	423	GLN
1	6-A	430	GLN
1	6-A	454	ASN
1	6-A	457	ASN
1	6-A	559	HIS
1	6-A	565	ASN
1	6-A	637	ASN
1	6-A	638	HIS
1	6-A	696	GLN

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Mol	Chain	Res	Type
1	6-A	762	GLN
1	6-A	770	ASN
2	6-B	269	ASN
2	6-B	317	ASN
2	6-B	348	ASN
2	6-B	386	ASN
2	6-B	423	ASN
2	6-B	430	HIS
2	6-B	434	GLN
2	6-B	452	GLN
2	6-B	461	ASN
2	6-B	465	ASN
2	6-B	521	GLN
2	6-B	530	ASN
2	6-B	534	ASN
2	6-B	573	ASN
2	6-B	575	ASN
2	6-B	588	ASN
2	6-B	596	ASN
2	6-B	629	ASN
2	6-B	645	ASN
2	6-B	669	GLN
2	6-B	756	GLN
2	6-B	767	ASN
2	6-B	808	ASN
3	6-C	9	GLN
3	6-C	15	ASN
3	6-C	38	GLN
3	6-C	121	ASN
3	6-C	206	ASN
3	6-C	225	GLN
3	6-C	240	ASN
3	6-C	311	ASN
3	6-C	339	GLN
3	6-C	340	GLN
3	6-C	353	HIS
3	6-C	355	ASN
3	6-C	385	ASN
3	6-C	392	ASN
3	6-C	414	GLN
3	6-C	442	GLN
3	6-D	9	GLN

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Mol	Chain	Res	Type
3	6-D	15	ASN
3	6-D	24	GLN
3	6-D	38	GLN
3	6-D	107	ASN
3	6-D	132	ASN
3	6-D	183	GLN
3	6-D	211	ASN
3	6-D	219	ASN
3	6-D	229	GLN
3	6-D	289	HIS
3	6-D	303	ASN
3	6-D	330	GLN
3	6-D	353	HIS
3	6-D	368	ASN
3	6-D	406	ASN
3	6-D	417	GLN
3	6-D	431	GLN
1	7-A	136	GLN
1	7-A	175	GLN
1	7-A	191	ASN
1	7-A	277	GLN
1	7-A	389	ASN
1	7-A	449	HIS
1	7-A	454	ASN
1	7-A	455	ASN
1	7-A	470	GLN
1	7-A	559	HIS
1	7-A	589	GLN
1	7-A	595	HIS
1	7-A	607	ASN
1	7-A	633	HIS
1	7-A	637	ASN
1	7-A	638	HIS
1	7-A	698	GLN
2	7-B	206	GLN
2	7-B	215	ASN
2	7-B	232	GLN
2	7-B	290	ASN
2	7-B	303	HIS
2	7-B	386	ASN
2	7-B	387	GLN
2	7-B	458	ASN

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Mol	Chain	Res	Type
2	7-B	461	ASN
2	7-B	465	ASN
2	7-B	466	GLN
2	7-B	573	ASN
2	7-B	601	GLN
2	7-B	608	ASN
2	7-B	654	ASN
2	7-B	669	GLN
2	7-B	808	ASN
3	7-C	29	HIS
3	7-C	60	ASN
3	7-C	121	ASN
3	7-C	132	ASN
3	7-C	186	ASN
3	7-C	225	GLN
3	7-C	226	HIS
3	7-C	240	ASN
3	7-C	266	HIS
3	7-C	281	HIS
3	7-C	286	HIS
3	7-C	289	HIS
3	7-C	303	ASN
3	7-C	311	ASN
3	7-C	317	ASN
3	7-C	355	ASN
3	7-C	385	ASN
3	7-C	406	ASN
3	7-C	431	GLN
3	7-C	442	GLN
3	7-D	115	ASN
3	7-D	153	ASN
3	7-D	229	GLN
3	7-D	281	HIS
3	7-D	325	ASN
3	7-D	379	ASN
3	7-D	392	ASN
3	7-D	417	GLN
1	8-A	175	GLN
1	8-A	252	GLN
1	8-A	273	ASN
1	8-A	274	ASN
1	8-A	293	ASN

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Mol	Chain	Res	Type
1	8-A	411	GLN
1	8-A	417	ASN
1	8-A	421	HIS
1	8-A	452	ASN
1	8-A	473	ASN
1	8-A	589	GLN
1	8-A	595	HIS
1	8-A	607	ASN
1	8-A	638	HIS
1	8-A	674	ASN
1	8-A	686	ASN
1	8-A	781	ASN
2	8-B	206	GLN
2	8-B	208	GLN
2	8-B	232	GLN
2	8-B	262	GLN
2	8-B	367	ASN
2	8-B	380	HIS
2	8-B	386	ASN
2	8-B	420	GLN
2	8-B	497	ASN
2	8-B	509	ASN
2	8-B	534	ASN
2	8-B	550	HIS
2	8-B	573	ASN
2	8-B	601	GLN
2	8-B	608	ASN
2	8-B	629	ASN
2	8-B	642	GLN
2	8-B	720	ASN
2	8-B	734	ASN
2	8-B	778	ASN
2	8-B	806	ASN
2	8-B	808	ASN
3	8-C	12	GLN
3	8-C	16	HIS
3	8-C	91	ASN
3	8-C	289	HIS
3	8-C	317	ASN
3	8-C	325	ASN
3	8-C	385	ASN
3	8-C	389	ASN

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Mol	Chain	Res	Type
3	8-C	418	ASN
3	8-C	431	GLN
3	8-C	442	GLN
3	8-D	9	GLN
3	8-D	12	GLN
3	8-D	15	ASN
3	8-D	16	HIS
3	8-D	121	ASN
3	8-D	132	ASN
3	8-D	153	ASN
3	8-D	206	ASN
3	8-D	211	ASN
3	8-D	219	ASN
3	8-D	225	GLN
3	8-D	240	ASN
3	8-D	266	HIS
3	8-D	353	HIS
3	8-D	370	ASN
3	8-D	414	GLN
3	8-D	417	GLN
3	8-D	418	ASN
3	8-D	442	GLN
1	9-A	258	ASN
1	9-A	273	ASN
1	9-A	277	GLN
1	9-A	289	GLN
1	9-A	297	GLN
1	9-A	323	GLN
1	9-A	369	ASN
1	9-A	452	ASN
1	9-A	470	GLN
1	9-A	485	GLN
1	9-A	559	HIS
1	9-A	649	GLN
1	9-A	650	ASN
1	9-A	686	ASN
1	9-A	698	GLN
1	9-A	770	ASN
1	9-A	784	GLN
2	9-B	206	GLN
2	9-B	215	ASN
2	9-B	232	GLN

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Mol	Chain	Res	Type
2	9-B	262	GLN
2	9-B	290	ASN
2	9-B	380	HIS
2	9-B	430	HIS
2	9-B	434	GLN
2	9-B	452	GLN
2	9-B	459	HIS
2	9-B	462	GLN
2	9-B	575	ASN
2	9-B	588	ASN
2	9-B	597	ASN
2	9-B	640	GLN
2	9-B	642	GLN
2	9-B	643	GLN
2	9-B	645	ASN
2	9-B	780	ASN
2	9-B	806	ASN
2	9-B	832	ASN
3	9-C	16	HIS
3	9-C	24	GLN
3	9-C	29	HIS
3	9-C	60	ASN
3	9-C	116	GLN
3	9-C	225	GLN
3	9-C	226	HIS
3	9-C	320	ASN
3	9-C	325	ASN
3	9-C	385	ASN
3	9-C	406	ASN
3	9-C	442	GLN
3	9-D	103	ASN
3	9-D	116	GLN
3	9-D	186	ASN
3	9-D	219	ASN
3	9-D	229	GLN
3	9-D	266	HIS
3	9-D	289	HIS
3	9-D	303	ASN
3	9-D	339	GLN
3	9-D	353	HIS
3	9-D	368	ASN
3	9-D	385	ASN

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Mol	Chain	Res	Type
3	9-D	418	ASN
3	9-D	420	GLN
1	10-A	55	GLN
1	10-A	136	GLN
1	10-A	167	ASN
1	10-A	185	GLN
1	10-A	253	GLN
1	10-A	274	ASN
1	10-A	289	GLN
1	10-A	362	GLN
1	10-A	379	ASN
1	10-A	423	GLN
1	10-A	442	ASN
1	10-A	464	ASN
1	10-A	593	GLN
1	10-A	633	HIS
1	10-A	638	HIS
1	10-A	665	ASN
2	10-B	206	GLN
2	10-B	215	ASN
2	10-B	232	GLN
2	10-B	262	GLN
2	10-B	303	HIS
2	10-B	322	HIS
2	10-B	333	ASN
2	10-B	459	HIS
2	10-B	466	GLN
2	10-B	479	ASN
2	10-B	497	ASN
2	10-B	573	ASN
2	10-B	597	ASN
2	10-B	601	GLN
2	10-B	645	ASN
2	10-B	734	ASN
2	10-B	778	ASN
2	10-B	780	ASN
2	10-B	799	ASN
2	10-B	806	ASN
2	10-B	832	ASN
3	10-C	16	HIS
3	10-C	24	GLN
3	10-C	81	ASN

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Mol	Chain	Res	Type
3	10-C	91	ASN
3	10-C	115	ASN
3	10-C	153	ASN
3	10-C	186	ASN
3	10-C	206	ASN
3	10-C	211	ASN
3	10-C	266	HIS
3	10-C	286	HIS
3	10-C	289	HIS
3	10-C	311	ASN
3	10-C	312	ASN
3	10-C	320	ASN
3	10-C	325	ASN
3	10-C	389	ASN
3	10-C	392	ASN
3	10-C	405	ASN
3	10-D	24	GLN
3	10-D	132	ASN
3	10-D	140	HIS
3	10-D	225	GLN
3	10-D	226	HIS
3	10-D	289	HIS
3	10-D	317	ASN
3	10-D	366	GLN
3	10-D	368	ASN
3	10-D	385	ASN
3	10-D	389	ASN
3	10-D	442	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

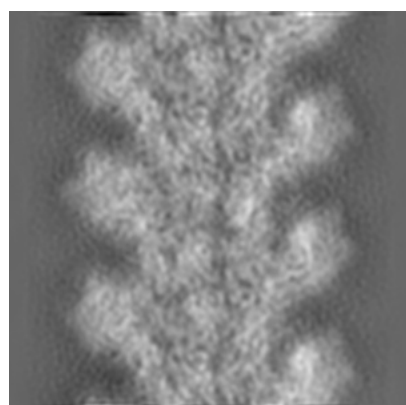
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2799. These allow visual inspection of the internal detail of the map and identification of artifacts.

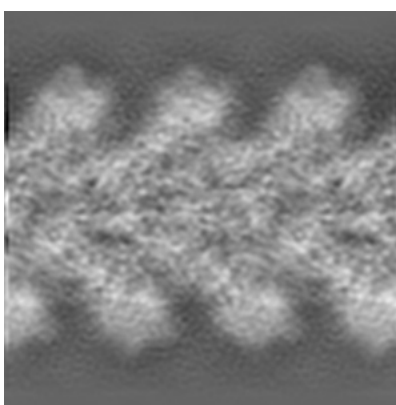
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

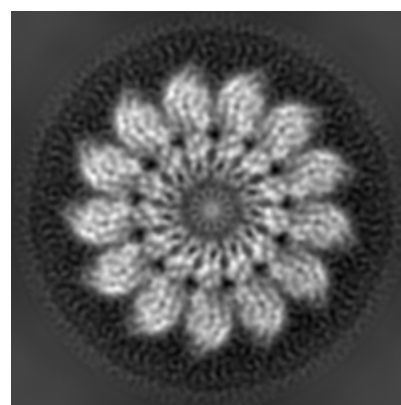
6.1.1 Primary map



X



Y

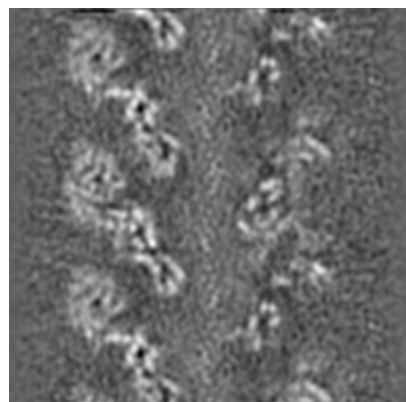


Z

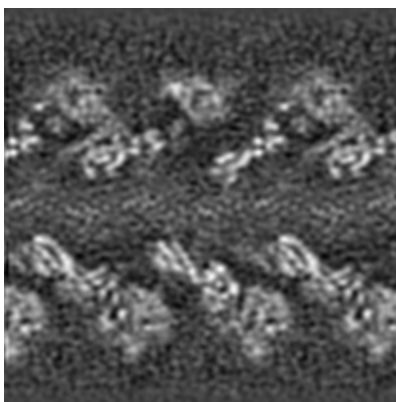
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

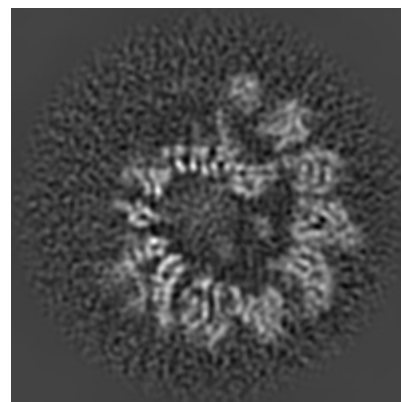
6.2.1 Primary map



X Index: 106



Y Index: 106

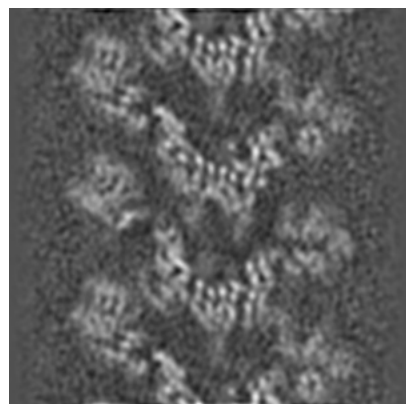


Z Index: 106

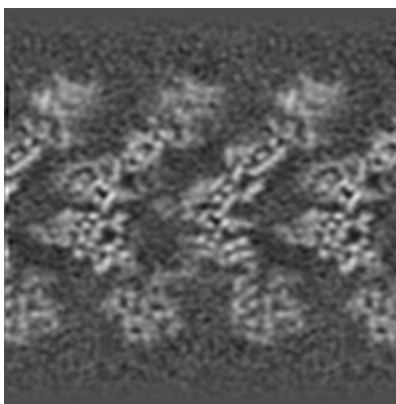
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

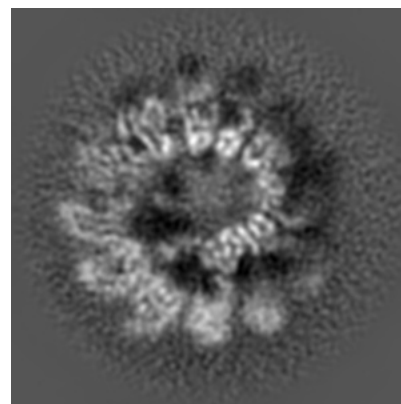
6.3.1 Primary map



X Index: 131



Y Index: 135

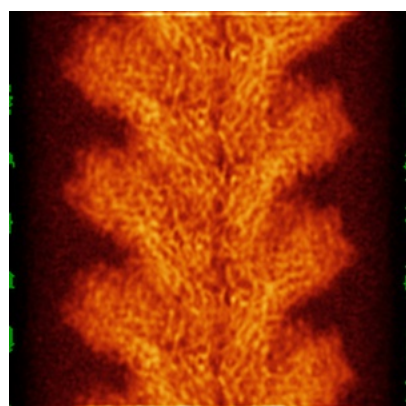


Z Index: 1

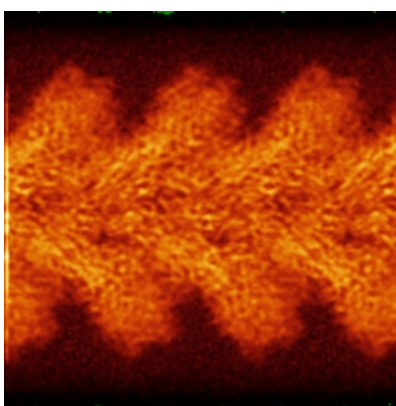
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

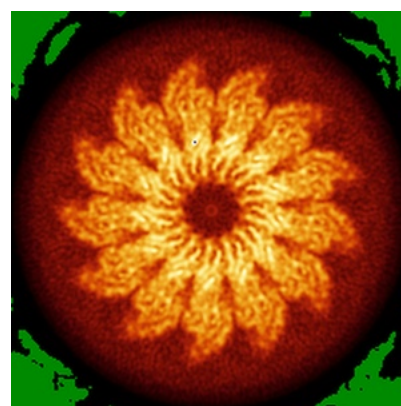
6.4.1 Primary map



X



Y

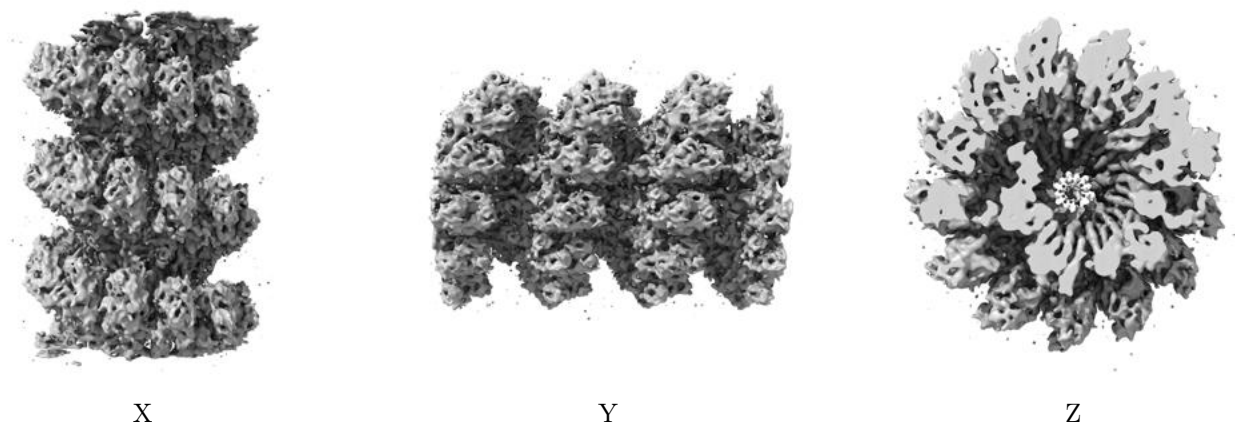


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

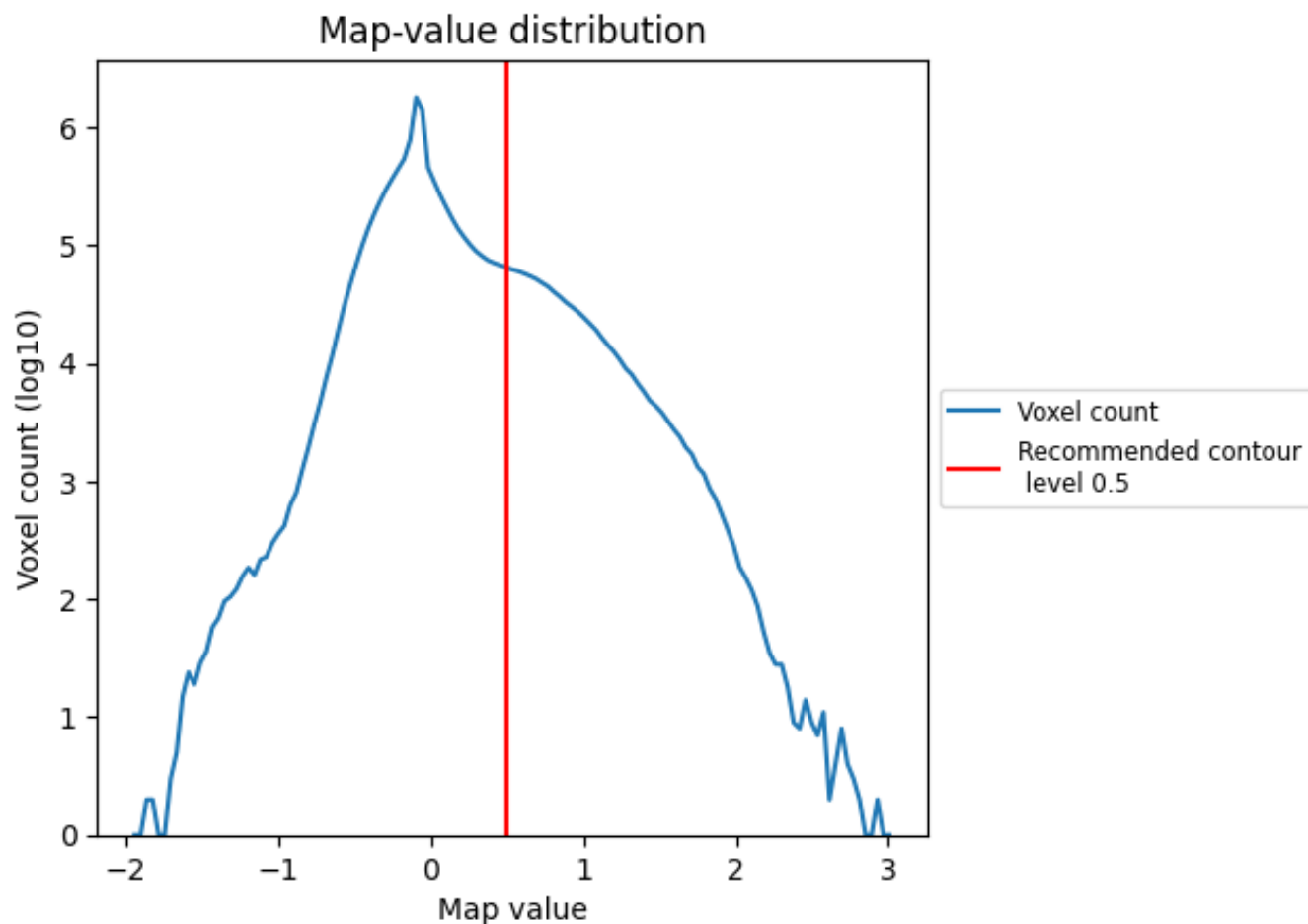
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

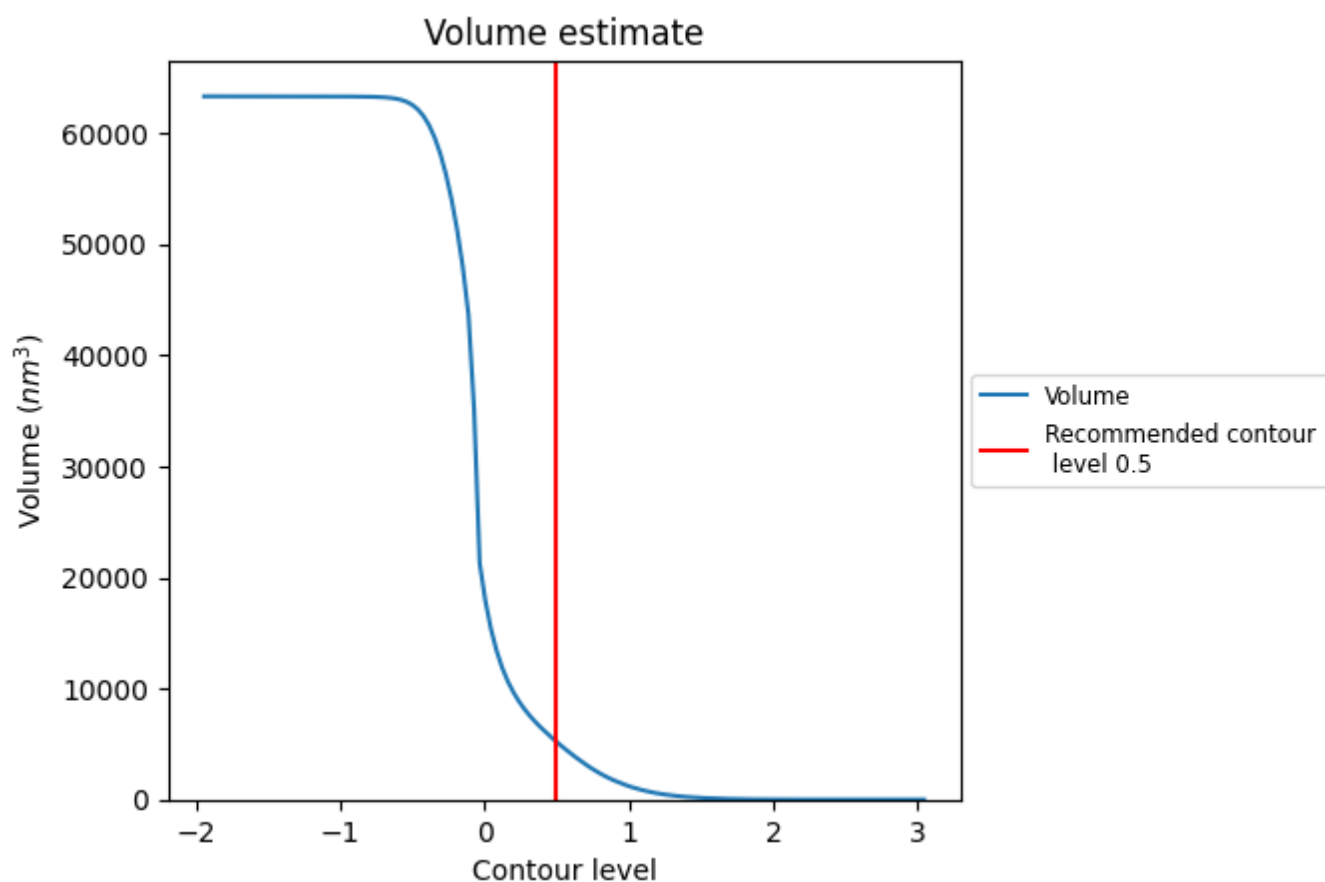
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

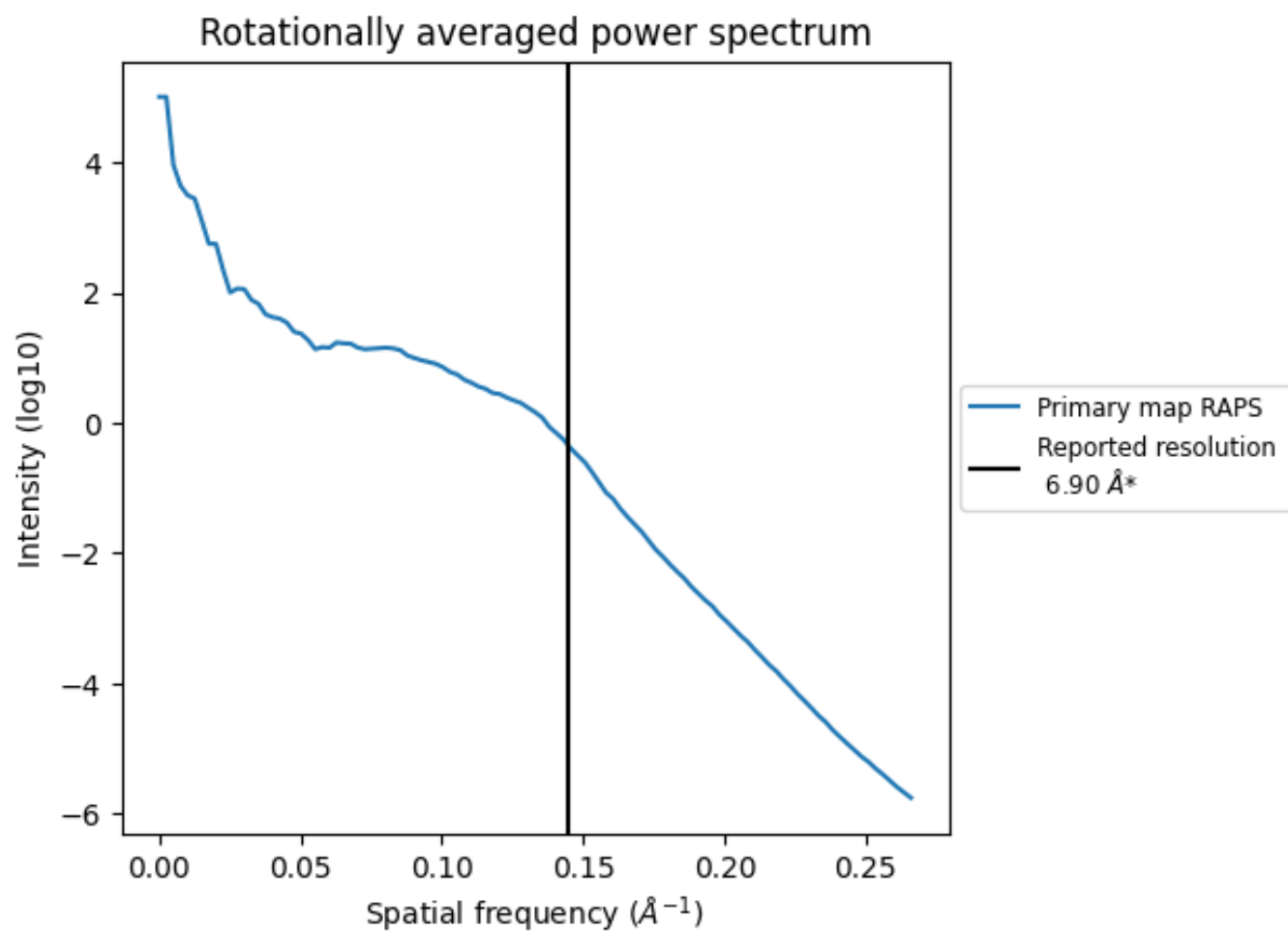
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5183 nm³; this corresponds to an approximate mass of 4682 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.145 Å⁻¹

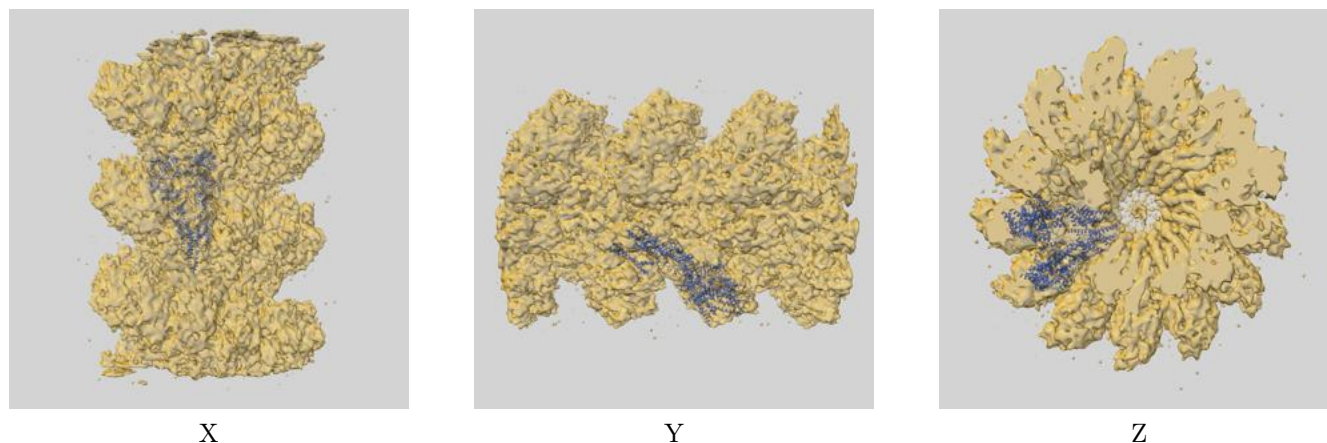
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

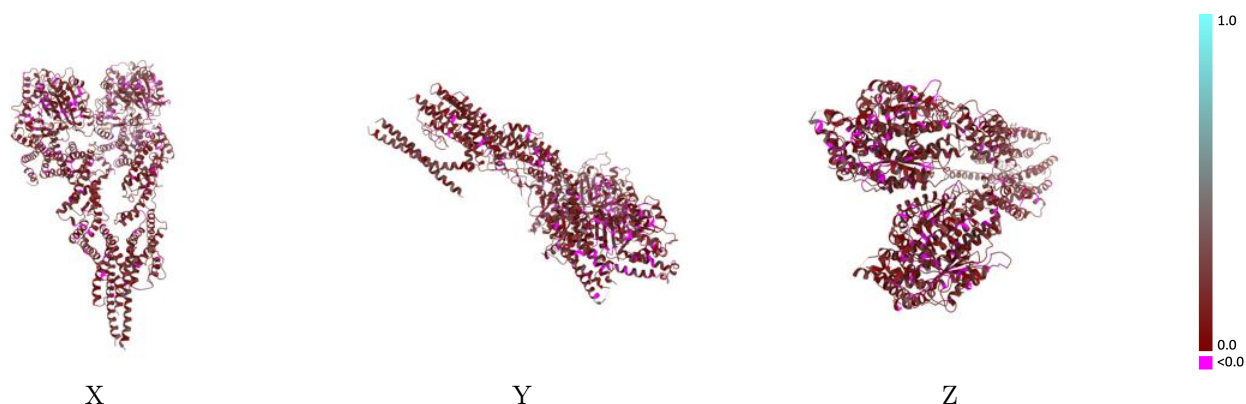
This section contains information regarding the fit between EMDB map EMD-2799 and PDB model 5FLZ. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



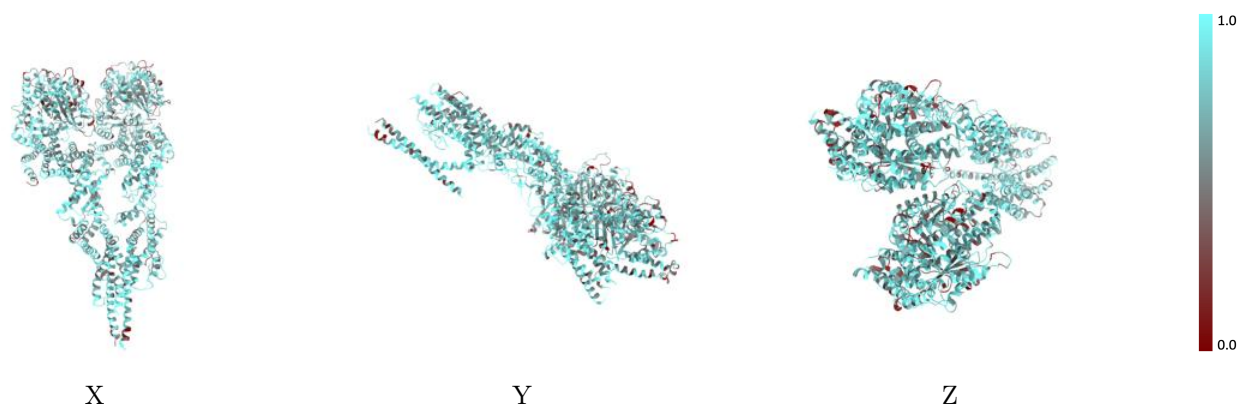
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



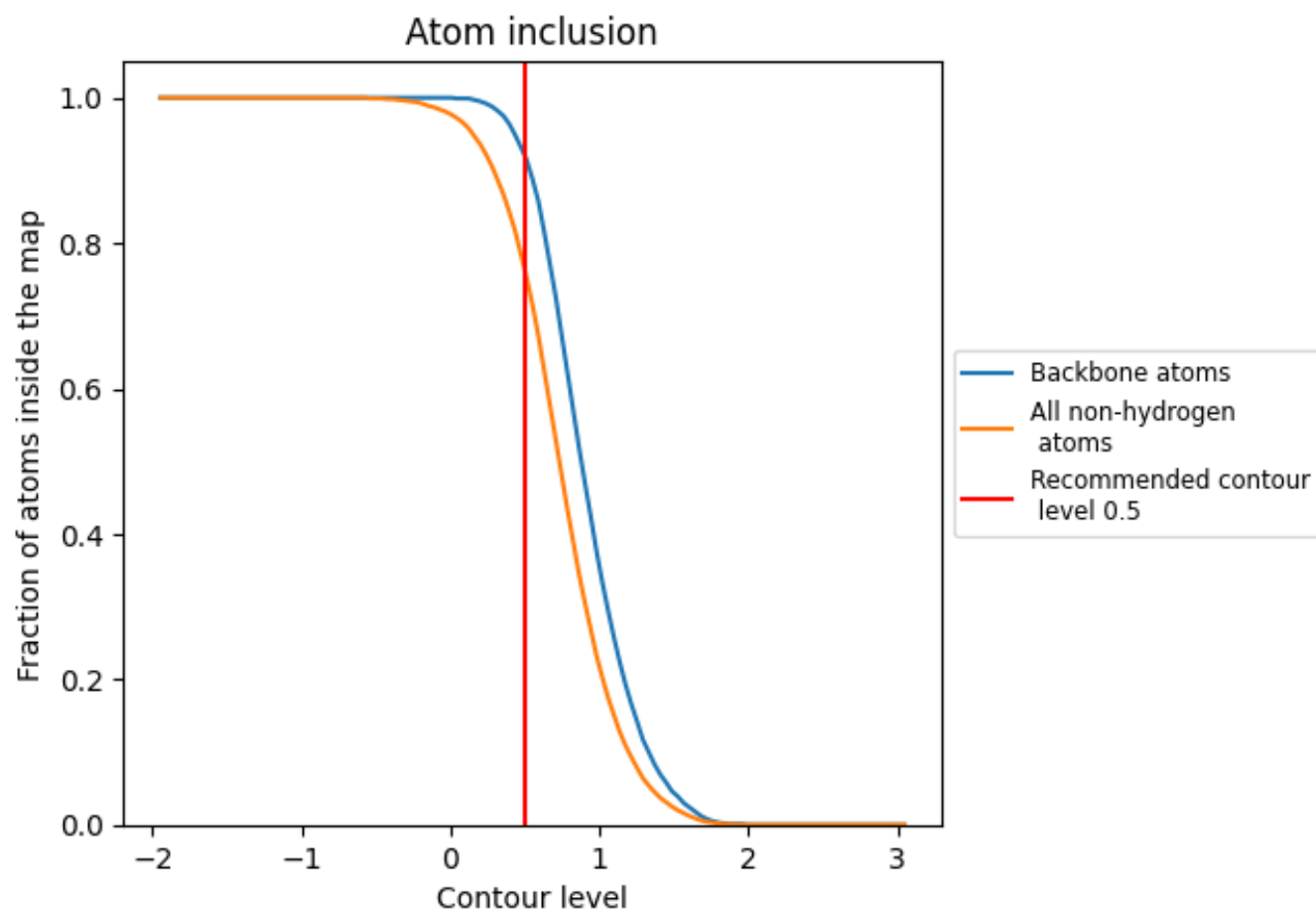
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7620	0.1530
A	0.7890	0.1640
B	0.8100	0.1630
C	0.7210	0.1380
D	0.7020	0.1300
E	0.7590	0.2320
F	0.7410	0.2410

