Full wwPDB EM Validation Report

Nov 18, 2024 – 11:40 AM JST

PDB ID	:	8WYJ
EMDB ID	:	EMD-37930
Title	:	The global map of Omicron Subvariants Spike with two antibodies
Authors	:	Yan, R.H.; Wang, A.J.; Yang, H.N.
Deposited on	:	2023-10-31
Resolution	:	3.10 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:

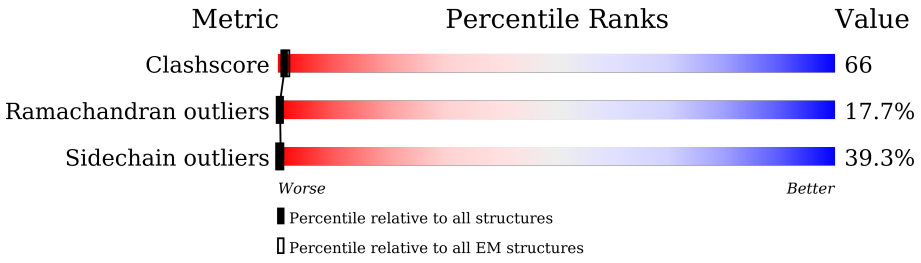
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	A	1123	6% 22% 42% 24% · 8%
1	B	1123	· 21% 39% 25% 7% 8%
1	C	1123	8% 25% 37% 24% 5% 8%
2	D	125	53% 10% 36% 42% 11%
2	H	125	50% 13% 43% 33% 11%
2	Q	125	· 10% 43% 35% 11%
3	E	127	80% 17% 46% 29% 8%
3	I	127	85% 13% 45% 31% 11%

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Mol	Chain	Length	Quality of chain
3	S	127	45% 14% 50% 28% 8%
4	F	106	84% 15% 37% 41% 8%
4	J	106	74% 14% 42% 35% 8%
4	R	106	7% 11% 42% 39% 8%
5	G	104	95% 19% 44% 22% 14%
5	K	104	86% 19% 45% 27% 9%
5	T	104	38% 15% 47% 25% 12%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 34491 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1030	Total	C	N	O	S	0	0
			8083	5183	1342	1522	36		
1	B	1030	Total	C	N	O	S	0	0
			8083	5183	1342	1522	36		
1	C	1030	Total	C	N	O	S	0	0
			8083	5183	1342	1522	36		

There are 207 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	conflict	UNP P0DTC2
A	24	THR	ARG	conflict	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	conflict	UNP P0DTC2
A	50	LEU	SER	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	127	PHE	VAL	conflict	UNP P0DTC2
A	142	ASP	GLY	conflict	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	157	SER	PHE	conflict	UNP P0DTC2
A	158	GLY	ARG	conflict	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	211	ILE	LEU	conflict	UNP P0DTC2
A	212	GLY	VAL	conflict	UNP P0DTC2
A	215	PHE	LEU	conflict	UNP P0DTC2
A	245	ASN	HIS	conflict	UNP P0DTC2
A	264	ASP	ALA	conflict	UNP P0DTC2
A	332	VAL	ILE	conflict	UNP P0DTC2
A	339	HIS	GLY	conflict	UNP P0DTC2
A	356	THR	LYS	conflict	UNP P0DTC2
A	371	PHE	SER	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	376	ALA	THR	conflict	UNP P0DTC2
A	403	LYS	ARG	conflict	UNP P0DTC2
A	405	ASN	ASP	conflict	UNP P0DTC2
A	408	SER	ARG	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	445	HIS	VAL	conflict	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	450	ASP	ASN	conflict	UNP P0DTC2
A	452	TRP	LEU	conflict	UNP P0DTC2
A	460	LYS	ASN	conflict	UNP P0DTC2
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	481	LYS	ASN	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	483	LYS	GLU	conflict	UNP P0DTC2
A	485	PRO	PHE	conflict	UNP P0DTC2
A	497	ARG	GLN	conflict	UNP P0DTC2
A	500	TYR	ASN	conflict	UNP P0DTC2
A	504	HIS	TYR	conflict	UNP P0DTC2
A	553	LYS	GLU	conflict	UNP P0DTC2
A	569	VAL	ALA	conflict	UNP P0DTC2
A	613	GLY	ASP	conflict	UNP P0DTC2
A	620	SER	PRO	conflict	UNP P0DTC2
A	654	TYR	HIS	conflict	UNP P0DTC2
A	669	VAL	ILE	conflict	UNP P0DTC2
A	679	LYS	ASN	conflict	UNP P0DTC2
A	681	ARG	PRO	conflict	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	conflict	UNP P0DTC2
A	796	TYR	ASP	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	939	PHE	SER	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	conflict	UNP P0DTC2
A	969	LYS	ASN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1143	LEU	PRO	conflict	UNP P0DTC2
B	22	ILE	THR	conflict	UNP P0DTC2
B	24	THR	ARG	conflict	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	conflict	UNP P0DTC2
B	50	LEU	SER	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	127	PHE	VAL	conflict	UNP P0DTC2
B	142	ASP	GLY	conflict	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	conflict	UNP P0DTC2
B	158	GLY	ARG	conflict	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	211	ILE	LEU	conflict	UNP P0DTC2
B	212	GLY	VAL	conflict	UNP P0DTC2
B	215	PHE	LEU	conflict	UNP P0DTC2
B	245	ASN	HIS	conflict	UNP P0DTC2
B	264	ASP	ALA	conflict	UNP P0DTC2
B	332	VAL	ILE	conflict	UNP P0DTC2
B	339	HIS	GLY	conflict	UNP P0DTC2
B	356	THR	LYS	conflict	UNP P0DTC2
B	371	PHE	SER	conflict	UNP P0DTC2
B	373	PRO	SER	conflict	UNP P0DTC2
B	375	PHE	SER	conflict	UNP P0DTC2
B	376	ALA	THR	conflict	UNP P0DTC2
B	403	LYS	ARG	conflict	UNP P0DTC2
B	405	ASN	ASP	conflict	UNP P0DTC2
B	408	SER	ARG	conflict	UNP P0DTC2
B	417	ASN	LYS	conflict	UNP P0DTC2
B	440	LYS	ASN	conflict	UNP P0DTC2
B	445	HIS	VAL	conflict	UNP P0DTC2
B	446	SER	GLY	conflict	UNP P0DTC2
B	450	ASP	ASN	conflict	UNP P0DTC2
B	452	TRP	LEU	conflict	UNP P0DTC2
B	460	LYS	ASN	conflict	UNP P0DTC2
B	477	ASN	SER	conflict	UNP P0DTC2
B	478	LYS	THR	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	481	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	483	LYS	GLU	conflict	UNP P0DTC2
B	485	PRO	PHE	conflict	UNP P0DTC2
B	497	ARG	GLN	conflict	UNP P0DTC2
B	500	TYR	ASN	conflict	UNP P0DTC2
B	504	HIS	TYR	conflict	UNP P0DTC2
B	553	LYS	GLU	conflict	UNP P0DTC2
B	569	VAL	ALA	conflict	UNP P0DTC2
B	613	GLY	ASP	conflict	UNP P0DTC2
B	620	SER	PRO	conflict	UNP P0DTC2
B	654	TYR	HIS	conflict	UNP P0DTC2
B	669	VAL	ILE	conflict	UNP P0DTC2
B	679	LYS	ASN	conflict	UNP P0DTC2
B	681	ARG	PRO	conflict	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	conflict	UNP P0DTC2
B	796	TYR	ASP	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	939	PHE	SER	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	conflict	UNP P0DTC2
B	969	LYS	ASN	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1143	LEU	PRO	conflict	UNP P0DTC2
C	22	ILE	THR	conflict	UNP P0DTC2
C	24	THR	ARG	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	conflict	UNP P0DTC2
C	50	LEU	SER	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	127	PHE	VAL	conflict	UNP P0DTC2
C	142	ASP	GLY	conflict	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	157	SER	PHE	conflict	UNP P0DTC2
C	158	GLY	ARG	conflict	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	211	ILE	LEU	conflict	UNP P0DTC2
C	212	GLY	VAL	conflict	UNP P0DTC2
C	215	PHE	LEU	conflict	UNP P0DTC2
C	245	ASN	HIS	conflict	UNP P0DTC2
C	264	ASP	ALA	conflict	UNP P0DTC2
C	332	VAL	ILE	conflict	UNP P0DTC2
C	339	HIS	GLY	conflict	UNP P0DTC2
C	356	THR	LYS	conflict	UNP P0DTC2
C	371	PHE	SER	conflict	UNP P0DTC2
C	373	PRO	SER	conflict	UNP P0DTC2
C	375	PHE	SER	conflict	UNP P0DTC2
C	376	ALA	THR	conflict	UNP P0DTC2
C	403	LYS	ARG	conflict	UNP P0DTC2
C	405	ASN	ASP	conflict	UNP P0DTC2
C	408	SER	ARG	conflict	UNP P0DTC2
C	417	ASN	LYS	conflict	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2
C	445	HIS	VAL	conflict	UNP P0DTC2
C	446	SER	GLY	conflict	UNP P0DTC2
C	450	ASP	ASN	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	UNP P0DTC2
C	460	LYS	ASN	conflict	UNP P0DTC2
C	477	ASN	SER	conflict	UNP P0DTC2
C	478	LYS	THR	conflict	UNP P0DTC2
C	481	LYS	ASN	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	483	LYS	GLU	conflict	UNP P0DTC2
C	485	PRO	PHE	conflict	UNP P0DTC2
C	497	ARG	GLN	conflict	UNP P0DTC2
C	500	TYR	ASN	conflict	UNP P0DTC2
C	504	HIS	TYR	conflict	UNP P0DTC2
C	553	LYS	GLU	conflict	UNP P0DTC2
C	569	VAL	ALA	conflict	UNP P0DTC2
C	613	GLY	ASP	conflict	UNP P0DTC2
C	620	SER	PRO	conflict	UNP P0DTC2
C	654	TYR	HIS	conflict	UNP P0DTC2
C	669	VAL	ILE	conflict	UNP P0DTC2
C	679	LYS	ASN	conflict	UNP P0DTC2
C	681	ARG	PRO	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	conflict	UNP P0DTC2
C	796	TYR	ASP	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	939	PHE	SER	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	conflict	UNP P0DTC2
C	969	LYS	ASN	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1143	LEU	PRO	conflict	UNP P0DTC2

- Molecule 2 is a protein called SA55-HC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	125	Total	C	N	O	S	0	0
			924	586	156	177	5		
2	D	125	Total	C	N	O	S	0	0
			924	586	156	177	5		
2	H	125	Total	C	N	O	S	0	0
			924	586	156	177	5		

- Molecule 3 is a protein called S309-HC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	127	Total	C	N	O	S	0	0
			956	605	166	180	5		
3	E	127	Total	C	N	O	S	0	0
			956	605	166	180	5		
3	I	127	Total	C	N	O	S	0	0
			956	605	166	180	5		

- Molecule 4 is a protein called SA55_KC.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	106	Total	C	N	O	S	0	0
			796	505	134	154	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	106	Total	C	N	O	S	0	0
			796	505	134	154	3		
4	J	106	Total	C	N	O	S	0	0
			796	505	134	154	3		

- Molecule 5 is a protein called S309-KC.

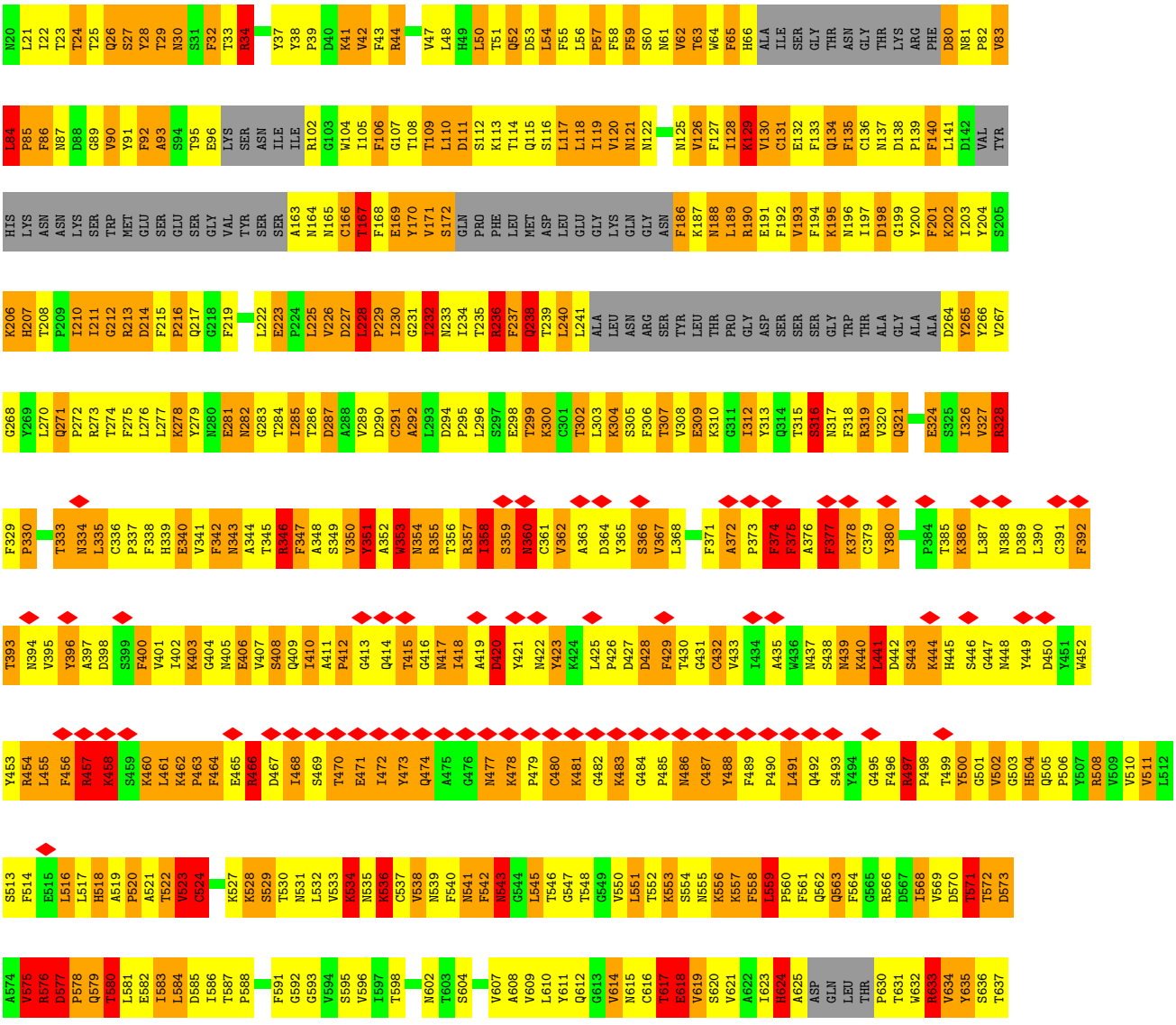
Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	104	Total	C	N	O	S	0	0
			738	466	134	136	2		
5	G	104	Total	C	N	O	S	0	0
			738	466	134	136	2		
5	K	104	Total	C	N	O	S	0	0
			738	466	134	136	2		

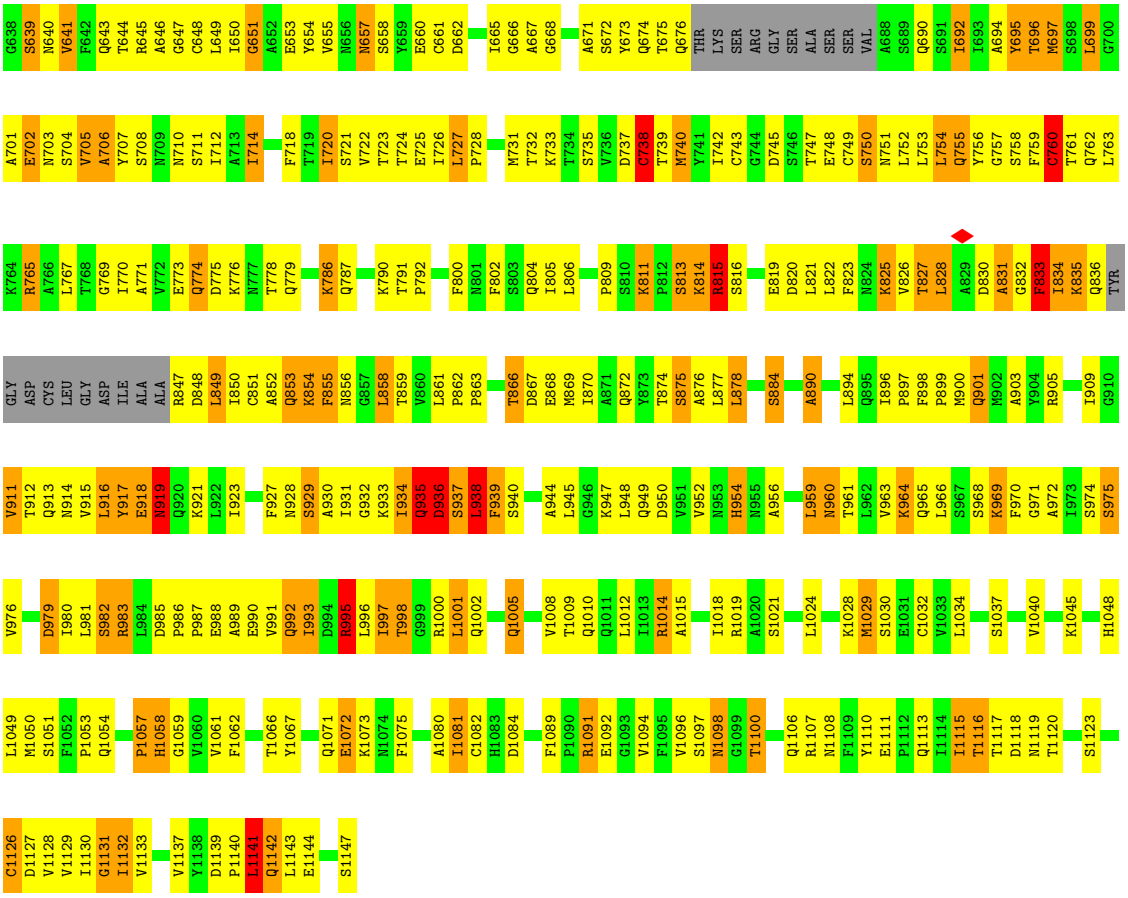
3 Residue-property plots (i)

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: Spike glycoprotein

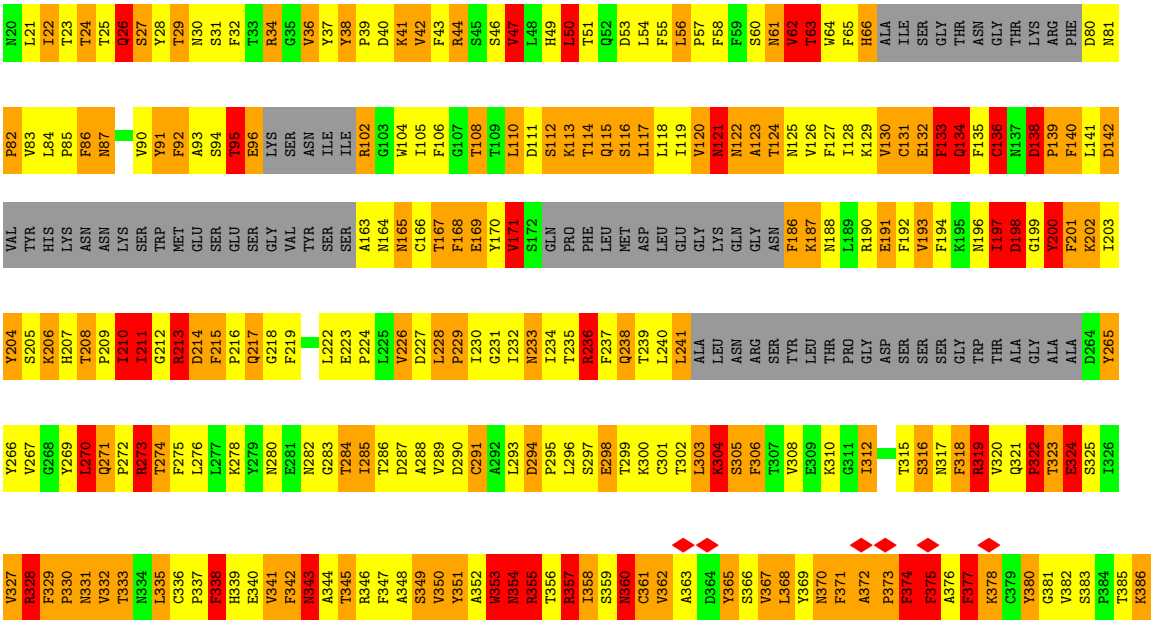
Chain A: 

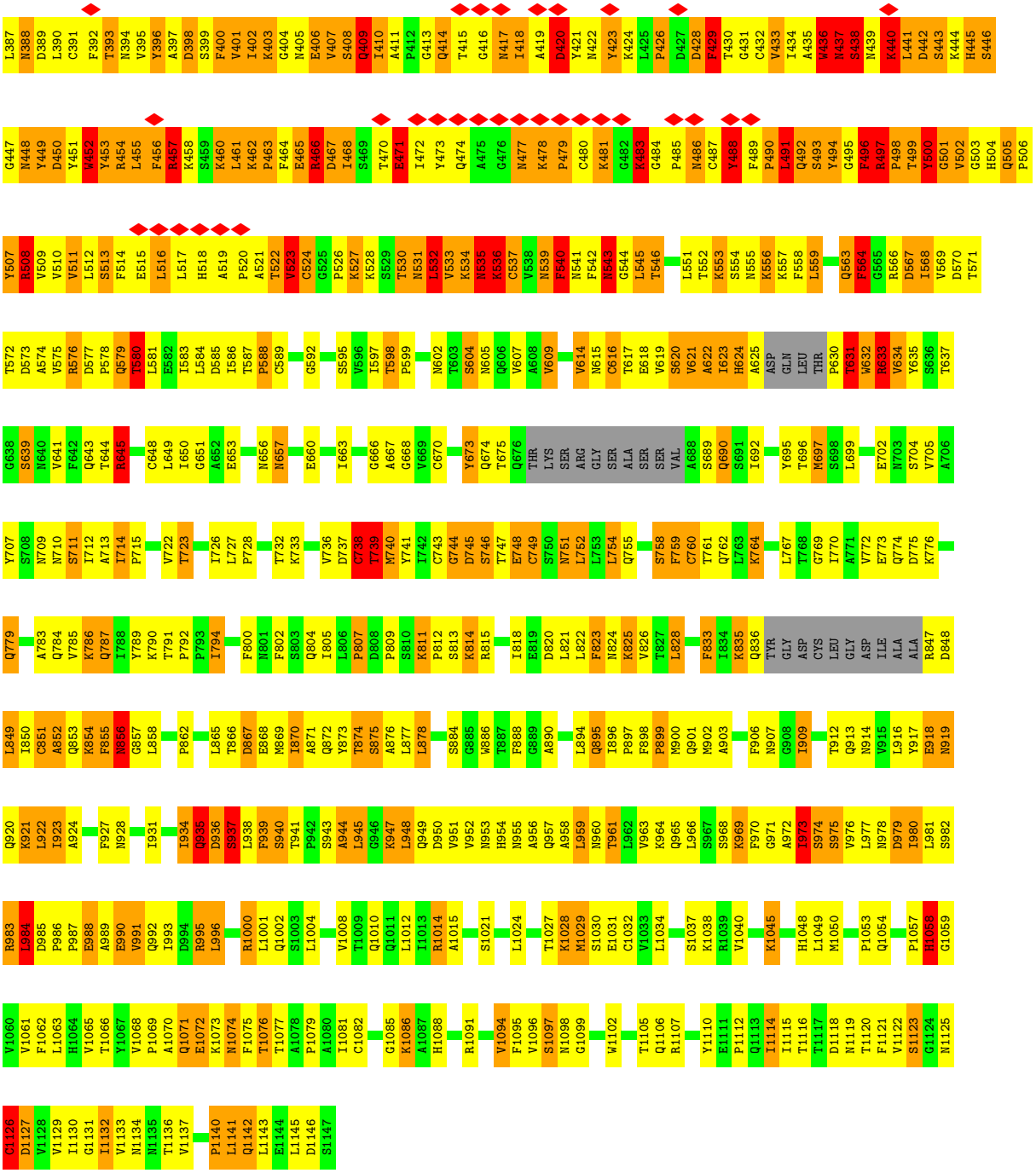




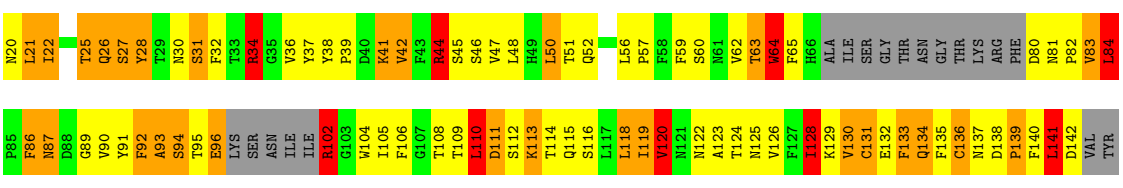
• Molecule 1: Spike glycoprotein

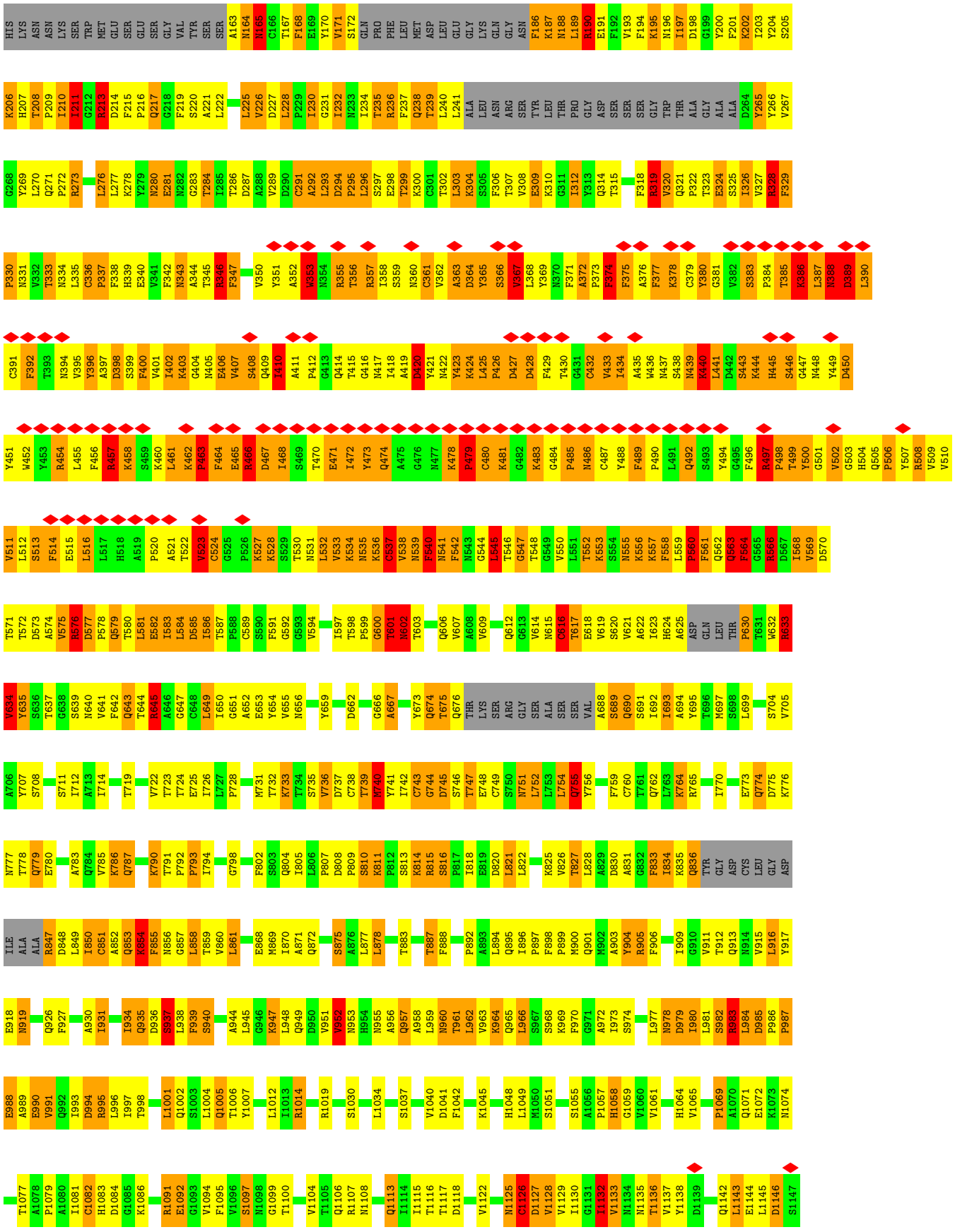
Chain B:





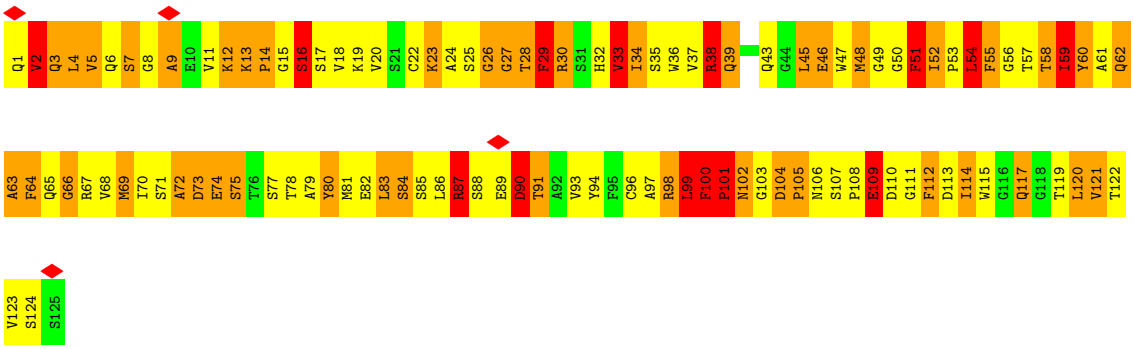
• Molecule 1: Spike glycoprotein





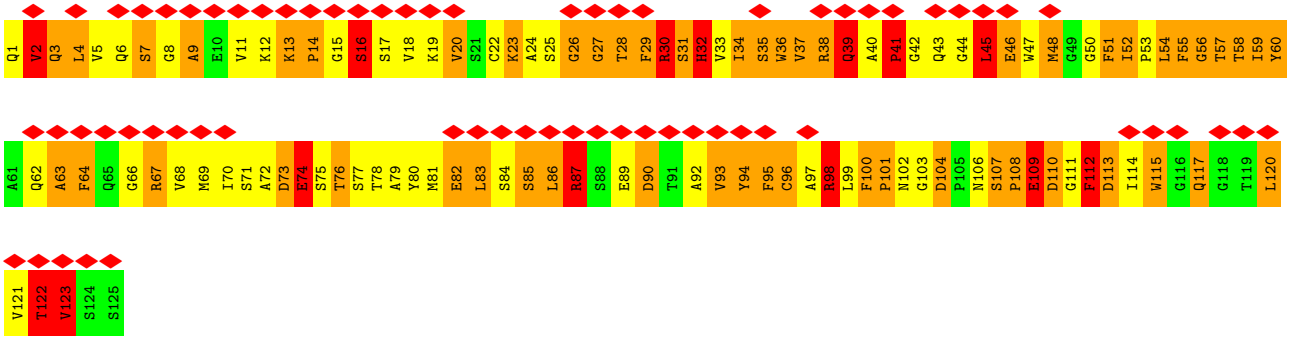
• Molecule 2: SA55-HC

Chain Q:



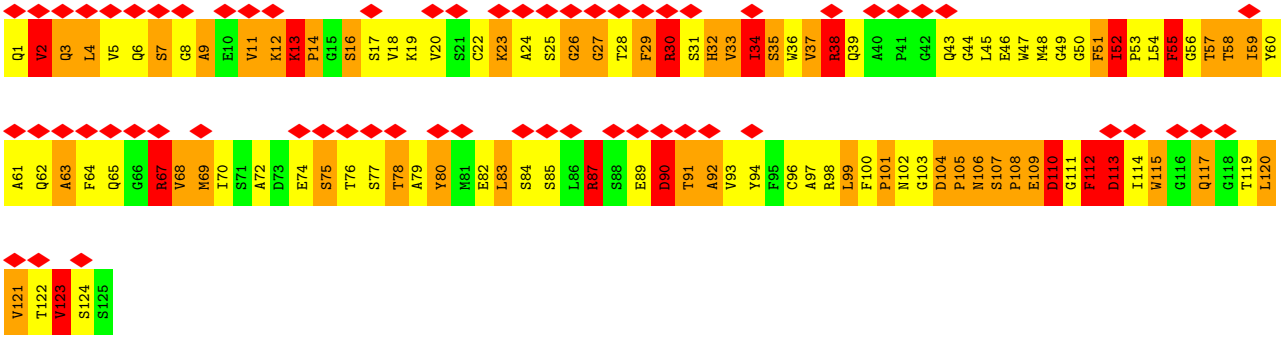
• Molecule 2: SA55-HC

Chain D:



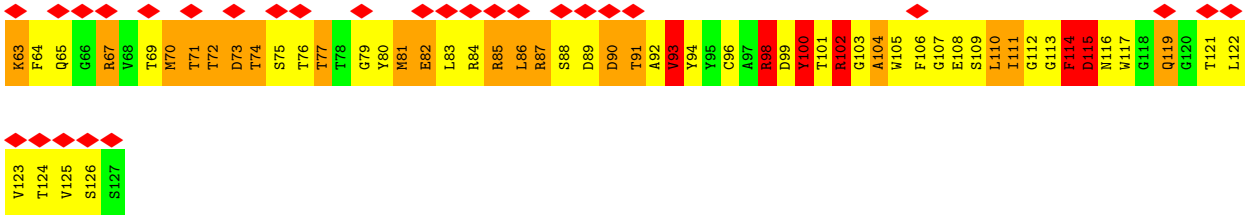
• Molecule 2: SA55-HC

Chain H:

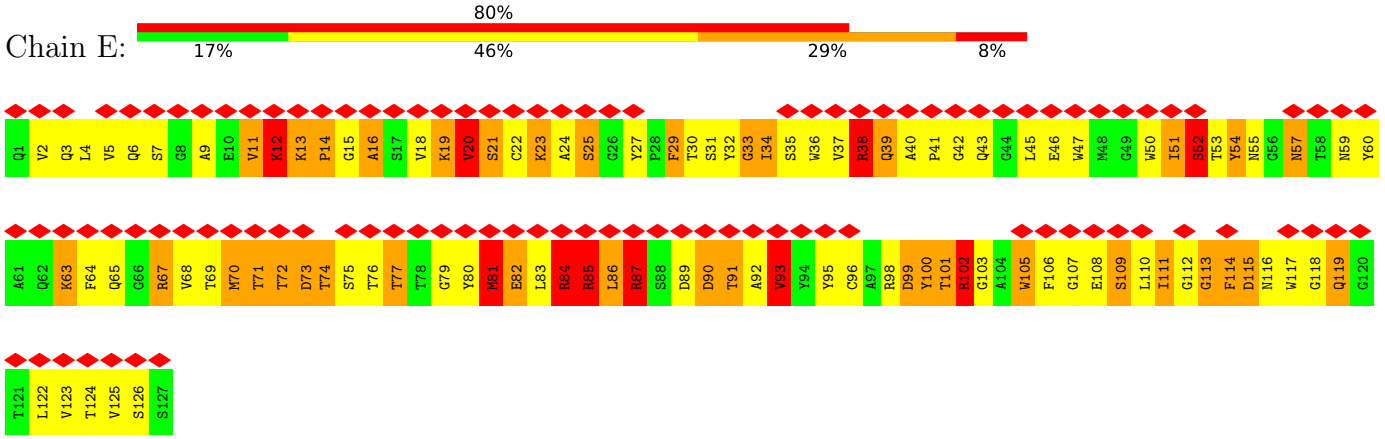


• Molecule 3: S309-HC

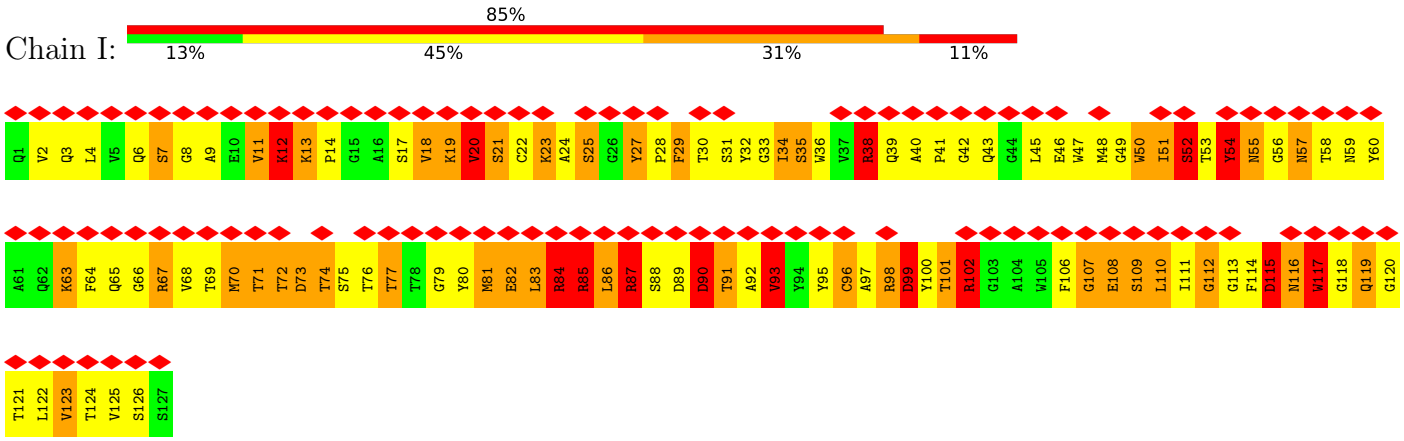
Chain S:



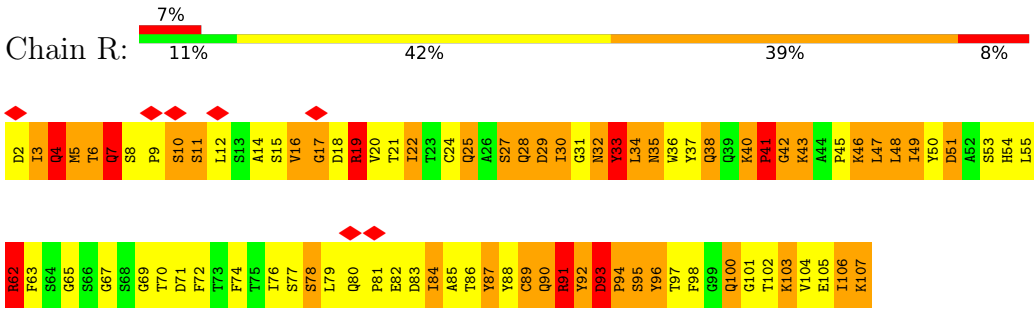
• Molecule 3: S309-HC



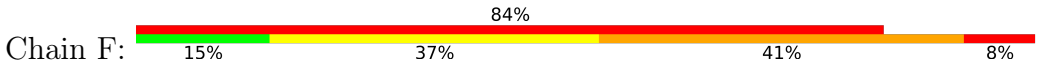
• Molecule 3: S309-HC

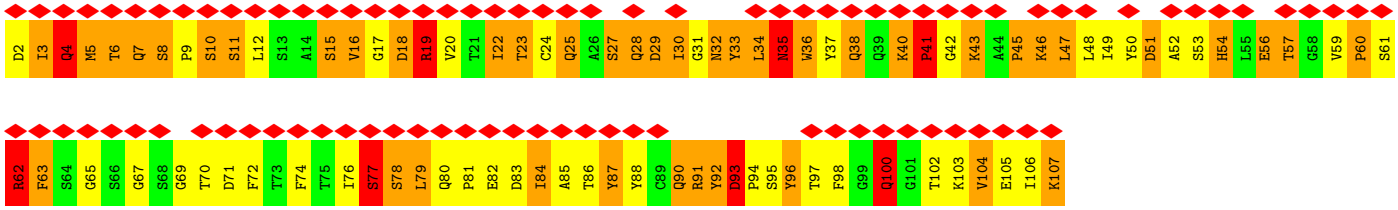


• Molecule 4: SA55_KC



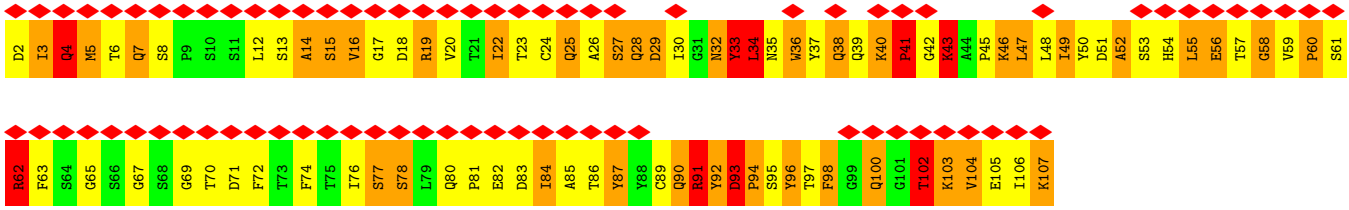
• Molecule 4: SA55_KC





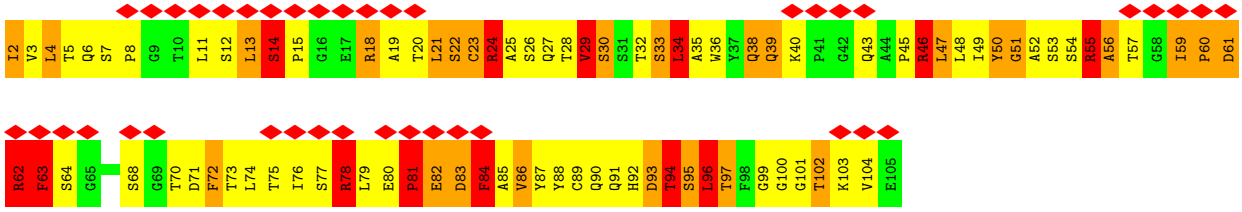
- Molecule 4: SA55_KC

Chain J:



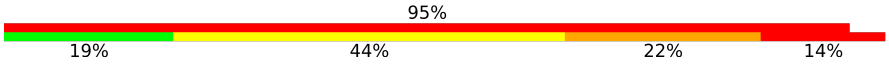
- Molecule 5: S309-KC

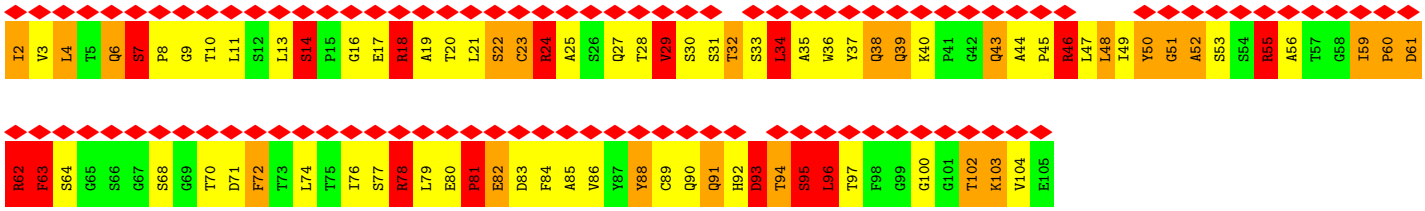
Chain T:



- Molecule 5: S309-KC

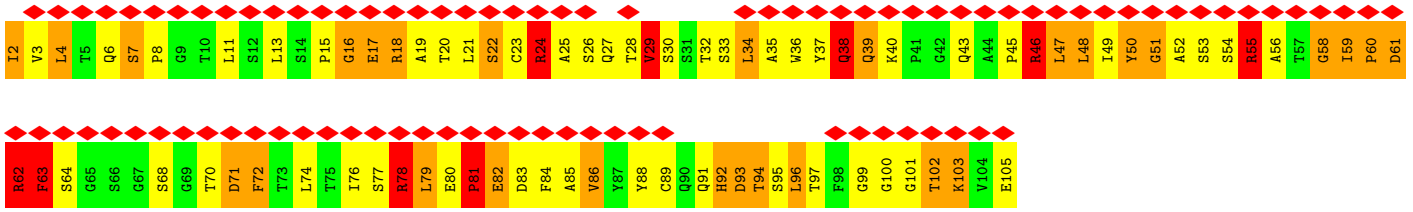
Chain G:





- Molecule 5: S309-KC

Chain K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	125226	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.5625	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.303	Depositor
Minimum map value	-1.180	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	448.19998, 448.19998, 448.19998	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.64	0/8277	0.81	0/11261
1	B	0.64	0/8277	0.84	0/11261
1	C	0.63	0/8277	0.83	0/11261
2	D	0.65	0/946	0.83	0/1285
2	H	0.64	0/946	0.85	0/1285
2	Q	0.66	0/946	0.85	0/1285
3	E	0.63	0/980	0.74	0/1334
3	I	0.61	0/980	0.78	0/1334
3	S	0.61	0/980	0.73	0/1334
4	F	0.64	0/815	0.84	0/1108
4	J	0.65	0/815	0.84	0/1108
4	R	0.65	0/815	0.84	0/1108
5	G	0.67	0/754	0.75	0/1026
5	K	0.65	0/754	0.74	0/1026
5	T	0.67	0/754	0.73	0/1026
All	All	0.64	0/35316	0.82	0/48042

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	24
1	B	0	16
1	C	0	28
2	D	0	3
2	H	0	4
2	Q	0	4
3	E	0	5
3	I	0	6
3	S	0	5
4	F	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	J	0	2
4	R	0	2
5	G	0	6
5	K	0	6
5	T	0	5
All	All	0	119

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (119) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1014	ARG	Sidechain
1	A	1019	ARG	Sidechain
1	A	102	ARG	Sidechain
1	A	1091	ARG	Sidechain
1	A	1107	ARG	Sidechain
1	A	190	ARG	Sidechain
1	A	236	ARG	Sidechain
1	A	319	ARG	Sidechain
1	A	328	ARG	Sidechain
1	A	34	ARG	Sidechain
1	A	346	ARG	Sidechain
1	A	355	ARG	Sidechain
1	A	357	ARG	Sidechain
1	A	44	ARG	Sidechain
1	A	454	ARG	Sidechain
1	A	457	ARG	Sidechain
1	A	466	ARG	Sidechain
1	A	497	ARG	Sidechain
1	A	576	ARG	Sidechain
1	A	633	ARG	Sidechain
1	A	765	ARG	Sidechain
1	A	815	ARG	Sidechain
1	A	983	ARG	Sidechain
1	A	995	ARG	Sidechain
1	B	1000	ARG	Sidechain
1	B	213	ARG	Sidechain
1	B	236	ARG	Sidechain
1	B	273	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	319	ARG	Sidechain
1	B	34	ARG	Sidechain
1	B	346	ARG	Sidechain
1	B	355	ARG	Sidechain
1	B	357	ARG	Sidechain
1	B	44	ARG	Sidechain
1	B	466	ARG	Sidechain
1	B	497	ARG	Sidechain
1	B	508	ARG	Sidechain
1	B	633	ARG	Sidechain
1	B	645	ARG	Sidechain
1	B	983	ARG	Sidechain
1	C	1014	ARG	Sidechain
1	C	1019	ARG	Sidechain
1	C	102	ARG	Sidechain
1	C	1091	ARG	Sidechain
1	C	1107	ARG	Sidechain
1	C	190	ARG	Sidechain
1	C	213	ARG	Sidechain
1	C	236	ARG	Sidechain
1	C	273	ARG	Sidechain
1	C	319	ARG	Sidechain
1	C	34	ARG	Sidechain
1	C	346	ARG	Sidechain
1	C	355	ARG	Sidechain
1	C	357	ARG	Sidechain
1	C	44	ARG	Sidechain
1	C	454	ARG	Sidechain
1	C	457	ARG	Sidechain
1	C	466	ARG	Sidechain
1	C	497	ARG	Sidechain
1	C	566	ARG	Sidechain
1	C	576	ARG	Sidechain
1	C	645	ARG	Sidechain
1	C	765	ARG	Sidechain
1	C	815	ARG	Sidechain
1	C	847	ARG	Sidechain
1	C	905	ARG	Sidechain
1	C	983	ARG	Sidechain
1	C	995	ARG	Sidechain
2	D	30	ARG	Sidechain
2	D	87	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	D	98	ARG	Sidechain
3	E	102	ARG	Sidechain
3	E	38	ARG	Sidechain
3	E	84	ARG	Sidechain
3	E	85	ARG	Sidechain
3	E	87	ARG	Sidechain
4	F	19	ARG	Sidechain
4	F	62	ARG	Sidechain
4	F	91	ARG	Sidechain
5	G	18	ARG	Sidechain
5	G	24	ARG	Sidechain
5	G	46	ARG	Sidechain
5	G	55	ARG	Sidechain
5	G	62	ARG	Sidechain
5	G	78	ARG	Sidechain
2	H	30	ARG	Sidechain
2	H	38	ARG	Sidechain
2	H	67	ARG	Sidechain
2	H	87	ARG	Sidechain
3	I	102	ARG	Sidechain
3	I	38	ARG	Sidechain
3	I	84	ARG	Sidechain
3	I	85	ARG	Sidechain
3	I	87	ARG	Sidechain
3	I	98	ARG	Sidechain
4	J	62	ARG	Sidechain
4	J	91	ARG	Sidechain
5	K	18	ARG	Sidechain
5	K	24	ARG	Sidechain
5	K	46	ARG	Sidechain
5	K	55	ARG	Sidechain
5	K	62	ARG	Sidechain
5	K	78	ARG	Sidechain
2	Q	30	ARG	Sidechain
2	Q	38	ARG	Sidechain
2	Q	87	ARG	Sidechain
2	Q	98	ARG	Sidechain
4	R	19	ARG	Sidechain
4	R	91	ARG	Sidechain
3	S	102	ARG	Sidechain
3	S	38	ARG	Sidechain
3	S	85	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	S	87	ARG	Sidechain
3	S	98	ARG	Sidechain
5	T	24	ARG	Sidechain
5	T	46	ARG	Sidechain
5	T	55	ARG	Sidechain
5	T	62	ARG	Sidechain
5	T	78	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8083	0	7910	911	0
1	B	8083	0	7908	1040	0
1	C	8083	0	7906	842	0
2	D	924	0	881	223	0
2	H	924	0	881	192	0
2	Q	924	0	881	229	0
3	E	956	0	894	140	0
3	I	956	0	894	176	0
3	S	956	0	894	132	0
4	F	796	0	737	146	0
4	J	796	0	737	132	0
4	R	796	0	737	149	0
5	G	738	0	686	137	0
5	K	738	0	686	107	0
5	T	738	0	686	142	0
All	All	34491	0	33318	4448	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 66.

All (4448) 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:357:ARG:HA	1:A:396:TYR:HA	1.19	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASN:HA	2:D:53:PRO:HB3	1.30	1.13
1:A:474:GLN:HA	1:A:483:LYS:HA	1.12	1.11
5:T:40:LYS:HD2	5:T:46:ARG:NH1	1.66	1.11
1:B:85:PRO:HA	1:B:236:ARG:HA	1.31	1.09
1:C:448:ASN:HB3	1:C:496:PHE:HB2	1.39	1.04
1:C:325:SER:O	1:C:539:ASN:HB2	1.57	1.03
1:B:502:VAL:HB	3:S:100:TYR:HB2	1.36	1.02
1:C:473:TYR:HB3	1:C:487:CYS:HB3	1.39	1.02
1:C:357:ARG:HA	1:C:396:TYR:HA	1.05	1.02
1:B:474:GLN:HB2	1:B:485:PRO:HD3	1.43	1.01
1:C:577:ASP:HB2	1:C:582:GLU:HB2	1.42	1.01
2:D:112:PHE:HD2	4:F:37:TYR:HH	1.03	1.00
5:G:56:ALA:H	5:G:59:ILE:HG13	1.23	0.99
2:D:24:ALA:HB2	2:D:30:ARG:HD2	1.45	0.98
2:D:100:PHE:H	2:D:101:PRO:HD2	1.29	0.98
5:T:62:ARG:HG3	5:T:77:SER:HB2	1.45	0.98
1:C:410:ILE:HG22	1:C:425:LEU:HD23	1.43	0.98
2:Q:33:VAL:HG22	2:Q:99:LEU:HB3	1.46	0.98
1:C:355:ARG:HA	1:C:398:ASP:HA	1.44	0.97
2:H:12:LYS:HB2	2:H:123:VAL:HG12	1.42	0.97
1:B:130:VAL:HG21	1:B:168:PHE:CE1	1.99	0.97
2:Q:102:ASN:HA	2:Q:109:GLU:HB2	1.47	0.96
1:C:106:PHE:HB3	1:C:234:ILE:HG23	1.45	0.96
4:J:19:ARG:HG2	4:J:77:SER:HA	1.47	0.95
1:B:131:CYS:HA	1:B:166:CYS:CB	1.96	0.95
1:B:474:GLN:HB3	1:B:484:GLY:HA2	1.48	0.95
4:J:34:LEU:HD22	4:J:74:PHE:HZ	1.32	0.94
1:C:357:ARG:CA	1:C:396:TYR:HA	1.96	0.94
1:C:312:ILE:HG12	1:C:597:ILE:HG13	1.49	0.94
5:T:35:ALA:HA	5:T:50:TYR:HA	1.48	0.94
1:B:497:ARG:HB2	1:B:498:PRO:HD3	1.50	0.94
1:B:616:CYS:HA	1:B:648:CYS:HB2	1.50	0.94
4:J:34:LEU:HD11	4:J:52:ALA:HB2	1.46	0.94
4:R:34:LEU:HA	4:R:91:ARG:HA	1.48	0.93
3:I:4:LEU:HD11	3:I:98:ARG:HB2	1.49	0.93
1:B:44:ARG:HB3	1:B:47:VAL:HG21	1.48	0.93
1:A:355:ARG:HD3	1:A:396:TYR:HB3	1.50	0.93
1:A:474:GLN:HA	1:A:483:LYS:CA	1.99	0.93
2:Q:108:PRO:HG2	4:R:33:TYR:CZ	2.04	0.93
5:G:55:ARG:HB2	5:G:59:ILE:HG13	1.49	0.93
1:C:322:PRO:HA	1:C:537:CYS:HB3	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:ASN:HB2	1:B:505:GLN:HE22	1.32	0.92
2:Q:108:PRO:HG2	4:R:33:TYR:OH	1.69	0.92
1:C:331:ASN:N	1:C:579:GLN:HB2	1.84	0.92
2:H:104:ASP:HB3	2:H:105:PRO:HD3	1.48	0.92
3:I:32:TYR:HE1	3:I:102:ARG:HA	1.35	0.92
2:Q:50:GLY:HA2	2:Q:59:ILE:HB	1.51	0.92
4:R:37:TYR:HE1	4:R:90:GLN:HB2	1.35	0.92
2:D:34:ILE:H	2:D:99:LEU:HB2	1.35	0.92
1:B:357:ARG:HG2	1:B:358:ILE:HG12	1.51	0.92
2:Q:56:GLY:HA3	2:Q:72:ALA:HB3	1.53	0.90
5:T:50:TYR:CE2	5:T:56:ALA:HA	2.06	0.90
5:G:49:ILE:HA	5:G:55:ARG:HA	1.54	0.90
2:D:54:LEU:HD11	2:D:99:LEU:HG	1.54	0.89
4:R:9:PRO:C	4:R:11:SER:H	1.75	0.89
5:T:40:LYS:HD2	5:T:46:ARG:HH12	1.35	0.89
1:C:357:ARG:HA	1:C:396:TYR:CA	2.00	0.89
1:C:719:THR:HA	1:C:926:GLN:HE22	1.37	0.88
1:B:770:ILE:HD11	1:B:1012:LEU:HG	1.55	0.88
1:B:403:LYS:HG2	1:B:405:ASN:H	1.39	0.88
2:Q:18:VAL:HB	2:Q:86:LEU:HD11	1.56	0.88
2:H:99:LEU:HD11	4:J:96:TYR:HE2	1.38	0.88
1:B:393:THR:HB	1:B:516:LEU:HA	1.55	0.88
1:C:195:LYS:HE2	1:C:197:ILE:HD11	1.52	0.87
1:B:65:PHE:HB2	1:B:265:TYR:HB3	1.54	0.87
1:A:127:PHE:HA	1:A:171:VAL:HG23	1.54	0.87
1:A:106:PHE:HB3	1:A:234:ILE:HG23	1.57	0.87
1:B:452:TRP:HA	1:B:493:SER:HA	1.55	0.86
1:B:472:ILE:HG13	1:B:489:PHE:HA	1.56	0.86
1:C:228:LEU:HB3	1:C:230:ILE:HD11	1.54	0.86
5:T:38:GLN:HB3	5:T:48:LEU:HD21	1.58	0.86
1:B:440:LYS:HD2	2:Q:57:THR:HA	1.58	0.86
1:A:472:ILE:HG13	1:A:490:PRO:HD3	1.56	0.85
1:A:869:MET:HB3	1:C:699:LEU:HD21	1.57	0.85
1:B:321:GLN:HB2	1:B:630:PRO:HG2	1.59	0.85
1:B:133:PHE:HB2	1:B:163:ALA:N	1.91	0.85
1:B:391:CYS:HB2	1:B:521:ALA:HB1	1.57	0.85
5:G:29:VAL:HG13	5:G:33:SER:HB2	1.58	0.85
1:B:118:LEU:HB3	1:B:129:LYS:HB3	1.56	0.85
4:R:81:PRO:HA	4:R:106:ILE:HG21	1.59	0.84
4:R:37:TYR:CE1	4:R:90:GLN:HB2	2.11	0.84
1:C:30:ASN:HD21	1:C:59:PHE:HD1	1.24	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:PRO:HA	1:C:537:CYS:CB	2.07	0.84
1:B:361:CYS:H	1:B:523:VAL:HA	1.40	0.84
5:K:17:GLU:O	5:K:78:ARG:HA	1.78	0.84
1:B:454:ARG:HA	1:B:492:GLN:H	1.41	0.84
5:T:55:ARG:HD2	5:T:59:ILE:HB	1.60	0.84
1:A:391:CYS:HB3	1:A:524:CYS:HA	1.60	0.83
1:B:712:ILE:O	1:B:1075:PHE:N	2.11	0.83
1:B:131:CYS:HA	1:B:166:CYS:HB3	1.58	0.83
2:H:50:GLY:HA2	2:H:54:LEU:HD21	1.60	0.83
4:J:7:GLN:NE2	4:J:71:ASP:CB	2.41	0.83
1:A:357:ARG:CA	1:A:396:TYR:HA	2.05	0.83
1:A:815:ARG:HB2	1:A:820:ASP:OD1	1.78	0.83
1:B:351:TYR:HB3	1:B:454:ARG:HB2	1.60	0.83
1:C:276:LEU:HD23	1:C:289:VAL:HG13	1.60	0.83
1:A:474:GLN:CA	1:A:483:LYS:HA	2.03	0.82
3:I:99:ASP:HA	3:I:114:PHE:O	1.78	0.82
4:J:34:LEU:HD22	4:J:74:PHE:CZ	2.14	0.82
5:G:35:ALA:HA	5:G:50:TYR:HA	1.59	0.82
4:F:81:PRO:HA	4:F:106:ILE:HG21	1.61	0.82
4:J:7:GLN:HE21	4:J:71:ASP:CB	1.93	0.82
1:B:194:PHE:HD1	1:B:203:ILE:HG23	1.45	0.82
1:C:471:GLU:N	1:C:490:PRO:HG3	1.95	0.82
1:C:752:LEU:HD23	1:C:993:ILE:HG21	1.60	0.82
3:I:48:MET:HB3	3:I:81:MET:HE1	1.62	0.82
1:B:737:ASP:HB3	1:B:740:MET:HB3	1.60	0.82
3:S:102:ARG:HH22	3:S:114:PHE:HA	1.45	0.82
1:B:111:ASP:HB2	1:B:113:LYS:HZ2	1.42	0.81
4:R:38:GLN:HB2	4:R:48:LEU:HD13	1.62	0.81
1:A:62:VAL:HG21	1:A:215:PHE:HE2	1.44	0.81
1:B:447:GLY:HA2	1:B:497:ARG:HA	1.62	0.81
1:C:432:CYS:HB3	1:C:512:LEU:HD12	1.61	0.81
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.62	0.81
2:Q:111:GLY:HA2	4:R:92:TYR:CE2	2.15	0.81
5:K:33:SER:HA	5:K:92:HIS:HB2	1.62	0.81
1:B:429:PHE:HD1	1:B:430:THR:H	1.26	0.81
2:D:35:SER:HB3	2:D:112:PHE:CZ	2.15	0.81
5:G:23:CYS:HB3	5:G:34:LEU:HD21	1.61	0.81
1:A:402:ILE:HD11	1:A:407:VAL:HA	1.61	0.81
2:D:86:LEU:HD23	2:D:90:ASP:HB3	1.62	0.81
3:E:102:ARG:HH11	3:E:103:GLY:HA2	1.45	0.81
1:A:353:TRP:H	1:A:353:TRP:HD1	1.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:LYS:HD2	1:A:939:PHE:HA	1.64	0.80
5:T:33:SER:HA	5:T:92:HIS:H	1.44	0.80
4:J:80:GLN:HB2	4:J:81:PRO:HD2	1.63	0.80
1:B:447:GLY:HA2	1:B:497:ARG:CA	2.10	0.80
1:B:713:ALA:HA	1:B:1074:ASN:HA	1.63	0.80
1:C:322:PRO:CA	1:C:537:CYS:HB3	2.11	0.80
1:B:299:THR:O	1:B:303:LEU:HG	1.81	0.80
1:B:440:LYS:CD	2:Q:57:THR:HA	2.12	0.80
1:C:353:TRP:HD1	1:C:353:TRP:H	1.28	0.80
1:C:412:PRO:HA	1:C:425:LEU:HD12	1.63	0.80
2:Q:54:LEU:HD22	2:Q:54:LEU:H	1.45	0.80
1:A:348:ALA:HB3	1:A:354:ASN:HB3	1.63	0.80
1:C:558:PHE:CG	1:C:583:ILE:HD12	2.16	0.80
2:H:99:LEU:HA	2:H:112:PHE:CE1	2.16	0.80
1:A:834:ILE:HG13	1:C:643:GLN:HE22	1.47	0.80
1:C:436:TRP:HH2	1:C:510:VAL:HG23	1.47	0.80
3:S:38:ARG:HB3	3:S:46:GLU:HB3	1.64	0.80
1:A:410:ILE:O	1:A:425:LEU:HD12	1.81	0.80
1:B:64:TRP:HH2	1:B:213:ARG:HD2	1.47	0.80
3:I:32:TYR:CE1	3:I:102:ARG:HA	2.16	0.80
2:H:13:LYS:HA	2:H:13:LYS:HZ2	1.46	0.79
2:H:12:LYS:HA	2:H:122:THR:O	1.82	0.79
1:A:519:ALA:HB1	1:A:520:PRO:HD2	1.64	0.79
3:I:4:LEU:CD1	3:I:98:ARG:HB2	2.12	0.79
1:C:438:SER:HB2	1:C:508:ARG:HD2	1.63	0.79
5:T:35:ALA:HB1	5:T:47:LEU:HD11	1.64	0.79
5:T:49:ILE:HG13	5:T:55:ARG:HG3	1.64	0.79
1:B:351:TYR:CB	1:B:454:ARG:HB2	2.13	0.79
3:I:41:PRO:HD3	3:I:92:ALA:HB2	1.65	0.79
5:K:62:ARG:HD2	5:K:77:SER:HB2	1.64	0.79
2:D:100:PHE:N	2:D:101:PRO:HD2	1.97	0.79
1:A:62:VAL:HG21	1:A:215:PHE:CE2	2.18	0.78
2:Q:53:PRO:HB2	2:Q:57:THR:HB	1.65	0.78
1:A:1126:CYS:HB3	1:A:1132:ILE:HD12	1.65	0.78
4:F:33:TYR:HB2	4:F:34:LEU:HD22	1.65	0.78
4:F:34:LEU:HD21	4:F:72:PHE:CD2	2.18	0.78
1:C:369:TYR:HA	1:C:374:PHE:CE2	2.18	0.78
1:C:545:LEU:HG	1:C:546:THR:HG23	1.65	0.78
2:Q:102:ASN:H	4:R:92:TYR:HB3	1.47	0.78
1:B:104:TRP:HE3	1:B:119:ILE:HG21	1.46	0.78
3:S:44:GLY:HA2	5:T:88:TYR:HE2	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:41:PRO:HD3	3:E:92:ALA:HB2	1.65	0.78
1:B:356:THR:HB	1:B:396:TYR:HB2	1.66	0.78
1:C:200:TYR:HB3	1:C:227:ASP:O	1.83	0.78
1:A:394:ASN:HA	1:A:523:VAL:HG11	1.64	0.78
1:B:190:ARG:HD2	1:B:207:HIS:HB3	1.65	0.78
1:C:822:LEU:HD22	1:C:945:LEU:HD21	1.63	0.78
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.64	0.78
1:B:140:PHE:HD2	1:B:241:LEU:HD21	1.46	0.78
1:C:502:VAL:HG12	3:I:100:TYR:CG	2.18	0.78
2:Q:111:GLY:HA3	4:R:50:TYR:CD2	2.19	0.78
1:B:197:ILE:HD11	1:B:202:LYS:HG3	1.64	0.77
3:S:41:PRO:HD3	3:S:92:ALA:HB2	1.65	0.77
1:C:457:ARG:HG2	1:C:458:LYS:HG2	1.66	0.77
1:C:462:LYS:H	1:C:462:LYS:HE2	1.48	0.77
1:A:107:GLY:H	1:A:234:ILE:HD12	1.47	0.77
5:T:34:LEU:HD22	5:T:52:ALA:HA	1.66	0.77
2:H:102:ASN:HA	2:H:109:GLU:HB2	1.67	0.77
3:E:39:GLN:O	3:E:92:ALA:HB1	1.83	0.77
1:C:808:ASP:HB3	1:C:811:LYS:HD2	1.66	0.77
1:A:610:LEU:HB2	1:A:649:LEU:HD12	1.66	0.76
1:B:853:GLN:HB3	1:B:858:LEU:HD12	1.66	0.76
4:F:81:PRO:HA	4:F:106:ILE:HG12	1.66	0.76
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.67	0.76
1:C:418:ILE:HA	1:C:422:ASN:HB2	1.68	0.76
1:C:455:LEU:HD13	1:C:492:GLN:HG3	1.67	0.76
1:A:371:PHE:HB2	1:A:374:PHE:HD2	1.50	0.76
1:A:131:CYS:HG	1:A:163:ALA:N	1.84	0.76
1:A:213:ARG:H	1:A:216:PRO:HG3	1.51	0.76
1:B:822:LEU:HD21	1:B:938:LEU:HD13	1.67	0.76
2:Q:105:PRO:HB3	2:Q:110:ASP:CB	2.16	0.76
1:B:437:ASN:HB3	1:B:508:ARG:HB2	1.67	0.76
4:F:15:SER:HA	4:F:18:ASP:HB3	1.66	0.76
3:E:24:ALA:HB1	3:E:27:TYR:CE2	2.20	0.76
1:A:64:TRP:CZ3	1:A:66:HIS:HB3	2.21	0.76
2:H:24:ALA:HB3	2:H:77:SER:HB3	1.68	0.76
1:C:339:HIS:CD2	1:C:367:VAL:HB	2.20	0.76
1:C:478:LYS:HB2	1:C:479:PRO:HD2	1.67	0.76
3:I:98:ARG:HD3	3:I:116:ASN:HB2	1.67	0.76
1:A:541:ASN:HA	1:A:546:THR:HA	1.67	0.75
1:B:496:PHE:HA	1:B:500:TYR:HD2	1.50	0.75
2:Q:4:LEU:HD21	2:Q:30:ARG:HD2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG12	1:A:267:VAL:HG23	1.67	0.75
1:A:135:PHE:CG	1:A:139:PRO:HB3	2.21	0.75
1:A:193:VAL:HG23	1:A:222:LEU:CD2	2.16	0.75
1:B:44:ARG:HB3	1:B:47:VAL:CG2	2.16	0.75
1:B:436:TRP:HH2	1:B:510:VAL:HG23	1.50	0.75
1:B:497:ARG:HB2	1:B:498:PRO:CD	2.15	0.75
1:A:542:PHE:HZ	1:A:584:LEU:HD22	1.50	0.75
2:Q:32:HIS:HA	2:Q:55:PHE:HB2	1.67	0.75
5:T:2:ILE:HG23	5:T:27:GLN:HG2	1.69	0.75
1:A:106:PHE:HB3	1:A:234:ILE:CG2	2.16	0.75
3:S:39:GLN:O	3:S:92:ALA:HB1	1.86	0.75
1:B:353:TRP:HD1	1:B:353:TRP:H	1.33	0.75
4:J:35:ASN:HA	4:J:50:TYR:HA	1.68	0.75
2:Q:22:CYS:HB2	2:Q:36:TRP:CH2	2.22	0.75
1:A:533:VAL:HG11	1:A:538:VAL:HG11	1.69	0.74
1:A:990:GLU:HA	1:A:993:ILE:HG22	1.66	0.74
3:E:108:GLU:C	3:E:110:LEU:H	1.91	0.74
5:G:2:ILE:HG23	5:G:27:GLN:HG2	1.69	0.74
2:H:22:CYS:HB2	2:H:36:TRP:CH2	2.22	0.74
3:I:106:PHE:HB3	3:I:109:SER:HB3	1.69	0.74
4:J:34:LEU:CD1	4:J:52:ALA:HB2	2.17	0.74
1:B:869:MET:C	1:B:871:ALA:H	1.89	0.74
2:H:55:PHE:HD1	2:H:74:GLU:HG3	1.51	0.74
1:B:496:PHE:HB2	1:B:505:GLN:HA	1.69	0.74
4:R:56:GLU:HG3	4:R:57:THR:N	2.03	0.74
2:H:12:LYS:HB2	2:H:123:VAL:CG1	2.15	0.74
1:C:558:PHE:CD2	1:C:576:ARG:HG3	2.22	0.74
2:H:111:GLY:HA3	4:J:50:TYR:CD2	2.23	0.74
1:B:370:ASN:HB2	4:R:94:PRO:HG3	1.67	0.74
5:K:2:ILE:HG23	5:K:27:GLN:HG2	1.69	0.74
1:A:371:PHE:HB2	1:A:374:PHE:CD2	2.23	0.74
4:J:16:VAL:HG13	4:J:107:LYS:HB2	1.68	0.74
1:C:424:LYS:HB2	1:C:461:LEU:HD12	1.69	0.74
1:C:726:ILE:HG13	1:C:1061:VAL:HG22	1.69	0.74
2:H:110:ASP:O	4:J:51:ASP:HB3	1.87	0.74
1:C:371:PHE:HB2	1:C:374:PHE:CD2	2.23	0.74
1:C:438:SER:HB2	1:C:508:ARG:CD	2.17	0.74
2:Q:24:ALA:HB3	2:Q:77:SER:HB3	1.68	0.74
1:A:343:ASN:HA	2:D:53:PRO:CB	2.14	0.74
1:A:545:LEU:HG	1:A:572:THR:HG21	1.68	0.74
1:A:554:SER:HB3	1:A:583:ILE:HG13	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:85:ALA:HB3	4:J:87:TYR:CE2	2.23	0.73
1:A:408:SER:C	1:A:410:ILE:N	2.38	0.73
2:Q:53:PRO:HG2	2:Q:58:THR:O	1.88	0.73
3:S:100:TYR:HA	3:S:114:PHE:CD2	2.23	0.73
4:F:85:ALA:HB3	4:F:87:TYR:CE2	2.23	0.73
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.35	0.73
1:B:336:CYS:SG	1:B:338:PHE:HB2	2.28	0.73
1:B:1110:TYR:CZ	1:B:1112:PRO:HG3	2.23	0.73
2:D:37:VAL:HG22	2:D:47:TRP:HA	1.69	0.73
1:A:188:ASN:H	1:A:211:ILE:HG12	1.54	0.73
1:A:355:ARG:CD	1:A:396:TYR:HB3	2.19	0.73
4:J:6:THR:H	4:J:25:GLN:HB3	1.53	0.73
2:D:100:PHE:HB2	2:D:111:GLY:O	1.88	0.73
1:B:378:LYS:HG2	1:B:380:TYR:CE2	2.23	0.73
2:D:37:VAL:HB	2:D:115:TRP:CZ3	2.24	0.73
1:A:614:VAL:HG11	1:A:619:VAL:HG13	1.70	0.73
1:B:805:ILE:HB	1:B:1054:GLN:HE22	1.52	0.73
4:R:85:ALA:HB3	4:R:87:TYR:CE2	2.23	0.73
1:A:472:ILE:HG22	1:A:483:LYS:HE3	1.69	0.73
1:B:616:CYS:HA	1:B:648:CYS:CB	2.16	0.73
1:C:497:ARG:HB3	1:C:498:PRO:HD2	1.71	0.73
3:S:100:TYR:HA	3:S:114:PHE:CG	2.24	0.73
1:A:356:THR:HB	1:A:397:ALA:HB3	1.71	0.73
4:R:16:VAL:HG12	4:R:81:PRO:HG3	1.69	0.73
1:C:27:SER:HB2	1:C:64:TRP:HB3	1.70	0.72
3:E:32:TYR:HB3	3:E:100:TYR:CE1	2.23	0.72
1:B:359:SER:HB3	1:B:394:ASN:HB2	1.70	0.72
1:C:1132:ILE:O	1:C:1133:VAL:HG23	1.89	0.72
5:T:49:ILE:HD11	5:T:63:PHE:O	1.89	0.72
1:A:360:ASN:HA	1:A:523:VAL:HA	1.70	0.72
1:C:556:LYS:HB2	1:C:583:ILE:HD13	1.71	0.72
2:Q:55:PHE:HD1	2:Q:74:GLU:HG3	1.52	0.72
2:Q:99:LEU:HA	2:Q:112:PHE:CE1	2.22	0.72
5:T:21:LEU:HD21	5:T:87:TYR:HB2	1.71	0.72
5:K:23:CYS:HB3	5:K:34:LEU:HD21	1.71	0.72
1:B:770:ILE:O	1:B:774:GLN:HG2	1.89	0.72
2:Q:105:PRO:HB3	2:Q:110:ASP:HB2	1.71	0.72
2:H:48:MET:HE1	2:H:94:TYR:HD1	1.53	0.72
1:B:409:GLN:HA	3:S:54:TYR:CZ	2.25	0.72
4:F:35:ASN:H	4:F:51:ASP:HA	1.55	0.72
2:H:34:ILE:O	2:H:54:LEU:HD13	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:32:HIS:HA	2:Q:55:PHE:CB	2.20	0.72
5:G:56:ALA:N	5:G:59:ILE:HG13	2.03	0.72
1:C:115:GLN:HA	1:C:131:CYS:O	1.90	0.72
1:C:392:PHE:HB3	1:C:516:LEU:HD22	1.72	0.72
1:C:474:GLN:HA	1:C:480:CYS:HB2	1.69	0.72
1:A:452:TRP:HB3	1:A:491:LEU:HD13	1.70	0.72
1:B:620:SER:HB3	1:B:623:ILE:HA	1.72	0.72
4:J:65:GLY:HA3	4:J:74:PHE:CD2	2.25	0.72
1:B:353:TRP:O	1:B:354:ASN:HB3	1.90	0.72
1:B:1070:ALA:O	1:B:1071:GLN:C	2.27	0.72
1:C:129:LYS:HB2	1:C:133:PHE:CZ	2.24	0.72
1:C:328:ARG:CG	1:C:542:PHE:HB2	2.20	0.72
1:C:1143:LEU:O	1:C:1146:ASP:HB2	1.89	0.72
4:F:34:LEU:HD11	4:F:72:PHE:CG	2.25	0.72
2:H:99:LEU:HD11	4:J:96:TYR:CE2	2.24	0.72
5:K:40:LYS:HG3	5:K:85:ALA:HB2	1.72	0.72
1:C:836:GLN:HB3	1:C:849:LEU:HD21	1.72	0.71
2:D:100:PHE:HB3	2:D:110:ASP:HB3	1.72	0.71
4:J:40:LYS:HB2	4:J:43:LYS:HE2	1.69	0.71
1:B:442:ASP:HB3	1:B:448:ASN:CG	2.11	0.71
5:T:38:GLN:HB2	5:T:87:TYR:CE2	2.25	0.71
5:K:51:GLY:H	5:K:92:HIS:HE1	1.37	0.71
1:B:462:LYS:HZ3	1:B:465:GLU:HG3	1.55	0.71
1:B:673:TYR:CD2	1:B:690:GLN:HG2	2.25	0.71
5:T:49:ILE:HA	5:T:55:ARG:HA	1.72	0.71
2:D:70:ILE:HA	2:D:81:MET:HA	1.73	0.71
1:C:105:ILE:O	1:C:237:PHE:HA	1.90	0.71
2:H:12:LYS:HB2	2:H:123:VAL:HA	1.72	0.71
1:A:1029:MET:HE2	1:A:1062:PHE:CE1	2.25	0.71
1:B:434:ILE:O	1:B:509:VAL:HA	1.90	0.71
4:F:65:GLY:HA3	4:F:74:PHE:CD2	2.25	0.71
1:B:133:PHE:CD2	1:B:163:ALA:HB3	2.25	0.71
3:S:44:GLY:HA2	5:T:88:TYR:CE2	2.26	0.71
3:S:93:VAL:HA	3:S:122:LEU:HA	1.71	0.71
5:T:62:ARG:HA	5:T:77:SER:HB2	1.71	0.71
2:H:12:LYS:O	2:H:13:LYS:HB2	1.90	0.71
1:A:213:ARG:HD2	1:A:216:PRO:HA	1.72	0.71
1:A:1081:ILE:HD12	1:A:1115:ILE:HD13	1.73	0.71
4:R:50:TYR:HB2	4:R:54:HIS:O	1.91	0.71
3:E:93:VAL:HA	3:E:122:LEU:HA	1.71	0.71
1:B:372:ALA:HB1	1:B:373:PRO:HD2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:THR:HG23	1:C:210:ILE:HD12	1.72	0.71
2:Q:99:LEU:HA	2:Q:112:PHE:CD1	2.26	0.71
4:F:35:ASN:HB2	4:F:90:GLN:HG2	1.72	0.71
3:I:72:THR:HB	3:I:79:GLY:HA2	1.73	0.71
1:B:438:SER:H	1:B:441:LEU:HB3	1.54	0.70
1:C:537:CYS:O	1:C:538:VAL:C	2.29	0.70
4:R:16:VAL:HA	4:R:81:PRO:HD3	1.73	0.70
3:E:72:THR:HB	3:E:79:GLY:HA2	1.73	0.70
2:H:12:LYS:CB	2:H:123:VAL:HA	2.21	0.70
1:A:557:LYS:HG3	1:B:282:ASN:HB3	1.73	0.70
4:R:65:GLY:HA3	4:R:74:PHE:CD2	2.25	0.70
2:H:102:ASN:HA	2:H:109:GLU:CB	2.22	0.70
1:A:477:ASN:N	1:A:482:GLY:HA2	2.06	0.70
1:A:561:PHE:CE1	1:B:224:PRO:HG2	2.26	0.70
1:B:540:PHE:CD2	1:B:551:LEU:HD21	2.26	0.70
5:G:11:LEU:HB2	5:G:104:VAL:HG13	1.74	0.70
1:B:474:GLN:CB	1:B:484:GLY:HA2	2.21	0.70
1:B:858:LEU:HD11	1:B:963:VAL:HG22	1.72	0.70
2:Q:47:TRP:CH2	2:Q:51:PHE:HA	2.26	0.70
2:Q:54:LEU:HG	2:Q:99:LEU:HD22	1.74	0.70
3:S:102:ARG:NH2	3:S:114:PHE:HA	2.07	0.70
4:R:67:GLY:HA3	4:R:72:PHE:HA	1.74	0.70
3:I:93:VAL:HA	3:I:122:LEU:HA	1.71	0.70
1:A:225:LEU:O	1:A:226:VAL:HB	1.91	0.70
1:B:736:VAL:HG21	1:B:1004:LEU:HD21	1.74	0.70
2:Q:38:ARG:HB2	2:Q:94:TYR:CE1	2.26	0.70
2:Q:102:ASN:CA	2:Q:109:GLU:HB2	2.21	0.70
1:A:340:GLU:HG2	1:A:341:VAL:HG13	1.73	0.70
1:C:747:THR:HG21	1:C:977:LEU:HD13	1.73	0.70
2:Q:55:PHE:HA	2:Q:74:GLU:OE1	1.91	0.70
4:F:18:ASP:O	4:F:79:LEU:HB2	1.92	0.70
2:H:52:ILE:HG22	2:H:101:PRO:HB2	1.74	0.70
1:B:117:LEU:HB2	1:B:234:ILE:HD11	1.74	0.70
1:B:142:ASP:HB3	1:B:241:LEU:HD23	1.72	0.70
2:Q:99:LEU:O	2:Q:100:PHE:HB2	1.89	0.70
3:S:107:GLY:HA2	3:S:111:ILE:HG12	1.72	0.70
4:F:56:GLU:HB3	4:F:60:PRO:HG2	1.72	0.70
5:K:17:GLU:H	5:K:79:LEU:HB2	1.56	0.70
5:K:35:ALA:HB1	5:K:47:LEU:HD13	1.74	0.70
1:A:115:GLN:HG3	1:A:165:ASN:HB2	1.74	0.70
1:C:93:ALA:O	1:C:94:SER:HB3	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:PRO:HG3	1:C:692:ILE:HD11	1.74	0.70
2:Q:59:ILE:HG23	2:Q:60:TYR:H	1.56	0.70
1:B:382:VAL:HG22	1:B:431:GLY:HA2	1.73	0.69
1:B:435:ALA:HA	1:B:508:ARG:O	1.92	0.69
1:B:437:ASN:HD22	1:B:508:ARG:N	1.90	0.69
4:J:67:GLY:HA3	4:J:72:PHE:HA	1.74	0.69
1:A:530:THR:HG22	1:A:531:ASN:H	1.57	0.69
1:A:770:ILE:HD11	1:A:1012:LEU:HG	1.74	0.69
2:D:101:PRO:HA	4:F:92:TYR:CD2	2.26	0.69
5:K:46:ARG:HH22	5:K:59:ILE:HD12	1.56	0.69
1:B:345:THR:N	2:Q:104:ASP:HA	2.06	0.69
1:B:350:VAL:C	1:B:352:ALA:H	1.95	0.69
3:I:108:GLU:C	3:I:110:LEU:H	1.93	0.69
5:K:48:LEU:HD12	5:K:49:ILE:HD12	1.74	0.69
1:B:112:SER:HB3	1:B:164:ASN:HD22	1.56	0.69
1:B:485:PRO:HD2	1:B:488:TYR:CD2	2.27	0.69
5:T:11:LEU:HD12	5:T:12:SER:H	1.58	0.69
5:T:56:ALA:HB3	5:T:59:ILE:HD11	1.73	0.69
3:I:2:VAL:HG22	3:I:27:TYR:HB3	1.73	0.69
1:A:518:HIS:ND1	1:A:518:HIS:N	2.41	0.69
2:Q:18:VAL:HG11	2:Q:121:VAL:HG11	1.74	0.69
3:S:72:THR:HB	3:S:79:GLY:HA2	1.73	0.69
5:G:19:ALA:HB3	5:G:76:ILE:HB	1.75	0.69
3:S:101:THR:O	3:S:114:PHE:HB3	1.93	0.69
2:D:18:VAL:HG12	2:D:83:LEU:HB2	1.74	0.69
2:D:64:PHE:HE1	2:D:68:VAL:HG23	1.58	0.69
2:H:51:PHE:CD1	2:H:59:ILE:HB	2.27	0.69
1:B:112:SER:C	1:B:132:GLU:HB3	2.13	0.69
1:C:57:PRO:O	1:C:60:SER:HB3	1.93	0.69
1:C:504:HIS:CD2	3:I:31:SER:HB3	2.28	0.69
3:I:19:LYS:HG2	3:I:82:GLU:HB3	1.74	0.69
1:B:95:THR:HB	1:B:186:PHE:CD2	2.27	0.69
1:B:236:ARG:HG3	1:B:237:PHE:H	1.58	0.69
1:B:496:PHE:HA	1:B:500:TYR:CD2	2.27	0.69
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.75	0.69
1:C:909:ILE:HD13	1:C:1049:LEU:HD21	1.75	0.69
4:R:6:THR:O	4:R:8:SER:N	2.25	0.69
2:D:34:ILE:H	2:D:99:LEU:CB	2.05	0.69
5:G:33:SER:O	5:G:34:LEU:HB2	1.93	0.69
1:A:375:PHE:HZ	3:E:54:TYR:HD2	1.40	0.69
1:A:409:GLN:HB3	1:A:418:ILE:HB	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ASP:HB3	1:B:448:ASN:OD1	1.93	0.69
2:Q:104:ASP:N	2:Q:105:PRO:HD2	2.08	0.69
1:B:345:THR:HA	2:Q:32:HIS:NE2	2.08	0.69
3:S:113:GLY:HA2	5:T:47:LEU:HD13	1.72	0.69
3:I:12:LYS:HE3	3:I:18:VAL:HB	1.75	0.69
1:A:361:CYS:O	1:A:362:VAL:C	2.30	0.68
1:A:421:TYR:HB3	1:A:457:ARG:CB	2.23	0.68
1:A:447:GLY:HA2	1:A:497:ARG:CZ	2.23	0.68
1:A:469:SER:C	1:A:471:GLU:H	1.96	0.68
5:T:79:LEU:HD13	5:T:84:PHE:HE1	1.58	0.68
1:A:336:CYS:HB3	1:A:364:ASP:H	1.58	0.68
1:A:421:TYR:HB3	1:A:457:ARG:HB3	1.75	0.68
1:A:558:PHE:O	1:A:562:GLN:HB2	1.94	0.68
1:B:37:TYR:HB3	1:B:193:VAL:HG11	1.75	0.68
1:B:95:THR:HB	1:B:186:PHE:HD2	1.58	0.68
3:S:19:LYS:HG2	3:S:82:GLU:HB3	1.73	0.68
2:D:36:TRP:HA	2:D:96:CYS:HA	1.75	0.68
3:E:102:ARG:HB3	3:E:111:ILE:HA	1.74	0.68
1:A:194:PHE:HD1	1:A:203:ILE:HG23	1.57	0.68
1:C:471:GLU:H	1:C:490:PRO:HG3	1.56	0.68
1:C:558:PHE:HD2	1:C:576:ARG:HG3	1.58	0.68
2:H:55:PHE:CD1	2:H:74:GLU:HG3	2.28	0.68
1:A:193:VAL:HG13	1:A:270:LEU:HD11	1.76	0.68
1:A:849:LEU:HD12	1:A:851:CYS:H	1.56	0.68
2:D:100:PHE:HB3	2:D:111:GLY:H	1.58	0.68
4:F:67:GLY:HA3	4:F:72:PHE:HA	1.74	0.68
1:B:25:THR:H	1:B:66:HIS:HB3	1.57	0.68
1:B:869:MET:O	1:B:871:ALA:N	2.27	0.68
1:B:1125:ASN:O	1:B:1127:ASP:N	2.27	0.68
1:C:355:ARG:CA	1:C:398:ASP:HA	2.23	0.68
1:A:752:LEU:HD21	1:A:990:GLU:HB3	1.75	0.68
1:B:821:LEU:HD21	1:B:939:PHE:HB2	1.74	0.68
2:H:32:HIS:HA	2:H:55:PHE:CB	2.23	0.68
1:A:353:TRP:CD1	1:A:466:ARG:HD3	2.29	0.68
1:A:398:ASP:HB2	1:A:511:VAL:HG23	1.76	0.68
1:A:703:ASN:O	1:B:789:TYR:HA	1.93	0.68
2:Q:48:MET:HG2	2:Q:68:VAL:HG11	1.76	0.68
2:D:54:LEU:HD12	2:D:55:PHE:H	1.56	0.68
2:H:13:LYS:H	2:H:123:VAL:CG1	2.07	0.68
2:H:29:PHE:HA	2:H:30:ARG:NH1	2.09	0.68
1:B:36:VAL:HG21	1:B:219:PHE:CZ	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:VAL:O	1:A:707:TYR:N	2.26	0.68
1:B:87:ASN:HB3	1:B:269:TYR:CE1	2.29	0.68
3:S:30:THR:HA	3:S:53:THR:HB	1.76	0.68
4:F:15:SER:HB2	4:F:106:ILE:CD1	2.24	0.68
2:H:105:PRO:HD3	2:H:110:ASP:HB2	1.75	0.68
3:I:2:VAL:HG13	3:I:27:TYR:CD2	2.29	0.68
1:A:488:TYR:HD1	1:A:489:PHE:H	1.41	0.67
1:C:577:ASP:HB2	1:C:582:GLU:CB	2.22	0.67
4:F:12:LEU:HD22	4:F:20:VAL:HG13	1.76	0.67
3:E:115:ASP:HA	3:E:117:TRP:HD1	1.59	0.67
2:H:49:GLY:HA2	2:H:60:TYR:H	1.58	0.67
3:I:51:ILE:O	3:I:52:SER:C	2.32	0.67
4:J:47:LEU:HD21	4:J:50:TYR:HB3	1.75	0.67
1:A:444:LYS:H	1:A:448:ASN:HB2	1.59	0.67
1:A:1115:ILE:HG23	1:A:1120:THR:HG21	1.76	0.67
1:B:133:PHE:H	1:B:164:ASN:HB2	1.59	0.67
1:C:91:TYR:O	1:C:92:PHE:HB2	1.94	0.67
1:C:291:CYS:O	1:C:292:ALA:C	2.31	0.67
1:C:522:THR:HG23	1:C:523:VAL:H	1.59	0.67
4:F:19:ARG:HG2	4:F:77:SER:HA	1.75	0.67
3:I:2:VAL:HG11	3:I:98:ARG:HD2	1.75	0.67
1:B:474:GLN:CB	1:B:485:PRO:HD3	2.23	0.67
1:C:21:LEU:HD13	1:C:22:ILE:H	1.60	0.67
4:R:34:LEU:HD23	4:R:35:ASN:H	1.58	0.67
1:A:497:ARG:HG3	1:A:498:PRO:HD2	1.76	0.67
1:A:712:ILE:HD13	1:A:1094:VAL:HG21	1.76	0.67
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	1.75	0.67
1:B:564:PHE:HE1	1:C:41:LYS:HD3	1.59	0.67
1:C:399:SER:HB3	1:C:510:VAL:HA	1.76	0.67
1:C:576:ARG:HG2	1:C:582:GLU:O	1.95	0.67
2:H:72:ALA:HB1	2:H:79:ALA:HA	1.76	0.67
1:A:835:LYS:HD2	1:C:645:ARG:HH12	1.59	0.67
3:E:98:ARG:HA	3:E:100:TYR:CZ	2.30	0.67
2:H:78:THR:HB	2:H:80:TYR:CE1	2.29	0.67
3:I:14:PRO:HG3	3:I:125:VAL:HB	1.75	0.67
1:B:805:ILE:HD12	1:B:878:LEU:HD21	1.77	0.67
1:C:616:CYS:HB2	1:C:643:GLN:CG	2.25	0.67
5:T:50:TYR:CZ	5:T:56:ALA:HA	2.30	0.67
5:K:47:LEU:HD21	5:K:50:TYR:HD2	1.59	0.67
5:G:6:GLN:HG3	5:G:100:GLY:H	1.60	0.67
1:A:193:VAL:HG23	1:A:222:LEU:HD23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:TYR:HA	1:A:457:ARG:HH11	1.60	0.67
1:B:120:VAL:HG22	1:B:121:ASN:H	1.58	0.67
1:B:1129:VAL:HG13	1:C:917:TYR:HB3	1.77	0.67
4:R:22:ILE:HG13	4:R:36:TRP:CZ3	2.30	0.67
5:K:6:GLN:HG2	5:K:100:GLY:H	1.58	0.67
1:B:330:PRO:HA	1:B:579:GLN:HE22	1.59	0.67
1:B:338:PHE:CZ	1:B:363:ALA:HB1	2.30	0.67
1:B:558:PHE:HZ	1:B:574:ALA:CB	2.08	0.67
1:B:986:PRO:HB2	1:B:987:PRO:HD3	1.77	0.67
1:C:396:TYR:HD1	1:C:396:TYR:H	1.43	0.67
1:C:534:LYS:O	1:C:535:ASN:C	2.33	0.67
4:R:9:PRO:C	4:R:11:SER:N	2.46	0.67
3:E:47:TRP:CH2	5:G:95:SER:HB3	2.30	0.67
5:G:48:LEU:HB2	5:G:49:ILE:HD12	1.76	0.67
1:A:214:ASP:HB2	1:A:266:TYR:CE1	2.30	0.66
1:B:876:ALA:O	1:B:877:LEU:HB2	1.94	0.66
1:C:368:LEU:HA	1:C:371:PHE:CZ	2.30	0.66
1:C:375:PHE:O	3:I:55:ASN:HB3	1.94	0.66
1:C:501:GLY:N	1:C:505:GLN:HG3	2.11	0.66
4:R:24:CYS:O	4:R:71:ASP:HA	1.95	0.66
4:J:86:THR:O	4:J:102:THR:N	2.25	0.66
1:A:722:VAL:HG23	1:A:930:ALA:HB3	1.77	0.66
1:C:357:ARG:HG2	1:C:358:ILE:H	1.60	0.66
1:C:460:LYS:HG3	1:C:461:LEU:N	2.11	0.66
1:C:615:ASN:O	1:C:617:THR:N	2.28	0.66
5:T:36:TRP:HB3	5:T:48:LEU:HD12	1.76	0.66
1:A:336:CYS:C	1:A:338:PHE:H	1.98	0.66
1:B:133:PHE:CD2	1:B:136:CYS:HB3	2.29	0.66
1:B:500:TYR:CD2	1:B:504:HIS:HD2	2.13	0.66
1:C:357:ARG:HH22	1:C:359:SER:HB3	1.60	0.66
2:D:54:LEU:HD11	2:D:99:LEU:CG	2.24	0.66
1:A:556:LYS:HG2	1:B:847:ARG:CZ	2.25	0.66
2:D:25:SER:C	2:D:27:GLY:H	1.98	0.66
3:E:4:LEU:HD11	3:E:98:ARG:HG3	1.77	0.66
2:H:97:ALA:HB2	2:H:115:TRP:CE3	2.29	0.66
3:I:34:ILE:H	3:I:100:TYR:HD2	1.42	0.66
1:A:410:ILE:HD11	1:A:423:TYR:CD1	2.30	0.66
1:B:707:TYR:HB2	1:C:883:THR:HG23	1.78	0.66
1:C:408:SER:HB3	1:C:509:VAL:HG11	1.77	0.66
1:C:416:GLY:O	1:C:420:ASP:HB2	1.95	0.66
2:H:6:GLN:H	2:H:117:GLN:CD	1.99	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13:LYS:HB3	2:H:16:SER:OG	1.96	0.66
3:I:12:LYS:HA	3:I:12:LYS:HE2	1.76	0.66
4:J:93:ASP:O	4:J:95:SER:N	2.28	0.66
1:A:429:PHE:HD1	1:A:430:THR:N	1.93	0.66
1:B:193:VAL:CG1	1:B:204:TYR:HB2	2.25	0.66
1:B:619:VAL:HG21	1:B:650:ILE:HD11	1.77	0.66
1:C:371:PHE:HB2	1:C:374:PHE:HD2	1.60	0.66
2:Q:35:SER:HB2	2:Q:49:GLY:HA3	1.78	0.66
3:S:98:ARG:HG3	3:S:116:ASN:HB2	1.76	0.66
5:T:34:LEU:HD21	5:T:36:TRP:CD1	2.30	0.66
1:A:316:SER:HB2	1:A:633:ARG:HD2	1.77	0.66
1:B:395:VAL:HA	1:B:514:PHE:HA	1.77	0.66
2:Q:6:GLN:H	2:Q:117:GLN:CD	1.99	0.66
2:D:99:LEU:HD21	4:F:96:TYR:OH	1.95	0.66
4:F:57:THR:O	4:F:60:PRO:HD2	1.96	0.66
5:G:7:SER:CB	5:G:8:PRO:HD2	2.26	0.66
1:A:194:PHE:CD1	1:A:203:ILE:HG23	2.30	0.66
1:A:326:ILE:CG2	1:A:533:VAL:HG23	2.25	0.66
1:C:120:VAL:HG22	1:C:122:ASN:HD22	1.60	0.66
2:D:99:LEU:HD22	2:D:101:PRO:HG2	1.77	0.66
2:H:51:PHE:HE1	2:H:58:THR:H	1.42	0.66
2:H:102:ASN:ND2	4:J:32:ASN:HB3	2.11	0.66
1:A:391:CYS:CB	1:A:524:CYS:HA	2.26	0.66
1:A:438:SER:HB3	1:A:508:ARG:HD2	1.77	0.66
1:B:226:VAL:HG11	1:B:228:LEU:HD22	1.77	0.66
1:C:462:LYS:HG2	1:C:465:GLU:HG3	1.78	0.66
4:R:3:ILE:HG13	4:R:97:THR:HG21	1.76	0.66
2:D:35:SER:HB2	2:D:99:LEU:HD23	1.77	0.66
2:H:12:LYS:HE2	2:H:13:LYS:CG	2.26	0.66
1:A:64:TRP:NE1	1:A:214:ASP:HB3	2.11	0.66
1:A:444:LYS:HZ1	1:A:445:HIS:H	1.43	0.66
1:B:354:ASN:HD22	1:B:399:SER:H	1.45	0.66
1:B:616:CYS:HB2	1:B:643:GLN:OE1	1.96	0.66
1:B:707:TYR:HB3	1:C:792:PRO:HG3	1.77	0.66
1:C:1104:VAL:CG2	1:C:1115:ILE:HG22	2.26	0.66
2:Q:25:SER:C	2:Q:27:GLY:H	1.98	0.66
2:Q:39:GLN:NE2	2:Q:45:LEU:HG	2.10	0.66
1:A:197:ILE:HB	1:A:202:LYS:HE3	1.77	0.65
1:A:1048:HIS:HE1	1:A:1051:SER:OG	1.79	0.65
1:B:566:ARG:HB2	1:C:42:VAL:CG1	2.25	0.65
1:C:463:PRO:O	1:C:464:PHE:HB2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:37:VAL:HG11	3:S:117:TRP:HH2	1.61	0.65
5:T:29:VAL:HG22	5:T:33:SER:CB	2.25	0.65
2:D:36:TRP:H	2:D:36:TRP:HD1	1.42	0.65
4:J:91:ARG:CZ	4:J:91:ARG:HB2	2.27	0.65
1:B:56:LEU:HD22	1:B:57:PRO:HD2	1.78	0.65
1:B:115:GLN:HG3	1:B:130:VAL:HG12	1.75	0.65
1:B:133:PHE:HD2	1:B:136:CYS:HB3	1.61	0.65
1:C:406:GLU:CB	1:C:409:GLN:HB2	2.26	0.65
1:C:448:ASN:HD21	1:C:451:TYR:HE2	1.44	0.65
5:T:38:GLN:HE21	5:T:85:ALA:HB3	1.61	0.65
5:T:59:ILE:HG22	5:T:63:PHE:CD1	2.31	0.65
2:H:25:SER:C	2:H:27:GLY:H	1.98	0.65
1:A:469:SER:O	1:A:471:GLU:N	2.30	0.65
1:B:318:PHE:CD1	1:B:631:THR:HG22	2.31	0.65
1:B:401:VAL:HG11	1:B:448:ASN:HD21	1.61	0.65
1:B:472:ILE:HB	1:B:483:LYS:HG3	1.78	0.65
1:B:833:PHE:HE2	1:B:851:CYS:HB2	1.60	0.65
2:Q:98:ARG:N	2:Q:114:ILE:O	2.30	0.65
1:B:356:THR:CB	1:B:396:TYR:HB2	2.26	0.65
1:B:408:SER:C	1:B:410:ILE:H	2.00	0.65
2:D:6:GLN:H	2:D:117:GLN:CD	1.99	0.65
2:D:20:VAL:HG11	2:D:94:TYR:CE1	2.31	0.65
4:F:34:LEU:HD23	4:F:52:ALA:HB2	1.77	0.65
1:A:497:ARG:HB3	1:A:499:THR:HB	1.78	0.65
1:A:502:VAL:HG23	5:G:92:HIS:CE1	2.32	0.65
1:C:447:GLY:HA3	1:C:449:TYR:CZ	2.31	0.65
1:C:993:ILE:HG23	1:C:997:ILE:HD13	1.78	0.65
1:A:661:CYS:HA	1:A:695:TYR:HE2	1.62	0.65
1:B:370:ASN:HB2	4:R:94:PRO:CG	2.26	0.65
5:T:39:GLN:HG3	5:T:45:PRO:HG3	1.79	0.65
3:I:50:TRP:HB3	3:I:59:ASN:H	1.61	0.65
1:B:448:ASN:C	1:B:450:ASP:H	1.98	0.65
1:C:171:VAL:HG22	1:C:172:SER:H	1.60	0.65
3:S:23:LYS:HE2	3:S:77:THR:HB	1.79	0.65
4:F:60:PRO:HA	4:F:63:PHE:CG	2.32	0.65
1:A:23:THR:HA	1:A:80:ASP:HA	1.79	0.65
1:A:429:PHE:HD1	1:A:430:THR:H	1.45	0.65
1:B:916:LEU:HD12	1:B:923:ILE:HG21	1.78	0.65
2:H:34:ILE:N	2:H:99:LEU:HB2	2.12	0.65
2:H:59:ILE:HG23	2:H:61:ALA:H	1.62	0.65
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:ASN:O	1:C:540:PHE:C	2.34	0.65
2:D:51:PHE:N	2:D:51:PHE:HD1	1.95	0.65
5:G:49:ILE:CA	5:G:55:ARG:HA	2.26	0.65
3:I:4:LEU:HD13	3:I:22:CYS:SG	2.37	0.65
4:J:92:TYR:O	4:J:93:ASP:HB2	1.97	0.65
5:K:35:ALA:HB2	5:K:92:HIS:NE2	2.12	0.65
1:A:452:TRP:CE3	1:A:491:LEU:HB3	2.30	0.65
1:A:964:LYS:HD3	1:C:569:VAL:HG12	1.78	0.65
1:B:265:TYR:O	1:B:267:VAL:HG23	1.96	0.65
1:B:448:ASN:C	1:B:450:ASP:N	2.48	0.65
1:C:460:LYS:HG3	1:C:461:LEU:H	1.60	0.65
1:C:616:CYS:HB2	1:C:643:GLN:HG2	1.78	0.65
1:C:1057:PRO:O	1:C:1058:HIS:HB2	1.97	0.65
2:D:54:LEU:CD1	2:D:55:PHE:H	2.10	0.65
1:A:668:GLY:O	1:A:697:MET:HG2	1.96	0.64
1:B:519:ALA:HB1	1:B:520:PRO:HD2	1.77	0.64
1:B:805:ILE:HB	1:B:1054:GLN:NE2	2.12	0.64
1:C:428:ASP:O	1:C:429:PHE:C	2.36	0.64
2:Q:109:GLU:HG3	4:R:92:TYR:HD2	1.62	0.64
3:S:4:LEU:HD13	3:S:22:CYS:SG	2.37	0.64
3:S:107:GLY:H	3:S:111:ILE:HD11	1.61	0.64
1:A:501:GLY:O	1:A:505:GLN:HG3	1.96	0.64
1:A:972:ALA:HA	1:A:992:GLN:NE2	2.12	0.64
1:B:204:TYR:HA	1:B:224:PRO:HA	1.78	0.64
1:B:318:PHE:CE1	1:B:631:THR:HG22	2.33	0.64
1:B:455:LEU:H	1:B:492:GLN:HB2	1.62	0.64
1:B:800:PHE:HD2	1:B:927:PHE:HD2	1.45	0.64
1:C:615:ASN:HA	1:C:643:GLN:NE2	2.13	0.64
2:D:4:LEU:HD12	2:D:96:CYS:HB2	1.79	0.64
5:G:55:ARG:HB2	5:G:59:ILE:CG1	2.26	0.64
4:J:34:LEU:HD23	4:J:72:PHE:CD2	2.32	0.64
1:A:722:VAL:HG21	1:A:931:ILE:HG12	1.78	0.64
1:C:319:ARG:HB2	1:C:632:TRP:HE3	1.60	0.64
1:C:330:PRO:C	1:C:579:GLN:HB2	2.17	0.64
1:C:578:PRO:O	1:C:579:GLN:C	2.36	0.64
5:G:34:LEU:HD22	5:G:72:PHE:HB2	1.78	0.64
2:H:36:TRP:O	2:H:48:MET:HB2	1.97	0.64
1:A:834:ILE:HD11	1:C:647:GLY:HA2	1.80	0.64
1:B:353:TRP:CH2	1:B:465:GLU:HB3	2.32	0.64
1:B:453:TYR:CE2	1:B:492:GLN:HB3	2.32	0.64
1:C:505:GLN:HB3	1:C:506:PRO:HD2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577:ASP:CB	1:C:582:GLU:HB2	2.25	0.64
5:G:48:LEU:O	5:G:56:ALA:HB2	1.98	0.64
3:I:35:SER:N	3:I:97:ALA:HB1	2.12	0.64
1:A:1057:PRO:O	1:A:1058:HIS:HB2	1.97	0.64
1:C:1083:HIS:HB2	1:C:1137:VAL:HG23	1.78	0.64
3:I:101:THR:H	3:I:114:PHE:HA	1.61	0.64
1:A:806:LEU:HA	1:A:878:LEU:HD21	1.78	0.64
1:B:193:VAL:HG23	1:B:270:LEU:HD21	1.79	0.64
1:B:312:ILE:HG13	1:B:595:SER:HB2	1.80	0.64
1:B:811:LYS:HG2	1:B:812:PRO:HD2	1.79	0.64
5:T:32:THR:O	5:T:92:HIS:HB2	1.98	0.64
3:I:23:LYS:HE2	3:I:77:THR:HB	1.79	0.64
3:I:30:THR:HA	3:I:53:THR:HB	1.79	0.64
4:J:38:GLN:HB3	4:J:48:LEU:HD13	1.79	0.64
1:A:128:ILE:HG12	1:A:170:TYR:HB3	1.79	0.64
1:B:381:GLY:HA3	1:B:429:PHE:HA	1.78	0.64
1:C:425:LEU:HD22	1:C:426:PRO:HD2	1.80	0.64
2:H:47:TRP:CZ2	2:H:51:PHE:HA	2.33	0.64
2:H:102:ASN:HD21	4:J:32:ASN:HB3	1.63	0.64
1:A:720:ILE:HG13	1:A:923:ILE:HG23	1.78	0.64
1:B:26:GLN:HE21	1:B:27:SER:H	1.44	0.64
1:B:353:TRP:HH2	1:B:461:LEU:HB3	1.62	0.64
1:B:973:ILE:HD13	1:B:984:LEU:HG	1.79	0.64
1:C:322:PRO:CB	1:C:537:CYS:HB3	2.27	0.64
5:G:56:ALA:HB3	5:G:59:ILE:HD11	1.77	0.64
5:K:19:ALA:HB3	5:K:76:ILE:HB	1.80	0.64
1:A:299:THR:O	1:A:303:LEU:HG	1.98	0.64
1:B:118:LEU:HB3	1:B:129:LYS:CB	2.27	0.64
1:C:420:ASP:HA	1:C:460:LYS:HD3	1.78	0.64
4:F:47:LEU:O	4:F:56:GLU:HG2	1.98	0.64
4:J:6:THR:HA	4:J:100:GLN:HE22	1.62	0.64
1:A:286:THR:O	1:A:287:ASP:HB2	1.97	0.64
1:A:396:TYR:HB2	1:A:513:SER:OG	1.97	0.64
1:B:342:PHE:HB3	1:B:371:PHE:HZ	1.63	0.64
1:B:343:ASN:HD22	1:B:343:ASN:N	1.95	0.64
1:C:444:LYS:HD3	1:C:446:SER:H	1.61	0.64
5:T:33:SER:HA	5:T:92:HIS:N	2.12	0.64
3:E:23:LYS:HE2	3:E:77:THR:HB	1.79	0.64
1:A:58:PHE:O	1:A:59:PHE:C	2.36	0.63
1:A:392:PHE:CD2	1:A:514:PHE:HB2	2.33	0.63
1:A:714:ILE:HD11	1:A:1094:VAL:HG11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ALA:N	1:B:414:GLN:HG2	2.13	0.63
1:C:338:PHE:HD2	1:C:364:ASP:C	2.01	0.63
2:Q:107:SER:HB2	2:Q:108:PRO:HD3	1.80	0.63
2:D:38:ARG:HH22	2:D:93:VAL:N	1.95	0.63
4:F:33:TYR:HA	4:F:91:ARG:CZ	2.28	0.63
4:J:6:THR:C	4:J:25:GLN:HB2	2.19	0.63
1:A:456:PHE:CE1	1:A:490:PRO:HA	2.32	0.63
1:B:359:SER:HB3	1:B:394:ASN:CB	2.28	0.63
1:B:414:GLN:HG3	3:S:54:TYR:CE2	2.33	0.63
1:B:981:LEU:HD21	1:B:989:ALA:HB1	1.80	0.63
1:C:380:TYR:CZ	1:C:412:PRO:HD3	2.33	0.63
2:D:51:PHE:CG	2:D:59:ILE:HB	2.32	0.63
4:F:7:GLN:HG2	4:F:25:GLN:HE21	1.63	0.63
4:F:59:VAL:HB	4:F:60:PRO:HD3	1.80	0.63
5:G:39:GLN:HB2	5:G:88:TYR:HE1	1.62	0.63
1:A:353:TRP:HZ2	1:A:461:LEU:HD22	1.62	0.63
1:C:502:VAL:CG1	3:I:100:TYR:CG	2.81	0.63
2:Q:102:ASN:HB2	4:R:93:ASP:N	2.14	0.63
3:E:95:TYR:HD2	3:E:117:TRP:HE3	1.47	0.63
1:A:462:LYS:HD3	1:A:463:PRO:HD2	1.80	0.63
1:B:95:THR:HB	1:B:186:PHE:HB3	1.79	0.63
1:B:371:PHE:HB2	1:B:374:PHE:CD2	2.33	0.63
1:C:197:ILE:HG13	1:C:202:LYS:HZ3	1.64	0.63
3:S:115:ASP:OD1	5:T:47:LEU:HB2	1.98	0.63
4:J:4:GLN:O	4:J:6:THR:N	2.31	0.63
1:B:620:SER:C	1:B:622:ALA:H	2.00	0.63
1:C:441:LEU:HD13	2:H:32:HIS:HB3	1.81	0.63
2:D:27:GLY:C	2:D:29:PHE:H	2.02	0.63
1:A:848:ASP:HB2	1:A:851:CYS:HB3	1.79	0.63
1:B:330:PRO:HA	1:B:579:GLN:NE2	2.13	0.63
1:C:436:TRP:CH2	1:C:510:VAL:HG23	2.33	0.63
5:T:79:LEU:HD21	5:T:104:VAL:HG11	1.81	0.63
3:E:67:ARG:NH2	3:E:85:ARG:HB2	2.13	0.63
1:B:804:GLN:O	1:B:818:ILE:HG13	1.99	0.63
1:B:981:LEU:CD2	1:B:989:ALA:HB1	2.28	0.63
1:C:376:ALA:HB3	1:C:435:ALA:HB3	1.79	0.63
2:H:102:ASN:HB2	4:J:93:ASP:N	2.14	0.63
1:B:113:LYS:HA	1:B:132:GLU:OE2	1.98	0.63
1:C:63:THR:O	1:C:64:TRP:HB2	1.99	0.63
4:R:16:VAL:HB	4:R:81:PRO:HD3	1.81	0.63
4:R:34:LEU:HD21	4:R:89:CYS:SG	2.39	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:50:TYR:C	5:T:52:ALA:H	2.02	0.63
2:H:93:VAL:HG22	2:H:120:LEU:HD13	1.80	0.63
5:K:35:ALA:HB2	5:K:92:HIS:CE1	2.34	0.63
1:A:718:PHE:HB3	1:A:1067:TYR:CE2	2.34	0.63
1:A:909:ILE:HD13	1:A:1049:LEU:HD21	1.80	0.63
1:B:57:PRO:HD3	1:B:271:GLN:OE1	1.99	0.63
1:B:620:SER:H	1:B:631:THR:HG21	1.62	0.63
1:B:914:ASN:O	1:B:918:GLU:HB2	1.99	0.63
1:C:805:ILE:O	1:C:816:SER:HB2	1.99	0.63
4:F:48:LEU:HD12	4:F:60:PRO:HG3	1.80	0.63
3:I:12:LYS:HG2	3:I:18:VAL:CG1	2.29	0.63
1:A:336:CYS:HB2	1:A:338:PHE:CD1	2.34	0.62
1:B:462:LYS:NZ	1:B:465:GLU:HG3	2.14	0.62
1:C:321:GLN:HE21	1:C:632:TRP:HB2	1.64	0.62
2:D:29:PHE:HD1	2:D:77:SER:HG	1.46	0.62
4:J:62:ARG:HG2	4:J:62:ARG:HH11	1.63	0.62
1:B:130:VAL:HG21	1:B:168:PHE:HE1	1.62	0.62
1:C:187:LYS:HD3	1:C:209:PRO:HA	1.81	0.62
1:C:381:GLY:HA3	1:C:429:PHE:CB	2.28	0.62
5:G:40:LYS:HA	5:G:85:ALA:CB	2.29	0.62
2:H:13:LYS:HB3	2:H:16:SER:HG	1.64	0.62
1:A:439:ASN:HB2	1:A:506:PRO:HD2	1.80	0.62
1:C:82:PRO:O	1:C:238:GLN:HG3	2.00	0.62
1:C:776:LYS:O	1:C:780:GLU:HG2	1.99	0.62
2:Q:93:VAL:HG22	2:Q:120:LEU:HD13	1.82	0.62
4:R:30:ILE:HG12	4:R:31:GLY:H	1.65	0.62
4:R:38:GLN:CB	4:R:48:LEU:HD13	2.29	0.62
5:G:50:TYR:C	5:G:52:ALA:N	2.50	0.62
1:A:64:TRP:HE1	1:A:214:ASP:HB3	1.63	0.62
1:A:295:PRO:HB3	1:A:596:VAL:HG22	1.81	0.62
1:A:445:HIS:CD2	2:D:73:ASP:HB3	2.35	0.62
1:A:877:LEU:HD22	1:A:1034:LEU:HD11	1.81	0.62
1:A:1080:ALA:HB3	1:A:1132:ILE:HG12	1.80	0.62
1:A:1141:LEU:O	1:A:1142:GLN:C	2.36	0.62
1:C:327:VAL:O	1:C:328:ARG:HB3	1.98	0.62
1:C:499:THR:HG21	5:K:50:TYR:HB2	1.80	0.62
1:C:831:ALA:HB1	1:C:851:CYS:O	1.98	0.62
4:R:3:ILE:HD11	4:R:5:MET:SD	2.40	0.62
3:E:51:ILE:O	3:E:52:SER:C	2.38	0.62
3:I:12:LYS:HG2	3:I:18:VAL:HG12	1.82	0.62
3:I:113:GLY:HA2	5:K:47:LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:THR:HG23	1:A:523:VAL:H	1.65	0.62
1:A:634:VAL:O	1:A:635:TYR:C	2.38	0.62
1:A:644:THR:HG22	1:A:646:ALA:H	1.64	0.62
1:B:114:THR:O	1:B:115:GLN:HB2	1.99	0.62
1:B:386:LYS:HA	1:B:389:ASP:HB2	1.82	0.62
1:B:727:LEU:HD21	1:B:1024:LEU:HD23	1.82	0.62
1:C:956:ALA:C	1:C:958:ALA:H	2.02	0.62
2:D:27:GLY:O	2:D:29:PHE:N	2.32	0.62
3:E:101:THR:HG22	3:E:114:PHE:CD1	2.34	0.62
1:A:535:ASN:O	1:A:536:LYS:C	2.38	0.62
1:B:373:PRO:O	1:B:374:PHE:C	2.38	0.62
1:B:453:TYR:N	1:B:492:GLN:O	2.30	0.62
2:Q:52:ILE:N	2:Q:53:PRO:HD3	2.15	0.62
2:Q:105:PRO:CG	2:Q:109:GLU:HA	2.30	0.62
1:A:96:GLU:C	1:A:186:PHE:HA	2.20	0.62
1:A:751:ASN:HA	1:A:754:LEU:HD22	1.81	0.62
1:A:1096:VAL:HG21	1:A:1110:TYR:HE1	1.65	0.62
1:B:329:PHE:O	1:B:579:GLN:NE2	2.32	0.62
1:C:439:ASN:OD1	1:C:505:GLN:HB3	1.98	0.62
2:Q:98:ARG:HG3	2:Q:113:ASP:HB2	1.80	0.62
2:D:51:PHE:HB3	2:D:59:ILE:HB	1.81	0.62
2:H:26:GLY:O	2:H:28:THR:N	2.33	0.62
2:H:28:THR:O	2:H:29:PHE:C	2.38	0.62
3:I:110:LEU:HB2	3:I:116:ASN:HD22	1.63	0.62
1:A:337:PRO:HD3	1:A:361:CYS:HB2	1.81	0.62
1:A:737:ASP:O	1:A:738:CYS:C	2.38	0.62
1:C:632:TRP:O	1:C:633:ARG:HB2	1.99	0.62
5:K:86:VAL:HG12	5:K:102:THR:H	1.64	0.62
1:A:452:TRP:CE2	1:A:493:SER:HB2	2.35	0.62
1:B:115:GLN:OE1	1:B:132:GLU:HG3	1.99	0.62
1:C:501:GLY:O	1:C:505:GLN:N	2.33	0.62
1:C:1126:CYS:O	1:C:1126:CYS:SG	2.57	0.62
3:S:24:ALA:HB1	3:S:27:TYR:CE2	2.34	0.62
4:R:90:GLN:HE21	4:R:91:ARG:H	1.47	0.62
2:D:44:GLY:O	2:D:46:GLU:N	2.33	0.62
3:I:24:ALA:HB1	3:I:27:TYR:CE2	2.35	0.62
1:B:543:ASN:HD21	1:B:578:PRO:HB3	1.64	0.62
1:B:578:PRO:HB2	1:B:579:GLN:NE2	2.14	0.62
1:C:329:PHE:CD1	1:C:330:PRO:HD2	2.35	0.62
2:D:51:PHE:N	2:D:51:PHE:CD1	2.68	0.62
2:D:83:LEU:HB3	2:D:86:LEU:HG	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:97:ALA:HB2	2:D:115:TRP:HA	1.82	0.62
4:F:62:ARG:HD3	4:F:62:ARG:H	1.65	0.62
4:J:16:VAL:CG1	4:J:107:LYS:HB2	2.30	0.62
1:A:662:ASP:HB3	1:A:671:ALA:O	2.00	0.61
1:B:91:TYR:HE1	1:B:191:GLU:HG3	1.65	0.61
4:R:12:LEU:HD22	4:R:20:VAL:HG13	1.82	0.61
1:A:121:ASN:HA	1:A:126:VAL:HG13	1.82	0.61
1:A:378:LYS:HG2	1:A:380:TYR:CD2	2.35	0.61
1:A:758:SER:HB2	1:A:761:THR:HG22	1.82	0.61
1:B:164:ASN:O	1:B:165:ASN:C	2.39	0.61
1:B:1057:PRO:O	1:B:1058:HIS:HB2	1.99	0.61
1:C:129:LYS:HB2	1:C:133:PHE:HZ	1.65	0.61
1:C:330:PRO:HD3	1:C:542:PHE:CD1	2.35	0.61
1:C:372:ALA:HB1	1:C:373:PRO:CD	2.29	0.61
1:C:438:SER:H	1:C:507:TYR:HA	1.64	0.61
1:C:853:GLN:O	1:C:855:PHE:N	2.33	0.61
5:K:63:PHE:HA	5:K:76:ILE:HA	1.82	0.61
1:A:295:PRO:HB3	1:A:596:VAL:CG2	2.31	0.61
1:A:336:CYS:SG	1:A:364:ASP:HB2	2.40	0.61
1:A:542:PHE:CZ	1:A:584:LEU:HD22	2.35	0.61
1:A:556:LYS:HB2	1:A:583:ILE:HG12	1.82	0.61
1:C:594:VAL:HG11	1:C:635:TYR:OH	1.99	0.61
1:C:744:GLY:C	1:C:746:SER:H	2.03	0.61
3:S:28:PRO:C	3:S:30:THR:H	2.03	0.61
1:B:29:THR:O	1:B:61:ASN:HA	1.99	0.61
1:B:372:ALA:HB1	1:B:373:PRO:CD	2.30	0.61
1:B:1029:MET:HG2	1:B:1062:PHE:CZ	2.36	0.61
1:C:903:ALA:HB2	1:C:916:LEU:HD22	1.81	0.61
2:Q:53:PRO:CB	2:Q:57:THR:HB	2.29	0.61
2:Q:100:PHE:N	2:Q:101:PRO:HD2	2.15	0.61
3:E:27:TYR:CZ	3:E:98:ARG:HD3	2.35	0.61
5:G:7:SER:HB3	5:G:8:PRO:HD2	1.83	0.61
4:J:62:ARG:HH12	4:J:76:ILE:HG23	1.65	0.61
1:A:386:LYS:HA	1:A:389:ASP:CG	2.21	0.61
1:A:853:GLN:O	1:A:854:LYS:C	2.39	0.61
1:A:969:LYS:O	1:A:971:GLY:N	2.33	0.61
1:A:970:PHE:CE2	1:A:1000:ARG:HG2	2.34	0.61
1:C:361:CYS:H	1:C:523:VAL:HA	1.66	0.61
1:C:406:GLU:HB3	1:C:409:GLN:HB2	1.81	0.61
1:C:743:CYS:O	1:C:745:ASP:N	2.33	0.61
5:T:40:LYS:CD	5:T:46:ARG:HH12	2.10	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:SER:HB3	2:D:108:PRO:HD3	1.82	0.61
4:F:34:LEU:HD11	4:F:72:PHE:HB2	1.81	0.61
2:H:99:LEU:HD12	2:H:112:PHE:CE1	2.36	0.61
1:A:271:GLN:HE21	1:A:273:ARG:HD3	1.64	0.61
1:A:372:ALA:HB1	1:A:373:PRO:CD	2.29	0.61
1:A:869:MET:HB3	1:C:699:LEU:CD2	2.29	0.61
1:B:443:SER:HB2	2:Q:29:PHE:CE2	2.36	0.61
1:B:869:MET:C	1:B:871:ALA:N	2.52	0.61
1:C:849:LEU:CB	1:C:852:ALA:HB2	2.30	0.61
3:E:110:LEU:HB3	3:E:113:GLY:O	2.01	0.61
4:F:95:SER:O	4:F:97:THR:N	2.32	0.61
1:A:356:THR:CB	1:A:397:ALA:HB3	2.30	0.61
1:B:236:ARG:HG3	1:B:237:PHE:N	2.15	0.61
1:B:522:THR:HG23	1:B:523:VAL:H	1.66	0.61
1:C:189:LEU:O	1:C:190:ARG:C	2.38	0.61
1:C:869:MET:C	1:C:871:ALA:H	2.03	0.61
4:R:90:GLN:CD	4:R:96:TYR:HB3	2.20	0.61
2:D:35:SER:CB	2:D:112:PHE:CZ	2.84	0.61
1:A:894:LEU:HD21	1:C:1072:GLU:HB3	1.82	0.61
1:B:329:PHE:CE2	1:B:527:LYS:HG3	2.36	0.61
1:B:339:HIS:HA	1:B:342:PHE:CB	2.31	0.61
4:F:92:TYR:HA	4:F:96:TYR:CD1	2.35	0.61
3:I:49:GLY:HA3	3:I:70:MET:SD	2.41	0.61
1:A:440:LYS:HZ2	5:G:93:ASP:CG	2.03	0.61
1:B:403:LYS:HG3	1:B:504:HIS:HA	1.82	0.61
1:B:624:HIS:O	1:B:625:ALA:C	2.39	0.61
1:C:961:THR:HA	1:C:964:LYS:HG2	1.81	0.61
2:Q:37:VAL:HG22	2:Q:47:TRP:HA	1.82	0.61
2:H:99:LEU:HA	2:H:112:PHE:HE1	1.64	0.61
3:I:39:GLN:O	3:I:92:ALA:HB1	2.00	0.61
1:A:360:ASN:CA	1:A:523:VAL:HA	2.30	0.61
1:A:377:PHE:HA	1:A:433:VAL:O	2.01	0.61
1:A:936:ASP:O	1:A:937:SER:C	2.39	0.61
1:A:1081:ILE:HG12	1:A:1133:VAL:HG22	1.83	0.61
1:B:543:ASN:OD1	1:B:578:PRO:HG3	2.01	0.61
1:C:44:ARG:HG2	1:C:47:VAL:HG11	1.81	0.61
1:C:388:ASN:O	1:C:389:ASP:C	2.39	0.61
1:C:404:GLY:HA2	1:C:407:VAL:HG22	1.83	0.61
1:C:556:LYS:HB2	1:C:583:ILE:CD1	2.30	0.61
2:D:37:VAL:HB	2:D:115:TRP:CH2	2.35	0.61
2:H:37:VAL:HG11	2:H:45:LEU:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:VAL:HG12	1:A:268:GLY:HA3	1.83	0.60
1:C:375:PHE:HE2	3:I:54:TYR:HB3	1.66	0.60
1:C:406:GLU:HB3	1:C:409:GLN:HE21	1.66	0.60
2:Q:59:ILE:HG23	2:Q:60:TYR:N	2.16	0.60
2:Q:102:ASN:HA	2:Q:109:GLU:CB	2.28	0.60
5:T:81:PRO:O	5:T:82:GLU:C	2.40	0.60
2:D:35:SER:HB3	2:D:112:PHE:HZ	1.62	0.60
2:H:111:GLY:HA3	4:J:50:TYR:HD2	1.66	0.60
3:I:34:ILE:HB	3:I:51:ILE:HG22	1.82	0.60
1:A:894:LEU:CD2	1:C:1072:GLU:HB3	2.31	0.60
1:B:331:ASN:O	1:B:332:VAL:C	2.39	0.60
1:B:410:ILE:HG12	1:B:418:ILE:HG21	1.83	0.60
1:C:328:ARG:HG2	1:C:542:PHE:HB2	1.83	0.60
1:C:358:ILE:HG13	1:C:395:VAL:O	2.01	0.60
1:C:1083:HIS:CD2	1:C:1137:VAL:HB	2.35	0.60
2:D:20:VAL:HG21	2:D:81:MET:HE2	1.83	0.60
5:G:86:VAL:CG1	5:G:102:THR:H	2.13	0.60
3:I:91:THR:HG23	3:I:125:VAL:H	1.65	0.60
1:A:350:VAL:C	1:A:352:ALA:H	2.04	0.60
1:B:350:VAL:C	1:B:352:ALA:N	2.54	0.60
1:C:410:ILE:CG2	1:C:425:LEU:HD23	2.25	0.60
1:C:614:VAL:HG21	1:C:619:VAL:HG13	1.84	0.60
2:Q:30:ARG:HA	2:Q:30:ARG:HH11	1.63	0.60
2:D:98:ARG:O	2:D:112:PHE:HD1	1.83	0.60
3:E:114:PHE:CD1	5:G:47:LEU:HD22	2.36	0.60
2:H:51:PHE:HB3	2:H:59:ILE:CB	2.32	0.60
4:J:69:GLY:O	4:J:71:ASP:N	2.34	0.60
1:B:56:LEU:HD23	1:B:270:LEU:HD13	1.82	0.60
1:B:381:GLY:HA3	1:B:429:PHE:CB	2.31	0.60
1:B:386:LYS:HA	1:B:389:ASP:CG	2.20	0.60
2:Q:36:TRP:H	2:Q:49:GLY:HA3	1.66	0.60
2:Q:59:ILE:HG12	2:Q:60:TYR:N	2.16	0.60
2:Q:72:ALA:HB1	2:Q:79:ALA:HB1	1.82	0.60
3:S:2:VAL:HG22	3:S:27:TYR:HB3	1.82	0.60
1:A:373:PRO:O	1:A:374:PHE:C	2.39	0.60
1:A:408:SER:HB3	3:E:54:TYR:HE1	1.65	0.60
1:A:828:LEU:HA	1:A:850:ILE:HG13	1.82	0.60
1:B:361:CYS:N	1:B:523:VAL:HA	2.16	0.60
1:B:1116:THR:HG23	1:B:1118:ASP:H	1.65	0.60
1:B:187:LYS:NZ	1:B:188:ASN:HB3	2.17	0.60
1:B:443:SER:HB3	1:B:448:ASN:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:TYR:HD1	1:C:468:ILE:HA	1.66	0.60
1:C:619:VAL:O	1:C:623:ILE:HB	2.02	0.60
2:Q:108:PRO:CG	4:R:33:TYR:CZ	2.82	0.60
4:F:34:LEU:HD11	4:F:72:PHE:CB	2.31	0.60
1:A:277:LEU:HB3	1:A:285:ILE:HG23	1.84	0.60
1:A:813:SER:HB2	1:A:815:ARG:HG3	1.84	0.60
1:B:87:ASN:HB3	1:B:269:TYR:HE1	1.66	0.60
1:B:196:ASN:HA	1:B:201:PHE:HA	1.83	0.60
1:B:339:HIS:CB	1:B:367:VAL:HB	2.30	0.60
1:B:350:VAL:HG12	1:B:453:TYR:HA	1.83	0.60
1:B:1085:GLY:HA2	1:B:1126:CYS:SG	2.42	0.60
1:B:1141:LEU:C	1:B:1143:LEU:H	2.05	0.60
1:C:128:ILE:CG2	1:C:170:TYR:HB3	2.31	0.60
1:C:351:TYR:HE2	1:C:452:TRP:HB2	1.66	0.60
2:D:56:GLY:O	2:D:57:THR:C	2.40	0.60
3:I:117:TRP:N	3:I:117:TRP:CD1	2.68	0.60
1:B:375:PHE:HD1	1:B:435:ALA:HB3	1.67	0.60
1:B:767:LEU:HD23	1:B:770:ILE:HD12	1.84	0.60
1:B:858:LEU:HD13	1:B:959:LEU:HD22	1.83	0.60
1:C:634:VAL:O	1:C:635:TYR:C	2.39	0.60
3:S:30:THR:O	3:S:54:TYR:HD1	1.85	0.60
2:D:39:GLN:HB2	2:D:45:LEU:HG	1.84	0.60
2:H:30:ARG:HG3	2:H:34:ILE:HD13	1.82	0.60
2:H:104:ASP:CB	2:H:105:PRO:HD3	2.26	0.60
5:K:56:ALA:HB3	5:K:59:ILE:HD11	1.83	0.60
1:A:354:ASN:H	1:A:466:ARG:NH1	2.00	0.60
1:A:501:GLY:HA2	3:E:100:TYR:O	2.02	0.60
1:A:822:LEU:HD22	1:A:945:LEU:HD21	1.84	0.60
1:B:391:CYS:CB	1:B:521:ALA:HB1	2.29	0.60
1:B:426:PRO:HB3	1:B:463:PRO:HB3	1.83	0.60
5:K:55:ARG:NH1	5:K:59:ILE:HG12	2.17	0.60
1:A:135:PHE:CD2	1:A:139:PRO:HB3	2.37	0.60
1:A:139:PRO:O	1:A:140:PHE:C	2.40	0.60
1:A:193:VAL:HG12	1:A:193:VAL:O	2.01	0.60
1:A:410:ILE:O	1:A:410:ILE:HG23	2.02	0.60
1:A:634:VAL:O	1:A:636:SER:N	2.34	0.60
1:B:447:GLY:CA	1:B:497:ARG:HA	2.31	0.60
1:C:358:ILE:O	1:C:394:ASN:HB2	2.02	0.60
1:C:395:VAL:HG13	1:C:514:PHE:CA	2.31	0.60
5:G:60:PRO:O	5:G:61:ASP:C	2.40	0.60
2:H:30:ARG:HD2	2:H:74:GLU:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:117:TRP:CH2	5:K:45:PRO:HB2	2.37	0.60
1:B:415:THR:O	1:B:419:ALA:HB3	2.02	0.59
1:B:558:PHE:HZ	1:B:574:ALA:HB1	1.67	0.59
1:B:981:LEU:CD2	1:B:989:ALA:CB	2.79	0.59
1:C:186:PHE:O	1:C:210:ILE:HG12	2.02	0.59
1:C:438:SER:CB	1:C:508:ARG:HD2	2.32	0.59
2:D:55:PHE:HZ	2:D:75:SER:HB3	1.67	0.59
4:F:69:GLY:O	4:F:71:ASP:N	2.34	0.59
5:G:49:ILE:HD13	5:G:74:LEU:HD13	1.83	0.59
2:H:59:ILE:C	2:H:61:ALA:H	2.05	0.59
3:I:54:TYR:O	3:I:55:ASN:C	2.39	0.59
1:A:386:LYS:HA	1:A:389:ASP:HB2	1.82	0.59
1:A:588:PRO:HG2	1:B:855:PHE:HB3	1.83	0.59
1:B:508:ARG:HH11	1:B:508:ARG:HG2	1.67	0.59
4:R:16:VAL:CA	4:R:81:PRO:HD3	2.32	0.59
4:R:50:TYR:HE1	4:R:56:GLU:HA	1.67	0.59
5:G:31:SER:C	5:G:33:SER:H	2.04	0.59
3:I:106:PHE:HB3	3:I:109:SER:CB	2.32	0.59
1:A:278:LYS:O	1:A:279:TYR:C	2.40	0.59
1:B:396:TYR:O	1:B:513:SER:N	2.35	0.59
1:B:414:GLN:HG3	3:S:54:TYR:HE2	1.64	0.59
1:B:440:LYS:HD2	2:Q:57:THR:HG23	1.82	0.59
1:C:188:ASN:H	1:C:210:ILE:HG23	1.66	0.59
2:Q:55:PHE:CD1	2:Q:74:GLU:HG3	2.35	0.59
4:R:76:ILE:HD11	4:R:87:TYR:HE1	1.68	0.59
5:G:59:ILE:HG22	5:G:63:PHE:CD1	2.37	0.59
2:H:89:GLU:O	2:H:90:ASP:C	2.41	0.59
1:A:410:ILE:HD11	1:A:423:TYR:CG	2.37	0.59
1:B:421:TYR:HB3	1:B:457:ARG:HE	1.66	0.59
1:B:422:ASN:ND2	1:B:453:TYR:O	2.36	0.59
1:B:631:THR:O	1:B:632:TRP:C	2.41	0.59
1:C:402:ILE:HG13	1:C:407:VAL:HA	1.83	0.59
1:C:436:TRP:CE2	1:C:508:ARG:HB3	2.37	0.59
1:C:654:TYR:HA	1:C:694:ALA:O	2.01	0.59
2:Q:60:TYR:HE1	2:Q:70:ILE:HD13	1.67	0.59
3:S:115:ASP:O	3:S:116:ASN:C	2.40	0.59
3:E:15:GLY:HA2	3:E:86:LEU:O	2.02	0.59
3:I:111:ILE:C	3:I:113:GLY:H	2.06	0.59
4:J:16:VAL:HG22	4:J:107:LYS:HA	1.83	0.59
1:A:95:THR:HG22	1:A:211:ILE:HD11	1.82	0.59
1:B:91:TYR:CE1	1:B:191:GLU:HG3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ILE:HA	1:B:494:TYR:CE2	2.38	0.59
1:C:194:PHE:HB3	1:C:201:PHE:CE1	2.37	0.59
1:C:539:ASN:HD21	1:C:548:THR:HG23	1.65	0.59
5:K:59:ILE:HB	5:K:63:PHE:CE1	2.37	0.59
1:A:32:PHE:HA	1:A:59:PHE:HD1	1.67	0.59
1:A:203:ILE:HB	1:A:226:VAL:HG12	1.84	0.59
1:B:102:ARG:HD2	1:B:241:LEU:O	2.03	0.59
1:B:299:THR:HA	1:B:302:THR:OG1	2.02	0.59
1:B:405:ASN:HD21	3:S:102:ARG:N	2.01	0.59
1:B:442:ASP:OD2	1:B:506:PRO:HB2	2.02	0.59
1:B:445:HIS:C	1:B:447:GLY:H	2.06	0.59
1:C:353:TRP:HB3	1:C:423:TYR:CE2	2.37	0.59
1:C:441:LEU:HB2	2:H:55:PHE:CE2	2.37	0.59
3:S:91:THR:HG23	3:S:125:VAL:H	1.65	0.59
3:S:102:ARG:HA	3:S:102:ARG:NE	2.18	0.59
5:T:55:ARG:HH11	5:T:56:ALA:H	1.49	0.59
2:D:35:SER:CB	2:D:112:PHE:HZ	2.15	0.59
4:F:40:LYS:O	4:F:41:PRO:C	2.40	0.59
4:F:86:THR:HB	4:F:88:TYR:HE1	1.67	0.59
1:A:575:VAL:HG22	1:A:586:ILE:HD11	1.85	0.59
1:B:743:CYS:O	1:B:744:GLY:C	2.41	0.59
1:C:64:TRP:HE3	1:C:65:PHE:N	2.01	0.59
1:C:385:THR:C	1:C:387:LEU:H	2.05	0.59
1:C:1125:ASN:HD22	1:C:1127:ASP:H	1.49	0.59
2:Q:51:PHE:CD1	2:Q:53:PRO:HD3	2.37	0.59
3:E:91:THR:HG23	3:E:125:VAL:H	1.65	0.59
5:G:81:PRO:O	5:G:82:GLU:C	2.40	0.59
1:A:128:ILE:O	1:A:129:LYS:HB3	2.01	0.59
1:B:348:ALA:HB3	1:B:354:ASN:HB2	1.85	0.59
1:B:597:ILE:HG23	1:B:663:ILE:HG21	1.85	0.59
1:B:758:SER:O	1:B:759:PHE:C	2.39	0.59
1:C:188:ASN:H	1:C:210:ILE:HD13	1.66	0.59
4:R:40:LYS:O	4:R:41:PRO:C	2.40	0.59
5:T:60:PRO:O	5:T:61:ASP:C	2.40	0.59
3:E:2:VAL:HG13	3:E:27:TYR:CE2	2.38	0.59
3:E:102:ARG:NH1	3:E:103:GLY:HA2	2.17	0.59
1:A:129:LYS:HB3	1:A:169:GLU:HG2	1.85	0.59
1:B:381:GLY:HA3	1:B:429:PHE:HB3	1.85	0.59
1:B:978:ASN:O	1:B:982:SER:N	2.35	0.59
1:B:1079:PRO:HD2	1:B:1131:GLY:O	2.03	0.59
1:C:308:VAL:CG2	1:C:598:THR:HG21	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:TRP:CD1	1:C:353:TRP:N	2.70	0.59
1:C:1083:HIS:HB2	1:C:1137:VAL:CG2	2.33	0.59
4:R:69:GLY:O	4:R:71:ASP:N	2.34	0.59
2:D:27:GLY:C	2:D:29:PHE:N	2.54	0.59
2:D:54:LEU:HD11	2:D:99:LEU:CB	2.33	0.59
4:J:3:ILE:HA	4:J:27:SER:HB3	1.85	0.59
5:K:6:GLN:O	5:K:7:SER:C	2.41	0.59
5:K:49:ILE:HD11	5:K:64:SER:HA	1.83	0.59
5:K:62:ARG:HH12	5:K:80:GLU:H	1.51	0.59
1:A:62:VAL:HG12	1:A:268:GLY:CA	2.33	0.59
1:C:187:LYS:HD3	1:C:209:PRO:CA	2.32	0.59
1:C:322:PRO:HB3	1:C:537:CYS:HB3	1.85	0.59
3:E:68:VAL:HA	3:E:84:ARG:HE	1.68	0.59
3:E:89:ASP:O	3:E:91:THR:N	2.36	0.59
2:H:54:LEU:HB2	2:H:99:LEU:HD22	1.84	0.59
5:K:81:PRO:O	5:K:82:GLU:C	2.40	0.59
1:A:30:ASN:HD22	1:A:59:PHE:HA	1.67	0.58
1:A:129:LYS:HD3	1:A:131:CYS:HB3	1.85	0.58
1:B:381:GLY:HA3	1:B:429:PHE:CA	2.33	0.58
1:B:447:GLY:C	1:B:449:TYR:N	2.56	0.58
1:B:478:LYS:HB3	1:B:486:ASN:H	1.68	0.58
3:S:99:ASP:O	3:S:114:PHE:HB2	2.03	0.58
5:T:6:GLN:HE22	5:T:36:TRP:HZ3	1.51	0.58
2:H:51:PHE:H	2:H:54:LEU:CG	2.16	0.58
3:I:89:ASP:O	3:I:91:THR:N	2.36	0.58
4:J:40:LYS:O	4:J:41:PRO:C	2.40	0.58
1:A:326:ILE:HG23	1:A:533:VAL:HG23	1.85	0.58
1:A:353:TRP:CE2	1:A:466:ARG:HA	2.38	0.58
1:B:112:SER:N	1:B:134:GLN:HA	2.18	0.58
1:B:822:LEU:C	1:B:824:ASN:H	2.06	0.58
1:B:976:VAL:HG12	1:B:978:ASN:H	1.68	0.58
1:C:298:GLU:O	1:C:302:THR:HG23	2.02	0.58
5:T:21:LEU:HB2	5:T:74:LEU:HB3	1.84	0.58
5:T:56:ALA:HB3	5:T:59:ILE:CD1	2.33	0.58
2:D:24:ALA:HB2	2:D:30:ARG:CD	2.28	0.58
3:E:108:GLU:C	3:E:110:LEU:N	2.56	0.58
4:F:3:ILE:HA	4:F:27:SER:HB3	1.85	0.58
2:H:51:PHE:HB3	2:H:59:ILE:HB	1.84	0.58
3:I:101:THR:OG1	3:I:102:ARG:N	2.36	0.58
1:A:329:PHE:H	1:A:529:SER:HA	1.68	0.58
1:B:338:PHE:CE1	1:B:363:ALA:HB1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:THR:O	1:B:325:SER:N	2.34	0.58
1:B:465:GLU:CD	1:B:466:ARG:H	2.06	0.58
1:B:853:GLN:O	1:B:854:LYS:C	2.41	0.58
2:Q:36:TRP:H	2:Q:49:GLY:CA	2.17	0.58
2:Q:120:LEU:O	2:Q:122:THR:N	2.36	0.58
5:T:79:LEU:HD11	5:T:104:VAL:HG12	1.86	0.58
2:D:50:GLY:O	2:D:59:ILE:HG22	2.03	0.58
2:D:111:GLY:HA3	4:F:50:TYR:CD2	2.37	0.58
4:F:9:PRO:HD3	4:F:23:THR:OG1	2.04	0.58
4:J:37:TYR:CD1	4:J:47:LEU:HD23	2.38	0.58
4:J:103:LYS:O	4:J:104:VAL:C	2.41	0.58
5:K:50:TYR:C	5:K:52:ALA:H	2.07	0.58
1:B:713:ALA:HA	1:B:1073:LYS:O	2.04	0.58
1:B:833:PHE:CE2	1:B:851:CYS:HB2	2.38	0.58
1:B:950:ASP:HB3	1:B:954:HIS:CE1	2.38	0.58
1:C:308:VAL:HG22	1:C:601:THR:HG23	1.85	0.58
2:D:29:PHE:O	2:D:31:SER:N	2.37	0.58
3:E:110:LEU:HD22	3:E:115:ASP:HB2	1.85	0.58
2:H:54:LEU:HD23	2:H:57:THR:H	1.68	0.58
1:B:42:VAL:O	1:B:43:PHE:C	2.42	0.58
1:B:106:PHE:HB3	1:B:234:ILE:CG2	2.34	0.58
1:C:329:PHE:CG	1:C:528:LYS:HA	2.38	0.58
1:C:377:PHE:CZ	1:C:434:ILE:HD13	2.37	0.58
3:S:6:GLN:HB2	3:S:119:GLN:NE2	2.19	0.58
1:A:115:GLN:HE22	1:A:131:CYS:HA	1.68	0.58
1:A:352:ALA:O	1:A:353:TRP:C	2.41	0.58
1:A:441:LEU:HD11	1:A:508:ARG:NH1	2.19	0.58
1:A:737:ASP:HB3	1:A:740:MET:HB2	1.85	0.58
1:A:996:LEU:O	1:A:997:ILE:C	2.42	0.58
1:B:410:ILE:HG23	1:B:418:ILE:HG22	1.86	0.58
1:B:444:LYS:HB3	1:B:498:PRO:HB3	1.86	0.58
2:Q:33:VAL:C	2:Q:99:LEU:HB2	2.24	0.58
4:F:6:THR:C	4:F:8:SER:H	2.06	0.58
2:H:33:VAL:HG13	2:H:99:LEU:HB3	1.86	0.58
2:H:54:LEU:CD2	2:H:57:THR:H	2.17	0.58
3:I:48:MET:HB3	3:I:81:MET:CE	2.32	0.58
1:A:137:ASN:O	1:A:139:PRO:HD3	2.04	0.58
1:A:200:TYR:HA	1:A:229:PRO:HA	1.86	0.58
1:B:323:THR:C	1:B:325:SER:H	2.07	0.58
1:B:472:ILE:HG13	1:B:490:PRO:HD3	1.85	0.58
1:C:56:LEU:O	1:C:57:PRO:C	2.40	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:PRO:HB3	1:C:463:PRO:HB3	1.85	0.58
2:D:32:HIS:HA	2:D:55:PHE:HB2	1.86	0.58
2:D:100:PHE:N	2:D:101:PRO:CD	2.67	0.58
2:D:101:PRO:O	2:D:102:ASN:C	2.42	0.58
3:I:36:TRP:CE3	3:I:96:CYS:HA	2.38	0.58
1:A:454:ARG:HD2	1:A:457:ARG:HA	1.86	0.58
1:A:632:TRP:O	1:A:633:ARG:HB2	2.03	0.58
1:A:1029:MET:HE2	1:A:1062:PHE:HE1	1.69	0.58
1:B:447:GLY:O	1:B:449:TYR:N	2.37	0.58
1:B:822:LEU:HD22	1:B:945:LEU:HD21	1.86	0.58
1:C:187:LYS:CD	1:C:209:PRO:HB3	2.33	0.58
1:C:329:PHE:CD1	1:C:528:LYS:HA	2.38	0.58
1:C:558:PHE:CD2	1:C:583:ILE:HD12	2.38	0.58
1:C:959:LEU:HD12	1:C:960:ASN:HD22	1.69	0.58
2:Q:111:GLY:HA2	4:R:92:TYR:HE2	1.67	0.58
3:E:102:ARG:HG2	3:E:111:ILE:HD13	1.86	0.58
2:H:59:ILE:HG23	2:H:61:ALA:N	2.17	0.58
5:K:15:PRO:O	5:K:16:GLY:C	2.42	0.58
1:A:309:GLU:HG2	1:A:313:TYR:OH	2.04	0.58
1:A:334:ASN:HA	4:F:30:ILE:HD11	1.85	0.58
1:B:420:ASP:HA	1:B:460:LYS:NZ	2.19	0.58
1:B:457:ARG:HA	1:B:473:TYR:HA	1.86	0.58
5:G:13:LEU:O	5:G:14:SER:C	2.42	0.58
4:J:40:LYS:HB2	4:J:43:LYS:CE	2.33	0.58
5:K:2:ILE:CG2	5:K:25:ALA:HB1	2.34	0.58
1:A:64:TRP:CE3	1:A:66:HIS:HB3	2.38	0.57
1:A:335:LEU:CB	4:F:31:GLY:HA3	2.34	0.57
1:A:916:LEU:O	1:A:918:GLU:N	2.37	0.57
1:B:444:LYS:HA	1:B:498:PRO:HA	1.86	0.57
5:T:39:GLN:HB3	5:T:86:VAL:HG23	1.85	0.57
2:D:102:ASN:HD22	4:F:92:TYR:HB3	1.69	0.57
2:H:1:GLN:O	2:H:2:VAL:C	2.42	0.57
3:I:36:TRP:HZ2	3:I:79:GLY:HA3	1.68	0.57
4:J:14:ALA:HB3	4:J:105:GLU:O	2.04	0.57
1:A:503:GLY:C	1:A:505:GLN:H	2.07	0.57
1:A:809:PRO:HA	1:A:814:LYS:HD2	1.85	0.57
1:B:284:THR:O	1:B:286:THR:N	2.37	0.57
1:B:353:TRP:HZ2	1:B:461:LEU:HD22	1.69	0.57
1:B:405:ASN:HD21	3:S:102:ARG:H	1.50	0.57
1:B:406:GLU:HG3	1:B:418:ILE:HG12	1.85	0.57
1:B:424:LYS:HB2	1:B:461:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:ILE:CG2	1:B:948:LEU:HG	2.35	0.57
1:B:981:LEU:HD21	1:B:989:ALA:CB	2.34	0.57
2:Q:71:SER:OG	5:T:30:SER:HB3	2.05	0.57
2:Q:111:GLY:HA3	4:R:50:TYR:HD2	1.64	0.57
3:S:89:ASP:O	3:S:91:THR:N	2.36	0.57
2:H:32:HIS:HA	2:H:55:PHE:CG	2.39	0.57
1:A:296:LEU:HA	1:A:299:THR:HG23	1.86	0.57
1:A:328:ARG:HG3	1:A:578:PRO:HG2	1.86	0.57
1:B:93:ALA:HB3	1:B:266:TYR:HD1	1.70	0.57
1:B:128:ILE:HG13	1:B:170:TYR:HB3	1.86	0.57
1:B:228:LEU:O	1:B:230:ILE:HG12	2.05	0.57
1:C:445:HIS:HA	1:C:498:PRO:HD3	1.86	0.57
2:D:54:LEU:CD1	2:D:99:LEU:HG	2.33	0.57
3:E:102:ARG:HD2	3:E:105:TRP:HZ3	1.69	0.57
1:A:81:ASN:HA	1:A:265:TYR:CE2	2.39	0.57
1:A:1081:ILE:HG12	1:A:1133:VAL:CG2	2.35	0.57
1:B:300:LYS:C	1:B:302:THR:N	2.55	0.57
1:B:981:LEU:HG	1:B:993:ILE:HD11	1.86	0.57
1:C:131:CYS:H	1:C:133:PHE:HE1	1.50	0.57
2:Q:108:PRO:O	2:Q:109:GLU:HB3	2.04	0.57
5:T:93:ASP:O	5:T:94:THR:C	2.43	0.57
4:J:33:TYR:HB2	4:J:34:LEU:HG	1.86	0.57
5:K:34:LEU:HD22	5:K:72:PHE:HB2	1.86	0.57
1:A:47:VAL:HG12	1:A:48:LEU:H	1.69	0.57
1:A:82:PRO:HB2	1:A:84:LEU:HD13	1.86	0.57
1:A:404:GLY:HA2	1:A:407:VAL:HG23	1.85	0.57
1:A:979:ASP:O	1:A:982:SER:N	2.38	0.57
1:B:199:GLY:O	1:B:200:TYR:C	2.42	0.57
1:B:342:PHE:CE2	1:B:512:LEU:HD21	2.39	0.57
1:C:327:VAL:O	1:C:328:ARG:HD3	2.04	0.57
4:R:84:ILE:HG22	4:R:105:GLU:HA	1.86	0.57
5:T:91:GLN:O	5:T:96:LEU:HA	2.04	0.57
3:I:51:ILE:HD12	3:I:58:THR:HG22	1.86	0.57
1:A:105:ILE:O	1:A:237:PHE:HA	2.04	0.57
1:A:540:PHE:HB2	1:A:551:LEU:HD11	1.87	0.57
1:A:976:VAL:HB	1:A:979:ASP:HB3	1.85	0.57
1:B:140:PHE:CD2	1:B:241:LEU:HD21	2.34	0.57
1:B:403:LYS:HD3	1:B:405:ASN:HB2	1.85	0.57
1:B:410:ILE:HG23	1:B:418:ILE:CG2	2.34	0.57
1:B:501:GLY:O	1:B:502:VAL:C	2.42	0.57
1:C:187:LYS:HD3	1:C:209:PRO:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:ASN:O	1:C:440:LYS:C	2.41	0.57
2:Q:13:LYS:O	2:Q:14:PRO:C	2.43	0.57
4:R:19:ARG:HA	4:R:76:ILE:O	2.05	0.57
2:D:62:GLN:O	2:D:63:ALA:C	2.42	0.57
5:G:95:SER:O	5:G:96:LEU:HB2	2.03	0.57
1:A:472:ILE:HA	1:A:490:PRO:HG3	1.87	0.57
1:A:522:THR:O	1:A:523:VAL:C	2.42	0.57
1:A:608:ALA:HB1	1:A:651:GLY:HA3	1.85	0.57
1:B:448:ASN:HB3	1:B:496:PHE:CD1	2.40	0.57
1:C:328:ARG:HG2	1:C:329:PHE:N	2.19	0.57
1:C:500:TYR:H	1:C:505:GLN:HE21	1.52	0.57
4:R:3:ILE:HA	4:R:27:SER:HB3	1.85	0.57
2:D:37:VAL:HG13	2:D:46:GLU:O	2.05	0.57
2:D:50:GLY:H	2:D:59:ILE:H	1.53	0.57
3:E:47:TRP:HB2	5:G:96:LEU:O	2.04	0.57
3:E:76:THR:O	3:E:77:THR:C	2.43	0.57
5:G:78:ARG:HD2	5:G:80:GLU:H	1.69	0.57
1:A:62:VAL:CG2	1:A:215:PHE:HE2	2.17	0.57
1:A:359:SER:O	1:A:360:ASN:C	2.43	0.57
1:A:477:ASN:H	1:A:482:GLY:HA2	1.70	0.57
1:A:534:LYS:HG3	1:A:553:LYS:NZ	2.20	0.57
1:A:917:TYR:O	1:A:918:GLU:HB2	2.04	0.57
1:B:564:PHE:CZ	1:C:42:VAL:HG22	2.39	0.57
1:C:138:ASP:O	1:C:140:PHE:N	2.37	0.57
2:Q:24:ALA:HB1	2:Q:30:ARG:HE	1.69	0.57
3:S:82:GLU:CD	3:S:82:GLU:H	2.07	0.57
2:H:51:PHE:CG	2:H:59:ILE:HB	2.40	0.57
1:A:355:ARG:HA	1:A:397:ALA:O	2.04	0.57
1:A:357:ARG:HA	1:A:396:TYR:CA	2.14	0.57
1:A:368:LEU:HA	1:A:371:PHE:CZ	2.40	0.57
1:B:378:LYS:HG2	1:B:380:TYR:CD2	2.40	0.57
1:B:416:GLY:O	1:B:420:ASP:HB2	2.05	0.57
1:B:454:ARG:HA	1:B:492:GLN:N	2.18	0.57
1:B:1086:LYS:HB2	1:B:1122:VAL:HG13	1.85	0.57
1:C:849:LEU:HB2	1:C:852:ALA:HB2	1.86	0.57
2:Q:1:GLN:O	2:Q:2:VAL:C	2.42	0.57
3:S:2:VAL:HG13	3:S:27:TYR:CD2	2.39	0.57
4:R:12:LEU:O	4:R:104:VAL:HA	2.05	0.57
5:T:6:GLN:NE2	5:T:36:TRP:HZ3	2.03	0.57
3:I:106:PHE:O	3:I:108:GLU:N	2.38	0.57
4:J:12:LEU:HD13	4:J:104:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:GLU:HB2	1:B:536:LYS:HD2	1.87	0.57
1:B:614:VAL:HG21	1:B:619:VAL:HG12	1.86	0.57
1:B:712:ILE:HD13	1:B:1094:VAL:HG21	1.85	0.57
1:B:940:SER:O	1:B:941:THR:C	2.43	0.57
1:C:369:TYR:HA	1:C:374:PHE:CZ	2.40	0.57
1:C:574:ALA:HA	1:C:585:ASP:HA	1.85	0.57
1:C:712:ILE:HD13	1:C:1094:VAL:HG21	1.87	0.57
2:Q:26:GLY:O	2:Q:28:THR:N	2.37	0.57
5:T:4:LEU:HD12	5:T:23:CYS:SG	2.45	0.57
2:D:51:PHE:HD1	2:D:51:PHE:H	1.53	0.57
3:E:114:PHE:HB2	5:G:37:TYR:OH	2.05	0.57
1:A:43:PHE:HE1	1:A:283:GLY:HA3	1.70	0.56
1:A:213:ARG:CD	1:A:216:PRO:HA	2.34	0.56
1:A:469:SER:C	1:A:471:GLU:N	2.57	0.56
1:B:502:VAL:CB	3:S:100:TYR:HB2	2.25	0.56
1:C:86:PHE:HA	1:C:90:VAL:CG1	2.35	0.56
2:D:48:MET:HG2	2:D:68:VAL:HG11	1.86	0.56
5:G:39:GLN:HG3	5:G:45:PRO:HG3	1.86	0.56
3:I:76:THR:O	3:I:77:THR:C	2.43	0.56
1:A:43:PHE:CE1	1:A:283:GLY:HA3	2.40	0.56
1:A:271:GLN:CD	1:A:272:PRO:HD2	2.25	0.56
1:B:447:GLY:C	1:B:449:TYR:H	2.09	0.56
1:B:1141:LEU:O	1:B:1143:LEU:N	2.35	0.56
1:C:323:THR:O	1:C:325:SER:N	2.38	0.56
2:Q:99:LEU:HG	2:Q:101:PRO:HD2	1.87	0.56
3:S:47:TRP:CD2	5:T:95:SER:HB2	2.40	0.56
3:S:76:THR:O	3:S:77:THR:C	2.43	0.56
5:T:33:SER:HA	5:T:92:HIS:HB2	1.86	0.56
3:E:60:TYR:CE2	3:E:69:THR:HA	2.41	0.56
4:F:35:ASN:O	4:F:36:TRP:HB2	2.04	0.56
3:I:36:TRP:N	3:I:97:ALA:HB2	2.20	0.56
4:J:93:ASP:CB	4:J:94:PRO:HD2	2.36	0.56
5:K:62:ARG:HD3	5:K:78:ARG:HG2	1.87	0.56
5:K:68:SER:HA	5:K:72:PHE:CE2	2.40	0.56
1:A:39:PRO:HD2	1:A:285:ILE:HD11	1.88	0.56
1:A:114:THR:O	1:A:132:GLU:HB2	2.05	0.56
1:A:472:ILE:HG23	1:A:473:TYR:N	2.20	0.56
1:A:934:ILE:O	1:A:935:GLN:C	2.43	0.56
1:B:353:TRP:CZ3	1:B:423:TYR:HA	2.40	0.56
1:B:372:ALA:O	1:B:374:PHE:N	2.36	0.56
1:C:34:ARG:HB2	1:C:34:ARG:CZ	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:THR:O	1:C:602:ASN:C	2.43	0.56
1:C:854:LYS:H	1:C:854:LYS:CD	2.16	0.56
1:C:1144:GLU:C	1:C:1146:ASP:H	2.08	0.56
2:Q:33:VAL:HG22	2:Q:100:PHE:N	2.19	0.56
4:R:7:GLN:HE22	4:R:88:TYR:HA	1.70	0.56
2:D:13:LYS:O	2:D:14:PRO:C	2.43	0.56
5:G:47:LEU:HD21	5:G:50:TYR:HD2	1.70	0.56
5:G:59:ILE:O	5:G:60:PRO:C	2.41	0.56
2:H:14:PRO:HB3	2:H:87:ARG:HA	1.87	0.56
2:H:23:LYS:HD3	2:H:25:SER:H	1.70	0.56
2:H:49:GLY:HA2	2:H:60:TYR:N	2.19	0.56
3:I:60:TYR:CE2	3:I:69:THR:HA	2.40	0.56
4:J:61:SER:O	4:J:63:PHE:N	2.38	0.56
1:A:231:GLY:O	1:A:232:ILE:HG12	2.04	0.56
1:A:500:TYR:C	3:E:102:ARG:HH21	2.08	0.56
1:B:80:ASP:O	1:B:82:PRO:HD3	2.05	0.56
1:B:386:LYS:HA	1:B:389:ASP:CB	2.36	0.56
1:C:449:TYR:C	1:C:451:TYR:H	2.09	0.56
1:C:735:SER:HB3	1:C:861:LEU:HD21	1.87	0.56
2:D:23:LYS:HD3	2:D:25:SER:H	1.70	0.56
4:F:22:ILE:HG12	4:F:74:PHE:O	2.05	0.56
4:F:33:TYR:HA	4:F:91:ARG:NE	2.21	0.56
4:F:81:PRO:HA	4:F:106:ILE:CG2	2.33	0.56
1:A:353:TRP:CD1	1:A:353:TRP:N	2.67	0.56
1:A:554:SER:HB3	1:A:583:ILE:CG1	2.34	0.56
1:B:370:ASN:HD22	4:R:94:PRO:HB3	1.70	0.56
1:B:401:VAL:HG11	1:B:448:ASN:ND2	2.21	0.56
1:B:441:LEU:O	1:B:442:ASP:HB2	2.05	0.56
1:B:448:ASN:HD22	1:B:506:PRO:HB3	1.71	0.56
1:B:599:PRO:HG3	1:B:692:ILE:HD11	1.88	0.56
1:B:807:PRO:CG	1:B:875:SER:HB2	2.36	0.56
1:B:939:PHE:O	1:B:940:SER:C	2.43	0.56
1:C:833:PHE:O	1:C:834:ILE:C	2.43	0.56
3:S:32:TYR:HE1	3:S:102:ARG:HA	1.70	0.56
5:T:32:THR:C	5:T:92:HIS:HB2	2.25	0.56
5:T:38:GLN:CB	5:T:48:LEU:HD21	2.34	0.56
5:T:90:GLN:HB3	5:T:96:LEU:HD12	1.86	0.56
2:D:102:ASN:H	2:D:109:GLU:HB2	1.71	0.56
2:D:114:ILE:HG22	2:D:115:TRP:O	2.05	0.56
3:E:106:PHE:HB3	3:E:109:SER:HB3	1.87	0.56
4:F:40:LYS:HZ1	4:F:59:VAL:HG21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:71:THR:O	3:I:80:TYR:N	2.39	0.56
4:J:6:THR:C	4:J:8:SER:H	2.08	0.56
1:A:105:ILE:HG22	1:A:110:LEU:HD21	1.88	0.56
1:A:375:PHE:CZ	3:E:54:TYR:HD2	2.21	0.56
1:A:440:LYS:NZ	5:G:93:ASP:CB	2.69	0.56
1:A:828:LEU:HD13	1:A:952:VAL:HG11	1.88	0.56
1:B:295:PRO:HD3	1:B:635:TYR:HB2	1.87	0.56
1:B:391:CYS:HB2	1:B:521:ALA:CB	2.31	0.56
1:C:361:CYS:SG	1:C:362:VAL:N	2.79	0.56
3:S:18:VAL:O	3:S:82:GLU:HA	2.05	0.56
5:T:91:GLN:O	5:T:96:LEU:HD13	2.06	0.56
2:H:74:GLU:HA	2:H:78:THR:O	2.06	0.56
4:J:35:ASN:O	4:J:36:TRP:HB2	2.06	0.56
1:B:449:TYR:CZ	1:B:495:GLY:HA2	2.40	0.56
1:C:352:ALA:O	1:C:353:TRP:C	2.44	0.56
2:Q:78:THR:HB	2:Q:80:TYR:CE2	2.40	0.56
5:K:16:GLY:HA2	5:K:79:LEU:O	2.05	0.56
1:A:64:TRP:O	1:A:65:PHE:C	2.43	0.56
1:A:1142:GLN:O	1:A:1143:LEU:C	2.43	0.56
1:C:81:ASN:ND2	1:C:238:GLN:HG2	2.21	0.56
1:C:188:ASN:N	1:C:210:ILE:HG23	2.20	0.56
1:C:339:HIS:H	1:C:342:PHE:HD2	1.53	0.56
1:C:373:PRO:O	1:C:374:PHE:C	2.43	0.56
2:Q:3:GLN:HG2	2:Q:25:SER:HB2	1.88	0.56
4:R:90:GLN:HE22	4:R:92:TYR:HD1	1.52	0.56
2:D:1:GLN:O	2:D:2:VAL:C	2.42	0.56
2:D:38:ARG:N	2:D:48:MET:HB2	2.21	0.56
5:G:49:ILE:HG12	5:G:64:SER:HA	1.87	0.56
2:H:49:GLY:HA3	2:H:70:ILE:HD13	1.87	0.56
5:K:6:GLN:HE22	5:K:88:TYR:HA	1.70	0.56
1:A:86:PHE:HB2	1:A:237:PHE:CD1	2.41	0.56
1:A:398:ASP:CB	1:A:511:VAL:HG23	2.35	0.56
1:A:472:ILE:CG1	1:A:490:PRO:HD3	2.32	0.56
1:A:496:PHE:CG	1:A:506:PRO:HG3	2.40	0.56
1:B:422:ASN:OD1	1:B:454:ARG:HB3	2.06	0.56
1:B:452:TRP:CA	1:B:493:SER:HA	2.29	0.56
1:B:478:LYS:N	1:B:485:PRO:HA	2.20	0.56
1:B:1110:TYR:CE2	1:B:1112:PRO:HG3	2.40	0.56
1:C:381:GLY:HA3	1:C:429:PHE:HB3	1.88	0.56
1:C:773:GLU:O	1:C:775:ASP:N	2.39	0.56
3:S:60:TYR:CE2	3:S:69:THR:HA	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:72:PHE:N	5:T:72:PHE:CD1	2.72	0.56
2:D:4:LEU:HD11	2:D:30:ARG:HH22	1.71	0.56
2:D:20:VAL:HG11	2:D:94:TYR:HE1	1.69	0.56
2:D:51:PHE:HE1	2:D:57:THR:HB	1.70	0.56
3:E:71:THR:O	3:E:80:TYR:N	2.39	0.56
5:G:39:GLN:HB2	5:G:88:TYR:CE1	2.39	0.56
5:G:49:ILE:HG13	5:G:55:ARG:HA	1.88	0.56
1:A:339:HIS:HA	1:A:342:PHE:HB2	1.88	0.56
1:A:416:GLY:O	1:A:420:ASP:HB2	2.06	0.56
1:A:533:VAL:HG11	1:A:538:VAL:CG1	2.35	0.56
1:B:49:HIS:O	1:B:276:LEU:HD12	2.06	0.56
1:B:194:PHE:CD1	1:B:203:ILE:HG23	2.33	0.56
1:C:337:PRO:HG2	1:C:363:ALA:HA	1.87	0.56
2:D:32:HIS:HA	2:D:55:PHE:CB	2.36	0.56
4:F:37:TYR:CE1	4:F:47:LEU:HD23	2.40	0.56
5:G:68:SER:HA	5:G:72:PHE:CE2	2.40	0.56
2:H:14:PRO:HG3	2:H:87:ARG:O	2.06	0.56
4:J:7:GLN:N	4:J:25:GLN:HB2	2.21	0.56
1:A:452:TRP:HE3	1:A:491:LEU:HB3	1.70	0.55
1:A:1037:SER:H	1:A:1048:HIS:CD2	2.24	0.55
1:B:27:SER:HB3	1:B:64:TRP:HB3	1.88	0.55
1:B:115:GLN:CG	1:B:130:VAL:HG12	2.36	0.55
1:C:395:VAL:HG13	1:C:514:PHE:HA	1.87	0.55
1:C:948:LEU:HD21	1:C:1059:GLY:HA3	1.88	0.55
2:Q:69:MET:C	2:Q:70:ILE:HD12	2.26	0.55
3:S:71:THR:O	3:S:80:TYR:N	2.39	0.55
4:R:50:TYR:CE1	4:R:56:GLU:HB2	2.41	0.55
5:T:68:SER:HA	5:T:72:PHE:CE2	2.41	0.55
3:E:37:VAL:HG21	3:E:117:TRP:CH2	2.41	0.55
2:H:13:LYS:H	2:H:123:VAL:HG13	1.71	0.55
5:K:92:HIS:O	5:K:93:ASP:C	2.43	0.55
1:A:672:SER:O	1:A:692:ILE:HA	2.06	0.55
1:B:112:SER:HB3	1:B:164:ASN:ND2	2.21	0.55
1:B:1070:ALA:O	1:B:1072:GLU:N	2.38	0.55
1:C:227:ASP:O	1:C:228:LEU:C	2.43	0.55
1:C:653:GLU:HG2	1:C:653:GLU:O	2.06	0.55
2:Q:15:GLY:O	2:Q:16:SER:C	2.44	0.55
5:T:2:ILE:HA	5:T:27:GLN:HE21	1.71	0.55
5:T:55:ARG:CD	5:T:59:ILE:HB	2.35	0.55
5:T:68:SER:HA	5:T:72:PHE:CZ	2.42	0.55
5:G:2:ILE:HA	5:G:27:GLN:HE21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:46:LYS:NZ	4:J:59:VAL:HB	2.21	0.55
1:A:65:PHE:CZ	1:A:84:LEU:HD11	2.40	0.55
1:A:386:LYS:HA	1:A:389:ASP:CB	2.36	0.55
1:A:481:LYS:HD3	1:A:483:LYS:HD2	1.87	0.55
1:A:858:LEU:HD13	1:A:959:LEU:HD22	1.87	0.55
1:B:49:HIS:CG	1:B:50:LEU:H	2.25	0.55
1:B:619:VAL:C	1:B:621:VAL:H	2.09	0.55
1:B:644:THR:HG22	1:B:645:ARG:N	2.21	0.55
1:B:854:LYS:O	1:B:856:ASN:N	2.39	0.55
1:B:877:LEU:HD23	1:B:888:PHE:HE2	1.72	0.55
1:B:984:LEU:HD13	1:B:988:GLU:HG3	1.88	0.55
1:C:666:GLY:O	1:C:667:ALA:HB3	2.06	0.55
3:S:115:ASP:HB3	3:S:117:TRP:HD1	1.71	0.55
3:E:113:GLY:O	3:E:114:PHE:C	2.44	0.55
2:H:12:LYS:HE2	2:H:13:LYS:HG2	1.87	0.55
2:H:78:THR:HB	2:H:80:TYR:HE1	1.72	0.55
3:I:29:PHE:HB3	3:I:74:THR:HA	1.87	0.55
5:K:2:ILE:HA	5:K:27:GLN:HE21	1.71	0.55
1:A:37:TYR:O	1:A:38:TYR:C	2.45	0.55
1:A:356:THR:HB	1:A:397:ALA:CB	2.35	0.55
1:A:950:ASP:O	1:A:954:HIS:HB2	2.05	0.55
1:C:200:TYR:O	1:C:202:LYS:HG2	2.05	0.55
1:C:927:PHE:CZ	1:C:931:ILE:HD12	2.41	0.55
2:Q:105:PRO:CB	2:Q:110:ASP:HB2	2.37	0.55
1:A:34:ARG:HG2	1:A:91:TYR:OH	2.06	0.55
1:A:483:LYS:O	1:A:488:TYR:HB2	2.06	0.55
1:A:834:ILE:HG13	1:C:643:GLN:NE2	2.20	0.55
1:B:142:ASP:H	1:B:241:LEU:HD23	1.71	0.55
1:B:339:HIS:HA	1:B:342:PHE:HB2	1.88	0.55
1:B:359:SER:O	1:B:360:ASN:C	2.45	0.55
1:B:441:LEU:HD13	2:Q:32:HIS:CG	2.42	0.55
1:C:64:TRP:CD1	1:C:266:TYR:HE2	2.25	0.55
1:C:170:TYR:CG	1:C:171:VAL:N	2.74	0.55
1:C:353:TRP:HZ2	1:C:461:LEU:HD22	1.70	0.55
1:C:448:ASN:C	1:C:450:ASP:H	2.10	0.55
2:Q:23:LYS:HD3	2:Q:25:SER:H	1.70	0.55
2:Q:64:PHE:CD1	2:Q:68:VAL:HB	2.42	0.55
5:T:8:PRO:HB2	5:T:102:THR:OG1	2.06	0.55
4:F:91:ARG:O	4:F:92:TYR:HB2	2.06	0.55
2:H:27:GLY:O	2:H:28:THR:C	2.45	0.55
4:J:62:ARG:N	4:J:62:ARG:HD3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LYS:HB2	1:A:305:SER:O	2.07	0.55
1:A:334:ASN:O	1:A:362:VAL:HB	2.07	0.55
1:A:731:MET:H	1:A:774:GLN:HG3	1.70	0.55
1:B:39:PRO:HG3	1:B:51:THR:HG21	1.89	0.55
1:B:367:VAL:C	1:B:369:TYR:H	2.08	0.55
1:C:347:PHE:HB2	1:C:401:VAL:HG23	1.89	0.55
1:C:479:PRO:HB2	1:C:486:ASN:HB2	1.89	0.55
1:C:568:ILE:HG12	1:C:569:VAL:HG22	1.87	0.55
3:S:50:TRP:CZ2	3:S:100:TYR:CE1	2.93	0.55
3:I:73:ASP:OD2	3:I:76:THR:HG23	2.07	0.55
1:A:120:VAL:HG23	1:A:127:PHE:HB3	1.87	0.55
1:A:127:PHE:HE2	1:A:129:LYS:HG2	1.72	0.55
1:A:289:VAL:HG11	1:A:300:LYS:CG	2.37	0.55
1:A:661:CYS:HA	1:A:695:TYR:CE2	2.41	0.55
1:B:227:ASP:O	1:B:228:LEU:C	2.44	0.55
1:B:1094:VAL:HG13	1:B:1105:THR:HG23	1.88	0.55
1:C:27:SER:O	1:C:28:TYR:HB2	2.07	0.55
1:C:196:ASN:ND2	1:C:201:PHE:HD1	2.05	0.55
1:C:375:PHE:CG	1:C:507:TYR:HE2	2.25	0.55
1:C:504:HIS:HB2	3:I:31:SER:O	2.07	0.55
5:T:91:GLN:H	5:T:96:LEU:HD12	1.71	0.55
2:D:3:GLN:HG2	2:D:25:SER:HB2	1.88	0.55
2:H:109:GLU:OE1	4:J:32:ASN:HA	2.07	0.55
3:I:108:GLU:C	3:I:110:LEU:N	2.59	0.55
1:A:852:ALA:HB1	1:A:855:PHE:CZ	2.42	0.55
1:B:219:PHE:HE2	1:B:288:ALA:HB3	1.72	0.55
1:B:365:TYR:CD1	1:B:388:ASN:HA	2.42	0.55
1:B:454:ARG:HH21	1:B:491:LEU:HD23	1.71	0.55
2:Q:105:PRO:HB3	2:Q:110:ASP:HB3	1.88	0.55
2:H:69:MET:C	2:H:70:ILE:HD12	2.26	0.55
3:I:96:CYS:SG	3:I:118:GLY:HA3	2.45	0.55
1:B:616:CYS:O	1:B:619:VAL:HG22	2.06	0.55
2:Q:4:LEU:HD12	2:Q:96:CYS:HB3	1.89	0.55
2:Q:101:PRO:HG3	4:R:92:TYR:CE1	2.42	0.55
4:R:60:PRO:HG2	4:R:62:ARG:HH21	1.71	0.55
4:R:93:ASP:O	4:R:95:SER:N	2.36	0.55
5:T:6:GLN:HG3	5:T:8:PRO:HG2	1.88	0.55
5:G:46:ARG:HH11	5:G:48:LEU:HD23	1.72	0.55
3:I:12:LYS:HG3	3:I:86:LEU:HG	1.89	0.55
1:A:65:PHE:HB2	1:A:265:TYR:O	2.07	0.55
1:A:104:TRP:HA	1:A:238:GLN:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LEU:HB3	1:A:120:VAL:HG22	1.89	0.55
1:A:440:LYS:HZ1	5:G:93:ASP:CB	2.20	0.55
1:A:500:TYR:CG	3:E:102:ARG:HD3	2.42	0.55
1:A:935:GLN:O	1:A:939:PHE:HB3	2.07	0.55
1:B:112:SER:CB	1:B:164:ASN:HD22	2.19	0.55
1:B:280:ASN:OD1	1:B:284:THR:N	2.40	0.55
1:B:483:LYS:O	1:B:487:CYS:HA	2.06	0.55
1:B:498:PRO:O	1:B:499:THR:C	2.45	0.55
1:B:898:PHE:O	1:B:900:MET:N	2.39	0.55
1:C:438:SER:OG	1:C:506:PRO:HB2	2.07	0.55
1:C:854:LYS:H	1:C:854:LYS:HD2	1.72	0.55
1:C:1097:SER:C	1:C:1099:GLY:H	2.09	0.55
2:D:15:GLY:O	2:D:16:SER:C	2.44	0.55
2:D:52:ILE:HD12	2:D:53:PRO:HD3	1.87	0.55
3:E:34:ILE:N	3:E:51:ILE:HG22	2.22	0.55
3:E:67:ARG:HH22	3:E:85:ARG:HB2	1.70	0.55
3:E:73:ASP:OD2	3:E:76:THR:HG23	2.07	0.55
4:F:81:PRO:CA	4:F:106:ILE:HG21	2.33	0.55
3:I:2:VAL:HG21	3:I:98:ARG:NH1	2.22	0.55
1:A:189:LEU:HB3	1:A:208:THR:OG1	2.07	0.54
1:A:333:THR:HB	1:A:362:VAL:CG2	2.37	0.54
1:B:274:THR:O	1:B:291:CYS:SG	2.64	0.54
1:B:397:ALA:HB1	1:B:510:VAL:HG13	1.90	0.54
1:B:534:LYS:O	1:B:536:LYS:N	2.40	0.54
2:Q:112:PHE:O	4:R:47:LEU:HD12	2.07	0.54
4:R:14:ALA:O	4:R:106:ILE:HA	2.07	0.54
1:A:335:LEU:HB2	4:F:31:GLY:HA3	1.90	0.54
1:A:616:CYS:O	1:A:617:THR:C	2.44	0.54
1:B:106:PHE:HB3	1:B:234:ILE:HG21	1.89	0.54
1:B:122:ASN:O	1:B:124:THR:N	2.40	0.54
1:B:376:ALA:O	1:B:434:ILE:HG23	2.07	0.54
1:B:421:TYR:HA	1:B:457:ARG:NH1	2.20	0.54
1:B:751:ASN:HA	1:B:754:LEU:HD21	1.90	0.54
1:B:1126:CYS:HA	1:B:1132:ILE:HD13	1.89	0.54
1:C:818:ILE:HA	1:C:821:LEU:HD23	1.88	0.54
2:Q:37:VAL:HB	2:Q:115:TRP:CZ3	2.43	0.54
2:Q:89:GLU:O	2:Q:91:THR:N	2.40	0.54
3:S:98:ARG:HB2	3:S:116:ASN:HB2	1.90	0.54
5:T:47:LEU:HD23	5:T:48:LEU:N	2.21	0.54
2:H:3:GLN:HG2	2:H:25:SER:HB2	1.88	0.54
1:B:30:ASN:HA	1:B:60:SER:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:ILE:HD11	1:B:1096:VAL:HG11	1.89	0.54
2:Q:51:PHE:HD1	2:Q:51:PHE:H	1.55	0.54
2:D:51:PHE:HE1	2:D:58:THR:H	1.55	0.54
5:K:63:PHE:HD2	5:K:76:ILE:HG23	1.71	0.54
1:A:200:TYR:O	1:A:201:PHE:C	2.46	0.54
1:A:554:SER:HB2	1:A:585:ASP:HB2	1.89	0.54
1:B:299:THR:HA	1:B:302:THR:HG1	1.72	0.54
1:B:707:TYR:HB3	1:C:792:PRO:CG	2.37	0.54
1:B:973:ILE:CD1	1:B:984:LEU:HG	2.38	0.54
1:B:1029:MET:HG2	1:B:1062:PHE:CE1	2.42	0.54
1:C:362:VAL:O	1:C:364:ASP:N	2.41	0.54
1:C:985:ASP:O	1:C:988:GLU:HG2	2.08	0.54
2:Q:105:PRO:HG3	2:Q:109:GLU:HA	1.89	0.54
3:S:53:THR:O	3:S:54:TYR:C	2.45	0.54
4:R:15:SER:C	4:R:17:GLY:H	2.09	0.54
2:D:37:VAL:HB	2:D:115:TRP:HZ3	1.72	0.54
2:D:64:PHE:CE1	2:D:67:ARG:HB3	2.42	0.54
2:D:107:SER:CB	2:D:108:PRO:HD3	2.37	0.54
3:I:11:VAL:HA	3:I:124:THR:OG1	2.07	0.54
3:I:48:MET:SD	3:I:81:MET:HE1	2.48	0.54
3:I:55:ASN:OD1	3:I:56:GLY:N	2.40	0.54
4:J:85:ALA:O	4:J:103:LYS:HA	2.08	0.54
1:A:701:ALA:HB3	1:B:787:GLN:HG3	1.89	0.54
1:B:616:CYS:N	1:B:643:GLN:OE1	2.40	0.54
1:C:353:TRP:CD1	1:C:466:ARG:HD3	2.42	0.54
1:C:737:ASP:HB3	1:C:740:MET:HB3	1.90	0.54
1:C:742:ILE:HD13	1:C:1001:LEU:HG	1.88	0.54
4:F:59:VAL:O	4:F:61:SER:N	2.41	0.54
4:J:90:GLN:HG2	4:J:97:THR:O	2.07	0.54
1:A:207:HIS:O	1:A:208:THR:C	2.46	0.54
1:A:411:ALA:O	1:A:413:GLY:N	2.41	0.54
1:A:444:LYS:HE3	1:A:446:SER:H	1.73	0.54
1:A:503:GLY:C	1:A:505:GLN:N	2.61	0.54
1:B:380:TYR:HE1	1:B:433:VAL:HG12	1.73	0.54
1:C:92:PHE:HZ	1:C:239:THR:HB	1.71	0.54
1:C:188:ASN:HD21	1:C:190:ARG:HD2	1.73	0.54
1:C:195:LYS:CE	1:C:197:ILE:HD11	2.32	0.54
3:S:15:GLY:HA2	3:S:86:LEU:O	2.07	0.54
4:R:4:GLN:O	4:R:5:MET:C	2.46	0.54
2:D:97:ALA:HB2	2:D:115:TRP:CD2	2.43	0.54
3:I:32:TYR:HE1	3:I:102:ARG:CA	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:119:GLN:HG2	3:I:120:GLY:N	2.21	0.54
4:J:93:ASP:HB3	4:J:94:PRO:HD2	1.88	0.54
1:A:360:ASN:HA	1:A:523:VAL:CA	2.37	0.54
1:A:391:CYS:HB2	1:A:521:ALA:HB3	1.90	0.54
1:A:392:PHE:N	1:A:521:ALA:HB1	2.23	0.54
1:A:1029:MET:O	1:A:1034:LEU:HD13	2.08	0.54
1:B:206:LYS:HB3	1:B:222:LEU:CD2	2.38	0.54
1:C:560:PRO:O	1:C:561:PHE:HB3	2.08	0.54
2:Q:30:ARG:O	2:Q:33:VAL:HG12	2.08	0.54
5:T:18:ARG:NH1	5:T:77:SER:HA	2.23	0.54
2:D:51:PHE:CB	2:D:59:ILE:HB	2.37	0.54
2:H:51:PHE:H	2:H:54:LEU:HG	1.72	0.54
1:A:91:TYR:O	1:A:93:ALA:N	2.40	0.54
1:A:407:VAL:HB	3:E:54:TYR:CE2	2.42	0.54
1:B:42:VAL:O	1:B:44:ARG:HG3	2.08	0.54
1:B:344:ALA:HA	2:Q:104:ASP:HA	1.89	0.54
1:C:188:ASN:ND2	1:C:190:ARG:HD2	2.22	0.54
1:C:559:LEU:O	1:C:561:PHE:N	2.40	0.54
3:S:73:ASP:OD2	3:S:76:THR:HG23	2.07	0.54
2:D:38:ARG:O	2:D:46:GLU:HG2	2.07	0.54
3:I:51:ILE:O	3:I:53:THR:N	2.40	0.54
5:K:88:TYR:CD2	5:K:101:GLY:HA2	2.43	0.54
1:A:83:VAL:HB	1:A:236:ARG:HH11	1.72	0.54
1:A:318:PHE:CE1	1:A:592:GLY:HA3	2.42	0.54
1:A:321:GLN:HB2	1:A:630:PRO:HB2	1.90	0.54
1:A:394:ASN:HA	1:A:523:VAL:CG1	2.37	0.54
1:A:398:ASP:O	1:A:511:VAL:N	2.35	0.54
1:A:478:LYS:H	1:A:479:PRO:HD2	1.72	0.54
1:B:81:ASN:OD1	1:B:238:GLN:HB2	2.06	0.54
1:C:339:HIS:HA	1:C:342:PHE:HB2	1.90	0.54
1:C:351:TYR:HB2	1:C:454:ARG:HH21	1.73	0.54
3:S:115:ASP:HB3	3:S:117:TRP:CD1	2.42	0.54
3:E:87:ARG:HH21	3:E:87:ARG:HB2	1.73	0.54
4:F:22:ILE:HG13	4:F:36:TRP:CH2	2.43	0.54
3:I:50:TRP:HD1	3:I:52:SER:H	1.56	0.54
1:A:296:LEU:HD12	1:A:598:THR:HG21	1.89	0.54
1:A:324:GLU:H	1:A:538:VAL:HG12	1.73	0.54
1:A:378:LYS:HG2	1:A:380:TYR:CE2	2.42	0.54
1:A:608:ALA:CB	1:A:651:GLY:HA3	2.38	0.54
1:A:890:ALA:O	1:C:1069:PRO:HD2	2.08	0.54
1:B:131:CYS:HA	1:B:166:CYS:HB2	1.84	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:SER:HB3	1:B:651:GLY:HA2	1.89	0.54
1:B:713:ALA:CA	1:B:1074:ASN:HA	2.37	0.54
1:B:758:SER:O	1:B:760:CYS:N	2.40	0.54
1:C:786:LYS:HG2	1:C:787:GLN:HG2	1.89	0.54
2:Q:64:PHE:HD1	2:Q:68:VAL:HB	1.73	0.54
3:S:19:LYS:HE3	3:S:80:TYR:HB3	1.90	0.54
4:R:16:VAL:HG13	4:R:107:LYS:HE3	1.90	0.54
2:D:8:GLY:O	2:D:9:ALA:C	2.47	0.54
4:F:35:ASN:HA	4:F:50:TYR:O	2.08	0.54
5:G:50:TYR:O	5:G:52:ALA:N	2.41	0.54
2:H:37:VAL:CG1	2:H:45:LEU:HB3	2.37	0.54
2:H:52:ILE:HB	2:H:53:PRO:HD3	1.90	0.54
1:A:380:TYR:N	1:A:380:TYR:CD1	2.76	0.53
1:A:557:LYS:HZ2	1:A:557:LYS:H	1.56	0.53
1:B:351:TYR:O	1:B:468:ILE:HA	2.07	0.53
1:B:916:LEU:CD1	1:B:923:ILE:HG21	2.38	0.53
1:C:486:ASN:O	1:C:487:CYS:C	2.47	0.53
1:C:558:PHE:CD1	1:C:583:ILE:HD12	2.43	0.53
1:C:634:VAL:HG13	1:C:635:TYR:H	1.73	0.53
2:Q:48:MET:CG	2:Q:64:PHE:HE1	2.21	0.53
2:Q:56:GLY:CA	2:Q:72:ALA:HB3	2.32	0.53
3:E:100:TYR:C	3:E:101:THR:HG23	2.27	0.53
4:F:35:ASN:N	4:F:51:ASP:HA	2.20	0.53
5:G:50:TYR:C	5:G:52:ALA:H	2.10	0.53
3:I:19:LYS:HE3	3:I:80:TYR:HB3	1.90	0.53
3:I:114:PHE:O	3:I:116:ASN:N	2.36	0.53
4:J:76:ILE:HD11	4:J:87:TYR:HE1	1.72	0.53
1:A:34:ARG:HE	1:A:215:PHE:HB3	1.73	0.53
1:A:189:LEU:HB2	1:A:210:ILE:O	2.07	0.53
1:A:385:THR:C	1:A:387:LEU:H	2.11	0.53
1:B:108:THR:HA	1:B:235:THR:HG22	1.91	0.53
1:B:448:ASN:O	1:B:450:ASP:N	2.41	0.53
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.41	0.53
1:C:104:TRP:O	1:C:105:ILE:HG13	2.08	0.53
3:S:32:TYR:HD1	3:S:101:THR:HG23	1.72	0.53
3:E:112:GLY:HA3	5:G:50:TYR:CE2	2.44	0.53
4:F:24:CYS:O	4:F:71:ASP:HA	2.08	0.53
5:G:59:ILE:O	5:G:61:ASP:N	2.41	0.53
2:H:34:ILE:HG13	2:H:97:ALA:O	2.07	0.53
2:H:89:GLU:O	2:H:91:THR:N	2.40	0.53
1:A:53:ASP:HB2	1:A:55:PHE:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ILE:HG12	1:A:488:TYR:HB3	1.89	0.53
1:A:1117:THR:HG22	1:A:1137:VAL:HG12	1.89	0.53
1:B:328:ARG:HD2	1:B:578:PRO:HG2	1.89	0.53
1:B:445:HIS:HA	1:B:497:ARG:HB2	1.90	0.53
1:B:445:HIS:CD2	1:B:498:PRO:HG3	2.43	0.53
1:C:109:THR:C	1:C:110:LEU:HG	2.29	0.53
2:Q:100:PHE:O	2:Q:105:PRO:HD3	2.06	0.53
3:S:83:LEU:HD23	3:S:86:LEU:HD22	1.90	0.53
5:T:55:ARG:HH11	5:T:55:ARG:HB3	1.73	0.53
4:J:15:SER:O	4:J:18:ASP:HB2	2.08	0.53
1:A:171:VAL:HG22	1:A:172:SER:H	1.73	0.53
1:A:276:LEU:HD23	1:A:306:PHE:CE1	2.43	0.53
1:A:366:SER:C	1:A:368:LEU:H	2.12	0.53
1:A:396:TYR:HD1	1:A:396:TYR:H	1.55	0.53
1:A:702:GLU:HG3	1:A:703:ASN:N	2.24	0.53
1:B:462:LYS:HB2	1:B:463:PRO:HD2	1.90	0.53
1:B:571:THR:O	1:B:572:THR:C	2.45	0.53
1:C:168:PHE:CE1	1:C:228:LEU:HD22	2.44	0.53
1:C:187:LYS:HA	1:C:209:PRO:HA	1.90	0.53
2:Q:51:PHE:H	2:Q:59:ILE:HG13	1.74	0.53
2:Q:72:ALA:HA	2:Q:80:TYR:H	1.72	0.53
5:T:6:GLN:HG2	5:T:101:GLY:O	2.08	0.53
5:T:38:GLN:HG2	5:T:46:ARG:HH11	1.73	0.53
5:T:79:LEU:O	5:T:80:GLU:C	2.47	0.53
2:D:47:TRP:CZ2	4:F:96:TYR:CE2	2.97	0.53
2:D:51:PHE:HB3	2:D:59:ILE:CB	2.38	0.53
2:H:64:PHE:CE2	2:H:68:VAL:HG23	2.43	0.53
4:J:81:PRO:C	4:J:83:ASP:H	2.12	0.53
5:K:49:ILE:HA	5:K:55:ARG:HA	1.89	0.53
1:A:106:PHE:HA	1:A:236:ARG:O	2.09	0.53
1:A:127:PHE:CE2	1:A:129:LYS:HG2	2.43	0.53
1:A:227:ASP:O	1:A:228:LEU:C	2.47	0.53
1:A:337:PRO:HD2	1:A:361:CYS:SG	2.48	0.53
1:A:819:GLU:O	1:A:823:PHE:HD1	1.91	0.53
1:B:395:VAL:HG13	1:B:514:PHE:CA	2.38	0.53
1:B:722:VAL:HG11	1:B:931:ILE:HD12	1.89	0.53
1:C:104:TRP:HE3	1:C:119:ILE:CG2	2.21	0.53
1:C:355:ARG:HD3	1:C:396:TYR:HD2	1.74	0.53
5:T:72:PHE:N	5:T:72:PHE:HD1	2.06	0.53
2:H:32:HIS:HA	2:H:55:PHE:HB2	1.90	0.53
2:H:74:GLU:O	2:H:75:SER:C	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:49:ILE:CD1	5:K:64:SER:HA	2.39	0.53
1:A:80:ASP:O	1:A:81:ASN:C	2.46	0.53
1:A:437:ASN:HD21	1:A:505:GLN:HB3	1.73	0.53
1:A:800:PHE:HA	1:A:928:ASN:OD1	2.08	0.53
1:A:989:ALA:C	1:A:991:VAL:H	2.11	0.53
1:B:714:ILE:CD1	1:B:1096:VAL:HG11	2.38	0.53
1:C:120:VAL:O	1:C:126:VAL:HA	2.07	0.53
5:K:53:SER:O	5:K:54:SER:C	2.45	0.53
1:A:335:LEU:H	4:F:30:ILE:HD13	1.73	0.53
1:B:564:PHE:HD1	1:B:564:PHE:H	1.55	0.53
1:B:620:SER:HB3	1:B:623:ILE:CA	2.38	0.53
1:C:406:GLU:O	1:C:409:GLN:N	2.42	0.53
1:C:833:PHE:CG	1:C:836:GLN:HA	2.43	0.53
2:Q:47:TRP:HH2	2:Q:51:PHE:HA	1.73	0.53
4:R:95:SER:O	4:R:97:THR:N	2.41	0.53
5:T:62:ARG:HA	5:T:77:SER:CB	2.38	0.53
3:E:19:LYS:HE3	3:E:80:TYR:HB3	1.91	0.53
3:I:59:ASN:ND2	3:I:60:TYR:H	2.07	0.53
4:J:48:LEU:HD11	4:J:59:VAL:HG21	1.91	0.53
1:A:48:LEU:HD23	1:A:278:LYS:HA	1.90	0.53
1:B:133:PHE:HB3	1:B:136:CYS:HG	1.73	0.53
1:B:329:PHE:CD2	1:B:527:LYS:HG3	2.44	0.53
1:B:342:PHE:HB3	1:B:371:PHE:CZ	2.44	0.53
1:B:769:GLY:HA2	1:B:772:VAL:HG22	1.91	0.53
1:B:1097:SER:C	1:B:1099:GLY:H	2.11	0.53
1:C:189:LEU:HB2	1:C:208:THR:O	2.07	0.53
1:C:984:LEU:HD12	1:C:988:GLU:HG3	1.90	0.53
1:C:1104:VAL:HG23	1:C:1115:ILE:HG22	1.90	0.53
2:Q:89:GLU:O	2:Q:90:ASP:C	2.47	0.53
3:I:17:SER:HA	3:I:86:LEU:HD23	1.91	0.53
3:I:102:ARG:HG2	3:I:109:SER:O	2.09	0.53
1:A:115:GLN:NE2	1:A:131:CYS:HA	2.23	0.53
1:A:214:ASP:HB2	1:A:266:TYR:CZ	2.44	0.53
1:A:498:PRO:HA	5:G:92:HIS:NE2	2.24	0.53
1:B:344:ALA:HA	2:Q:104:ASP:N	2.24	0.53
1:B:408:SER:O	1:B:410:ILE:N	2.41	0.53
1:B:440:LYS:HB3	2:Q:73:ASP:HA	1.90	0.53
1:B:1094:VAL:HG13	1:B:1105:THR:CG2	2.39	0.53
1:C:409:GLN:HB3	1:C:418:ILE:HB	1.90	0.53
1:C:540:PHE:CZ	1:C:578:PRO:HD3	2.44	0.53
1:C:557:LYS:H	1:C:583:ILE:HD13	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:743:CYS:O	1:C:747:THR:HG23	2.08	0.53
2:Q:100:PHE:N	2:Q:101:PRO:CD	2.72	0.53
2:D:122:THR:O	2:D:123:VAL:HG13	2.09	0.53
3:E:95:TYR:CD2	3:E:117:TRP:HE3	2.26	0.53
1:A:361:CYS:O	1:A:361:CYS:SG	2.67	0.53
1:A:361:CYS:H	1:A:523:VAL:HA	1.74	0.53
1:A:398:ASP:HB2	1:A:511:VAL:CG2	2.39	0.53
1:B:371:PHE:N	1:B:371:PHE:CD1	2.77	0.53
1:B:426:PRO:HG3	1:B:463:PRO:HB3	1.91	0.53
1:B:878:LEU:HD11	1:B:1054:GLN:NE2	2.23	0.53
1:C:125:ASN:ND2	1:C:171:VAL:HG23	2.24	0.53
1:C:337:PRO:CG	1:C:363:ALA:HA	2.39	0.53
1:C:346:ARG:HA	1:C:508:ARG:NH2	2.23	0.53
1:C:428:ASP:HB3	1:C:430:THR:HG23	1.90	0.53
1:C:802:PHE:HZ	1:C:898:PHE:CZ	2.26	0.53
1:C:901:GLN:O	1:C:905:ARG:HG3	2.09	0.53
5:T:59:ILE:O	5:T:61:ASP:N	2.42	0.53
2:D:33:VAL:HG21	2:D:98:ARG:HH11	1.73	0.53
3:E:2:VAL:HG13	3:E:27:TYR:CD2	2.44	0.53
5:G:80:GLU:O	5:G:81:PRO:C	2.48	0.53
1:A:135:PHE:O	1:A:139:PRO:HA	2.09	0.52
1:A:353:TRP:CZ2	1:A:461:LEU:HD22	2.43	0.52
1:A:673:TYR:CE2	1:A:690:GLN:HG2	2.44	0.52
1:B:342:PHE:CE1	1:B:510:VAL:HG11	2.45	0.52
1:B:343:ASN:HB2	2:Q:103:GLY:HA3	1.91	0.52
1:B:371:PHE:HB2	1:B:374:PHE:HD2	1.73	0.52
1:B:385:THR:C	1:B:387:LEU:H	2.12	0.52
1:C:308:VAL:HG21	1:C:598:THR:HG21	1.90	0.52
1:C:353:TRP:CE2	1:C:466:ARG:HA	2.44	0.52
1:C:541:ASN:HA	1:C:545:LEU:HA	1.90	0.52
1:C:989:ALA:O	1:C:990:GLU:C	2.47	0.52
2:Q:106:ASN:ND2	2:Q:108:PRO:HD2	2.24	0.52
3:S:59:ASN:ND2	3:S:60:TYR:H	2.07	0.52
2:D:86:LEU:HB3	2:D:90:ASP:CG	2.29	0.52
4:F:33:TYR:HA	4:F:91:ARG:HE	1.74	0.52
2:H:8:GLY:O	2:H:9:ALA:C	2.47	0.52
3:I:50:TRP:HD1	3:I:51:ILE:H	1.56	0.52
4:J:53:SER:O	4:J:55:LEU:HG	2.09	0.52
1:B:291:CYS:C	1:B:293:LEU:H	2.11	0.52
1:B:327:VAL:HG13	1:B:328:ARG:N	2.24	0.52
1:B:405:ASN:ND2	3:S:102:ARG:H	2.06	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:VAL:CG1	1:C:228:LEU:HG	2.40	0.52
1:C:479:PRO:HA	1:C:483:LYS:HZ1	1.73	0.52
1:C:538:VAL:HG23	1:C:539:ASN:N	2.25	0.52
4:R:35:ASN:HB2	4:R:50:TYR:O	2.09	0.52
5:T:12:SER:C	5:T:14:SER:H	2.12	0.52
2:D:2:VAL:O	2:D:114:ILE:HD13	2.09	0.52
1:A:26:GLN:O	1:A:27:SER:HB3	2.08	0.52
1:B:131:CYS:CA	1:B:166:CYS:HB3	2.36	0.52
1:B:215:PHE:C	1:B:217:GLN:H	2.11	0.52
1:B:351:TYR:HB2	1:B:454:ARG:HB2	1.88	0.52
1:B:353:TRP:CD1	1:B:353:TRP:N	2.76	0.52
1:B:620:SER:C	1:B:622:ALA:N	2.63	0.52
3:S:107:GLY:HA2	3:S:111:ILE:CG1	2.38	0.52
4:R:47:LEU:HD21	4:R:50:TYR:HA	1.91	0.52
2:D:51:PHE:CD1	2:D:54:LEU:HB3	2.44	0.52
3:E:12:LYS:HD3	3:E:16:ALA:HB3	1.91	0.52
3:E:68:VAL:HA	3:E:82:GLU:O	2.09	0.52
5:G:78:ARG:HD2	5:G:80:GLU:N	2.25	0.52
2:H:29:PHE:HA	2:H:30:ARG:HH12	1.73	0.52
1:A:58:PHE:CE1	1:A:275:PHE:HE2	2.28	0.52
1:A:347:PHE:O	1:A:348:ALA:C	2.47	0.52
1:B:94:SER:HB2	1:B:190:ARG:HB2	1.91	0.52
1:B:492:GLN:NE2	1:B:493:SER:H	2.08	0.52
1:C:188:ASN:O	1:C:207:HIS:HD2	1.92	0.52
1:C:403:LYS:HD2	1:C:504:HIS:NE2	2.24	0.52
1:C:409:GLN:O	1:C:411:ALA:N	2.41	0.52
1:C:497:ARG:HB3	1:C:498:PRO:CD	2.39	0.52
1:C:731:MET:HB2	1:C:955:ASN:HD21	1.74	0.52
1:C:739:THR:O	1:C:741:TYR:N	2.42	0.52
4:R:35:ASN:OD1	4:R:37:TYR:CE1	2.62	0.52
3:E:2:VAL:HG21	3:E:98:ARG:NH1	2.25	0.52
1:A:447:GLY:HA2	1:A:497:ARG:NE	2.24	0.52
1:B:37:TYR:O	1:B:38:TYR:C	2.47	0.52
1:B:130:VAL:HG23	1:B:169:GLU:OE2	2.10	0.52
1:B:321:GLN:HB2	1:B:630:PRO:CG	2.37	0.52
1:C:48:LEU:HG	1:C:278:LYS:HG3	1.92	0.52
1:C:189:LEU:HD22	1:C:210:ILE:HG22	1.92	0.52
1:C:759:PHE:O	1:C:760:CYS:C	2.47	0.52
2:Q:8:GLY:O	2:Q:9:ALA:C	2.47	0.52
2:D:100:PHE:O	2:D:103:GLY:N	2.40	0.52
4:F:6:THR:HB	4:F:100:GLN:HE22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:76:ILE:HD11	4:F:87:TYR:CE1	2.44	0.52
2:H:3:GLN:O	2:H:4:LEU:C	2.48	0.52
5:K:80:GLU:O	5:K:81:PRO:C	2.48	0.52
1:A:336:CYS:HB2	1:A:338:PHE:CG	2.44	0.52
1:A:453:TYR:C	1:A:491:LEU:HD22	2.30	0.52
1:B:353:TRP:CH2	1:B:423:TYR:HA	2.45	0.52
1:B:449:TYR:HD1	1:B:493:SER:HB2	1.74	0.52
1:B:521:ALA:O	1:B:522:THR:C	2.48	0.52
1:B:712:ILE:HG21	1:B:1096:VAL:HG12	1.91	0.52
1:C:384:PRO:O	1:C:387:LEU:HD22	2.08	0.52
1:C:435:ALA:HA	1:C:508:ARG:O	2.09	0.52
3:S:112:GLY:HA3	5:T:50:TYR:CE2	2.44	0.52
2:D:97:ALA:CB	2:D:115:TRP:HA	2.40	0.52
5:G:31:SER:O	5:G:33:SER:N	2.35	0.52
3:I:39:GLN:HB2	3:I:45:LEU:HD23	1.91	0.52
1:A:897:PRO:HG3	1:C:1077:THR:HG21	1.90	0.52
1:A:1139:ASP:CG	1:A:1142:GLN:HG2	2.30	0.52
1:B:429:PHE:O	1:B:430:THR:HB	2.10	0.52
1:B:457:ARG:HA	1:B:473:TYR:HB2	1.92	0.52
1:B:1088:HIS:CG	1:B:1137:VAL:HG21	2.45	0.52
1:C:501:GLY:HA2	3:I:100:TYR:O	2.09	0.52
2:Q:37:VAL:HB	2:Q:115:TRP:HZ3	1.74	0.52
3:S:51:ILE:HA	3:S:58:THR:HG22	1.92	0.52
2:D:34:ILE:O	2:D:99:LEU:HB2	2.09	0.52
3:E:13:LYS:O	3:E:14:PRO:C	2.47	0.52
3:E:13:LYS:O	3:E:15:GLY:N	2.42	0.52
3:E:36:TRP:CZ3	3:E:96:CYS:HB3	2.44	0.52
2:H:54:LEU:HD12	2:H:99:LEU:HD22	1.92	0.52
1:A:420:ASP:O	1:A:460:LYS:HA	2.09	0.52
1:B:533:VAL:HG11	1:B:536:LYS:HD2	1.92	0.52
1:C:113:LYS:O	1:C:132:GLU:HB3	2.10	0.52
3:S:88:SER:HA	3:S:125:VAL:HG21	1.92	0.52
2:D:39:GLN:HA	2:D:45:LEU:HA	1.91	0.52
3:E:27:TYR:CD1	3:E:32:TYR:CD2	2.98	0.52
5:G:72:PHE:N	5:G:72:PHE:CD1	2.78	0.52
2:H:33:VAL:HG12	2:H:98:ARG:HE	1.75	0.52
2:H:62:GLN:O	2:H:63:ALA:C	2.49	0.52
4:J:6:THR:H	4:J:25:GLN:CB	2.20	0.52
4:J:62:ARG:HD3	4:J:62:ARG:H	1.75	0.52
1:A:420:ASP:HA	1:A:460:LYS:HD3	1.92	0.52
1:B:426:PRO:HB3	1:B:463:PRO:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:ASN:C	1:B:441:LEU:H	2.13	0.52
1:B:825:LYS:HD2	1:B:939:PHE:HA	1.91	0.52
1:C:852:ALA:O	1:C:853:GLN:C	2.49	0.52
2:Q:3:GLN:O	2:Q:4:LEU:C	2.48	0.52
5:T:13:LEU:O	5:T:14:SER:C	2.47	0.52
5:T:22:SER:HA	5:T:73:THR:HA	1.92	0.52
5:T:35:ALA:CA	5:T:50:TYR:HA	2.30	0.52
3:E:39:GLN:HB2	3:E:45:LEU:HD23	1.92	0.52
3:I:6:GLN:HB2	3:I:119:GLN:HE22	1.75	0.52
3:I:110:LEU:HB2	3:I:116:ASN:ND2	2.24	0.52
1:A:480:CYS:O	1:A:483:LYS:HG2	2.10	0.52
1:A:767:LEU:HD23	1:A:770:ILE:HD12	1.91	0.52
1:A:825:LYS:HD3	1:A:945:LEU:HD13	1.92	0.52
1:B:64:TRP:CH2	1:B:213:ARG:HD2	2.36	0.52
1:B:119:ILE:O	1:B:120:VAL:HB	2.09	0.52
1:B:168:PHE:CG	1:B:169:GLU:N	2.75	0.52
1:B:210:ILE:HG22	1:B:212:GLY:O	2.10	0.52
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.91	0.52
1:B:398:ASP:OD2	1:B:511:VAL:HB	2.09	0.52
1:B:943:SER:O	1:B:944:ALA:C	2.48	0.52
1:C:377:PHE:HA	1:C:433:VAL:O	2.10	0.52
1:C:751:ASN:HA	1:C:754:LEU:HD11	1.90	0.52
5:T:50:TYR:C	5:T:52:ALA:N	2.63	0.52
2:D:106:ASN:O	2:D:107:SER:C	2.48	0.52
3:E:84:ARG:HB3	3:E:85:ARG:NE	2.25	0.52
1:A:230:ILE:HG22	1:A:231:GLY:H	1.75	0.51
1:A:237:PHE:O	1:A:238:GLN:HB3	2.09	0.51
1:B:269:TYR:O	1:B:270:LEU:C	2.47	0.51
1:C:28:TYR:HA	1:C:62:VAL:O	2.10	0.51
1:C:985:ASP:O	1:C:986:PRO:C	2.49	0.51
3:S:6:GLN:HB2	3:S:119:GLN:HE22	1.75	0.51
4:R:38:GLN:HG3	4:R:87:TYR:CE1	2.45	0.51
5:K:6:GLN:OE1	5:K:99:GLY:HA3	2.10	0.51
5:K:38:GLN:O	5:K:39:GLN:HB2	2.10	0.51
1:A:402:ILE:CD1	1:A:407:VAL:HA	2.37	0.51
1:A:496:PHE:O	1:A:497:ARG:HB2	2.10	0.51
1:A:561:PHE:CZ	1:B:224:PRO:HG2	2.45	0.51
1:A:1129:VAL:HG13	1:B:917:TYR:HB3	1.90	0.51
1:B:197:ILE:O	1:B:198:ASP:C	2.47	0.51
3:S:50:TRP:CZ2	3:S:100:TYR:CD1	2.98	0.51
2:D:97:ALA:HA	2:D:114:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:PHE:H	2:D:101:PRO:CD	2.12	0.51
4:J:77:SER:O	4:J:78:SER:C	2.47	0.51
1:A:472:ILE:HG13	1:A:490:PRO:CD	2.36	0.51
1:A:472:ILE:HA	1:A:490:PRO:CG	2.41	0.51
1:B:273:ARG:HB2	1:B:275:PHE:HE1	1.75	0.51
1:B:542:PHE:O	1:B:545:LEU:HG	2.10	0.51
1:B:714:ILE:HB	1:B:1075:PHE:CE2	2.45	0.51
1:B:850:ILE:O	1:B:852:ALA:N	2.43	0.51
1:C:410:ILE:HG22	1:C:425:LEU:CD2	2.29	0.51
1:C:741:TYR:OH	1:C:962:LEU:HD22	2.10	0.51
1:C:965:GLN:HG2	1:C:970:PHE:HZ	1.75	0.51
1:C:979:ASP:O	1:C:980:ILE:C	2.47	0.51
4:R:10:SER:O	4:R:11:SER:C	2.48	0.51
2:D:3:GLN:O	2:D:4:LEU:C	2.48	0.51
2:D:95:PHE:CD1	4:F:45:PRO:HG2	2.45	0.51
4:F:86:THR:HB	4:F:88:TYR:CE1	2.46	0.51
5:K:29:VAL:HG13	5:K:33:SER:HB2	1.92	0.51
1:A:330:PRO:HG2	1:A:527:LYS:HB2	1.92	0.51
1:A:827:THR:C	1:A:828:LEU:HG	2.28	0.51
1:B:209:PRO:O	1:B:210:ILE:C	2.48	0.51
1:B:352:ALA:O	1:B:353:TRP:C	2.49	0.51
1:B:448:ASN:HB3	1:B:496:PHE:CE1	2.45	0.51
1:B:748:GLU:HB3	1:B:751:ASN:HD21	1.74	0.51
1:C:546:THR:O	1:C:547:GLY:C	2.49	0.51
4:R:7:GLN:NE2	4:R:88:TYR:HA	2.26	0.51
4:R:37:TYR:CZ	4:R:98:PHE:CE2	2.99	0.51
2:D:97:ALA:HB2	2:D:115:TRP:CE3	2.46	0.51
3:E:59:ASN:ND2	3:E:60:TYR:H	2.07	0.51
4:F:63:PHE:N	4:F:63:PHE:HD1	2.08	0.51
4:F:93:ASP:O	4:F:95:SER:N	2.39	0.51
2:H:100:PHE:HB2	2:H:111:GLY:O	2.10	0.51
1:A:39:PRO:HD2	1:A:285:ILE:CD1	2.40	0.51
1:A:305:SER:C	1:A:307:THR:H	2.14	0.51
1:A:341:VAL:HG21	1:A:397:ALA:HB1	1.92	0.51
1:A:454:ARG:HH12	1:A:469:SER:N	2.08	0.51
1:A:485:PRO:C	1:A:487:CYS:H	2.14	0.51
1:A:763:LEU:HD21	1:A:1005:GLN:HG3	1.93	0.51
1:A:898:PHE:O	1:A:900:MET:N	2.44	0.51
1:B:305:SER:OG	1:B:306:PHE:N	2.41	0.51
1:B:409:GLN:HB3	1:B:418:ILE:HB	1.93	0.51
1:B:477:ASN:HA	1:B:485:PRO:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:PHE:HZ	1:B:574:ALA:HB3	1.75	0.51
1:C:37:TYR:O	1:C:39:PRO:N	2.43	0.51
1:C:187:LYS:HD3	1:C:209:PRO:CB	2.40	0.51
1:C:540:PHE:HZ	1:C:578:PRO:HD3	1.76	0.51
1:C:833:PHE:CD1	1:C:836:GLN:HA	2.46	0.51
2:Q:34:ILE:H	2:Q:54:LEU:HB3	1.75	0.51
2:H:105:PRO:CD	2:H:110:ASP:HB2	2.40	0.51
3:I:35:SER:H	3:I:97:ALA:HB1	1.73	0.51
4:J:29:ASP:OD1	4:J:91:ARG:HG2	2.10	0.51
5:K:86:VAL:HG22	5:K:103:LYS:HD3	1.91	0.51
1:A:86:PHE:H	1:A:236:ARG:HA	1.75	0.51
1:A:90:VAL:C	1:A:92:PHE:H	2.14	0.51
1:A:500:TYR:O	3:E:101:THR:OG1	2.29	0.51
1:A:528:LYS:NZ	1:A:529:SER:H	2.09	0.51
1:B:120:VAL:HG11	1:B:127:PHE:CE2	2.46	0.51
1:B:295:PRO:HG3	1:B:635:TYR:CD1	2.46	0.51
1:B:436:TRP:O	1:B:508:ARG:HB2	2.09	0.51
1:B:938:LEU:HD11	1:B:1061:VAL:HG11	1.93	0.51
1:C:37:TYR:O	1:C:38:TYR:C	2.48	0.51
4:R:31:GLY:O	4:R:91:ARG:NH1	2.43	0.51
5:T:6:GLN:OE1	5:T:88:TYR:HA	2.10	0.51
5:T:80:GLU:O	5:T:81:PRO:C	2.48	0.51
2:D:25:SER:O	2:D:27:GLY:N	2.43	0.51
2:D:69:MET:HG3	5:G:28:THR:CB	2.40	0.51
3:E:108:GLU:O	3:E:110:LEU:N	2.43	0.51
2:H:74:GLU:O	2:H:77:SER:N	2.44	0.51
5:K:55:ARG:HH12	5:K:58:GLY:H	1.58	0.51
1:A:38:TYR:O	1:A:39:PRO:C	2.49	0.51
1:A:438:SER:CB	1:A:508:ARG:HD2	2.40	0.51
1:A:897:PRO:HG3	1:C:1077:THR:CG2	2.41	0.51
1:A:1040:VAL:HB	1:B:1030:SER:O	2.11	0.51
1:B:208:THR:C	1:B:210:ILE:H	2.14	0.51
1:B:1040:VAL:HB	1:C:1030:SER:O	2.11	0.51
1:C:104:TRP:H	1:C:119:ILE:HG23	1.74	0.51
1:C:987:PRO:HG2	1:C:988:GLU:OE1	2.11	0.51
3:S:13:LYS:O	3:S:15:GLY:N	2.39	0.51
3:S:41:PRO:O	3:S:42:GLY:C	2.49	0.51
5:T:51:GLY:O	5:T:52:ALA:HB3	2.11	0.51
2:D:17:SER:CB	2:D:85:SER:H	2.24	0.51
5:G:49:ILE:HA	5:G:55:ARG:CA	2.36	0.51
3:I:41:PRO:O	3:I:42:GLY:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:TYR:CD1	1:A:265:TYR:N	2.79	0.51
1:A:528:LYS:HZ2	1:A:529:SER:H	1.59	0.51
1:A:748:GLU:O	1:A:752:LEU:HD12	2.10	0.51
1:B:472:ILE:H	1:B:483:LYS:HE3	1.75	0.51
1:B:1048:HIS:HA	1:B:1066:THR:HG22	1.93	0.51
1:C:64:TRP:CE3	1:C:65:PHE:N	2.79	0.51
1:C:522:THR:O	1:C:523:VAL:C	2.49	0.51
2:Q:25:SER:C	2:Q:27:GLY:N	2.64	0.51
2:Q:25:SER:O	2:Q:27:GLY:N	2.43	0.51
5:T:47:LEU:HD23	5:T:48:LEU:H	1.76	0.51
2:H:24:ALA:HB3	2:H:77:SER:CB	2.39	0.51
3:I:50:TRP:CZ3	5:K:95:SER:HA	2.45	0.51
1:A:239:THR:O	1:A:240:LEU:C	2.49	0.51
1:A:440:LYS:HZ1	5:G:93:ASP:HB3	1.75	0.51
1:A:500:TYR:O	3:E:102:ARG:NE	2.44	0.51
1:A:625:ALA:HB3	1:A:630:PRO:N	2.26	0.51
1:A:833:PHE:CE1	1:A:836:GLN:HA	2.46	0.51
1:B:339:HIS:HA	1:B:342:PHE:HB3	1.93	0.51
1:B:802:PHE:CE1	1:B:927:PHE:HE2	2.28	0.51
3:S:12:LYS:HD3	3:S:16:ALA:HB3	1.93	0.51
4:F:63:PHE:N	4:F:63:PHE:CD1	2.79	0.51
2:H:25:SER:O	2:H:27:GLY:N	2.43	0.51
4:J:40:LYS:O	4:J:43:LYS:HB2	2.11	0.51
1:A:129:LYS:CB	1:A:169:GLU:HG2	2.40	0.51
1:A:343:ASN:ND2	2:D:52:ILE:HB	2.26	0.51
1:A:453:TYR:HE2	1:A:455:LEU:HD22	1.75	0.51
1:A:504:HIS:ND1	1:A:504:HIS:N	2.58	0.51
1:A:615:ASN:O	1:A:616:CYS:C	2.48	0.51
1:B:91:TYR:CG	1:B:91:TYR:O	2.63	0.51
1:B:114:THR:HG22	1:B:232:ILE:HD11	1.93	0.51
1:B:370:ASN:OD1	2:Q:52:ILE:HB	2.11	0.51
1:B:439:ASN:HB2	1:B:505:GLN:NE2	2.14	0.51
1:B:496:PHE:HB2	1:B:505:GLN:CA	2.39	0.51
1:C:310:LYS:HA	1:C:598:THR:O	2.10	0.51
1:C:887:THR:HG21	1:C:894:LEU:HD12	1.93	0.51
1:C:1132:ILE:HG23	1:C:1133:VAL:N	2.26	0.51
2:Q:91:THR:HA	2:Q:121:VAL:O	2.10	0.51
4:R:76:ILE:HD11	4:R:87:TYR:CE1	2.45	0.51
5:T:38:GLN:HG2	5:T:46:ARG:NH1	2.26	0.51
3:E:12:LYS:HD3	3:E:13:LYS:H	1.76	0.51
3:E:101:THR:OG1	3:E:102:ARG:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:60:PRO:HA	4:F:63:PHE:CD2	2.46	0.51
2:H:25:SER:C	2:H:27:GLY:N	2.65	0.51
4:J:93:ASP:C	4:J:95:SER:H	2.13	0.51
5:K:51:GLY:O	5:K:52:ALA:HB3	2.11	0.51
1:A:541:ASN:O	1:A:542:PHE:C	2.49	0.50
1:A:831:ALA:C	1:A:833:PHE:H	2.14	0.50
1:A:866:THR:C	1:A:868:GLU:H	2.13	0.50
1:B:215:PHE:CZ	1:B:218:GLY:HA3	2.46	0.50
1:B:347:PHE:O	1:B:400:PHE:HA	2.11	0.50
1:B:553:LYS:HD2	1:B:554:SER:H	1.76	0.50
1:B:770:ILE:HG23	1:B:1015:ALA:CB	2.41	0.50
1:B:935:GLN:O	1:B:936:ASP:C	2.49	0.50
1:B:948:LEU:HD21	1:B:1059:GLY:HA3	1.93	0.50
1:B:1102:TRP:CZ2	1:B:1133:VAL:HG11	2.46	0.50
1:C:128:ILE:HG21	1:C:170:TYR:HB3	1.93	0.50
1:C:197:ILE:HG13	1:C:202:LYS:NZ	2.25	0.50
1:C:364:ASP:C	1:C:366:SER:H	2.13	0.50
1:C:438:SER:N	1:C:506:PRO:O	2.44	0.50
1:C:510:VAL:HG12	1:C:512:LEU:HD23	1.93	0.50
1:C:533:VAL:HG23	1:C:534:LYS:HG2	1.92	0.50
2:Q:36:TRP:N	2:Q:49:GLY:HA3	2.26	0.50
3:S:98:ARG:CG	3:S:116:ASN:HB2	2.41	0.50
2:D:52:ILE:CD1	4:F:94:PRO:HD3	2.41	0.50
5:G:34:LEU:HD22	5:G:72:PHE:CG	2.46	0.50
2:H:99:LEU:HA	2:H:112:PHE:CD1	2.45	0.50
3:I:23:LYS:HA	3:I:77:THR:O	2.12	0.50
3:I:39:GLN:HB2	3:I:95:TYR:HE2	1.76	0.50
1:A:193:VAL:O	1:A:194:PHE:C	2.46	0.50
1:A:405:ASN:ND2	1:A:504:HIS:HB3	2.26	0.50
1:B:104:TRP:CE3	1:B:119:ILE:HG21	2.37	0.50
1:C:36:VAL:O	1:C:221:ALA:HA	2.10	0.50
1:C:214:ASP:O	1:C:215:PHE:C	2.49	0.50
1:C:456:PHE:HB2	1:C:473:TYR:CZ	2.46	0.50
1:C:478:LYS:O	1:C:479:PRO:C	2.49	0.50
1:C:502:VAL:HG12	3:I:100:TYR:CB	2.40	0.50
4:R:36:TRP:HB2	4:R:49:ILE:HB	1.91	0.50
5:T:62:ARG:CZ	5:T:62:ARG:HB2	2.41	0.50
2:D:36:TRP:CD1	2:D:36:TRP:N	2.78	0.50
5:G:63:PHE:HD2	5:G:76:ILE:HD12	1.76	0.50
3:I:18:VAL:O	3:I:82:GLU:HA	2.10	0.50
5:K:2:ILE:HG22	5:K:25:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:79:LEU:HD13	5:K:84:PHE:HE1	1.77	0.50
1:A:37:TYR:O	1:A:39:PRO:N	2.44	0.50
1:A:85:PRO:O	1:A:87:ASN:N	2.43	0.50
1:A:911:VAL:HG12	1:A:915:VAL:HG21	1.92	0.50
1:B:472:ILE:CG2	1:B:484:GLY:HA3	2.41	0.50
1:C:319:ARG:O	1:C:320:VAL:C	2.49	0.50
1:C:421:TYR:HD1	1:C:457:ARG:HH12	1.60	0.50
1:C:559:LEU:HG	1:C:562:GLN:NE2	2.26	0.50
1:C:743:CYS:C	1:C:745:ASP:H	2.15	0.50
1:C:822:LEU:HD23	1:C:945:LEU:HD11	1.93	0.50
2:Q:33:VAL:HG22	2:Q:100:PHE:H	1.77	0.50
5:T:35:ALA:HB2	5:T:92:HIS:CE1	2.47	0.50
5:T:38:GLN:HG2	5:T:46:ARG:NE	2.26	0.50
2:D:45:LEU:HB3	4:F:98:PHE:CD2	2.47	0.50
4:F:15:SER:HB2	4:F:106:ILE:HD11	1.92	0.50
5:G:59:ILE:HG22	5:G:63:PHE:HD1	1.76	0.50
3:I:88:SER:HA	3:I:125:VAL:HG21	1.92	0.50
3:I:114:PHE:HB2	5:K:37:TYR:OH	2.12	0.50
5:K:36:TRP:O	5:K:48:LEU:HG	2.11	0.50
1:A:29:THR:O	1:A:62:VAL:N	2.33	0.50
1:A:195:LYS:HE3	1:A:197:ILE:HD13	1.93	0.50
1:A:215:PHE:C	1:A:217:GLN:H	2.14	0.50
1:A:568:ILE:O	1:A:569:VAL:C	2.50	0.50
1:B:120:VAL:HG11	1:B:127:PHE:CZ	2.47	0.50
1:B:567:ASP:OD2	1:B:569:VAL:HG22	2.11	0.50
1:C:41:LYS:O	1:C:42:VAL:C	2.50	0.50
1:C:292:ALA:O	1:C:294:ASP:N	2.45	0.50
1:C:441:LEU:HB2	2:H:55:PHE:HE2	1.76	0.50
1:C:624:HIS:CG	1:C:625:ALA:N	2.79	0.50
2:Q:97:ALA:HA	2:Q:115:TRP:HA	1.93	0.50
5:T:28:THR:O	5:T:29:VAL:C	2.50	0.50
2:D:30:ARG:NE	2:D:78:THR:O	2.44	0.50
2:D:86:LEU:HB3	2:D:90:ASP:OD2	2.11	0.50
5:K:72:PHE:N	5:K:72:PHE:CD1	2.78	0.50
1:A:338:PHE:CZ	1:A:363:ALA:HB1	2.47	0.50
1:A:391:CYS:HB2	1:A:521:ALA:CB	2.42	0.50
1:A:521:ALA:O	1:A:522:THR:C	2.50	0.50
1:B:106:PHE:HA	1:B:236:ARG:O	2.10	0.50
1:B:343:ASN:HD22	1:B:343:ASN:H	1.58	0.50
1:B:362:VAL:HG13	1:B:526:PRO:HD3	1.93	0.50
1:B:367:VAL:C	1:B:369:TYR:N	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:HIS:O	1:B:624:HIS:CG	2.63	0.50
1:B:986:PRO:HB2	1:B:987:PRO:CD	2.40	0.50
1:C:327:VAL:HG21	1:C:532:LEU:H	1.76	0.50
1:C:342:PHE:C	1:C:343:ASN:HD22	2.14	0.50
1:C:400:PHE:HE2	1:C:423:TYR:HD2	1.59	0.50
1:C:623:ILE:O	1:C:624:HIS:C	2.50	0.50
3:S:63:LYS:O	3:S:64:PHE:C	2.50	0.50
4:R:90:GLN:NE2	4:R:91:ARG:H	2.09	0.50
5:T:59:ILE:O	5:T:60:PRO:C	2.50	0.50
2:D:38:ARG:HB2	2:D:48:MET:CB	2.42	0.50
2:D:73:ASP:O	2:D:75:SER:N	2.44	0.50
2:D:102:ASN:ND2	2:D:109:GLU:HB3	2.26	0.50
5:G:61:ASP:O	5:G:62:ARG:C	2.50	0.50
4:J:14:ALA:O	4:J:106:ILE:HA	2.12	0.50
4:J:49:ILE:HG23	4:J:55:LEU:HD23	1.93	0.50
1:A:644:THR:HG22	1:A:646:ALA:N	2.26	0.50
1:A:948:LEU:CD2	1:A:1059:GLY:HA3	2.42	0.50
1:B:454:ARG:HD3	1:B:457:ARG:HD3	1.92	0.50
1:B:1116:THR:H	1:B:1119:ASN:HD21	1.59	0.50
1:C:131:CYS:HA	1:C:165:ASN:O	2.12	0.50
1:C:439:ASN:O	1:C:441:LEU:N	2.44	0.50
1:C:457:ARG:HH11	1:C:458:LYS:H	1.58	0.50
1:C:616:CYS:HB2	1:C:643:GLN:HG3	1.94	0.50
1:C:951:VAL:C	1:C:953:ASN:H	2.14	0.50
5:T:11:LEU:HB3	5:T:104:VAL:HA	1.94	0.50
2:D:57:THR:O	2:D:58:THR:HB	2.12	0.50
4:F:62:ARG:HB2	4:F:77:SER:HB2	1.92	0.50
5:G:49:ILE:HD12	5:G:49:ILE:H	1.77	0.50
3:I:73:ASP:O	3:I:76:THR:N	2.45	0.50
1:A:312:ILE:HG13	1:A:595:SER:HB3	1.94	0.50
1:A:398:ASP:O	1:A:510:VAL:HA	2.12	0.50
1:A:409:GLN:HG2	1:A:418:ILE:HB	1.92	0.50
1:B:849:LEU:HG	1:B:851:CYS:SG	2.52	0.50
1:B:888:PHE:CZ	1:B:1034:LEU:HG	2.46	0.50
1:C:404:GLY:C	1:C:406:GLU:N	2.65	0.50
1:C:739:THR:O	1:C:740:MET:C	2.50	0.50
1:C:749:CYS:O	1:C:752:LEU:HB2	2.12	0.50
2:Q:34:ILE:HG22	2:Q:56:GLY:H	1.75	0.50
2:Q:78:THR:HB	2:Q:80:TYR:HE2	1.76	0.50
3:S:32:TYR:CE1	3:S:102:ARG:HA	2.47	0.50
4:R:9:PRO:O	4:R:11:SER:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:38:GLN:HG3	4:R:87:TYR:CZ	2.47	0.50
3:I:83:LEU:HD23	3:I:86:LEU:HD22	1.92	0.50
5:K:93:ASP:O	5:K:95:SER:N	2.45	0.50
1:A:353:TRP:HB3	1:A:423:TYR:CD2	2.46	0.50
1:A:748:GLU:CD	1:A:748:GLU:H	2.12	0.50
1:B:38:TYR:OH	1:B:284:THR:HA	2.11	0.50
1:B:312:ILE:CG1	1:B:595:SER:HB2	2.42	0.50
1:B:403:LYS:HB3	1:B:494:TYR:CE1	2.45	0.50
1:B:818:ILE:O	1:B:818:ILE:HG22	2.12	0.50
1:C:633:ARG:NH1	1:C:633:ARG:HA	2.27	0.50
1:C:896:ILE:O	1:C:897:PRO:C	2.49	0.50
4:R:61:SER:O	4:R:63:PHE:N	2.40	0.50
3:E:23:LYS:HA	3:E:77:THR:O	2.11	0.50
5:K:28:THR:O	5:K:29:VAL:C	2.50	0.50
1:A:192:PHE:HB3	1:A:194:PHE:CE1	2.46	0.50
1:A:722:VAL:HG23	1:A:930:ALA:CB	2.41	0.50
1:A:753:LEU:HD11	1:A:1001:LEU:HD12	1.94	0.50
1:A:1030:SER:O	1:C:1040:VAL:HB	2.11	0.50
1:B:115:GLN:O	1:B:116:SER:C	2.49	0.50
1:B:337:PRO:CG	1:B:358:ILE:HG21	2.42	0.50
1:B:343:ASN:ND2	1:B:371:PHE:HE1	2.10	0.50
1:B:353:TRP:HH2	1:B:461:LEU:CB	2.25	0.50
1:B:356:THR:HB	1:B:396:TYR:CB	2.40	0.50
1:B:398:ASP:N	1:B:511:VAL:O	2.45	0.50
1:B:452:TRP:HA	1:B:493:SER:CA	2.35	0.50
1:B:738:CYS:C	1:B:740:MET:H	2.14	0.50
1:B:977:LEU:CD2	1:B:996:LEU:HD23	2.42	0.50
1:B:977:LEU:O	1:B:981:LEU:HB2	2.12	0.50
1:C:502:VAL:HG12	3:I:100:TYR:HB3	1.94	0.50
1:C:773:GLU:C	1:C:775:ASP:H	2.15	0.50
3:S:19:LYS:CG	3:S:82:GLU:HB3	2.40	0.50
4:R:12:LEU:HD13	4:R:104:VAL:HG22	1.94	0.50
5:T:25:ALA:C	5:T:27:GLN:H	2.15	0.50
4:F:92:TYR:HA	4:F:96:TYR:HD1	1.77	0.50
2:H:51:PHE:N	2:H:54:LEU:HD11	2.26	0.50
1:A:294:ASP:HB2	1:A:295:PRO:CD	2.42	0.49
1:A:354:ASN:H	1:A:466:ARG:HH12	1.58	0.49
1:A:408:SER:C	1:A:410:ILE:H	2.13	0.49
1:A:551:LEU:HB3	1:A:584:LEU:HD23	1.93	0.49
1:A:554:SER:HB2	1:A:585:ASP:CB	2.42	0.49
1:A:569:VAL:HG11	1:B:963:VAL:HG12	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ASP:O	1:A:739:THR:N	2.45	0.49
1:A:755:GLN:C	1:A:757:GLY:H	2.15	0.49
1:A:972:ALA:HB2	1:A:995:ARG:HB3	1.94	0.49
1:B:344:ALA:HA	2:Q:104:ASP:CA	2.42	0.49
1:B:347:PHE:CZ	1:B:508:ARG:HG3	2.47	0.49
1:B:351:TYR:CD2	1:B:491:LEU:HB3	2.47	0.49
1:B:386:LYS:CA	1:B:389:ASP:HB2	2.41	0.49
1:B:418:ILE:HD11	1:B:494:TYR:OH	2.12	0.49
1:B:740:MET:O	1:B:740:MET:HG3	2.11	0.49
1:C:479:PRO:O	1:C:481:LYS:N	2.45	0.49
1:C:1048:HIS:HE1	1:C:1051:SER:HB2	1.77	0.49
4:R:38:GLN:NE2	4:R:87:TYR:OH	2.44	0.49
2:D:25:SER:C	2:D:27:GLY:N	2.64	0.49
2:D:74:GLU:HB2	2:D:78:THR:O	2.12	0.49
3:E:4:LEU:HD13	3:E:22:CYS:SG	2.52	0.49
5:G:56:ALA:H	5:G:59:ILE:CG1	2.10	0.49
2:H:17:SER:CB	2:H:85:SER:H	2.25	0.49
2:H:18:VAL:HG11	2:H:121:VAL:HG21	1.93	0.49
2:H:51:PHE:HB3	2:H:59:ILE:HG21	1.94	0.49
2:H:102:ASN:ND2	2:H:109:GLU:OE1	2.44	0.49
1:A:203:ILE:HD11	1:A:228:LEU:HD11	1.94	0.49
1:A:296:LEU:O	1:A:299:THR:N	2.41	0.49
1:A:351:TYR:CG	1:A:491:LEU:HD11	2.47	0.49
1:A:363:ALA:HB2	1:A:523:VAL:HG23	1.94	0.49
1:A:408:SER:O	1:A:409:GLN:C	2.51	0.49
1:B:335:LEU:O	1:B:362:VAL:N	2.44	0.49
1:B:375:PHE:CD1	1:B:435:ALA:HB3	2.48	0.49
1:B:470:THR:O	1:B:471:GLU:C	2.50	0.49
1:B:726:ILE:HG12	1:B:945:LEU:HD23	1.93	0.49
1:B:1028:LYS:HG2	1:B:1032:CYS:SG	2.52	0.49
1:C:27:SER:HB2	1:C:64:TRP:CB	2.38	0.49
1:C:318:PHE:CZ	1:C:592:GLY:HA3	2.47	0.49
1:C:360:ASN:HA	1:C:522:THR:OG1	2.12	0.49
1:C:421:TYR:HA	1:C:457:ARG:NH2	2.26	0.49
1:C:441:LEU:HD22	2:H:32:HIS:HB3	1.94	0.49
1:C:479:PRO:HA	1:C:483:LYS:NZ	2.27	0.49
1:C:480:CYS:HA	1:C:484:GLY:O	2.12	0.49
1:C:617:THR:HA	1:C:620:SER:OG	2.12	0.49
2:Q:33:VAL:O	2:Q:33:VAL:HG13	2.11	0.49
3:S:115:ASP:CB	3:S:117:TRP:HD1	2.25	0.49
4:R:22:ILE:HG12	4:R:74:PHE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:HIS:ND1	2:D:55:PHE:HB2	2.27	0.49
3:E:115:ASP:HA	3:E:117:TRP:CD1	2.44	0.49
4:F:34:LEU:HG	4:F:74:PHE:CZ	2.47	0.49
4:J:62:ARG:HH12	4:J:76:ILE:CG2	2.24	0.49
5:K:24:ARG:HG3	5:K:71:ASP:CB	2.42	0.49
5:K:37:TYR:O	5:K:48:LEU:HD21	2.12	0.49
1:A:43:PHE:CG	1:A:43:PHE:O	2.63	0.49
1:A:409:GLN:O	1:A:419:ALA:HB2	2.13	0.49
1:A:441:LEU:HD13	2:D:54:LEU:O	2.12	0.49
1:A:834:ILE:HD11	1:C:647:GLY:CA	2.41	0.49
1:A:854:LYS:HB3	1:C:591:PHE:CE1	2.48	0.49
1:B:130:VAL:HG21	1:B:168:PHE:CD1	2.45	0.49
1:B:440:LYS:NZ	2:Q:71:SER:HA	2.28	0.49
1:C:168:PHE:CD2	1:C:230:ILE:HD13	2.47	0.49
1:C:410:ILE:HG21	1:C:423:TYR:CD1	2.47	0.49
1:C:956:ALA:C	1:C:958:ALA:N	2.66	0.49
4:R:16:VAL:CG1	4:R:81:PRO:HG3	2.38	0.49
4:R:30:ILE:HG12	4:R:31:GLY:N	2.27	0.49
4:R:48:LEU:O	4:R:56:GLU:HB3	2.12	0.49
3:I:34:ILE:HG23	3:I:97:ALA:HB3	1.94	0.49
3:I:48:MET:CB	3:I:81:MET:HE1	2.40	0.49
3:I:106:PHE:HD2	3:I:109:SER:N	2.10	0.49
4:J:4:GLN:O	4:J:6:THR:HG23	2.11	0.49
1:A:128:ILE:HG12	1:A:170:TYR:HD2	1.77	0.49
1:A:392:PHE:HA	1:A:516:LEU:HD22	1.94	0.49
1:A:441:LEU:HB2	2:D:55:PHE:HB3	1.93	0.49
1:A:872:GLN:HB2	1:C:699:LEU:CD1	2.41	0.49
1:B:193:VAL:O	1:B:194:PHE:C	2.50	0.49
1:B:344:ALA:HA	2:Q:103:GLY:C	2.33	0.49
1:B:478:LYS:O	1:B:479:PRO:C	2.50	0.49
1:B:644:THR:HG22	1:B:645:ARG:H	1.76	0.49
1:C:215:PHE:O	1:C:217:GLN:N	2.46	0.49
1:C:367:VAL:O	1:C:368:LEU:HD12	2.12	0.49
1:C:457:ARG:NE	1:C:458:LYS:H	2.11	0.49
1:C:836:GLN:HB3	1:C:849:LEU:CD2	2.40	0.49
1:C:849:LEU:HB3	1:C:852:ALA:HB2	1.93	0.49
3:S:23:LYS:HA	3:S:77:THR:O	2.12	0.49
3:S:29:PHE:CD2	3:S:77:THR:HA	2.47	0.49
3:S:36:TRP:CZ3	3:S:96:CYS:HB3	2.48	0.49
2:H:30:ARG:NH2	2:H:75:SER:HA	2.28	0.49
3:I:11:VAL:O	3:I:12:LYS:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:47:TRP:HZ2	3:I:50:TRP:HE3	1.60	0.49
3:I:63:LYS:O	3:I:64:PHE:C	2.50	0.49
4:J:14:ALA:HB2	4:J:104:VAL:HG13	1.95	0.49
1:A:386:LYS:CA	1:A:389:ASP:HB2	2.42	0.49
1:B:959:LEU:O	1:B:963:VAL:HG23	2.13	0.49
1:B:973:ILE:HD11	1:B:980:ILE:HG23	1.94	0.49
1:C:91:TYR:HE2	1:C:215:PHE:CZ	2.31	0.49
1:C:194:PHE:CE1	1:C:203:ILE:HG23	2.47	0.49
1:C:324:GLU:O	1:C:326:ILE:N	2.43	0.49
1:C:357:ARG:HG2	1:C:358:ILE:N	2.27	0.49
1:C:471:GLU:C	1:C:490:PRO:HD3	2.33	0.49
1:C:577:ASP:HB2	1:C:582:GLU:N	2.28	0.49
1:C:577:ASP:H	1:C:582:GLU:N	2.10	0.49
1:C:898:PHE:O	1:C:900:MET:N	2.46	0.49
1:C:1095:PHE:CD1	1:C:1104:VAL:HG22	2.47	0.49
2:Q:2:VAL:HB	2:Q:30:ARG:NH2	2.27	0.49
2:Q:62:GLN:O	2:Q:63:ALA:C	2.50	0.49
4:R:42:GLY:O	4:R:43:LYS:HB2	2.12	0.49
5:T:86:VAL:HA	5:T:102:THR:O	2.12	0.49
2:D:40:ALA:O	2:D:42:GLY:N	2.46	0.49
3:E:63:LYS:O	3:E:64:PHE:C	2.50	0.49
3:E:73:ASP:O	3:E:76:THR:N	2.45	0.49
3:I:7:SER:HB3	3:I:21:SER:HB3	1.95	0.49
4:J:93:ASP:H	4:J:96:TYR:HE1	1.59	0.49
5:K:6:GLN:NE2	5:K:102:THR:HG22	2.28	0.49
5:K:96:LEU:O	5:K:97:THR:C	2.50	0.49
1:A:112:SER:CB	1:A:134:GLN:HA	2.42	0.49
1:A:214:ASP:HA	1:A:266:TYR:CE2	2.47	0.49
1:A:502:VAL:HB	3:E:100:TYR:HA	1.94	0.49
1:B:92:PHE:HD1	1:B:93:ALA:H	1.59	0.49
1:B:127:PHE:HA	1:B:171:VAL:HG13	1.95	0.49
1:B:428:ASP:O	1:B:429:PHE:C	2.50	0.49
1:B:437:ASN:ND2	1:B:508:ARG:HD3	2.28	0.49
1:B:444:LYS:O	1:B:446:SER:N	2.45	0.49
1:B:449:TYR:CE2	1:B:495:GLY:HA2	2.47	0.49
1:B:454:ARG:HG3	1:B:490:PRO:C	2.32	0.49
1:B:472:ILE:HG22	1:B:484:GLY:HA3	1.95	0.49
1:B:759:PHE:H	1:B:762:GLN:HE21	1.61	0.49
1:C:462:LYS:HE2	1:C:462:LYS:N	2.22	0.49
1:C:831:ALA:CB	1:C:851:CYS:HB2	2.43	0.49
1:C:939:PHE:CG	1:C:940:SER:N	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:SER:OG	2:D:8:GLY:N	2.46	0.49
3:E:41:PRO:O	3:E:42:GLY:C	2.49	0.49
4:F:15:SER:HB2	4:F:106:ILE:HD12	1.93	0.49
5:G:20:THR:HA	5:G:74:LEU:O	2.13	0.49
4:J:34:LEU:HD12	4:J:34:LEU:O	2.13	0.49
1:A:271:GLN:NE2	1:A:273:ARG:HD3	2.26	0.49
1:A:328:ARG:HD3	1:A:328:ARG:HA	1.50	0.49
1:A:726:ILE:CG2	1:A:948:LEU:HG	2.43	0.49
1:B:21:LEU:HG	1:B:23:THR:HG23	1.94	0.49
1:B:86:PHE:HE2	1:B:196:ASN:N	2.09	0.49
1:B:127:PHE:HD1	1:B:128:ILE:O	1.95	0.49
1:B:228:LEU:O	1:B:230:ILE:N	2.45	0.49
1:B:321:GLN:O	1:B:322:PRO:C	2.51	0.49
1:B:330:PRO:CA	1:B:579:GLN:HE22	2.25	0.49
1:B:368:LEU:HD12	1:B:371:PHE:CZ	2.48	0.49
1:B:619:VAL:C	1:B:621:VAL:N	2.66	0.49
1:C:404:GLY:O	1:C:407:VAL:HG23	2.12	0.49
4:R:37:TYR:HE1	4:R:90:GLN:CB	2.16	0.49
2:D:99:LEU:HA	2:D:112:PHE:CE1	2.47	0.49
4:F:63:PHE:CE1	4:F:76:ILE:HG23	2.46	0.49
2:H:38:ARG:HB2	2:H:48:MET:SD	2.53	0.49
4:J:59:VAL:HG22	4:J:63:PHE:CZ	2.47	0.49
5:K:34:LEU:HD22	5:K:72:PHE:CG	2.48	0.49
1:A:336:CYS:C	1:A:338:PHE:N	2.62	0.49
1:A:479:PRO:C	1:A:481:LYS:H	2.16	0.49
1:B:120:VAL:HG12	1:B:127:PHE:O	2.13	0.49
1:B:139:PRO:O	1:B:140:PHE:HD1	1.96	0.49
1:B:187:LYS:HZ3	1:B:188:ASN:HB3	1.75	0.49
1:B:330:PRO:HA	1:B:579:GLN:OE1	2.13	0.49
1:B:741:TYR:CZ	1:B:966:LEU:HD13	2.48	0.49
1:C:347:PHE:HB2	1:C:401:VAL:CG2	2.42	0.49
3:S:73:ASP:O	3:S:76:THR:N	2.45	0.49
4:R:19:ARG:HG2	4:R:76:ILE:O	2.12	0.49
2:D:40:ALA:O	2:D:41:PRO:C	2.51	0.49
4:F:81:PRO:CA	4:F:106:ILE:HG12	2.41	0.49
5:G:47:LEU:HD21	5:G:50:TYR:CD2	2.48	0.49
5:G:93:ASP:O	5:G:94:THR:C	2.51	0.49
2:H:33:VAL:HG13	2:H:99:LEU:CB	2.42	0.49
2:H:60:TYR:CE1	2:H:69:MET:HA	2.47	0.49
3:I:29:PHE:CD2	3:I:77:THR:HA	2.48	0.49
3:I:108:GLU:O	3:I:110:LEU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:7:SER:O	5:K:8:PRO:C	2.51	0.49
1:A:165:ASN:O	1:A:166:CYS:C	2.51	0.49
1:A:339:HIS:HB3	1:A:343:ASN:OD1	2.13	0.49
1:A:351:TYR:CD2	1:A:491:LEU:HD11	2.47	0.49
1:A:454:ARG:HH12	1:A:468:ILE:C	2.16	0.49
1:B:26:GLN:O	1:B:27:SER:HB2	2.13	0.49
1:B:112:SER:H	1:B:113:LYS:HZ1	1.61	0.49
1:B:324:GLU:HB2	1:B:536:LYS:CD	2.42	0.49
1:B:395:VAL:HG13	1:B:514:PHE:HA	1.95	0.49
1:B:438:SER:HA	1:B:506:PRO:O	2.12	0.49
1:B:462:LYS:H	1:B:465:GLU:HB2	1.77	0.49
1:B:737:ASP:O	1:B:739:THR:N	2.46	0.49
1:B:877:LEU:HD13	1:B:1029:MET:HE1	1.95	0.49
1:C:328:ARG:CD	1:C:542:PHE:HB2	2.43	0.49
1:C:455:LEU:HB2	1:C:492:GLN:NE2	2.28	0.49
1:C:539:ASN:ND2	1:C:548:THR:HG23	2.27	0.49
1:C:985:ASP:HB2	1:C:988:GLU:OE1	2.13	0.49
2:Q:54:LEU:O	2:Q:55:PHE:C	2.51	0.49
2:Q:99:LEU:HA	2:Q:112:PHE:HE1	1.73	0.49
5:T:5:THR:OG1	5:T:24:ARG:HB3	2.13	0.49
2:D:4:LEU:CD1	2:D:96:CYS:HB2	2.42	0.49
3:E:13:LYS:O	3:E:16:ALA:N	2.40	0.49
5:G:28:THR:O	5:G:29:VAL:C	2.50	0.49
1:A:83:VAL:HG12	1:A:236:ARG:HG3	1.94	0.49
1:A:396:TYR:N	1:A:396:TYR:CD1	2.81	0.49
1:B:377:PHE:CE2	1:B:434:ILE:HG12	2.47	0.49
1:B:977:LEU:HD21	1:B:996:LEU:HD23	1.95	0.49
1:C:309:GLU:O	1:C:310:LYS:C	2.51	0.49
1:C:633:ARG:O	1:C:634:VAL:C	2.50	0.49
2:Q:24:ALA:HB1	2:Q:30:ARG:NE	2.28	0.49
2:Q:99:LEU:HD23	2:Q:100:PHE:H	1.77	0.49
2:Q:105:PRO:HG2	2:Q:109:GLU:HA	1.95	0.49
4:R:16:VAL:CB	4:R:81:PRO:HD3	2.42	0.49
5:T:96:LEU:O	5:T:97:THR:C	2.51	0.49
2:D:18:VAL:HG12	2:D:83:LEU:CB	2.43	0.49
2:D:48:MET:SD	2:D:68:VAL:HG11	2.53	0.49
3:E:98:ARG:HB2	3:E:116:ASN:CB	2.42	0.49
4:J:24:CYS:O	4:J:71:ASP:HA	2.13	0.49
5:K:20:THR:HA	5:K:74:LEU:O	2.13	0.49
1:B:95:THR:O	1:B:186:PHE:HA	2.13	0.48
1:B:131:CYS:O	1:B:132:GLU:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:GLN:O	1:B:135:PHE:C	2.52	0.48
1:C:323:THR:C	1:C:325:SER:N	2.65	0.48
1:C:374:PHE:C	1:C:376:ALA:H	2.16	0.48
2:Q:32:HIS:O	2:Q:54:LEU:HD23	2.13	0.48
2:Q:52:ILE:N	2:Q:53:PRO:CD	2.76	0.48
2:Q:54:LEU:HD13	2:Q:54:LEU:N	2.28	0.48
2:Q:65:GLN:O	2:Q:66:GLY:C	2.51	0.48
1:A:353:TRP:CZ2	1:A:466:ARG:HA	2.48	0.48
1:A:372:ALA:C	1:A:374:PHE:H	2.15	0.48
1:B:241:LEU:HD13	1:B:241:LEU:N	2.28	0.48
1:B:660:GLU:O	1:B:695:TYR:CE1	2.66	0.48
1:B:939:PHE:CG	1:B:940:SER:N	2.81	0.48
1:C:211:ILE:N	1:C:213:ARG:HH12	2.10	0.48
1:C:292:ALA:O	1:C:293:LEU:C	2.51	0.48
1:C:296:LEU:O	1:C:297:SER:C	2.51	0.48
1:C:326:ILE:HB	1:C:328:ARG:HH12	1.77	0.48
1:C:396:TYR:CD1	1:C:396:TYR:N	2.77	0.48
1:C:575:VAL:O	1:C:583:ILE:HA	2.13	0.48
1:C:825:LYS:NZ	1:C:944:ALA:HB3	2.27	0.48
2:Q:7:SER:OG	2:Q:8:GLY:N	2.46	0.48
2:Q:33:VAL:CG2	2:Q:99:LEU:HB3	2.31	0.48
4:R:34:LEU:CA	4:R:91:ARG:HA	2.32	0.48
4:F:12:LEU:HD13	4:F:104:VAL:HG22	1.95	0.48
2:H:106:ASN:O	2:H:107:SER:C	2.51	0.48
2:H:107:SER:HB3	2:H:108:PRO:HD3	1.95	0.48
5:K:23:CYS:HB2	5:K:36:TRP:CH2	2.48	0.48
5:K:60:PRO:O	5:K:61:ASP:C	2.51	0.48
1:A:53:ASP:HB2	1:A:55:PHE:CE1	2.48	0.48
1:A:56:LEU:O	1:A:57:PRO:C	2.51	0.48
1:B:65:PHE:HB2	1:B:265:TYR:CB	2.37	0.48
1:B:577:ASP:O	1:B:581:LEU:N	2.46	0.48
1:B:620:SER:CB	1:B:623:ILE:H	2.26	0.48
1:B:1119:ASN:OD1	1:B:1120:THR:HG23	2.13	0.48
1:C:90:VAL:HG12	1:C:269:TYR:CE1	2.49	0.48
4:R:34:LEU:H	4:R:91:ARG:NE	2.11	0.48
2:D:26:GLY:O	2:D:28:THR:N	2.47	0.48
2:D:34:ILE:HG23	2:D:56:GLY:HA2	1.96	0.48
2:D:72:ALA:HB2	2:D:80:TYR:HB2	1.96	0.48
4:F:46:LYS:HE3	4:F:46:LYS:HB2	1.63	0.48
5:K:62:ARG:CD	5:K:78:ARG:H	2.26	0.48
1:A:32:PHE:HA	1:A:59:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ILE:HG13	1:A:240:LEU:HD22	1.95	0.48
1:A:450:ASP:O	1:A:452:TRP:HD1	1.97	0.48
1:A:502:VAL:HG23	5:G:92:HIS:NE2	2.29	0.48
1:B:324:GLU:HG2	1:B:533:VAL:HG11	1.95	0.48
1:B:490:PRO:HG2	1:B:491:LEU:HD23	1.96	0.48
1:B:1086:LYS:HB2	1:B:1122:VAL:CG1	2.43	0.48
2:Q:37:VAL:HG21	2:Q:115:TRP:HH2	1.78	0.48
2:Q:54:LEU:O	2:Q:57:THR:N	2.46	0.48
2:Q:90:ASP:O	2:Q:91:THR:C	2.51	0.48
3:S:114:PHE:O	3:S:115:ASP:C	2.52	0.48
4:R:90:GLN:HA	4:R:97:THR:O	2.13	0.48
5:T:11:LEU:HD23	5:T:104:VAL:HG13	1.94	0.48
2:D:3:GLN:HG2	2:D:25:SER:CB	2.44	0.48
1:A:393:THR:H	1:A:516:LEU:HD13	1.78	0.48
1:C:188:ASN:HB2	1:C:210:ILE:HD13	1.96	0.48
1:C:693:ILE:HG13	1:C:693:ILE:O	2.13	0.48
1:C:935:GLN:O	1:C:936:ASP:C	2.51	0.48
2:Q:70:ILE:HG13	2:Q:81:MET:HB2	1.94	0.48
2:Q:103:GLY:C	2:Q:105:PRO:HD2	2.34	0.48
3:S:7:SER:HB3	3:S:21:SER:HB3	1.95	0.48
4:R:7:GLN:NE2	4:R:101:GLY:HA2	2.28	0.48
5:T:62:ARG:HB3	5:T:63:PHE:H	1.42	0.48
3:E:87:ARG:HB2	3:E:87:ARG:NH2	2.28	0.48
4:F:81:PRO:HA	4:F:106:ILE:CG1	2.40	0.48
5:G:33:SER:HB3	5:G:91:GLN:HA	1.95	0.48
5:G:50:TYR:CE2	5:G:56:ALA:HA	2.48	0.48
2:H:7:SER:OG	2:H:8:GLY:N	2.46	0.48
3:I:98:ARG:CD	3:I:116:ASN:HB2	2.41	0.48
3:I:107:GLY:O	3:I:109:SER:N	2.46	0.48
1:A:85:PRO:HA	1:A:236:ARG:CZ	2.44	0.48
1:A:326:ILE:HG22	1:A:531:ASN:O	2.14	0.48
1:A:499:THR:HG23	5:G:50:TYR:CZ	2.48	0.48
1:A:500:TYR:CD2	3:E:102:ARG:HD3	2.48	0.48
1:A:724:THR:CG2	1:A:934:ILE:HD12	2.44	0.48
1:B:37:TYR:O	1:B:39:PRO:N	2.46	0.48
1:B:408:SER:C	1:B:410:ILE:N	2.67	0.48
1:B:409:GLN:HA	3:S:54:TYR:OH	2.14	0.48
1:B:445:HIS:C	1:B:447:GLY:N	2.67	0.48
1:B:770:ILE:HG23	1:B:1015:ALA:HB2	1.95	0.48
1:C:193:VAL:HG13	1:C:270:LEU:HD11	1.96	0.48
1:C:421:TYR:HA	1:C:457:ARG:HH22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:TRP:CZ2	1:C:508:ARG:HB3	2.49	0.48
1:C:577:ASP:HB2	1:C:581:LEU:C	2.34	0.48
2:D:101:PRO:HB3	4:F:92:TYR:CD1	2.49	0.48
2:D:112:PHE:O	2:D:113:ASP:C	2.51	0.48
5:G:62:ARG:HA	5:G:77:SER:HB2	1.94	0.48
3:I:69:THR:HG22	3:I:71:THR:HG22	1.96	0.48
1:A:444:LYS:HE3	1:A:444:LYS:HB3	1.65	0.48
1:A:534:LYS:HA	1:A:551:LEU:O	2.14	0.48
1:A:985:ASP:OD1	1:A:985:ASP:N	2.47	0.48
1:A:1037:SER:H	1:A:1048:HIS:HD2	1.61	0.48
1:A:1089:PHE:CE1	1:A:1123:SER:HB3	2.49	0.48
1:B:56:LEU:O	1:B:57:PRO:C	2.52	0.48
1:B:120:VAL:HG13	1:B:121:ASN:N	2.29	0.48
1:C:45:SER:O	1:C:46:SER:C	2.52	0.48
1:C:190:ARG:HG3	1:C:207:HIS:CD2	2.49	0.48
3:S:37:VAL:HG21	3:S:117:TRP:CH2	2.49	0.48
4:R:6:THR:HA	4:R:100:GLN:HE22	1.78	0.48
4:J:95:SER:O	4:J:97:THR:N	2.45	0.48
1:A:24:THR:HG22	1:A:25:THR:H	1.79	0.48
1:A:273:ARG:HB2	1:A:275:PHE:HE1	1.79	0.48
1:A:289:VAL:HG11	1:A:300:LYS:HG2	1.96	0.48
1:A:387:LEU:HD12	1:A:387:LEU:HA	1.75	0.48
1:A:453:TYR:O	1:A:491:LEU:HA	2.14	0.48
1:A:701:ALA:H	1:B:786:LYS:NZ	2.12	0.48
1:A:854:LYS:HB3	1:C:591:PHE:CZ	2.48	0.48
1:B:133:PHE:HB3	1:B:136:CYS:SG	2.53	0.48
1:B:495:GLY:O	1:B:497:ARG:HG2	2.14	0.48
1:B:927:PHE:CG	1:B:927:PHE:O	2.60	0.48
1:C:46:SER:N	1:C:280:ASN:O	2.46	0.48
1:C:375:PHE:HE2	3:I:54:TYR:CB	2.26	0.48
1:C:385:THR:C	1:C:387:LEU:N	2.66	0.48
1:C:530:THR:HG22	1:C:531:ASN:H	1.78	0.48
1:C:556:LYS:HB2	1:C:583:ILE:CG1	2.43	0.48
2:Q:3:GLN:HG2	2:Q:25:SER:CB	2.44	0.48
3:S:69:THR:HG22	3:S:71:THR:HG22	1.96	0.48
2:D:4:LEU:HD21	2:D:30:ARG:HH22	1.78	0.48
4:F:56:GLU:HB3	4:F:60:PRO:CG	2.43	0.48
3:I:107:GLY:C	3:I:109:SER:N	2.65	0.48
1:A:65:PHE:HE2	1:A:267:VAL:CG1	2.27	0.48
1:A:360:ASN:HB3	1:A:522:THR:OG1	2.14	0.48
1:A:1097:SER:OG	1:A:1098:ASN:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:TRP:O	1:B:437:ASN:HB3	2.13	0.48
1:B:555:ASN:O	1:B:556:LYS:C	2.52	0.48
1:C:104:TRP:HE3	1:C:119:ILE:HG21	1.78	0.48
1:C:226:VAL:HG11	1:C:228:LEU:HG	1.96	0.48
1:C:402:ILE:HG13	1:C:407:VAL:CA	2.43	0.48
1:C:535:ASN:O	1:C:536:LYS:HB3	2.13	0.48
4:R:92:TYR:HA	4:R:96:TYR:CD1	2.49	0.48
5:T:38:GLN:HG3	5:T:39:GLN:N	2.28	0.48
2:D:115:TRP:HB2	4:F:45:PRO:O	2.14	0.48
2:H:47:TRP:CZ2	4:J:96:TYR:CD2	3.02	0.48
4:J:76:ILE:HD11	4:J:87:TYR:CE1	2.48	0.48
5:K:55:ARG:NH1	5:K:58:GLY:H	2.11	0.48
1:A:318:PHE:CZ	1:A:614:VAL:HG22	2.49	0.48
1:A:480:CYS:C	1:A:482:GLY:H	2.18	0.48
1:A:632:TRP:O	1:A:633:ARG:CB	2.61	0.48
1:B:342:PHE:HZ	1:B:512:LEU:HD11	1.79	0.48
1:B:420:ASP:HA	1:B:460:LYS:HZ3	1.76	0.48
1:B:457:ARG:CZ	1:B:458:LYS:HB2	2.43	0.48
1:B:545:LEU:HD13	1:B:564:PHE:HB3	1.96	0.48
1:C:334:ASN:HD21	1:C:336:CYS:HB3	1.79	0.48
1:C:398:ASP:OD2	1:C:511:VAL:HB	2.14	0.48
1:C:540:PHE:O	1:C:547:GLY:N	2.46	0.48
4:R:87:TYR:HB2	4:R:102:THR:HG1	1.79	0.48
5:T:62:ARG:O	5:T:64:SER:N	2.47	0.48
2:D:24:ALA:CB	2:D:30:ARG:HD2	2.30	0.48
2:D:38:ARG:HB3	2:D:46:GLU:HG2	1.94	0.48
4:F:9:PRO:HD2	4:F:102:THR:CG2	2.44	0.48
4:F:93:ASP:C	4:F:95:SER:H	2.16	0.48
2:H:2:VAL:HG13	2:H:114:ILE:HD13	1.96	0.48
2:H:39:GLN:O	2:H:92:ALA:HB1	2.13	0.48
5:K:40:LYS:HG3	5:K:85:ALA:CB	2.42	0.48
1:A:333:THR:HB	1:A:362:VAL:HG21	1.96	0.47
1:A:374:PHE:O	1:A:376:ALA:N	2.47	0.47
1:A:409:GLN:CB	1:A:418:ILE:HB	2.43	0.47
1:A:571:THR:O	1:A:572:THR:C	2.50	0.47
1:B:131:CYS:O	1:B:163:ALA:N	2.46	0.47
1:B:500:TYR:CE2	1:B:504:HIS:HD2	2.32	0.47
1:B:577:ASP:HB3	1:B:580:THR:HB	1.96	0.47
1:C:108:THR:HA	1:C:236:ARG:HH12	1.79	0.47
1:C:194:PHE:CD1	1:C:203:ILE:HG23	2.49	0.47
1:C:396:TYR:O	1:C:513:SER:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:ARG:O	1:C:473:TYR:HE1	1.97	0.47
1:C:756:TYR:HE2	1:C:998:THR:CG2	2.27	0.47
1:C:793:PRO:HG2	1:C:794:ILE:HD12	1.94	0.47
2:Q:34:ILE:HG22	2:Q:56:GLY:N	2.29	0.47
3:S:67:ARG:HA	3:S:85:ARG:CZ	2.44	0.47
4:R:61:SER:C	4:R:63:PHE:H	2.18	0.47
4:F:63:PHE:CD2	4:F:76:ILE:HG12	2.49	0.47
4:F:84:ILE:HG22	4:F:105:GLU:HA	1.96	0.47
2:H:32:HIS:CE1	2:H:53:PRO:HA	2.49	0.47
4:J:90:GLN:HE21	4:J:91:ARG:N	2.12	0.47
1:A:116:SER:O	1:A:130:VAL:HA	2.14	0.47
1:A:326:ILE:HG21	1:A:533:VAL:HG23	1.96	0.47
1:A:755:GLN:H	1:A:755:GLN:HG2	1.48	0.47
1:A:969:LYS:O	1:A:970:PHE:C	2.52	0.47
1:A:971:GLY:HA3	1:A:995:ARG:CZ	2.44	0.47
1:B:345:THR:HB	2:Q:104:ASP:HB3	1.95	0.47
1:B:405:ASN:ND2	3:S:102:ARG:N	2.62	0.47
1:B:436:TRP:O	1:B:436:TRP:CG	2.67	0.47
1:B:472:ILE:HA	1:B:490:PRO:HG3	1.96	0.47
1:B:481:LYS:HD3	1:B:481:LYS:HA	1.61	0.47
1:B:540:PHE:CE2	1:B:551:LEU:HD21	2.49	0.47
1:C:770:ILE:HD11	1:C:1012:LEU:HG	1.94	0.47
1:C:915:VAL:O	1:C:919:ASN:ND2	2.47	0.47
2:Q:87:ARG:HB3	2:Q:88:SER:H	1.58	0.47
5:T:79:LEU:HD13	5:T:84:PHE:CE1	2.44	0.47
3:E:6:GLN:HA	3:E:21:SER:O	2.14	0.47
4:F:5:MET:O	4:F:100:GLN:NE2	2.47	0.47
1:A:409:GLN:CG	1:A:418:ILE:HB	2.44	0.47
1:A:533:VAL:HB	1:A:538:VAL:HG21	1.96	0.47
1:A:566:ARG:HG2	1:A:570:ASP:HA	1.96	0.47
1:A:870:ILE:O	1:A:874:THR:HG23	2.14	0.47
1:B:387:LEU:HD12	1:B:387:LEU:HA	1.75	0.47
1:B:402:ILE:HD11	1:B:509:VAL:HG21	1.96	0.47
1:B:457:ARG:HD2	1:B:467:ASP:CG	2.34	0.47
1:B:631:THR:O	1:B:633:ARG:N	2.47	0.47
1:C:234:ILE:O	1:C:236:ARG:N	2.47	0.47
1:C:404:GLY:HA2	1:C:407:VAL:CG2	2.43	0.47
1:C:410:ILE:CG2	1:C:423:TYR:CD1	2.97	0.47
1:C:439:ASN:HD22	1:C:443:SER:HB3	1.78	0.47
2:Q:24:ALA:HB3	2:Q:77:SER:CB	2.39	0.47
2:Q:24:ALA:O	2:Q:27:GLY:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:59:ILE:CG2	2:Q:60:TYR:H	2.21	0.47
5:T:29:VAL:HG13	5:T:33:SER:HB2	1.95	0.47
5:T:33:SER:HA	5:T:92:HIS:CB	2.44	0.47
4:F:62:ARG:HB2	4:F:77:SER:CB	2.44	0.47
5:G:31:SER:C	5:G:33:SER:N	2.67	0.47
2:H:12:LYS:CE	2:H:13:LYS:HG2	2.45	0.47
4:J:7:GLN:OE1	4:J:23:THR:HB	2.14	0.47
1:A:41:LYS:O	1:A:42:VAL:C	2.52	0.47
1:A:439:ASN:C	1:A:441:LEU:H	2.18	0.47
1:A:474:GLN:O	1:A:474:GLN:HG3	2.14	0.47
1:A:617:THR:OG1	1:A:618:GLU:N	2.48	0.47
1:B:462:LYS:N	1:B:465:GLU:HB2	2.29	0.47
1:B:568:ILE:H	1:B:568:ILE:HG13	1.40	0.47
1:B:953:ASN:O	1:B:956:ALA:N	2.47	0.47
1:C:478:LYS:HE2	1:C:480:CYS:SG	2.54	0.47
1:C:600:GLY:O	1:C:602:ASN:N	2.47	0.47
1:C:649:LEU:HD21	1:C:652:ALA:HB3	1.96	0.47
4:R:20:VAL:HG11	4:R:104:VAL:CG2	2.45	0.47
2:D:31:SER:C	2:D:33:VAL:H	2.17	0.47
2:D:47:TRP:HZ3	4:F:95:SER:N	2.12	0.47
5:G:40:LYS:HA	5:G:85:ALA:HB2	1.95	0.47
2:H:34:ILE:HD12	2:H:98:ARG:HA	1.96	0.47
4:J:91:ARG:O	4:J:92:TYR:CG	2.68	0.47
5:K:50:TYR:C	5:K:52:ALA:N	2.67	0.47
1:B:213:ARG:O	1:B:216:PRO:HD3	2.15	0.47
1:B:353:TRP:CZ2	1:B:461:LEU:HD22	2.47	0.47
1:B:368:LEU:HD12	1:B:371:PHE:CE2	2.50	0.47
1:B:385:THR:HG23	1:B:386:LYS:HD2	1.96	0.47
1:B:454:ARG:O	1:B:455:LEU:C	2.53	0.47
1:B:670:CYS:HB2	1:B:695:TYR:CE1	2.48	0.47
1:B:744:GLY:O	1:B:745:ASP:C	2.53	0.47
1:C:140:PHE:CG	1:C:141:LEU:N	2.82	0.47
1:C:483:LYS:HB3	1:C:483:LYS:HE3	1.40	0.47
1:C:737:ASP:O	1:C:738:CYS:C	2.52	0.47
1:C:755:GLN:HE21	1:C:755:GLN:HB2	1.46	0.47
1:C:854:LYS:HZ1	1:C:860:VAL:HG23	1.80	0.47
3:S:102:ARG:NH2	3:S:116:ASN:OD1	2.48	0.47
2:D:9:ALA:HA	2:D:120:LEU:HB2	1.96	0.47
2:D:23:LYS:HA	2:D:78:THR:HA	1.97	0.47
2:D:67:ARG:CZ	2:D:67:ARG:HB2	2.43	0.47
3:E:32:TYR:HB3	3:E:100:TYR:HE1	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:3:ILE:HG23	4:F:97:THR:HG21	1.95	0.47
5:G:7:SER:CB	5:G:8:PRO:CD	2.93	0.47
2:H:3:GLN:HG2	2:H:25:SER:CB	2.44	0.47
2:H:12:LYS:CA	2:H:122:THR:O	2.60	0.47
2:H:51:PHE:HB3	2:H:59:ILE:CG2	2.44	0.47
5:K:51:GLY:H	5:K:92:HIS:CE1	2.25	0.47
5:K:62:ARG:HB3	5:K:63:PHE:H	1.53	0.47
1:A:91:TYR:O	1:A:91:TYR:CG	2.67	0.47
1:A:235:THR:HG22	1:A:236:ARG:NE	2.29	0.47
1:A:939:PHE:CG	1:A:940:SER:N	2.82	0.47
1:B:345:THR:H	2:Q:104:ASP:HA	1.78	0.47
1:B:426:PRO:CG	1:B:463:PRO:HB3	2.44	0.47
1:B:896:ILE:O	1:B:897:PRO:C	2.52	0.47
1:B:898:PHE:C	1:B:900:MET:H	2.18	0.47
1:C:131:CYS:N	1:C:133:PHE:HE1	2.13	0.47
1:C:271:GLN:HB3	1:C:272:PRO:HD2	1.96	0.47
1:C:338:PHE:C	1:C:340:GLU:H	2.18	0.47
1:C:402:ILE:HD11	1:C:509:VAL:HG23	1.96	0.47
1:C:675:THR:O	1:C:676:GLN:HG3	2.14	0.47
4:R:63:PHE:CZ	4:R:76:ILE:HD13	2.50	0.47
2:D:51:PHE:CE1	2:D:54:LEU:HA	2.49	0.47
3:E:32:TYR:HE1	3:E:102:ARG:O	1.98	0.47
4:F:15:SER:CA	4:F:18:ASP:HB3	2.40	0.47
3:I:51:ILE:HA	3:I:58:THR:HG22	1.96	0.47
3:I:54:TYR:O	3:I:56:GLY:N	2.48	0.47
3:I:82:GLU:CD	3:I:82:GLU:H	2.18	0.47
4:J:57:THR:O	4:J:59:VAL:N	2.48	0.47
1:A:32:PHE:CD1	1:A:32:PHE:N	2.82	0.47
1:A:472:ILE:HG12	1:A:487:CYS:O	2.15	0.47
1:A:666:GLY:O	1:A:667:ALA:HB3	2.14	0.47
1:A:853:GLN:HE22	1:A:854:LYS:HE3	1.78	0.47
1:A:1129:VAL:HB	1:A:1132:ILE:HG13	1.96	0.47
1:B:131:CYS:HB3	1:B:163:ALA:N	2.30	0.47
1:B:133:PHE:HA	1:B:164:ASN:CG	2.35	0.47
1:B:193:VAL:O	1:B:193:VAL:HG22	2.14	0.47
1:B:197:ILE:HD12	1:B:200:TYR:HD2	1.80	0.47
1:B:291:CYS:C	1:B:293:LEU:N	2.68	0.47
1:B:374:PHE:O	1:B:376:ALA:N	2.48	0.47
1:B:402:ILE:C	1:B:496:PHE:HE2	2.18	0.47
1:B:500:TYR:O	1:B:501:GLY:C	2.52	0.47
1:B:673:TYR:CE2	1:B:690:GLN:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:VAL:HG22	1:C:122:ASN:H	1.80	0.47
1:C:188:ASN:C	1:C:190:ARG:H	2.17	0.47
1:C:328:ARG:HD2	1:C:542:PHE:N	2.29	0.47
1:C:401:VAL:HG22	1:C:508:ARG:HG3	1.94	0.47
1:C:436:TRP:O	1:C:438:SER:N	2.48	0.47
1:C:872:GLN:O	1:C:872:GLN:HG2	2.15	0.47
1:C:888:PHE:CZ	1:C:1034:LEU:HG	2.49	0.47
1:C:984:LEU:HG	1:C:988:GLU:HB2	1.95	0.47
4:R:21:THR:HA	4:R:74:PHE:O	2.15	0.47
4:R:29:ASP:O	4:R:91:ARG:NH1	2.48	0.47
4:R:59:VAL:HG22	4:R:63:PHE:CZ	2.50	0.47
4:R:90:GLN:HG3	4:R:98:PHE:CZ	2.50	0.47
2:D:48:MET:SD	2:D:94:TYR:CD2	3.08	0.47
2:D:71:SER:O	2:D:72:ALA:HB2	2.14	0.47
3:E:117:TRP:HB3	5:G:44:ALA:HB1	1.96	0.47
4:F:62:ARG:HG2	4:F:76:ILE:HG23	1.97	0.47
2:H:23:LYS:HD3	2:H:25:SER:N	2.30	0.47
2:H:33:VAL:O	2:H:34:ILE:HB	2.13	0.47
2:H:34:ILE:HG21	2:H:74:GLU:OE2	2.14	0.47
3:I:113:GLY:O	3:I:116:ASN:ND2	2.47	0.47
4:J:6:THR:N	4:J:25:GLN:CB	2.77	0.47
4:J:39:GLN:HA	4:J:45:PRO:HA	1.97	0.47
4:J:47:LEU:HD13	4:J:56:GLU:OE2	2.15	0.47
5:K:33:SER:HB3	5:K:91:GLN:HA	1.97	0.47
1:A:85:PRO:O	1:A:86:PHE:C	2.51	0.47
1:A:206:LYS:HB2	1:A:222:LEU:HA	1.95	0.47
1:A:395:VAL:HA	1:A:514:PHE:HA	1.96	0.47
1:B:299:THR:CA	1:B:302:THR:OG1	2.62	0.47
1:B:371:PHE:HA	2:Q:52:ILE:HG21	1.96	0.47
1:B:429:PHE:C	1:B:431:GLY:H	2.18	0.47
1:B:500:TYR:CD2	1:B:504:HIS:CD2	3.00	0.47
1:B:619:VAL:HG11	1:B:648:CYS:HB3	1.97	0.47
1:B:712:ILE:HB	1:B:1077:THR:HB	1.97	0.47
1:C:210:ILE:HG13	1:C:213:ARG:NH1	2.30	0.47
1:C:744:GLY:C	1:C:746:SER:N	2.69	0.47
1:C:828:LEU:H	1:C:828:LEU:HD12	1.79	0.47
1:C:930:ALA:O	1:C:934:ILE:HD13	2.15	0.47
1:C:985:ASP:H	1:C:988:GLU:HG3	1.80	0.47
2:Q:23:LYS:HD3	2:Q:25:SER:N	2.30	0.47
5:T:50:TYR:O	5:T:52:ALA:N	2.48	0.47
5:T:95:SER:O	5:T:96:LEU:HD22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:ILE:HG23	2:D:56:GLY:CA	2.44	0.47
2:D:45:LEU:HB3	4:F:98:PHE:CE2	2.50	0.47
3:I:48:MET:HG2	3:I:64:PHE:CE2	2.50	0.47
4:J:56:GLU:CG	4:J:57:THR:H	2.28	0.47
1:A:326:ILE:HG12	1:A:539:ASN:O	2.15	0.47
1:A:385:THR:HG23	1:A:386:LYS:HD2	1.96	0.47
1:A:393:THR:CB	1:A:517:LEU:H	2.28	0.47
1:A:559:LEU:O	1:A:561:PHE:N	2.48	0.47
1:A:1141:LEU:O	1:A:1144:GLU:N	2.48	0.47
1:B:95:THR:O	1:B:96:GLU:C	2.53	0.47
1:B:286:THR:OG1	1:B:287:ASP:N	2.48	0.47
1:B:318:PHE:CZ	1:B:320:VAL:HG23	2.49	0.47
1:B:443:SER:HB2	2:Q:29:PHE:CZ	2.49	0.47
1:B:448:ASN:ND2	1:B:506:PRO:HB3	2.30	0.47
1:B:457:ARG:HG2	1:B:458:LYS:N	2.29	0.47
1:B:823:PHE:CD1	1:B:1057:PRO:HG3	2.50	0.47
1:B:1114:ILE:O	1:B:1119:ASN:ND2	2.46	0.47
1:C:447:GLY:H	1:C:497:ARG:HG3	1.80	0.47
1:C:454:ARG:CD	1:C:457:ARG:HB2	2.44	0.47
1:C:870:ILE:O	1:C:870:ILE:HG22	2.15	0.47
1:C:949:GLN:HA	1:C:952:VAL:HG23	1.97	0.47
5:T:53:SER:O	5:T:54:SER:C	2.52	0.47
2:D:23:LYS:C	2:D:25:SER:H	2.18	0.47
3:E:69:THR:HG22	3:E:71:THR:HG22	1.96	0.47
4:F:3:ILE:HD13	4:F:28:GLN:NE2	2.30	0.47
5:G:29:VAL:HG13	5:G:33:SER:CB	2.40	0.47
2:H:112:PHE:N	4:J:92:TYR:OH	2.48	0.47
3:I:38:ARG:NH1	3:I:90:ASP:HA	2.30	0.47
5:K:49:ILE:HG13	5:K:55:ARG:HG3	1.96	0.47
1:A:53:ASP:H	1:A:55:PHE:HE1	1.63	0.47
1:A:403:LYS:HG2	1:A:403:LYS:O	2.14	0.47
1:A:409:GLN:HG2	1:A:419:ALA:H	1.79	0.47
1:A:540:PHE:O	1:A:547:GLY:N	2.48	0.47
1:A:654:TYR:HA	1:A:694:ALA:O	2.15	0.47
1:B:65:PHE:HD2	1:B:265:TYR:CD1	2.32	0.47
1:B:133:PHE:N	1:B:164:ASN:HB2	2.27	0.47
1:B:465:GLU:CG	1:B:466:ARG:H	2.28	0.47
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.96	0.47
1:B:807:PRO:HG2	1:B:875:SER:HB2	1.97	0.47
1:C:387:LEU:HD12	1:C:387:LEU:HA	1.71	0.47
1:C:472:ILE:HA	1:C:489:PHE:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:17:SER:HA	3:S:86:LEU:HD23	1.97	0.47
2:D:48:MET:SD	2:D:94:TYR:HD2	2.38	0.47
3:E:6:GLN:OE1	3:E:95:TYR:HA	2.15	0.47
3:E:73:ASP:H	3:E:76:THR:HG1	1.61	0.47
4:F:50:TYR:HE1	4:F:56:GLU:HA	1.80	0.47
2:H:103:GLY:N	2:H:109:GLU:HA	2.30	0.47
3:I:114:PHE:C	3:I:116:ASN:H	2.19	0.47
4:J:4:GLN:O	4:J:5:MET:C	2.53	0.47
4:J:22:ILE:HG12	4:J:74:PHE:O	2.15	0.47
1:A:27:SER:OG	1:A:28:TYR:N	2.47	0.46
1:A:412:PRO:HB3	1:A:427:ASP:HA	1.97	0.46
1:A:497:ARG:HB3	1:A:500:TYR:H	1.80	0.46
1:A:505:GLN:NE2	5:G:92:HIS:CD2	2.84	0.46
1:B:135:PHE:O	1:B:136:CYS:C	2.53	0.46
1:B:337:PRO:HB3	1:B:357:ARG:NH1	2.30	0.46
1:B:349:SER:HB2	1:B:451:TYR:HB3	1.97	0.46
1:B:370:ASN:HD22	2:Q:51:PHE:HB2	1.79	0.46
1:B:424:LYS:HB3	1:B:461:LEU:HB2	1.96	0.46
1:B:456:PHE:CD1	1:B:456:PHE:N	2.81	0.46
1:B:807:PRO:HG3	1:B:875:SER:HB2	1.97	0.46
1:B:909:ILE:HD13	1:B:1049:LEU:HD21	1.96	0.46
1:C:105:ILE:HD12	1:C:240:LEU:HD21	1.96	0.46
1:C:673:TYR:HD1	1:C:692:ILE:HG12	1.79	0.46
1:C:728:PRO:HD3	1:C:947:LYS:HD2	1.97	0.46
5:T:99:GLY:C	5:T:101:GLY:H	2.17	0.46
2:D:55:PHE:CZ	2:D:75:SER:HB3	2.50	0.46
2:D:84:SER:O	2:D:85:SER:C	2.53	0.46
3:E:51:ILE:HD12	3:E:70:MET:HB3	1.96	0.46
1:A:699:LEU:HD23	1:B:872:GLN:CD	2.36	0.46
1:B:32:PHE:HB2	1:B:217:GLN:HB2	1.97	0.46
1:B:228:LEU:HD12	1:B:228:LEU:HA	1.68	0.46
1:B:341:VAL:HA	2:Q:103:GLY:HA2	1.98	0.46
1:B:397:ALA:HA	1:B:512:LEU:HA	1.97	0.46
1:B:428:ASP:OD1	1:B:428:ASP:N	2.48	0.46
1:B:437:ASN:ND2	1:B:442:ASP:OD2	2.39	0.46
1:B:439:ASN:C	1:B:441:LEU:N	2.69	0.46
1:B:447:GLY:HA2	1:B:497:ARG:CB	2.45	0.46
1:B:454:ARG:HA	1:B:490:PRO:O	2.14	0.46
1:B:779:GLN:O	1:B:783:ALA:HB3	2.15	0.46
1:B:1069:PRO:HD2	1:C:892:PRO:HD2	1.96	0.46
1:C:90:VAL:HG11	1:C:237:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:LYS:HA	1:C:134:GLN:HE22	1.80	0.46
1:C:132:GLU:N	1:C:132:GLU:OE1	2.48	0.46
1:C:206:LYS:HB2	1:C:222:LEU:HA	1.96	0.46
1:C:345:THR:OG1	1:C:441:LEU:HD11	2.15	0.46
1:C:391:CYS:HB3	1:C:521:ALA:HB1	1.96	0.46
1:C:896:ILE:O	1:C:896:ILE:HG23	2.15	0.46
3:S:67:ARG:HA	3:S:85:ARG:HE	1.80	0.46
2:D:24:ALA:O	2:D:27:GLY:N	2.48	0.46
2:D:86:LEU:HD21	2:D:121:VAL:HG11	1.97	0.46
5:G:39:GLN:HG3	5:G:45:PRO:CG	2.46	0.46
5:G:48:LEU:HA	5:G:59:ILE:HD12	1.96	0.46
2:H:34:ILE:HD12	2:H:98:ARG:HD2	1.97	0.46
3:I:19:LYS:HD2	3:I:82:GLU:OE2	2.15	0.46
4:J:6:THR:N	4:J:25:GLN:HB3	2.28	0.46
1:A:211:ILE:HD12	1:A:212:GLY:H	1.80	0.46
1:A:271:GLN:HB3	1:A:273:ARG:HG2	1.98	0.46
1:A:1028:LYS:O	1:A:1032:CYS:HB2	2.15	0.46
1:B:102:ARG:HH21	1:B:241:LEU:C	2.19	0.46
1:B:333:THR:HA	4:R:30:ILE:CD1	2.45	0.46
1:B:497:ARG:CB	1:B:498:PRO:CD	2.90	0.46
1:B:534:LYS:O	1:B:535:ASN:C	2.54	0.46
1:B:898:PHE:N	1:B:899:PRO:HD2	2.30	0.46
1:B:1045:LYS:HE2	1:B:1045:LYS:HB2	1.51	0.46
2:Q:38:ARG:HB2	2:Q:94:TYR:CD1	2.50	0.46
5:T:49:ILE:HD13	5:T:74:LEU:HD13	1.97	0.46
5:T:61:ASP:O	5:T:62:ARG:C	2.53	0.46
5:T:62:ARG:HD3	5:T:78:ARG:HG3	1.97	0.46
2:D:23:LYS:HD3	2:D:25:SER:N	2.30	0.46
3:E:73:ASP:HB3	3:E:76:THR:HG23	1.98	0.46
3:E:95:TYR:HE2	5:G:44:ALA:HB1	1.80	0.46
2:H:24:ALA:O	2:H:27:GLY:N	2.48	0.46
2:H:25:SER:OG	2:H:26:GLY:N	2.49	0.46
2:H:35:SER:HB2	2:H:50:GLY:HA3	1.97	0.46
5:K:21:LEU:HD23	5:K:102:THR:OG1	2.16	0.46
1:A:284:THR:O	1:A:286:THR:N	2.48	0.46
1:A:339:HIS:HA	1:A:342:PHE:CG	2.50	0.46
1:A:344:ALA:HA	2:D:103:GLY:O	2.15	0.46
1:A:528:LYS:HA	1:A:528:LYS:HD2	1.81	0.46
1:B:368:LEU:HD13	1:B:368:LEU:N	2.30	0.46
1:B:460:LYS:NZ	1:B:460:LYS:HA	2.30	0.46
1:B:478:LYS:H	1:B:485:PRO:CB	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:GLY:HA3	1:B:488:TYR:HB2	1.96	0.46
1:B:578:PRO:HB2	1:B:579:GLN:HE22	1.80	0.46
1:C:383:SER:O	1:C:387:LEU:HD13	2.15	0.46
1:C:402:ILE:O	1:C:506:PRO:HA	2.15	0.46
1:C:499:THR:O	3:I:101:THR:HG21	2.14	0.46
1:C:632:TRP:O	1:C:633:ARG:CB	2.63	0.46
1:C:756:TYR:HE2	1:C:998:THR:HG22	1.81	0.46
1:C:825:LYS:HE3	1:C:939:PHE:O	2.15	0.46
1:C:1083:HIS:CE1	1:C:1137:VAL:H	2.33	0.46
4:R:60:PRO:HG2	4:R:62:ARG:NH2	2.30	0.46
3:E:60:TYR:OH	3:E:70:MET:N	2.48	0.46
4:F:38:GLN:HB3	4:F:48:LEU:HD13	1.96	0.46
4:F:50:TYR:HB2	4:F:54:HIS:HB3	1.97	0.46
5:G:38:GLN:CB	5:G:48:LEU:HD21	2.45	0.46
5:G:49:ILE:HD11	5:G:63:PHE:O	2.16	0.46
2:H:33:VAL:HG13	2:H:99:LEU:N	2.31	0.46
4:J:3:ILE:HD12	4:J:4:GLN:H	1.80	0.46
5:K:37:TYR:CD2	5:K:46:ARG:C	2.89	0.46
1:A:328:ARG:HB3	1:A:542:PHE:HD1	1.80	0.46
1:A:543:ASN:HD22	1:A:543:ASN:HA	1.61	0.46
1:A:825:LYS:O	1:A:827:THR:N	2.49	0.46
1:B:25:THR:O	1:B:26:GLN:HB2	2.16	0.46
1:B:206:LYS:HB3	1:B:222:LEU:HD22	1.96	0.46
1:B:323:THR:HG23	1:B:624:HIS:HE2	1.81	0.46
1:B:441:LEU:HD13	2:Q:32:HIS:CB	2.45	0.46
1:B:828:LEU:HB2	1:B:952:VAL:HG11	1.98	0.46
1:C:44:ARG:CG	1:C:47:VAL:HG11	2.43	0.46
1:C:63:THR:HG1	1:C:65:PHE:HE2	1.63	0.46
1:C:133:PHE:H	1:C:163:ALA:HA	1.79	0.46
1:C:385:THR:O	1:C:387:LEU:N	2.48	0.46
1:C:448:ASN:C	1:C:450:ASP:N	2.68	0.46
1:C:835:LYS:O	1:C:836:GLN:HB2	2.15	0.46
2:Q:100:PHE:HD1	2:Q:100:PHE:HA	1.67	0.46
4:R:7:GLN:HE21	4:R:7:GLN:HB2	1.41	0.46
4:R:49:ILE:HG21	4:R:74:PHE:HE2	1.79	0.46
3:E:53:THR:O	3:E:54:TYR:C	2.53	0.46
4:F:40:LYS:O	4:F:43:LYS:HB2	2.16	0.46
5:G:17:GLU:C	5:G:78:ARG:HA	2.36	0.46
2:H:108:PRO:O	2:H:109:GLU:HB3	2.16	0.46
4:J:32:ASN:O	4:J:33:TYR:HB3	2.16	0.46
5:K:49:ILE:HG13	5:K:55:ARG:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:CYS:O	1:A:292:ALA:HB2	2.15	0.46
1:A:478:LYS:H	1:A:479:PRO:CD	2.28	0.46
1:A:496:PHE:O	1:A:497:ARG:NE	2.48	0.46
1:A:989:ALA:C	1:A:991:VAL:N	2.69	0.46
1:B:90:VAL:HG21	1:B:237:PHE:CZ	2.50	0.46
1:B:217:GLN:HE21	1:B:218:GLY:H	1.63	0.46
1:B:359:SER:O	1:B:523:VAL:HG13	2.15	0.46
1:B:429:PHE:HD1	1:B:430:THR:N	2.05	0.46
1:B:564:PHE:CE1	1:C:41:LYS:HD3	2.46	0.46
1:B:1027:THR:O	1:B:1031:GLU:HG3	2.15	0.46
1:C:327:VAL:HG13	1:C:538:VAL:HB	1.97	0.46
1:C:417:ASN:HD22	1:C:421:TYR:HD2	1.63	0.46
1:C:436:TRP:HH2	1:C:510:VAL:CG2	2.24	0.46
1:C:676:GLN:N	1:C:689:SER:O	2.48	0.46
2:Q:22:CYS:O	2:Q:79:ALA:N	2.45	0.46
2:Q:23:LYS:C	2:Q:25:SER:H	2.18	0.46
2:Q:38:ARG:O	2:Q:46:GLU:HG3	2.15	0.46
3:S:39:GLN:O	3:S:39:GLN:HG3	2.16	0.46
5:T:7:SER:O	5:T:8:PRO:C	2.54	0.46
2:D:48:MET:CG	2:D:68:VAL:HG11	2.46	0.46
2:D:52:ILE:H	2:D:52:ILE:HG13	1.43	0.46
2:D:98:ARG:HD2	2:D:113:ASP:HB2	1.97	0.46
3:E:4:LEU:HD11	3:E:98:ARG:CG	2.44	0.46
3:E:99:ASP:HA	3:E:114:PHE:HB3	1.98	0.46
4:F:40:LYS:NZ	4:F:59:VAL:HG11	2.31	0.46
5:G:79:LEU:O	5:G:80:GLU:C	2.53	0.46
2:H:22:CYS:O	2:H:79:ALA:N	2.48	0.46
2:H:36:TRP:HZ2	2:H:79:ALA:C	2.19	0.46
2:H:54:LEU:HD12	2:H:99:LEU:CD2	2.45	0.46
2:H:54:LEU:O	2:H:55:PHE:HB2	2.15	0.46
5:K:37:TYR:HA	5:K:47:LEU:HA	1.96	0.46
5:K:62:ARG:O	5:K:63:PHE:C	2.53	0.46
5:K:92:HIS:HB3	5:K:93:ASP:H	1.48	0.46
1:A:29:THR:N	1:A:62:VAL:O	2.49	0.46
1:A:657:ASN:N	1:A:657:ASN:OD1	2.47	0.46
1:A:916:LEU:HA	1:A:923:ILE:CD1	2.45	0.46
1:B:129:LYS:HA	1:B:129:LYS:NZ	2.31	0.46
1:B:347:PHE:O	1:B:348:ALA:C	2.53	0.46
1:B:989:ALA:C	1:B:991:VAL:H	2.18	0.46
1:C:210:ILE:HB	1:C:213:ARG:HH11	1.81	0.46
1:C:295:PRO:HD3	1:C:635:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:VAL:HG23	1:C:400:PHE:CE2	2.50	0.46
2:Q:17:SER:CB	2:Q:85:SER:H	2.29	0.46
2:Q:108:PRO:HG2	4:R:33:TYR:HH	1.77	0.46
5:T:21:LEU:HD23	5:T:102:THR:HG21	1.97	0.46
5:T:50:TYR:CE1	5:T:54:SER:HB2	2.50	0.46
3:E:29:PHE:O	3:E:53:THR:HB	2.16	0.46
4:F:32:ASN:O	4:F:33:TYR:HB3	2.14	0.46
5:G:21:LEU:HD23	5:G:102:THR:OG1	2.16	0.46
5:G:36:TRP:O	5:G:47:LEU:HD12	2.16	0.46
2:H:30:ARG:H	2:H:30:ARG:HD3	1.81	0.46
1:A:133:PHE:O	1:A:135:PHE:N	2.48	0.46
1:A:206:LYS:HB3	1:A:208:THR:HG23	1.98	0.46
1:A:448:ASN:O	1:A:495:GLY:HA2	2.15	0.46
1:A:571:THR:O	1:A:573:ASP:N	2.49	0.46
1:A:747:THR:O	1:A:748:GLU:C	2.54	0.46
1:B:210:ILE:HG23	1:B:215:PHE:HB3	1.97	0.46
1:B:329:PHE:CE1	1:B:543:ASN:HA	2.51	0.46
1:B:444:LYS:O	1:B:447:GLY:N	2.49	0.46
1:B:462:LYS:HZ3	1:B:462:LYS:H	1.62	0.46
1:B:504:HIS:NE2	3:S:111:ILE:HG22	2.31	0.46
1:B:532:LEU:HD11	1:B:584:LEU:HD11	1.98	0.46
1:C:351:TYR:O	1:C:353:TRP:HD1	1.98	0.46
1:C:420:ASP:HA	1:C:460:LYS:CD	2.44	0.46
1:C:585:ASP:O	1:C:586:ILE:HG12	2.16	0.46
1:C:833:PHE:CE1	1:C:836:GLN:HG3	2.51	0.46
3:S:30:THR:OG1	3:S:54:TYR:HA	2.16	0.46
3:S:73:ASP:HB3	3:S:76:THR:HG23	1.98	0.46
3:S:73:ASP:H	3:S:76:THR:HG1	1.63	0.46
4:R:36:TRP:N	4:R:49:ILE:O	2.42	0.46
2:D:92:ALA:HA	2:D:121:VAL:O	2.16	0.46
2:D:109:GLU:OE1	4:F:32:ASN:HA	2.16	0.46
3:E:114:PHE:HD1	3:E:114:PHE:H	1.63	0.46
4:F:37:TYR:HE1	4:F:47:LEU:HD23	1.80	0.46
2:H:51:PHE:HE1	2:H:57:THR:HB	1.81	0.46
4:J:14:ALA:HB2	4:J:20:VAL:HG21	1.97	0.46
1:A:453:TYR:CZ	1:A:492:GLN:HB2	2.51	0.46
1:A:486:ASN:O	1:A:487:CYS:HB2	2.15	0.46
1:A:491:LEU:HD22	1:A:491:LEU:HA	1.78	0.46
1:A:758:SER:HB3	1:C:964:LYS:HE3	1.98	0.46
1:A:996:LEU:O	1:A:998:THR:N	2.49	0.46
1:B:456:PHE:O	1:B:457:ARG:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:PHE:N	1:B:564:PHE:CD1	2.84	0.46
1:B:985:ASP:HB3	1:B:986:PRO:HD2	1.97	0.46
1:C:287:ASP:HB3	1:C:306:PHE:CE2	2.51	0.46
1:C:328:ARG:HD2	1:C:541:ASN:H	1.80	0.46
1:C:351:TYR:CD1	1:C:468:ILE:HA	2.49	0.46
1:C:356:THR:C	1:C:397:ALA:H	2.20	0.46
1:C:358:ILE:CG2	1:C:523:VAL:HG11	2.46	0.46
1:C:379:CYS:SG	1:C:384:PRO:HA	2.56	0.46
1:C:577:ASP:O	1:C:578:PRO:C	2.54	0.46
1:C:1095:PHE:CE1	1:C:1104:VAL:HG22	2.51	0.46
2:Q:25:SER:OG	2:Q:26:GLY:N	2.49	0.46
3:I:19:LYS:HA	3:I:81:MET:C	2.35	0.46
4:J:3:ILE:HD13	4:J:28:GLN:NE2	2.30	0.46
1:A:56:LEU:HD13	1:A:268:GLY:O	2.15	0.46
1:A:273:ARG:HH21	1:A:292:ALA:HB3	1.81	0.46
1:A:335:LEU:HB3	4:F:31:GLY:HA3	1.97	0.46
1:A:697:MET:HE2	1:A:697:MET:HB2	1.80	0.46
1:A:822:LEU:CD2	1:A:945:LEU:HD21	2.44	0.46
1:B:57:PRO:HD3	1:B:271:GLN:CD	2.36	0.46
1:B:85:PRO:HD2	1:B:269:TYR:OH	2.16	0.46
1:B:200:TYR:HB3	1:B:229:PRO:HA	1.97	0.46
1:B:540:PHE:HE1	1:B:545:LEU:O	1.97	0.46
1:B:620:SER:HA	1:B:631:THR:OG1	2.16	0.46
1:B:743:CYS:O	1:B:745:ASP:N	2.49	0.46
1:B:1125:ASN:ND2	1:B:1127:ASP:HB2	2.31	0.46
1:C:205:SER:HB3	1:C:225:LEU:HD22	1.98	0.46
1:C:540:PHE:HB3	1:C:547:GLY:HA3	1.98	0.46
1:C:1082:CYS:HB3	1:C:1126:CYS:HB2	1.45	0.46
4:F:15:SER:HA	4:F:18:ASP:CB	2.39	0.46
2:H:72:ALA:C	2:H:74:GLU:H	2.19	0.46
3:I:57:ASN:OD1	3:I:57:ASN:N	2.49	0.46
3:I:67:ARG:HA	3:I:85:ARG:HE	1.80	0.46
1:A:417:ASN:HD22	1:A:417:ASN:HA	1.63	0.45
1:A:442:ASP:O	1:A:443:SER:C	2.54	0.45
1:A:836:GLN:NE2	1:A:854:LYS:H	2.14	0.45
1:A:1144:GLU:O	1:A:1147:SER:N	2.46	0.45
1:B:213:ARG:HB2	1:B:213:ARG:CZ	2.46	0.45
1:B:289:VAL:HG23	1:B:306:PHE:CZ	2.51	0.45
1:B:298:GLU:O	1:B:302:THR:HG23	2.16	0.45
1:B:333:THR:HA	4:R:30:ILE:HD12	1.98	0.45
1:B:365:TYR:CE1	1:B:388:ASN:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:LYS:HA	1:B:460:LYS:HZ2	1.80	0.45
2:Q:98:ARG:HB3	2:Q:114:ILE:H	1.81	0.45
2:D:47:TRP:CZ2	2:D:51:PHE:HA	2.51	0.45
2:D:51:PHE:CE1	2:D:57:THR:HB	2.49	0.45
2:H:35:SER:HB3	2:H:99:LEU:HD13	1.98	0.45
2:H:48:MET:HB3	2:H:49:GLY:H	1.64	0.45
1:A:219:PHE:HE2	1:A:285:ILE:O	1.99	0.45
1:A:281:GLU:C	1:A:283:GLY:N	2.69	0.45
1:A:353:TRP:HB3	1:A:423:TYR:HD2	1.81	0.45
1:A:454:ARG:O	1:A:455:LEU:C	2.53	0.45
1:A:646:ALA:HB2	1:B:862:PRO:HG3	1.98	0.45
1:B:339:HIS:CE1	4:R:94:PRO:CD	2.99	0.45
1:B:573:ASP:OD1	1:C:855:PHE:HZ	1.99	0.45
1:B:625:ALA:O	1:B:630:PRO:HB3	2.16	0.45
1:B:826:VAL:HB	1:B:1057:PRO:HG2	1.97	0.45
1:B:996:LEU:O	1:B:1000:ARG:HB2	2.16	0.45
1:C:34:ARG:HG3	1:C:191:GLU:OE1	2.16	0.45
1:C:811:LYS:HE2	1:C:811:LYS:HB3	1.71	0.45
1:C:854:LYS:HE3	1:C:854:LYS:HB3	1.77	0.45
4:R:3:ILE:HD12	4:R:4:GLN:H	1.80	0.45
5:G:92:HIS:O	5:G:93:ASP:C	2.54	0.45
4:J:6:THR:O	4:J:8:SER:N	2.46	0.45
4:J:46:LYS:HB2	4:J:46:LYS:HE3	1.69	0.45
1:A:50:LEU:HD23	1:A:50:LEU:HA	1.78	0.45
1:A:82:PRO:HB2	1:A:84:LEU:CD1	2.46	0.45
1:A:339:HIS:HA	1:A:342:PHE:CB	2.45	0.45
1:A:521:ALA:O	1:A:524:CYS:N	2.50	0.45
1:B:57:PRO:O	1:B:60:SER:HB2	2.17	0.45
1:B:355:ARG:H	1:B:355:ARG:HG2	1.59	0.45
1:B:385:THR:C	1:B:387:LEU:N	2.70	0.45
1:B:752:LEU:HD12	1:B:993:ILE:HG21	1.97	0.45
1:B:1140:PRO:O	1:B:1141:LEU:C	2.54	0.45
1:C:374:PHE:C	1:C:376:ALA:N	2.70	0.45
1:C:485:PRO:O	1:C:486:ASN:C	2.55	0.45
1:C:534:LYS:HA	1:C:534:LYS:NZ	2.31	0.45
1:C:810:SER:OG	1:C:811:LYS:N	2.49	0.45
1:C:978:ASN:O	1:C:979:ASP:C	2.54	0.45
2:Q:52:ILE:H	2:Q:53:PRO:HD3	1.81	0.45
4:R:6:THR:O	4:R:7:GLN:C	2.55	0.45
5:T:50:TYR:HE1	5:T:54:SER:HB2	1.81	0.45
4:F:3:ILE:HD12	4:F:4:GLN:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:82:GLU:O	2:H:83:LEU:C	2.55	0.45
1:A:365:TYR:HA	1:A:368:LEU:HD22	1.98	0.45
1:A:499:THR:HG23	5:G:50:TYR:OH	2.17	0.45
1:A:722:VAL:HG11	1:A:931:ILE:HD13	1.98	0.45
1:A:972:ALA:HA	1:A:992:GLN:HE21	1.78	0.45
1:B:267:VAL:O	1:B:267:VAL:HG12	2.16	0.45
1:B:754:LEU:HD12	1:B:755:GLN:HG2	1.98	0.45
1:B:773:GLU:C	1:B:775:ASP:H	2.20	0.45
1:B:938:LEU:HD23	1:B:938:LEU:HA	1.82	0.45
1:B:959:LEU:HD23	1:B:959:LEU:HA	1.70	0.45
1:B:979:ASP:O	1:B:980:ILE:C	2.55	0.45
1:C:129:LYS:O	1:C:130:VAL:HB	2.16	0.45
1:C:206:LYS:O	1:C:208:THR:HG22	2.16	0.45
1:C:321:GLN:NE2	1:C:632:TRP:HB2	2.30	0.45
1:C:374:PHE:O	1:C:376:ALA:N	2.49	0.45
1:C:375:PHE:CD2	1:C:507:TYR:HE2	2.35	0.45
1:C:378:LYS:HE3	1:C:378:LYS:HB2	1.82	0.45
1:C:533:VAL:HG23	1:C:534:LYS:N	2.30	0.45
1:C:1104:VAL:HG22	1:C:1115:ILE:HG22	1.98	0.45
3:S:100:TYR:CD1	5:T:96:LEU:CD2	3.00	0.45
4:R:3:ILE:HD13	4:R:28:GLN:NE2	2.30	0.45
4:R:20:VAL:HG11	4:R:104:VAL:HG22	1.97	0.45
5:T:2:ILE:CG2	5:T:25:ALA:HB1	2.46	0.45
5:T:40:LYS:HA	5:T:85:ALA:HB2	1.98	0.45
2:H:23:LYS:C	2:H:25:SER:H	2.18	0.45
3:I:4:LEU:O	3:I:118:GLY:HA2	2.17	0.45
1:A:238:GLN:HE21	1:A:238:GLN:N	2.14	0.45
1:A:318:PHE:CZ	1:A:592:GLY:HA3	2.51	0.45
1:A:338:PHE:O	1:A:339:HIS:HB2	2.17	0.45
1:A:471:GLU:O	1:A:490:PRO:HG2	2.16	0.45
1:A:758:SER:HB2	1:A:761:THR:CG2	2.45	0.45
1:B:298:GLU:O	1:B:302:THR:CG2	2.64	0.45
1:B:437:ASN:OD1	1:B:441:LEU:HB3	2.16	0.45
1:B:499:THR:O	1:B:500:TYR:C	2.55	0.45
1:B:566:ARG:HB2	1:C:42:VAL:HG11	1.98	0.45
1:C:136:CYS:O	1:C:139:PRO:HD3	2.17	0.45
1:C:203:ILE:O	1:C:204:TYR:C	2.54	0.45
1:C:406:GLU:O	1:C:407:VAL:C	2.54	0.45
1:C:473:TYR:HB3	1:C:487:CYS:CB	2.29	0.45
2:Q:60:TYR:CE1	2:Q:70:ILE:HD13	2.49	0.45
2:D:30:ARG:NH2	2:D:34:ILE:HD12	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:ILE:CG2	2:D:56:GLY:N	2.79	0.45
2:D:69:MET:O	2:D:82:GLU:N	2.49	0.45
3:E:54:TYR:CG	3:E:55:ASN:N	2.84	0.45
3:E:72:THR:OG1	3:E:73:ASP:N	2.50	0.45
5:G:18:ARG:HA	5:G:78:ARG:HA	1.99	0.45
3:I:6:GLN:HB2	3:I:119:GLN:NE2	2.30	0.45
4:J:32:ASN:O	4:J:33:TYR:CB	2.62	0.45
5:K:53:SER:O	5:K:55:ARG:N	2.50	0.45
1:A:129:LYS:CB	1:A:169:GLU:HA	2.47	0.45
1:A:319:ARG:HB2	1:A:319:ARG:HH11	1.79	0.45
1:A:609:VAL:O	1:A:650:ILE:N	2.50	0.45
1:A:648:CYS:SG	1:A:650:ILE:HG12	2.57	0.45
1:A:927:PHE:O	1:A:929:SER:N	2.49	0.45
1:A:1073:LYS:HG2	1:A:1075:PHE:CZ	2.51	0.45
1:B:38:TYR:CE2	1:B:285:ILE:HG13	2.52	0.45
1:B:122:ASN:O	1:B:123:ALA:C	2.55	0.45
1:B:422:ASN:ND2	1:B:454:ARG:O	2.42	0.45
1:B:450:ASP:N	1:B:450:ASP:OD1	2.50	0.45
1:B:453:TYR:HD2	1:B:493:SER:C	2.20	0.45
1:B:480:CYS:O	1:B:480:CYS:SG	2.75	0.45
1:B:539:ASN:O	1:B:540:PHE:CB	2.65	0.45
1:B:633:ARG:HA	1:B:633:ARG:CZ	2.47	0.45
1:C:331:ASN:H	1:C:579:GLN:HB2	1.75	0.45
1:C:350:VAL:HG22	1:C:422:ASN:HB3	1.98	0.45
1:C:505:GLN:CB	1:C:506:PRO:HD2	2.46	0.45
1:C:978:ASN:O	1:C:982:SER:N	2.46	0.45
2:Q:38:ARG:HB3	2:Q:48:MET:SD	2.57	0.45
2:D:4:LEU:HD21	2:D:30:ARG:NH2	2.32	0.45
2:D:25:SER:OG	2:D:26:GLY:N	2.49	0.45
3:E:11:VAL:HA	3:E:124:THR:OG1	2.17	0.45
3:E:71:THR:O	3:E:72:THR:HB	2.16	0.45
3:E:95:TYR:HE2	5:G:44:ALA:CB	2.29	0.45
4:F:4:GLN:O	4:F:6:THR:HG22	2.16	0.45
5:G:19:ALA:O	5:G:76:ILE:N	2.50	0.45
5:G:34:LEU:HD22	5:G:72:PHE:CB	2.44	0.45
5:G:93:ASP:O	5:G:95:SER:N	2.49	0.45
2:H:90:ASP:O	2:H:91:THR:C	2.54	0.45
1:A:287:ASP:HB3	1:A:306:PHE:CE2	2.51	0.45
1:A:409:GLN:O	1:A:418:ILE:HG22	2.16	0.45
1:A:822:LEU:HD23	1:A:945:LEU:HD11	1.99	0.45
1:A:986:PRO:N	1:A:987:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLU:HA	1:B:186:PHE:CD1	2.52	0.45
1:B:300:LYS:O	1:B:302:THR:N	2.49	0.45
1:B:452:TRP:HD1	1:B:492:GLN:C	2.20	0.45
1:C:400:PHE:HE2	1:C:423:TYR:CD2	2.34	0.45
1:C:786:LYS:CD	1:C:786:LYS:H	2.30	0.45
3:S:28:PRO:C	3:S:30:THR:N	2.70	0.45
3:S:60:TYR:OH	3:S:70:MET:N	2.48	0.45
3:E:92:ALA:O	3:E:93:VAL:C	2.55	0.45
4:F:35:ASN:O	4:F:36:TRP:CB	2.64	0.45
3:I:12:LYS:HG2	3:I:18:VAL:HG11	1.99	0.45
3:I:111:ILE:O	3:I:113:GLY:N	2.49	0.45
5:K:91:GLN:O	5:K:92:HIS:C	2.55	0.45
1:A:112:SER:HB2	1:A:134:GLN:HA	1.99	0.45
1:A:118:LEU:O	1:A:120:VAL:N	2.50	0.45
1:A:317:ASN:ND2	1:A:593:GLY:HA2	2.31	0.45
1:A:385:THR:C	1:A:387:LEU:N	2.69	0.45
1:A:445:HIS:N	2:D:73:ASP:OD2	2.49	0.45
1:A:1119:ASN:OD1	1:A:1120:THR:HG23	2.17	0.45
1:B:140:PHE:CG	1:B:141:LEU:N	2.85	0.45
1:B:170:TYR:CD2	1:B:228:LEU:HD11	2.52	0.45
1:B:298:GLU:O	1:B:302:THR:OG1	2.34	0.45
1:B:441:LEU:O	1:B:442:ASP:CB	2.65	0.45
1:B:867:ASP:OD1	1:B:867:ASP:N	2.49	0.45
1:C:132:GLU:OE2	1:C:164:ASN:HB2	2.17	0.45
1:C:289:VAL:HG12	1:C:306:PHE:CE2	2.51	0.45
1:C:424:LYS:NZ	1:C:425:LEU:H	2.14	0.45
1:C:616:CYS:SG	1:C:643:GLN:HG2	2.57	0.45
1:C:858:LEU:HD11	1:C:963:VAL:CG2	2.46	0.45
1:C:1079:PRO:HB2	1:C:1129:VAL:CG1	2.47	0.45
2:Q:89:GLU:H	2:Q:89:GLU:HG3	1.57	0.45
3:E:102:ARG:HD2	3:E:105:TRP:CZ3	2.50	0.45
4:F:63:PHE:CE2	4:F:76:ILE:HG12	2.51	0.45
4:F:93:ASP:C	4:F:95:SER:N	2.70	0.45
2:H:12:LYS:HB3	2:H:123:VAL:HA	1.96	0.45
3:I:92:ALA:O	3:I:93:VAL:C	2.55	0.45
1:A:81:ASN:HB2	1:A:238:GLN:HB2	1.98	0.45
1:A:234:ILE:HG22	1:A:235:THR:N	2.32	0.45
1:A:327:VAL:HG23	1:A:530:THR:HG21	1.98	0.45
1:A:342:PHE:N	1:A:342:PHE:CD1	2.83	0.45
1:A:356:THR:CA	1:A:397:ALA:HB3	2.46	0.45
1:A:444:LYS:H	1:A:448:ASN:CB	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:LEU:HD13	1:A:939:PHE:CB	2.47	0.45
1:A:1072:GLU:HB3	1:B:894:LEU:CD2	2.46	0.45
1:B:128:ILE:HG12	1:B:170:TYR:O	2.17	0.45
1:B:345:THR:HA	2:Q:32:HIS:CE1	2.51	0.45
1:B:345:THR:O	1:B:508:ARG:NH2	2.50	0.45
1:B:420:ASP:HB3	1:B:421:TYR:CD2	2.52	0.45
1:B:996:LEU:HD12	1:B:996:LEU:HA	1.79	0.45
1:C:92:PHE:CZ	1:C:239:THR:HB	2.50	0.45
1:C:281:GLU:H	1:C:281:GLU:HG3	1.68	0.45
1:C:454:ARG:HD2	1:C:457:ARG:HB2	1.99	0.45
1:C:624:HIS:NE2	1:C:630:PRO:HD3	2.32	0.45
1:C:972:ALA:O	1:C:973:ILE:C	2.55	0.45
1:C:1005:GLN:HE21	1:C:1005:GLN:HB2	1.58	0.45
3:S:11:VAL:HA	3:S:124:THR:OG1	2.17	0.45
3:S:72:THR:OG1	3:S:73:ASP:N	2.50	0.45
4:R:38:GLN:HE22	4:R:40:LYS:HZ2	1.65	0.45
4:R:91:ARG:O	4:R:92:TYR:CB	2.65	0.45
3:E:118:GLY:O	3:E:119:GLN:C	2.55	0.45
1:A:112:SER:HB2	1:A:133:PHE:O	2.16	0.45
1:A:276:LEU:CD1	1:A:304:LYS:HG3	2.47	0.45
1:A:350:VAL:C	1:A:352:ALA:N	2.70	0.45
1:A:358:ILE:O	1:A:359:SER:HB3	2.17	0.45
1:A:457:ARG:HD2	1:A:467:ASP:CB	2.46	0.45
1:A:577:ASP:OD1	1:A:584:LEU:HD13	2.17	0.45
1:A:834:ILE:HD11	1:C:647:GLY:N	2.32	0.45
1:A:917:TYR:O	1:A:918:GLU:CB	2.65	0.45
1:A:917:TYR:HB3	1:C:1129:VAL:HG13	1.99	0.45
1:B:104:TRP:HE3	1:B:119:ILE:CG2	2.24	0.45
1:B:193:VAL:HG13	1:B:204:TYR:HB2	1.98	0.45
1:B:329:PHE:CG	1:B:330:PRO:HD2	2.52	0.45
1:B:392:PHE:HD2	1:B:395:VAL:CG2	2.30	0.45
1:B:422:ASN:O	1:B:423:TYR:HB2	2.17	0.45
1:B:532:LEU:HD21	1:B:542:PHE:CE1	2.52	0.45
1:B:923:ILE:O	1:B:923:ILE:HD13	2.16	0.45
1:C:616:CYS:CB	1:C:643:GLN:HG2	2.46	0.45
1:C:736:VAL:HA	1:C:857:GLY:O	2.17	0.45
1:C:973:ILE:HD11	1:C:980:ILE:HA	1.98	0.45
4:R:103:LYS:HA	4:R:103:LYS:HD3	1.79	0.45
4:R:106:ILE:O	4:R:107:LYS:HB3	2.17	0.45
5:T:19:ALA:HB3	5:T:76:ILE:HB	1.97	0.45
5:T:91:GLN:NE2	5:T:94:THR:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:29:PHE:C	2:D:30:ARG:HG2	2.36	0.45
2:D:37:VAL:CG1	2:D:45:LEU:HD23	2.47	0.45
2:D:83:LEU:HG	2:D:86:LEU:HD21	1.99	0.45
2:D:85:SER:O	2:D:87:ARG:N	2.50	0.45
2:D:94:TYR:N	2:D:94:TYR:CD1	2.85	0.45
2:H:49:GLY:HA2	2:H:60:TYR:CA	2.47	0.45
2:H:51:PHE:CB	2:H:59:ILE:HB	2.47	0.45
5:K:48:LEU:HD11	5:K:74:LEU:HD22	1.99	0.45
1:A:34:ARG:HH12	1:A:189:LEU:HD11	1.81	0.44
1:A:343:ASN:CG	2:D:52:ILE:HB	2.38	0.44
1:A:422:ASN:O	1:A:423:TYR:HB2	2.17	0.44
1:A:460:LYS:HE3	1:A:460:LYS:HB2	1.68	0.44
1:A:465:GLU:HB3	1:A:466:ARG:H	1.58	0.44
1:A:813:SER:HB2	1:A:815:ARG:HD2	1.98	0.44
1:A:898:PHE:HB3	1:A:899:PRO:CD	2.47	0.44
1:B:633:ARG:HA	1:B:633:ARG:NE	2.24	0.44
1:B:822:LEU:C	1:B:824:ASN:N	2.71	0.44
1:B:872:GLN:HG3	1:B:872:GLN:O	2.18	0.44
1:B:1029:MET:HG2	1:B:1062:PHE:HZ	1.81	0.44
1:C:235:THR:HB	1:C:236:ARG:NH1	2.32	0.44
1:C:326:ILE:HG22	1:C:541:ASN:ND2	2.32	0.44
1:C:328:ARG:HG3	1:C:540:PHE:CE1	2.52	0.44
1:C:339:HIS:HD2	1:C:367:VAL:HB	1.77	0.44
1:C:984:LEU:HD13	1:C:984:LEU:HA	1.74	0.44
2:Q:27:GLY:O	2:Q:28:THR:C	2.56	0.44
4:R:6:THR:HA	4:R:100:GLN:NE2	2.31	0.44
4:R:46:LYS:HE3	4:R:46:LYS:HB2	1.88	0.44
2:D:30:ARG:NE	2:D:74:GLU:OE2	2.50	0.44
3:E:102:ARG:CB	3:E:111:ILE:HA	2.45	0.44
4:F:35:ASN:N	4:F:35:ASN:ND2	2.65	0.44
3:I:71:THR:O	3:I:72:THR:HB	2.16	0.44
3:I:73:ASP:HB3	3:I:76:THR:HG23	1.98	0.44
1:A:105:ILE:HB	1:A:110:LEU:HD11	1.98	0.44
1:A:522:THR:O	1:A:524:CYS:HB2	2.17	0.44
1:A:792:PRO:CG	1:C:707:TYR:HB3	2.46	0.44
1:A:938:LEU:HD22	1:A:944:ALA:HB1	1.99	0.44
1:B:90:VAL:HG21	1:B:237:PHE:CE1	2.52	0.44
1:B:336:CYS:C	1:B:338:PHE:H	2.21	0.44
1:B:436:TRP:HZ3	1:B:509:VAL:HA	1.82	0.44
1:B:631:THR:O	1:B:633:ARG:HB2	2.17	0.44
1:B:634:VAL:O	1:B:635:TYR:C	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ARG:CB	1:C:398:ASP:HA	2.47	0.44
1:C:764:LYS:HE3	1:C:764:LYS:HB2	1.35	0.44
1:C:808:ASP:CB	1:C:811:LYS:HD2	2.44	0.44
2:Q:22:CYS:HB3	2:Q:79:ALA:HB3	1.98	0.44
2:Q:47:TRP:CZ2	2:Q:51:PHE:HA	2.52	0.44
2:Q:99:LEU:HA	2:Q:112:PHE:HD1	1.81	0.44
2:Q:111:GLY:HA2	4:R:92:TYR:CZ	2.52	0.44
3:S:19:LYS:HA	3:S:81:MET:O	2.17	0.44
4:R:76:ILE:HB	4:R:79:LEU:HD21	1.99	0.44
5:T:18:ARG:HH12	5:T:77:SER:HA	1.82	0.44
5:T:62:ARG:HG3	5:T:77:SER:CB	2.32	0.44
5:T:76:ILE:O	5:T:77:SER:C	2.56	0.44
2:D:52:ILE:HG21	4:F:93:ASP:HA	1.98	0.44
2:D:98:ARG:HB3	2:D:113:ASP:HB2	1.99	0.44
3:I:34:ILE:N	3:I:100:TYR:CD2	2.84	0.44
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.86	0.44
1:A:328:ARG:HD3	1:A:530:THR:H	1.83	0.44
1:A:408:SER:OG	1:A:409:GLN:N	2.50	0.44
1:A:420:ASP:HA	1:A:460:LYS:HG3	2.00	0.44
1:A:550:VAL:O	1:A:552:THR:HG23	2.18	0.44
1:A:557:LYS:HZ3	1:A:557:LYS:HG2	1.63	0.44
1:A:610:LEU:HB2	1:A:649:LEU:CD1	2.43	0.44
1:B:215:PHE:CD1	1:B:217:GLN:HG3	2.52	0.44
1:B:426:PRO:CB	1:B:463:PRO:HB3	2.46	0.44
1:B:540:PHE:CD1	1:B:540:PHE:C	2.91	0.44
1:B:759:PHE:N	1:B:762:GLN:HE21	2.14	0.44
1:B:935:GLN:H	1:B:935:GLN:HG2	1.60	0.44
1:B:972:ALA:O	1:B:973:ILE:C	2.55	0.44
1:B:995:ARG:H	1:B:995:ARG:HG2	1.65	0.44
1:B:1125:ASN:CG	1:B:1127:ASP:HB2	2.38	0.44
1:C:25:THR:HB	1:C:26:GLN:H	1.45	0.44
1:C:39:PRO:HG3	1:C:51:THR:HG21	1.99	0.44
1:C:109:THR:HG22	1:C:113:LYS:HD3	1.98	0.44
1:C:503:GLY:HA3	3:I:33:GLY:N	2.32	0.44
1:C:904:TYR:CD1	1:C:904:TYR:C	2.91	0.44
2:Q:82:GLU:O	2:Q:83:LEU:C	2.54	0.44
4:R:8:SER:O	4:R:102:THR:HG22	2.18	0.44
5:T:7:SER:N	5:T:8:PRO:HD2	2.31	0.44
5:T:29:VAL:HG22	5:T:33:SER:HB3	1.99	0.44
5:T:52:ALA:CB	5:T:72:PHE:HD2	2.29	0.44
2:D:33:VAL:HA	2:D:99:LEU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:86:LEU:HD13	3:E:86:LEU:HA	1.77	0.44
2:H:38:ARG:HH12	2:H:89:GLU:HB2	1.82	0.44
2:H:101:PRO:O	2:H:104:ASP:HB2	2.17	0.44
3:I:12:LYS:HD3	3:I:13:LYS:N	2.32	0.44
1:A:281:GLU:C	1:A:283:GLY:H	2.20	0.44
1:A:352:ALA:HA	1:A:466:ARG:HE	1.82	0.44
1:A:408:SER:HB3	3:E:54:TYR:CE1	2.50	0.44
1:A:558:PHE:CE2	1:A:576:ARG:HG2	2.52	0.44
1:A:724:THR:HG21	1:A:934:ILE:HG23	2.00	0.44
1:A:742:ILE:HD11	1:A:1001:LEU:HG	1.99	0.44
1:B:62:VAL:HG11	1:B:266:TYR:HB3	1.99	0.44
1:B:233:ASN:OD1	1:B:233:ASN:N	2.50	0.44
1:B:351:TYR:HB2	1:B:454:ARG:NE	2.33	0.44
1:B:558:PHE:CE2	1:B:563:GLN:O	2.70	0.44
1:B:822:LEU:HD22	1:B:945:LEU:HD11	1.98	0.44
1:B:970:PHE:HD2	1:B:996:LEU:HD12	1.81	0.44
1:C:38:TYR:OH	1:C:284:THR:HG22	2.18	0.44
1:C:138:ASP:O	1:C:139:PRO:C	2.56	0.44
1:C:304:LYS:HE3	1:C:304:LYS:HB2	1.77	0.44
1:C:374:PHE:CG	1:C:377:PHE:HD2	2.35	0.44
1:C:418:ILE:HA	1:C:422:ASN:HD22	1.83	0.44
1:C:585:ASP:OD1	1:C:585:ASP:N	2.50	0.44
1:C:744:GLY:O	1:C:746:SER:N	2.46	0.44
1:C:973:ILE:HG13	1:C:974:SER:N	2.33	0.44
3:S:71:THR:O	3:S:72:THR:HB	2.16	0.44
3:S:92:ALA:O	3:S:93:VAL:C	2.55	0.44
4:R:37:TYR:CZ	4:R:98:PHE:HE2	2.35	0.44
5:T:6:GLN:NE2	5:T:87:TYR:O	2.51	0.44
2:D:45:LEU:CB	4:F:98:PHE:CD2	3.00	0.44
2:D:101:PRO:HG3	4:F:92:TYR:CE1	2.52	0.44
3:E:7:SER:HB3	3:E:21:SER:HB3	1.98	0.44
5:G:55:ARG:HB2	5:G:56:ALA:H	1.65	0.44
2:H:67:ARG:O	2:H:69:MET:N	2.50	0.44
3:I:115:ASP:HB3	5:K:46:ARG:HA	1.98	0.44
5:K:37:TYR:CE1	5:K:47:LEU:HB2	2.52	0.44
5:K:62:ARG:NH1	5:K:80:GLU:H	2.15	0.44
1:A:203:ILE:CD1	1:A:228:LEU:HD11	2.47	0.44
1:A:281:GLU:O	1:A:283:GLY:N	2.50	0.44
1:A:290:ASP:O	1:A:292:ALA:N	2.49	0.44
1:A:366:SER:C	1:A:368:LEU:N	2.71	0.44
1:A:396:TYR:HD1	1:A:513:SER:O	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:SER:OG	1:A:975:SER:N	2.51	0.44
1:B:92:PHE:CE1	1:B:265:TYR:HA	2.52	0.44
1:B:748:GLU:HB3	1:B:751:ASN:ND2	2.32	0.44
1:B:934:ILE:HD12	1:B:934:ILE:HA	1.70	0.44
1:B:1126:CYS:HA	1:B:1132:ILE:CD1	2.47	0.44
1:C:303:LEU:O	1:C:304:LYS:C	2.55	0.44
1:C:355:ARG:HB2	1:C:398:ASP:HA	1.99	0.44
1:C:426:PRO:HB2	1:C:427:ASP:H	1.55	0.44
1:C:481:LYS:HG3	1:C:481:LYS:O	2.18	0.44
1:C:489:PHE:CG	1:C:490:PRO:HD2	2.53	0.44
1:C:577:ASP:HB3	1:C:581:LEU:N	2.32	0.44
1:C:586:ILE:HG22	1:C:586:ILE:O	2.17	0.44
1:C:953:ASN:C	1:C:955:ASN:H	2.19	0.44
2:Q:33:VAL:N	2:Q:55:PHE:H	2.15	0.44
2:Q:99:LEU:CG	2:Q:101:PRO:HD2	2.47	0.44
4:F:76:ILE:HD11	4:F:87:TYR:HE1	1.82	0.44
2:H:13:LYS:N	2:H:123:VAL:CG1	2.78	0.44
2:H:49:GLY:HA2	2:H:60:TYR:HA	2.00	0.44
1:A:58:PHE:O	1:A:60:SER:N	2.51	0.44
1:A:305:SER:OG	1:A:307:THR:O	2.33	0.44
1:A:403:LYS:HE2	3:E:102:ARG:HH12	1.82	0.44
1:A:608:ALA:HA	1:A:651:GLY:HA3	1.99	0.44
1:A:969:LYS:HE2	1:A:974:SER:HA	2.00	0.44
1:B:201:PHE:O	1:B:201:PHE:CG	2.70	0.44
1:B:764:LYS:HB3	1:B:764:LYS:HE3	1.59	0.44
1:C:326:ILE:HG22	1:C:541:ASN:HD21	1.81	0.44
1:C:327:VAL:HB	1:C:530:THR:O	2.17	0.44
1:C:364:ASP:C	1:C:366:SER:N	2.71	0.44
1:C:365:TYR:CD1	1:C:388:ASN:HB3	2.53	0.44
1:C:402:ILE:HA	1:C:494:TYR:CE2	2.53	0.44
3:S:67:ARG:HA	3:S:85:ARG:NE	2.33	0.44
3:S:98:ARG:HG3	3:S:116:ASN:CB	2.44	0.44
2:D:39:GLN:C	2:D:39:GLN:HE21	2.21	0.44
2:D:39:GLN:HE21	2:D:40:ALA:N	2.16	0.44
2:D:55:PHE:C	2:D:57:THR:H	2.20	0.44
4:F:6:THR:C	4:F:8:SER:N	2.69	0.44
2:H:98:ARG:HG3	2:H:100:PHE:CE2	2.51	0.44
3:I:72:THR:OG1	3:I:73:ASP:N	2.50	0.44
4:J:60:PRO:HB2	4:J:63:PHE:HE1	1.81	0.44
1:A:167:THR:O	1:A:168:PHE:C	2.55	0.44
1:A:192:PHE:O	1:A:194:PHE:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:NH1	1:A:532:LEU:HD13	2.32	0.44
1:A:363:ALA:HB2	1:A:523:VAL:CG2	2.48	0.44
1:A:635:TYR:CD2	1:A:635:TYR:O	2.71	0.44
1:A:654:TYR:O	1:A:655:VAL:C	2.56	0.44
1:A:855:PHE:HB3	1:A:856:ASN:H	1.63	0.44
1:A:909:ILE:HG13	1:A:911:VAL:HG23	2.00	0.44
1:B:122:ASN:ND2	1:B:125:ASN:H	2.16	0.44
1:B:219:PHE:CE2	1:B:288:ALA:HB3	2.53	0.44
1:B:310:LYS:HG2	1:B:663:ILE:HD11	2.00	0.44
1:B:323:THR:HB	1:B:537:CYS:O	2.17	0.44
1:B:353:TRP:CZ3	1:B:465:GLU:N	2.85	0.44
1:B:398:ASP:O	1:B:511:VAL:N	2.43	0.44
1:B:500:TYR:CG	1:B:504:HIS:HD2	2.35	0.44
1:B:809:PRO:HA	1:B:814:LYS:NZ	2.33	0.44
1:B:851:CYS:C	1:B:853:GLN:H	2.21	0.44
1:C:106:PHE:HB2	1:C:234:ILE:HD13	2.00	0.44
1:C:109:THR:HG21	1:C:113:LYS:HZ2	1.83	0.44
1:C:125:ASN:HD21	1:C:171:VAL:HG23	1.82	0.44
1:C:195:LYS:HD3	1:C:204:TYR:CE1	2.52	0.44
1:C:284:THR:H	1:C:284:THR:HG1	1.63	0.44
1:C:312:ILE:CG1	1:C:597:ILE:HG13	2.34	0.44
1:C:447:GLY:HA2	1:C:497:ARG:HH21	1.83	0.44
1:C:564:PHE:CD1	1:C:564:PHE:N	2.85	0.44
2:Q:48:MET:CG	2:Q:68:VAL:HG11	2.45	0.44
3:S:29:PHE:HB2	3:S:77:THR:HG23	1.99	0.44
5:T:60:PRO:O	5:T:62:ARG:N	2.51	0.44
2:D:104:ASP:HB2	2:D:110:ASP:HB2	2.00	0.44
2:D:111:GLY:O	2:D:113:ASP:N	2.51	0.44
3:E:32:TYR:CG	3:E:98:ARG:HD2	2.52	0.44
2:H:4:LEU:CD2	2:H:24:ALA:HA	2.48	0.44
3:I:54:TYR:HB3	3:I:55:ASN:H	1.61	0.44
4:J:37:TYR:HD1	4:J:47:LEU:HD23	1.82	0.44
5:K:22:SER:HB3	5:K:24:ARG:CZ	2.47	0.44
5:K:37:TYR:HB3	5:K:38:GLN:H	1.63	0.44
1:A:170:TYR:CG	1:A:171:VAL:N	2.86	0.44
1:A:298:GLU:O	1:A:302:THR:HG22	2.18	0.44
1:A:339:HIS:NE2	1:A:371:PHE:HE1	2.16	0.44
1:A:420:ASP:HB3	1:A:421:TYR:CD2	2.52	0.44
1:A:438:SER:C	1:A:440:LYS:N	2.70	0.44
1:A:477:ASN:HD21	1:A:484:GLY:H	1.63	0.44
1:A:485:PRO:C	1:A:487:CYS:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:LEU:HA	1:A:728:PRO:HD3	1.83	0.44
1:A:758:SER:O	1:A:760:CYS:N	2.45	0.44
1:B:49:HIS:CD2	1:B:50:LEU:H	2.36	0.44
1:B:111:ASP:HB2	1:B:113:LYS:NZ	2.22	0.44
1:B:166:CYS:SG	1:B:167:THR:N	2.89	0.44
1:B:403:LYS:HG2	1:B:404:GLY:N	2.32	0.44
1:B:504:HIS:CE1	3:S:111:ILE:HG22	2.53	0.44
1:B:770:ILE:O	1:B:770:ILE:HG22	2.18	0.44
1:B:969:LYS:HE2	1:B:969:LYS:HB3	1.77	0.44
1:B:1141:LEU:C	1:B:1143:LEU:N	2.71	0.44
1:C:338:PHE:CD2	1:C:364:ASP:C	2.89	0.44
1:C:361:CYS:SG	1:C:523:VAL:HG12	2.58	0.44
1:C:365:TYR:CE1	1:C:388:ASN:HA	2.52	0.44
3:S:106:PHE:HD2	3:S:109:SER:N	2.15	0.44
2:D:46:GLU:HG3	2:D:47:TRP:N	2.33	0.44
2:D:47:TRP:CH2	2:D:51:PHE:HA	2.53	0.44
2:D:101:PRO:HA	4:F:92:TYR:CE2	2.53	0.44
4:F:15:SER:CB	4:F:106:ILE:HD12	2.48	0.44
5:G:39:GLN:CB	5:G:88:TYR:HE1	2.30	0.44
5:G:46:ARG:HG3	5:G:46:ARG:O	2.18	0.44
3:I:40:ALA:O	3:I:41:PRO:C	2.56	0.44
3:I:60:TYR:OH	3:I:70:MET:N	2.48	0.44
4:J:84:ILE:HG22	4:J:105:GLU:HA	1.98	0.44
1:A:92:PHE:CD2	1:A:237:PHE:HE2	2.36	0.44
1:B:341:VAL:O	1:B:344:ALA:HB2	2.17	0.44
1:B:558:PHE:CZ	1:B:574:ALA:HB1	2.48	0.44
1:B:563:GLN:HB2	1:B:564:PHE:H	1.59	0.44
1:B:566:ARG:HG2	1:B:570:ASP:OD1	2.18	0.44
1:B:737:ASP:CB	1:B:740:MET:HB3	2.38	0.44
1:B:906:PHE:O	1:B:907:ASN:C	2.56	0.44
1:C:81:ASN:HA	1:C:82:PRO:HD3	1.83	0.44
1:C:406:GLU:HB3	1:C:409:GLN:NE2	2.33	0.44
1:C:427:ASP:O	1:C:428:ASP:C	2.57	0.44
1:C:965:GLN:HG2	1:C:970:PHE:CZ	2.53	0.44
1:C:995:ARG:CZ	1:C:995:ARG:HB3	2.48	0.44
2:Q:2:VAL:HG11	2:Q:98:ARG:HG2	1.98	0.44
4:R:90:GLN:HE21	4:R:91:ARG:N	2.15	0.44
5:T:22:SER:HA	5:T:72:PHE:O	2.18	0.44
2:D:39:GLN:NE2	2:D:45:LEU:HA	2.33	0.44
4:F:77:SER:O	4:F:79:LEU:N	2.50	0.44
3:I:2:VAL:HG13	3:I:27:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:107:GLY:HA2	3:I:111:ILE:CG1	2.47	0.44
4:J:92:TYR:HD1	4:J:92:TYR:HA	1.63	0.44
5:K:34:LEU:HD13	5:K:72:PHE:CE1	2.53	0.44
5:K:68:SER:HA	5:K:72:PHE:CZ	2.53	0.44
1:A:200:TYR:CA	1:A:229:PRO:HA	2.47	0.43
1:A:458:LYS:HA	1:A:458:LYS:HD2	1.66	0.43
1:A:563:GLN:H	1:A:563:GLN:HG3	1.53	0.43
1:A:576:ARG:O	1:A:582:GLU:N	2.51	0.43
1:A:696:THR:O	1:A:697:MET:C	2.57	0.43
1:A:849:LEU:HB2	1:A:850:ILE:H	1.63	0.43
1:A:898:PHE:O	1:A:899:PRO:C	2.54	0.43
1:B:323:THR:C	1:B:325:SER:N	2.72	0.43
1:B:457:ARG:HA	1:B:473:TYR:CA	2.46	0.43
1:C:186:PHE:CZ	1:C:211:ILE:HA	2.53	0.43
1:C:869:MET:C	1:C:871:ALA:N	2.66	0.43
1:C:966:LEU:HD12	1:C:966:LEU:HA	1.70	0.43
1:C:1002:GLN:HG2	1:C:1002:GLN:O	2.18	0.43
3:S:13:LYS:HD3	3:S:13:LYS:HA	1.72	0.43
3:E:73:ASP:O	3:E:74:THR:C	2.57	0.43
1:A:34:ARG:NH2	1:A:216:PRO:HD2	2.33	0.43
1:A:271:GLN:HE21	1:A:271:GLN:HB3	1.67	0.43
1:A:355:ARG:HH21	1:A:357:ARG:HB2	1.83	0.43
1:A:725:GLU:O	1:A:1061:VAL:HA	2.19	0.43
1:A:966:LEU:HD23	1:A:1000:ARG:HD2	2.00	0.43
1:B:130:VAL:O	1:B:166:CYS:HB2	2.17	0.43
1:B:202:LYS:HE3	1:B:202:LYS:HB3	1.61	0.43
1:B:330:PRO:HA	1:B:579:GLN:CD	2.38	0.43
1:B:350:VAL:O	1:B:352:ALA:N	2.51	0.43
1:B:747:THR:C	1:B:749:CYS:H	2.20	0.43
1:B:825:LYS:HB3	1:B:825:LYS:HE3	1.59	0.43
1:C:278:LYS:HB3	1:C:278:LYS:HE3	1.82	0.43
1:C:365:TYR:CE1	1:C:388:ASN:HB3	2.53	0.43
1:C:449:TYR:O	1:C:451:TYR:N	2.51	0.43
2:Q:49:GLY:C	2:Q:59:ILE:HG21	2.39	0.43
2:Q:105:PRO:HB2	2:Q:106:ASN:OD1	2.17	0.43
4:R:77:SER:O	4:R:78:SER:C	2.56	0.43
5:T:91:GLN:NE2	5:T:94:THR:HB	2.33	0.43
3:E:57:ASN:N	3:E:57:ASN:OD1	2.49	0.43
2:H:59:ILE:C	2:H:61:ALA:N	2.71	0.43
3:I:73:ASP:H	3:I:76:THR:HG1	1.66	0.43
4:J:22:ILE:HG13	4:J:36:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TRP:CD1	1:A:214:ASP:HB3	2.53	0.43
1:A:522:THR:HG23	1:A:523:VAL:N	2.30	0.43
1:A:633:ARG:HA	1:A:633:ARG:HH11	1.82	0.43
1:A:811:LYS:HG3	1:A:820:ASP:OD2	2.18	0.43
1:A:898:PHE:H	1:C:707:TYR:HE2	1.63	0.43
1:B:55:PHE:HB2	1:B:275:PHE:CZ	2.54	0.43
1:B:56:LEU:N	1:B:270:LEU:HD12	2.33	0.43
1:B:328:ARG:HB2	1:B:329:PHE:H	1.49	0.43
1:B:342:PHE:CZ	1:B:512:LEU:HD21	2.53	0.43
1:B:365:TYR:CD1	1:B:365:TYR:N	2.86	0.43
1:B:392:PHE:C	1:B:394:ASN:N	2.72	0.43
1:B:437:ASN:OD1	1:B:438:SER:N	2.51	0.43
1:B:609:VAL:O	1:B:649:LEU:HD12	2.18	0.43
1:B:850:ILE:O	1:B:853:GLN:HG3	2.18	0.43
1:B:958:ALA:C	1:B:960:ASN:H	2.20	0.43
1:C:102:ARG:NH1	1:C:241:LEU:HD12	2.33	0.43
1:C:138:ASP:N	1:C:139:PRO:HD3	2.33	0.43
2:Q:4:LEU:CD2	2:Q:24:ALA:HA	2.48	0.43
4:R:16:VAL:HA	4:R:81:PRO:CD	2.46	0.43
4:R:18:ASP:CG	4:R:19:ARG:H	2.22	0.43
5:T:11:LEU:HD12	5:T:12:SER:N	2.30	0.43
3:E:2:VAL:HG22	3:E:27:TYR:HB3	1.99	0.43
4:F:81:PRO:C	4:F:83:ASP:H	2.22	0.43
4:F:84:ILE:HG23	4:F:106:ILE:HB	1.99	0.43
4:F:93:ASP:CB	4:F:94:PRO:HD2	2.49	0.43
5:G:32:THR:O	5:G:92:HIS:HB3	2.18	0.43
5:G:62:ARG:CB	5:G:77:SER:HB2	2.49	0.43
5:G:103:LYS:HA	5:G:103:LYS:HD2	1.64	0.43
2:H:93:VAL:HA	2:H:119:THR:O	2.17	0.43
3:I:101:THR:HB	3:I:112:GLY:N	2.32	0.43
1:A:276:LEU:HD13	1:A:304:LYS:HG3	2.00	0.43
1:A:440:LYS:NZ	5:G:93:ASP:HB3	2.33	0.43
1:A:497:ARG:O	1:A:498:PRO:C	2.56	0.43
1:A:508:ARG:HH12	2:D:32:HIS:CE1	2.36	0.43
1:A:557:LYS:HZ2	1:A:557:LYS:N	2.16	0.43
1:B:66:HIS:C	1:B:80:ASP:HB3	2.38	0.43
1:B:360:ASN:H	1:B:522:THR:HG23	1.84	0.43
1:B:452:TRP:HA	1:B:493:SER:HB3	2.00	0.43
1:B:554:SER:HB2	1:B:585:ASP:HB2	1.99	0.43
1:B:699:LEU:HD12	1:C:872:GLN:CD	2.38	0.43
1:B:711:SER:HA	1:B:1076:THR:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ASN:O	1:C:207:HIS:CD2	2.72	0.43
1:C:188:ASN:HB3	1:C:189:LEU:H	1.65	0.43
1:C:410:ILE:H	1:C:410:ILE:HG13	1.47	0.43
1:C:773:GLU:C	1:C:775:ASP:N	2.72	0.43
1:C:986:PRO:HB2	1:C:987:PRO:HD3	2.00	0.43
3:E:101:THR:HG22	3:E:114:PHE:HA	2.01	0.43
4:F:47:LEU:HD23	4:F:47:LEU:HA	1.81	0.43
5:G:34:LEU:N	5:G:91:GLN:HA	2.33	0.43
5:G:86:VAL:HG13	5:G:102:THR:H	1.82	0.43
3:I:2:VAL:HG13	3:I:27:TYR:HD2	1.81	0.43
3:I:2:VAL:HG11	3:I:98:ARG:CD	2.46	0.43
3:I:18:VAL:C	3:I:82:GLU:HA	2.39	0.43
1:A:129:LYS:HZ3	1:A:130:VAL:H	1.67	0.43
1:A:355:ARG:HG2	1:A:397:ALA:O	2.19	0.43
1:A:497:ARG:C	1:A:499:THR:N	2.70	0.43
1:A:530:THR:HG22	1:A:531:ASN:N	2.28	0.43
1:A:558:PHE:CD2	1:A:576:ARG:HG2	2.53	0.43
1:A:561:PHE:CE1	1:B:41:LYS:HB3	2.54	0.43
1:A:588:PRO:HG2	1:B:855:PHE:CG	2.53	0.43
1:A:708:SER:C	1:A:710:ASN:N	2.71	0.43
1:A:936:ASP:OD1	1:A:936:ASP:N	2.51	0.43
1:B:111:ASP:CG	1:B:113:LYS:HD2	2.39	0.43
1:B:1116:THR:H	1:B:1119:ASN:ND2	2.16	0.43
1:C:356:THR:O	1:C:397:ALA:N	2.42	0.43
1:C:820:ASP:C	1:C:822:LEU:N	2.72	0.43
2:Q:38:ARG:HG2	2:Q:46:GLU:HG3	2.01	0.43
3:S:101:THR:O	3:S:102:ARG:HB2	2.18	0.43
3:E:20:VAL:HB	3:E:21:SER:H	1.56	0.43
4:F:47:LEU:HD11	4:F:50:TYR:HA	2.00	0.43
5:K:4:LEU:HD13	5:K:4:LEU:HA	1.91	0.43
5:K:33:SER:CA	5:K:92:HIS:HB2	2.39	0.43
1:A:63:THR:HG22	1:A:64:TRP:H	1.83	0.43
1:A:296:LEU:HB2	1:A:607:VAL:HG11	2.00	0.43
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.42	0.43
1:A:361:CYS:N	1:A:523:VAL:HA	2.33	0.43
1:A:496:PHE:CB	1:A:506:PRO:HG3	2.49	0.43
1:A:568:ILE:H	1:A:568:ILE:HD12	1.82	0.43
1:A:909:ILE:CG1	1:A:911:VAL:HG23	2.48	0.43
1:A:919:ASN:HD22	1:A:919:ASN:HA	1.62	0.43
1:A:985:ASP:OD1	1:A:988:GLU:HB3	2.19	0.43
1:B:86:PHE:CE2	1:B:196:ASN:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:GLU:OE1	1:B:166:CYS:HA	2.18	0.43
1:B:319:ARG:O	1:B:320:VAL:C	2.57	0.43
1:B:802:PHE:CE1	1:B:927:PHE:CE2	3.07	0.43
1:B:870:ILE:HG22	1:B:870:ILE:O	2.19	0.43
1:C:96:GLU:H	1:C:188:ASN:CG	2.22	0.43
1:C:323:THR:C	1:C:325:SER:H	2.20	0.43
1:C:376:ALA:CB	1:C:435:ALA:HB3	2.46	0.43
1:C:438:SER:HG	1:C:506:PRO:HB2	1.83	0.43
1:C:877:LEU:HD22	1:C:1034:LEU:HD11	2.00	0.43
1:C:993:ILE:HG22	1:C:994:ASP:N	2.34	0.43
2:Q:112:PHE:O	2:Q:113:ASP:C	2.57	0.43
4:F:37:TYR:HD1	4:F:47:LEU:HA	1.84	0.43
5:G:22:SER:HB3	5:G:24:ARG:CZ	2.49	0.43
5:G:34:LEU:H	5:G:91:GLN:HA	1.83	0.43
2:H:47:TRP:HZ2	2:H:51:PHE:HA	1.79	0.43
2:H:89:GLU:H	2:H:89:GLU:HG3	1.62	0.43
4:J:16:VAL:HG21	4:J:107:LYS:HD2	2.00	0.43
4:J:35:ASN:O	4:J:36:TRP:CB	2.66	0.43
1:A:89:GLY:O	1:A:90:VAL:HG13	2.18	0.43
1:A:129:LYS:HZ3	1:A:129:LYS:HB2	1.83	0.43
1:A:440:LYS:HA	1:A:440:LYS:HD2	1.70	0.43
1:A:444:LYS:HE2	2:D:76:THR:HG23	2.00	0.43
1:A:551:LEU:CD2	1:A:586:ILE:HG12	2.48	0.43
1:A:653:GLU:H	1:A:653:GLU:HG2	1.57	0.43
1:B:92:PHE:HB2	1:B:194:PHE:CE2	2.54	0.43
1:B:375:PHE:HB3	1:B:435:ALA:O	2.18	0.43
1:B:413:GLY:N	1:B:426:PRO:O	2.52	0.43
1:B:462:LYS:O	1:B:463:PRO:C	2.57	0.43
1:B:564:PHE:CG	1:B:564:PHE:O	2.70	0.43
1:B:740:MET:HG2	1:B:857:GLY:CA	2.48	0.43
1:B:752:LEU:HD13	1:B:990:GLU:HG3	2.00	0.43
1:B:949:GLN:O	1:B:950:ASP:C	2.57	0.43
1:C:171:VAL:HG22	1:C:172:SER:N	2.29	0.43
1:C:280:ASN:HB3	1:C:286:THR:HG21	2.00	0.43
1:C:439:ASN:C	1:C:441:LEU:N	2.71	0.43
1:C:471:GLU:O	1:C:472:ILE:C	2.57	0.43
1:C:1125:ASN:C	1:C:1127:ASP:H	2.22	0.43
3:S:73:ASP:O	3:S:74:THR:C	2.57	0.43
3:S:110:LEU:HD12	3:S:116:ASN:H	1.83	0.43
4:R:81:PRO:C	4:R:83:ASP:H	2.22	0.43
4:R:91:ARG:O	4:R:92:TYR:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:GLY:HA3	2:H:72:ALA:HB3	2.00	0.43
3:I:29:PHE:HB2	3:I:77:THR:HG23	1.99	0.43
4:J:22:ILE:HG13	4:J:36:TRP:CH2	2.54	0.43
4:J:22:ILE:N	4:J:74:PHE:O	2.51	0.43
4:J:96:TYR:N	4:J:96:TYR:CD1	2.87	0.43
1:A:284:THR:O	1:A:286:THR:HG23	2.18	0.43
1:A:748:GLU:OE2	1:A:981:LEU:HD13	2.19	0.43
1:A:870:ILE:O	1:A:870:ILE:HG22	2.18	0.43
1:A:964:LYS:HE2	1:A:964:LYS:HB2	1.68	0.43
1:B:112:SER:HA	1:B:133:PHE:C	2.39	0.43
1:B:273:ARG:NH2	1:B:290:ASP:OD1	2.50	0.43
1:B:353:TRP:HE1	1:B:467:ASP:HB3	1.84	0.43
1:B:501:GLY:O	1:B:504:HIS:CE1	2.72	0.43
1:B:532:LEU:HD22	1:B:532:LEU:HA	1.70	0.43
1:B:637:THR:O	1:B:650:ILE:HG21	2.18	0.43
1:B:754:LEU:H	1:B:754:LEU:HG	1.60	0.43
1:B:906:PHE:O	1:B:909:ILE:HG12	2.19	0.43
1:C:399:SER:HB3	1:C:510:VAL:HG22	1.99	0.43
1:C:403:LYS:HG2	1:C:504:HIS:CD2	2.54	0.43
1:C:409:GLN:C	1:C:411:ALA:N	2.72	0.43
1:C:445:HIS:CE1	1:C:498:PRO:HG3	2.53	0.43
1:C:655:VAL:HG23	1:C:695:TYR:HB3	2.01	0.43
1:C:833:PHE:HE2	1:C:851:CYS:SG	2.42	0.43
2:Q:93:VAL:HA	2:Q:119:THR:O	2.17	0.43
3:S:47:TRP:CH2	3:S:49:GLY:HA2	2.53	0.43
5:T:29:VAL:CG1	5:T:33:SER:HB2	2.49	0.43
4:F:77:SER:O	4:F:78:SER:C	2.56	0.43
3:I:98:ARG:HH21	3:I:116:ASN:HB3	1.83	0.43
5:K:50:TYR:O	5:K:52:ALA:N	2.52	0.43
1:A:38:TYR:CD2	1:A:285:ILE:HG13	2.53	0.43
1:A:129:LYS:HB2	1:A:169:GLU:HA	2.00	0.43
1:A:542:PHE:CE2	1:A:575:VAL:HG21	2.53	0.43
1:A:611:TYR:O	1:A:647:GLY:HA3	2.18	0.43
1:A:702:GLU:CD	1:B:790:LYS:HG3	2.39	0.43
1:A:862:PRO:HA	1:A:863:PRO:HD3	1.93	0.43
1:A:948:LEU:HD21	1:A:1059:GLY:HA3	2.00	0.43
1:B:119:ILE:HG13	1:B:120:VAL:H	1.83	0.43
1:B:133:PHE:O	1:B:135:PHE:N	2.52	0.43
1:B:324:GLU:HG3	1:B:533:VAL:HG21	2.00	0.43
1:B:339:HIS:CG	1:B:367:VAL:HB	2.53	0.43
1:B:357:ARG:O	1:B:358:ILE:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:CYS:O	1:B:740:MET:N	2.52	0.43
1:B:776:LYS:HB3	1:B:776:LYS:HE2	1.85	0.43
1:B:950:ASP:O	1:B:952:VAL:N	2.52	0.43
1:C:44:ARG:O	1:C:283:GLY:HA2	2.19	0.43
1:C:355:ARG:HB2	1:C:398:ASP:CA	2.48	0.43
1:C:810:SER:O	1:C:811:LYS:C	2.57	0.43
1:C:986:PRO:HB2	1:C:987:PRO:CD	2.48	0.43
2:Q:24:ALA:O	2:Q:25:SER:C	2.57	0.43
2:Q:102:ASN:N	2:Q:109:GLU:HB2	2.33	0.43
3:S:33:GLY:HA3	3:S:50:TRP:CH2	2.54	0.43
2:D:106:ASN:ND2	2:D:109:GLU:O	2.52	0.43
2:D:120:LEU:HD13	2:D:120:LEU:HA	1.82	0.43
2:H:44:GLY:O	2:H:45:LEU:C	2.56	0.43
5:K:34:LEU:O	5:K:35:ALA:C	2.56	0.43
5:K:103:LYS:HA	5:K:103:LYS:HD2	1.47	0.43
1:A:115:GLN:HB3	1:A:130:VAL:CG2	2.49	0.43
1:A:127:PHE:CG	1:A:128:ILE:N	2.87	0.43
1:A:336:CYS:SG	1:A:338:PHE:HB2	2.58	0.43
1:A:500:TYR:CE2	3:E:105:TRP:CZ3	3.07	0.43
1:B:300:LYS:O	1:B:301:CYS:C	2.57	0.43
1:B:380:TYR:CD1	1:B:380:TYR:N	2.87	0.43
1:B:854:LYS:HB2	1:B:854:LYS:HE3	1.69	0.43
1:B:916:LEU:O	1:B:918:GLU:N	2.51	0.43
1:C:106:PHE:HA	1:C:236:ARG:O	2.19	0.43
1:C:733:LYS:HB2	1:C:733:LYS:HE2	1.81	0.43
1:C:898:PHE:HB3	1:C:899:PRO:CD	2.49	0.43
1:C:959:LEU:HD12	1:C:960:ASN:ND2	2.34	0.43
2:Q:28:THR:O	2:Q:29:PHE:C	2.57	0.43
4:R:15:SER:O	4:R:17:GLY:N	2.52	0.43
5:T:25:ALA:C	5:T:27:GLN:N	2.73	0.43
2:D:17:SER:HA	2:D:86:LEU:HD12	2.01	0.43
2:D:24:ALA:O	2:D:25:SER:C	2.57	0.43
5:G:94:THR:O	5:G:96:LEU:N	2.52	0.43
2:H:67:ARG:HD2	2:H:87:ARG:HG3	2.01	0.43
1:A:339:HIS:CD2	1:A:342:PHE:HD2	2.37	0.42
1:A:356:THR:N	1:A:397:ALA:HB3	2.34	0.42
1:A:786:LYS:H	1:A:786:LYS:HG2	1.54	0.42
1:B:411:ALA:HB3	1:B:414:GLN:HG2	2.01	0.42
1:B:657:ASN:OD1	1:B:657:ASN:N	2.52	0.42
1:B:744:GLY:O	1:B:746:SER:N	2.52	0.42
1:B:961:THR:HG21	1:C:762:GLN:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:ARG:HE	1:C:467:ASP:HB3	1.83	0.42
1:C:552:THR:O	1:C:584:LEU:HB2	2.19	0.42
1:C:770:ILE:O	1:C:774:GLN:HG2	2.19	0.42
1:C:936:ASP:HA	1:C:939:PHE:CD2	2.54	0.42
2:Q:39:GLN:HE22	2:Q:45:LEU:HG	1.83	0.42
2:Q:93:VAL:HG12	2:Q:94:TYR:N	2.34	0.42
4:R:19:ARG:CA	4:R:79:LEU:HD12	2.49	0.42
4:R:37:TYR:HA	4:R:48:LEU:H	1.84	0.42
4:R:67:GLY:HA3	4:R:72:PHE:CA	2.48	0.42
3:E:38:ARG:O	3:E:46:GLU:N	2.52	0.42
5:G:86:VAL:HB	5:G:88:TYR:CE1	2.54	0.42
2:H:11:VAL:HB	2:H:12:LYS:H	1.52	0.42
1:A:42:VAL:HG11	1:C:566:ARG:HH12	1.84	0.42
1:A:351:TYR:HB3	1:A:453:TYR:HA	2.02	0.42
1:A:392:PHE:O	1:A:393:THR:C	2.58	0.42
1:A:403:LYS:HG3	1:A:504:HIS:HB3	2.00	0.42
1:A:462:LYS:O	1:A:463:PRO:C	2.58	0.42
1:A:735:SER:OG	1:A:861:LEU:HD11	2.19	0.42
1:A:770:ILE:HG23	1:A:1015:ALA:CB	2.49	0.42
1:A:869:MET:CB	1:C:699:LEU:HD21	2.39	0.42
1:B:308:VAL:HG21	1:B:598:THR:HG21	2.01	0.42
1:B:329:PHE:CG	1:B:330:PRO:CD	3.02	0.42
1:B:447:GLY:H	1:B:497:ARG:HB3	1.85	0.42
1:B:563:GLN:NE2	1:B:576:ARG:HD2	2.35	0.42
1:B:1095:PHE:HZ	1:B:1120:THR:HG22	1.84	0.42
1:C:189:LEU:O	1:C:191:GLU:N	2.52	0.42
1:C:318:PHE:CE2	1:C:592:GLY:HA3	2.54	0.42
1:C:338:PHE:O	1:C:340:GLU:N	2.45	0.42
1:C:386:LYS:O	1:C:387:LEU:C	2.57	0.42
1:C:814:LYS:HA	1:C:814:LYS:HD3	1.59	0.42
2:Q:123:VAL:HG23	2:Q:124:SER:N	2.34	0.42
4:R:57:THR:C	4:R:59:VAL:N	2.71	0.42
5:T:35:ALA:HB2	5:T:92:HIS:HE1	1.84	0.42
3:E:36:TRP:HA	3:E:95:TYR:O	2.19	0.42
3:E:40:ALA:O	3:E:41:PRO:C	2.56	0.42
4:F:9:PRO:HD2	4:F:102:THR:HG22	2.01	0.42
5:G:13:LEU:HD13	5:G:13:LEU:HA	1.83	0.42
2:H:87:ARG:N	2:H:90:ASP:OD2	2.39	0.42
4:J:93:ASP:O	4:J:96:TYR:CE1	2.72	0.42
1:A:338:PHE:CD2	1:A:368:LEU:HD11	2.54	0.42
1:A:396:TYR:N	1:A:513:SER:O	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ALA:HB3	1:A:414:GLN:CG	2.42	0.42
1:A:654:TYR:O	1:A:654:TYR:CG	2.68	0.42
1:A:814:LYS:HE3	1:A:814:LYS:HB3	1.46	0.42
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.69	0.42
1:B:116:SER:O	1:B:117:LEU:C	2.57	0.42
1:B:141:LEU:HD23	1:B:141:LEU:HA	1.76	0.42
1:B:329:PHE:CD1	1:B:543:ASN:HA	2.54	0.42
1:B:338:PHE:HB3	1:B:339:HIS:H	1.41	0.42
1:B:361:CYS:HB3	1:B:362:VAL:H	1.40	0.42
1:B:393:THR:H	1:B:516:LEU:HD13	1.84	0.42
1:B:471:GLU:HA	1:B:483:LYS:HZ1	1.84	0.42
1:B:874:THR:HG23	1:B:1053:PRO:O	2.19	0.42
1:B:916:LEU:O	1:B:917:TYR:C	2.58	0.42
1:B:943:SER:OG	1:B:944:ALA:N	2.52	0.42
1:B:1143:LEU:HD23	1:B:1143:LEU:HA	1.79	0.42
1:C:83:VAL:O	1:C:84:LEU:C	2.57	0.42
1:C:408:SER:HB3	1:C:509:VAL:CG1	2.48	0.42
1:C:457:ARG:HD2	1:C:467:ASP:CG	2.39	0.42
1:C:553:LYS:HB3	1:C:553:LYS:HE2	1.53	0.42
1:C:566:ARG:HD2	1:C:570:ASP:HA	2.01	0.42
4:R:15:SER:OG	4:R:107:LYS:HE3	2.19	0.42
4:R:86:THR:HA	4:R:103:LYS:HD3	2.01	0.42
2:D:73:ASP:C	2:D:75:SER:H	2.22	0.42
5:G:68:SER:HA	5:G:72:PHE:CZ	2.53	0.42
3:I:19:LYS:CG	3:I:82:GLU:HB3	2.45	0.42
1:A:118:LEU:C	1:A:120:VAL:N	2.72	0.42
1:A:121:ASN:O	1:A:122:ASN:HB2	2.20	0.42
1:A:402:ILE:HB	1:A:406:GLU:OE1	2.20	0.42
1:A:558:PHE:HE2	1:A:575:VAL:O	2.02	0.42
1:B:62:VAL:HB	1:B:63:THR:H	1.65	0.42
1:B:120:VAL:O	1:B:121:ASN:HB3	2.19	0.42
1:B:710:ASN:O	1:B:1076:THR:HG23	2.19	0.42
1:B:898:PHE:C	1:B:900:MET:N	2.73	0.42
1:C:110:LEU:HD12	1:C:111:ASP:O	2.19	0.42
1:C:395:VAL:HA	1:C:513:SER:O	2.19	0.42
1:C:456:PHE:CE1	1:C:490:PRO:HA	2.54	0.42
1:C:633:ARG:HA	1:C:633:ARG:CZ	2.49	0.42
1:C:741:TYR:CZ	1:C:966:LEU:HD13	2.55	0.42
1:C:798:GLY:HA3	1:C:899:PRO:HD3	1.99	0.42
2:Q:101:PRO:HB3	4:R:92:TYR:CD1	2.54	0.42
2:Q:105:PRO:HG3	2:Q:110:ASP:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:LEU:CD2	2:D:24:ALA:HA	2.48	0.42
4:F:77:SER:HB3	4:F:78:SER:H	1.67	0.42
5:G:47:LEU:CD2	5:G:50:TYR:HD2	2.32	0.42
3:I:47:TRP:NE1	3:I:49:GLY:O	2.53	0.42
5:K:62:ARG:HD2	5:K:78:ARG:H	1.83	0.42
1:A:91:TYR:CE2	1:A:215:PHE:CE1	3.08	0.42
1:A:316:SER:HB2	1:A:317:ASN:H	1.57	0.42
1:A:362:VAL:O	1:A:364:ASP:OD1	2.36	0.42
1:A:409:GLN:HG3	1:A:415:THR:O	2.19	0.42
1:A:421:TYR:HB3	1:A:457:ARG:HB2	1.99	0.42
1:A:499:THR:HG22	3:E:111:ILE:HG22	2.00	0.42
1:A:833:PHE:HE1	1:A:836:GLN:HA	1.82	0.42
1:A:1131:GLY:O	1:A:1132:ILE:C	2.58	0.42
1:B:95:THR:CB	1:B:186:PHE:HD2	2.27	0.42
1:B:122:ASN:HD22	1:B:124:THR:HB	1.84	0.42
1:B:190:ARG:CD	1:B:207:HIS:HB3	2.41	0.42
1:B:356:THR:HG22	1:B:397:ALA:O	2.18	0.42
1:B:714:ILE:HA	1:B:715:PRO:HD3	1.89	0.42
1:C:86:PHE:CD2	1:C:90:VAL:HG22	2.54	0.42
1:C:308:VAL:O	1:C:601:THR:OG1	2.38	0.42
1:C:338:PHE:CE2	1:C:363:ALA:HB1	2.55	0.42
1:C:419:ALA:HB1	1:C:424:LYS:HD2	2.01	0.42
1:C:441:LEU:HB2	2:H:55:PHE:CD2	2.55	0.42
1:C:523:VAL:HG23	1:C:524:CYS:H	1.85	0.42
2:Q:51:PHE:HD1	2:Q:51:PHE:N	2.17	0.42
3:S:28:PRO:HD2	3:S:32:TYR:HE2	1.85	0.42
2:D:22:CYS:HB3	2:D:79:ALA:HB3	2.01	0.42
2:D:38:ARG:CZ	2:D:92:ALA:H	2.33	0.42
2:D:51:PHE:CD2	2:D:53:PRO:HD2	2.54	0.42
3:E:16:ALA:O	3:E:86:LEU:N	2.50	0.42
5:G:46:ARG:CZ	5:G:59:ILE:HG23	2.50	0.42
5:G:50:TYR:O	5:G:51:GLY:C	2.58	0.42
2:H:24:ALA:O	2:H:25:SER:C	2.57	0.42
3:I:31:SER:O	3:I:32:TYR:CG	2.73	0.42
4:J:90:GLN:HE21	4:J:91:ARG:H	1.66	0.42
5:K:84:PHE:HB3	5:K:105:GLU:CB	2.50	0.42
1:A:33:THR:HB	1:A:219:PHE:HD1	1.85	0.42
1:A:195:LYS:HE3	1:A:197:ILE:CD1	2.49	0.42
1:A:749:CYS:O	1:A:750:SER:C	2.57	0.42
1:A:813:SER:HB2	1:A:815:ARG:CG	2.48	0.42
1:B:394:ASN:ND2	1:B:515:GLU:OE1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:PHE:O	1:B:544:GLY:N	2.52	0.42
1:B:927:PHE:HE1	1:B:931:ILE:HD13	1.84	0.42
1:C:614:VAL:O	1:C:643:GLN:NE2	2.52	0.42
1:C:708:SER:HB3	1:C:711:SER:HB2	2.00	0.42
1:C:779:GLN:HE21	1:C:779:GLN:HB3	1.42	0.42
1:C:807:PRO:HG3	1:C:875:SER:HB2	2.01	0.42
2:Q:71:SER:O	2:Q:73:ASP:N	2.53	0.42
2:Q:101:PRO:O	2:Q:105:PRO:CD	2.67	0.42
4:R:87:TYR:HB2	4:R:102:THR:OG1	2.18	0.42
2:D:17:SER:CB	2:D:85:SER:N	2.82	0.42
3:E:67:ARG:O	3:E:84:ARG:N	2.53	0.42
5:G:2:ILE:CG2	5:G:25:ALA:HB1	2.49	0.42
5:G:6:GLN:HG3	5:G:100:GLY:N	2.30	0.42
5:G:46:ARG:HH11	5:G:48:LEU:CD2	2.31	0.42
3:I:69:THR:N	3:I:84:ARG:HE	2.17	0.42
4:J:5:MET:HE3	4:J:24:CYS:SG	2.59	0.42
4:J:49:ILE:CD1	4:J:63:PHE:HB3	2.50	0.42
4:J:80:GLN:HB2	4:J:81:PRO:CD	2.44	0.42
1:A:128:ILE:HG23	1:A:170:TYR:O	2.20	0.42
1:A:375:PHE:CZ	3:E:54:TYR:CD2	3.05	0.42
1:A:421:TYR:CD2	1:A:455:LEU:O	2.73	0.42
1:A:520:PRO:HB2	1:A:521:ALA:H	1.54	0.42
1:A:1053:PRO:O	1:A:1054:GLN:HG2	2.20	0.42
1:B:24:THR:H	1:B:80:ASP:HB2	1.84	0.42
1:B:192:PHE:HB3	1:B:194:PHE:CE1	2.54	0.42
1:B:353:TRP:CH2	1:B:461:LEU:HB3	2.48	0.42
1:B:583:ILE:N	1:B:583:ILE:HD13	2.35	0.42
1:B:714:ILE:HG13	1:B:1075:PHE:CD2	2.54	0.42
1:C:36:VAL:HG11	1:C:219:PHE:HE1	1.83	0.42
1:C:95:THR:HA	1:C:188:ASN:HB3	2.02	0.42
1:C:102:ARG:HH12	1:C:241:LEU:HD12	1.83	0.42
1:C:132:GLU:O	1:C:133:PHE:HB2	2.19	0.42
1:C:189:LEU:N	1:C:210:ILE:CG2	2.83	0.42
1:C:331:ASN:N	1:C:579:GLN:CB	2.70	0.42
1:C:414:GLN:HE21	1:C:414:GLN:HB3	1.58	0.42
1:C:779:GLN:O	1:C:783:ALA:HB3	2.20	0.42
1:C:820:ASP:C	1:C:822:LEU:H	2.23	0.42
1:C:887:THR:CG2	1:C:894:LEU:HD12	2.50	0.42
2:Q:32:HIS:HA	2:Q:55:PHE:CG	2.55	0.42
2:Q:72:ALA:HB1	2:Q:79:ALA:CB	2.50	0.42
3:S:98:ARG:HB2	3:S:114:PHE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:49:ILE:HG23	5:T:53:SER:O	2.19	0.42
2:D:52:ILE:HD11	4:F:94:PRO:HD3	2.02	0.42
2:D:101:PRO:HA	4:F:92:TYR:CG	2.54	0.42
3:E:67:ARG:HA	3:E:84:ARG:HB2	2.01	0.42
5:G:4:LEU:HD12	5:G:23:CYS:SG	2.60	0.42
3:I:48:MET:CE	3:I:81:MET:HE1	2.49	0.42
4:J:98:PHE:N	4:J:98:PHE:CD1	2.88	0.42
1:A:54:LEU:HD12	1:A:54:LEU:HA	1.85	0.42
1:A:66:HIS:HB2	1:A:264:ASP:CB	2.50	0.42
1:A:540:PHE:O	1:A:546:THR:HA	2.19	0.42
1:A:557:LYS:H	1:A:557:LYS:NZ	2.17	0.42
1:A:598:THR:HG22	1:A:607:VAL:HG12	2.01	0.42
1:A:1116:THR:HG22	1:A:1140:PRO:HD3	2.02	0.42
1:B:106:PHE:C	1:B:234:ILE:HG12	2.40	0.42
1:B:217:GLN:HE21	1:B:218:GLY:N	2.18	0.42
1:B:295:PRO:HB2	1:B:607:VAL:HG21	2.02	0.42
1:B:357:ARG:HG2	1:B:358:ILE:CG1	2.37	0.42
1:B:536:LYS:O	1:B:537:CYS:C	2.57	0.42
1:B:641:VAL:HG22	1:B:650:ILE:HG12	2.01	0.42
1:B:921:LYS:H	1:B:921:LYS:HG2	1.71	0.42
1:B:1140:PRO:O	1:B:1143:LEU:HB2	2.20	0.42
1:C:118:LEU:C	1:C:119:ILE:HG22	2.40	0.42
1:C:122:ASN:O	1:C:124:THR:N	2.53	0.42
1:C:133:PHE:HB3	1:C:135:PHE:CD2	2.54	0.42
1:C:833:PHE:HB2	1:C:836:GLN:N	2.35	0.42
1:C:1144:GLU:C	1:C:1146:ASP:N	2.72	0.42
2:Q:27:GLY:HA2	2:Q:77:SER:HB3	2.01	0.42
3:S:28:PRO:HG2	3:S:31:SER:HB3	2.02	0.42
4:R:57:THR:O	4:R:58:GLY:C	2.56	0.42
5:G:91:GLN:HE21	5:G:97:THR:H	1.67	0.42
3:I:6:GLN:OE1	3:I:118:GLY:HA3	2.20	0.42
3:I:67:ARG:HA	3:I:85:ARG:CZ	2.50	0.42
3:I:111:ILE:C	3:I:113:GLY:N	2.71	0.42
5:K:86:VAL:HA	5:K:103:LYS:HA	2.02	0.42
1:A:299:THR:HG22	1:A:315:THR:HG21	2.01	0.42
1:A:338:PHE:HZ	1:A:363:ALA:HB1	1.85	0.42
1:A:423:TYR:HH	1:A:464:PHE:HE1	1.64	0.42
1:A:519:ALA:HB1	1:A:520:PRO:CD	2.44	0.42
1:A:835:LYS:HB3	1:A:835:LYS:HE2	1.59	0.42
1:A:874:THR:O	1:A:876:ALA:N	2.53	0.42
1:A:992:GLN:HE21	1:A:992:GLN:HB3	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1024:LEU:O	1:A:1028:LYS:HB2	2.20	0.42
1:B:34:ARG:NH1	1:B:218:GLY:O	2.53	0.42
1:B:192:PHE:HB3	1:B:194:PHE:CZ	2.55	0.42
1:B:339:HIS:HB3	1:B:367:VAL:HB	2.01	0.42
1:B:478:LYS:H	1:B:485:PRO:HB3	1.85	0.42
1:B:522:THR:O	1:B:523:VAL:C	2.58	0.42
1:B:972:ALA:O	1:B:974:SER:N	2.53	0.42
1:C:225:LEU:HD12	1:C:225:LEU:HA	1.90	0.42
1:C:230:ILE:O	1:C:232:ILE:N	2.52	0.42
1:C:330:PRO:HD3	1:C:542:PHE:CG	2.55	0.42
1:C:375:PHE:CE2	3:I:54:TYR:HB3	2.50	0.42
1:C:402:ILE:HD11	1:C:509:VAL:CG2	2.50	0.42
1:C:498:PRO:O	1:C:500:TYR:N	2.53	0.42
1:C:892:PRO:O	1:C:894:LEU:HG	2.19	0.42
1:C:898:PHE:O	1:C:899:PRO:C	2.57	0.42
1:C:983:ARG:O	1:C:984:LEU:HD22	2.20	0.42
1:C:996:LEU:O	1:C:997:ILE:C	2.58	0.42
1:C:997:ILE:O	1:C:1001:LEU:HB2	2.19	0.42
2:Q:59:ILE:CG1	2:Q:60:TYR:H	2.31	0.42
2:Q:101:PRO:HB3	4:R:92:TYR:CG	2.55	0.42
3:S:2:VAL:HG21	3:S:98:ARG:NH2	2.35	0.42
4:R:38:GLN:CD	4:R:40:LYS:HZ3	2.23	0.42
4:F:5:MET:HE1	4:F:91:ARG:CD	2.50	0.42
4:F:35:ASN:HB2	4:F:90:GLN:CG	2.44	0.42
1:A:408:SER:O	1:A:410:ILE:HB	2.20	0.42
1:A:706:ALA:HB3	1:B:895:GLN:NE2	2.35	0.42
1:A:739:THR:O	1:A:740:MET:C	2.57	0.42
1:A:866:THR:C	1:A:868:GLU:N	2.73	0.42
1:A:903:ALA:HB1	1:A:913:GLN:HG2	2.01	0.42
1:B:230:ILE:C	1:B:232:ILE:H	2.22	0.42
1:B:339:HIS:CE1	1:B:370:ASN:HB3	2.55	0.42
1:B:374:PHE:HA	1:B:436:TRP:CB	2.49	0.42
1:B:436:TRP:N	1:B:436:TRP:CE3	2.88	0.42
1:B:502:VAL:O	3:S:101:THR:N	2.53	0.42
1:B:767:LEU:HG	1:B:1008:VAL:HG22	2.02	0.42
1:B:773:GLU:C	1:B:775:ASP:N	2.73	0.42
1:B:896:ILE:O	1:B:896:ILE:HG23	2.20	0.42
1:C:34:ARG:HB2	1:C:34:ARG:NH2	2.35	0.42
1:C:438:SER:O	1:C:440:LYS:N	2.52	0.42
1:C:851:CYS:C	1:C:853:GLN:H	2.23	0.42
1:C:1040:VAL:O	1:C:1042:PHE:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:88:SER:O	2:Q:89:GLU:C	2.58	0.42
2:Q:108:PRO:O	2:Q:109:GLU:CB	2.67	0.42
2:D:83:LEU:O	2:D:84:SER:C	2.57	0.42
3:E:101:THR:CB	3:E:111:ILE:O	2.68	0.42
2:H:51:PHE:CE1	2:H:57:THR:HB	2.55	0.42
4:J:6:THR:C	4:J:8:SER:N	2.71	0.42
4:J:93:ASP:C	4:J:95:SER:N	2.70	0.42
1:A:23:THR:HA	1:A:80:ASP:CA	2.48	0.41
1:A:62:VAL:HG12	1:A:268:GLY:HA2	2.02	0.41
1:A:90:VAL:C	1:A:92:PHE:N	2.74	0.41
1:A:408:SER:O	1:A:410:ILE:N	2.53	0.41
1:A:916:LEU:O	1:A:917:TYR:C	2.58	0.41
1:A:935:GLN:HE21	1:A:935:GLN:HB3	1.74	0.41
1:B:36:VAL:HG21	1:B:219:PHE:CE2	2.54	0.41
1:B:444:LYS:O	1:B:497:ARG:HA	2.20	0.41
1:B:496:PHE:CD1	1:B:496:PHE:N	2.86	0.41
1:B:554:SER:HB3	1:B:583:ILE:HG22	2.02	0.41
1:B:920:GLN:HG2	1:B:920:GLN:O	2.20	0.41
1:B:922:LEU:O	1:B:924:ALA:N	2.53	0.41
1:B:936:ASP:O	1:B:937:SER:C	2.57	0.41
1:C:87:ASN:O	1:C:89:GLY:N	2.46	0.41
1:C:342:PHE:CG	1:C:371:PHE:CZ	3.08	0.41
1:C:365:TYR:CZ	1:C:388:ASN:HA	2.55	0.41
1:C:372:ALA:C	1:C:374:PHE:H	2.23	0.41
1:C:376:ALA:HB3	1:C:435:ALA:CB	2.46	0.41
1:C:416:GLY:H	1:C:419:ALA:HB3	1.85	0.41
1:C:538:VAL:HG23	1:C:539:ASN:H	1.85	0.41
2:Q:72:ALA:CB	2:Q:80:TYR:H	2.33	0.41
3:S:102:ARG:NH2	3:S:110:LEU:O	2.53	0.41
4:R:15:SER:C	4:R:17:GLY:N	2.74	0.41
4:R:34:LEU:O	4:R:51:ASP:HA	2.20	0.41
3:E:29:PHE:HB2	3:E:74:THR:HA	2.02	0.41
4:F:16:VAL:CG1	4:F:107:LYS:HA	2.50	0.41
2:H:32:HIS:HA	2:H:55:PHE:CA	2.50	0.41
2:H:93:VAL:HG12	2:H:94:TYR:N	2.34	0.41
2:H:115:TRP:HZ2	4:J:37:TYR:CE2	2.38	0.41
3:I:68:VAL:HB	3:I:83:LEU:HD12	2.02	0.41
1:A:52:GLN:HG2	1:A:274:THR:OG1	2.19	0.41
1:A:167:THR:HB	1:A:168:PHE:H	1.66	0.41
1:A:277:LEU:HD13	1:A:285:ILE:HD13	2.01	0.41
1:A:618:GLU:O	1:A:620:SER:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:GLU:C	1:A:620:SER:N	2.74	0.41
1:A:932:GLY:O	1:A:933:LYS:C	2.57	0.41
1:B:26:GLN:HG2	1:B:65:PHE:CD1	2.55	0.41
1:B:382:VAL:CG2	1:B:431:GLY:HA2	2.44	0.41
1:B:439:ASN:HD22	1:B:499:THR:N	2.18	0.41
1:B:478:LYS:H	1:B:485:PRO:HA	1.83	0.41
1:B:919:ASN:OD1	1:B:919:ASN:N	2.53	0.41
1:B:1068:VAL:HA	1:B:1069:PRO:HD3	1.89	0.41
2:Q:38:ARG:O	2:Q:46:GLU:N	2.48	0.41
3:S:15:GLY:C	3:S:86:LEU:H	2.23	0.41
3:S:48:MET:HE2	3:S:48:MET:HB3	1.94	0.41
2:D:60:TYR:CD1	2:D:60:TYR:N	2.86	0.41
3:E:36:TRP:CD1	3:E:81:MET:HG3	2.55	0.41
4:F:72:PHE:HB3	4:F:74:PHE:HE1	1.85	0.41
5:G:29:VAL:HG22	5:G:33:SER:OG	2.20	0.41
5:G:38:GLN:HB2	5:G:48:LEU:HD21	2.01	0.41
2:H:23:LYS:HG2	2:H:78:THR:HG23	2.02	0.41
3:I:20:VAL:HB	3:I:21:SER:H	1.56	0.41
4:J:86:THR:HG22	4:J:103:LYS:HD2	2.03	0.41
1:A:129:LYS:HG3	1:A:130:VAL:N	2.34	0.41
1:A:133:PHE:HB2	1:A:163:ALA:HB2	2.02	0.41
1:A:329:PHE:CB	1:A:330:PRO:HD2	2.42	0.41
1:A:350:VAL:O	1:A:352:ALA:N	2.52	0.41
1:A:621:VAL:O	1:A:624:HIS:HB2	2.20	0.41
1:B:206:LYS:HB3	1:B:222:LEU:HD23	2.02	0.41
1:B:406:GLU:HB3	1:B:494:TYR:OH	2.19	0.41
1:B:443:SER:OG	1:B:444:LYS:N	2.53	0.41
1:B:712:ILE:CD1	1:B:1094:VAL:HG21	2.50	0.41
1:C:111:ASP:OD2	1:C:112:SER:N	2.53	0.41
1:C:189:LEU:HA	1:C:189:LEU:HD13	1.76	0.41
1:C:424:LYS:HD2	1:C:424:LYS:HA	1.68	0.41
1:C:440:LYS:HA	1:C:440:LYS:HD2	1.93	0.41
1:C:1051:SER:HB2	1:C:1064:HIS:HD2	1.85	0.41
1:C:1135:ASN:ND2	1:C:1136:THR:H	2.18	0.41
2:Q:115:TRP:CG	4:R:45:PRO:HB2	2.55	0.41
3:S:16:ALA:N	3:S:86:LEU:HB2	2.35	0.41
3:S:38:ARG:HD3	3:S:94:TYR:CE1	2.56	0.41
3:S:40:ALA:O	3:S:41:PRO:C	2.56	0.41
3:S:64:PHE:O	3:S:65:GLN:C	2.59	0.41
5:T:6:GLN:O	5:T:7:SER:C	2.59	0.41
5:T:79:LEU:HD21	5:T:104:VAL:CG1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:SER:O	2:D:33:VAL:N	2.48	0.41
3:E:102:ARG:HB2	3:E:103:GLY:H	1.66	0.41
2:H:55:PHE:HD1	2:H:74:GLU:CG	2.28	0.41
4:J:16:VAL:HG13	4:J:107:LYS:CB	2.44	0.41
1:A:65:PHE:HE2	1:A:267:VAL:HG12	1.85	0.41
1:A:117:LEU:HG	1:A:119:ILE:HG12	2.02	0.41
1:A:203:ILE:O	1:A:203:ILE:HG22	2.19	0.41
1:B:108:THR:H	1:B:114:THR:HG21	1.86	0.41
1:B:297:SER:O	1:B:299:THR:N	2.54	0.41
1:B:344:ALA:C	2:Q:104:ASP:HA	2.40	0.41
1:B:554:SER:OG	1:B:555:ASN:N	2.53	0.41
1:B:616:CYS:O	1:B:617:THR:C	2.57	0.41
1:B:714:ILE:N	1:B:1073:LYS:O	2.49	0.41
1:B:792:PRO:HB2	1:B:794:ILE:HD13	2.01	0.41
1:B:947:LYS:H	1:B:947:LYS:HG2	1.61	0.41
1:C:404:GLY:O	1:C:405:ASN:C	2.59	0.41
1:C:953:ASN:C	1:C:955:ASN:N	2.73	0.41
1:C:1132:ILE:HG23	1:C:1133:VAL:H	1.84	0.41
3:S:103:GLY:O	3:S:104:ALA:HB2	2.20	0.41
4:R:72:PHE:HB3	4:R:74:PHE:HE1	1.85	0.41
5:T:55:ARG:HG2	5:T:59:ILE:HG13	2.02	0.41
5:T:96:LEU:HA	5:T:96:LEU:HD13	1.68	0.41
4:F:81:PRO:O	4:F:83:ASP:N	2.51	0.41
5:G:43:GLN:H	5:G:43:GLN:HG2	1.66	0.41
2:H:27:GLY:HA2	2:H:77:SER:HB3	2.01	0.41
2:H:47:TRP:CE2	4:J:96:TYR:CD2	3.08	0.41
3:I:34:ILE:N	3:I:100:TYR:HD2	2.12	0.41
3:I:66:GLY:O	3:I:84:ARG:NH2	2.53	0.41
4:J:72:PHE:HB3	4:J:74:PHE:HE1	1.85	0.41
1:A:56:LEU:HD22	1:A:91:TYR:CB	2.51	0.41
1:A:320:VAL:O	1:A:321:GLN:HB2	2.21	0.41
1:A:343:ASN:HB2	1:A:344:ALA:H	1.63	0.41
1:A:464:PHE:HD1	1:A:464:PHE:HA	1.68	0.41
1:A:591:PHE:CE1	1:B:854:LYS:HG2	2.56	0.41
1:B:348:ALA:O	1:B:400:PHE:HA	2.20	0.41
1:B:498:PRO:O	1:B:500:TYR:N	2.54	0.41
1:B:532:LEU:HD21	1:B:542:PHE:HE1	1.84	0.41
1:B:553:LYS:HD2	1:B:554:SER:N	2.35	0.41
1:B:604:SER:HB3	1:B:673:TYR:CE2	2.56	0.41
1:B:668:GLY:O	1:B:697:MET:HG2	2.20	0.41
1:B:702:GLU:CG	1:C:790:LYS:HD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:LEU:HD12	1:B:727:LEU:HA	1.83	0.41
1:C:299:THR:HG23	1:C:315:THR:HG22	2.02	0.41
1:C:379:CYS:O	1:C:381:GLY:N	2.54	0.41
2:Q:48:MET:HE3	2:Q:48:MET:HB3	1.53	0.41
2:Q:60:TYR:O	2:Q:61:ALA:C	2.57	0.41
2:Q:67:ARG:HA	2:Q:84:SER:O	2.20	0.41
3:S:108:GLU:C	3:S:110:LEU:H	2.24	0.41
5:T:2:ILE:O	5:T:4:LEU:N	2.53	0.41
3:E:98:ARG:HG2	3:E:100:TYR:OH	2.21	0.41
4:F:31:GLY:O	4:F:91:ARG:NH1	2.53	0.41
5:G:6:GLN:O	5:G:7:SER:C	2.58	0.41
5:G:51:GLY:C	5:G:53:SER:N	2.74	0.41
3:I:73:ASP:O	3:I:74:THR:C	2.57	0.41
4:J:39:GLN:HB2	4:J:45:PRO:HG3	2.03	0.41
4:J:82:GLU:C	4:J:84:ILE:N	2.73	0.41
5:K:2:ILE:O	5:K:4:LEU:N	2.53	0.41
5:K:4:LEU:HD12	5:K:23:CYS:SG	2.61	0.41
5:K:48:LEU:HG	5:K:48:LEU:H	1.76	0.41
1:A:386:LYS:O	1:A:389:ASP:N	2.54	0.41
1:A:819:GLU:HA	1:A:822:LEU:HD12	2.02	0.41
1:A:830:ASP:O	1:A:832:GLY:N	2.53	0.41
1:B:215:PHE:C	1:B:217:GLN:N	2.74	0.41
1:B:339:HIS:HE1	1:B:370:ASN:CB	2.32	0.41
1:B:392:PHE:HD2	1:B:395:VAL:HG21	1.85	0.41
1:B:433:VAL:HB	1:B:511:VAL:HA	2.02	0.41
1:B:458:LYS:HA	1:B:458:LYS:HD3	1.90	0.41
1:B:666:GLY:O	1:B:667:ALA:HB3	2.20	0.41
1:B:800:PHE:HD2	1:B:927:PHE:CD2	2.33	0.41
1:B:969:LYS:HG2	1:C:755:GLN:HG3	2.03	0.41
1:B:981:LEU:HD23	1:B:989:ALA:HB1	2.02	0.41
1:C:50:LEU:HD23	1:C:276:LEU:HB2	2.03	0.41
1:C:133:PHE:HA	1:C:135:PHE:CE2	2.55	0.41
1:C:353:TRP:HE1	1:C:467:ASP:H	1.69	0.41
1:C:365:TYR:HB3	1:C:368:LEU:HD22	2.03	0.41
1:C:466:ARG:HD3	1:C:466:ARG:HA	1.78	0.41
1:C:466:ARG:HD2	1:C:468:ILE:CG2	2.50	0.41
5:T:20:THR:HA	5:T:75:THR:HA	2.02	0.41
2:D:78:THR:HB	2:D:79:ALA:H	1.74	0.41
3:E:33:GLY:C	3:E:51:ILE:HG22	2.41	0.41
5:G:2:ILE:O	5:G:4:LEU:N	2.53	0.41
5:G:23:CYS:HB2	5:G:36:TRP:CH2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:51:GLY:O	5:G:53:SER:N	2.54	0.41
3:I:64:PHE:O	3:I:65:GLN:C	2.59	0.41
5:K:24:ARG:HG3	5:K:71:ASP:HA	2.01	0.41
1:A:109:THR:HG22	1:A:110:LEU:H	1.86	0.41
1:A:129:LYS:HB2	1:A:129:LYS:HE2	1.88	0.41
1:A:214:ASP:O	1:A:215:PHE:CD1	2.74	0.41
1:A:231:GLY:C	1:A:232:ILE:HG12	2.41	0.41
1:A:408:SER:HA	1:A:410:ILE:HG22	2.03	0.41
1:A:534:LYS:HE3	1:A:534:LYS:HB3	1.45	0.41
1:A:579:GLN:O	1:A:581:LEU:N	2.54	0.41
1:A:588:PRO:HG2	1:B:855:PHE:CB	2.49	0.41
1:A:773:GLU:C	1:A:775:ASP:N	2.73	0.41
1:B:131:CYS:O	1:B:133:PHE:N	2.54	0.41
1:B:303:LEU:O	1:B:305:SER:N	2.54	0.41
1:B:353:TRP:NE1	1:B:467:ASP:N	2.66	0.41
1:B:386:LYS:O	1:B:389:ASP:N	2.54	0.41
1:B:403:LYS:HA	1:B:505:GLN:O	2.21	0.41
1:B:418:ILE:HD11	1:B:494:TYR:HH	1.85	0.41
1:B:437:ASN:O	1:B:507:TYR:HA	2.20	0.41
1:B:498:PRO:C	1:B:500:TYR:N	2.71	0.41
1:B:564:PHE:HD1	1:B:564:PHE:N	2.16	0.41
1:B:922:LEU:C	1:B:924:ALA:H	2.24	0.41
1:C:122:ASN:OD1	1:C:125:ASN:HB3	2.20	0.41
1:C:186:PHE:N	1:C:186:PHE:CD1	2.89	0.41
1:C:187:LYS:HD2	1:C:209:PRO:HB3	2.02	0.41
1:C:387:LEU:HA	1:C:390:LEU:HD12	2.02	0.41
1:C:676:GLN:HB2	1:C:689:SER:HB3	2.03	0.41
1:C:833:PHE:HB2	1:C:836:GLN:H	1.85	0.41
2:Q:48:MET:HG2	2:Q:64:PHE:HE1	1.86	0.41
2:Q:104:ASP:N	2:Q:105:PRO:CD	2.81	0.41
4:R:38:GLN:NE2	4:R:40:LYS:HD3	2.35	0.41
2:D:51:PHE:HB3	2:D:59:ILE:CG2	2.50	0.41
2:D:70:ILE:HG13	2:D:81:MET:HG3	2.01	0.41
5:G:62:ARG:CA	5:G:77:SER:HB2	2.51	0.41
2:H:2:VAL:HG11	2:H:98:ARG:HG2	2.02	0.41
2:H:54:LEU:HD12	2:H:99:LEU:HD13	2.03	0.41
3:I:73:ASP:N	3:I:76:THR:OG1	2.51	0.41
1:A:305:SER:C	1:A:307:THR:N	2.74	0.41
1:A:579:GLN:O	1:A:580:THR:C	2.58	0.41
1:B:117:LEU:HD13	1:B:117:LEU:HA	1.82	0.41
1:B:294:ASP:OD2	1:B:296:LEU:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LEU:O	1:B:304:LYS:C	2.59	0.41
1:B:327:VAL:HG13	1:B:328:ARG:H	1.86	0.41
1:B:442:ASP:HB3	1:B:448:ASN:ND2	2.34	0.41
1:B:955:ASN:HA	1:B:1014:ARG:HH12	1.84	0.41
1:C:186:PHE:N	1:C:186:PHE:HD1	2.19	0.41
1:C:308:VAL:HG22	1:C:601:THR:CG2	2.51	0.41
1:C:379:CYS:O	1:C:380:TYR:C	2.58	0.41
1:C:447:GLY:HA2	1:C:496:PHE:O	2.19	0.41
1:C:481:LYS:HE3	1:C:483:LYS:HE2	2.03	0.41
1:C:575:VAL:O	1:C:584:LEU:N	2.53	0.41
1:C:814:LYS:HZ3	1:C:814:LYS:HG2	1.78	0.41
1:C:990:GLU:O	1:C:991:VAL:C	2.58	0.41
1:C:1006:THR:O	1:C:1007:TYR:C	2.59	0.41
2:Q:15:GLY:O	2:Q:85:SER:HA	2.21	0.41
2:Q:51:PHE:CD1	2:Q:59:ILE:HG13	2.56	0.41
3:E:6:GLN:HE21	3:E:6:GLN:HB3	1.66	0.41
3:E:64:PHE:O	3:E:65:GLN:C	2.59	0.41
3:E:68:VAL:HB	3:E:83:LEU:HA	2.03	0.41
4:F:19:ARG:CG	4:F:77:SER:HA	2.48	0.41
4:F:37:TYR:CD1	4:F:47:LEU:HA	2.55	0.41
5:G:10:THR:O	5:G:11:LEU:HD23	2.21	0.41
2:H:107:SER:CB	2:H:108:PRO:HD3	2.51	0.41
4:J:35:ASN:OD1	4:J:90:GLN:HB3	2.20	0.41
1:A:84:LEU:O	1:A:86:PHE:N	2.53	0.41
1:A:112:SER:C	1:A:132:GLU:HB3	2.40	0.41
1:A:117:LEU:HD12	1:A:118:LEU:H	1.86	0.41
1:A:195:LYS:HE2	1:A:204:TYR:CE1	2.56	0.41
1:A:222:LEU:O	1:A:223:GLU:C	2.59	0.41
1:A:303:LEU:O	1:A:304:LYS:C	2.58	0.41
1:A:347:PHE:CD2	1:A:508:ARG:HG2	2.56	0.41
1:A:348:ALA:HB3	1:A:354:ASN:CB	2.42	0.41
1:A:349:SER:O	1:A:352:ALA:N	2.53	0.41
1:A:405:ASN:ND2	3:E:31:SER:HB3	2.36	0.41
1:A:410:ILE:O	1:A:410:ILE:CG2	2.67	0.41
1:A:470:THR:O	1:A:471:GLU:C	2.59	0.41
1:A:528:LYS:HZ1	1:A:529:SER:HB2	1.85	0.41
1:A:616:CYS:HA	1:A:619:VAL:HG23	2.03	0.41
1:A:639:SER:OG	1:A:640:ASN:N	2.53	0.41
1:A:767:LEU:HG	1:A:1008:VAL:HG13	2.02	0.41
1:A:834:ILE:HD12	1:A:834:ILE:HA	1.75	0.41
1:A:980:ILE:H	1:A:980:ILE:HG13	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:LEU:HD12	1:B:21:LEU:HA	1.93	0.41
1:B:167:THR:HB	1:B:168:PHE:H	1.54	0.41
1:B:271:GLN:HB2	1:B:272:PRO:HD2	2.02	0.41
1:B:335:LEU:HB3	1:B:336:CYS:H	1.72	0.41
1:B:338:PHE:O	1:B:339:HIS:C	2.59	0.41
1:B:353:TRP:HZ3	1:B:465:GLU:N	2.19	0.41
1:B:417:ASN:O	1:B:418:ILE:C	2.59	0.41
1:B:503:GLY:HA3	3:S:101:THR:HA	2.02	0.41
1:B:569:VAL:HG23	1:B:571:THR:HG23	2.02	0.41
1:B:811:LYS:O	1:B:814:LYS:NZ	2.54	0.41
1:B:903:ALA:HB1	1:B:913:GLN:HG2	2.03	0.41
1:B:1095:PHE:CZ	1:B:1120:THR:HG22	2.55	0.41
1:C:82:PRO:HB2	1:C:84:LEU:HG	2.03	0.41
1:C:138:ASP:N	1:C:139:PRO:CD	2.84	0.41
1:C:439:ASN:HD21	1:C:506:PRO:HD2	1.86	0.41
1:C:473:TYR:HB2	1:C:488:TYR:O	2.20	0.41
1:C:532:LEU:HB3	1:C:538:VAL:HG11	2.02	0.41
1:C:666:GLY:O	1:C:667:ALA:CB	2.69	0.41
2:Q:70:ILE:HG13	2:Q:81:MET:CB	2.51	0.41
2:Q:102:ASN:ND2	2:Q:109:GLU:OE2	2.53	0.41
3:S:19:LYS:HA	3:S:81:MET:C	2.40	0.41
3:S:55:ASN:H	3:S:55:ASN:HD22	1.69	0.41
4:R:35:ASN:OD1	4:R:37:TYR:HE1	2.02	0.41
5:T:12:SER:C	5:T:14:SER:N	2.74	0.41
2:D:41:PRO:HB2	2:D:43:GLN:HE21	1.85	0.41
3:E:32:TYR:CD1	3:E:98:ARG:HD2	2.55	0.41
4:F:29:ASP:HB3	4:F:91:ARG:NH1	2.36	0.41
2:H:37:VAL:HB	2:H:115:TRP:CZ3	2.56	0.41
2:H:99:LEU:HD23	2:H:101:PRO:HD3	2.03	0.41
3:I:36:TRP:CA	3:I:97:ALA:HB2	2.51	0.41
3:I:68:VAL:HG21	3:I:81:MET:HE2	2.02	0.41
3:I:119:GLN:CG	3:I:120:GLY:N	2.84	0.41
4:J:38:GLN:HG3	4:J:87:TYR:CE1	2.56	0.41
5:K:38:GLN:HE21	5:K:39:GLN:N	2.19	0.41
1:A:236:ARG:HB2	1:A:237:PHE:H	1.75	0.41
1:A:454:ARG:NH1	1:A:469:SER:O	2.54	0.41
1:A:756:TYR:HE2	1:A:998:THR:HG23	1.86	0.41
1:A:811:LYS:HA	1:A:811:LYS:HD3	1.69	0.41
1:A:956:ALA:O	1:A:960:ASN:HB3	2.21	0.41
1:A:979:ASP:C	1:A:981:LEU:N	2.73	0.41
1:A:989:ALA:O	1:A:991:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:PHE:HE1	1:B:631:THR:HG22	1.85	0.41
1:B:361:CYS:HB2	1:B:523:VAL:HG13	2.03	0.41
1:B:403:LYS:HD2	1:B:406:GLU:HB2	2.03	0.41
1:B:447:GLY:HA2	1:B:497:ARG:N	2.36	0.41
1:B:531:ASN:CG	1:B:532:LEU:H	2.25	0.41
1:B:723:THR:O	1:B:1063:LEU:HA	2.20	0.41
1:B:856:ASN:HD22	1:B:856:ASN:HA	1.67	0.41
1:B:980:ILE:HD13	1:B:992:GLN:HB3	2.02	0.41
1:B:1077:THR:CG2	1:C:897:PRO:HG2	2.51	0.41
1:C:312:ILE:O	1:C:312:ILE:HG22	2.20	0.41
1:C:582:GLU:HB3	1:C:584:LEU:HD23	2.02	0.41
1:C:688:ALA:O	1:C:690:GLN:HG2	2.20	0.41
1:C:809:PRO:HA	1:C:814:LYS:HD2	2.01	0.41
1:C:833:PHE:HB2	1:C:836:GLN:CA	2.51	0.41
1:C:1113:GLN:HE21	1:C:1113:GLN:HB2	1.61	0.41
2:Q:55:PHE:CE1	2:Q:75:SER:N	2.89	0.41
3:S:20:VAL:HB	3:S:21:SER:H	1.56	0.41
3:S:51:ILE:HG13	3:S:70:MET:HB3	2.03	0.41
4:R:61:SER:C	4:R:63:PHE:N	2.74	0.41
5:T:90:GLN:HB3	5:T:91:GLN:H	1.72	0.41
2:D:14:PRO:HD3	2:D:123:VAL:HG11	2.03	0.41
4:F:38:GLN:HG3	4:F:87:TYR:CE1	2.56	0.41
4:F:47:LEU:HB3	4:F:56:GLU:OE2	2.21	0.41
2:H:93:VAL:HG13	2:H:119:THR:O	2.21	0.41
2:H:101:PRO:HB3	4:J:96:TYR:OH	2.21	0.41
2:H:112:PHE:O	2:H:113:ASP:C	2.59	0.41
3:I:38:ARG:HG2	3:I:46:GLU:HB3	2.03	0.41
3:I:39:GLN:HB2	3:I:95:TYR:CE2	2.56	0.41
3:I:51:ILE:HD12	3:I:58:THR:CG2	2.50	0.41
1:A:24:THR:HG21	1:A:65:PHE:HB3	2.02	0.40
1:A:86:PHE:HB2	1:A:237:PHE:CE1	2.56	0.40
1:A:197:ILE:HG22	1:A:198:ASP:OD2	2.21	0.40
1:A:345:THR:OG1	1:A:346:ARG:N	2.55	0.40
1:A:347:PHE:HB3	1:A:400:PHE:N	2.36	0.40
1:A:372:ALA:O	1:A:374:PHE:N	2.47	0.40
1:A:378:LYS:O	1:A:433:VAL:HG22	2.21	0.40
1:A:753:LEU:HD13	1:A:997:ILE:HG12	2.03	0.40
1:A:933:LYS:O	1:A:934:ILE:C	2.59	0.40
1:A:1048:HIS:HA	1:A:1066:THR:HG22	2.01	0.40
1:B:24:THR:HB	1:B:66:HIS:C	2.41	0.40
1:B:58:PHE:CE1	1:B:275:PHE:HE2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASP:HB2	1:B:113:LYS:HD2	2.02	0.40
1:B:392:PHE:O	1:B:393:THR:C	2.59	0.40
1:B:527:LYS:HA	1:B:527:LYS:HD2	1.65	0.40
1:B:743:CYS:SG	1:B:749:CYS:C	2.99	0.40
1:B:922:LEU:C	1:B:924:ALA:N	2.75	0.40
1:C:94:SER:HA	1:C:265:TYR:H	1.86	0.40
1:C:338:PHE:C	1:C:340:GLU:N	2.75	0.40
1:C:499:THR:HG21	5:K:50:TYR:CG	2.56	0.40
1:C:534:LYS:O	1:C:536:LYS:N	2.53	0.40
1:C:826:VAL:HB	1:C:1057:PRO:HG2	2.03	0.40
1:C:980:ILE:O	1:C:984:LEU:HB2	2.21	0.40
2:Q:12:LYS:HZ2	2:Q:12:LYS:HA	1.86	0.40
5:T:48:LEU:HD11	5:T:87:TYR:HD2	1.86	0.40
2:D:67:ARG:CD	2:D:87:ARG:H	2.34	0.40
3:E:19:LYS:HD2	3:E:82:GLU:OE2	2.21	0.40
4:F:9:PRO:O	4:F:10:SER:HB3	2.21	0.40
2:H:30:ARG:H	2:H:30:ARG:CD	2.34	0.40
2:H:51:PHE:CD2	2:H:53:PRO:HD2	2.56	0.40
2:H:65:GLN:O	2:H:69:MET:HG3	2.21	0.40
3:I:29:PHE:CG	3:I:77:THR:HA	2.56	0.40
4:J:58:GLY:O	4:J:59:VAL:C	2.60	0.40
4:J:62:ARG:HG2	4:J:62:ARG:O	2.21	0.40
1:A:91:TYR:CE1	1:A:191:GLU:HB3	2.55	0.40
1:A:193:VAL:CG1	1:A:270:LEU:HD11	2.48	0.40
1:A:339:HIS:HE2	1:A:371:PHE:HE1	1.69	0.40
1:A:435:ALA:HA	1:A:508:ARG:O	2.21	0.40
1:A:461:LEU:HB3	1:A:465:GLU:HB2	2.02	0.40
1:A:540:PHE:O	1:A:540:PHE:CG	2.74	0.40
1:A:802:PHE:HZ	1:A:898:PHE:CZ	2.39	0.40
1:B:368:LEU:HA	1:B:371:PHE:CZ	2.57	0.40
1:B:660:GLU:O	1:B:695:TYR:CZ	2.74	0.40
1:C:188:ASN:HB2	1:C:210:ILE:CD1	2.51	0.40
1:C:329:PHE:CE1	1:C:527:LYS:O	2.74	0.40
1:C:338:PHE:CZ	1:C:363:ALA:HB1	2.57	0.40
1:C:500:TYR:CB	1:C:505:GLN:HG2	2.51	0.40
1:C:539:ASN:HA	1:C:547:GLY:O	2.21	0.40
1:C:741:TYR:CZ	1:C:962:LEU:HD22	2.56	0.40
1:C:878:LEU:HD23	1:C:878:LEU:O	2.22	0.40
1:C:1082:CYS:SG	1:C:1132:ILE:HG12	2.62	0.40
4:R:81:PRO:O	4:R:83:ASP:N	2.51	0.40
2:D:37:VAL:HG12	2:D:45:LEU:HD23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:MET:O	2:D:81:MET:HG3	2.21	0.40
4:F:62:ARG:NE	4:F:78:SER:O	2.55	0.40
5:G:88:TYR:CD1	5:G:88:TYR:N	2.87	0.40
5:G:90:GLN:HB3	5:G:91:GLN:H	1.54	0.40
2:H:59:ILE:O	2:H:61:ALA:N	2.53	0.40
3:I:4:LEU:HB2	3:I:117:TRP:O	2.21	0.40
4:J:7:GLN:NE2	4:J:24:CYS:O	2.54	0.40
4:J:46:LYS:CE	4:J:59:VAL:HB	2.51	0.40
5:K:25:ALA:C	5:K:27:GLN:H	2.25	0.40
1:A:429:PHE:O	1:A:431:GLY:N	2.45	0.40
1:A:449:TYR:CD1	1:A:495:GLY:HA3	2.56	0.40
1:A:559:LEU:O	1:A:560:PRO:C	2.59	0.40
1:A:708:SER:C	1:A:710:ASN:H	2.25	0.40
1:A:769:GLY:C	1:A:771:ALA:H	2.25	0.40
1:A:898:PHE:N	1:C:707:TYR:HE2	2.20	0.40
1:A:915:VAL:O	1:A:919:ASN:HB2	2.21	0.40
1:A:1126:CYS:HB3	1:A:1132:ILE:HG21	2.03	0.40
1:B:372:ALA:H	2:Q:52:ILE:HG21	1.85	0.40
1:B:402:ILE:O	1:B:506:PRO:HA	2.21	0.40
1:B:541:ASN:HA	1:B:546:THR:HA	2.03	0.40
1:B:622:ALA:C	1:B:624:HIS:N	2.75	0.40
1:B:632:TRP:O	1:B:633:ARG:HD2	2.22	0.40
1:C:398:ASP:OD1	1:C:398:ASP:N	2.53	0.40
1:C:448:ASN:ND2	1:C:451:TYR:HE2	2.16	0.40
1:C:478:LYS:O	1:C:481:LYS:HG2	2.21	0.40
1:C:563:GLN:HB2	1:C:564:PHE:H	1.64	0.40
1:C:621:VAL:O	1:C:622:ALA:C	2.59	0.40
1:C:674:GLN:NE2	1:C:693:ILE:HD11	2.36	0.40
2:Q:2:VAL:HG13	2:Q:114:ILE:HD13	2.03	0.40
2:Q:4:LEU:HD22	2:Q:4:LEU:HA	1.93	0.40
2:Q:35:SER:CB	2:Q:49:GLY:HA3	2.47	0.40
2:Q:60:TYR:CA	2:Q:63:ALA:HB3	2.51	0.40
2:Q:97:ALA:HA	2:Q:114:ILE:O	2.22	0.40
4:R:35:ASN:ND2	4:R:92:TYR:OH	2.54	0.40
5:T:21:LEU:HD13	5:T:74:LEU:HD23	2.03	0.40
2:D:34:ILE:N	2:D:99:LEU:H	2.19	0.40
5:G:61:ASP:O	5:G:63:PHE:N	2.54	0.40
3:I:7:SER:OG	3:I:8:GLY:N	2.54	0.40
3:I:22:CYS:HB2	3:I:96:CYS:HB2	1.86	0.40
3:I:34:ILE:O	3:I:50:TRP:HA	2.22	0.40
3:I:39:GLN:O	3:I:40:ALA:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:67:GLY:HA3	4:J:72:PHE:CA	2.48	0.40
5:K:34:LEU:HD22	5:K:72:PHE:CB	2.50	0.40
1:A:199:GLY:O	1:A:201:PHE:N	2.54	0.40
1:A:238:GLN:HG2	1:A:240:LEU:HD23	2.03	0.40
1:A:379:CYS:HA	1:A:432:CYS:HA	2.04	0.40
1:A:408:SER:HB2	3:E:54:TYR:OH	2.21	0.40
1:A:576:ARG:O	1:A:581:LEU:HA	2.22	0.40
1:A:914:ASN:O	1:A:918:GLU:HB2	2.22	0.40
1:B:138:ASP:HB3	1:B:139:PRO:HD3	2.03	0.40
1:B:409:GLN:HE22	1:B:417:ASN:H	1.69	0.40
1:B:865:LEU:HD22	1:B:869:MET:SD	2.62	0.40
1:B:969:LYS:O	1:B:971:GLY:N	2.55	0.40
1:C:65:PHE:CG	1:C:265:TYR:CE2	3.09	0.40
1:C:502:VAL:HG11	3:I:100:TYR:CD1	2.56	0.40
1:C:556:LYS:CB	1:C:583:ILE:HG12	2.51	0.40
1:C:786:LYS:H	1:C:786:LYS:CE	2.35	0.40
1:C:850:ILE:H	1:C:850:ILE:HG13	1.48	0.40
2:Q:38:ARG:HG2	2:Q:46:GLU:CG	2.51	0.40
3:S:98:ARG:CB	3:S:116:ASN:HB2	2.51	0.40
3:E:101:THR:HB	3:E:111:ILE:O	2.21	0.40
4:F:11:SER:OG	4:F:12:LEU:N	2.54	0.40
4:F:59:VAL:CB	4:F:60:PRO:HD3	2.50	0.40
2:H:113:ASP:HB3	2:H:114:ILE:H	1.67	0.40
3:I:27:TYR:CD1	3:I:32:TYR:CE2	3.09	0.40
1:A:105:ILE:CG2	1:A:110:LEU:HD21	2.49	0.40
1:A:128:ILE:HG12	1:A:170:TYR:CD2	2.56	0.40
1:A:192:PHE:C	1:A:194:PHE:H	2.23	0.40
1:A:328:ARG:NE	1:A:530:THR:O	2.54	0.40
1:A:428:ASP:O	1:A:429:PHE:C	2.58	0.40
1:A:703:ASN:HB2	1:B:787:GLN:HG2	2.03	0.40
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.86	0.40
1:A:1141:LEU:O	1:A:1144:GLU:HG2	2.22	0.40
1:B:49:HIS:CG	1:B:50:LEU:N	2.89	0.40
1:B:110:LEU:HB3	1:B:135:PHE:CG	2.57	0.40
1:B:211:ILE:HG23	1:B:214:ASP:OD1	2.22	0.40
1:B:339:HIS:CA	1:B:342:PHE:HB2	2.50	0.40
1:B:559:LEU:HD12	1:B:559:LEU:HA	1.91	0.40
1:B:916:LEU:O	1:B:919:ASN:N	2.54	0.40
1:B:921:LYS:HE2	1:B:921:LYS:HB3	1.85	0.40
1:B:969:LYS:O	1:B:970:PHE:C	2.60	0.40
1:B:1094:VAL:HG22	1:B:1096:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:TRP:CZ2	1:C:422:ASN:O	2.75	0.40
1:C:418:ILE:HG23	1:C:423:TYR:H	1.86	0.40
1:C:502:VAL:CG1	3:I:100:TYR:CD1	3.05	0.40
1:C:633:ARG:HA	1:C:633:ARG:NE	2.31	0.40
1:C:911:VAL:HG12	1:C:912:THR:H	1.87	0.40
1:C:936:ASP:O	1:C:937:SER:C	2.60	0.40
2:Q:5:VAL:HG22	2:Q:25:SER:HB3	2.04	0.40
2:Q:51:PHE:CD1	2:Q:51:PHE:N	2.88	0.40
3:S:115:ASP:OD1	3:S:115:ASP:N	2.47	0.40
4:R:16:VAL:CG1	4:R:107:LYS:HD2	2.51	0.40
5:T:81:PRO:O	5:T:83:ASP:N	2.55	0.40
2:D:38:ARG:NH2	2:D:92:ALA:H	2.19	0.40
2:D:115:TRP:CG	4:F:45:PRO:HB2	2.56	0.40
3:E:114:PHE:H	5:G:47:LEU:HD23	1.86	0.40
4:F:40:LYS:HG3	4:F:43:LYS:HD2	2.02	0.40
5:G:62:ARG:HA	5:G:77:SER:CB	2.52	0.40
5:G:88:TYR:H	5:G:88:TYR:HD1	1.68	0.40
3:I:28:PRO:C	3:I:30:THR:H	2.25	0.40
3:I:122:LEU:HD12	3:I:123:VAL: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	A	1012/1123 (90%)	589 (58%)	291 (29%)	132 (13%)	0	1
1	B	1012/1123 (90%)	597 (59%)	242 (24%)	173 (17%)	0	0
1	C	1012/1123 (90%)	582 (58%)	289 (29%)	141 (14%)	0	1
2	D	123/125 (98%)	47 (38%)	40 (32%)	36 (29%)	0	0
2	H	123/125 (98%)	45 (37%)	46 (37%)	32 (26%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	123/125 (98%)	50 (41%)	45 (37%)	28 (23%)	0	0
3	E	125/127 (98%)	63 (50%)	36 (29%)	26 (21%)	0	0
3	I	125/127 (98%)	65 (52%)	31 (25%)	29 (23%)	0	0
3	S	125/127 (98%)	68 (54%)	31 (25%)	26 (21%)	0	0
4	F	104/106 (98%)	48 (46%)	31 (30%)	25 (24%)	0	0
4	J	104/106 (98%)	47 (45%)	32 (31%)	25 (24%)	0	0
4	R	104/106 (98%)	50 (48%)	23 (22%)	31 (30%)	0	0
5	G	102/104 (98%)	48 (47%)	29 (28%)	25 (24%)	0	0
5	K	102/104 (98%)	44 (43%)	34 (33%)	24 (24%)	0	0
5	T	102/104 (98%)	39 (38%)	39 (38%)	24 (24%)	0	0
All	All	4398/4755 (92%)	2382 (54%)	1239 (28%)	777 (18%)	0	0

All (777) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	59	PHE
1	A	92	PHE
1	A	226	VAL
1	A	292	ALA
1	A	362	VAL
1	A	377	PHE
1	A	412	PRO
1	A	423	TYR
1	A	458	LYS
1	A	466	ARG
1	A	470	THR
1	A	522	THR
1	A	568	ILE
1	A	579	GLN
1	A	639	SER
1	A	660	GLU
1	A	706	ALA
1	A	738	CYS
1	A	833	PHE
1	A	854	LYS
1	A	918	GLU
1	A	919	ASN

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Mol	Chain	Res	Type
1	A	936	ASP
1	A	937	SER
1	B	26	GLN
1	B	63	THR
1	B	115	GLN
1	B	120	VAL
1	B	123	ALA
1	B	138	ASP
1	B	304	LYS
1	B	322	PRO
1	B	323	THR
1	B	328	ARG
1	B	331	ASN
1	B	332	VAL
1	B	333	THR
1	B	360	ASN
1	B	361	CYS
1	B	377	PHE
1	B	409	GLN
1	B	423	TYR
1	B	442	ASP
1	B	445	HIS
1	B	448	ASN
1	B	457	ARG
1	B	465	GLU
1	B	468	ILE
1	B	479	PRO
1	B	490	PRO
1	B	497	ARG
1	B	523	VAL
1	B	539	ASN
1	B	540	PHE
1	B	615	ASN
1	B	622	ALA
1	B	631	THR
1	B	759	PHE
1	B	760	CYS
1	B	870	ILE
1	B	940	SER
1	B	1123	SER
1	B	1126	CYS
1	C	28	TYR

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Mol	Chain	Res	Type
1	C	32	PHE
1	C	63	THR
1	C	64	TRP
1	C	92	PHE
1	C	94	SER
1	C	116	SER
1	C	130	VAL
1	C	139	PRO
1	C	141	LEU
1	C	291	CYS
1	C	292	ALA
1	C	293	LEU
1	C	328	ARG
1	C	333	THR
1	C	361	CYS
1	C	457	ARG
1	C	479	PRO
1	C	480	CYS
1	C	539	ASN
1	C	560	PRO
1	C	561	PHE
1	C	563	GLN
1	C	564	PHE
1	C	573	ASP
1	C	579	GLN
1	C	583	ILE
1	C	616	CYS
1	C	633	ARG
1	C	854	LYS
1	C	991	VAL
1	C	1092	GLU
1	C	1128	VAL
1	C	1132	ILE
2	Q	9	ALA
2	Q	16	SER
2	Q	29	PHE
2	Q	48	MET
2	Q	90	ASP
2	Q	100	PHE
2	Q	102	ASN
2	Q	109	GLU
3	S	31	SER

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Mol	Chain	Res	Type
3	S	52	SER
3	S	53	THR
3	S	90	ASP
3	S	102	ARG
3	S	104	ALA
3	S	126	SER
4	R	11	SER
4	R	43	LYS
4	R	53	SER
4	R	92	TYR
4	R	96	TYR
5	T	15	PRO
5	T	34	LEU
5	T	55	ARG
5	T	60	PRO
5	T	61	ASP
5	T	63	PHE
5	T	71	ASP
5	T	84	PHE
5	T	96	LEU
2	D	9	ALA
2	D	16	SER
2	D	30	ARG
2	D	31	SER
2	D	34	ILE
2	D	41	PRO
2	D	45	LEU
2	D	57	THR
2	D	58	THR
2	D	63	ALA
2	D	107	SER
2	D	123	VAL
3	E	14	PRO
3	E	52	SER
3	E	87	ARG
3	E	90	ASP
3	E	102	ARG
3	E	126	SER
4	F	36	TRP
4	F	53	SER
5	G	7	SER
5	G	34	LEU

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Mol	Chain	Res	Type
5	G	55	ARG
5	G	60	PRO
5	G	61	ASP
5	G	62	ARG
5	G	71	ASP
5	G	91	GLN
5	G	93	ASP
5	G	94	THR
5	G	96	LEU
2	H	9	ALA
2	H	11	VAL
2	H	13	LYS
2	H	27	GLY
2	H	29	PHE
2	H	34	ILE
2	H	63	ALA
2	H	90	ASP
2	H	107	SER
2	H	109	GLU
2	H	124	SER
3	I	51	ILE
3	I	52	SER
3	I	54	TYR
3	I	90	ASP
3	I	99	ASP
3	I	115	ASP
3	I	126	SER
4	J	5	MET
4	J	27	SER
4	J	34	LEU
4	J	36	TRP
4	J	62	ARG
4	J	92	TYR
4	J	93	ASP
4	J	104	VAL
5	K	39	GLN
5	K	71	ASP
5	K	92	HIS
5	K	93	ASP
5	K	94	THR
5	K	96	LEU
1	A	65	PHE

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Mol	Chain	Res	Type
1	A	111	ASP
1	A	113	LYS
1	A	134	GLN
1	A	140	PHE
1	A	188	ASN
1	A	193	VAL
1	A	230	ILE
1	A	237	PHE
1	A	287	ASP
1	A	351	TYR
1	A	353	TRP
1	A	360	ASN
1	A	372	ALA
1	A	374	PHE
1	A	408	SER
1	A	410	ILE
1	A	420	ASP
1	A	426	PRO
1	A	441	LEU
1	A	463	PRO
1	A	520	PRO
1	A	536	LYS
1	A	543	ASN
1	A	564	PHE
1	A	571	THR
1	A	633	ARG
1	A	635	TYR
1	A	641	VAL
1	A	826	VAL
1	A	831	ALA
1	A	855	PHE
1	A	890	ALA
1	A	917	TYR
1	A	938	LEU
1	A	997	ILE
1	A	1058	HIS
1	A	1100	THR
1	A	1141	LEU
1	A	1142	GLN
1	B	27	SER
1	B	53	ASP
1	B	62	VAL

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Mol	Chain	Res	Type
1	B	116	SER
1	B	132	GLU
1	B	133	PHE
1	B	134	GLN
1	B	200	TYR
1	B	210	ILE
1	B	285	ILE
1	B	324	GLU
1	B	343	ASN
1	B	349	SER
1	B	354	ASN
1	B	358	ILE
1	B	374	PHE
1	B	407	VAL
1	B	420	ASP
1	B	426	PRO
1	B	437	ASN
1	B	477	ASN
1	B	488	TYR
1	B	491	LEU
1	B	496	PHE
1	B	501	GLY
1	B	502	VAL
1	B	522	THR
1	B	535	ASN
1	B	536	LYS
1	B	537	CYS
1	B	564	PHE
1	B	580	THR
1	B	632	TRP
1	B	744	GLY
1	B	835	LYS
1	B	848	ASP
1	B	851	CYS
1	B	856	ASN
1	B	890	ALA
1	B	928	ASN
1	B	936	ASP
1	B	937	SER
1	B	939	PHE
1	B	944	ALA
1	B	973	ILE

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Mol	Chain	Res	Type
1	B	1142	GLN
1	C	22	ILE
1	C	27	SER
1	C	110	LEU
1	C	113	LYS
1	C	190	ARG
1	C	211	ILE
1	C	231	GLY
1	C	320	VAL
1	C	353	TRP
1	C	363	ALA
1	C	372	ALA
1	C	374	PHE
1	C	380	TYR
1	C	410	ILE
1	C	420	ASP
1	C	426	PRO
1	C	428	ASP
1	C	437	ASN
1	C	440	LYS
1	C	498	PRO
1	C	523	VAL
1	C	538	VAL
1	C	540	PHE
1	C	547	GLY
1	C	555	ASN
1	C	566	ARG
1	C	571	THR
1	C	580	THR
1	C	601	THR
1	C	634	VAL
1	C	639	SER
1	C	667	ALA
1	C	744	GLY
1	C	774	GLN
1	C	810	SER
1	C	827	THR
1	C	937	SER
1	C	938	LEU
1	C	1058	HIS
2	Q	27	GLY
2	Q	33	VAL

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Mol	Chain	Res	Type
2	Q	66	GLY
2	Q	99	LEU
2	Q	101	PRO
2	Q	105	PRO
2	Q	117	GLN
2	Q	121	VAL
3	S	25	SER
3	S	54	TYR
3	S	63	LYS
3	S	72	THR
3	S	111	ILE
3	S	115	ASP
4	R	7	GLN
4	R	10	SER
4	R	16	VAL
4	R	25	GLN
4	R	27	SER
4	R	32	ASN
4	R	42	GLY
4	R	48	LEU
4	R	51	ASP
4	R	62	ARG
4	R	87	TYR
4	R	91	ARG
5	T	3	VAL
5	T	26	SER
5	T	51	GLY
5	T	62	ARG
5	T	82	GLU
5	T	94	THR
2	D	27	GLY
2	D	28	THR
2	D	32	HIS
2	D	35	SER
2	D	74	GLU
2	D	86	LEU
2	D	109	GLU
2	D	112	PHE
2	D	115	TRP
3	E	25	SER
3	E	33	GLY
3	E	54	TYR

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Mol	Chain	Res	Type
3	E	63	LYS
3	E	72	THR
3	E	109	SER
3	E	113	GLY
4	F	6	THR
4	F	17	GLY
4	F	27	SER
4	F	35	ASN
4	F	78	SER
4	F	87	TYR
5	G	3	VAL
5	G	16	GLY
5	G	32	THR
5	G	52	ALA
5	G	63	PHE
5	G	82	GLU
2	H	68	VAL
2	H	113	ASP
2	H	115	TRP
3	I	25	SER
3	I	55	ASN
3	I	63	LYS
3	I	72	THR
3	I	87	ARG
3	I	107	GLY
3	I	108	GLU
3	I	109	SER
4	J	26	ALA
4	J	33	TYR
4	J	58	GLY
4	J	60	PRO
4	J	87	TYR
5	K	3	VAL
5	K	16	GLY
5	K	38	GLN
5	K	51	GLY
5	K	55	ARG
5	K	82	GLU
1	A	32	PHE
1	A	86	PHE
1	A	129	LYS
1	A	167	THR

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Mol	Chain	Res	Type
1	A	171	VAL
1	A	201	PHE
1	A	232	ILE
1	A	285	ILE
1	A	330	PRO
1	A	334	ASN
1	A	375	PHE
1	A	487	CYS
1	A	551	LEU
1	A	572	THR
1	A	580	THR
1	A	697	MET
1	A	743	CYS
1	A	759	PHE
1	A	760	CYS
1	A	1127	ASP
1	B	82	PRO
1	B	95	THR
1	B	114	THR
1	B	136	CYS
1	B	139	PRO
1	B	315	THR
1	B	316	SER
1	B	335	LEU
1	B	351	TYR
1	B	353	TRP
1	B	366	SER
1	B	373	PRO
1	B	375	PHE
1	B	429	PHE
1	B	438	SER
1	B	440	LYS
1	B	449	TYR
1	B	452	TRP
1	B	453	TYR
1	B	454	ARG
1	B	498	PRO
1	B	530	THR
1	B	532	LEU
1	B	543	ASN
1	B	588	PRO
1	B	620	SER

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Mol	Chain	Res	Type
1	B	633	ARG
1	B	634	VAL
1	B	738	CYS
1	B	739	THR
1	B	852	ALA
1	B	855	PHE
1	B	984	LEU
1	B	1071	GLN
1	B	1140	PRO
1	C	42	VAL
1	C	93	ALA
1	C	123	ALA
1	C	165	ASN
1	C	280	ASN
1	C	319	ARG
1	C	330	PRO
1	C	337	PRO
1	C	375	PHE
1	C	386	LYS
1	C	389	ASP
1	C	407	VAL
1	C	450	ASP
1	C	463	PRO
1	C	465	GLU
1	C	485	PRO
1	C	486	ASN
1	C	497	ARG
1	C	499	THR
1	C	537	CYS
1	C	558	PHE
1	C	740	MET
1	C	940	SER
1	C	952	VAL
1	C	957	GLN
1	C	978	ASN
1	C	1145	LEU
2	Q	2	VAL
2	Q	7	SER
2	Q	14	PRO
2	Q	54	LEU
2	Q	59	ILE
2	Q	63	ALA

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Mol	Chain	Res	Type
2	Q	72	ALA
2	Q	91	THR
3	S	9	ALA
3	S	15	GLY
4	R	41	PRO
4	R	95	SER
5	T	43	GLN
5	T	56	ALA
5	T	97	THR
2	D	2	VAL
2	D	7	SER
2	D	14	PRO
2	D	67	ARG
2	D	87	ARG
2	D	108	PRO
2	D	122	THR
3	E	9	ALA
3	E	82	GLU
3	E	105	TRP
3	E	107	GLY
4	F	10	SER
4	F	41	PRO
4	F	45	PRO
4	F	51	ASP
4	F	77	SER
4	F	92	TYR
4	F	100	GLN
5	G	9	GLY
5	G	43	GLN
2	H	2	VAL
2	H	7	SER
2	H	92	ALA
2	H	99	LEU
2	H	104	ASP
3	I	9	ALA
3	I	12	LYS
3	I	117	TRP
4	J	4	GLN
4	J	14	ALA
4	J	17	GLY
4	J	41	PRO
4	J	43	LYS

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Mol	Chain	Res	Type
4	J	103	LYS
5	K	17	GLU
5	K	43	GLN
5	K	58	GLY
5	K	60	PRO
5	K	63	PHE
1	A	170	TYR
1	A	238	GLN
1	A	281	GLU
1	A	321	GLN
1	A	358	ILE
1	A	359	SER
1	A	440	LYS
1	A	478	LYS
1	A	534	LYS
1	A	559	LEU
1	A	577	ASP
1	A	578	PRO
1	A	624	HIS
1	A	634	VAL
1	A	825	LYS
1	B	50	LEU
1	B	121	ASN
1	B	165	ASN
1	B	198	ASP
1	B	229	PRO
1	B	270	LEU
1	B	338	PHE
1	B	436	TRP
1	B	483	LYS
1	B	517	LEU
1	B	524	CYS
1	B	556	LYS
1	B	639	SER
1	B	745	ASP
1	B	935	GLN
1	B	945	LEU
1	B	979	ASP
1	B	1141	LEU
1	C	31	SER
1	C	84	LEU
1	C	228	LEU

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Mol	Chain	Res	Type
1	C	324	GLU
1	C	367	VAL
1	C	390	LEU
1	C	464	PHE
1	C	603	THR
1	C	635	TYR
1	C	689	SER
1	C	1130	ILE
1	C	1133	VAL
2	Q	62	GLN
2	Q	87	ARG
3	S	7	SER
3	S	14	PRO
3	S	16	ALA
3	S	20	VAL
3	S	29	PHE
3	S	100	TYR
3	S	114	PHE
4	R	4	GLN
4	R	5	MET
4	R	33	TYR
4	R	57	THR
4	R	82	GLU
5	T	70	THR
5	T	95	SER
2	D	39	GLN
2	D	85	SER
2	D	117	GLN
3	E	12	LYS
3	E	16	ALA
3	E	20	VAL
3	E	93	VAL
3	E	119	GLN
4	F	4	GLN
4	F	11	SER
4	F	82	GLU
4	F	93	ASP
5	G	51	GLY
5	G	95	SER
2	H	55	PHE
2	H	76	THR
2	H	108	PRO

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Mol	Chain	Res	Type
2	H	117	GLN
2	H	121	VAL
3	I	7	SER
3	I	20	VAL
3	I	34	ILE
3	I	96	CYS
4	J	42	GLY
4	J	52	ALA
4	J	100	GLN
5	K	26	SER
5	K	61	ASP
1	A	84	LEU
1	A	93	ALA
1	A	282	ASN
1	A	316	SER
1	A	347	PHE
1	A	497	ARG
1	A	524	CYS
1	A	617	THR
1	A	618	GLU
1	A	651	GLY
1	A	875	SER
1	A	935	GLN
1	A	1092	GLU
1	A	1131	GLY
1	B	42	VAL
1	B	87	ASN
1	B	124	THR
1	B	167	THR
1	B	171	VAL
1	B	303	LEU
1	B	372	ALA
1	B	455	LEU
1	B	494	TYR
1	B	500	TYR
1	B	531	ASN
1	B	623	ILE
1	B	823	PHE
1	B	975	SER
1	B	1058	HIS
1	B	1098	ASN
1	B	1115	ILE

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Mol	Chain	Res	Type
1	C	171	VAL
1	C	235	THR
1	C	388	ASN
1	C	439	ASN
1	C	481	LYS
1	C	535	ASN
1	C	545	LEU
1	C	600	GLY
1	C	649	LEU
1	C	755	GLN
1	C	777	ASN
1	C	1041	ASP
1	C	1071	GLN
3	S	105	TRP
4	R	70	THR
4	R	100	GLN
2	D	56	GLY
2	D	66	GLY
2	D	101	PRO
2	D	110	ASP
3	E	81	MET
3	E	114	PHE
4	F	42	GLY
4	F	56	GLU
4	F	70	THR
4	F	104	VAL
5	G	14	SER
5	G	70	THR
2	H	105	PRO
2	H	110	ASP
2	H	112	PHE
3	I	85	ARG
3	I	102	ARG
4	J	70	THR
4	J	102	THR
5	K	70	THR
5	K	102	THR
1	A	85	PRO
1	A	106	PHE
1	A	126	VAL
1	A	228	LEU
1	A	229	PRO

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Mol	Chain	Res	Type
1	A	471	GLU
1	A	720	ILE
1	A	853	GLN
1	A	884	SER
1	B	197	ILE
1	B	283	GLY
1	B	463	PRO
1	B	471	GLU
1	B	899	PRO
1	C	216	PRO
1	C	344	ALA
1	C	347	PHE
1	C	472	ILE
1	C	489	PHE
1	C	602	ASN
1	C	793	PRO
1	C	979	ASP
1	C	1126	CYS
2	Q	26	GLY
2	Q	51	PHE
3	S	67	ARG
4	R	38	GLN
5	T	29	VAL
5	T	100	GLY
2	D	26	GLY
3	E	67	ARG
4	F	43	LYS
5	G	29	VAL
2	H	26	GLY
2	H	52	ILE
3	I	67	ARG
3	I	83	LEU
3	I	93	VAL
4	J	94	PRO
5	K	29	VAL
1	A	57	PRO
1	B	22	ILE
1	B	330	PRO
1	C	651	GLY
5	T	14	SER
1	A	575	VAL
1	A	1115	ILE

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Mol	Chain	Res	Type
1	B	211	ILE
1	B	362	VAL
1	B	621	VAL
1	C	544	GLY
4	R	59	VAL
4	R	94	PRO
4	F	60	PRO
1	A	216	PRO
1	A	367	VAL
1	A	523	VAL
1	A	1057	PRO
1	B	38	TYR
1	B	47	VAL
1	B	980	ILE
1	C	120	VAL
4	R	17	GLY
4	R	93	ASP
5	T	81	PRO
5	G	81	PRO
3	I	112	GLY
5	K	7	SER
5	K	81	PRO
1	A	212	GLY
1	B	193	VAL
1	B	231	GLY
1	B	951	VAL
1	B	1132	ILE
1	C	520	PRO
1	C	987	PRO
2	H	14	PRO
2	H	101	PRO
1	A	934	ILE
1	B	592	GLY
1	C	128	ILE
1	C	506	PRO
3	S	18	VAL
3	S	93	VAL
3	E	18	VAL
2	H	123	VAL
3	I	18	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	903/978 (92%)	586 (65%)	317 (35%)	0	0
1	B	903/978 (92%)	555 (62%)	348 (38%)	0	0
1	C	903/978 (92%)	572 (63%)	331 (37%)	0	0
2	D	96/102 (94%)	47 (49%)	49 (51%)	0	0
2	H	96/102 (94%)	53 (55%)	43 (45%)	0	0
2	Q	96/102 (94%)	51 (53%)	45 (47%)	0	0
3	E	94/103 (91%)	52 (55%)	42 (45%)	0	0
3	I	94/103 (91%)	51 (54%)	43 (46%)	0	0
3	S	94/103 (91%)	52 (55%)	42 (45%)	0	0
4	F	81/92 (88%)	41 (51%)	40 (49%)	0	0
4	J	81/92 (88%)	43 (53%)	38 (47%)	0	0
4	R	81/92 (88%)	47 (58%)	34 (42%)	0	0
5	G	69/86 (80%)	37 (54%)	32 (46%)	0	0
5	K	69/86 (80%)	41 (59%)	28 (41%)	0	0
5	T	69/86 (80%)	35 (51%)	34 (49%)	0	0
All	All	3729/4083 (91%)	2263 (61%)	1466 (39%)	0	0

All (1466) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	22	ILE
1	A	24	THR
1	A	26	GLN
1	A	28	TYR
1	A	29	THR
1	A	30	ASN
1	A	34	ARG
1	A	41	LYS
1	A	42	VAL

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Mol	Chain	Res	Type
1	A	44	ARG
1	A	50	LEU
1	A	51	THR
1	A	52	GLN
1	A	54	LEU
1	A	61	ASN
1	A	62	VAL
1	A	63	THR
1	A	80	ASP
1	A	83	VAL
1	A	84	LEU
1	A	90	VAL
1	A	108	THR
1	A	109	THR
1	A	110	LEU
1	A	111	ASP
1	A	117	LEU
1	A	118	LEU
1	A	119	ILE
1	A	120	VAL
1	A	121	ASN
1	A	125	ASN
1	A	128	ILE
1	A	129	LYS
1	A	130	VAL
1	A	131	CYS
1	A	135	PHE
1	A	136	CYS
1	A	138	ASP
1	A	141	LEU
1	A	164	ASN
1	A	166	CYS
1	A	167	THR
1	A	169	GLU
1	A	172	SER
1	A	186	PHE
1	A	187	LYS
1	A	189	LEU
1	A	190	ARG
1	A	195	LYS
1	A	196	ASN
1	A	198	ASP

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Mol	Chain	Res	Type
1	A	202	LYS
1	A	206	LYS
1	A	207	HIS
1	A	210	ILE
1	A	211	ILE
1	A	213	ARG
1	A	214	ASP
1	A	223	GLU
1	A	225	LEU
1	A	227	ASP
1	A	228	LEU
1	A	232	ILE
1	A	233	ASN
1	A	236	ARG
1	A	238	GLN
1	A	240	LEU
1	A	241	LEU
1	A	265	TYR
1	A	271	GLN
1	A	278	LYS
1	A	282	ASN
1	A	291	CYS
1	A	299	THR
1	A	300	LYS
1	A	302	THR
1	A	304	LYS
1	A	307	THR
1	A	308	VAL
1	A	309	GLU
1	A	310	LYS
1	A	312	ILE
1	A	316	SER
1	A	324	GLU
1	A	326	ILE
1	A	327	VAL
1	A	328	ARG
1	A	333	THR
1	A	335	LEU
1	A	340	GLU
1	A	342	PHE
1	A	343	ASN
1	A	346	ARG

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Mol	Chain	Res	Type
1	A	350	VAL
1	A	351	TYR
1	A	353	TRP
1	A	354	ASN
1	A	358	ILE
1	A	360	ASN
1	A	366	SER
1	A	367	VAL
1	A	374	PHE
1	A	375	PHE
1	A	377	PHE
1	A	378	LYS
1	A	380	TYR
1	A	386	LYS
1	A	388	ASN
1	A	390	LEU
1	A	392	PHE
1	A	393	THR
1	A	396	TYR
1	A	400	PHE
1	A	401	VAL
1	A	403	LYS
1	A	406	GLU
1	A	415	THR
1	A	417	ASN
1	A	418	ILE
1	A	420	ASP
1	A	428	ASP
1	A	429	PHE
1	A	432	CYS
1	A	439	ASN
1	A	441	LEU
1	A	443	SER
1	A	444	LYS
1	A	455	LEU
1	A	456	PHE
1	A	457	ARG
1	A	458	LYS
1	A	460	LYS
1	A	461	LEU
1	A	462	LYS
1	A	464	PHE

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Mol	Chain	Res	Type
1	A	466	ARG
1	A	468	ILE
1	A	472	ILE
1	A	473	TYR
1	A	474	GLN
1	A	477	ASN
1	A	480	CYS
1	A	481	LYS
1	A	483	LYS
1	A	486	ASN
1	A	488	TYR
1	A	491	LEU
1	A	497	ARG
1	A	500	TYR
1	A	502	VAL
1	A	504	HIS
1	A	508	ARG
1	A	511	VAL
1	A	516	LEU
1	A	518	HIS
1	A	523	VAL
1	A	524	CYS
1	A	528	LYS
1	A	529	SER
1	A	534	LYS
1	A	536	LYS
1	A	537	CYS
1	A	538	VAL
1	A	541	ASN
1	A	542	PHE
1	A	543	ASN
1	A	545	LEU
1	A	548	THR
1	A	553	LYS
1	A	555	ASN
1	A	556	LYS
1	A	557	LYS
1	A	558	PHE
1	A	559	LEU
1	A	563	GLN
1	A	571	THR
1	A	573	ASP

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Mol	Chain	Res	Type
1	A	575	VAL
1	A	576	ARG
1	A	577	ASP
1	A	580	THR
1	A	583	ILE
1	A	584	LEU
1	A	587	THR
1	A	602	ASN
1	A	604	SER
1	A	612	GLN
1	A	614	VAL
1	A	617	THR
1	A	618	GLU
1	A	619	VAL
1	A	623	ILE
1	A	624	HIS
1	A	631	THR
1	A	637	THR
1	A	641	VAL
1	A	643	GLN
1	A	645	ARG
1	A	657	ASN
1	A	658	SER
1	A	665	ILE
1	A	674	GLN
1	A	675	THR
1	A	676	GLN
1	A	692	ILE
1	A	695	TYR
1	A	696	THR
1	A	699	LEU
1	A	702	GLU
1	A	704	SER
1	A	705	VAL
1	A	711	SER
1	A	714	ILE
1	A	721	SER
1	A	723	THR
1	A	727	LEU
1	A	732	THR
1	A	733	LYS
1	A	738	CYS

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Mol	Chain	Res	Type
1	A	740	MET
1	A	745	ASP
1	A	750	SER
1	A	754	LEU
1	A	755	GLN
1	A	760	CYS
1	A	762	GLN
1	A	765	ARG
1	A	774	GLN
1	A	776	LYS
1	A	778	THR
1	A	779	GLN
1	A	786	LYS
1	A	787	GLN
1	A	790	LYS
1	A	791	THR
1	A	804	GLN
1	A	811	LYS
1	A	813	SER
1	A	814	LYS
1	A	815	ARG
1	A	816	SER
1	A	827	THR
1	A	828	LEU
1	A	833	PHE
1	A	834	ILE
1	A	835	LYS
1	A	847	ARG
1	A	849	LEU
1	A	858	LEU
1	A	859	THR
1	A	866	THR
1	A	867	ASP
1	A	875	SER
1	A	878	LEU
1	A	884	SER
1	A	896	ILE
1	A	901	GLN
1	A	911	VAL
1	A	912	THR
1	A	916	LEU
1	A	919	ASN

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Mol	Chain	Res	Type
1	A	921	LYS
1	A	929	SER
1	A	935	GLN
1	A	936	ASP
1	A	938	LEU
1	A	939	PHE
1	A	947	LYS
1	A	949	GLN
1	A	954	HIS
1	A	959	LEU
1	A	960	ASN
1	A	961	THR
1	A	963	VAL
1	A	964	LYS
1	A	965	GLN
1	A	968	SER
1	A	969	LYS
1	A	975	SER
1	A	979	ASP
1	A	982	SER
1	A	983	ARG
1	A	992	GLN
1	A	993	ILE
1	A	995	ARG
1	A	998	THR
1	A	1001	LEU
1	A	1002	GLN
1	A	1005	GLN
1	A	1009	THR
1	A	1010	GLN
1	A	1014	ARG
1	A	1018	ILE
1	A	1021	SER
1	A	1029	MET
1	A	1045	LYS
1	A	1050	MET
1	A	1071	GLN
1	A	1072	GLU
1	A	1081	ILE
1	A	1082	CYS
1	A	1084	ASP
1	A	1091	ARG

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Mol	Chain	Res	Type
1	A	1098	ASN
1	A	1100	THR
1	A	1106	GLN
1	A	1108	ASN
1	A	1111	GLU
1	A	1113	GLN
1	A	1116	THR
1	A	1118	ASP
1	A	1126	CYS
1	A	1128	VAL
1	A	1130	ILE
1	A	1132	ILE
1	A	1141	LEU
1	B	22	ILE
1	B	24	THR
1	B	26	GLN
1	B	28	TYR
1	B	29	THR
1	B	31	SER
1	B	36	VAL
1	B	40	ASP
1	B	41	LYS
1	B	46	SER
1	B	47	VAL
1	B	50	LEU
1	B	54	LEU
1	B	56	LEU
1	B	61	ASN
1	B	62	VAL
1	B	63	THR
1	B	66	HIS
1	B	83	VAL
1	B	84	LEU
1	B	86	PHE
1	B	91	TYR
1	B	92	PHE
1	B	95	THR
1	B	96	GLU
1	B	102	ARG
1	B	105	ILE
1	B	108	THR
1	B	110	LEU

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Mol	Chain	Res	Type
1	B	112	SER
1	B	113	LYS
1	B	117	LEU
1	B	121	ASN
1	B	122	ASN
1	B	126	VAL
1	B	130	VAL
1	B	131	CYS
1	B	133	PHE
1	B	134	GLN
1	B	136	CYS
1	B	138	ASP
1	B	140	PHE
1	B	142	ASP
1	B	168	PHE
1	B	169	GLU
1	B	171	VAL
1	B	186	PHE
1	B	187	LYS
1	B	191	GLU
1	B	197	ILE
1	B	198	ASP
1	B	200	TYR
1	B	201	PHE
1	B	202	LYS
1	B	204	TYR
1	B	205	SER
1	B	206	LYS
1	B	208	THR
1	B	210	ILE
1	B	211	ILE
1	B	213	ARG
1	B	214	ASP
1	B	215	PHE
1	B	217	GLN
1	B	223	GLU
1	B	226	VAL
1	B	228	LEU
1	B	233	ASN
1	B	236	ARG
1	B	238	GLN
1	B	239	THR

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Mol	Chain	Res	Type
1	B	240	LEU
1	B	241	LEU
1	B	265	TYR
1	B	270	LEU
1	B	271	GLN
1	B	273	ARG
1	B	274	THR
1	B	278	LYS
1	B	284	THR
1	B	291	CYS
1	B	294	ASP
1	B	298	GLU
1	B	304	LYS
1	B	305	SER
1	B	306	PHE
1	B	312	ILE
1	B	316	SER
1	B	317	ASN
1	B	318	PHE
1	B	319	ARG
1	B	322	PRO
1	B	324	GLU
1	B	327	VAL
1	B	328	ARG
1	B	329	PHE
1	B	338	PHE
1	B	340	GLU
1	B	341	VAL
1	B	342	PHE
1	B	343	ASN
1	B	345	THR
1	B	350	VAL
1	B	353	TRP
1	B	354	ASN
1	B	355	ARG
1	B	357	ARG
1	B	360	ASN
1	B	365	TYR
1	B	367	VAL
1	B	368	LEU
1	B	370	ASN
1	B	371	PHE

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Mol	Chain	Res	Type
1	B	374	PHE
1	B	375	PHE
1	B	377	PHE
1	B	378	LYS
1	B	380	TYR
1	B	383	SER
1	B	386	LYS
1	B	388	ASN
1	B	390	LEU
1	B	393	THR
1	B	396	TYR
1	B	398	ASP
1	B	400	PHE
1	B	401	VAL
1	B	402	ILE
1	B	403	LYS
1	B	406	GLU
1	B	407	VAL
1	B	408	SER
1	B	409	GLN
1	B	410	ILE
1	B	414	GLN
1	B	417	ASN
1	B	418	ILE
1	B	420	ASP
1	B	428	ASP
1	B	429	PHE
1	B	432	CYS
1	B	433	VAL
1	B	436	TRP
1	B	437	ASN
1	B	438	SER
1	B	440	LYS
1	B	441	LEU
1	B	443	SER
1	B	446	SER
1	B	450	ASP
1	B	452	TRP
1	B	456	PHE
1	B	457	ARG
1	B	460	LYS
1	B	461	LEU

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Mol	Chain	Res	Type
1	B	462	LYS
1	B	464	PHE
1	B	466	ARG
1	B	467	ASP
1	B	471	GLU
1	B	478	LYS
1	B	481	LYS
1	B	483	LYS
1	B	486	ASN
1	B	488	TYR
1	B	491	LEU
1	B	492	GLN
1	B	493	SER
1	B	496	PHE
1	B	497	ARG
1	B	499	THR
1	B	500	TYR
1	B	505	GLN
1	B	507	TYR
1	B	508	ARG
1	B	511	VAL
1	B	513	SER
1	B	516	LEU
1	B	518	HIS
1	B	523	VAL
1	B	524	CYS
1	B	527	LYS
1	B	528	LYS
1	B	530	THR
1	B	532	LEU
1	B	533	VAL
1	B	534	LYS
1	B	535	ASN
1	B	536	LYS
1	B	540	PHE
1	B	543	ASN
1	B	545	LEU
1	B	546	THR
1	B	552	THR
1	B	553	LYS
1	B	557	LYS
1	B	559	LEU

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Mol	Chain	Res	Type
1	B	563	GLN
1	B	564	PHE
1	B	567	ASP
1	B	568	ILE
1	B	575	VAL
1	B	576	ARG
1	B	579	GLN
1	B	580	THR
1	B	586	ILE
1	B	587	THR
1	B	588	PRO
1	B	589	CYS
1	B	598	THR
1	B	602	ASN
1	B	604	SER
1	B	605	ASN
1	B	609	VAL
1	B	614	VAL
1	B	616	CYS
1	B	618	GLU
1	B	624	HIS
1	B	631	THR
1	B	633	ARG
1	B	645	ARG
1	B	653	GLU
1	B	656	ASN
1	B	657	ASN
1	B	673	TYR
1	B	674	GLN
1	B	675	THR
1	B	689	SER
1	B	690	GLN
1	B	696	THR
1	B	697	MET
1	B	704	SER
1	B	705	VAL
1	B	709	ASN
1	B	711	SER
1	B	714	ILE
1	B	723	THR
1	B	728	PRO
1	B	732	THR

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Mol	Chain	Res	Type
1	B	733	LYS
1	B	738	CYS
1	B	739	THR
1	B	740	MET
1	B	746	SER
1	B	748	GLU
1	B	749	CYS
1	B	751	ASN
1	B	752	LEU
1	B	754	LEU
1	B	758	SER
1	B	761	THR
1	B	764	LYS
1	B	779	GLN
1	B	784	GLN
1	B	785	VAL
1	B	786	LYS
1	B	787	GLN
1	B	791	THR
1	B	794	ILE
1	B	807	PRO
1	B	811	LYS
1	B	813	SER
1	B	814	LYS
1	B	815	ARG
1	B	820	ASP
1	B	825	LYS
1	B	828	LEU
1	B	833	PHE
1	B	835	LYS
1	B	836	GLN
1	B	849	LEU
1	B	854	LYS
1	B	856	ASN
1	B	866	THR
1	B	867	ASP
1	B	868	GLU
1	B	873	TYR
1	B	874	THR
1	B	875	SER
1	B	878	LEU
1	B	884	SER

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Mol	Chain	Res	Type
1	B	886	TRP
1	B	895	GLN
1	B	901	GLN
1	B	902	MET
1	B	909	ILE
1	B	912	THR
1	B	918	GLU
1	B	919	ASN
1	B	921	LYS
1	B	922	LEU
1	B	923	ILE
1	B	934	ILE
1	B	935	GLN
1	B	937	SER
1	B	947	LYS
1	B	948	LEU
1	B	957	GLN
1	B	959	LEU
1	B	961	THR
1	B	964	LYS
1	B	965	GLN
1	B	968	SER
1	B	969	LYS
1	B	973	ILE
1	B	974	SER
1	B	975	SER
1	B	983	ARG
1	B	984	LEU
1	B	988	GLU
1	B	990	GLU
1	B	991	VAL
1	B	995	ARG
1	B	996	LEU
1	B	1001	LEU
1	B	1002	GLN
1	B	1010	GLN
1	B	1014	ARG
1	B	1021	SER
1	B	1028	LYS
1	B	1029	MET
1	B	1037	SER
1	B	1038	LYS

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Mol	Chain	Res	Type
1	B	1045	LYS
1	B	1050	MET
1	B	1058	HIS
1	B	1072	GLU
1	B	1074	ASN
1	B	1076	THR
1	B	1081	ILE
1	B	1082	CYS
1	B	1086	LYS
1	B	1091	ARG
1	B	1094	VAL
1	B	1097	SER
1	B	1106	GLN
1	B	1107	ARG
1	B	1114	ILE
1	B	1121	PHE
1	B	1123	SER
1	B	1126	CYS
1	B	1127	ASP
1	B	1130	ILE
1	B	1134	ASN
1	B	1136	THR
1	B	1142	GLN
1	B	1145	LEU
1	B	1146	ASP
1	C	20	ASN
1	C	21	LEU
1	C	25	THR
1	C	26	GLN
1	C	31	SER
1	C	34	ARG
1	C	41	LYS
1	C	44	ARG
1	C	50	LEU
1	C	52	GLN
1	C	64	TRP
1	C	80	ASP
1	C	83	VAL
1	C	84	LEU
1	C	86	PHE
1	C	87	ASN
1	C	96	GLU

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Mol	Chain	Res	Type
1	C	102	ARG
1	C	110	LEU
1	C	111	ASP
1	C	114	THR
1	C	118	LEU
1	C	119	ILE
1	C	120	VAL
1	C	128	ILE
1	C	131	CYS
1	C	133	PHE
1	C	134	GLN
1	C	136	CYS
1	C	137	ASN
1	C	141	LEU
1	C	142	ASP
1	C	164	ASN
1	C	165	ASN
1	C	167	THR
1	C	168	PHE
1	C	186	PHE
1	C	187	LYS
1	C	188	ASN
1	C	189	LEU
1	C	195	LYS
1	C	197	ILE
1	C	198	ASP
1	C	202	LYS
1	C	206	LYS
1	C	208	THR
1	C	210	ILE
1	C	211	ILE
1	C	213	ARG
1	C	217	GLN
1	C	220	SER
1	C	225	LEU
1	C	226	VAL
1	C	230	ILE
1	C	232	ILE
1	C	238	GLN
1	C	239	THR
1	C	265	TYR
1	C	267	VAL

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Mol	Chain	Res	Type
1	C	273	ARG
1	C	276	LEU
1	C	277	LEU
1	C	281	GLU
1	C	284	THR
1	C	294	ASP
1	C	295	PRO
1	C	296	LEU
1	C	299	THR
1	C	300	LYS
1	C	303	LEU
1	C	304	LYS
1	C	307	THR
1	C	309	GLU
1	C	312	ILE
1	C	314	GLN
1	C	319	ARG
1	C	326	ILE
1	C	328	ARG
1	C	329	PHE
1	C	333	THR
1	C	335	LEU
1	C	336	CYS
1	C	343	ASN
1	C	346	ARG
1	C	353	TRP
1	C	356	THR
1	C	364	ASP
1	C	365	TYR
1	C	366	SER
1	C	367	VAL
1	C	374	PHE
1	C	377	PHE
1	C	378	LYS
1	C	383	SER
1	C	385	THR
1	C	386	LYS
1	C	387	LEU
1	C	388	ASN
1	C	389	ASP
1	C	392	PHE
1	C	396	TYR

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Mol	Chain	Res	Type
1	C	398	ASP
1	C	400	PHE
1	C	402	ILE
1	C	403	LYS
1	C	406	GLU
1	C	408	SER
1	C	410	ILE
1	C	415	THR
1	C	420	ASP
1	C	423	TYR
1	C	424	LYS
1	C	425	LEU
1	C	427	ASP
1	C	432	CYS
1	C	433	VAL
1	C	434	ILE
1	C	440	LYS
1	C	441	LEU
1	C	443	SER
1	C	444	LYS
1	C	445	HIS
1	C	446	SER
1	C	458	LYS
1	C	461	LEU
1	C	462	LYS
1	C	463	PRO
1	C	466	ARG
1	C	467	ASP
1	C	468	ILE
1	C	470	THR
1	C	471	GLU
1	C	473	TYR
1	C	474	GLN
1	C	478	LYS
1	C	479	PRO
1	C	483	LYS
1	C	492	GLN
1	C	497	ARG
1	C	500	TYR
1	C	502	VAL
1	C	508	ARG
1	C	511	VAL

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Mol	Chain	Res	Type
1	C	513	SER
1	C	514	PHE
1	C	515	GLU
1	C	516	LEU
1	C	523	VAL
1	C	524	CYS
1	C	527	LYS
1	C	528	LYS
1	C	532	LEU
1	C	533	VAL
1	C	534	LYS
1	C	536	LYS
1	C	537	CYS
1	C	540	PHE
1	C	541	ASN
1	C	542	PHE
1	C	545	LEU
1	C	550	VAL
1	C	552	THR
1	C	553	LYS
1	C	555	ASN
1	C	556	LYS
1	C	557	LYS
1	C	560	PRO
1	C	563	GLN
1	C	564	PHE
1	C	566	ARG
1	C	568	ILE
1	C	569	VAL
1	C	572	THR
1	C	575	VAL
1	C	576	ARG
1	C	577	ASP
1	C	581	LEU
1	C	582	GLU
1	C	584	LEU
1	C	585	ASP
1	C	586	ILE
1	C	587	THR
1	C	589	CYS
1	C	601	THR
1	C	602	ASN

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Mol	Chain	Res	Type
1	C	606	GLN
1	C	607	VAL
1	C	609	VAL
1	C	612	GLN
1	C	616	CYS
1	C	617	THR
1	C	618	GLU
1	C	630	PRO
1	C	633	ARG
1	C	634	VAL
1	C	637	THR
1	C	640	ASN
1	C	641	VAL
1	C	642	PHE
1	C	643	GLN
1	C	644	THR
1	C	645	ARG
1	C	650	ILE
1	C	656	ASN
1	C	659	TYR
1	C	662	ASP
1	C	674	GLN
1	C	675	THR
1	C	690	GLN
1	C	691	SER
1	C	693	ILE
1	C	697	MET
1	C	704	SER
1	C	705	VAL
1	C	714	ILE
1	C	723	THR
1	C	724	THR
1	C	725	GLU
1	C	732	THR
1	C	733	LYS
1	C	736	VAL
1	C	739	THR
1	C	740	MET
1	C	743	CYS
1	C	745	ASP
1	C	747	THR
1	C	748	GLU

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Mol	Chain	Res	Type
1	C	751	ASN
1	C	752	LEU
1	C	754	LEU
1	C	755	GLN
1	C	764	LYS
1	C	778	THR
1	C	779	GLN
1	C	785	VAL
1	C	786	LYS
1	C	787	GLN
1	C	790	LYS
1	C	791	THR
1	C	804	GLN
1	C	811	LYS
1	C	813	SER
1	C	814	LYS
1	C	815	ARG
1	C	816	SER
1	C	821	LEU
1	C	827	THR
1	C	830	ASP
1	C	833	PHE
1	C	834	ILE
1	C	836	GLN
1	C	847	ARG
1	C	848	ASP
1	C	850	ILE
1	C	851	CYS
1	C	853	GLN
1	C	854	LYS
1	C	855	PHE
1	C	856	ASN
1	C	858	LEU
1	C	859	THR
1	C	861	LEU
1	C	868	GLU
1	C	875	SER
1	C	878	LEU
1	C	887	THR
1	C	895	GLN
1	C	904	TYR
1	C	906	PHE

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Mol	Chain	Res	Type
1	C	913	GLN
1	C	916	LEU
1	C	918	GLU
1	C	919	ASN
1	C	931	ILE
1	C	934	ILE
1	C	935	GLN
1	C	937	SER
1	C	939	PHE
1	C	947	LYS
1	C	952	VAL
1	C	957	GLN
1	C	960	ASN
1	C	961	THR
1	C	962	LEU
1	C	964	LYS
1	C	966	LEU
1	C	968	SER
1	C	969	LYS
1	C	980	ILE
1	C	981	LEU
1	C	982	SER
1	C	983	ARG
1	C	984	LEU
1	C	985	ASP
1	C	988	GLU
1	C	990	GLU
1	C	994	ASP
1	C	1001	LEU
1	C	1004	LEU
1	C	1005	GLN
1	C	1014	ARG
1	C	1037	SER
1	C	1045	LYS
1	C	1055	SER
1	C	1069	PRO
1	C	1074	ASN
1	C	1081	ILE
1	C	1082	CYS
1	C	1084	ASP
1	C	1086	LYS
1	C	1091	ARG

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Mol	Chain	Res	Type
1	C	1092	GLU
1	C	1097	SER
1	C	1100	THR
1	C	1106	GLN
1	C	1108	ASN
1	C	1113	GLN
1	C	1116	THR
1	C	1117	THR
1	C	1118	ASP
1	C	1122	VAL
1	C	1125	ASN
1	C	1126	CYS
1	C	1127	ASP
1	C	1128	VAL
1	C	1132	ILE
1	C	1136	THR
1	C	1138	TYR
1	C	1142	GLN
1	C	1143	LEU
1	C	1146	ASP
2	Q	2	VAL
2	Q	3	GLN
2	Q	4	LEU
2	Q	5	VAL
2	Q	11	VAL
2	Q	12	LYS
2	Q	13	LYS
2	Q	16	SER
2	Q	19	LYS
2	Q	20	VAL
2	Q	23	LYS
2	Q	28	THR
2	Q	29	PHE
2	Q	33	VAL
2	Q	34	ILE
2	Q	38	ARG
2	Q	39	GLN
2	Q	43	GLN
2	Q	45	LEU
2	Q	46	GLU
2	Q	51	PHE
2	Q	52	ILE

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Mol	Chain	Res	Type
2	Q	54	LEU
2	Q	55	PHE
2	Q	58	THR
2	Q	59	ILE
2	Q	60	TYR
2	Q	64	PHE
2	Q	69	MET
2	Q	73	ASP
2	Q	74	GLU
2	Q	75	SER
2	Q	80	TYR
2	Q	83	LEU
2	Q	84	SER
2	Q	87	ARG
2	Q	90	ASP
2	Q	99	LEU
2	Q	100	PHE
2	Q	101	PRO
2	Q	104	ASP
2	Q	109	GLU
2	Q	112	PHE
2	Q	114	ILE
2	Q	120	LEU
3	S	3	GLN
3	S	11	VAL
3	S	12	LYS
3	S	13	LYS
3	S	19	LYS
3	S	20	VAL
3	S	21	SER
3	S	23	LYS
3	S	25	SER
3	S	27	TYR
3	S	29	PHE
3	S	34	ILE
3	S	35	SER
3	S	38	ARG
3	S	43	GLN
3	S	48	MET
3	S	50	TRP
3	S	52	SER
3	S	54	TYR

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Mol	Chain	Res	Type
3	S	70	MET
3	S	71	THR
3	S	73	ASP
3	S	74	THR
3	S	75	SER
3	S	77	THR
3	S	81	MET
3	S	82	GLU
3	S	84	ARG
3	S	86	LEU
3	S	87	ARG
3	S	90	ASP
3	S	91	THR
3	S	93	VAL
3	S	98	ARG
3	S	100	TYR
3	S	102	ARG
3	S	110	LEU
3	S	114	PHE
3	S	115	ASP
3	S	119	GLN
3	S	121	THR
3	S	123	VAL
4	R	2	ASP
4	R	3	ILE
4	R	4	GLN
4	R	6	THR
4	R	7	GLN
4	R	19	ARG
4	R	22	ILE
4	R	25	GLN
4	R	28	GLN
4	R	29	ASP
4	R	30	ILE
4	R	32	ASN
4	R	33	TYR
4	R	34	LEU
4	R	35	ASN
4	R	40	LYS
4	R	41	PRO
4	R	46	LYS
4	R	47	LEU

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Mol	Chain	Res	Type
4	R	49	ILE
4	R	55	LEU
4	R	56	GLU
4	R	59	VAL
4	R	61	SER
4	R	62	ARG
4	R	78	SER
4	R	80	GLN
4	R	84	ILE
4	R	89	CYS
4	R	90	GLN
4	R	93	ASP
4	R	103	LYS
4	R	106	ILE
4	R	107	LYS
5	T	2	ILE
5	T	4	LEU
5	T	13	LEU
5	T	14	SER
5	T	18	ARG
5	T	21	LEU
5	T	22	SER
5	T	23	CYS
5	T	24	ARG
5	T	29	VAL
5	T	30	SER
5	T	33	SER
5	T	34	LEU
5	T	38	GLN
5	T	39	GLN
5	T	46	ARG
5	T	47	LEU
5	T	50	TYR
5	T	57	THR
5	T	59	ILE
5	T	62	ARG
5	T	63	PHE
5	T	72	PHE
5	T	78	ARG
5	T	81	PRO
5	T	83	ASP
5	T	84	PHE

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Mol	Chain	Res	Type
5	T	86	VAL
5	T	89	CYS
5	T	93	ASP
5	T	94	THR
5	T	96	LEU
5	T	102	THR
5	T	103	LYS
2	D	2	VAL
2	D	3	GLN
2	D	4	LEU
2	D	5	VAL
2	D	11	VAL
2	D	12	LYS
2	D	13	LYS
2	D	16	SER
2	D	19	LYS
2	D	20	VAL
2	D	23	LYS
2	D	29	PHE
2	D	30	ARG
2	D	32	HIS
2	D	36	TRP
2	D	37	VAL
2	D	38	ARG
2	D	39	GLN
2	D	41	PRO
2	D	45	LEU
2	D	46	GLU
2	D	48	MET
2	D	51	PHE
2	D	52	ILE
2	D	54	LEU
2	D	55	PHE
2	D	59	ILE
2	D	60	TYR
2	D	64	PHE
2	D	73	ASP
2	D	74	GLU
2	D	76	THR
2	D	82	GLU
2	D	83	LEU
2	D	89	GLU

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Mol	Chain	Res	Type
2	D	90	ASP
2	D	93	VAL
2	D	94	TYR
2	D	95	PHE
2	D	96	CYS
2	D	98	ARG
2	D	100	PHE
2	D	104	ASP
2	D	109	GLU
2	D	112	PHE
2	D	113	ASP
2	D	120	LEU
2	D	122	THR
2	D	123	VAL
3	E	3	GLN
3	E	5	VAL
3	E	11	VAL
3	E	12	LYS
3	E	13	LYS
3	E	19	LYS
3	E	20	VAL
3	E	21	SER
3	E	23	LYS
3	E	25	SER
3	E	29	PHE
3	E	30	THR
3	E	34	ILE
3	E	35	SER
3	E	38	ARG
3	E	39	GLN
3	E	43	GLN
3	E	50	TRP
3	E	51	ILE
3	E	52	SER
3	E	57	ASN
3	E	70	MET
3	E	71	THR
3	E	73	ASP
3	E	74	THR
3	E	75	SER
3	E	77	THR
3	E	81	MET

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Mol	Chain	Res	Type
3	E	84	ARG
3	E	85	ARG
3	E	86	LEU
3	E	87	ARG
3	E	90	ASP
3	E	91	THR
3	E	93	VAL
3	E	99	ASP
3	E	100	TYR
3	E	101	THR
3	E	102	ARG
3	E	111	ILE
3	E	115	ASP
3	E	123	VAL
4	F	2	ASP
4	F	3	ILE
4	F	4	GLN
4	F	5	MET
4	F	7	GLN
4	F	8	SER
4	F	15	SER
4	F	16	VAL
4	F	18	ASP
4	F	19	ARG
4	F	22	ILE
4	F	23	THR
4	F	25	GLN
4	F	28	GLN
4	F	29	ASP
4	F	30	ILE
4	F	32	ASN
4	F	33	TYR
4	F	34	LEU
4	F	35	ASN
4	F	38	GLN
4	F	40	LYS
4	F	41	PRO
4	F	46	LYS
4	F	47	LEU
4	F	49	ILE
4	F	54	HIS
4	F	57	THR

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Mol	Chain	Res	Type
4	F	62	ARG
4	F	63	PHE
4	F	77	SER
4	F	79	LEU
4	F	80	GLN
4	F	84	ILE
4	F	90	GLN
4	F	93	ASP
4	F	96	TYR
4	F	100	GLN
4	F	103	LYS
4	F	107	LYS
5	G	2	ILE
5	G	4	LEU
5	G	6	GLN
5	G	7	SER
5	G	14	SER
5	G	18	ARG
5	G	22	SER
5	G	23	CYS
5	G	24	ARG
5	G	29	VAL
5	G	30	SER
5	G	34	LEU
5	G	38	GLN
5	G	39	GLN
5	G	46	ARG
5	G	48	LEU
5	G	50	TYR
5	G	55	ARG
5	G	59	ILE
5	G	63	PHE
5	G	72	PHE
5	G	78	ARG
5	G	81	PRO
5	G	83	ASP
5	G	84	PHE
5	G	88	TYR
5	G	89	CYS
5	G	93	ASP
5	G	95	SER
5	G	96	LEU

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Mol	Chain	Res	Type
5	G	102	THR
5	G	103	LYS
2	H	2	VAL
2	H	3	GLN
2	H	4	LEU
2	H	5	VAL
2	H	12	LYS
2	H	13	LYS
2	H	16	SER
2	H	19	LYS
2	H	20	VAL
2	H	23	LYS
2	H	30	ARG
2	H	31	SER
2	H	32	HIS
2	H	33	VAL
2	H	34	ILE
2	H	35	SER
2	H	37	VAL
2	H	38	ARG
2	H	43	GLN
2	H	46	GLU
2	H	51	PHE
2	H	52	ILE
2	H	55	PHE
2	H	57	THR
2	H	58	THR
2	H	59	ILE
2	H	67	ARG
2	H	69	MET
2	H	75	SER
2	H	78	THR
2	H	80	TYR
2	H	83	LEU
2	H	84	SER
2	H	87	ARG
2	H	90	ASP
2	H	91	THR
2	H	96	CYS
2	H	106	ASN
2	H	110	ASP
2	H	112	PHE

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Mol	Chain	Res	Type
2	H	113	ASP
2	H	120	LEU
2	H	123	VAL
3	I	3	GLN
3	I	11	VAL
3	I	12	LYS
3	I	13	LYS
3	I	19	LYS
3	I	20	VAL
3	I	21	SER
3	I	23	LYS
3	I	25	SER
3	I	27	TYR
3	I	29	PHE
3	I	35	SER
3	I	38	ARG
3	I	43	GLN
3	I	50	TRP
3	I	52	SER
3	I	54	TYR
3	I	57	ASN
3	I	70	MET
3	I	71	THR
3	I	73	ASP
3	I	74	THR
3	I	75	SER
3	I	77	THR
3	I	81	MET
3	I	82	GLU
3	I	84	ARG
3	I	85	ARG
3	I	86	LEU
3	I	87	ARG
3	I	90	ASP
3	I	91	THR
3	I	93	VAL
3	I	99	ASP
3	I	101	THR
3	I	102	ARG
3	I	110	LEU
3	I	115	ASP
3	I	116	ASN

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Mol	Chain	Res	Type
3	I	117	TRP
3	I	119	GLN
3	I	121	THR
3	I	123	VAL
4	J	2	ASP
4	J	3	ILE
4	J	4	GLN
4	J	7	GLN
4	J	13	SER
4	J	15	SER
4	J	16	VAL
4	J	19	ARG
4	J	22	ILE
4	J	25	GLN
4	J	28	GLN
4	J	29	ASP
4	J	30	ILE
4	J	32	ASN
4	J	33	TYR
4	J	34	LEU
4	J	38	GLN
4	J	40	LYS
4	J	41	PRO
4	J	43	LYS
4	J	46	LYS
4	J	47	LEU
4	J	49	ILE
4	J	54	HIS
4	J	55	LEU
4	J	56	GLU
4	J	62	ARG
4	J	77	SER
4	J	78	SER
4	J	84	ILE
4	J	89	CYS
4	J	90	GLN
4	J	91	ARG
4	J	93	ASP
4	J	96	TYR
4	J	98	PHE
4	J	102	THR
4	J	107	LYS

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Mol	Chain	Res	Type
5	K	2	ILE
5	K	4	LEU
5	K	11	LEU
5	K	13	LEU
5	K	18	ARG
5	K	22	SER
5	K	24	ARG
5	K	29	VAL
5	K	30	SER
5	K	32	THR
5	K	34	LEU
5	K	38	GLN
5	K	46	ARG
5	K	47	LEU
5	K	48	LEU
5	K	50	TYR
5	K	59	ILE
5	K	62	ARG
5	K	63	PHE
5	K	72	PHE
5	K	78	ARG
5	K	79	LEU
5	K	81	PRO
5	K	83	ASP
5	K	86	VAL
5	K	89	CYS
5	K	94	THR
5	K	103	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (146) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	61	ASN
1	A	66	HIS
1	A	121	ASN
1	A	134	GLN
1	A	137	ASN
1	A	196	ASN
1	A	217	GLN
1	A	238	GLN
1	A	271	GLN

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Mol	Chain	Res	Type
1	A	317	ASN
1	A	321	GLN
1	A	331	ASN
1	A	354	ASN
1	A	370	ASN
1	A	405	ASN
1	A	414	GLN
1	A	417	ASN
1	A	437	ASN
1	A	505	GLN
1	A	541	ASN
1	A	543	ASN
1	A	579	GLN
1	A	602	ASN
1	A	640	ASN
1	A	643	GLN
1	A	779	GLN
1	A	853	GLN
1	A	901	GLN
1	A	919	ASN
1	A	949	GLN
1	A	955	ASN
1	A	965	GLN
1	A	992	GLN
1	A	1011	GLN
1	A	1048	HIS
1	A	1098	ASN
1	A	1101	HIS
1	A	1142	GLN
1	B	20	ASN
1	B	26	GLN
1	B	49	HIS
1	B	87	ASN
1	B	122	ASN
1	B	164	ASN
1	B	217	GLN
1	B	314	GLN
1	B	317	ASN
1	B	334	ASN
1	B	343	ASN
1	B	354	ASN
1	B	405	ASN

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Mol	Chain	Res	Type
1	B	417	ASN
1	B	445	HIS
1	B	492	GLN
1	B	504	HIS
1	B	563	GLN
1	B	579	GLN
1	B	640	ASN
1	B	676	GLN
1	B	690	GLN
1	B	751	ASN
1	B	762	GLN
1	B	774	GLN
1	B	779	GLN
1	B	784	GLN
1	B	787	GLN
1	B	907	ASN
1	B	913	GLN
1	B	1002	GLN
1	B	1010	GLN
1	B	1054	GLN
1	B	1071	GLN
1	B	1142	GLN
1	C	122	ASN
1	C	134	GLN
1	C	165	ASN
1	C	196	ASN
1	C	207	HIS
1	C	233	ASN
1	C	317	ASN
1	C	343	ASN
1	C	405	ASN
1	C	414	GLN
1	C	448	ASN
1	C	474	GLN
1	C	539	ASN
1	C	562	GLN
1	C	602	ASN
1	C	606	GLN
1	C	643	GLN
1	C	657	ASN
1	C	674	GLN
1	C	690	GLN

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Mol	Chain	Res	Type
1	C	710	ASN
1	C	755	GLN
1	C	779	GLN
1	C	804	GLN
1	C	856	ASN
1	C	914	ASN
1	C	919	ASN
1	C	926	GLN
1	C	954	HIS
1	C	957	GLN
1	C	960	ASN
1	C	978	ASN
1	C	1005	GLN
1	C	1023	ASN
1	C	1048	HIS
1	C	1064	HIS
1	C	1113	GLN
1	C	1125	ASN
1	C	1135	ASN
2	Q	3	GLN
2	Q	6	GLN
2	Q	39	GLN
2	Q	102	ASN
3	S	59	ASN
4	R	4	GLN
4	R	28	GLN
4	R	35	ASN
4	R	90	GLN
5	T	27	GLN
5	T	38	GLN
5	T	91	GLN
2	D	3	GLN
2	D	39	GLN
2	D	102	ASN
3	E	59	ASN
3	E	116	ASN
4	F	4	GLN
5	G	27	GLN
5	G	91	GLN
2	H	3	GLN
2	H	39	GLN
2	H	102	ASN

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Mol	Chain	Res	Type
3	I	59	ASN
3	I	116	ASN
4	J	4	GLN
4	J	32	ASN
4	J	54	HIS
4	J	90	GLN
4	J	100	GLN
5	K	27	GLN
5	K	91	GLN
5	K	92	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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.

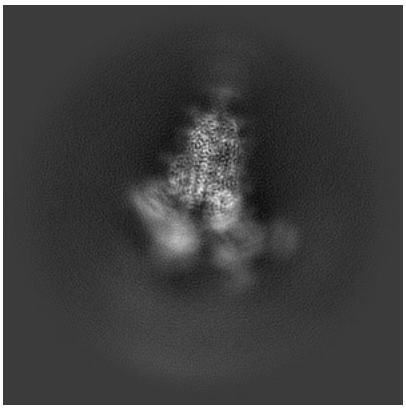
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37930. These allow visual inspection of the internal detail of the map and identification of artifacts.

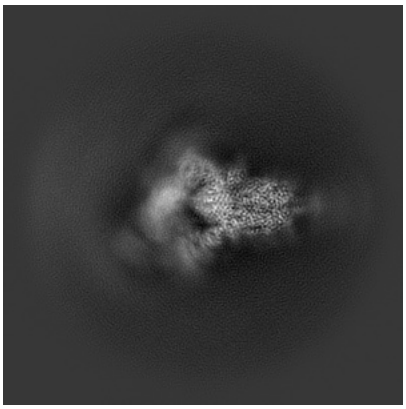
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

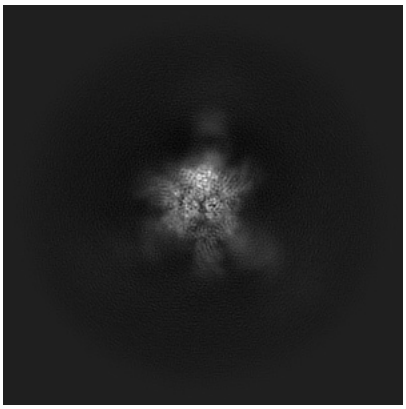
6.1.1 Primary map



X

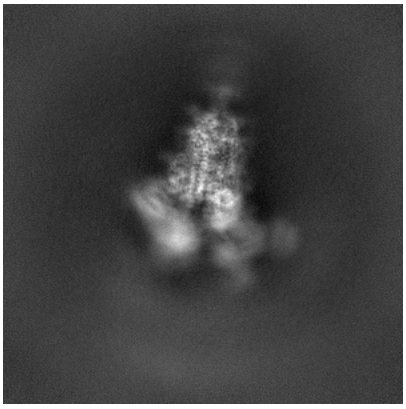


Y

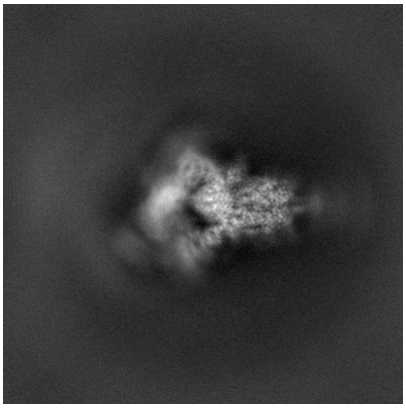


Z

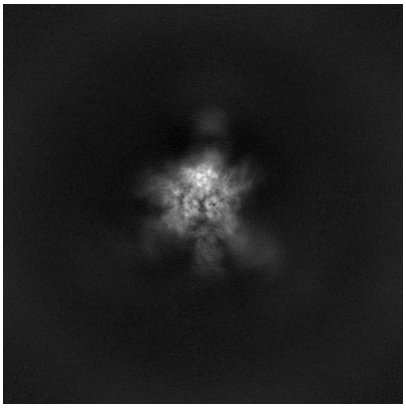
6.1.2 Raw map



X



Y



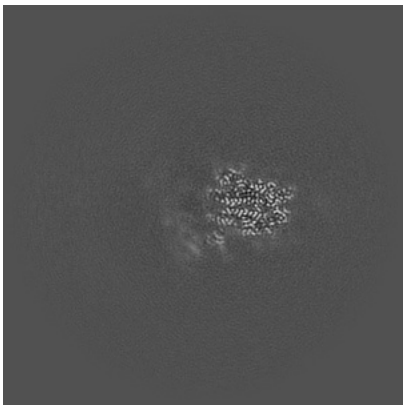
Z

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

6.2 Central slices (i)

6.2.1 Primary map

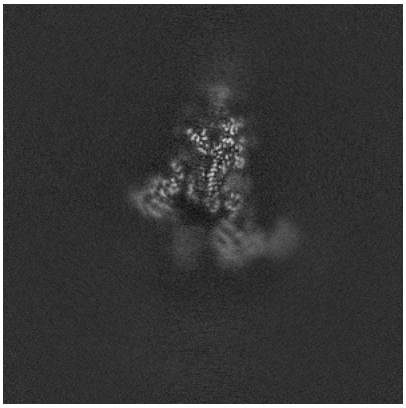
X Index: 270



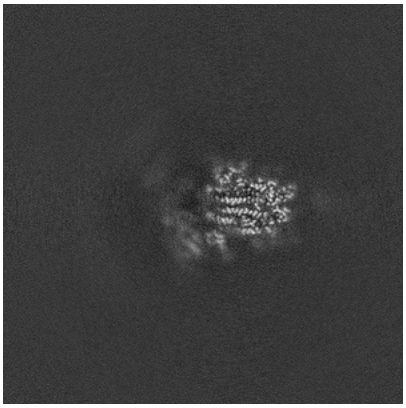
Y Index: 270

Z Index: 270

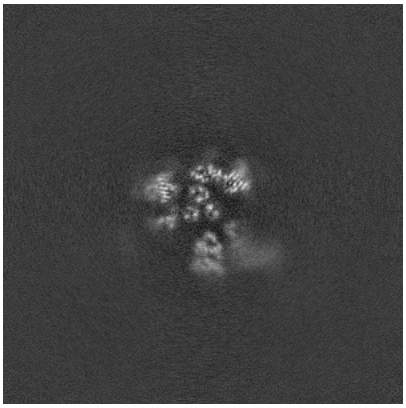
6.2.2 Raw map



X Index: 270



Y Index: 270



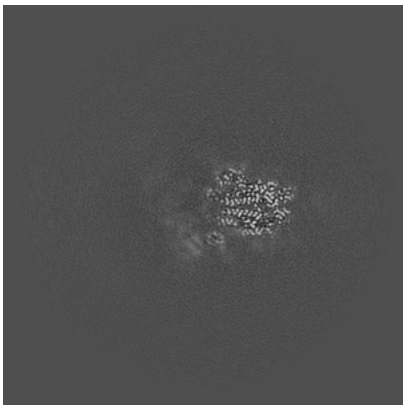
Z Index: 270

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

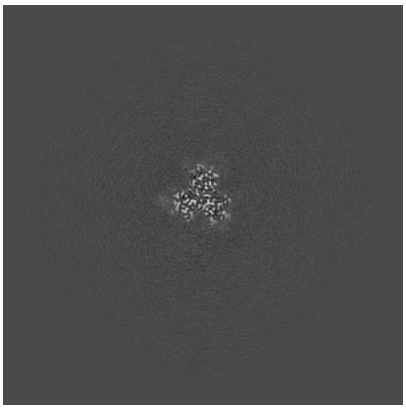
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 278



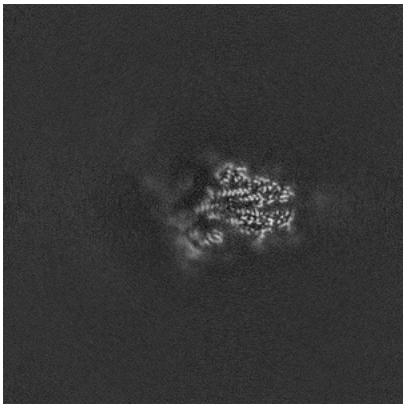
Y Index: 271



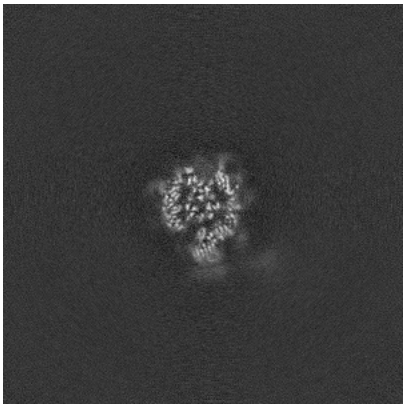
Z Index: 343

6.3.2 Raw map

X Index: 277



Y Index: 275

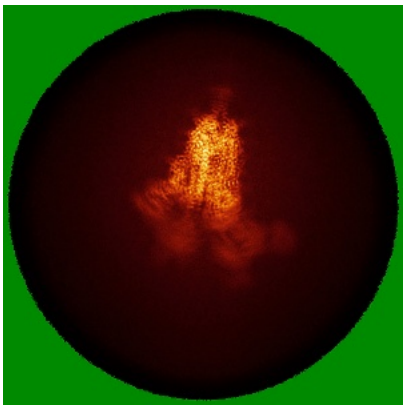


Z Index: 288

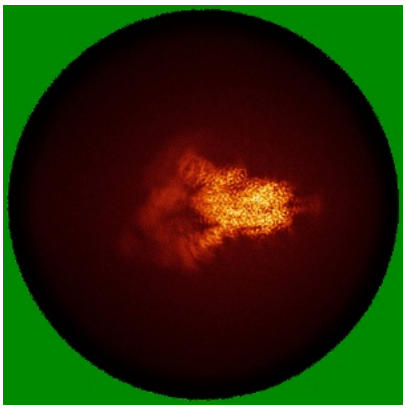
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

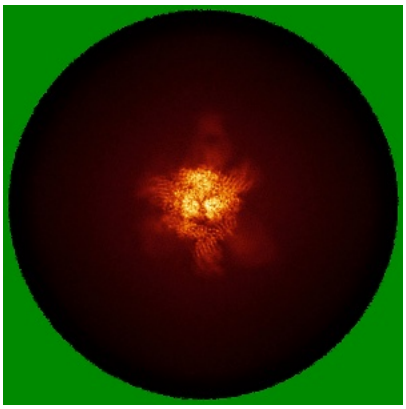
6.4.1 Primary map



X

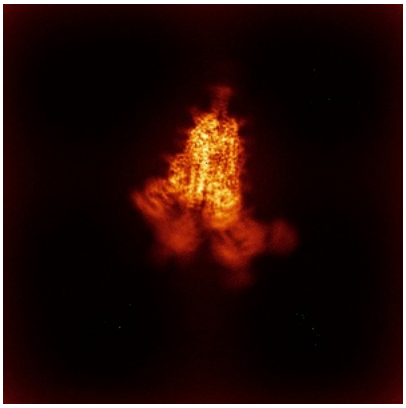


Y

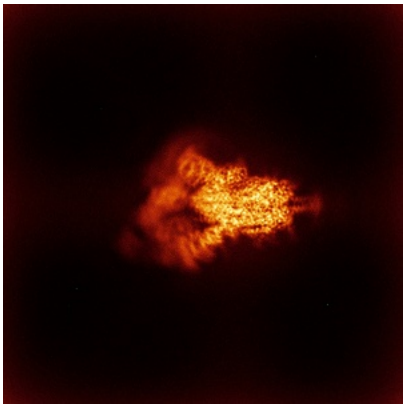


Z

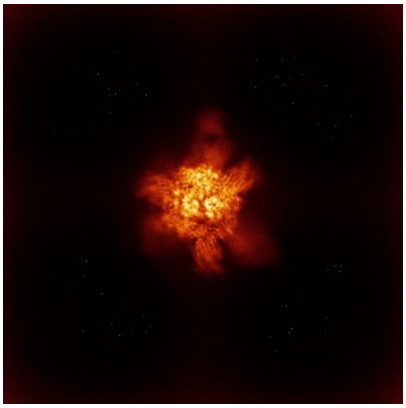
6.4.2 Raw map



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

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X

Y

Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

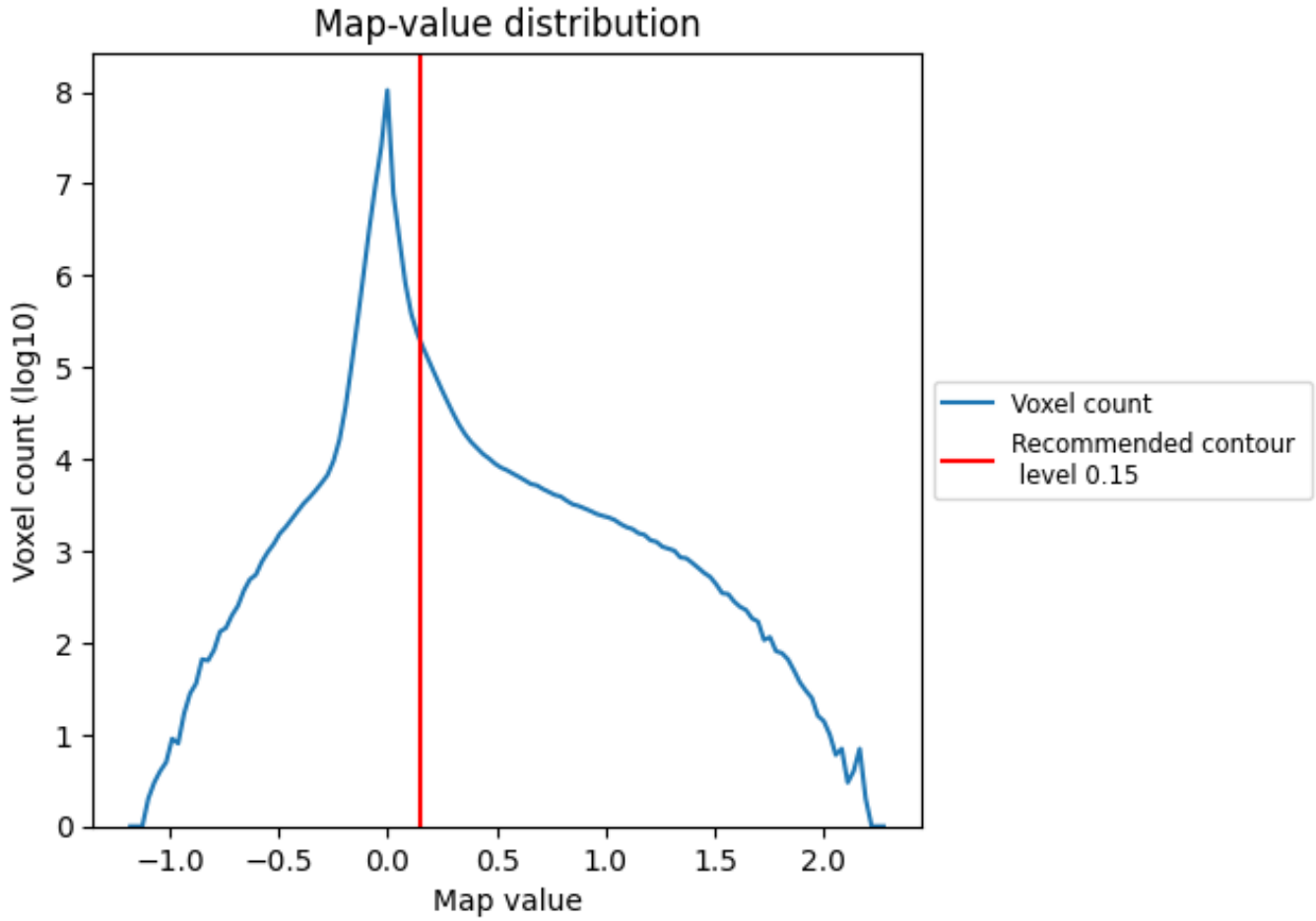
6.6 Mask visualisation (i)

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

7 Map analysis

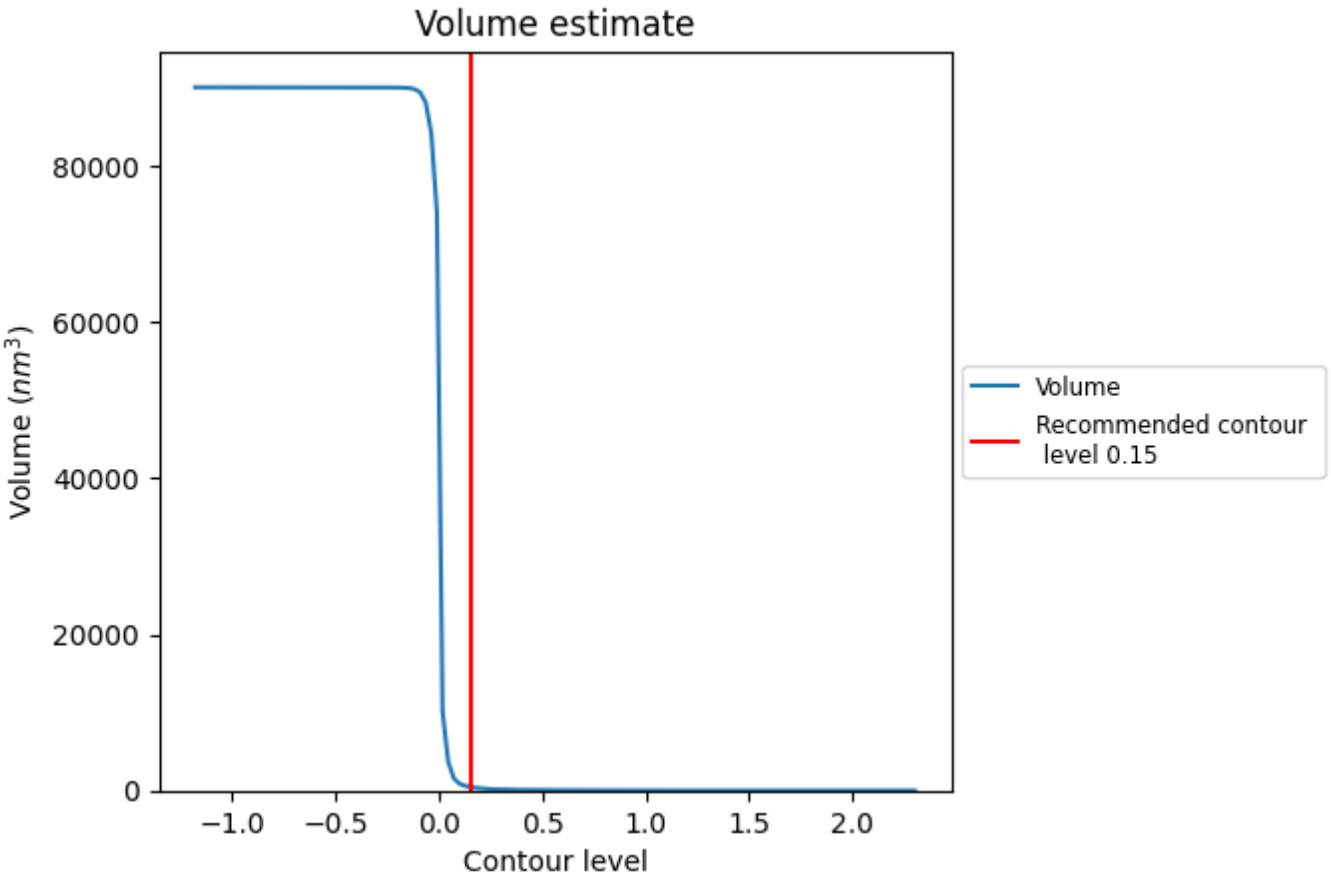
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

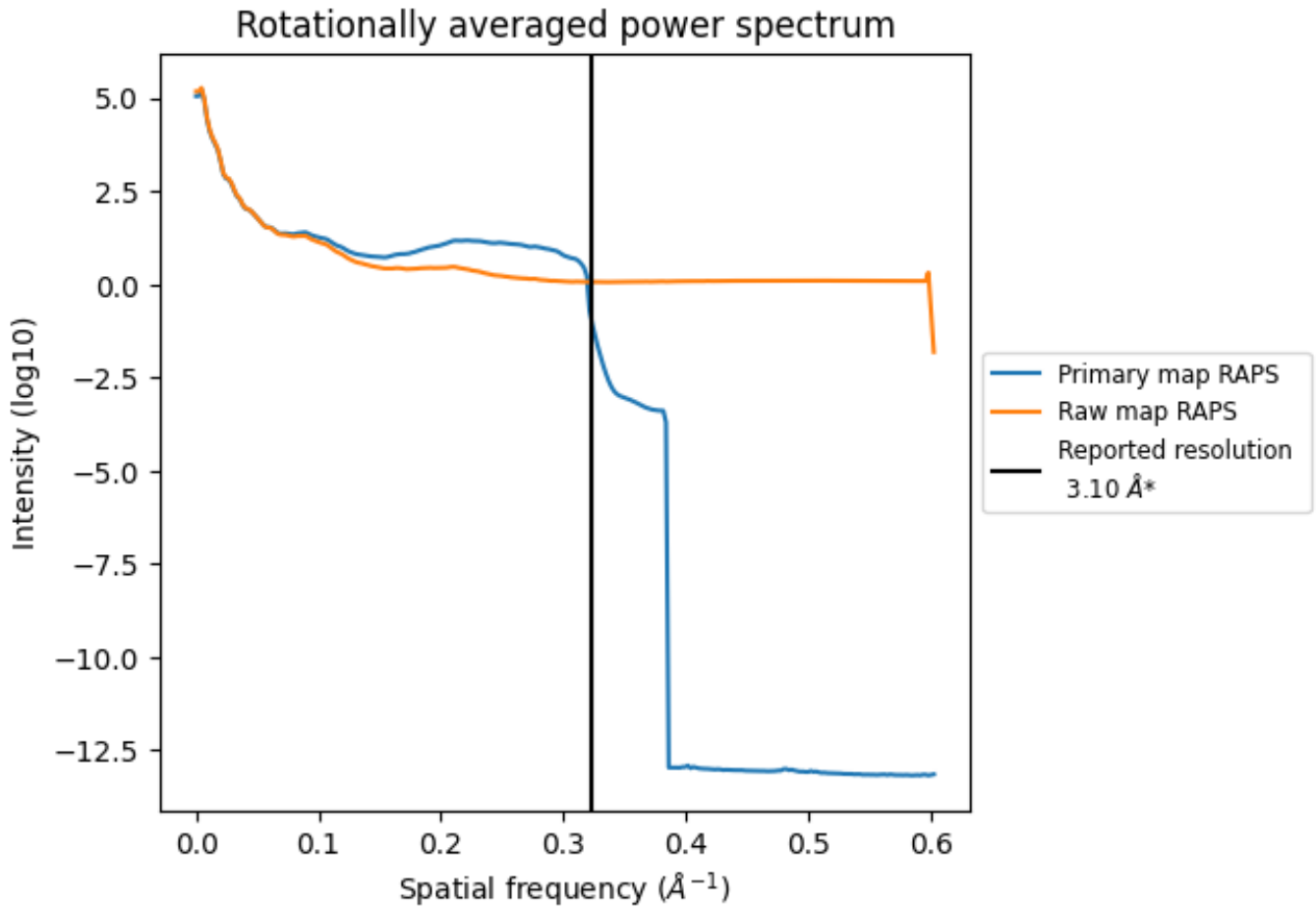
7.2 Volume estimate



The volume at the recommended contour level is 464 nm^3; this corresponds to an approximate mass of 419 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 (i)

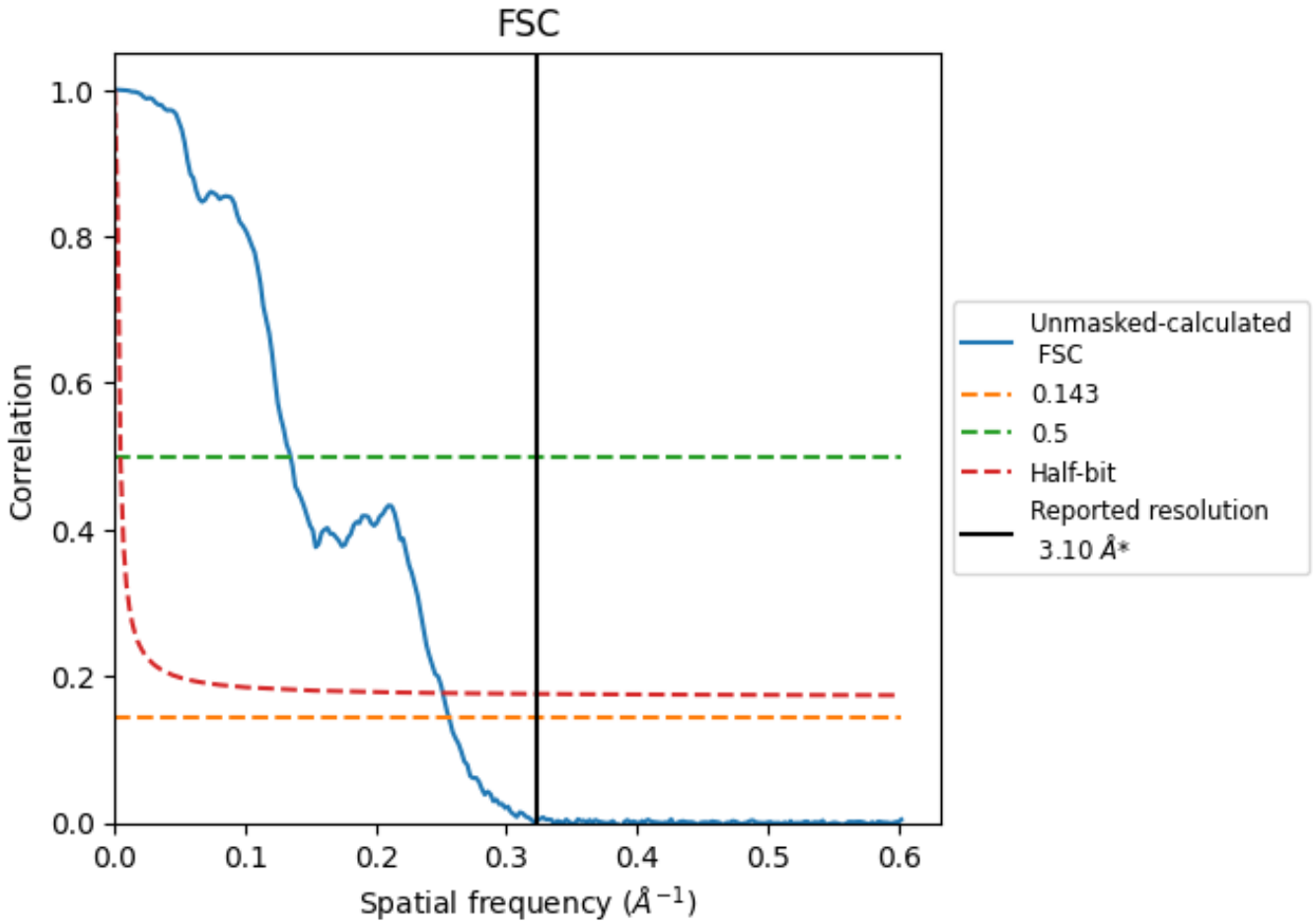


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

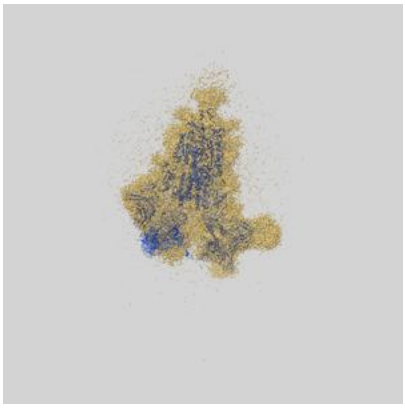
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	7.43	3.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.1 by more than 10 %

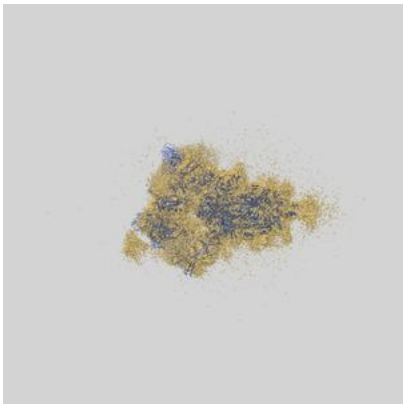
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37930 and PDB model 8WYJ. Per-residue inclusion information can be found in section 3 on page 11.

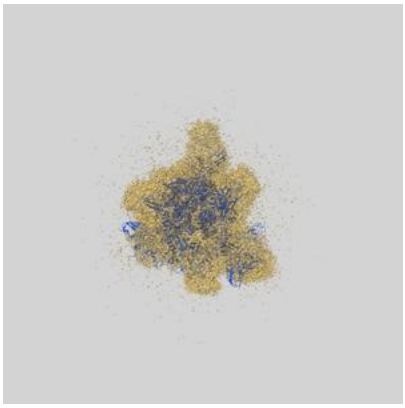
9.1 Map-model overlay



X



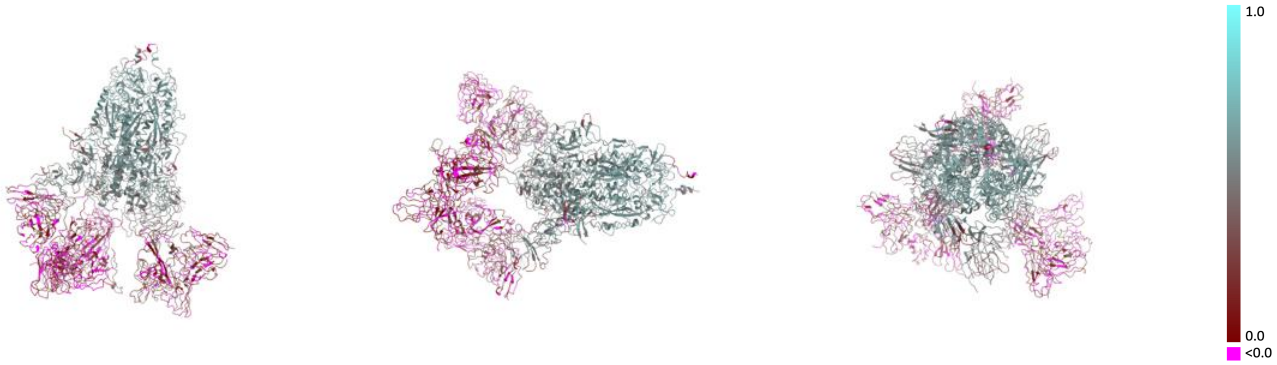
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

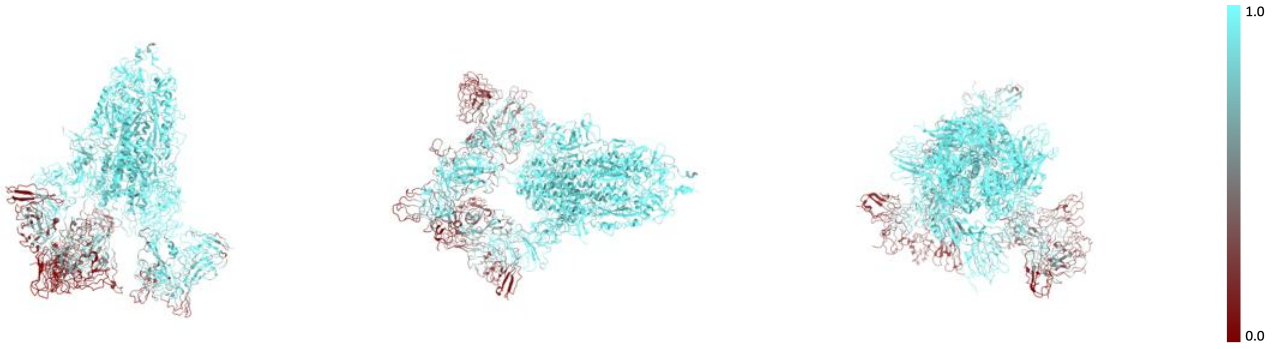
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

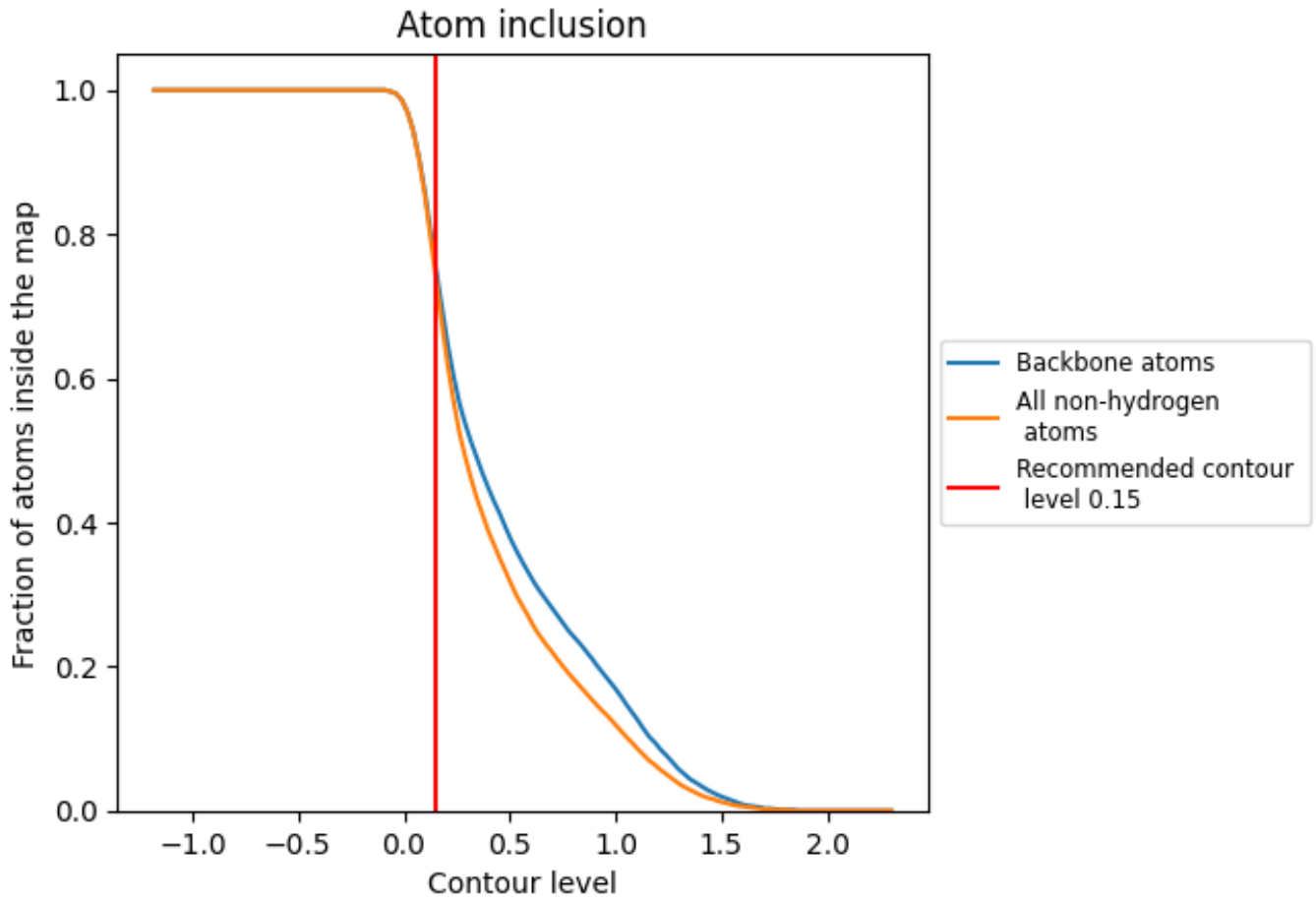
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 74% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7400	0.3380
A	0.8810	0.4350
B	0.9130	0.4380
C	0.8600	0.4460
D	0.4440	0.1590
E	0.1820	0.0730
F	0.2150	0.0980
G	0.1040	0.0560
H	0.4260	0.0800
I	0.1550	0.0590
J	0.2980	0.1100
K	0.1570	0.0990
Q	0.8160	0.0940
R	0.8300	0.1120
S	0.4970	0.1000
T	0.5650	0.1180