



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 05:59 AM UTC

PDB ID : 8WYH / pdb_00008wyh
EMDB ID : EMD-37928
Title : The global map of Omicron Subvariants Spike with ACE2
Authors : Yan, R.H.; Wang, A.J.; Yang, H.N.
Deposited on : 2023-10-31
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

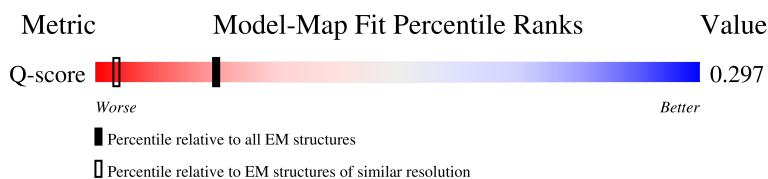
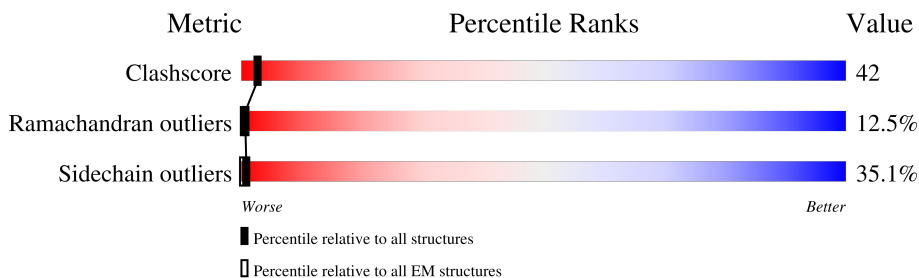
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1123	
1	B	1123	
1	C	1123	
2	T	597	

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Mol	Chain	Length	Quality of chain
2	X	597	<div><div></div><div>36%</div><div>18%</div><div>42%</div><div>32%</div><div>7%</div></div>
2	Z	597	<div><div></div><div>51%</div><div>19%</div><div>42%</div><div>32%</div><div>7%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 38852 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	1029	Total	C	N	O	S	0	0
			8076	5178	1341	1521	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

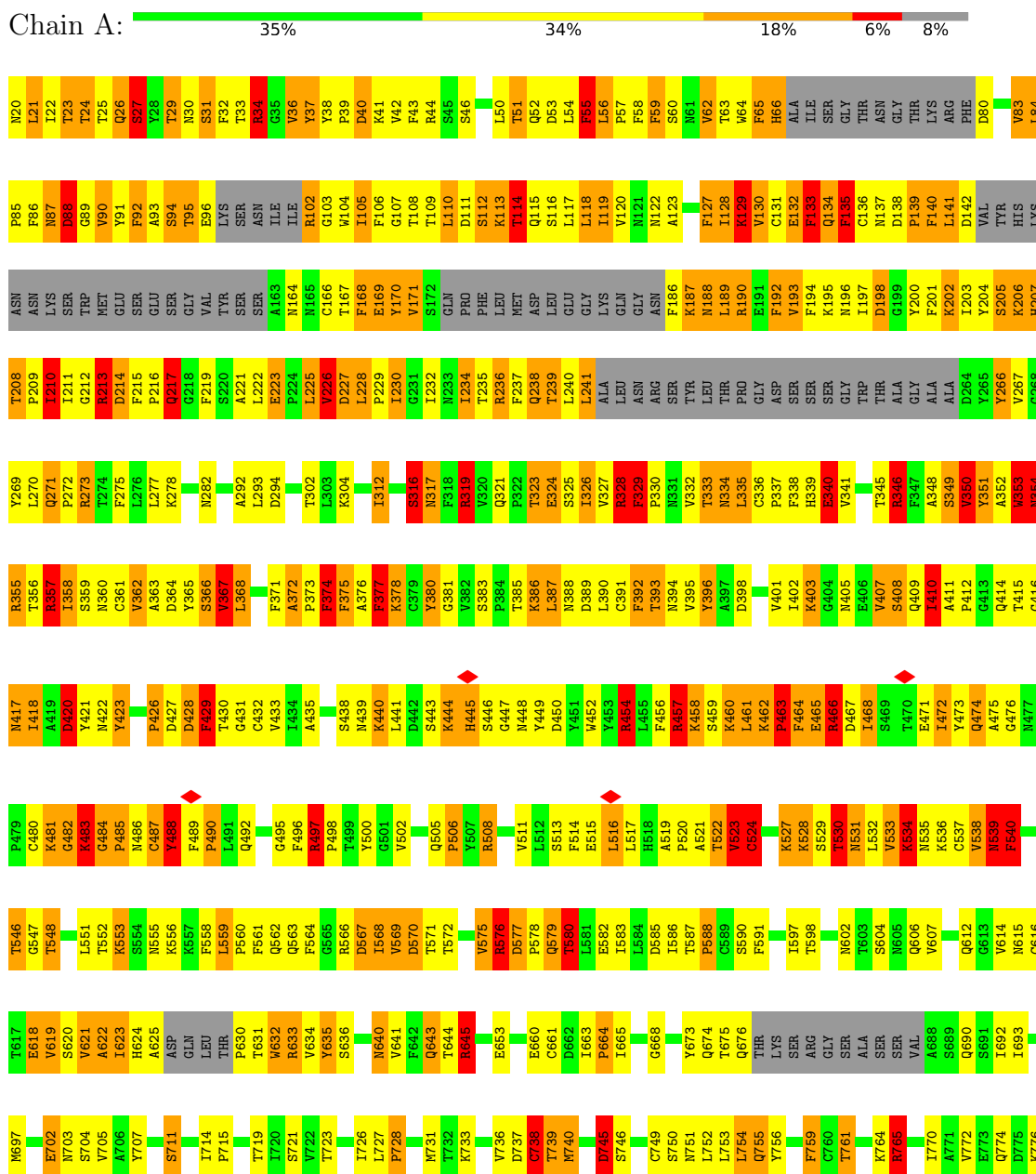
- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

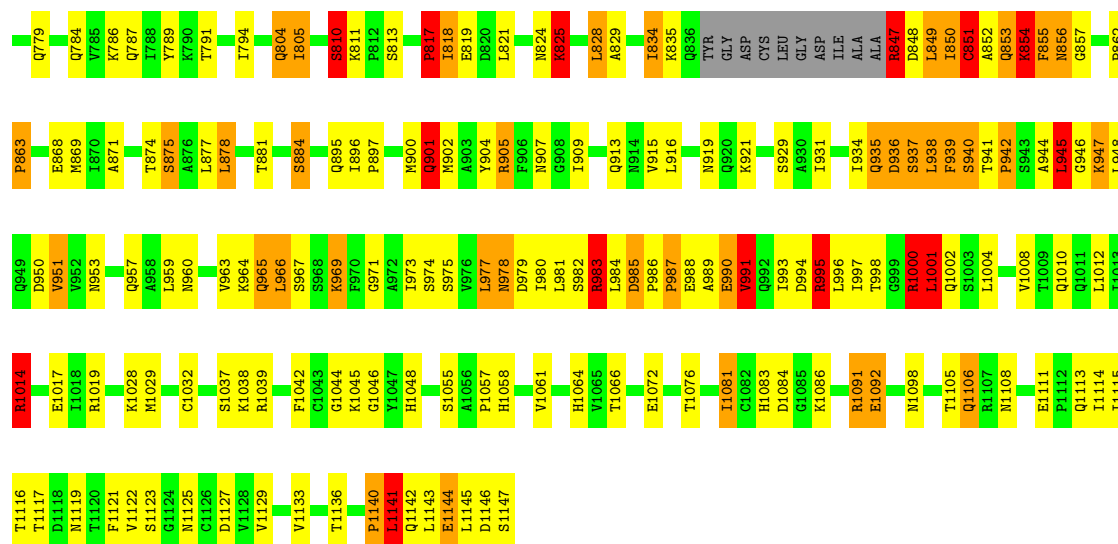
Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		
2	X	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		
2	Z	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

3 Residue-property plots

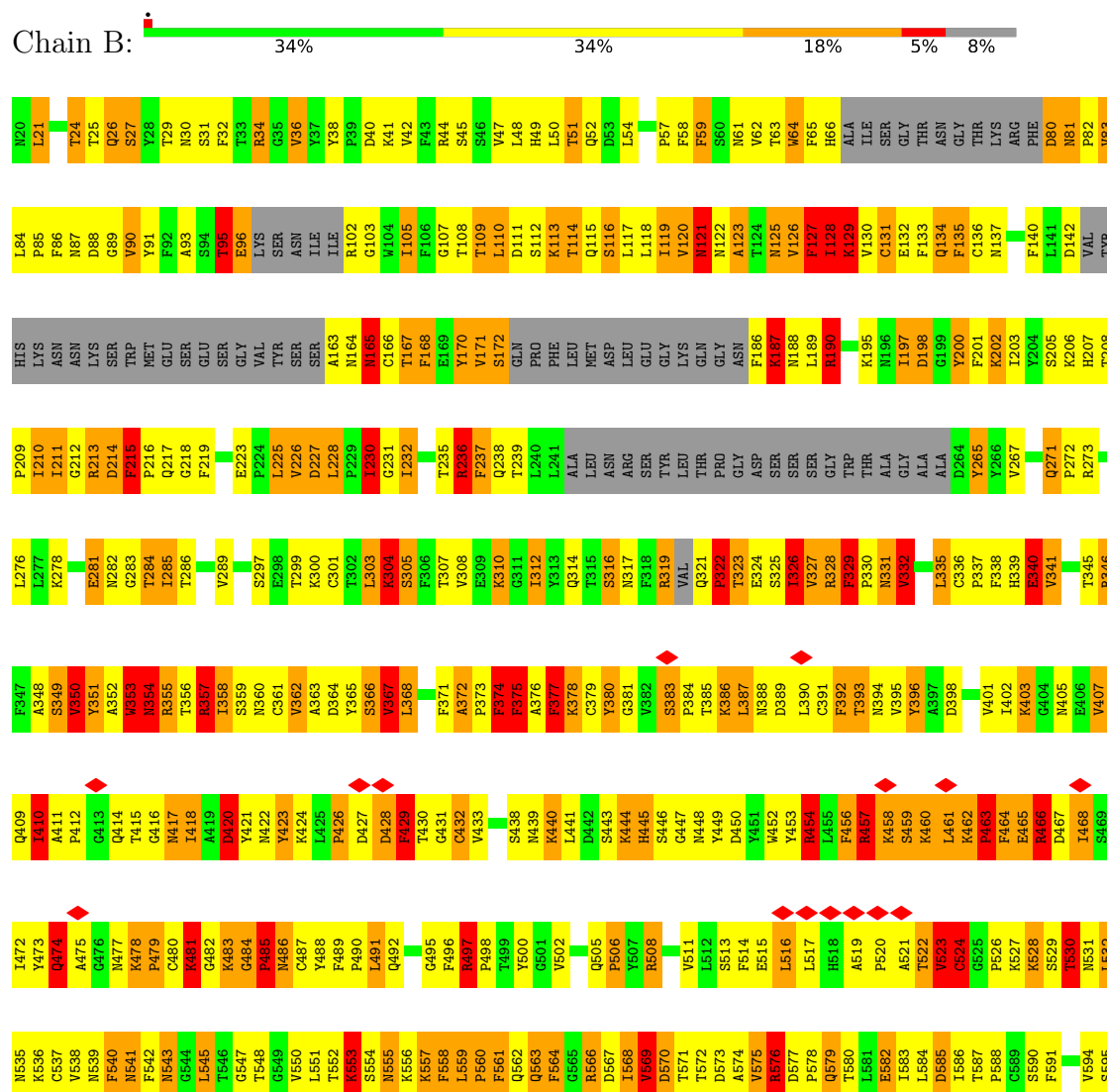
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

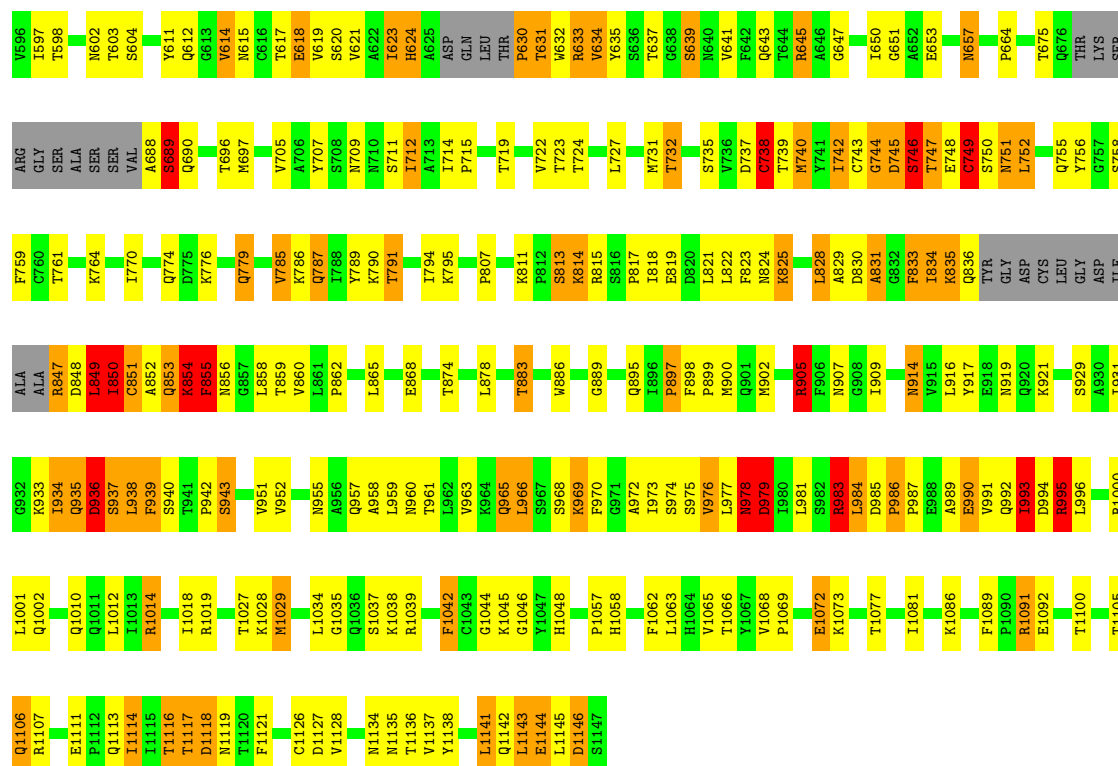
• Molecule 1: Spike glycoprotein



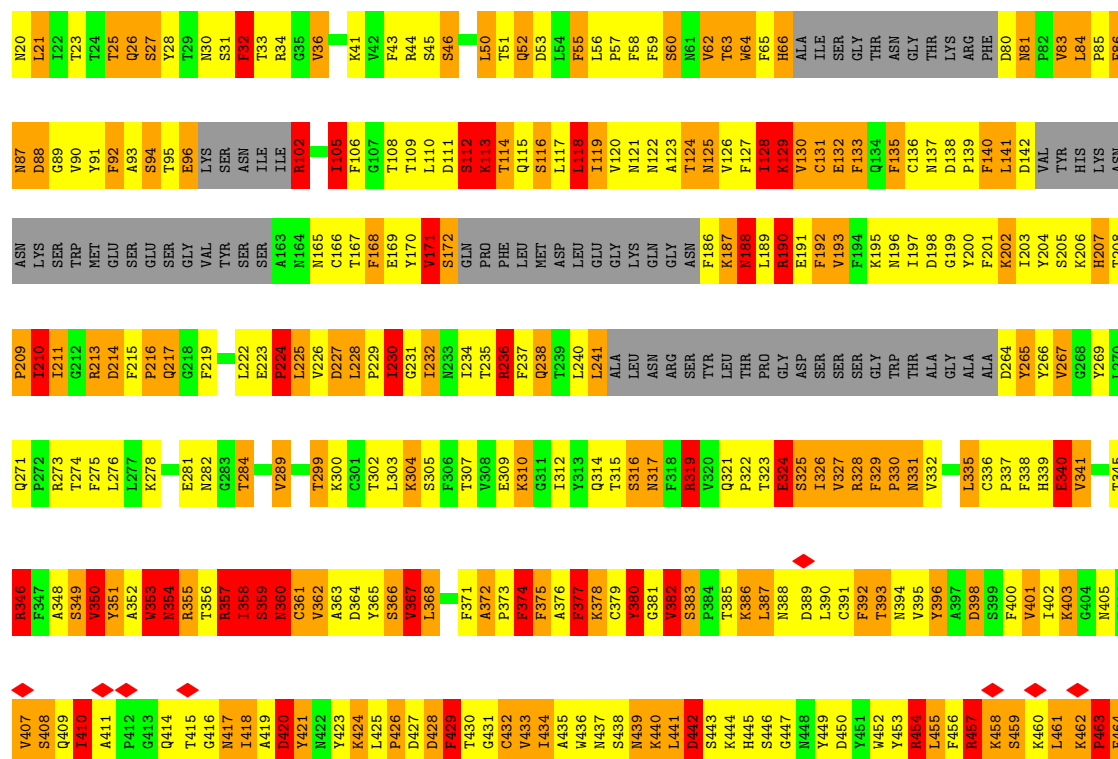


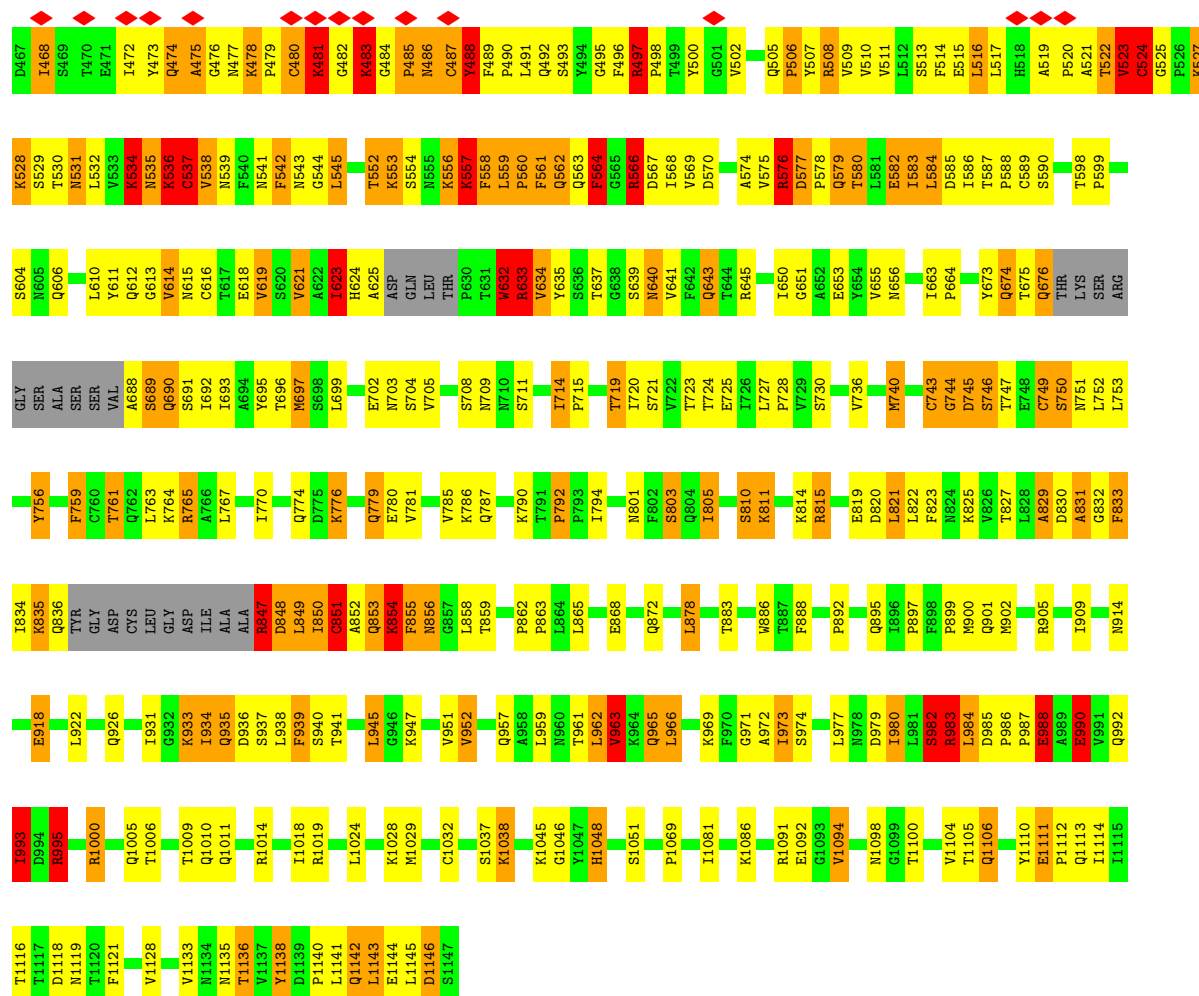
- Molecule 1: Spike glycoprotein



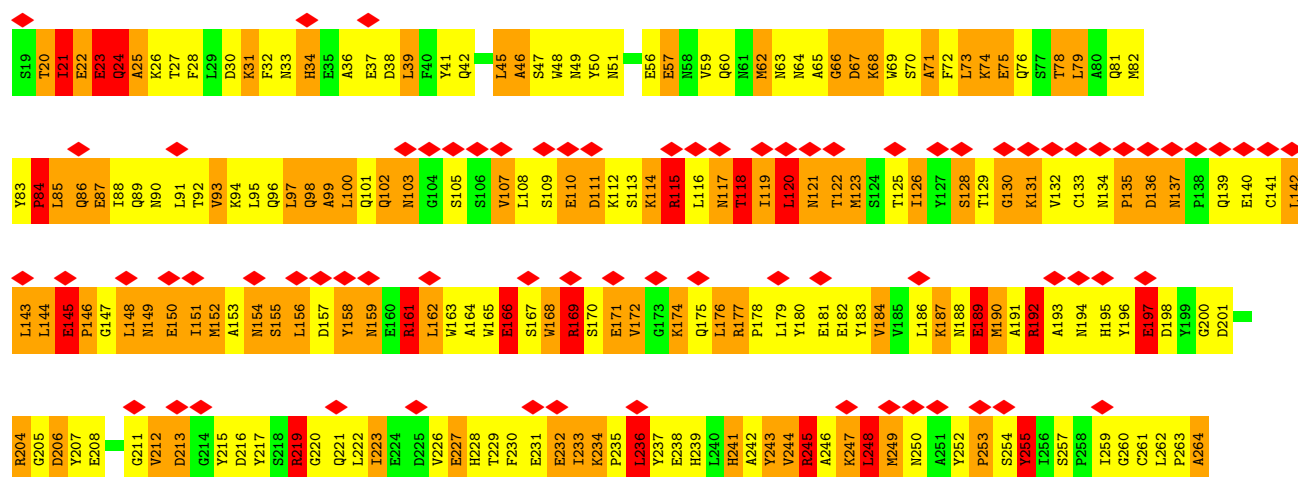
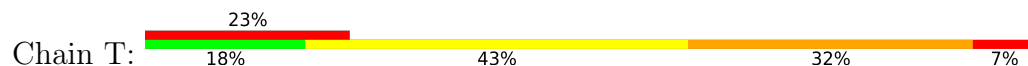


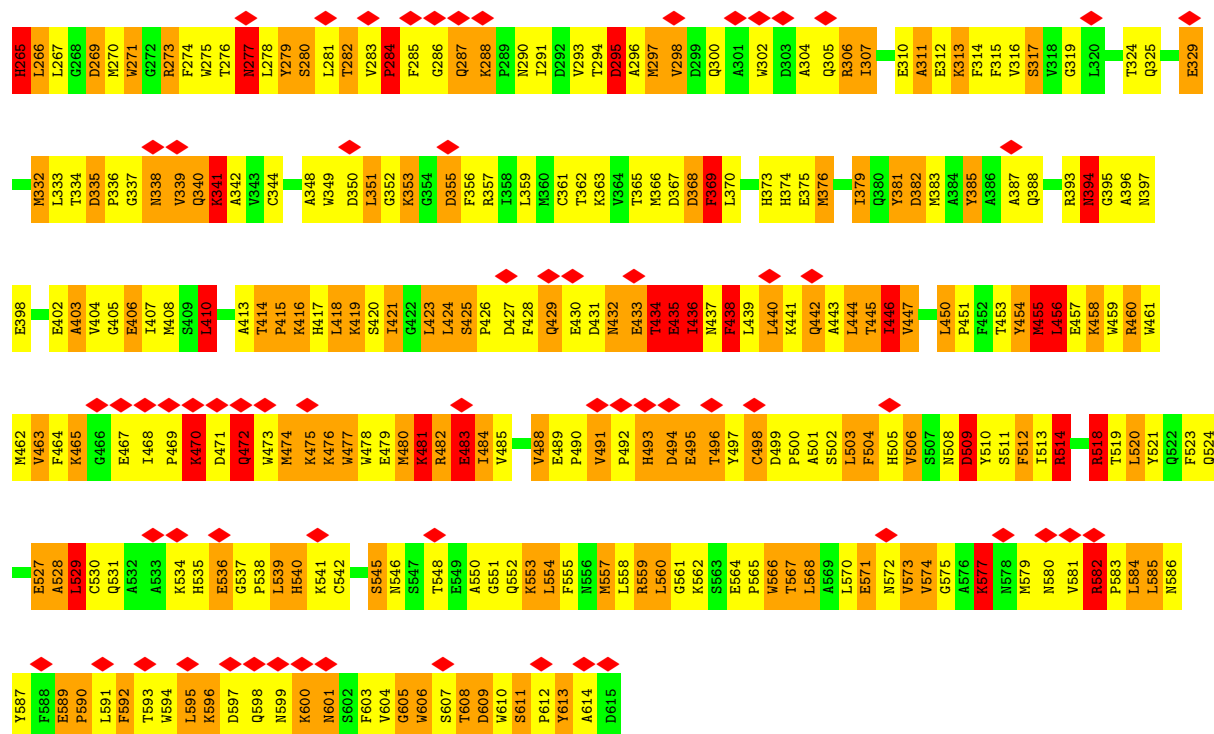
• Molecule 1: Spike glycoprotein



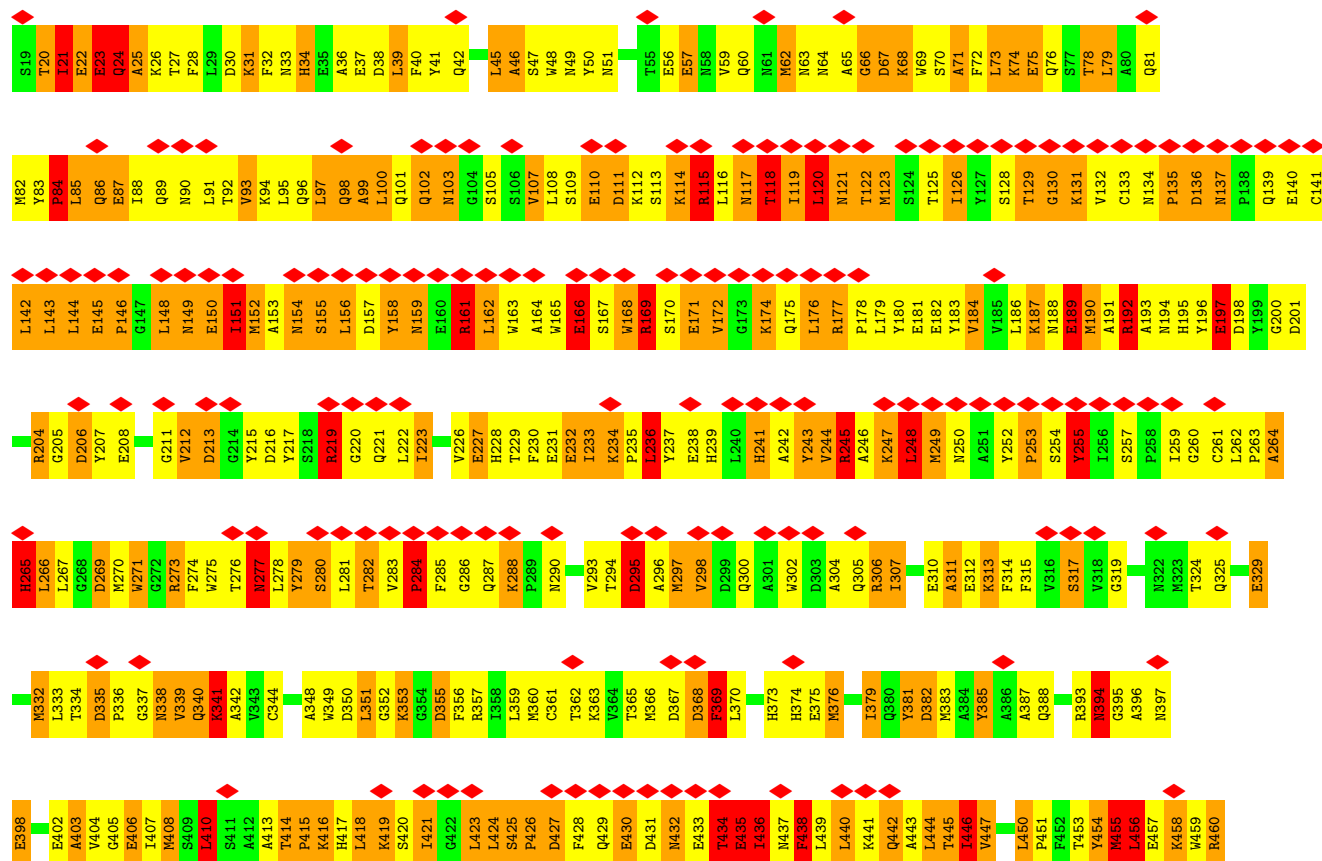
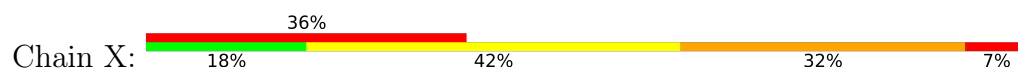


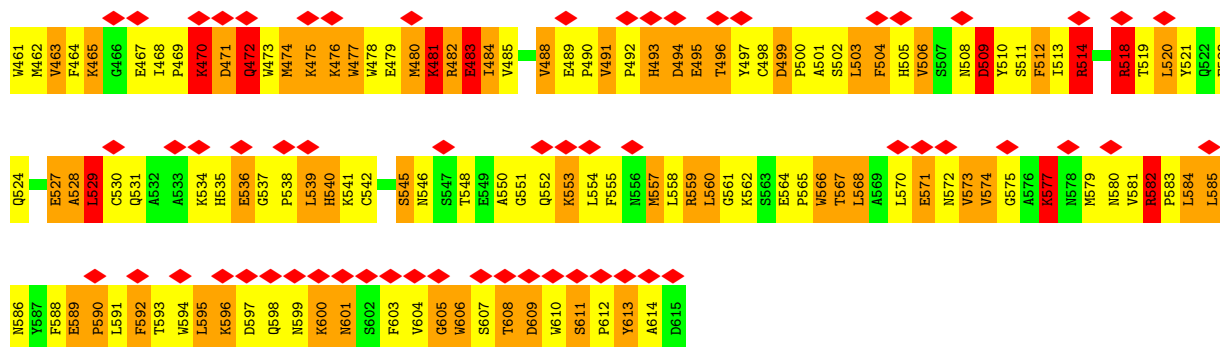
• Molecule 2: Angiotensin-converting enzyme 2



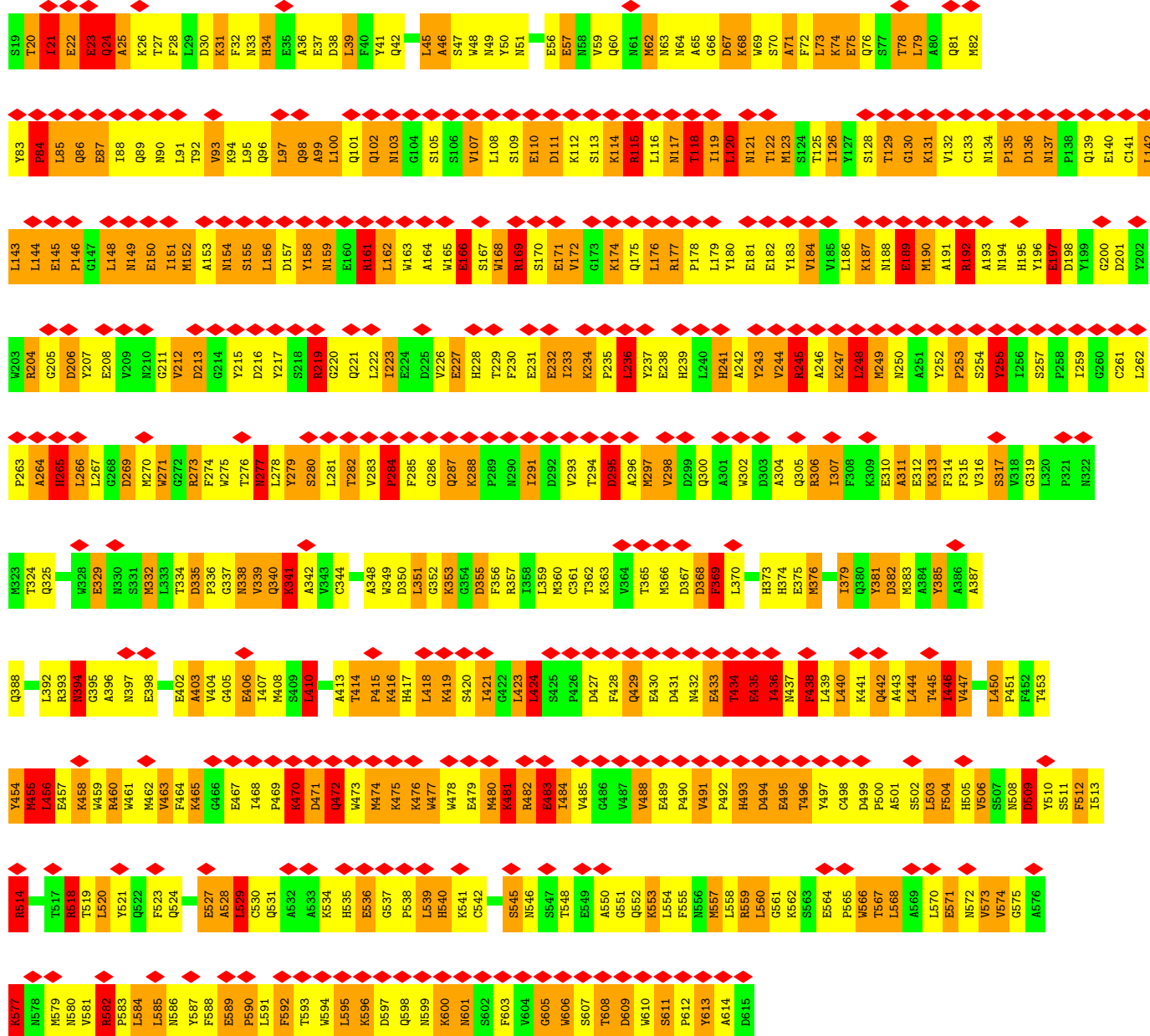
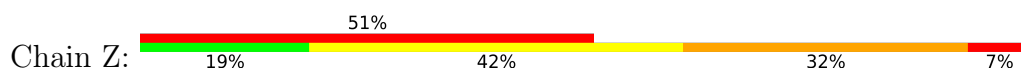


• Molecule 2: Angiotensin-converting enzyme 2





• Molecule 2: Angiotensin-converting enzyme 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50714	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 ($e^-/\text{\AA}^2$)	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	3.196	Depositor
Minimum map value	-1.695	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	359.1, 359.1, 359.1	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	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	1.00	6/8277 (0.1%)	1.35	50/11261 (0.4%)
1	B	0.98	3/8269 (0.0%)	1.34	53/11248 (0.5%)
1	C	1.00	7/8277 (0.1%)	1.34	41/11261 (0.4%)
2	T	0.84	0/5007	1.25	32/6803 (0.5%)
2	X	0.85	0/5007	1.25	32/6803 (0.5%)
2	Z	0.84	0/5007	1.25	31/6803 (0.5%)
All	All	0.94	16/39844 (0.0%)	1.31	239/54179 (0.4%)

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	26
1	B	0	27
1	C	0	27
2	T	0	15
2	X	0	15
2	Z	0	15
All	All	0	125

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	897	PRO	C-O	-6.75	1.15	1.23
1	A	316	SER	CA-CB	-6.47	1.49	1.54
1	B	715	PRO	C-O	-6.25	1.16	1.23
1	C	897	PRO	C-O	-5.92	1.16	1.23
1	A	884	SER	CA-CB	-5.85	1.45	1.54
1	B	664	PRO	C-O	-5.65	1.19	1.24
1	C	728	PRO	C-O	-5.50	1.17	1.23
1	A	728	PRO	C-O	-5.47	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1069	PRO	C-O	-5.40	1.17	1.23
1	C	109	THR	N-CA	5.37	1.49	1.46
1	C	892	PRO	C-O	-5.37	1.18	1.23
1	B	897	PRO	C-O	-5.36	1.17	1.23
1	C	899	PRO	C-O	-5.22	1.17	1.24
1	A	715	PRO	C-O	-5.08	1.17	1.23
1	A	863	PRO	C-O	-5.03	1.17	1.23
1	C	664	PRO	C-O	-5.01	1.17	1.23

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	444	LEU	N-CA-C	-9.06	100.86	114.64
2	T	444	LEU	N-CA-C	-9.04	100.90	114.64
2	Z	444	LEU	N-CA-C	-9.04	100.90	114.64
1	A	540	PHE	N-CA-C	8.98	123.58	108.13
2	X	434	THR	N-CA-C	-8.93	101.29	112.72
1	A	506	PRO	CB-CA-C	-8.77	103.42	111.40
1	B	506	PRO	CB-CA-C	-8.77	103.42	111.40
2	T	434	THR	N-CA-C	-8.76	101.28	112.93
2	Z	434	THR	N-CA-C	-8.76	101.28	112.93
1	C	506	PRO	CB-CA-C	-8.72	103.46	111.40
2	T	406	GLU	N-CA-C	-8.65	102.65	113.55
2	X	406	GLU	N-CA-C	-8.62	102.69	113.55
1	A	540	PHE	CA-CB-CG	8.61	122.41	113.80
2	Z	406	GLU	N-CA-C	-8.59	102.73	113.55
1	A	966	LEU	N-CA-C	-8.42	103.01	113.28
1	B	909	ILE	N-CA-C	-8.36	104.32	113.43
1	C	619	VAL	N-CA-C	-7.90	103.50	113.22
1	B	966	LEU	N-CA-C	-7.78	103.36	113.17
1	A	427	ASP	N-CA-C	-7.76	104.70	114.56
1	B	427	ASP	N-CA-C	-7.71	104.77	114.56
2	Z	529	LEU	N-CA-C	-7.70	103.78	113.02
2	X	529	LEU	N-CA-C	-7.68	103.81	113.02
2	T	529	LEU	N-CA-C	-7.67	103.81	113.02
2	T	135	PRO	N-CA-C	-7.51	104.96	114.35
2	Z	135	PRO	N-CA-C	-7.49	104.98	114.35
1	B	618	GLU	N-CA-C	-7.46	103.30	113.30
2	X	135	PRO	N-CA-C	-7.46	105.03	114.35
1	B	749	CYS	N-CA-C	-7.19	104.51	113.28
1	B	934	ILE	N-CA-C	-7.18	104.77	111.45
1	A	819	GLU	N-CA-C	-7.12	104.33	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	479	PRO	N-CA-C	-7.09	103.18	113.75
1	A	1121	PHE	CA-CB-CG	7.01	120.81	113.80
1	C	993	ILE	N-CA-C	-7.00	105.02	111.67
1	B	1116	THR	CB-CA-C	-6.97	100.66	111.74
1	B	1121	PHE	CA-CB-CG	6.77	120.57	113.80
1	A	759	PHE	N-CA-C	-6.76	105.10	113.15
1	C	962	LEU	N-CA-C	-6.76	105.56	113.88
1	B	759	PHE	N-CA-C	-6.71	104.22	112.88
2	Z	248	LEU	N-CA-C	-6.67	104.28	112.88
1	B	1048	HIS	CA-CB-CG	6.66	120.46	113.80
1	A	1001	LEU	N-CA-C	-6.65	105.20	113.38
2	T	248	LEU	N-CA-C	-6.64	104.32	112.88
2	X	248	LEU	N-CA-C	-6.63	104.32	112.88
1	A	302	THR	N-CA-C	-6.62	105.21	113.55
2	T	426	PRO	N-CA-C	-6.62	104.90	113.57
2	X	376	MET	N-CA-C	-6.61	105.35	113.41
1	C	524	CYS	CB-CA-C	-6.60	107.94	115.79
2	Z	376	MET	N-CA-C	-6.59	105.38	113.41
2	T	376	MET	N-CA-C	-6.58	105.38	113.41
1	C	299	THR	N-CA-C	-6.56	103.96	112.23
1	C	749	CYS	N-CA-C	-6.55	105.15	113.02
1	C	1121	PHE	CA-CB-CG	6.53	120.33	113.80
2	T	21	ILE	N-CA-C	-6.52	103.16	112.35
2	X	21	ILE	N-CA-C	-6.50	103.18	112.35
2	Z	21	ILE	N-CA-C	-6.49	103.20	112.35
1	A	524	CYS	CB-CA-C	-6.48	108.08	115.79
2	T	249	MET	N-CA-C	-6.44	105.35	113.72
2	Z	249	MET	N-CA-C	-6.43	105.36	113.72
2	X	249	MET	N-CA-C	-6.40	105.39	113.72
1	B	1118	ASP	N-CA-C	-6.39	104.70	114.16
1	A	805	ILE	N-CA-C	-6.37	107.66	113.71
2	X	514	ARG	N-CA-C	-6.34	105.53	113.20
2	Z	514	ARG	N-CA-C	-6.33	105.53	113.18
2	T	514	ARG	N-CA-C	-6.32	105.56	113.20
1	A	539	ASN	CA-C-N	-6.31	111.89	121.86
1	A	539	ASN	C-N-CA	-6.31	111.89	121.86
1	C	1048	HIS	CA-CB-CG	6.28	120.08	113.80
2	T	513	ILE	N-CA-C	-6.28	107.01	113.10
2	X	605	GLY	CA-C-O	-6.28	117.20	122.29
1	B	620	SER	N-CA-C	-6.27	104.68	113.20
2	X	513	ILE	N-CA-C	-6.27	107.02	113.10
2	Z	518	ARG	N-CA-C	-6.25	105.79	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	518	ARG	N-CA-C	-6.24	105.80	113.41
2	T	605	GLY	CA-C-O	-6.23	117.24	122.29
2	Z	513	ILE	N-CA-C	-6.23	107.06	113.10
1	A	909	ILE	N-CA-C	-6.23	106.64	113.43
1	C	1038	LYS	N-CA-C	-6.22	104.85	112.88
2	X	518	ARG	N-CA-C	-6.22	105.82	113.41
1	C	302	THR	N-CA-C	-6.21	105.36	113.12
1	A	756	TYR	N-CA-C	-6.20	105.48	113.16
1	B	965	GLN	N-CA-C	-6.19	103.42	113.19
1	C	330	PRO	CB-CA-C	-6.18	101.73	112.06
1	C	1146	ASP	N-CA-C	-6.18	105.76	113.55
2	Z	605	GLY	CA-C-O	-6.18	117.28	122.29
1	A	905	ARG	N-CA-C	-6.17	105.78	113.38
2	Z	241	HIS	N-CA-C	-6.15	105.04	112.54
2	T	241	HIS	N-CA-C	-6.13	105.06	112.54
1	B	573	ASP	N-CA-C	-6.11	105.35	114.64
1	B	761	THR	N-CA-C	-6.11	105.99	113.50
2	X	241	HIS	N-CA-C	-6.09	105.11	112.54
1	B	756	TYR	N-CA-C	-6.09	107.08	114.75
2	T	369	PHE	N-CA-C	-6.08	104.57	112.23
2	Z	369	PHE	N-CA-C	-6.08	104.58	112.23
1	B	952	VAL	N-CA-C	-6.07	105.83	112.80
1	B	849	LEU	O-C-N	6.06	125.32	120.83
1	B	995	ARG	N-CA-C	-6.06	105.38	112.89
1	B	446	SER	N-CA-C	-6.05	105.62	114.39
2	X	369	PHE	N-CA-C	-6.04	104.61	112.23
1	B	1042	PHE	N-CA-C	-6.02	104.65	112.23
2	Z	219	ARG	N-CA-C	-6.01	104.59	113.61
2	X	219	ARG	N-CA-C	-6.00	104.62	113.61
1	A	446	SER	N-CA-C	-6.00	105.70	114.39
1	C	1098	ASN	CB-CA-C	-6.00	103.67	111.40
2	T	219	ARG	N-CA-C	-5.99	104.63	113.61
1	B	1046	GLY	CA-C-O	-5.98	116.56	121.76
1	A	1044	GLY	CA-C-O	-5.96	117.81	122.52
1	C	886	TRP	N-CA-C	-5.92	105.37	112.59
2	X	512	PHE	CA-CB-CG	5.89	119.69	113.80
2	Z	512	PHE	CA-CB-CG	5.88	119.68	113.80
2	T	512	PHE	CA-CB-CG	5.86	119.66	113.80
1	A	745	ASP	N-CA-C	-5.84	106.29	113.41
1	C	656	ASN	N-CA-C	-5.82	105.94	114.39
1	A	817	PRO	N-CA-CB	-5.80	97.15	103.25
1	B	986	PRO	N-CA-C	5.79	117.77	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	664	PRO	CB-CA-C	-5.79	104.18	111.71
1	A	37	TYR	CA-C-O	-5.77	114.60	120.71
1	B	1089	PHE	CA-CB-CG	5.77	119.57	113.80
1	B	502	VAL	N-CA-C	-5.75	106.79	111.91
1	B	664	PRO	N-CA-CB	-5.75	99.70	102.92
1	A	463	PRO	N-CA-CB	-5.71	97.25	103.25
1	C	502	VAL	N-CA-C	-5.71	106.83	111.91
2	X	410	LEU	N-CA-C	-5.70	105.43	112.72
1	B	664	PRO	CB-CA-C	-5.69	107.09	111.87
1	A	502	VAL	N-CA-C	-5.69	106.85	111.91
1	A	934	ILE	N-CA-C	-5.67	104.82	111.00
1	C	965	GLN	N-CA-C	-5.67	106.41	113.15
2	Z	410	LEU	N-CA-C	-5.67	105.47	112.72
1	B	463	PRO	N-CA-CB	-5.66	97.30	103.25
2	T	66	GLY	N-CA-C	-5.66	108.12	114.40
1	C	939	PHE	N-CA-C	-5.66	105.21	111.71
2	T	410	LEU	N-CA-C	-5.66	105.48	112.72
1	C	463	PRO	N-CA-CB	-5.64	97.32	103.25
1	B	807	PRO	CB-CA-C	-5.64	104.48	111.64
2	X	66	GLY	N-CA-C	-5.63	108.15	114.40
2	Z	66	GLY	N-CA-C	-5.62	108.16	114.40
1	A	490	PRO	N-CA-C	5.62	120.93	113.40
1	C	359	SER	CA-C-O	-5.62	116.44	121.67
1	C	805	ILE	N-CA-C	-5.61	107.80	113.47
1	A	192	PHE	CB-CA-C	-5.61	102.82	111.74
2	Z	482	ARG	N-CA-C	-5.60	105.17	112.23
1	A	358	ILE	CA-C-O	-5.58	117.27	121.68
1	C	490	PRO	N-CA-C	5.58	120.88	113.40
1	B	1035	GLY	CA-C-O	-5.57	116.20	121.60
2	X	426	PRO	N-CA-C	-5.57	106.60	113.84
1	C	139	PRO	N-CA-C	-5.56	103.91	113.70
2	X	482	ARG	N-CA-C	-5.56	105.22	112.23
1	A	89	GLY	CA-C-O	-5.55	118.46	122.45
2	T	482	ARG	N-CA-C	-5.55	105.24	112.23
2	Z	381	TYR	N-CA-C	-5.54	105.15	111.14
2	T	381	TYR	N-CA-C	-5.54	105.16	111.14
2	X	381	TYR	N-CA-C	-5.53	105.16	111.14
1	B	358	ILE	CA-C-O	-5.53	117.31	121.68
1	C	623	ILE	N-CA-C	-5.53	104.18	111.09
1	A	784	GLN	N-CA-C	-5.51	106.01	114.16
1	B	1044	GLY	CA-C-O	-5.50	118.17	122.52
1	C	909	ILE	N-CA-C	-5.50	106.99	113.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	368	ASP	N-CA-C	-5.49	106.48	114.12
2	X	368	ASP	N-CA-C	-5.49	106.48	114.12
1	A	1046	GLY	CA-C-O	-5.48	117.00	121.76
1	C	761	THR	N-CA-C	-5.48	106.73	113.41
2	Z	368	ASP	N-CA-C	-5.47	106.51	114.12
1	C	137	ASN	N-CA-C	-5.46	105.42	111.71
1	B	850	ILE	N-CA-C	-5.45	107.96	113.47
1	A	621	VAL	N-CA-C	-5.45	98.01	109.34
1	A	965	GLN	N-CA-C	-5.44	105.26	112.94
1	A	1042	PHE	N-CA-C	-5.42	104.92	112.45
1	A	1064	HIS	CA-CB-CG	5.41	119.21	113.80
1	C	1119	ASN	N-CA-C	-5.41	106.46	113.16
1	C	1140	PRO	N-CA-CB	-5.39	99.23	102.79
2	T	26	LYS	N-CA-C	-5.38	105.35	112.34
1	B	951	VAL	N-CA-C	-5.37	107.57	113.43
2	X	26	LYS	N-CA-C	-5.37	105.36	112.34
1	B	340	GLU	N-CA-C	-5.35	106.45	112.87
2	Z	26	LYS	N-CA-C	-5.34	105.39	112.34
1	C	340	GLU	N-CA-C	-5.33	106.48	112.87
2	X	166	GLU	N-CA-C	-5.32	105.93	112.90
1	B	547	GLY	CA-C-O	-5.32	117.80	122.16
1	A	901	GLN	N-CA-C	-5.31	105.94	112.90
2	T	166	GLU	N-CA-C	-5.30	105.95	112.90
1	C	888	PHE	CA-CB-CG	5.29	119.09	113.80
1	C	753	LEU	N-CA-C	-5.28	107.38	113.88
2	Z	166	GLU	N-CA-C	-5.28	105.99	112.90
1	A	340	GLU	N-CA-C	-5.28	106.54	112.87
2	Z	566	TRP	N-CA-C	-5.28	105.53	111.28
1	C	990	GLU	N-CA-C	-5.27	105.67	112.68
2	X	438	PHE	N-CA-C	-5.27	106.11	112.54
1	B	529	SER	CB-CA-C	-5.26	109.49	117.07
2	X	566	TRP	N-CA-C	-5.26	105.55	111.28
1	A	942	PRO	N-CA-CB	-5.25	97.74	103.25
2	T	566	TRP	N-CA-C	-5.25	105.56	111.28
1	C	872	GLN	N-CA-C	-5.24	106.73	113.23
2	T	438	PHE	N-CA-C	-5.24	106.15	112.54
2	X	481	LYS	N-CA-C	-5.24	106.83	113.43
2	Z	438	PHE	N-CA-C	-5.24	106.15	112.54
2	Z	481	LYS	N-CA-C	-5.24	106.83	113.43
1	B	540	PHE	N-CA-C	5.24	115.96	108.74
2	Z	367	ASP	N-CA-C	-5.23	106.29	113.30
2	T	481	LYS	N-CA-C	-5.23	106.84	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	485	PRO	N-CA-CB	-5.21	97.78	103.25
2	T	367	ASP	N-CA-C	-5.20	106.33	113.30
1	B	886	TRP	N-CA-C	-5.20	106.25	112.59
1	B	807	PRO	N-CA-C	5.20	119.73	111.26
1	B	1106	GLN	N-CA-C	-5.19	103.68	110.53
1	B	1038	LYS	N-CA-C	-5.18	106.36	113.30
2	X	367	ASP	N-CA-C	-5.18	106.36	113.30
1	B	529	SER	O-C-N	5.17	125.34	121.47
1	B	218	GLY	CA-C-O	-5.15	118.45	122.52
1	A	986	PRO	N-CA-C	5.15	116.98	110.70
1	A	947	LYS	N-CA-C	-5.14	107.18	113.50
1	B	862	PRO	N-CA-CB	-5.14	100.55	103.22
1	B	817	PRO	N-CA-CB	-5.13	98.35	103.48
2	X	613	TYR	N-CA-C	-5.12	107.09	113.55
1	A	55	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	915	VAL	N-CA-C	-5.12	105.53	113.16
2	T	284	PRO	N-CA-CB	-5.12	97.88	103.25
1	B	1119	ASN	N-CA-C	-5.11	105.41	113.02
1	A	368	LEU	N-CA-C	-5.10	105.90	111.82
1	B	368	LEU	N-CA-C	-5.10	105.90	111.82
2	Z	284	PRO	N-CA-CB	-5.10	97.89	103.25
1	A	468	ILE	N-CA-C	-5.09	108.32	113.47
1	C	368	LEU	N-CA-C	-5.09	105.91	111.82
2	X	284	PRO	N-CA-CB	-5.09	97.91	103.25
1	A	275	PHE	CA-CB-CG	5.08	118.88	113.80
1	B	468	ILE	N-CA-C	-5.08	108.34	113.47
2	T	613	TYR	N-CA-C	-5.07	107.16	113.55
1	A	1000	ARG	N-CA-C	-5.07	107.08	114.12
1	A	1098	ASN	CB-CA-C	-5.07	103.42	111.17
1	C	468	ILE	N-CA-C	-5.06	108.36	113.47
2	Z	613	TYR	N-CA-C	-5.05	107.18	113.55
1	C	1112	PRO	N-CA-C	5.04	118.80	111.03
1	B	751	ASN	N-CA-C	-5.03	107.70	113.88
1	C	759	PHE	N-CA-C	-5.03	108.18	114.56
2	T	557	MET	N-CA-C	-5.03	106.50	113.18
2	Z	557	MET	N-CA-C	-5.02	106.51	113.18
1	C	988	GLU	N-CA-C	-5.01	107.82	114.04
2	X	557	MET	N-CA-C	-5.01	106.52	113.18
1	A	622	ALA	N-CA-C	-5.01	99.51	108.13
1	C	1046	GLY	CA-C-O	-5.00	116.49	120.79
1	A	945	LEU	N-CA-C	-5.00	106.40	113.20

There are no chirality outliers.

All (125) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1000	ARG	Sidechain
1	A	1014	ARG	Sidechain
1	A	1019	ARG	Sidechain
1	A	1039	ARG	Sidechain
1	A	1091	ARG	Sidechain
1	A	213	ARG	Sidechain
1	A	236	ARG	Sidechain
1	A	273	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	454	ARG	Sidechain
1	A	457	ARG	Sidechain
1	A	466	ARG	Sidechain
1	A	497	ARG	Sidechain
1	A	527	LYS	Mainchain
1	A	566	ARG	Sidechain
1	A	576	ARG	Sidechain
1	A	645	ARG	Sidechain
1	A	765	ARG	Sidechain
1	A	847	ARG	Sidechain
1	A	983	ARG	Sidechain
1	A	995	ARG	Sidechain
1	B	1014	ARG	Sidechain
1	B	1019	ARG	Sidechain
1	B	102	ARG	Sidechain
1	B	1039	ARG	Sidechain
1	B	1091	ARG	Sidechain
1	B	1107	ARG	Sidechain
1	B	190	ARG	Sidechain
1	B	236	ARG	Sidechain
1	B	319	ARG	Sidechain
1	B	328	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	454	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	457	ARG	Sidechain
1	B	466	ARG	Sidechain
1	B	497	ARG	Sidechain
1	B	566	ARG	Sidechain
1	B	576	ARG	Sidechain
1	B	645	ARG	Sidechain
1	B	815	ARG	Sidechain
1	B	847	ARG	Sidechain
1	B	905	ARG	Sidechain
1	B	983	ARG	Sidechain
1	B	995	ARG	Sidechain
1	C	1000	ARG	Sidechain
1	C	1014	ARG	Sidechain
1	C	1019	ARG	Sidechain
1	C	102	ARG	Sidechain
1	C	1091	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	328	ARG	Sidechain
1	C	34	ARG	Sidechain
1	C	346	ARG	Sidechain
1	C	355	ARG	Sidechain
1	C	357	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	983	ARG	Sidechain
1	C	995	ARG	Sidechain
2	T	115	ARG	Sidechain
2	T	161	ARG	Sidechain
2	T	169	ARG	Sidechain
2	T	177	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	T	192	ARG	Sidechain
2	T	204	ARG	Sidechain
2	T	219	ARG	Sidechain
2	T	245	ARG	Sidechain
2	T	273	ARG	Sidechain
2	T	393	ARG	Sidechain
2	T	460	ARG	Sidechain
2	T	514	ARG	Sidechain
2	T	518	ARG	Sidechain
2	T	559	ARG	Sidechain
2	T	582	ARG	Sidechain
2	X	115	ARG	Sidechain
2	X	161	ARG	Sidechain
2	X	169	ARG	Sidechain
2	X	177	ARG	Sidechain
2	X	192	ARG	Sidechain
2	X	204	ARG	Sidechain
2	X	219	ARG	Sidechain
2	X	245	ARG	Sidechain
2	X	273	ARG	Sidechain
2	X	393	ARG	Sidechain
2	X	460	ARG	Sidechain
2	X	514	ARG	Sidechain
2	X	518	ARG	Sidechain
2	X	559	ARG	Sidechain
2	X	582	ARG	Sidechain
2	Z	115	ARG	Sidechain
2	Z	161	ARG	Sidechain
2	Z	169	ARG	Sidechain
2	Z	177	ARG	Sidechain
2	Z	192	ARG	Sidechain
2	Z	204	ARG	Sidechain
2	Z	219	ARG	Sidechain
2	Z	245	ARG	Sidechain
2	Z	273	ARG	Sidechain
2	Z	393	ARG	Sidechain
2	Z	460	ARG	Sidechain
2	Z	514	ARG	Sidechain
2	Z	518	ARG	Sidechain
2	Z	559	ARG	Sidechain
2	Z	582	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8083	0	7912	580	0
1	B	8076	0	7900	535	0
1	C	8083	0	7910	565	0
2	T	4870	0	4643	530	0
2	X	4870	0	4643	529	0
2	Z	4870	0	4643	505	0
All	All	38852	0	37651	3192	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 42.

All (3192) 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:476:GLY:HA3	1:A:484:GLY:HA3	1.14	1.12
2:X:145:GLU:HB3	2:X:146:PRO:HD3	1.43	1.00
2:T:145:GLU:HB3	2:T:146:PRO:HD3	1.43	0.98
1:A:361:CYS:H	1:A:523:VAL:HA	1.28	0.98
2:Z:145:GLU:HB3	2:Z:146:PRO:HD3	1.44	0.98
1:A:186:PHE:HE1	1:A:187:LYS:HZ1	0.96	0.95
1:B:361:CYS:H	1:B:523:VAL:HA	1.28	0.94
1:A:336:CYS:HB3	1:A:363:ALA:HA	1.50	0.93
2:T:133:CYS:HA	2:T:141:CYS:HA	1.51	0.93
1:A:381:GLY:HA3	1:A:429:PHE:HA	1.49	0.92
2:Z:133:CYS:HA	2:Z:141:CYS:HA	1.51	0.92
1:A:482:GLY:HA3	1:A:487:CYS:HA	1.50	0.92
1:B:381:GLY:HA3	1:B:429:PHE:HA	1.50	0.92
1:C:357:ARG:HA	1:C:396:TYR:HA	1.52	0.91
1:B:336:CYS:HB3	1:B:363:ALA:HA	1.50	0.91
2:X:133:CYS:HA	2:X:141:CYS:HA	1.51	0.90
1:A:357:ARG:HA	1:A:396:TYR:HA	1.52	0.90
1:B:454:ARG:HG2	1:B:490:PRO:HB2	1.53	0.90
1:A:482:GLY:CA	1:A:487:CYS:HA	2.01	0.90
1:B:357:ARG:HA	1:B:396:TYR:HA	1.52	0.89
2:T:70:SER:HA	2:T:73:LEU:HD12	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:491:VAL:HG22	2:X:492:PRO:HD2	1.54	0.89
1:A:188:ASN:HA	1:A:209:PRO:HA	1.52	0.89
2:X:70:SER:HA	2:X:73:LEU:HD12	1.54	0.88
2:Z:491:VAL:HG22	2:Z:492:PRO:HD2	1.54	0.88
2:T:491:VAL:HG22	2:T:492:PRO:HD2	1.54	0.87
1:C:421:TYR:HB3	1:C:457:ARG:HB2	1.56	0.87
2:Z:70:SER:HA	2:Z:73:LEU:HD12	1.54	0.87
1:A:476:GLY:HA3	1:A:484:GLY:CA	2.04	0.87
1:B:24:THR:HB	1:B:80:ASP:N	1.90	0.86
1:A:393:THR:H	1:A:516:LEU:HD13	1.41	0.86
2:X:144:LEU:HA	2:X:148:LEU:HB2	1.58	0.85
2:Z:144:LEU:HA	2:Z:148:LEU:HB2	1.58	0.85
2:T:144:LEU:HA	2:T:148:LEU:HB2	1.57	0.85
1:B:393:THR:H	1:B:516:LEU:HD13	1.41	0.85
1:C:62:VAL:HG11	1:C:215:PHE:HZ	1.42	0.85
1:C:478:LYS:HB3	1:C:479:PRO:HD2	1.59	0.85
1:C:480:CYS:HB2	1:C:483:LYS:HG2	1.59	0.84
1:A:186:PHE:HE1	1:A:187:LYS:NZ	1.76	0.84
2:Z:161:ARG:HB3	2:Z:265:HIS:HB2	1.60	0.84
2:X:164:ALA:HA	2:X:167:SER:HB2	1.60	0.83
2:X:161:ARG:HB3	2:X:265:HIS:HB2	1.60	0.83
1:B:478:LYS:H	1:B:481:LYS:HA	1.42	0.83
1:C:393:THR:H	1:C:516:LEU:HD13	1.41	0.83
2:X:413:ALA:HA	2:X:418:LEU:HD21	1.61	0.82
1:C:353:TRP:CD1	1:C:353:TRP:H	1.97	0.82
1:A:422:ASN:HD21	1:A:454:ARG:H	1.26	0.82
1:C:353:TRP:H	1:C:353:TRP:HD1	1.27	0.82
2:Z:413:ALA:HA	2:Z:418:LEU:HD21	1.61	0.82
1:B:519:ALA:HB1	1:B:520:PRO:HD2	1.62	0.81
2:Z:164:ALA:HA	2:Z:167:SER:HB2	1.60	0.81
1:A:381:GLY:HA3	1:A:429:PHE:CA	2.10	0.81
2:T:164:ALA:HA	2:T:167:SER:HB2	1.60	0.81
1:B:353:TRP:HD1	1:B:353:TRP:H	1.27	0.81
1:B:353:TRP:H	1:B:353:TRP:CD1	1.97	0.81
2:T:161:ARG:HB3	2:T:265:HIS:HB2	1.60	0.81
1:B:381:GLY:HA3	1:B:429:PHE:CA	2.11	0.81
1:C:611:TYR:HE2	1:C:633:ARG:HD3	1.46	0.81
1:A:519:ALA:HB1	1:A:520:PRO:HD2	1.62	0.80
2:T:413:ALA:HA	2:T:418:LEU:HD21	1.61	0.80
1:A:193:VAL:HG23	1:A:204:TYR:HB2	1.63	0.80
1:A:353:TRP:CD1	1:A:353:TRP:H	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:ALA:HB1	1:C:520:PRO:HD2	1.62	0.80
1:A:353:TRP:H	1:A:353:TRP:HD1	1.28	0.79
1:B:422:ASN:HD21	1:B:454:ARG:H	1.26	0.79
1:A:482:GLY:HA3	1:A:487:CYS:CA	2.11	0.79
2:X:336:PRO:HB3	2:X:342:ALA:HB3	1.64	0.79
1:A:476:GLY:CA	1:A:484:GLY:HA3	2.05	0.79
2:X:134:ASN:HB2	2:X:140:GLU:HB2	1.65	0.79
2:T:336:PRO:HB3	2:T:342:ALA:HB3	1.64	0.79
2:Z:134:ASN:HB2	2:Z:140:GLU:HB2	1.65	0.79
1:B:558:PHE:HZ	1:B:574:ALA:HB3	1.47	0.78
2:Z:336:PRO:HB3	2:Z:342:ALA:HB3	1.64	0.77
2:T:134:ASN:HB2	2:T:140:GLU:HB2	1.65	0.77
1:B:131:CYS:HA	1:B:166:CYS:HA	1.66	0.77
1:C:111:ASP:HA	1:C:135:PHE:HE1	1.49	0.77
1:B:473:TYR:HB2	1:B:490:PRO:HD3	1.67	0.77
1:C:331:ASN:HA	1:C:579:GLN:HG3	1.67	0.77
1:C:576:ARG:HB2	1:C:583:ILE:HD13	1.67	0.77
1:A:319:ARG:HG2	1:A:632:TRP:HE3	1.48	0.77
1:A:117:LEU:HB2	1:A:232:ILE:HD13	1.67	0.77
1:A:847:ARG:NH1	1:C:556:LYS:HB3	2.00	0.77
1:A:371:PHE:HB2	1:A:374:PHE:HD2	1.50	0.76
1:C:371:PHE:HB2	1:C:374:PHE:HD2	1.50	0.76
1:B:24:THR:HG23	1:B:66:HIS:H	1.50	0.76
2:X:336:PRO:HB3	2:X:342:ALA:CB	2.16	0.76
2:Z:336:PRO:HB3	2:Z:342:ALA:CB	2.16	0.76
2:X:611:SER:HB2	2:X:614:ALA:HB3	1.68	0.76
2:Z:611:SER:HB2	2:Z:614:ALA:HB3	1.68	0.76
1:A:478:LYS:O	1:A:483:LYS:HA	1.86	0.76
2:T:135:PRO:HD3	2:T:163:TRP:CZ2	2.20	0.76
2:Z:150:GLU:O	2:Z:154:ASN:HB2	1.86	0.76
2:X:81:GLN:HG3	2:X:101:GLN:HG2	1.69	0.76
2:T:150:GLU:O	2:T:154:ASN:HB2	1.86	0.75
2:X:135:PRO:HD3	2:X:163:TRP:CZ2	2.20	0.75
1:C:434:ILE:O	1:C:509:VAL:HA	1.86	0.75
1:C:482:GLY:H	1:C:483:LYS:HE3	1.50	0.75
2:X:150:GLU:O	2:X:154:ASN:HB2	1.86	0.75
2:Z:553:LYS:HE2	2:Z:573:VAL:HA	1.69	0.75
1:C:118:LEU:HB2	1:C:133:PHE:HE2	1.51	0.75
2:T:336:PRO:HB3	2:T:342:ALA:CB	2.16	0.75
2:Z:135:PRO:HD3	2:Z:163:TRP:CZ2	2.20	0.75
1:C:25:THR:HG23	1:C:80:ASP:HB3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1105:THR:HG23	1:C:1111:GLU:H	1.50	0.75
1:C:357:ARG:NH2	1:C:358:ILE:O	2.20	0.75
1:C:483:LYS:HA	1:C:488:TYR:HD2	1.52	0.75
2:Z:81:GLN:HG3	2:Z:101:GLN:HG2	1.69	0.75
1:B:429:PHE:HD1	1:B:430:THR:H	1.33	0.75
1:B:489:PHE:CZ	1:B:491:LEU:HB2	2.22	0.74
1:B:24:THR:CG2	1:B:65:PHE:HB3	2.16	0.74
1:A:24:THR:HA	1:A:80:ASP:HB3	1.69	0.74
1:B:984:LEU:HD23	1:B:985:ASP:H	1.52	0.74
1:A:396:TYR:HD1	1:A:396:TYR:H	1.35	0.74
1:B:371:PHE:HB2	1:B:374:PHE:HD2	1.50	0.74
1:C:382:VAL:HG21	1:C:431:GLY:HA2	1.68	0.74
1:C:401:VAL:HG21	1:C:442:ASP:OD2	1.87	0.74
1:C:522:THR:HG23	1:C:523:VAL:H	1.53	0.74
2:Z:404:VAL:HG21	2:Z:558:LEU:HD11	1.69	0.74
1:A:522:THR:HG23	1:A:523:VAL:H	1.53	0.74
2:T:611:SER:HB2	2:T:614:ALA:HB3	1.68	0.74
1:B:371:PHE:HB2	1:B:374:PHE:CD2	2.23	0.74
1:B:396:TYR:HD1	1:B:396:TYR:H	1.35	0.74
1:C:62:VAL:HG11	1:C:215:PHE:CZ	2.22	0.74
2:T:81:GLN:HG3	2:T:101:GLN:HG2	1.69	0.74
1:A:112:SER:HA	1:A:133:PHE:HA	1.70	0.73
1:A:130:VAL:HG12	1:A:168:PHE:HD1	1.53	0.73
1:A:429:PHE:HD1	1:A:430:THR:H	1.33	0.73
1:C:210:ILE:HG22	1:C:216:PRO:HG2	1.69	0.73
1:B:456:PHE:CE1	1:B:490:PRO:HA	2.23	0.73
1:C:362:VAL:HG13	1:C:525:GLY:HA2	1.70	0.73
2:T:553:LYS:HE2	2:T:573:VAL:HA	1.69	0.73
1:B:522:THR:HG23	1:B:523:VAL:H	1.53	0.73
1:A:271:GLN:HG2	1:A:272:PRO:HD2	1.71	0.73
1:A:371:PHE:HB2	1:A:374:PHE:CD2	2.23	0.73
1:C:132:GLU:O	1:C:133:PHE:HB2	1.88	0.73
1:C:458:LYS:HE2	1:C:474:GLN:HE22	1.52	0.73
1:C:534:LYS:O	1:C:536:LYS:HG2	1.89	0.72
1:C:1143:LEU:O	1:C:1146:ASP:HB2	1.89	0.72
2:X:553:LYS:HE2	2:X:573:VAL:HA	1.68	0.72
1:A:620:SER:HB3	1:A:623:ILE:HA	1.70	0.72
2:X:133:CYS:HA	2:X:141:CYS:CA	2.19	0.72
2:Z:263:PRO:HB2	2:Z:265:HIS:HE1	1.54	0.72
2:T:404:VAL:HG21	2:T:558:LEU:HD11	1.69	0.72
1:B:329:PHE:CD2	1:B:330:PRO:HD3	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:LEU:HD21	1:B:1141:LEU:HD23	1.71	0.72
1:C:371:PHE:HB2	1:C:374:PHE:CD2	2.23	0.72
2:Z:133:CYS:HA	2:Z:141:CYS:CA	2.19	0.72
2:T:478:TRP:HE1	2:T:493:HIS:HB2	1.55	0.72
2:X:404:VAL:HG21	2:X:558:LEU:HD11	1.69	0.72
1:A:847:ARG:HH12	1:C:556:LYS:HE2	1.55	0.72
1:B:456:PHE:CZ	1:B:488:TYR:HB3	2.24	0.72
1:C:396:TYR:HD1	1:C:396:TYR:H	1.34	0.72
2:T:133:CYS:HA	2:T:141:CYS:CA	2.19	0.72
2:Z:456:LEU:HD12	2:Z:477:TRP:HH2	1.55	0.72
2:X:263:PRO:HB2	2:X:265:HIS:HE1	1.54	0.71
2:Z:478:TRP:HE1	2:Z:493:HIS:HB2	1.55	0.71
2:T:263:PRO:HB2	2:T:265:HIS:HE1	1.54	0.71
2:Z:144:LEU:HD12	2:Z:148:LEU:HB3	1.72	0.71
1:A:190:ARG:HB3	1:A:192:PHE:CE1	2.25	0.71
2:X:470:LYS:HA	2:X:473:TRP:CD2	2.25	0.71
2:Z:143:LEU:HD22	2:Z:144:LEU:H	1.55	0.71
1:C:482:GLY:N	1:C:483:LYS:HE3	2.06	0.71
2:X:144:LEU:HD12	2:X:148:LEU:HB3	1.72	0.71
1:A:540:PHE:HB3	1:A:547:GLY:C	2.15	0.71
1:C:536:LYS:O	1:C:537:CYS:C	2.33	0.71
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.39	0.71
2:T:470:LYS:HA	2:T:473:TRP:CD2	2.25	0.71
2:X:478:TRP:HE1	2:X:493:HIS:HB2	1.55	0.71
2:Z:470:LYS:HA	2:Z:473:TRP:CD2	2.25	0.71
1:C:556:LYS:HD2	1:C:583:ILE:CG2	2.21	0.71
2:T:72:PHE:O	2:T:76:GLN:HG2	1.91	0.71
2:T:176:LEU:HA	2:T:179:LEU:HB2	1.73	0.71
2:T:456:LEU:HD12	2:T:477:TRP:HH2	1.55	0.71
2:X:456:LEU:HD12	2:X:477:TRP:HH2	1.55	0.71
1:A:403:LYS:HG3	1:A:405:ASN:H	1.56	0.70
2:T:115:ARG:HH12	2:T:118:THR:HB	1.56	0.70
2:X:115:ARG:HH12	2:X:118:THR:HB	1.56	0.70
2:X:176:LEU:HA	2:X:179:LEU:HB2	1.73	0.70
1:C:611:TYR:CE2	1:C:633:ARG:HD3	2.26	0.70
2:T:257:SER:HB3	2:T:610:TRP:CE2	2.26	0.70
2:Z:115:ARG:HH12	2:Z:118:THR:HB	1.56	0.70
1:B:130:VAL:HG11	1:B:230:ILE:HG21	1.73	0.70
1:C:403:LYS:HG3	1:C:405:ASN:H	1.56	0.70
2:T:241:HIS:O	2:T:245:ARG:HB2	1.91	0.70
1:C:462:LYS:H	1:C:462:LYS:HE2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1144:GLU:C	1:A:1146:ASP:H	2.00	0.70
1:B:361:CYS:N	1:B:523:VAL:HA	2.06	0.70
2:Z:257:SER:HB3	2:Z:610:TRP:CE2	2.26	0.70
1:A:333:THR:O	1:A:334:ASN:C	2.35	0.70
1:C:25:THR:O	1:C:26:GLN:HB2	1.90	0.70
2:T:144:LEU:HA	2:T:148:LEU:CB	2.22	0.70
1:C:1006:THR:O	1:C:1010:GLN:HG2	1.92	0.70
2:T:129:THR:O	2:T:131:LYS:HG2	1.92	0.70
2:X:72:PHE:O	2:X:76:GLN:HG2	1.91	0.70
2:X:143:LEU:HD22	2:X:144:LEU:H	1.55	0.70
2:X:257:SER:HB3	2:X:610:TRP:CE2	2.26	0.70
1:A:201:PHE:HD2	1:A:203:ILE:HD11	1.56	0.69
1:B:120:VAL:HG22	1:B:121:ASN:H	1.56	0.69
2:T:144:LEU:HD12	2:T:148:LEU:HB3	1.74	0.69
2:Z:538:PRO:HB2	2:Z:541:LYS:HG3	1.74	0.69
2:Z:241:HIS:O	2:Z:245:ARG:HB2	1.92	0.69
1:C:833:PHE:CG	1:C:836:GLN:HA	2.27	0.69
2:X:573:VAL:O	2:X:574:VAL:C	2.35	0.69
1:A:474:GLN:HA	1:A:483:LYS:HG3	1.73	0.69
1:B:381:GLY:CA	1:B:429:PHE:HA	2.22	0.69
1:C:119:ILE:H	1:C:119:ILE:HD12	1.56	0.69
1:C:483:LYS:HD2	1:C:484:GLY:N	2.07	0.69
1:B:189:LEU:HB2	1:B:210:ILE:HG12	1.73	0.69
1:C:142:ASP:HB3	1:C:241:LEU:O	1.93	0.69
2:Z:72:PHE:O	2:Z:76:GLN:HG2	1.91	0.69
1:A:86:PHE:HB2	1:A:235:THR:C	2.17	0.69
1:A:361:CYS:N	1:A:523:VAL:HA	2.06	0.69
1:C:478:LYS:HB2	1:C:484:GLY:HA2	1.73	0.69
2:T:538:PRO:HB2	2:T:541:LYS:HG3	1.74	0.69
1:A:834:ILE:HD11	1:C:613:GLY:HA2	1.75	0.69
1:A:1116:THR:HG22	1:A:1117:THR:H	1.56	0.69
2:X:241:HIS:O	2:X:245:ARG:HB2	1.91	0.69
2:Z:176:LEU:HA	2:Z:179:LEU:HB2	1.73	0.69
2:Z:288:LYS:HD2	2:Z:433:GLU:HB2	1.74	0.69
2:Z:573:VAL:O	2:Z:574:VAL:C	2.35	0.69
1:A:201:PHE:CD2	1:A:203:ILE:HD11	2.28	0.69
1:B:378:LYS:HG2	1:B:380:TYR:CE2	2.28	0.69
1:C:825:LYS:HE2	1:C:939:PHE:HA	1.72	0.69
2:X:538:PRO:HB2	2:X:541:LYS:HG3	1.74	0.69
1:A:462:LYS:H	1:A:462:LYS:HE2	1.58	0.69
1:A:540:PHE:O	1:A:546:THR:HA	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:CYS:HB3	1:C:363:ALA:HA	1.75	0.69
1:C:128:ILE:O	1:C:129:LYS:HB3	1.93	0.68
2:Z:340:GLN:O	2:Z:341:LYS:C	2.37	0.68
1:A:973:ILE:HG13	1:A:984:LEU:HD11	1.75	0.68
2:T:573:VAL:O	2:T:574:VAL:C	2.35	0.68
2:Z:144:LEU:HA	2:Z:148:LEU:CB	2.24	0.68
1:B:403:LYS:HG3	1:B:405:ASN:H	1.57	0.68
2:X:293:VAL:HG22	2:X:424:LEU:HD23	1.75	0.68
2:X:340:GLN:O	2:X:341:LYS:C	2.37	0.68
2:Z:22:GLU:O	2:Z:24:GLN:N	2.24	0.68
1:B:321:GLN:O	1:B:323:THR:N	2.27	0.68
1:C:130:VAL:HG13	1:C:168:PHE:HB3	1.75	0.68
1:C:214:ASP:O	1:C:215:PHE:C	2.34	0.68
1:A:349:SER:O	1:A:351:TYR:N	2.27	0.68
1:A:575:VAL:HG22	1:A:586:ILE:HD11	1.74	0.68
1:A:378:LYS:HG2	1:A:380:TYR:CE2	2.28	0.68
1:B:462:LYS:HE2	1:B:462:LYS:H	1.58	0.68
1:C:121:ASN:HA	1:C:126:VAL:HG13	1.76	0.68
1:B:853:GLN:O	1:B:854:LYS:C	2.37	0.68
2:T:84:PRO:HB2	2:T:87:GLU:OE2	1.94	0.68
1:A:102:ARG:HG3	1:A:141:LEU:HD22	1.75	0.68
1:C:349:SER:O	1:C:351:TYR:N	2.27	0.68
1:B:349:SER:O	1:B:351:TYR:N	2.27	0.68
2:X:259:ILE:HG22	2:X:603:PHE:CD2	2.29	0.68
1:A:540:PHE:CE2	1:A:551:LEU:HD21	2.29	0.67
2:X:144:LEU:HA	2:X:148:LEU:CB	2.24	0.67
1:C:358:ILE:HG21	1:C:523:VAL:HG11	1.76	0.67
1:C:940:SER:O	1:C:941:THR:C	2.37	0.67
2:Z:84:PRO:HB2	2:Z:87:GLU:OE2	1.94	0.67
2:Z:259:ILE:HG22	2:Z:603:PHE:CD2	2.29	0.67
1:A:540:PHE:HE2	1:A:551:LEU:HD21	1.59	0.67
2:X:84:PRO:HB2	2:X:87:GLU:OE2	1.94	0.67
2:Z:189:GLU:HA	2:Z:192:ARG:HE	1.59	0.67
1:A:632:TRP:O	1:A:633:ARG:C	2.38	0.67
2:T:259:ILE:HG22	2:T:603:PHE:CD2	2.29	0.67
1:B:853:GLN:HB3	1:B:858:LEU:HD12	1.75	0.67
1:B:1111:GLU:HG3	1:B:1111:GLU:O	1.94	0.67
2:Z:462:MET:O	2:Z:463:VAL:C	2.38	0.67
2:T:143:LEU:HD22	2:T:144:LEU:H	1.58	0.67
2:T:340:GLN:O	2:T:341:LYS:C	2.37	0.67
1:A:128:ILE:HD13	1:A:228:LEU:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:GLY:CA	1:A:429:PHE:HA	2.22	0.67
2:T:285:PHE:C	2:T:287:GLN:H	2.03	0.66
2:T:462:MET:O	2:T:463:VAL:C	2.38	0.66
1:A:445:HIS:CD2	1:A:498:PRO:HG3	2.31	0.66
1:B:445:HIS:CD2	1:B:498:PRO:HG3	2.30	0.66
1:A:373:PRO:O	1:A:374:PHE:C	2.39	0.66
1:A:386:LYS:HA	1:A:389:ASP:CG	2.21	0.66
1:B:542:PHE:HD1	1:B:578:PRO:HD3	1.60	0.66
1:C:545:LEU:HD11	1:C:575:VAL:HG21	1.76	0.66
2:X:189:GLU:HA	2:X:192:ARG:HE	1.59	0.66
2:Z:285:PHE:C	2:Z:287:GLN:H	2.03	0.66
1:A:188:ASN:HD22	1:A:190:ARG:HG3	1.60	0.66
1:B:463:PRO:O	1:B:464:PHE:HB2	1.95	0.66
1:C:386:LYS:HA	1:C:389:ASP:CG	2.21	0.66
1:C:556:LYS:HD3	1:C:558:PHE:CE1	2.31	0.66
1:A:463:PRO:O	1:A:464:PHE:HB2	1.95	0.66
1:C:121:ASN:ND2	1:C:126:VAL:HG22	2.11	0.66
1:A:86:PHE:CE1	1:A:234:ILE:HD11	2.31	0.66
1:C:118:LEU:HB2	1:C:133:PHE:CE2	2.30	0.66
1:A:64:TRP:O	1:A:65:PHE:C	2.39	0.66
1:B:373:PRO:O	1:B:374:PHE:C	2.38	0.66
2:X:168:TRP:HA	2:X:172:VAL:HG23	1.78	0.66
1:A:107:GLY:CA	1:A:234:ILE:HA	2.25	0.66
1:C:463:PRO:O	1:C:464:PHE:HB2	1.95	0.66
1:C:556:LYS:CD	1:C:583:ILE:HG21	2.25	0.66
1:C:1105:THR:CG2	1:C:1111:GLU:H	2.09	0.66
2:T:119:ILE:O	2:T:120:LEU:C	2.39	0.66
1:A:103:GLY:H	1:A:240:LEU:HB2	1.60	0.66
1:A:644:THR:HG22	1:A:645:ARG:H	1.60	0.66
1:B:328:ARG:O	1:B:329:PHE:HB3	1.95	0.66
1:C:849:LEU:O	1:C:850:ILE:C	2.39	0.66
2:Z:168:TRP:HA	2:Z:172:VAL:HG23	1.78	0.66
1:B:321:GLN:N	1:B:322:PRO:HD2	2.11	0.66
1:C:853:GLN:O	1:C:854:LYS:C	2.39	0.66
2:T:189:GLU:HA	2:T:192:ARG:HE	1.59	0.66
2:X:119:ILE:O	2:X:120:LEU:C	2.39	0.66
2:Z:119:ILE:O	2:Z:120:LEU:C	2.39	0.66
1:C:391:CYS:HB3	1:C:524:CYS:HA	1.78	0.65
2:T:351:LEU:H	2:T:351:LEU:HD12	1.61	0.65
2:X:91:LEU:HD23	2:X:94:LYS:HE2	1.78	0.65
2:X:351:LEU:H	2:X:351:LEU:HD12	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:462:MET:O	2:X:463:VAL:C	2.38	0.65
1:A:111:ASP:HA	1:A:134:GLN:HE22	1.60	0.65
1:A:118:LEU:O	1:A:119:ILE:C	2.38	0.65
1:B:386:LYS:HA	1:B:389:ASP:CG	2.21	0.65
1:A:116:SER:N	1:A:132:GLU:HB3	2.11	0.65
1:B:391:CYS:HB3	1:B:524:CYS:HA	1.78	0.65
1:C:610:LEU:HD23	1:C:612:GLN:HG2	1.77	0.65
1:A:849:LEU:HG	1:A:851:CYS:H	1.61	0.65
1:C:350:VAL:C	1:C:352:ALA:H	2.04	0.65
2:X:285:PHE:C	2:X:287:GLN:H	2.05	0.65
1:B:95:THR:HB	1:B:186:PHE:HB3	1.79	0.65
1:B:127:PHE:HA	1:B:171:VAL:HG13	1.77	0.65
1:C:130:VAL:CG1	1:C:168:PHE:HB3	2.26	0.65
1:A:20:ASN:C	1:A:22:ILE:H	2.04	0.65
1:B:128:ILE:HG21	1:B:228:LEU:HD21	1.79	0.65
1:B:989:ALA:C	1:B:991:VAL:H	2.05	0.65
1:C:822:LEU:HD22	1:C:945:LEU:HD21	1.79	0.65
2:T:22:GLU:O	2:T:24:GLN:N	2.24	0.65
1:A:751:ASN:HA	1:A:754:LEU:HD22	1.79	0.65
2:Z:453:THR:HA	2:Z:512:PHE:HE2	1.62	0.65
1:A:138:ASP:C	1:A:140:PHE:H	2.05	0.65
2:T:453:THR:HA	2:T:512:PHE:HE2	1.62	0.65
2:Z:144:LEU:O	2:Z:145:GLU:C	2.40	0.65
1:B:226:VAL:HG22	1:B:227:ASP:H	1.61	0.65
2:T:91:LEU:HD23	2:T:94:LYS:HE2	1.78	0.65
2:T:135:PRO:HD3	2:T:163:TRP:CE2	2.32	0.65
2:Z:135:PRO:HD3	2:Z:163:TRP:CE2	2.32	0.65
2:Z:351:LEU:H	2:Z:351:LEU:HD12	1.61	0.65
1:A:350:VAL:C	1:A:352:ALA:H	2.04	0.65
1:C:86:PHE:HB2	1:C:237:PHE:CD1	2.32	0.65
2:X:135:PRO:HD3	2:X:163:TRP:CE2	2.32	0.65
1:A:90:VAL:HG22	1:A:92:PHE:HB2	1.77	0.64
1:B:623:ILE:O	1:B:624:HIS:C	2.38	0.64
1:B:134:GLN:O	1:B:135:PHE:C	2.40	0.64
1:C:421:TYR:HA	1:C:457:ARG:HH11	1.62	0.64
2:T:168:TRP:HA	2:T:172:VAL:HG23	1.78	0.64
2:Z:21:ILE:HD12	2:Z:22:GLU:H	1.61	0.64
1:A:106:PHE:HB3	1:A:234:ILE:HG13	1.79	0.64
1:A:319:ARG:HG2	1:A:632:TRP:CE3	2.31	0.64
1:A:480:CYS:SG	1:A:481:LYS:N	2.69	0.64
1:B:190:ARG:HD2	1:B:207:HIS:CD2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:PHE:O	1:C:432:CYS:SG	2.56	0.64
2:X:285:PHE:HB3	2:X:287:GLN:NE2	2.13	0.64
2:X:453:THR:HA	2:X:512:PHE:HE2	1.62	0.64
1:A:106:PHE:CD2	1:A:234:ILE:HD12	2.32	0.64
2:X:152:MET:HG3	2:X:270:MET:HA	1.80	0.64
2:Z:45:LEU:O	2:Z:46:ALA:C	2.41	0.64
1:A:391:CYS:HB3	1:A:524:CYS:HA	1.78	0.64
1:C:36:VAL:HG11	1:C:219:PHE:CE1	2.33	0.64
1:C:619:VAL:O	1:C:623:ILE:HB	1.98	0.64
1:C:639:SER:HB3	1:C:651:GLY:HA2	1.80	0.64
1:A:188:ASN:ND2	1:A:190:ARG:HG3	2.12	0.64
1:C:531:ASN:O	1:C:532:LEU:HB3	1.98	0.64
1:C:538:VAL:HG13	1:C:539:ASN:O	1.97	0.64
1:C:557:LYS:O	1:C:559:LEU:N	2.31	0.64
2:X:21:ILE:HD12	2:X:22:GLU:H	1.61	0.64
1:C:429:PHE:HB2	1:C:514:PHE:HE1	1.62	0.64
2:T:158:TYR:HD1	2:T:159:ASN:H	1.45	0.64
2:X:144:LEU:O	2:X:145:GLU:C	2.40	0.64
2:Z:91:LEU:HD23	2:Z:94:LYS:HE2	1.78	0.64
1:C:373:PRO:O	1:C:374:PHE:C	2.38	0.64
2:Z:279:TYR:CD1	2:Z:441:LYS:HD3	2.33	0.64
1:B:93:ALA:HB1	1:B:189:LEU:HD11	1.80	0.64
1:C:776:LYS:O	1:C:780:GLU:HG3	1.98	0.64
2:T:45:LEU:O	2:T:46:ALA:C	2.41	0.64
2:Z:158:TYR:HD1	2:Z:159:ASN:H	1.45	0.64
2:T:21:ILE:HD12	2:T:22:GLU:H	1.61	0.63
2:T:152:MET:HG3	2:T:270:MET:HA	1.80	0.63
2:T:231:GLU:HA	2:T:234:LYS:HD3	1.80	0.63
2:Z:133:CYS:CA	2:Z:141:CYS:HA	2.27	0.63
2:Z:135:PRO:HB3	2:Z:163:TRP:CD1	2.33	0.63
2:Z:477:TRP:CD2	2:Z:500:PRO:HG3	2.33	0.63
2:Z:152:MET:HG3	2:Z:270:MET:HA	1.80	0.63
1:B:133:PHE:O	1:B:134:GLN:C	2.41	0.63
2:X:45:LEU:O	2:X:46:ALA:C	2.41	0.63
1:A:352:ALA:O	1:A:353:TRP:C	2.42	0.63
2:T:263:PRO:HB2	2:T:265:HIS:CE1	2.33	0.63
2:T:279:TYR:CD1	2:T:441:LYS:HD3	2.33	0.63
2:T:611:SER:CB	2:T:614:ALA:HB3	2.29	0.63
2:X:231:GLU:HA	2:X:234:LYS:HD3	1.80	0.63
2:X:22:GLU:O	2:X:24:GLN:N	2.24	0.63
1:A:616:CYS:H	1:A:643:GLN:HE22	1.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:VAL:C	1:B:352:ALA:H	2.04	0.63
1:B:522:THR:O	1:B:523:VAL:C	2.41	0.63
1:C:362:VAL:HA	1:C:523:VAL:O	1.99	0.63
2:T:455:MET:O	2:T:456:LEU:C	2.41	0.63
2:X:455:MET:O	2:X:456:LEU:C	2.41	0.63
1:A:140:PHE:CZ	1:A:142:ASP:HA	2.33	0.63
1:B:109:THR:HG23	1:B:114:THR:HB	1.79	0.63
2:X:158:TYR:HD1	2:X:159:ASN:H	1.45	0.63
2:X:421:ILE:HG23	2:X:423:LEU:HB2	1.81	0.63
2:Z:419:LYS:HA	2:Z:424:LEU:HB3	1.80	0.63
1:A:372:ALA:HB1	1:A:373:PRO:CD	2.29	0.63
1:A:522:THR:O	1:A:523:VAL:C	2.41	0.63
1:C:632:TRP:O	1:C:633:ARG:C	2.41	0.63
2:Z:455:MET:O	2:Z:456:LEU:C	2.41	0.63
2:Z:611:SER:CB	2:Z:614:ALA:HB3	2.29	0.63
1:A:201:PHE:HE1	1:A:234:ILE:HD13	1.64	0.62
1:A:971:GLY:O	1:A:995:ARG:HG2	1.99	0.62
1:B:352:ALA:O	1:B:353:TRP:C	2.42	0.62
1:C:372:ALA:HB1	1:C:373:PRO:CD	2.29	0.62
1:A:133:PHE:HD1	1:A:135:PHE:H	1.46	0.62
1:C:90:VAL:HG12	1:C:91:TYR:O	1.98	0.62
1:C:358:ILE:HG12	1:C:523:VAL:HG11	1.81	0.62
1:C:556:LYS:CD	1:C:583:ILE:CG2	2.77	0.62
2:T:571:GLU:O	2:T:572:ASN:C	2.42	0.62
2:Z:263:PRO:HB2	2:Z:265:HIS:CE1	2.33	0.62
1:A:206:LYS:HD2	1:A:208:THR:HG23	1.80	0.62
1:B:372:ALA:HB1	1:B:373:PRO:CD	2.29	0.62
2:T:468:ILE:HD13	2:T:476:LYS:HG3	1.82	0.62
2:X:133:CYS:CA	2:X:141:CYS:HA	2.27	0.62
2:X:233:ILE:O	2:X:234:LYS:C	2.41	0.62
2:Z:421:ILE:HG23	2:Z:423:LEU:HB2	1.81	0.62
1:A:853:GLN:O	1:A:855:PHE:N	2.31	0.62
1:B:454:ARG:CG	1:B:490:PRO:HB2	2.29	0.62
1:C:396:TYR:N	1:C:396:TYR:CD1	2.67	0.62
1:C:1144:GLU:C	1:C:1146:ASP:H	2.08	0.62
2:X:279:TYR:CD1	2:X:441:LYS:HD3	2.33	0.62
2:Z:231:GLU:HA	2:Z:234:LYS:HD3	1.80	0.62
1:B:396:TYR:N	1:B:396:TYR:CD1	2.67	0.62
1:C:327:VAL:HA	1:C:529:SER:OG	1.99	0.62
1:C:382:VAL:O	1:C:383:SER:C	2.42	0.62
2:X:264:ALA:O	2:X:265:HIS:C	2.43	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:468:ILE:HD13	2:X:476:LYS:HG3	1.82	0.62
1:B:276:LEU:HD11	1:B:304:LYS:HG3	1.81	0.62
1:C:123:ALA:O	1:C:124:THR:C	2.42	0.62
2:T:25:ALA:C	2:T:27:THR:N	2.57	0.62
2:X:263:PRO:HB2	2:X:265:HIS:CE1	2.33	0.62
2:X:611:SER:CB	2:X:614:ALA:HB3	2.29	0.62
1:A:115:GLN:C	1:A:132:GLU:HB3	2.24	0.62
1:A:853:GLN:C	1:A:855:PHE:H	2.07	0.62
1:C:324:GLU:O	1:C:325:SER:HB2	1.98	0.62
2:X:135:PRO:HB3	2:X:163:TRP:CD1	2.34	0.62
2:X:261:CYS:HB2	2:X:488:VAL:HG12	1.82	0.62
2:Z:143:LEU:HD22	2:Z:144:LEU:N	2.14	0.62
1:B:770:ILE:O	1:B:774:GLN:HG2	2.00	0.62
1:C:352:ALA:O	1:C:353:TRP:C	2.42	0.62
1:C:522:THR:O	1:C:523:VAL:C	2.41	0.62
2:T:233:ILE:O	2:T:234:LYS:C	2.41	0.62
1:B:117:LEU:HD11	1:B:232:ILE:HG12	1.80	0.62
1:B:393:THR:CB	1:B:517:LEU:H	2.13	0.62
2:T:22:GLU:C	2:T:24:GLN:H	2.08	0.62
2:X:143:LEU:HD22	2:X:144:LEU:N	2.13	0.62
2:X:243:TYR:O	2:X:244:VAL:C	2.43	0.62
1:B:353:TRP:CD1	1:B:353:TRP:N	2.67	0.62
1:C:393:THR:CB	1:C:517:LEU:H	2.13	0.62
2:Z:478:TRP:HA	2:Z:478:TRP:CE3	2.35	0.62
1:A:393:THR:CB	1:A:517:LEU:H	2.13	0.61
1:B:378:LYS:HG2	1:B:380:TYR:CZ	2.35	0.61
1:B:973:ILE:HD12	1:B:983:ARG:HH12	1.65	0.61
2:X:25:ALA:C	2:X:27:THR:N	2.57	0.61
2:X:99:ALA:O	2:X:101:GLN:N	2.33	0.61
2:Z:99:ALA:O	2:Z:101:GLN:N	2.33	0.61
2:Z:571:GLU:O	2:Z:572:ASN:C	2.42	0.61
1:A:482:GLY:C	1:A:487:CYS:HA	2.25	0.61
1:A:622:ALA:O	1:A:624:HIS:N	2.33	0.61
1:C:91:TYR:O	1:C:92:PHE:HB2	2.00	0.61
1:C:393:THR:HA	1:C:520:PRO:O	2.00	0.61
2:T:135:PRO:HB3	2:T:163:TRP:CD1	2.33	0.61
2:T:478:TRP:HA	2:T:478:TRP:CE3	2.35	0.61
2:X:22:GLU:C	2:X:24:GLN:H	2.08	0.61
2:X:285:PHE:O	2:X:287:GLN:N	2.33	0.61
1:A:386:LYS:HA	1:A:389:ASP:HB2	1.82	0.61
1:C:353:TRP:CD1	1:C:353:TRP:N	2.67	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:856:ASN:HD22	1:C:963:VAL:HG12	1.65	0.61
2:Z:474:MET:CE	2:Z:493:HIS:HB3	2.31	0.61
1:A:192:PHE:HB3	1:A:194:PHE:CE1	2.35	0.61
1:A:989:ALA:O	1:A:991:VAL:N	2.31	0.61
1:B:377:PHE:HA	1:B:433:VAL:O	2.01	0.61
1:B:712:ILE:CG1	1:B:1077:THR:HB	2.30	0.61
1:B:1116:THR:O	1:B:1118:ASP:N	2.33	0.61
1:C:542:PHE:CZ	1:C:584:LEU:HD11	2.36	0.61
1:A:87:ASN:O	1:A:88:ASP:C	2.44	0.61
1:A:193:VAL:HG12	1:A:270:LEU:HD11	1.81	0.61
1:A:391:CYS:CB	1:A:524:CYS:HA	2.30	0.61
1:A:474:GLN:CB	1:A:483:LYS:HG3	2.31	0.61
1:B:391:CYS:CB	1:B:524:CYS:HA	2.30	0.61
1:B:743:CYS:O	1:B:745:ASP:N	2.34	0.61
1:C:329:PHE:CG	1:C:527:LYS:O	2.54	0.61
1:C:381:GLY:O	1:C:382:VAL:C	2.42	0.61
1:C:386:LYS:HA	1:C:389:ASP:HB2	1.82	0.61
2:T:99:ALA:O	2:T:101:GLN:N	2.33	0.61
2:X:474:MET:CE	2:X:493:HIS:HB3	2.31	0.61
2:Z:264:ALA:O	2:Z:265:HIS:C	2.43	0.61
1:A:907:ASN:HD21	1:A:913:GLN:HG3	1.66	0.61
1:B:36:VAL:HG21	1:B:219:PHE:CZ	2.35	0.61
1:B:484:GLY:HA3	2:X:83:TYR:CE2	2.36	0.61
2:T:261:CYS:HB2	2:T:488:VAL:HG12	1.82	0.61
2:T:264:ALA:O	2:T:265:HIS:C	2.43	0.61
2:X:454:TYR:O	2:X:455:MET:C	2.44	0.61
1:A:377:PHE:HA	1:A:433:VAL:O	2.01	0.61
1:B:329:PHE:HB2	1:B:542:PHE:HA	1.83	0.61
1:C:335:LEU:O	1:C:361:CYS:HB2	2.01	0.61
2:T:243:TYR:O	2:T:244:VAL:C	2.43	0.61
2:X:476:LYS:O	2:X:477:TRP:C	2.44	0.61
2:Z:338:ASN:C	2:Z:340:GLN:H	2.08	0.61
1:B:386:LYS:HA	1:B:389:ASP:HB2	1.81	0.61
1:B:393:THR:HA	1:B:520:PRO:O	2.00	0.61
1:C:227:ASP:O	1:C:228:LEU:C	2.43	0.61
1:C:429:PHE:HD1	1:C:430:THR:H	1.48	0.61
2:T:336:PRO:O	2:T:337:GLY:C	2.43	0.61
2:Z:243:TYR:O	2:Z:244:VAL:C	2.43	0.61
1:A:136:CYS:C	1:A:138:ASP:H	2.08	0.61
1:A:393:THR:HA	1:A:520:PRO:O	2.00	0.61
1:A:473:TYR:CG	1:A:474:GLN:N	2.67	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:ILE:O	1:A:853:GLN:HG3	2.01	0.61
1:B:428:ASP:O	1:B:429:PHE:C	2.44	0.61
1:C:554:SER:HB2	1:C:556:LYS:HD2	1.83	0.61
2:T:421:ILE:HG23	2:T:423:LEU:HB2	1.81	0.61
2:T:476:LYS:O	2:T:477:TRP:C	2.44	0.61
2:X:482:ARG:HH21	2:X:488:VAL:HG23	1.66	0.61
2:Z:22:GLU:C	2:Z:24:GLN:H	2.08	0.61
2:Z:336:PRO:O	2:Z:337:GLY:C	2.43	0.61
2:Z:468:ILE:HD13	2:Z:476:LYS:HG3	1.82	0.61
2:Z:476:LYS:O	2:Z:477:TRP:C	2.44	0.61
1:A:378:LYS:HG2	1:A:380:TYR:CZ	2.35	0.61
1:A:428:ASP:O	1:A:429:PHE:C	2.44	0.61
2:T:474:MET:CE	2:T:493:HIS:HB3	2.31	0.61
2:X:118:THR:O	2:X:119:ILE:C	2.44	0.61
2:Z:261:CYS:HB2	2:Z:488:VAL:HG12	1.82	0.61
1:A:475:ALA:HB3	1:A:485:PRO:HG3	1.83	0.60
1:B:107:GLY:HA2	1:B:232:ILE:HD11	1.83	0.60
1:B:227:ASP:O	1:B:228:LEU:C	2.43	0.60
1:B:496:PHE:CG	1:B:506:PRO:HG3	2.36	0.60
1:C:111:ASP:HA	1:C:135:PHE:CE1	2.34	0.60
2:T:134:ASN:CB	2:T:140:GLU:HB2	2.31	0.60
2:X:338:ASN:C	2:X:340:GLN:H	2.08	0.60
2:Z:233:ILE:O	2:Z:234:LYS:C	2.41	0.60
2:Z:239:HIS:O	2:Z:242:ALA:HB3	2.01	0.60
2:Z:482:ARG:HH21	2:Z:488:VAL:HG23	1.66	0.60
1:A:353:TRP:CD1	1:A:353:TRP:N	2.67	0.60
2:T:239:HIS:O	2:T:242:ALA:HB3	2.02	0.60
2:T:311:ALA:O	2:T:312:GLU:C	2.44	0.60
2:T:454:TYR:O	2:T:455:MET:C	2.44	0.60
2:X:311:ALA:O	2:X:312:GLU:C	2.44	0.60
2:X:571:GLU:O	2:X:572:ASN:C	2.42	0.60
2:Z:180:TYR:O	2:Z:184:VAL:HG23	2.02	0.60
2:Z:454:TYR:O	2:Z:455:MET:C	2.44	0.60
2:X:415:PRO:HB3	2:X:428:PHE:CE2	2.36	0.60
2:X:488:VAL:HG21	2:X:612:PRO:HD2	1.83	0.60
2:Z:118:THR:O	2:Z:119:ILE:C	2.44	0.60
1:A:85:PRO:HB2	1:A:87:ASN:HD21	1.66	0.60
1:A:396:TYR:N	1:A:396:TYR:CD1	2.67	0.60
1:B:50:LEU:HD21	1:B:301:CYS:SG	2.41	0.60
1:C:264:ASP:O	1:C:265:TYR:C	2.44	0.60
1:C:624:HIS:O	1:C:625:ALA:C	2.43	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:239:HIS:HB3	2:Z:595:LEU:HD13	1.83	0.60
1:C:87:ASN:O	1:C:88:ASP:C	2.45	0.60
1:C:756:TYR:HB3	1:C:759:PHE:HD2	1.66	0.60
2:T:239:HIS:HB3	2:T:595:LEU:HD13	1.83	0.60
2:T:482:ARG:HH21	2:T:488:VAL:HG23	1.66	0.60
2:X:239:HIS:O	2:X:242:ALA:HB3	2.02	0.60
2:X:478:TRP:HA	2:X:478:TRP:CE3	2.35	0.60
1:A:496:PHE:CG	1:A:506:PRO:HG3	2.36	0.60
1:C:850:ILE:HG23	1:C:851:CYS:H	1.66	0.60
2:X:180:TYR:O	2:X:184:VAL:HG23	2.02	0.60
2:X:196:TYR:O	2:X:197:GLU:C	2.45	0.60
1:B:83:VAL:HB	1:B:236:ARG:CZ	2.32	0.60
1:B:688:ALA:O	1:B:689:SER:C	2.45	0.60
2:T:143:LEU:HD22	2:T:144:LEU:N	2.15	0.60
2:T:338:ASN:C	2:T:340:GLN:H	2.08	0.60
2:X:336:PRO:O	2:X:337:GLY:C	2.43	0.60
2:Z:83:TYR:O	2:Z:84:PRO:C	2.44	0.60
2:Z:488:VAL:HG21	2:Z:612:PRO:HD2	1.83	0.60
1:B:557:LYS:O	1:B:558:PHE:C	2.45	0.60
2:T:196:TYR:O	2:T:197:GLU:C	2.45	0.60
2:Z:311:ALA:O	2:Z:312:GLU:C	2.44	0.60
1:A:90:VAL:HG22	1:A:92:PHE:H	1.66	0.60
1:B:831:ALA:HA	1:B:851:CYS:HA	1.83	0.60
1:C:496:PHE:CG	1:C:506:PRO:HG3	2.36	0.60
1:C:719:THR:HA	1:C:926:GLN:HE22	1.66	0.60
2:T:72:PHE:O	2:T:75:GLU:HG3	2.02	0.60
2:T:83:TYR:O	2:T:84:PRO:C	2.44	0.60
2:X:239:HIS:HB3	2:X:595:LEU:HD13	1.83	0.60
2:Z:450:LEU:HD21	2:Z:519:THR:HG21	1.84	0.60
1:A:22:ILE:HG22	1:A:23:THR:H	1.67	0.59
1:A:198:ASP:HB2	1:A:200:TYR:CZ	2.36	0.59
1:B:357:ARG:HB2	1:B:396:TYR:CD2	2.37	0.59
1:B:1138:TYR:CE1	1:B:1143:LEU:HD23	2.37	0.59
2:T:118:THR:O	2:T:119:ILE:C	2.44	0.59
2:Z:22:GLU:C	2:Z:24:GLN:N	2.60	0.59
2:Z:196:TYR:O	2:Z:197:GLU:C	2.45	0.59
1:C:752:LEU:CD2	1:C:990:GLU:HG3	2.32	0.59
2:X:72:PHE:O	2:X:75:GLU:HG3	2.02	0.59
2:X:83:TYR:O	2:X:84:PRO:C	2.45	0.59
2:X:22:GLU:C	2:X:24:GLN:N	2.61	0.59
2:X:134:ASN:CG	2:X:135:PRO:HD2	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:HB2	1:A:396:TYR:CD2	2.38	0.59
1:B:456:PHE:HZ	1:B:488:TYR:HB3	1.67	0.59
1:C:378:LYS:HG2	1:C:380:TYR:CE2	2.38	0.59
1:C:556:LYS:HD3	1:C:583:ILE:HG21	1.85	0.59
2:T:22:GLU:C	2:T:24:GLN:N	2.60	0.59
2:T:145:GLU:CB	2:T:146:PRO:HD3	2.25	0.59
2:T:180:TYR:O	2:T:184:VAL:HG23	2.02	0.59
1:A:615:ASN:O	1:A:618:GLU:HG2	2.02	0.59
1:C:977:LEU:HD11	1:C:1000:ARG:HH22	1.68	0.59
2:Z:284:PRO:HG2	2:Z:437:ASN:HA	1.85	0.59
2:Z:581:VAL:HG22	2:Z:585:LEU:HD12	1.85	0.59
1:C:319:ARG:HG3	1:C:632:TRP:HB2	1.85	0.59
2:T:456:LEU:HD12	2:T:477:TRP:CH2	2.37	0.59
1:A:202:LYS:H	1:A:202:LYS:HZ3	1.50	0.59
1:B:120:VAL:HG11	1:B:127:PHE:CD2	2.38	0.59
1:B:480:CYS:O	1:B:481:LYS:C	2.45	0.59
2:T:134:ASN:CG	2:T:135:PRO:HD2	2.27	0.59
2:T:469:PRO:O	2:T:470:LYS:C	2.46	0.59
2:T:581:VAL:HG22	2:T:585:LEU:HD12	1.85	0.59
2:Z:25:ALA:C	2:Z:27:THR:N	2.57	0.59
2:Z:72:PHE:O	2:Z:75:GLU:HG3	2.02	0.59
1:A:485:PRO:HG3	1:A:488:TYR:CD2	2.38	0.59
1:B:381:GLY:HA3	1:B:429:PHE:CB	2.33	0.59
1:B:545:LEU:HD11	1:B:575:VAL:HG11	1.84	0.59
1:C:87:ASN:O	1:C:89:GLY:N	2.36	0.59
2:T:208:GLU:OE2	2:T:219:ARG:NH1	2.36	0.59
2:X:469:PRO:O	2:X:470:LYS:C	2.46	0.59
2:X:581:VAL:HG22	2:X:585:LEU:HD12	1.85	0.59
1:B:559:LEU:O	1:B:561:PHE:N	2.34	0.59
1:C:393:THR:N	1:C:516:LEU:HD13	2.16	0.59
2:T:133:CYS:CA	2:T:141:CYS:HA	2.27	0.59
2:T:488:VAL:HG21	2:T:612:PRO:HD2	1.83	0.59
2:X:71:ALA:O	2:X:74:LYS:HG3	2.03	0.59
2:X:134:ASN:CB	2:X:140:GLU:HB2	2.31	0.59
2:Z:134:ASN:CG	2:Z:135:PRO:HD2	2.27	0.59
1:C:357:ARG:HB2	1:C:396:TYR:CD2	2.38	0.59
1:C:821:LEU:O	1:C:825:LYS:HG3	2.03	0.59
2:T:424:LEU:HD22	2:T:425:SER:H	1.68	0.59
2:X:71:ALA:O	2:X:72:PHE:C	2.46	0.59
2:X:477:TRP:CD2	2:X:500:PRO:HG3	2.37	0.59
2:Z:71:ALA:O	2:Z:72:PHE:C	2.46	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:134:ASN:CB	2:Z:140:GLU:HB2	2.32	0.59
2:Z:456:LEU:HD12	2:Z:477:TRP:CH2	2.37	0.59
1:A:620:SER:O	1:A:622:ALA:N	2.35	0.58
1:A:622:ALA:O	1:A:623:ILE:C	2.46	0.58
1:B:643:GLN:NE2	1:C:834:ILE:HG12	2.17	0.58
1:A:381:GLY:HA3	1:A:429:PHE:CB	2.32	0.58
1:B:489:PHE:HD1	1:B:490:PRO:HD2	1.67	0.58
1:C:331:ASN:HA	1:C:579:GLN:CG	2.32	0.58
2:T:71:ALA:O	2:T:72:PHE:C	2.46	0.58
2:T:176:LEU:CA	2:T:179:LEU:HB2	2.33	0.58
2:T:450:LEU:HD21	2:T:519:THR:HG21	1.84	0.58
2:X:247:LYS:NZ	2:X:282:THR:HA	2.19	0.58
2:X:284:PRO:HG2	2:X:437:ASN:HA	1.85	0.58
2:X:450:LEU:HD21	2:X:519:THR:HG21	1.84	0.58
2:Z:570:LEU:O	2:Z:573:VAL:N	2.36	0.58
1:B:366:SER:C	1:B:368:LEU:H	2.12	0.58
2:X:176:LEU:CA	2:X:179:LEU:HB2	2.33	0.58
2:X:208:GLU:OE2	2:X:219:ARG:NH1	2.36	0.58
2:Z:176:LEU:CA	2:Z:179:LEU:HB2	2.33	0.58
2:T:474:MET:HE2	2:T:497:TYR:HB2	1.86	0.58
1:B:125:ASN:HB2	1:B:171:VAL:HG12	1.86	0.58
1:C:833:PHE:CD2	1:C:836:GLN:HA	2.39	0.58
1:C:1005:GLN:O	1:C:1009:THR:HG23	2.04	0.58
2:T:284:PRO:HG2	2:T:437:ASN:HA	1.85	0.58
1:B:331:ASN:C	1:B:579:GLN:HG2	2.29	0.58
1:C:429:PHE:HB2	1:C:514:PHE:CE1	2.39	0.58
1:C:556:LYS:HD2	1:C:583:ILE:HG22	1.85	0.58
2:T:540:HIS:HA	2:T:587:TYR:CE2	2.37	0.58
2:Z:208:GLU:OE2	2:Z:219:ARG:NH1	2.36	0.58
1:B:385:THR:C	1:B:387:LEU:H	2.11	0.58
1:B:454:ARG:HG2	1:B:490:PRO:CB	2.31	0.58
1:B:852:ALA:O	1:B:853:GLN:C	2.46	0.58
1:C:460:LYS:HG3	1:C:461:LEU:H	1.69	0.58
1:C:554:SER:HB2	1:C:556:LYS:CD	2.33	0.58
2:X:505:HIS:CD2	2:X:505:HIS:H	2.22	0.58
1:C:102:ARG:HA	1:C:102:ARG:HH11	1.69	0.58
1:C:378:LYS:HG2	1:C:380:TYR:CD2	2.39	0.58
1:B:942:PRO:O	1:B:943:SER:HB2	2.04	0.58
1:C:338:PHE:CZ	1:C:363:ALA:HB1	2.38	0.58
1:C:983:ARG:HH21	1:C:983:ARG:HB2	1.69	0.58
2:T:247:LYS:NZ	2:T:282:THR:HA	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ASP:HA	1:A:266:TYR:CE2	2.39	0.58
2:T:475:LYS:O	2:T:479:GLU:HG3	2.04	0.58
2:T:570:LEU:O	2:T:573:VAL:N	2.36	0.58
2:X:191:ALA:O	2:X:192:ARG:C	2.47	0.58
2:Z:453:THR:HA	2:Z:512:PHE:CE2	2.39	0.58
1:A:139:PRO:O	1:A:140:PHE:C	2.47	0.57
1:A:269:TYR:O	1:A:270:LEU:HD23	2.04	0.57
1:A:616:CYS:H	1:A:643:GLN:NE2	2.01	0.57
1:B:528:LYS:HA	1:B:528:LYS:HZ2	1.69	0.57
1:C:385:THR:C	1:C:387:LEU:H	2.11	0.57
2:T:71:ALA:O	2:T:74:LYS:HG3	2.03	0.57
2:T:189:GLU:O	2:T:190:MET:C	2.47	0.57
2:T:505:HIS:H	2:T:505:HIS:CD2	2.22	0.57
2:Z:469:PRO:O	2:Z:470:LYS:C	2.46	0.57
1:A:325:SER:O	1:A:327:VAL:HG23	2.04	0.57
1:A:326:ILE:HB	1:A:531:ASN:O	2.03	0.57
1:B:322:PRO:O	1:B:323:THR:C	2.48	0.57
1:C:770:ILE:O	1:C:774:GLN:HG2	2.03	0.57
2:X:591:LEU:C	2:X:593:THR:H	2.12	0.57
2:Z:432:ASN:HA	2:Z:435:GLU:HG3	1.86	0.57
2:Z:489:GLU:HB2	2:Z:491:VAL:O	2.04	0.57
1:A:193:VAL:HG22	1:A:222:LEU:CD2	2.34	0.57
1:B:362:VAL:HG13	1:B:526:PRO:N	2.19	0.57
1:B:484:GLY:O	1:B:485:PRO:C	2.47	0.57
1:C:187:LYS:HA	1:C:210:ILE:HD11	1.86	0.57
1:C:437:ASN:HD21	1:C:505:GLN:HB3	1.69	0.57
1:C:479:PRO:O	1:C:483:LYS:HD3	2.04	0.57
2:T:611:SER:HB3	2:T:614:ALA:H	1.70	0.57
1:A:30:ASN:HA	1:A:60:SER:O	2.04	0.57
1:A:133:PHE:HD2	1:A:164:ASN:HB2	1.69	0.57
1:B:86:PHE:HB2	1:B:237:PHE:HD2	1.69	0.57
1:C:193:VAL:HG12	1:C:222:LEU:HD23	1.85	0.57
2:X:489:GLU:HB2	2:X:491:VAL:O	2.04	0.57
2:X:570:LEU:O	2:X:573:VAL:N	2.36	0.57
2:Z:591:LEU:C	2:Z:593:THR:H	2.12	0.57
1:A:335:LEU:O	1:A:361:CYS:HB2	2.04	0.57
1:B:957:GLN:HE22	1:C:765:ARG:HD2	1.69	0.57
1:C:480:CYS:O	1:C:481:LYS:C	2.47	0.57
1:C:736:VAL:HG22	1:C:858:LEU:HD22	1.86	0.57
2:T:145:GLU:HB3	2:T:146:PRO:CD	2.27	0.57
2:T:550:ALA:O	2:T:551:GLY:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:586:ASN:O	2:T:589:GLU:HB2	2.05	0.57
2:X:159:ASN:O	2:X:162:LEU:N	2.37	0.57
2:X:189:GLU:O	2:X:190:MET:C	2.47	0.57
2:Z:142:LEU:HD12	2:Z:148:LEU:HD13	1.86	0.57
2:Z:159:ASN:O	2:Z:162:LEU:N	2.37	0.57
1:A:855:PHE:CD1	1:C:588:PRO:HG2	2.40	0.57
1:B:29:THR:O	1:B:61:ASN:HA	2.05	0.57
1:B:577:ASP:CG	1:B:582:GLU:HB2	2.29	0.57
2:T:439:LEU:O	2:T:441:LYS:N	2.38	0.57
2:T:489:GLU:HB2	2:T:491:VAL:O	2.04	0.57
2:X:222:LEU:O	2:X:223:ILE:C	2.47	0.57
2:Z:241:HIS:HB3	2:Z:606:TRP:CH2	2.39	0.57
2:Z:247:LYS:NZ	2:Z:282:THR:HA	2.19	0.57
2:Z:274:PHE:CD2	2:Z:445:THR:HG22	2.39	0.57
2:Z:474:MET:HE2	2:Z:497:TYR:HB2	1.86	0.57
2:Z:475:LYS:O	2:Z:479:GLU:HG3	2.04	0.57
2:Z:611:SER:HB3	2:Z:614:ALA:H	1.70	0.57
2:T:159:ASN:O	2:T:162:LEU:N	2.37	0.57
2:X:424:LEU:O	2:X:425:SER:C	2.48	0.57
2:X:435:GLU:O	2:X:437:ASN:N	2.38	0.57
2:X:439:LEU:O	2:X:441:LYS:N	2.38	0.57
2:X:475:LYS:O	2:X:479:GLU:HG3	2.04	0.57
2:Z:530:CYS:O	2:Z:531:GLN:C	2.47	0.57
1:A:202:LYS:H	1:A:202:LYS:NZ	2.03	0.57
1:B:319:ARG:CZ	1:B:322:PRO:HD2	2.34	0.57
1:C:228:LEU:HB3	1:C:230:ILE:HG12	1.87	0.57
1:C:419:ALA:HB1	1:C:424:LYS:HD2	1.86	0.57
2:T:274:PHE:CD2	2:T:445:THR:HG22	2.39	0.57
2:T:591:LEU:C	2:T:593:THR:H	2.12	0.57
2:X:125:THR:O	2:X:126:ILE:C	2.48	0.57
2:X:453:THR:HA	2:X:512:PHE:CE2	2.39	0.57
1:A:366:SER:C	1:A:368:LEU:H	2.12	0.57
1:A:393:THR:N	1:A:516:LEU:HD13	2.16	0.57
1:C:366:SER:C	1:C:368:LEU:H	2.12	0.57
1:C:445:HIS:CE1	1:C:498:PRO:HG3	2.40	0.57
1:C:833:PHE:HE2	1:C:851:CYS:SG	2.27	0.57
2:X:274:PHE:CD2	2:X:445:THR:HG22	2.39	0.57
2:X:279:TYR:CE1	2:X:441:LYS:HB2	2.40	0.57
2:X:611:SER:HB3	2:X:614:ALA:H	1.69	0.57
2:Z:71:ALA:O	2:Z:74:LYS:HG3	2.03	0.57
2:Z:189:GLU:O	2:Z:190:MET:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:THR:C	1:A:387:LEU:H	2.11	0.57
1:B:386:LYS:HA	1:B:389:ASP:CB	2.35	0.57
2:T:222:LEU:O	2:T:223:ILE:C	2.47	0.57
2:X:67:ASP:O	2:X:68:LYS:C	2.48	0.57
2:X:335:ASP:HB2	2:X:336:PRO:HD2	1.87	0.57
2:Z:23:GLU:C	2:Z:25:ALA:H	2.13	0.57
2:Z:435:GLU:O	2:Z:437:ASN:N	2.38	0.57
2:Z:505:HIS:H	2:Z:505:HIS:CD2	2.22	0.57
1:A:368:LEU:HA	1:A:371:PHE:CZ	2.40	0.56
2:T:435:GLU:O	2:T:437:ASN:N	2.38	0.56
2:X:142:LEU:HD12	2:X:148:LEU:HD13	1.86	0.56
2:X:474:MET:HE2	2:X:497:TYR:HB2	1.85	0.56
2:Z:191:ALA:O	2:Z:192:ARG:C	2.47	0.56
1:A:394:ASN:HA	1:A:523:VAL:HG21	1.87	0.56
1:C:438:SER:O	1:C:439:ASN:C	2.48	0.56
1:C:985:ASP:O	1:C:988:GLU:HG2	2.05	0.56
2:T:142:LEU:HD12	2:T:148:LEU:HD13	1.86	0.56
2:T:191:ALA:O	2:T:192:ARG:C	2.47	0.56
2:T:270:MET:HG3	2:T:271:TRP:N	2.20	0.56
2:T:530:CYS:O	2:T:531:GLN:C	2.47	0.56
2:Z:222:LEU:O	2:Z:223:ILE:C	2.47	0.56
1:B:444:LYS:O	1:B:498:PRO:HD3	2.05	0.56
1:B:489:PHE:CD1	1:B:490:PRO:HD2	2.40	0.56
1:C:394:ASN:HA	1:C:523:VAL:HG21	1.87	0.56
1:C:455:LEU:HD22	1:C:492:GLN:HG3	1.86	0.56
2:T:143:LEU:HD13	2:T:145:GLU:H	1.70	0.56
2:T:279:TYR:CE1	2:T:441:LYS:HB2	2.40	0.56
2:T:474:MET:HE1	2:T:499:ASP:OD2	2.05	0.56
2:X:23:GLU:C	2:X:25:ALA:H	2.13	0.56
2:X:241:HIS:HB3	2:X:606:TRP:CH2	2.39	0.56
2:X:270:MET:HG3	2:X:271:TRP:N	2.20	0.56
2:Z:67:ASP:O	2:Z:68:LYS:C	2.48	0.56
2:Z:550:ALA:O	2:Z:551:GLY:C	2.47	0.56
1:A:386:LYS:HA	1:A:389:ASP:CB	2.36	0.56
1:B:325:SER:C	1:B:326:ILE:HG12	2.28	0.56
2:T:67:ASP:O	2:T:68:LYS:C	2.48	0.56
2:X:129:THR:O	2:X:130:GLY:C	2.49	0.56
2:Z:439:LEU:O	2:Z:441:LYS:N	2.38	0.56
2:Z:490:PRO:O	2:Z:613:TYR:HB3	2.05	0.56
1:A:200:TYR:HB3	1:A:229:PRO:HA	1.87	0.56
1:A:312:ILE:HD12	1:A:597:ILE:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:LEU:HA	1:C:371:PHE:CZ	2.40	0.56
1:C:386:LYS:HA	1:C:389:ASP:CB	2.36	0.56
1:C:436:TRP:CZ2	1:C:508:ARG:HB3	2.41	0.56
2:T:71:ALA:O	2:T:74:LYS:HE3	2.06	0.56
2:T:125:THR:O	2:T:126:ILE:C	2.48	0.56
2:T:241:HIS:HB3	2:T:606:TRP:CH2	2.40	0.56
2:X:351:LEU:HD11	2:X:357:ARG:HD2	1.88	0.56
2:X:490:PRO:O	2:X:613:TYR:HB3	2.06	0.56
2:X:530:CYS:O	2:X:531:GLN:C	2.47	0.56
1:A:444:LYS:O	1:A:498:PRO:HD3	2.05	0.56
1:B:368:LEU:HA	1:B:371:PHE:CZ	2.40	0.56
1:B:394:ASN:HA	1:B:523:VAL:HG21	1.87	0.56
1:B:1144:GLU:C	1:B:1146:ASP:H	2.14	0.56
1:C:215:PHE:O	1:C:216:PRO:C	2.49	0.56
1:C:235:THR:C	1:C:236:ARG:HG2	2.30	0.56
1:C:557:LYS:O	1:C:558:PHE:C	2.48	0.56
2:T:115:ARG:O	2:T:119:ILE:HG13	2.06	0.56
2:T:490:PRO:O	2:T:613:TYR:HB3	2.06	0.56
2:Z:129:THR:O	2:Z:130:GLY:C	2.49	0.56
2:Z:351:LEU:HD11	2:Z:357:ARG:HD2	1.88	0.56
2:Z:482:ARG:NH2	2:Z:488:VAL:HG23	2.21	0.56
1:A:474:GLN:CA	1:A:483:LYS:HG3	2.36	0.56
1:A:1028:LYS:O	1:A:1032:CYS:HB2	2.05	0.56
1:C:167:THR:O	1:C:168:PHE:HB2	2.04	0.56
2:T:317:SER:C	2:T:319:GLY:H	2.13	0.56
2:T:335:ASP:HB2	2:T:336:PRO:HD2	1.87	0.56
2:T:472:GLN:O	2:T:473:TRP:C	2.48	0.56
2:X:115:ARG:O	2:X:119:ILE:HG13	2.06	0.56
2:X:456:LEU:HD12	2:X:477:TRP:CH2	2.37	0.56
2:Z:125:THR:O	2:Z:126:ILE:C	2.48	0.56
2:Z:279:TYR:CE1	2:Z:441:LYS:HB2	2.40	0.56
2:Z:317:SER:C	2:Z:319:GLY:H	2.13	0.56
1:A:86:PHE:HD1	1:A:237:PHE:CZ	2.24	0.56
1:B:82:PRO:O	1:B:83:VAL:C	2.48	0.56
1:B:416:GLY:O	1:B:420:ASP:HB2	2.06	0.56
1:C:483:LYS:HB3	1:C:488:TYR:HB2	1.87	0.56
2:T:482:ARG:NH2	2:T:488:VAL:HG23	2.21	0.56
2:X:245:ARG:HA	2:X:262:LEU:HD21	1.88	0.56
2:X:482:ARG:NH2	2:X:488:VAL:HG23	2.21	0.56
2:Z:245:ARG:HA	2:Z:262:LEU:HD21	1.88	0.56
2:Z:472:GLN:O	2:Z:473:TRP:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:O	1:A:57:PRO:C	2.47	0.56
1:A:129:LYS:HB2	1:A:169:GLU:OE2	2.05	0.56
1:A:213:ARG:HB3	1:A:216:PRO:HB3	1.86	0.56
1:A:761:THR:HG23	1:A:765:ARG:HH11	1.69	0.56
1:B:936:ASP:O	1:B:937:SER:C	2.49	0.56
2:T:74:LYS:HE3	2:T:75:GLU:HG2	1.88	0.56
2:X:71:ALA:O	2:X:74:LYS:HE3	2.06	0.56
2:Z:270:MET:HG3	2:Z:271:TRP:N	2.20	0.56
1:A:482:GLY:HA3	1:A:487:CYS:C	2.31	0.56
1:A:540:PHE:CE1	1:A:545:LEU:HD23	2.41	0.56
1:B:319:ARG:NH2	1:B:322:PRO:HD2	2.21	0.56
1:C:576:ARG:HG3	1:C:576:ARG:HH21	1.70	0.56
2:X:472:GLN:O	2:X:473:TRP:C	2.48	0.56
1:A:416:GLY:O	1:A:420:ASP:HB2	2.06	0.55
1:A:485:PRO:HA	2:T:79:LEU:HD21	1.87	0.55
1:A:620:SER:CB	1:A:623:ILE:HA	2.36	0.55
1:A:850:ILE:O	1:A:852:ALA:N	2.39	0.55
1:B:110:LEU:HA	1:B:135:PHE:CD1	2.41	0.55
1:B:337:PRO:HG2	1:B:358:ILE:HD13	1.88	0.55
1:C:416:GLY:O	1:C:420:ASP:HB2	2.06	0.55
1:C:441:LEU:HD11	1:C:508:ARG:NH1	2.21	0.55
1:C:454:ARG:CZ	1:C:491:LEU:HD21	2.35	0.55
2:T:23:GLU:C	2:T:25:ALA:H	2.13	0.55
2:X:145:GLU:HB3	2:X:146:PRO:CD	2.28	0.55
2:Z:432:ASN:C	2:Z:434:THR:H	2.14	0.55
1:A:201:PHE:O	1:A:203:ILE:HG13	2.06	0.55
1:A:420:ASP:HA	1:A:460:LYS:HD3	1.88	0.55
1:C:53:ASP:HB2	1:C:55:PHE:CZ	2.42	0.55
1:C:616:CYS:SG	1:C:643:GLN:HG2	2.46	0.55
2:T:278:LEU:O	2:T:280:SER:N	2.39	0.55
2:X:31:LYS:O	2:X:32:PHE:C	2.50	0.55
2:Z:73:LEU:O	2:Z:74:LYS:C	2.50	0.55
2:Z:145:GLU:HB3	2:Z:146:PRO:CD	2.28	0.55
1:A:619:VAL:O	1:A:623:ILE:N	2.40	0.55
1:B:111:ASP:HB3	1:B:113:LYS:NZ	2.21	0.55
1:C:372:ALA:C	1:C:374:PHE:H	2.15	0.55
2:Z:450:LEU:HB2	2:Z:451:PRO:HD3	1.89	0.55
1:A:64:TRP:O	1:A:66:HIS:N	2.39	0.55
1:B:228:LEU:HD23	1:B:230:ILE:HD11	1.88	0.55
1:C:117:LEU:HD23	1:C:119:ILE:HD11	1.88	0.55
1:C:358:ILE:HB	1:C:395:VAL:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:462:LYS:HE2	1:C:462:LYS:N	2.22	0.55
2:T:553:LYS:HD3	2:T:573:VAL:HG12	1.88	0.55
2:X:73:LEU:O	2:X:74:LYS:C	2.50	0.55
2:X:278:LEU:O	2:X:280:SER:N	2.39	0.55
2:Z:71:ALA:O	2:Z:74:LYS:HE3	2.06	0.55
2:Z:335:ASP:HB2	2:Z:336:PRO:HD2	1.87	0.55
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.35	0.55
1:A:559:LEU:O	1:A:561:PHE:N	2.40	0.55
1:C:417:ASN:ND2	1:C:421:TYR:HE1	2.03	0.55
2:T:36:ALA:O	2:T:37:GLU:C	2.50	0.55
2:T:153:ALA:HB2	2:T:277:ASN:HD22	1.72	0.55
2:X:153:ALA:HB2	2:X:277:ASN:HD22	1.72	0.55
2:X:181:GLU:HB3	2:X:470:LYS:NZ	2.22	0.55
2:Z:68:LYS:O	2:Z:69:TRP:C	2.50	0.55
2:Z:115:ARG:O	2:Z:119:ILE:HG13	2.06	0.55
2:Z:228:HIS:HA	2:Z:231:GLU:OE2	2.06	0.55
2:Z:247:LYS:HA	2:Z:250:ASN:ND2	2.22	0.55
1:A:86:PHE:HB2	1:A:235:THR:HA	1.89	0.55
1:A:994:ASP:HA	1:A:997:ILE:HG22	1.88	0.55
1:B:203:ILE:HB	1:B:226:VAL:HG12	1.88	0.55
1:B:210:ILE:HD13	1:B:216:PRO:HD3	1.89	0.55
1:B:403:LYS:HD3	1:B:405:ASN:HB2	1.88	0.55
1:C:21:LEU:HB3	1:C:80:ASP:OD1	2.06	0.55
1:C:111:ASP:O	1:C:112:SER:C	2.49	0.55
1:C:230:ILE:HD12	1:C:232:ILE:HD13	1.86	0.55
1:C:478:LYS:HB3	1:C:479:PRO:CD	2.35	0.55
2:T:247:LYS:HA	2:T:250:ASN:ND2	2.22	0.55
2:T:453:THR:HA	2:T:512:PHE:CE2	2.39	0.55
2:X:97:LEU:O	2:X:98:GLN:C	2.49	0.55
2:Z:88:ILE:HG22	2:Z:94:LYS:HG2	1.89	0.55
2:Z:237:TYR:CD1	2:Z:451:PRO:HG2	2.42	0.55
1:A:86:PHE:HA	1:A:237:PHE:CE1	2.42	0.55
1:B:571:THR:O	1:B:572:THR:C	2.50	0.55
1:B:631:THR:O	1:B:633:ARG:N	2.39	0.55
1:C:403:LYS:HD3	1:C:405:ASN:HB2	1.88	0.55
2:T:31:LYS:O	2:T:32:PHE:C	2.50	0.55
2:T:419:LYS:HA	2:T:424:LEU:HB3	1.88	0.55
2:X:381:TYR:CD2	2:X:404:VAL:HG11	2.42	0.55
2:X:432:ASN:ND2	2:X:436:ILE:HG12	2.22	0.55
2:Z:92:THR:HG22	2:Z:96:GLN:NE2	2.22	0.55
2:Z:167:SER:O	2:Z:168:TRP:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ALA:HB1	1:A:520:PRO:CD	2.35	0.55
1:B:712:ILE:HG12	1:B:1077:THR:HB	1.88	0.55
1:B:743:CYS:C	1:B:745:ASP:H	2.15	0.55
2:T:181:GLU:HB3	2:T:470:LYS:NZ	2.22	0.55
2:Z:97:LEU:O	2:Z:98:GLN:C	2.49	0.55
2:Z:501:ALA:HA	2:Z:506:VAL:HB	1.88	0.55
1:A:372:ALA:C	1:A:374:PHE:H	2.15	0.55
1:C:430:THR:O	1:C:514:PHE:HD1	1.89	0.55
2:T:97:LEU:O	2:T:98:GLN:C	2.49	0.55
2:T:274:PHE:HD2	2:T:445:THR:HG22	1.72	0.55
2:T:418:LEU:O	2:T:421:ILE:HG22	2.07	0.55
2:X:228:HIS:HA	2:X:231:GLU:OE2	2.06	0.55
2:X:237:TYR:CD1	2:X:451:PRO:HG2	2.42	0.55
2:Z:181:GLU:HB3	2:Z:470:LYS:NZ	2.22	0.55
2:Z:418:LEU:O	2:Z:421:ILE:HG22	2.07	0.55
1:A:907:ASN:ND2	1:A:913:GLN:HG3	2.22	0.55
1:B:303:LEU:O	1:B:304:LYS:C	2.49	0.55
1:B:393:THR:N	1:B:516:LEU:HD13	2.15	0.55
1:B:439:ASN:O	1:B:440:LYS:C	2.50	0.55
1:B:854:LYS:O	1:B:856:ASN:N	2.40	0.55
1:C:319:ARG:HE	1:C:321:GLN:HG2	1.72	0.55
2:T:245:ARG:HA	2:T:262:LEU:HD21	1.88	0.55
2:X:92:THR:HG22	2:X:96:GLN:NE2	2.22	0.55
2:X:418:LEU:O	2:X:421:ILE:HG22	2.07	0.55
2:Z:478:TRP:HA	2:Z:478:TRP:HE3	1.72	0.55
2:Z:492:PRO:HD3	2:Z:613:TYR:CD2	2.42	0.55
1:B:326:ILE:O	1:B:327:VAL:C	2.50	0.54
1:B:985:ASP:CG	1:B:986:PRO:HD2	2.32	0.54
1:C:349:SER:O	1:C:350:VAL:C	2.50	0.54
1:C:437:ASN:HA	1:C:507:TYR:HA	1.89	0.54
2:T:167:SER:O	2:T:168:TRP:HB2	2.07	0.54
2:T:237:TYR:CD1	2:T:451:PRO:HG2	2.42	0.54
2:X:68:LYS:O	2:X:69:TRP:C	2.50	0.54
2:X:317:SER:C	2:X:319:GLY:H	2.13	0.54
2:Z:69:TRP:CD1	2:Z:73:LEU:HD11	2.42	0.54
2:Z:278:LEU:O	2:Z:280:SER:N	2.39	0.54
1:A:87:ASN:HB2	1:A:269:TYR:CD1	2.42	0.54
1:A:337:PRO:HG2	1:A:358:ILE:HD13	1.88	0.54
1:B:126:VAL:HG23	1:B:172:SER:O	2.07	0.54
1:B:187:LYS:O	1:B:210:ILE:HB	2.08	0.54
1:B:554:SER:HB2	1:B:583:ILE:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:GLU:HG2	1:C:466:ARG:H	1.73	0.54
1:C:485:PRO:HA	2:Z:83:TYR:OH	2.07	0.54
2:T:228:HIS:HA	2:T:231:GLU:OE2	2.06	0.54
2:X:74:LYS:HE3	2:X:75:GLU:HG2	1.88	0.54
2:X:550:ALA:O	2:X:551:GLY:C	2.47	0.54
2:Z:313:LYS:O	2:Z:314:PHE:C	2.50	0.54
1:A:329:PHE:O	1:A:578:PRO:HG2	2.07	0.54
1:A:359:SER:HA	1:A:523:VAL:HG22	1.89	0.54
1:B:484:GLY:O	1:B:486:ASN:N	2.40	0.54
1:B:619:VAL:C	1:B:621:VAL:H	2.15	0.54
2:T:73:LEU:O	2:T:74:LYS:C	2.50	0.54
2:T:455:MET:HE1	2:T:481:LYS:HE3	1.90	0.54
2:X:81:GLN:C	2:X:83:TYR:H	2.15	0.54
2:Z:74:LYS:HE3	2:Z:75:GLU:HG2	1.88	0.54
1:A:329:PHE:CD2	1:A:527:LYS:HB3	2.42	0.54
1:A:422:ASN:ND2	1:A:454:ARG:H	2.01	0.54
1:B:235:THR:O	1:B:236:ARG:HG2	2.07	0.54
1:B:1116:THR:HG22	1:B:1138:TYR:HD2	1.73	0.54
1:C:276:LEU:HB3	1:C:289:VAL:HG22	1.88	0.54
2:T:81:GLN:C	2:T:83:TYR:H	2.15	0.54
2:T:351:LEU:HD11	2:T:357:ARG:HD2	1.88	0.54
2:X:247:LYS:HA	2:X:250:ASN:ND2	2.22	0.54
2:X:492:PRO:HD3	2:X:613:TYR:CD2	2.42	0.54
2:Z:36:ALA:O	2:Z:37:GLU:C	2.50	0.54
1:B:902:MET:HA	1:B:905:ARG:HD2	1.89	0.54
1:C:623:ILE:HD11	1:C:633:ARG:HH22	1.72	0.54
1:C:743:CYS:C	1:C:745:ASP:H	2.16	0.54
2:T:69:TRP:CD1	2:T:73:LEU:HD11	2.42	0.54
2:T:88:ILE:HG22	2:T:94:LYS:HG2	1.89	0.54
2:T:92:THR:HG22	2:T:96:GLN:NE2	2.22	0.54
2:T:215:TYR:HD1	2:T:577:LYS:NZ	2.05	0.54
2:T:492:PRO:HD3	2:T:613:TYR:CD2	2.42	0.54
2:Z:145:GLU:CB	2:Z:146:PRO:HD3	2.28	0.54
2:Z:591:LEU:O	2:Z:593:THR:N	2.41	0.54
1:A:380:TYR:CE2	1:A:412:PRO:HD2	2.43	0.54
1:A:474:GLN:HA	1:A:483:LYS:CG	2.36	0.54
1:A:478:LYS:HB3	1:A:484:GLY:N	2.22	0.54
1:A:640:ASN:ND2	1:A:640:ASN:H	2.06	0.54
1:B:380:TYR:CE2	1:B:412:PRO:HD2	2.43	0.54
1:B:743:CYS:C	1:B:745:ASP:N	2.63	0.54
1:C:118:LEU:O	1:C:119:ILE:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:TRP:CE2	1:C:508:ARG:HB3	2.42	0.54
1:C:982:SER:C	1:C:984:LEU:H	2.14	0.54
2:T:381:TYR:CD2	2:T:404:VAL:HG11	2.42	0.54
2:T:450:LEU:HB2	2:T:451:PRO:HD3	1.89	0.54
2:X:553:LYS:HD3	2:X:573:VAL:HG12	1.89	0.54
2:Z:153:ALA:HB2	2:Z:277:ASN:HD22	1.72	0.54
2:Z:230:PHE:HA	2:Z:233:ILE:HG13	1.90	0.54
2:Z:285:PHE:O	2:Z:287:GLN:N	2.41	0.54
2:Z:381:TYR:CD2	2:Z:404:VAL:HG11	2.42	0.54
2:Z:455:MET:HE1	2:Z:481:LYS:HE3	1.89	0.54
2:Z:553:LYS:HD3	2:Z:573:VAL:HG12	1.88	0.54
1:A:349:SER:O	1:A:350:VAL:C	2.50	0.54
1:A:475:ALA:HB3	1:A:485:PRO:CD	2.37	0.54
1:B:329:PHE:CG	1:B:330:PRO:N	2.75	0.54
1:B:438:SER:O	1:B:439:ASN:C	2.51	0.54
1:C:216:PRO:O	1:C:217:GLN:C	2.51	0.54
2:T:524:GLN:NE2	2:T:580:ASN:HB2	2.23	0.54
2:X:36:ALA:O	2:X:37:GLU:C	2.50	0.54
2:X:69:TRP:CD1	2:X:73:LEU:HD11	2.42	0.54
2:X:215:TYR:HD1	2:X:577:LYS:NZ	2.05	0.54
2:Z:31:LYS:O	2:Z:32:PHE:C	2.50	0.54
2:Z:274:PHE:HD2	2:Z:445:THR:HG22	1.72	0.54
1:B:462:LYS:HE2	1:B:462:LYS:N	2.22	0.54
1:C:228:LEU:H	1:C:228:LEU:HD12	1.73	0.54
1:C:480:CYS:HB2	1:C:483:LYS:CG	2.35	0.54
1:C:519:ALA:HB1	1:C:520:PRO:CD	2.35	0.54
2:T:230:PHE:HA	2:T:233:ILE:HG13	1.90	0.54
2:X:103:ASN:HB2	2:X:107:VAL:CG1	2.38	0.54
2:X:313:LYS:O	2:X:314:PHE:C	2.50	0.54
2:X:450:LEU:HB2	2:X:451:PRO:HD3	1.89	0.54
2:X:591:LEU:O	2:X:593:THR:N	2.41	0.54
1:A:568:ILE:O	1:A:569:VAL:C	2.50	0.54
1:A:620:SER:C	1:A:622:ALA:N	2.65	0.54
1:B:349:SER:O	1:B:350:VAL:C	2.50	0.54
1:B:465:GLU:HG2	1:B:466:ARG:H	1.73	0.54
1:B:937:SER:O	1:B:938:LEU:C	2.50	0.54
1:C:434:ILE:HB	1:C:436:TRP:HZ3	1.73	0.54
2:T:68:LYS:O	2:T:69:TRP:C	2.50	0.54
2:X:60:GLN:O	2:X:63:ASN:N	2.41	0.54
2:X:274:PHE:HD2	2:X:445:THR:HG22	1.72	0.54
2:X:523:PHE:CD2	2:X:584:LEU:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:215:TYR:HD1	2:Z:577:LYS:NZ	2.05	0.54
1:A:576:ARG:HA	1:A:582:GLU:O	2.08	0.54
1:A:904:TYR:N	1:A:904:TYR:CD1	2.75	0.54
1:B:639:SER:HB3	1:B:651:GLY:HA2	1.89	0.54
2:T:103:ASN:HB2	2:T:107:VAL:CG1	2.38	0.54
2:X:529:LEU:HD23	2:X:550:ALA:HB1	1.90	0.54
2:Z:523:PHE:CD2	2:Z:584:LEU:HB2	2.43	0.54
1:A:439:ASN:O	1:A:440:LYS:C	2.50	0.53
1:C:848:ASP:OD2	1:C:852:ALA:HB2	2.08	0.53
2:X:489:GLU:O	2:X:490:PRO:C	2.51	0.53
2:Z:236:LEU:O	2:Z:237:TYR:C	2.51	0.53
2:Z:275:TRP:HB3	2:Z:444:LEU:HD22	1.90	0.53
1:A:34:ARG:O	1:A:56:LEU:HD23	2.08	0.53
1:A:403:LYS:HD3	1:A:405:ASN:HB2	1.88	0.53
1:A:447:GLY:O	1:A:449:TYR:N	2.42	0.53
1:B:611:TYR:HB3	1:B:614:VAL:HG21	1.89	0.53
1:C:972:ALA:O	1:C:973:ILE:C	2.51	0.53
2:T:478:TRP:HA	2:T:478:TRP:HE3	1.72	0.53
2:X:88:ILE:HG22	2:X:94:LYS:HG2	1.89	0.53
2:X:230:PHE:HA	2:X:233:ILE:HG13	1.90	0.53
2:Z:524:GLN:NE2	2:Z:580:ASN:HB2	2.23	0.53
1:A:569:VAL:O	1:A:570:ASP:C	2.50	0.53
1:A:702:GLU:CG	1:B:790:LYS:HD3	2.38	0.53
1:B:281:GLU:C	1:B:283:GLY:H	2.15	0.53
1:B:372:ALA:C	1:B:374:PHE:H	2.15	0.53
1:B:747:THR:HG22	1:B:749:CYS:H	1.74	0.53
1:C:331:ASN:N	1:C:578:PRO:O	2.41	0.53
2:T:220:GLY:O	2:T:221:GLN:C	2.52	0.53
1:B:688:ALA:O	1:B:690:GLN:N	2.42	0.53
1:B:747:THR:HG22	1:B:749:CYS:N	2.21	0.53
1:C:541:ASN:O	1:C:542:PHE:C	2.51	0.53
1:C:554:SER:HB3	1:C:583:ILE:C	2.33	0.53
1:C:831:ALA:C	1:C:833:PHE:H	2.17	0.53
1:C:849:LEU:O	1:C:851:CYS:N	2.42	0.53
2:T:60:GLN:O	2:T:63:ASN:N	2.41	0.53
2:T:564:GLU:HB3	2:T:565:PRO:HD2	1.91	0.53
2:X:275:TRP:HB3	2:X:444:LEU:HD22	1.90	0.53
2:Z:489:GLU:O	2:Z:490:PRO:C	2.51	0.53
1:A:106:PHE:HB3	1:A:234:ILE:CG1	2.39	0.53
1:A:985:ASP:C	1:A:987:PRO:HD2	2.33	0.53
1:B:210:ILE:O	1:B:212:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:ASP:O	1:B:452:TRP:HD1	1.91	0.53
2:T:111:ASP:HA	2:T:114:LYS:HG3	1.91	0.53
2:T:236:LEU:O	2:T:237:TYR:C	2.51	0.53
2:T:489:GLU:O	2:T:490:PRO:C	2.51	0.53
2:X:167:SER:O	2:X:168:TRP:HB2	2.07	0.53
2:Z:416:LYS:O	2:Z:417:HIS:C	2.52	0.53
2:Z:529:LEU:HD23	2:Z:550:ALA:HB1	1.90	0.53
1:A:36:VAL:HG21	1:A:219:PHE:HE1	1.73	0.53
1:A:438:SER:O	1:A:439:ASN:C	2.51	0.53
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.57	0.53
1:B:478:LYS:HG3	1:B:482:GLY:H	1.74	0.53
1:C:197:ILE:HB	1:C:202:LYS:HE3	1.91	0.53
2:T:523:PHE:CD2	2:T:584:LEU:HB2	2.43	0.53
2:X:293:VAL:CG1	2:X:423:LEU:HD22	2.39	0.53
2:X:455:MET:HE1	2:X:481:LYS:HE3	1.90	0.53
1:A:465:GLU:HG2	1:A:466:ARG:H	1.73	0.53
1:A:632:TRP:CD1	1:A:632:TRP:C	2.86	0.53
1:B:536:LYS:O	1:B:537:CYS:C	2.51	0.53
1:B:594:VAL:HG11	1:B:635:TYR:OH	2.09	0.53
1:C:36:VAL:HG11	1:C:219:PHE:HE1	1.74	0.53
1:C:438:SER:HB3	1:C:508:ARG:HD2	1.89	0.53
1:C:454:ARG:O	1:C:455:LEU:C	2.51	0.53
2:T:283:VAL:O	2:T:284:PRO:C	2.52	0.53
2:X:237:TYR:CE1	2:X:451:PRO:HG2	2.44	0.53
2:X:419:LYS:HG2	2:X:426:PRO:HA	1.90	0.53
2:X:524:GLN:NE2	2:X:580:ASN:HB2	2.23	0.53
2:Z:220:GLY:O	2:Z:221:GLN:C	2.52	0.53
1:A:429:PHE:O	1:A:430:THR:HB	2.09	0.53
1:A:702:GLU:HG2	1:B:790:LYS:HD3	1.90	0.53
1:B:29:THR:HG22	1:B:30:ASN:H	1.72	0.53
1:B:359:SER:HA	1:B:523:VAL:HG22	1.90	0.53
1:B:429:PHE:O	1:B:430:THR:HB	2.09	0.53
2:T:91:LEU:O	2:T:92:THR:C	2.51	0.53
2:T:285:PHE:O	2:T:287:GLN:N	2.41	0.53
2:T:591:LEU:O	2:T:593:THR:N	2.41	0.53
2:X:91:LEU:O	2:X:92:THR:C	2.51	0.53
2:X:478:TRP:HA	2:X:478:TRP:HE3	1.72	0.53
2:Z:91:LEU:O	2:Z:92:THR:C	2.51	0.53
2:Z:217:TYR:CZ	2:Z:221:GLN:HG2	2.44	0.53
2:Z:293:VAL:CG1	2:Z:423:LEU:HD22	2.39	0.53
1:A:91:TYR:O	1:A:92:PHE:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1024:LEU:O	1:C:1028:LYS:HG3	2.09	0.53
2:T:529:LEU:HD23	2:T:550:ALA:HB1	1.90	0.53
2:X:236:LEU:O	2:X:237:TYR:C	2.51	0.53
2:X:276:THR:HB	2:X:445:THR:CG2	2.39	0.53
2:Z:237:TYR:CE1	2:Z:451:PRO:HG2	2.44	0.53
1:A:226:VAL:O	1:A:227:ASP:HB2	2.08	0.53
1:A:450:ASP:O	1:A:452:TRP:HD1	1.91	0.53
1:A:536:LYS:O	1:A:538:VAL:HG22	2.09	0.53
1:A:1140:PRO:O	1:A:1141:LEU:C	2.51	0.53
1:B:456:PHE:HE1	1:B:489:PHE:C	2.17	0.53
1:B:534:LYS:HG3	1:B:551:LEU:O	2.09	0.53
1:B:536:LYS:H	1:B:550:VAL:HG13	1.74	0.53
1:C:63:THR:O	1:C:65:PHE:N	2.41	0.53
1:C:423:TYR:CE2	1:C:425:LEU:HD21	2.44	0.53
1:C:452:TRP:HA	1:C:492:GLN:O	2.09	0.53
1:C:848:ASP:CG	1:C:852:ALA:HB2	2.33	0.53
2:T:275:TRP:HB3	2:T:444:LEU:HD22	1.90	0.53
2:T:313:LYS:O	2:T:314:PHE:C	2.50	0.53
2:Z:60:GLN:O	2:Z:63:ASN:N	2.41	0.53
2:Z:81:GLN:C	2:Z:83:TYR:H	2.15	0.53
2:Z:564:GLU:HB3	2:Z:565:PRO:HD2	1.90	0.53
1:B:856:ASN:HD22	1:B:963:VAL:HG13	1.73	0.52
1:C:56:LEU:HD12	1:C:269:TYR:O	2.08	0.52
2:T:103:ASN:HB2	2:T:107:VAL:HG12	1.91	0.52
2:T:237:TYR:CE1	2:T:451:PRO:HG2	2.44	0.52
2:T:580:ASN:HB3	2:T:583:PRO:HD2	1.92	0.52
2:Z:132:VAL:O	2:Z:141:CYS:HA	2.09	0.52
2:Z:276:THR:HB	2:Z:445:THR:CG2	2.39	0.52
1:A:201:PHE:CE1	1:A:234:ILE:HG21	2.44	0.52
1:A:559:LEU:C	1:A:561:PHE:H	2.17	0.52
1:A:805:ILE:HD12	1:A:878:LEU:HD21	1.90	0.52
1:B:321:GLN:N	1:B:322:PRO:CD	2.72	0.52
1:B:558:PHE:CZ	1:B:574:ALA:HB3	2.37	0.52
2:T:132:VAL:O	2:T:141:CYS:HA	2.09	0.52
2:T:217:TYR:CE1	2:T:221:GLN:HG2	2.45	0.52
2:Z:88:ILE:HG21	2:Z:93:VAL:HG22	1.92	0.52
2:Z:283:VAL:O	2:Z:284:PRO:C	2.52	0.52
1:A:462:LYS:HE2	1:A:462:LYS:N	2.22	0.52
1:A:482:GLY:O	1:A:483:LYS:HB2	2.10	0.52
1:A:673:TYR:CE2	1:A:690:GLN:HG2	2.44	0.52
1:B:358:ILE:HG22	1:B:359:SER:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:TRP:HB3	1:B:491:LEU:HD13	1.91	0.52
1:B:633:ARG:HE	1:B:634:VAL:N	2.06	0.52
1:B:940:SER:O	1:B:942:PRO:HD3	2.08	0.52
1:C:45:SER:O	1:C:46:SER:C	2.52	0.52
1:C:113:LYS:N	1:C:132:GLU:HG3	2.24	0.52
2:T:176:LEU:O	2:T:177:ARG:C	2.52	0.52
2:T:293:VAL:CG1	2:T:423:LEU:HD22	2.39	0.52
2:X:217:TYR:CZ	2:X:221:GLN:HG2	2.44	0.52
2:Z:103:ASN:HB2	2:Z:107:VAL:CG1	2.38	0.52
2:Z:215:TYR:HA	2:Z:577:LYS:NZ	2.25	0.52
2:Z:419:LYS:HA	2:Z:424:LEU:CB	2.39	0.52
2:Z:435:GLU:C	2:Z:437:ASN:N	2.68	0.52
1:A:214:ASP:C	1:A:216:PRO:HD3	2.35	0.52
1:A:230:ILE:HD13	1:A:232:ILE:HD12	1.91	0.52
1:B:122:ASN:O	1:B:123:ALA:C	2.53	0.52
1:B:456:PHE:CD1	1:B:490:PRO:HA	2.45	0.52
1:B:458:LYS:NZ	1:B:474:GLN:HE22	2.08	0.52
2:Z:111:ASP:HA	2:Z:114:LYS:HG3	1.91	0.52
2:Z:285:PHE:C	2:Z:287:GLN:N	2.68	0.52
2:Z:503:LEU:O	2:Z:504:PHE:C	2.53	0.52
1:A:349:SER:O	1:A:352:ALA:N	2.43	0.52
1:A:482:GLY:HA3	1:A:488:TYR:N	2.25	0.52
1:B:483:LYS:HB3	2:X:24:GLN:HA	1.91	0.52
1:B:831:ALA:HA	1:B:851:CYS:HB3	1.91	0.52
1:C:32:PHE:HE2	1:C:215:PHE:O	1.92	0.52
1:C:120:VAL:O	1:C:121:ASN:C	2.51	0.52
1:C:266:TYR:O	1:C:267:VAL:HB	2.10	0.52
1:C:805:ILE:HD12	1:C:878:LEU:HD21	1.91	0.52
1:C:959:LEU:O	1:C:962:LEU:N	2.35	0.52
2:T:434:THR:O	2:T:438:PHE:N	2.42	0.52
2:Z:217:TYR:CE1	2:Z:221:GLN:HG2	2.45	0.52
1:A:26:GLN:O	1:A:27:SER:HB3	2.08	0.52
1:A:63:THR:HG22	1:A:64:TRP:H	1.75	0.52
1:A:64:TRP:HE1	1:A:214:ASP:CB	2.22	0.52
1:A:736:VAL:HA	1:A:857:GLY:O	2.10	0.52
1:B:452:TRP:CE3	1:B:491:LEU:HB3	2.44	0.52
1:C:449:TYR:CE1	1:C:495:GLY:HA3	2.45	0.52
2:X:503:LEU:O	2:X:504:PHE:C	2.53	0.52
2:Z:434:THR:O	2:Z:438:PHE:N	2.42	0.52
1:A:358:ILE:HG22	1:A:359:SER:H	1.74	0.52
1:A:532:LEU:O	1:A:533:VAL:HB	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1091:ARG:C	1:A:1092:GLU:HG2	2.33	0.52
1:B:447:GLY:O	1:B:449:TYR:N	2.42	0.52
1:C:421:TYR:CB	1:C:457:ARG:HB2	2.35	0.52
1:C:475:ALA:O	2:Z:24:GLN:HG2	2.10	0.52
2:T:88:ILE:HG21	2:T:93:VAL:HG22	1.92	0.52
2:X:435:GLU:C	2:X:437:ASN:N	2.68	0.52
2:X:458:LYS:O	2:X:459:TRP:C	2.53	0.52
2:Z:103:ASN:HB2	2:Z:107:VAL:HG12	1.91	0.52
1:A:86:PHE:HB2	1:A:235:THR:CA	2.40	0.52
1:A:203:ILE:HB	1:A:226:VAL:HG23	1.91	0.52
1:B:86:PHE:HB2	1:B:237:PHE:CD2	2.44	0.52
2:T:217:TYR:CZ	2:T:221:GLN:HG2	2.44	0.52
2:T:276:THR:HB	2:T:445:THR:CG2	2.39	0.52
2:T:503:LEU:O	2:T:504:PHE:C	2.53	0.52
2:X:176:LEU:O	2:X:177:ARG:C	2.52	0.52
2:Z:580:ASN:HB3	2:Z:583:PRO:HD2	1.91	0.52
1:B:189:LEU:HB2	1:B:210:ILE:CG1	2.40	0.52
1:B:934:ILE:O	1:B:935:GLN:C	2.52	0.52
1:C:353:TRP:HB3	1:C:423:TYR:CE1	2.45	0.52
1:C:421:TYR:HB3	1:C:457:ARG:HD3	1.91	0.52
1:C:472:ILE:HG21	1:C:482:GLY:HA3	1.92	0.52
1:C:922:LEU:O	1:C:926:GLN:HG3	2.10	0.52
2:X:217:TYR:CE1	2:X:221:GLN:HG2	2.45	0.52
1:B:127:PHE:CA	1:B:171:VAL:HG13	2.40	0.52
1:B:707:TYR:HB2	1:C:883:THR:HG23	1.91	0.52
2:X:20:THR:HB	2:X:23:GLU:OE1	2.10	0.52
2:X:23:GLU:O	2:X:27:THR:HG23	2.10	0.52
1:A:186:PHE:N	1:A:212:GLY:HA3	2.25	0.51
1:A:1116:THR:HG22	1:A:1117:THR:N	2.25	0.51
1:A:1116:THR:CG2	1:A:1140:PRO:HD3	2.40	0.51
1:B:647:GLY:HA2	1:C:834:ILE:HD11	1.93	0.51
2:T:193:ALA:C	2:T:195:HIS:H	2.17	0.51
1:A:353:TRP:O	1:A:354:ASN:HB3	2.11	0.51
1:A:950:ASP:O	1:A:951:VAL:C	2.52	0.51
1:B:189:LEU:HD12	1:B:190:ARG:H	1.75	0.51
2:X:564:GLU:HB3	2:X:565:PRO:HD2	1.90	0.51
2:X:580:ASN:HB3	2:X:583:PRO:HD2	1.91	0.51
2:Z:247:LYS:HZ2	2:Z:282:THR:HA	1.74	0.51
1:A:37:TYR:O	1:A:39:PRO:N	2.42	0.51
1:B:478:LYS:HB3	1:B:479:PRO:HD2	1.91	0.51
1:B:489:PHE:CE2	1:B:491:LEU:HB2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:LYS:N	1:B:550:VAL:HG13	2.25	0.51
1:B:852:ALA:O	1:B:854:LYS:N	2.43	0.51
1:C:63:THR:O	1:C:64:TRP:C	2.53	0.51
1:C:95:THR:HG23	1:C:188:ASN:O	2.10	0.51
1:C:358:ILE:HG12	1:C:523:VAL:CG1	2.40	0.51
2:T:215:TYR:HA	2:T:577:LYS:NZ	2.25	0.51
2:T:277:ASN:OD1	2:T:277:ASN:N	2.44	0.51
2:X:415:PRO:O	2:X:419:LYS:HB2	2.10	0.51
2:X:416:LYS:O	2:X:417:HIS:C	2.52	0.51
2:Z:20:THR:HB	2:Z:23:GLU:OE1	2.10	0.51
2:Z:176:LEU:O	2:Z:177:ARG:C	2.52	0.51
2:Z:280:SER:O	2:Z:281:LEU:C	2.53	0.51
1:A:36:VAL:O	1:A:221:ALA:HA	2.10	0.51
1:A:111:ASP:HB2	1:A:113:LYS:HE3	1.91	0.51
1:A:127:PHE:CG	1:A:171:VAL:HG13	2.45	0.51
1:B:116:SER:HA	1:B:232:ILE:HD13	1.92	0.51
1:B:831:ALA:HA	1:B:851:CYS:CB	2.40	0.51
1:B:989:ALA:C	1:B:991:VAL:N	2.69	0.51
1:C:43:PHE:O	1:C:44:ARG:HG3	2.11	0.51
1:C:936:ASP:C	1:C:938:LEU:H	2.17	0.51
2:T:432:ASN:OD1	2:T:433:GLU:HG3	2.10	0.51
2:X:103:ASN:HB2	2:X:107:VAL:HG12	1.91	0.51
2:X:457:GLU:O	2:X:458:LYS:C	2.54	0.51
2:Z:188:ASN:HB3	2:Z:192:ARG:CZ	2.41	0.51
2:Z:193:ALA:C	2:Z:195:HIS:H	2.17	0.51
2:Z:439:LEU:C	2:Z:441:LYS:N	2.68	0.51
1:A:551:LEU:HD23	1:A:586:ILE:HG12	1.92	0.51
1:B:349:SER:O	1:B:352:ALA:N	2.43	0.51
1:C:349:SER:O	1:C:352:ALA:N	2.43	0.51
2:T:458:LYS:O	2:T:459:TRP:C	2.53	0.51
2:X:494:ASP:CG	2:X:496:THR:H	2.19	0.51
2:Z:215:TYR:HD1	2:Z:577:LYS:HZ1	1.58	0.51
2:Z:494:ASP:HB3	2:Z:497:TYR:CZ	2.45	0.51
1:A:188:ASN:HA	1:A:209:PRO:CA	2.35	0.51
1:A:533:VAL:O	1:A:534:LYS:HB3	2.09	0.51
1:A:789:TYR:HA	1:C:703:ASN:O	2.10	0.51
1:B:110:LEU:HD22	1:B:135:PHE:CE2	2.46	0.51
1:B:190:ARG:HD2	1:B:207:HIS:HD2	1.76	0.51
1:B:324:GLU:HG2	1:B:325:SER:N	2.26	0.51
1:B:353:TRP:O	1:B:354:ASN:HB3	2.11	0.51
1:B:576:ARG:HA	1:B:582:GLU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:PRO:HA	1:C:537:CYS:O	2.11	0.51
1:C:353:TRP:O	1:C:354:ASN:HB3	2.11	0.51
1:C:453:TYR:CE2	1:C:492:GLN:HB2	2.45	0.51
2:T:121:ASN:O	2:T:122:THR:C	2.54	0.51
2:T:494:ASP:HB3	2:T:497:TYR:CZ	2.46	0.51
2:X:220:GLY:O	2:X:221:GLN:C	2.52	0.51
2:Z:99:ALA:O	2:Z:100:LEU:C	2.54	0.51
2:Z:132:VAL:HB	2:Z:148:LEU:HD21	1.92	0.51
2:Z:474:MET:HE1	2:Z:493:HIS:HB3	1.93	0.51
1:A:904:TYR:N	1:A:904:TYR:HD1	2.09	0.51
1:A:1141:LEU:O	1:A:1142:GLN:C	2.53	0.51
1:B:1002:GLN:HE22	1:C:759:PHE:HE1	1.57	0.51
1:C:558:PHE:O	1:C:559:LEU:HG	2.10	0.51
1:C:821:LEU:HD22	1:C:939:PHE:CE1	2.45	0.51
2:T:20:THR:HB	2:T:23:GLU:OE1	2.10	0.51
2:T:280:SER:O	2:T:281:LEU:C	2.53	0.51
2:T:435:GLU:C	2:T:437:ASN:N	2.68	0.51
2:X:283:VAL:O	2:X:284:PRO:C	2.52	0.51
1:A:91:TYR:O	1:A:93:ALA:N	2.44	0.51
1:A:545:LEU:HB2	1:A:564:PHE:CE1	2.46	0.51
1:A:623:ILE:HG21	1:A:636:SER:OG	2.11	0.51
1:B:167:THR:O	1:B:168:PHE:HB2	2.11	0.51
1:B:197:ILE:HD11	1:B:202:LYS:HE2	1.92	0.51
1:B:284:THR:O	1:B:286:THR:HG23	2.11	0.51
1:B:338:PHE:C	1:B:340:GLU:H	2.19	0.51
1:B:386:LYS:CA	1:B:389:ASP:HB2	2.41	0.51
1:B:438:SER:HB3	1:B:508:ARG:HD2	1.93	0.51
1:C:116:SER:HB2	1:C:133:PHE:CD1	2.45	0.51
2:T:132:VAL:HB	2:T:148:LEU:HD21	1.92	0.51
2:T:188:ASN:HB3	2:T:192:ARG:CZ	2.41	0.51
2:T:414:THR:O	2:T:416:LYS:N	2.44	0.51
2:X:21:ILE:HD12	2:X:22:GLU:N	2.26	0.51
2:X:88:ILE:HG21	2:X:93:VAL:HG22	1.92	0.51
2:X:111:ASP:HA	2:X:114:LYS:HG3	1.91	0.51
2:X:193:ALA:C	2:X:195:HIS:H	2.17	0.51
2:X:215:TYR:HA	2:X:577:LYS:NZ	2.25	0.51
2:Z:457:GLU:O	2:Z:458:LYS:C	2.54	0.51
1:A:624:HIS:CG	1:A:625:ALA:N	2.79	0.51
1:C:439:ASN:O	1:C:440:LYS:C	2.54	0.51
1:C:833:PHE:HE2	1:C:851:CYS:HG	1.58	0.51
2:T:494:ASP:CG	2:T:496:THR:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:132:VAL:O	2:X:141:CYS:HA	2.09	0.51
2:X:188:ASN:HB3	2:X:192:ARG:CZ	2.41	0.51
2:X:414:THR:O	2:X:416:LYS:N	2.44	0.51
2:X:445:THR:C	2:X:446:ILE:HG12	2.36	0.51
2:X:494:ASP:HB3	2:X:497:TYR:CZ	2.46	0.51
2:Z:445:THR:C	2:Z:446:ILE:HG12	2.36	0.51
2:Z:584:LEU:C	2:Z:586:ASN:H	2.19	0.51
1:A:37:TYR:O	1:A:38:TYR:C	2.53	0.51
1:A:484:GLY:O	1:A:486:ASN:N	2.41	0.51
1:A:728:PRO:HA	1:A:948:LEU:HD21	1.92	0.51
1:B:519:ALA:HB1	1:B:520:PRO:CD	2.35	0.51
1:C:850:ILE:O	1:C:851:CYS:C	2.53	0.51
2:T:21:ILE:HD12	2:T:22:GLU:N	2.26	0.51
2:T:387:ALA:C	2:T:388:GLN:HG2	2.36	0.51
2:X:69:TRP:CE2	2:X:73:LEU:HD21	2.46	0.51
2:Z:315:PHE:CE1	2:Z:408:MET:HE3	2.46	0.51
1:A:127:PHE:CE1	1:A:171:VAL:HG22	2.46	0.50
1:A:192:PHE:O	1:A:193:VAL:C	2.54	0.50
1:A:438:SER:HB3	1:A:508:ARG:HD2	1.93	0.50
1:A:622:ALA:C	1:A:624:HIS:N	2.68	0.50
1:A:704:SER:HB3	1:B:790:LYS:HE2	1.93	0.50
1:A:855:PHE:O	1:A:856:ASN:HB2	2.12	0.50
1:B:214:ASP:O	1:B:215:PHE:C	2.54	0.50
1:B:558:PHE:CD2	1:B:563:GLN:O	2.64	0.50
1:C:133:PHE:HB3	1:C:135:PHE:CE2	2.46	0.50
2:T:439:LEU:C	2:T:441:LYS:N	2.68	0.50
2:X:582:ARG:O	2:X:583:PRO:C	2.53	0.50
2:Z:23:GLU:O	2:Z:27:THR:HG23	2.10	0.50
2:Z:70:SER:O	2:Z:71:ALA:C	2.54	0.50
2:Z:121:ASN:O	2:Z:122:THR:C	2.54	0.50
2:Z:415:PRO:O	2:Z:419:LYS:HB2	2.10	0.50
2:Z:607:SER:O	2:Z:609:ASP:N	2.45	0.50
1:A:118:LEU:O	1:A:120:VAL:HG23	2.11	0.50
1:A:386:LYS:CA	1:A:389:ASP:HB2	2.42	0.50
1:A:1129:VAL:HG13	1:B:917:TYR:HB3	1.94	0.50
1:C:102:ARG:HA	1:C:102:ARG:NH1	2.26	0.50
1:C:385:THR:C	1:C:387:LEU:N	2.69	0.50
2:T:90:ASN:O	2:T:93:VAL:HG13	2.11	0.50
2:T:287:GLN:HG3	2:T:288:LYS:HZ1	1.74	0.50
2:T:415:PRO:O	2:T:419:LYS:HB2	2.10	0.50
2:T:457:GLU:O	2:T:458:LYS:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:474:MET:HE1	2:T:493:HIS:HB3	1.93	0.50
2:X:280:SER:O	2:X:281:LEU:C	2.54	0.50
2:X:439:LEU:C	2:X:441:LYS:N	2.68	0.50
2:Z:414:THR:O	2:Z:416:LYS:N	2.44	0.50
2:Z:439:LEU:O	2:Z:440:LEU:C	2.54	0.50
1:A:936:ASP:OD1	1:A:936:ASP:N	2.39	0.50
1:B:633:ARG:O	1:B:634:VAL:HB	2.11	0.50
1:C:200:TYR:HB3	1:C:227:ASP:OD2	2.11	0.50
1:C:393:THR:HG22	1:C:394:ASN:N	2.27	0.50
1:C:674:GLN:HE21	1:C:693:ILE:HD11	1.75	0.50
1:C:852:ALA:HA	1:C:855:PHE:CE2	2.46	0.50
2:X:288:LYS:HG2	2:X:433:GLU:O	2.11	0.50
2:Z:472:GLN:HE22	2:Z:476:LYS:HG2	1.76	0.50
2:Z:494:ASP:CG	2:Z:496:THR:H	2.19	0.50
1:A:134:GLN:O	1:A:135:PHE:C	2.53	0.50
1:A:426:PRO:HB3	1:A:463:PRO:HB3	1.93	0.50
1:B:329:PHE:O	1:B:579:GLN:NE2	2.45	0.50
1:B:353:TRP:HB3	1:B:423:TYR:CD2	2.46	0.50
1:B:456:PHE:HE1	1:B:490:PRO:N	2.10	0.50
1:C:985:ASP:HB3	1:C:988:GLU:OE1	2.12	0.50
2:T:92:THR:HG22	2:T:96:GLN:HE22	1.77	0.50
2:T:416:LYS:O	2:T:417:HIS:C	2.52	0.50
2:T:582:ARG:O	2:T:583:PRO:C	2.53	0.50
2:T:607:SER:O	2:T:609:ASP:N	2.44	0.50
2:X:99:ALA:O	2:X:100:LEU:C	2.54	0.50
2:X:132:VAL:HB	2:X:148:LEU:HD21	1.93	0.50
2:X:304:ALA:O	2:X:307:ILE:HG12	2.12	0.50
2:Z:458:LYS:O	2:Z:459:TRP:C	2.53	0.50
1:A:43:PHE:O	1:A:44:ARG:HG3	2.11	0.50
1:A:105:ILE:HB	1:A:110:LEU:HD11	1.93	0.50
1:A:850:ILE:C	1:A:852:ALA:N	2.69	0.50
1:B:57:PRO:HG2	1:B:271:GLN:CD	2.35	0.50
1:C:821:LEU:HB2	1:C:939:PHE:CE2	2.47	0.50
2:T:304:ALA:O	2:T:307:ILE:HG12	2.12	0.50
2:X:170:SER:HB3	2:X:497:TYR:CE2	2.47	0.50
2:Z:462:MET:HE2	2:Z:468:ILE:HD11	1.93	0.50
1:A:632:TRP:O	1:A:634:VAL:N	2.45	0.50
1:B:385:THR:C	1:B:387:LEU:N	2.69	0.50
1:B:426:PRO:HB3	1:B:463:PRO:HB3	1.93	0.50
1:B:978:ASN:O	1:B:979:ASP:C	2.55	0.50
1:C:338:PHE:C	1:C:340:GLU:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:LYS:CA	1:C:389:ASP:HB2	2.42	0.50
2:T:23:GLU:O	2:T:27:THR:HG23	2.10	0.50
2:T:69:TRP:CE2	2:T:73:LEU:HD21	2.47	0.50
2:T:99:ALA:O	2:T:100:LEU:C	2.54	0.50
2:X:70:SER:O	2:X:71:ALA:C	2.54	0.50
2:X:215:TYR:HD1	2:X:577:LYS:HZ1	1.59	0.50
2:X:434:THR:O	2:X:438:PHE:N	2.42	0.50
2:X:439:LEU:O	2:X:440:LEU:C	2.54	0.50
2:X:474:MET:HE1	2:X:493:HIS:HB3	1.93	0.50
2:Z:387:ALA:C	2:Z:388:GLN:HG2	2.36	0.50
2:Z:582:ARG:O	2:Z:583:PRO:C	2.53	0.50
2:T:181:GLU:HB3	2:T:470:LYS:HZ1	1.77	0.50
2:T:414:THR:C	2:T:416:LYS:N	2.70	0.50
2:X:445:THR:O	2:X:446:ILE:HG12	2.12	0.50
2:X:462:MET:HE2	2:X:468:ILE:HD11	1.94	0.50
2:X:489:GLU:HG2	2:X:613:TYR:CE1	2.47	0.50
1:A:95:THR:HG23	1:A:189:LEU:HA	1.93	0.50
1:A:115:GLN:CA	1:A:132:GLU:HB3	2.42	0.50
1:A:197:ILE:H	1:A:202:LYS:NZ	2.09	0.50
1:A:540:PHE:O	1:A:546:THR:CG2	2.59	0.50
1:A:540:PHE:O	1:A:546:THR:HG22	2.11	0.50
1:A:633:ARG:NH2	1:A:635:TYR:CE2	2.80	0.50
1:B:422:ASN:ND2	1:B:454:ARG:H	2.01	0.50
1:C:30:ASN:HA	1:C:60:SER:O	2.11	0.50
1:C:534:LYS:O	1:C:535:ASN:C	2.53	0.50
1:C:599:PRO:HD3	1:C:692:ILE:HD11	1.94	0.50
1:C:833:PHE:O	1:C:833:PHE:HD1	1.95	0.50
2:X:132:VAL:HG21	2:X:167:SER:HB3	1.94	0.50
2:X:607:SER:O	2:X:609:ASP:N	2.45	0.50
1:A:136:CYS:C	1:A:138:ASP:N	2.70	0.50
1:A:194:PHE:CD1	1:A:203:ILE:HG23	2.47	0.50
1:A:350:VAL:C	1:A:352:ALA:N	2.70	0.50
1:A:353:TRP:HB3	1:A:423:TYR:CD2	2.46	0.50
1:B:330:PRO:HG3	1:B:527:LYS:HB2	1.94	0.50
1:C:379:CYS:O	1:C:380:TYR:C	2.55	0.50
1:C:740:MET:O	1:C:740:MET:HG3	2.12	0.50
2:T:315:PHE:CE1	2:T:408:MET:HE3	2.46	0.50
2:T:445:THR:C	2:T:446:ILE:HG12	2.36	0.50
2:T:445:THR:O	2:T:446:ILE:HG12	2.12	0.50
2:X:39:LEU:HD12	2:X:72:PHE:HB2	1.94	0.50
2:X:277:ASN:OD1	2:X:277:ASN:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:588:PHE:O	2:X:589:GLU:C	2.55	0.50
2:Z:170:SER:HB3	2:Z:497:TYR:CE2	2.47	0.50
1:A:168:PHE:CG	1:A:169:GLU:N	2.79	0.49
1:A:227:ASP:O	1:A:228:LEU:C	2.55	0.49
1:A:361:CYS:O	1:A:363:ALA:N	2.45	0.49
1:A:770:ILE:O	1:A:774:GLN:HG2	2.11	0.49
1:A:1083:HIS:CG	1:A:1083:HIS:O	2.64	0.49
1:B:201:PHE:HE2	1:B:203:ILE:HD11	1.77	0.49
1:B:210:ILE:O	1:B:211:ILE:C	2.53	0.49
1:C:425:LEU:HB3	1:C:426:PRO:HD2	1.94	0.49
1:C:752:LEU:HD22	1:C:990:GLU:HG3	1.93	0.49
2:X:122:THR:O	2:X:126:ILE:HG13	2.12	0.49
2:X:414:THR:HG21	2:X:542:CYS:O	2.12	0.49
2:Z:414:THR:HG21	2:Z:542:CYS:O	2.12	0.49
2:Z:432:ASN:HA	2:Z:435:GLU:CG	2.41	0.49
1:A:828:LEU:HG	1:A:829:ALA:N	2.26	0.49
1:B:322:PRO:O	1:B:324:GLU:N	2.45	0.49
1:B:350:VAL:C	1:B:352:ALA:N	2.70	0.49
1:B:737:ASP:O	1:B:738:CYS:C	2.54	0.49
1:B:978:ASN:O	1:B:981:LEU:N	2.45	0.49
1:C:122:ASN:HB2	1:C:127:PHE:HD1	1.76	0.49
1:C:198:ASP:C	1:C:200:TYR:H	2.20	0.49
1:C:853:GLN:O	1:C:855:PHE:N	2.44	0.49
2:T:70:SER:O	2:T:71:ALA:C	2.54	0.49
2:T:170:SER:HB3	2:T:497:TYR:CE2	2.47	0.49
2:X:121:ASN:O	2:X:122:THR:C	2.54	0.49
2:X:387:ALA:C	2:X:388:GLN:HG2	2.36	0.49
2:Z:69:TRP:CE2	2:Z:73:LEU:HD21	2.46	0.49
2:Z:291:ILE:HG21	2:Z:428:PHE:CZ	2.47	0.49
2:Z:463:VAL:HG23	2:Z:468:ILE:HD12	1.94	0.49
1:B:361:CYS:O	1:B:363:ALA:N	2.46	0.49
1:B:822:LEU:C	1:B:824:ASN:H	2.21	0.49
1:C:554:SER:HA	1:C:585:ASP:OD1	2.11	0.49
2:T:205:GLY:O	2:T:207:TYR:N	2.45	0.49
2:T:247:LYS:HZ2	2:T:282:THR:HA	1.76	0.49
2:T:291:ILE:HG21	2:T:428:PHE:CZ	2.47	0.49
2:T:414:THR:HG21	2:T:542:CYS:O	2.12	0.49
2:X:38:ASP:O	2:X:42:GLN:HG2	2.13	0.49
2:Z:132:VAL:HG21	2:Z:167:SER:HB3	1.94	0.49
2:Z:489:GLU:HG2	2:Z:613:TYR:CE1	2.47	0.49
1:A:711:SER:O	1:B:897:PRO:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	1.95	0.49
1:B:331:ASN:O	1:B:579:GLN:HG2	2.12	0.49
1:B:457:ARG:HH22	1:B:460:LYS:N	2.11	0.49
1:C:350:VAL:C	1:C:352:ALA:N	2.70	0.49
2:X:285:PHE:CD1	2:X:433:GLU:HB3	2.48	0.49
2:X:474:MET:HE1	2:X:499:ASP:OD2	2.12	0.49
2:Z:92:THR:HG22	2:Z:96:GLN:HE22	1.77	0.49
2:Z:205:GLY:O	2:Z:207:TYR:N	2.45	0.49
1:A:206:LYS:O	1:A:207:HIS:C	2.55	0.49
1:A:591:PHE:HZ	1:B:854:LYS:O	1.96	0.49
1:A:737:ASP:O	1:A:738:CYS:C	2.55	0.49
1:B:50:LEU:HG	1:B:276:LEU:HD12	1.93	0.49
1:B:87:ASN:C	1:B:89:GLY:H	2.21	0.49
1:B:393:THR:HG22	1:B:394:ASN:N	2.26	0.49
1:C:634:VAL:O	1:C:635:TYR:C	2.56	0.49
2:T:122:THR:O	2:T:126:ILE:HG13	2.12	0.49
2:T:228:HIS:O	2:T:229:THR:C	2.55	0.49
2:X:315:PHE:HE1	2:X:408:MET:HE3	1.78	0.49
2:Z:90:ASN:O	2:Z:93:VAL:HG13	2.11	0.49
1:A:804:GLN:O	1:A:818:ILE:HG23	2.12	0.49
1:B:321:GLN:C	1:B:323:THR:H	2.21	0.49
1:B:452:TRP:HZ3	1:B:491:LEU:O	1.96	0.49
1:C:95:THR:OG1	1:C:189:LEU:HA	2.13	0.49
1:C:428:ASP:O	1:C:429:PHE:C	2.55	0.49
2:T:25:ALA:C	2:T:27:THR:H	2.21	0.49
2:T:129:THR:O	2:T:130:GLY:C	2.55	0.49
2:T:132:VAL:HG21	2:T:167:SER:HB3	1.94	0.49
2:X:48:TRP:O	2:X:49:ASN:C	2.55	0.49
2:X:90:ASN:O	2:X:93:VAL:HG13	2.11	0.49
2:X:472:GLN:HE22	2:X:476:LYS:HG2	1.76	0.49
2:Z:36:ALA:HB1	2:Z:69:TRP:HH2	1.78	0.49
2:Z:445:THR:O	2:Z:446:ILE:HG12	2.12	0.49
1:A:127:PHE:HD1	1:A:128:ILE:H	1.61	0.49
1:A:136:CYS:HB2	1:A:139:PRO:HD3	1.93	0.49
1:A:338:PHE:C	1:A:340:GLU:H	2.19	0.49
1:A:489:PHE:CG	1:A:490:PRO:HD2	2.48	0.49
1:B:24:THR:HG21	1:B:65:PHE:HB3	1.92	0.49
1:B:188:ASN:HA	1:B:209:PRO:HA	1.95	0.49
1:B:392:PHE:O	1:B:393:THR:C	2.56	0.49
1:C:108:THR:OG1	1:C:235:THR:HG23	2.12	0.49
2:T:50:TYR:O	2:T:51:ASN:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:472:GLN:HE22	2:T:476:LYS:HG2	1.76	0.49
2:X:463:VAL:HG23	2:X:468:ILE:HD12	1.95	0.49
2:X:499:ASP:HB2	2:X:500:PRO:HD3	1.95	0.49
2:Z:122:THR:O	2:Z:126:ILE:HG13	2.12	0.49
2:Z:491:VAL:HG13	2:Z:492:PRO:O	2.13	0.49
2:Z:521:TYR:HE1	2:Z:579:MET:HB3	1.78	0.49
1:B:486:ASN:HD21	2:X:28:PHE:HD1	1.60	0.49
1:B:707:TYR:HB3	1:C:792:PRO:HG3	1.95	0.49
1:C:86:PHE:HB2	1:C:237:PHE:HD1	1.76	0.49
1:C:87:ASN:OD1	1:C:87:ASN:N	2.44	0.49
1:C:366:SER:C	1:C:368:LEU:N	2.71	0.49
1:C:821:LEU:HB2	1:C:939:PHE:CZ	2.47	0.49
2:T:36:ALA:HB1	2:T:69:TRP:HH2	1.78	0.49
2:T:39:LEU:HD12	2:T:72:PHE:HB2	1.94	0.49
2:T:489:GLU:HG2	2:T:613:TYR:CE1	2.47	0.49
2:X:462:MET:O	2:X:465:LYS:N	2.46	0.49
2:Z:39:LEU:HD12	2:Z:72:PHE:HB2	1.94	0.49
2:Z:50:TYR:O	2:Z:51:ASN:C	2.56	0.49
2:Z:228:HIS:O	2:Z:229:THR:C	2.56	0.49
2:Z:304:ALA:O	2:Z:307:ILE:HG12	2.12	0.49
1:A:213:ARG:HH22	1:A:215:PHE:H	1.60	0.49
1:A:392:PHE:O	1:A:393:THR:C	2.56	0.49
1:A:489:PHE:CD1	1:A:490:PRO:HD2	2.47	0.49
1:C:558:PHE:HZ	1:C:574:ALA:HB3	1.77	0.49
2:T:293:VAL:HG12	2:T:423:LEU:HD22	1.95	0.49
2:T:462:MET:O	2:T:465:LYS:N	2.46	0.49
2:X:36:ALA:HB1	2:X:69:TRP:HH2	1.78	0.49
2:X:116:LEU:O	2:X:117:ASN:C	2.56	0.49
2:X:205:GLY:O	2:X:207:TYR:N	2.45	0.49
2:X:315:PHE:CE1	2:X:408:MET:HE3	2.46	0.49
2:X:491:VAL:HG13	2:X:492:PRO:O	2.13	0.49
2:Z:149:ASN:O	2:Z:150:GLU:C	2.56	0.49
1:A:325:SER:O	1:A:326:ILE:C	2.56	0.49
1:A:408:SER:O	1:A:409:GLN:C	2.56	0.49
1:B:458:LYS:HE2	1:B:473:TYR:HE1	1.77	0.49
1:B:850:ILE:C	1:B:852:ALA:H	2.21	0.49
1:C:992:GLN:HA	1:C:995:ARG:HG3	1.94	0.49
2:X:50:TYR:O	2:X:51:ASN:C	2.56	0.49
2:X:149:ASN:O	2:X:150:GLU:C	2.56	0.49
2:X:228:HIS:O	2:X:231:GLU:HG2	2.13	0.49
2:Z:21:ILE:HD12	2:Z:22:GLU:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:560:LEU:O	2:Z:561:GLY:C	2.56	0.49
1:A:393:THR:HG22	1:A:394:ASN:N	2.27	0.48
1:A:622:ALA:HB3	1:A:624:HIS:ND1	2.28	0.48
1:B:90:VAL:HG13	1:B:91:TYR:O	2.13	0.48
1:B:120:VAL:HG13	1:B:121:ASN:N	2.28	0.48
1:B:740:MET:HG3	1:B:740:MET:O	2.11	0.48
1:C:86:PHE:CD1	1:C:86:PHE:C	2.91	0.48
1:C:95:THR:OG1	1:C:189:LEU:HD12	2.12	0.48
2:T:474:MET:HG3	2:T:495:GLU:HA	1.94	0.48
2:T:537:GLY:O	2:T:538:PRO:C	2.56	0.48
2:X:168:TRP:CE3	2:X:172:VAL:HG21	2.48	0.48
2:X:521:TYR:HE1	2:X:579:MET:HB3	1.78	0.48
1:B:358:ILE:HG22	1:B:359:SER:N	2.28	0.48
1:B:366:SER:C	1:B:368:LEU:N	2.71	0.48
1:B:488:TYR:CZ	2:X:31:LYS:HB3	2.48	0.48
1:B:632:TRP:O	1:B:633:ARG:C	2.54	0.48
1:C:204:TYR:CE2	1:C:224:PRO:HG3	2.48	0.48
1:C:486:ASN:O	1:C:487:CYS:C	2.55	0.48
2:T:38:ASP:O	2:T:42:GLN:HG2	2.13	0.48
2:T:463:VAL:HG23	2:T:468:ILE:HD12	1.94	0.48
2:T:521:TYR:HE1	2:T:579:MET:HB3	1.78	0.48
2:X:278:LEU:C	2:X:280:SER:N	2.71	0.48
2:Z:38:ASP:O	2:Z:42:GLN:HG2	2.13	0.48
2:Z:293:VAL:HG12	2:Z:423:LEU:HD22	1.95	0.48
2:Z:407:ILE:HG13	2:Z:408:MET:SD	2.53	0.48
1:A:358:ILE:HG22	1:A:359:SER:N	2.28	0.48
1:C:743:CYS:SG	1:C:749:CYS:C	2.96	0.48
1:C:744:GLY:O	1:C:746:SER:N	2.43	0.48
2:T:356:PHE:CE2	2:T:383:MET:HG2	2.48	0.48
2:T:462:MET:HE2	2:T:468:ILE:HD11	1.94	0.48
2:X:81:GLN:HE21	2:X:101:GLN:HA	1.78	0.48
2:Z:72:PHE:CE1	2:Z:76:GLN:HG3	2.49	0.48
2:Z:91:LEU:O	2:Z:95:LEU:HG	2.14	0.48
1:A:95:THR:HG21	1:A:186:PHE:N	2.29	0.48
1:B:58:PHE:O	1:B:59:PHE:C	2.55	0.48
1:B:95:THR:O	1:B:96:GLU:C	2.56	0.48
1:B:236:ARG:O	1:B:237:PHE:HB3	2.13	0.48
1:B:353:TRP:CZ2	1:B:466:ARG:HA	2.48	0.48
1:B:457:ARG:HH12	1:B:460:LYS:HA	1.77	0.48
1:B:833:PHE:C	1:B:835:LYS:H	2.22	0.48
1:C:66:HIS:CE1	1:C:264:ASP:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:TRP:CE2	1:C:493:SER:HB2	2.48	0.48
1:C:854:LYS:O	1:C:856:ASN:N	2.43	0.48
2:X:570:LEU:O	2:X:571:GLU:C	2.56	0.48
2:Z:48:TRP:O	2:Z:49:ASN:C	2.55	0.48
2:Z:474:MET:HG3	2:Z:495:GLU:HA	1.94	0.48
1:A:207:HIS:O	1:A:209:PRO:HD3	2.14	0.48
1:A:329:PHE:HB2	1:A:528:LYS:O	2.14	0.48
1:B:957:GLN:HE22	1:C:765:ARG:CD	2.26	0.48
1:C:105:ILE:HG23	1:C:106:PHE:N	2.29	0.48
2:T:91:LEU:O	2:T:95:LEU:HG	2.14	0.48
2:T:120:LEU:O	2:T:121:ASN:C	2.57	0.48
2:T:168:TRP:CE3	2:T:172:VAL:HG21	2.49	0.48
2:T:407:ILE:HG13	2:T:408:MET:SD	2.53	0.48
2:T:439:LEU:O	2:T:440:LEU:C	2.54	0.48
2:T:460:ARG:O	2:T:461:TRP:C	2.57	0.48
2:X:75:GLU:O	2:X:78:THR:HB	2.14	0.48
2:Z:414:THR:C	2:Z:416:LYS:N	2.70	0.48
1:B:385:THR:HG23	1:B:386:LYS:HD2	1.95	0.48
1:C:353:TRP:CZ2	1:C:466:ARG:HA	2.48	0.48
1:C:408:SER:O	1:C:409:GLN:C	2.56	0.48
2:T:101:GLN:O	2:T:102:GLN:C	2.56	0.48
2:T:112:LYS:O	2:T:113:SER:C	2.56	0.48
2:T:491:VAL:HG13	2:T:492:PRO:O	2.13	0.48
2:T:505:HIS:H	2:T:505:HIS:HD2	1.62	0.48
2:T:570:LEU:O	2:T:571:GLU:C	2.57	0.48
2:X:41:TYR:CE2	2:X:45:LEU:HD22	2.49	0.48
2:Z:228:HIS:O	2:Z:231:GLU:HG2	2.13	0.48
2:Z:462:MET:HE3	2:Z:467:GLU:HB3	1.95	0.48
2:Z:470:LYS:O	2:Z:472:GLN:N	2.45	0.48
1:A:366:SER:C	1:A:368:LEU:N	2.71	0.48
1:A:381:GLY:HA3	1:A:429:PHE:HB3	1.96	0.48
1:A:393:THR:HB	1:A:517:LEU:H	1.78	0.48
1:B:408:SER:O	1:B:409:GLN:C	2.56	0.48
1:B:439:ASN:OD1	1:B:505:GLN:HG2	2.14	0.48
1:B:819:GLU:O	1:B:823:PHE:HD1	1.96	0.48
1:C:424:LYS:O	1:C:463:PRO:HA	2.14	0.48
1:C:558:PHE:CE2	1:C:563:GLN:O	2.67	0.48
1:C:936:ASP:O	1:C:938:LEU:N	2.46	0.48
2:T:285:PHE:CD1	2:T:433:GLU:HB3	2.49	0.48
2:X:25:ALA:C	2:X:27:THR:H	2.21	0.48
2:X:116:LEU:HD12	2:X:119:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:275:TRP:CB	2:X:444:LEU:HD22	2.44	0.48
2:X:370:LEU:HD21	2:X:413:ALA:HB2	1.96	0.48
2:X:414:THR:C	2:X:416:LYS:N	2.70	0.48
2:X:465:LYS:HE3	2:X:465:LYS:HB3	1.53	0.48
2:X:504:PHE:O	2:X:505:HIS:C	2.57	0.48
1:A:328:ARG:H	1:A:328:ARG:HG2	1.46	0.48
1:A:385:THR:C	1:A:387:LEU:N	2.70	0.48
1:A:444:LYS:HB3	1:A:444:LYS:HE3	1.71	0.48
1:A:966:LEU:HD23	1:A:1000:ARG:HD3	1.96	0.48
1:B:36:VAL:HG11	1:B:219:PHE:HZ	1.78	0.48
1:B:522:THR:HG23	1:B:523:VAL:N	2.27	0.48
1:B:567:ASP:C	1:B:569:VAL:H	2.21	0.48
1:C:186:PHE:HD1	1:C:187:LYS:HB3	1.79	0.48
1:C:353:TRP:CE2	1:C:466:ARG:HA	2.49	0.48
1:C:392:PHE:O	1:C:393:THR:C	2.56	0.48
1:C:393:THR:HB	1:C:517:LEU:H	1.79	0.48
2:X:72:PHE:CE1	2:X:76:GLN:HG3	2.49	0.48
2:X:97:LEU:HD23	2:X:97:LEU:HA	1.71	0.48
2:Z:116:LEU:O	2:Z:117:ASN:C	2.56	0.48
2:Z:120:LEU:O	2:Z:121:ASN:C	2.57	0.48
2:Z:370:LEU:HD21	2:Z:413:ALA:HB2	1.96	0.48
1:A:20:ASN:O	1:A:22:ILE:N	2.47	0.48
1:A:103:GLY:N	1:A:240:LEU:HB2	2.28	0.48
1:A:352:ALA:O	1:A:354:ASN:N	2.47	0.48
1:A:374:PHE:O	1:A:376:ALA:N	2.47	0.48
1:B:393:THR:HB	1:B:517:LEU:H	1.78	0.48
2:T:41:TYR:CE2	2:T:45:LEU:HD22	2.49	0.48
2:T:149:ASN:O	2:T:150:GLU:C	2.56	0.48
2:X:92:THR:HG22	2:X:96:GLN:HE22	1.77	0.48
2:X:560:LEU:O	2:X:561:GLY:C	2.56	0.48
2:Z:168:TRP:CE3	2:Z:172:VAL:HG21	2.49	0.48
2:Z:462:MET:O	2:Z:465:LYS:N	2.46	0.48
2:Z:474:MET:HE1	2:Z:499:ASP:OD2	2.14	0.48
2:Z:504:PHE:O	2:Z:505:HIS:C	2.57	0.48
1:A:141:LEU:HD12	1:A:240:LEU:HB3	1.96	0.48
1:A:353:TRP:CE2	1:A:466:ARG:HA	2.49	0.48
1:A:1057:PRO:O	1:A:1058:HIS:HB2	2.14	0.48
1:B:542:PHE:CD1	1:B:578:PRO:HD3	2.44	0.48
1:B:744:GLY:O	1:B:746:SER:N	2.47	0.48
1:B:828:LEU:HG	1:B:829:ALA:N	2.25	0.48
1:C:114:THR:O	1:C:132:GLU:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1028:LYS:O	1:C:1032:CYS:HB2	2.14	0.48
2:T:116:LEU:HD12	2:T:119:ILE:HD12	1.96	0.48
2:X:120:LEU:O	2:X:121:ASN:C	2.57	0.48
2:X:356:PHE:CE2	2:X:383:MET:HG2	2.48	0.48
2:X:407:ILE:HG13	2:X:408:MET:SD	2.53	0.48
2:X:435:GLU:C	2:X:437:ASN:H	2.22	0.48
2:X:474:MET:HG3	2:X:495:GLU:HA	1.94	0.48
2:Z:278:LEU:C	2:Z:280:SER:N	2.71	0.48
1:A:353:TRP:CZ2	1:A:466:ARG:HA	2.48	0.47
1:A:439:ASN:OD1	1:A:505:GLN:HG2	2.14	0.47
1:A:749:CYS:HB2	1:A:977:LEU:HD21	1.96	0.47
1:A:834:ILE:CD1	1:C:613:GLY:HA2	2.44	0.47
1:B:83:VAL:O	1:B:236:ARG:NH1	2.47	0.47
1:B:112:SER:N	1:B:134:GLN:HA	2.29	0.47
1:B:1091:ARG:O	1:B:1092:GLU:HG2	2.13	0.47
1:C:396:TYR:HD1	1:C:513:SER:O	1.97	0.47
1:C:437:ASN:HB2	1:C:507:TYR:CE1	2.48	0.47
2:T:72:PHE:CE1	2:T:76:GLN:HG3	2.49	0.47
2:T:435:GLU:C	2:T:437:ASN:H	2.22	0.47
2:X:101:GLN:O	2:X:102:GLN:C	2.56	0.47
2:X:228:HIS:O	2:X:229:THR:C	2.55	0.47
2:X:527:GLU:O	2:X:528:ALA:HB2	2.14	0.47
2:X:537:GLY:O	2:X:538:PRO:C	2.56	0.47
2:Z:81:GLN:HE21	2:Z:101:GLN:HA	1.78	0.47
2:Z:275:TRP:CB	2:Z:444:LEU:HD22	2.44	0.47
2:Z:356:PHE:CE2	2:Z:383:MET:HG2	2.48	0.47
1:A:95:THR:CG2	1:A:189:LEU:HA	2.44	0.47
1:A:188:ASN:HD21	1:A:207:HIS:CB	2.26	0.47
1:A:271:GLN:HE21	1:A:271:GLN:HB3	1.52	0.47
1:B:189:LEU:O	1:B:190:ARG:HD3	2.15	0.47
1:C:171:VAL:O	1:C:172:SER:HB3	2.13	0.47
1:C:188:ASN:HD22	1:C:188:ASN:HA	1.51	0.47
1:C:326:ILE:C	1:C:327:VAL:HG22	2.39	0.47
1:C:1144:GLU:C	1:C:1146:ASP:N	2.72	0.47
2:T:215:TYR:HD1	2:T:577:LYS:HZ1	1.59	0.47
2:X:460:ARG:O	2:X:461:TRP:C	2.57	0.47
2:X:462:MET:HE3	2:X:467:GLU:HB3	1.95	0.47
2:X:609:ASP:O	2:X:610:TRP:C	2.57	0.47
2:Z:75:GLU:O	2:Z:78:THR:HB	2.14	0.47
2:Z:335:ASP:CB	2:Z:336:PRO:HD2	2.45	0.47
1:A:385:THR:HG23	1:A:386:LYS:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:ILE:O	1:A:624:HIS:C	2.56	0.47
1:B:238:GLN:HG2	1:B:239:THR:N	2.29	0.47
1:B:352:ALA:O	1:B:354:ASN:N	2.47	0.47
1:B:374:PHE:O	1:B:376:ALA:N	2.47	0.47
1:B:458:LYS:HA	1:B:458:LYS:HD3	1.61	0.47
1:C:232:ILE:HG13	1:C:234:ILE:HG13	1.96	0.47
1:C:530:THR:HG22	1:C:531:ASN:OD1	2.15	0.47
1:C:632:TRP:O	1:C:634:VAL:N	2.47	0.47
2:T:81:GLN:HE21	2:T:101:GLN:HA	1.78	0.47
2:T:169:ARG:HB2	2:T:169:ARG:HH21	1.80	0.47
2:T:285:PHE:C	2:T:287:GLN:N	2.68	0.47
2:T:315:PHE:HE1	2:T:408:MET:HE3	1.78	0.47
2:T:504:PHE:O	2:T:505:HIS:C	2.57	0.47
2:X:150:GLU:HG2	2:X:154:ASN:CG	2.39	0.47
2:Z:41:TYR:CE2	2:Z:45:LEU:HD22	2.49	0.47
2:Z:101:GLN:O	2:Z:102:GLN:C	2.56	0.47
2:Z:150:GLU:HG2	2:Z:154:ASN:CG	2.39	0.47
2:Z:276:THR:HB	2:Z:445:THR:HG23	1.96	0.47
2:Z:435:GLU:C	2:Z:437:ASN:H	2.22	0.47
1:B:84:LEU:HD12	1:B:265:TYR:OH	2.15	0.47
1:B:225:LEU:O	1:B:226:VAL:HB	2.14	0.47
1:B:395:VAL:HG22	1:B:514:PHE:HA	1.96	0.47
1:B:396:TYR:HD1	1:B:513:SER:O	1.97	0.47
1:C:536:LYS:O	1:C:538:VAL:N	2.47	0.47
1:C:934:ILE:O	1:C:935:GLN:C	2.57	0.47
2:T:48:TRP:O	2:T:49:ASN:C	2.55	0.47
2:T:162:LEU:O	2:T:166:GLU:N	2.44	0.47
2:T:253:PRO:HD2	2:T:255:TYR:HD2	1.80	0.47
2:T:335:ASP:CB	2:T:336:PRO:HD2	2.45	0.47
2:T:462:MET:HE3	2:T:467:GLU:HB3	1.95	0.47
2:T:584:LEU:C	2:T:586:ASN:H	2.22	0.47
2:X:520:LEU:O	2:X:524:GLN:HG3	2.14	0.47
2:Z:112:LYS:O	2:Z:113:SER:C	2.56	0.47
2:Z:250:ASN:C	2:Z:252:TYR:H	2.23	0.47
1:A:190:ARG:HB3	1:A:192:PHE:HE1	1.76	0.47
1:A:194:PHE:HD1	1:A:203:ILE:HG23	1.79	0.47
1:A:475:ALA:HB3	1:A:485:PRO:CG	2.43	0.47
1:C:385:THR:HG23	1:C:386:LYS:HD2	1.96	0.47
1:C:558:PHE:O	1:C:562:GLN:NE2	2.47	0.47
1:C:1105:THR:HG21	1:C:1110:TYR:HA	1.96	0.47
2:T:275:TRP:CB	2:T:444:LEU:HD22	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:414:THR:O	2:T:415:PRO:C	2.57	0.47
2:X:335:ASP:CB	2:X:336:PRO:HD2	2.45	0.47
2:X:472:GLN:NE2	2:X:476:LYS:HG2	2.30	0.47
2:X:476:LYS:O	2:X:480:MET:HG3	2.15	0.47
2:Z:277:ASN:OD1	2:Z:277:ASN:N	2.44	0.47
2:Z:591:LEU:C	2:Z:593:THR:N	2.72	0.47
1:B:830:ASP:HB3	1:B:831:ALA:H	1.45	0.47
1:C:395:VAL:HG22	1:C:514:PHE:HA	1.96	0.47
1:C:779:GLN:O	1:C:779:GLN:HG2	2.14	0.47
1:C:933:LYS:HB2	1:C:933:LYS:HE2	1.83	0.47
2:T:75:GLU:O	2:T:78:THR:HB	2.14	0.47
2:T:116:LEU:O	2:T:117:ASN:C	2.56	0.47
2:T:150:GLU:HG2	2:T:154:ASN:CG	2.39	0.47
2:T:205:GLY:O	2:T:206:ASP:C	2.58	0.47
2:T:228:HIS:O	2:T:231:GLU:HG2	2.13	0.47
2:T:259:ILE:O	2:T:607:SER:N	2.47	0.47
2:T:472:GLN:NE2	2:T:476:LYS:HG2	2.30	0.47
2:X:91:LEU:O	2:X:95:LEU:HG	2.14	0.47
2:X:239:HIS:HD2	2:X:592:PHE:HE1	1.62	0.47
2:Z:112:LYS:NZ	2:Z:189:GLU:HG2	2.29	0.47
2:Z:163:TRP:O	2:Z:167:SER:N	2.48	0.47
2:Z:520:LEU:O	2:Z:524:GLN:HG3	2.14	0.47
2:Z:539:LEU:C	2:Z:541:LYS:N	2.71	0.47
1:A:107:GLY:N	1:A:234:ILE:HA	2.29	0.47
1:A:521:ALA:O	1:A:522:THR:C	2.58	0.47
1:A:660:GLU:HG2	1:A:661:CYS:H	1.80	0.47
1:A:869:MET:HE1	1:C:697:MET:HG3	1.97	0.47
1:A:988:GLU:O	1:A:991:VAL:HG13	2.15	0.47
1:A:996:LEU:C	1:A:998:THR:H	2.22	0.47
1:B:312:ILE:HD12	1:B:597:ILE:HG12	1.97	0.47
1:B:391:CYS:C	1:B:521:ALA:HB1	2.40	0.47
1:B:428:ASP:OD1	1:B:428:ASP:N	2.48	0.47
1:B:483:LYS:HA	2:X:24:GLN:HG2	1.97	0.47
1:B:532:LEU:HD12	1:B:532:LEU:HA	1.77	0.47
1:B:852:ALA:HA	1:B:855:PHE:CZ	2.49	0.47
1:B:889:GLY:HA3	1:B:1034:LEU:HD23	1.97	0.47
1:B:939:PHE:CG	1:B:940:SER:N	2.83	0.47
1:C:374:PHE:O	1:C:376:ALA:N	2.47	0.47
1:C:476:GLY:CA	1:C:484:GLY:HA3	2.44	0.47
2:T:57:GLU:H	2:T:57:GLU:HG3	1.39	0.47
2:T:520:LEU:O	2:T:524:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:162:LEU:O	2:X:166:GLU:N	2.44	0.47
2:X:163:TRP:O	2:X:167:SER:N	2.48	0.47
2:X:169:ARG:HH21	2:X:169:ARG:HB2	1.79	0.47
2:X:253:PRO:HD2	2:X:255:TYR:HD2	1.80	0.47
2:X:264:ALA:HB3	2:X:490:PRO:CG	2.45	0.47
2:X:276:THR:O	2:X:278:LEU:N	2.47	0.47
2:Z:408:MET:C	2:Z:410:LEU:H	2.23	0.47
2:Z:460:ARG:O	2:Z:461:TRP:C	2.57	0.47
2:Z:465:LYS:HB3	2:Z:465:LYS:HE3	1.53	0.47
2:Z:570:LEU:O	2:Z:571:GLU:C	2.57	0.47
1:B:81:ASN:HB3	1:B:265:TYR:OH	2.14	0.47
1:B:128:ILE:O	1:B:129:LYS:HB2	2.15	0.47
1:B:486:ASN:O	1:B:487:CYS:C	2.56	0.47
1:C:26:GLN:O	1:C:27:SER:HB2	2.15	0.47
1:C:676:GLN:N	1:C:689:SER:O	2.48	0.47
2:T:116:LEU:HD12	2:T:116:LEU:HA	1.80	0.47
2:T:609:ASP:O	2:T:610:TRP:C	2.57	0.47
2:X:112:LYS:O	2:X:113:SER:C	2.56	0.47
2:X:205:GLY:C	2:X:207:TYR:N	2.73	0.47
2:X:276:THR:HB	2:X:445:THR:HG23	1.96	0.47
2:X:414:THR:O	2:X:415:PRO:C	2.57	0.47
2:X:593:THR:C	2:X:595:LEU:N	2.72	0.47
2:Z:25:ALA:C	2:Z:27:THR:H	2.21	0.47
2:Z:116:LEU:HD12	2:Z:119:ILE:HD12	1.96	0.47
2:Z:155:SER:OG	2:Z:156:LEU:N	2.48	0.47
2:Z:293:VAL:O	2:Z:294:THR:C	2.58	0.47
2:Z:609:ASP:O	2:Z:610:TRP:C	2.57	0.47
1:A:204:TYR:HB3	1:A:223:GLU:O	2.15	0.47
1:A:361:CYS:O	1:A:362:VAL:C	2.58	0.47
1:A:534:LYS:HG2	1:A:535:ASN:OD1	2.15	0.47
1:A:620:SER:OG	1:A:630:PRO:HD2	2.14	0.47
1:A:810:SER:OG	1:A:811:LYS:N	2.46	0.47
1:A:953:ASN:O	1:A:957:GLN:HG3	2.15	0.47
1:A:1144:GLU:O	1:A:1146:ASP:N	2.48	0.47
1:B:164:ASN:O	1:B:165:ASN:C	2.58	0.47
1:B:353:TRP:CE2	1:B:466:ARG:HA	2.49	0.47
1:B:854:LYS:HE2	1:B:854:LYS:HB3	1.71	0.47
2:T:112:LYS:NZ	2:T:189:GLU:HG2	2.29	0.47
2:T:239:HIS:HD2	2:T:592:PHE:HE1	1.63	0.47
2:T:370:LEU:HD21	2:T:413:ALA:HB2	1.96	0.47
2:T:408:MET:C	2:T:410:LEU:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:594:TRP:O	2:T:598:GLN:HB2	2.14	0.47
2:X:293:VAL:HG12	2:X:423:LEU:HD22	1.95	0.47
2:X:508:ASN:O	2:X:509:ASP:C	2.58	0.47
2:Z:315:PHE:HE1	2:Z:408:MET:HE3	1.78	0.47
2:Z:476:LYS:O	2:Z:480:MET:HG3	2.15	0.47
2:Z:593:THR:C	2:Z:595:LEU:N	2.72	0.47
2:Z:607:SER:O	2:Z:608:THR:C	2.58	0.47
1:A:58:PHE:O	1:A:59:PHE:C	2.57	0.47
1:A:118:LEU:O	1:A:120:VAL:N	2.48	0.47
1:A:847:ARG:NH1	1:C:556:LYS:HZ3	2.13	0.47
1:A:940:SER:O	1:A:941:THR:C	2.56	0.47
1:B:351:TYR:CE2	1:B:491:LEU:HD11	2.50	0.47
1:B:381:GLY:HA3	1:B:429:PHE:HB3	1.96	0.47
1:B:992:GLN:C	1:B:994:ASP:H	2.22	0.47
1:C:299:THR:O	1:C:303:LEU:HG	2.15	0.47
1:C:532:LEU:O	1:C:536:LYS:HD2	2.15	0.47
1:C:542:PHE:HZ	1:C:584:LEU:HD21	1.80	0.47
1:C:640:ASN:OD1	1:C:640:ASN:N	2.48	0.47
1:C:752:LEU:HD21	1:C:990:GLU:HG3	1.96	0.47
1:C:834:ILE:O	1:C:834:ILE:HG23	2.14	0.47
2:T:288:LYS:HD2	2:T:433:GLU:HB2	1.96	0.47
2:Z:253:PRO:HD2	2:Z:255:TYR:HD2	1.80	0.47
2:Z:470:LYS:HA	2:Z:473:TRP:CG	2.50	0.47
1:A:529:SER:O	1:A:530:THR:HG23	2.15	0.46
1:A:635:TYR:H	1:A:635:TYR:HD1	1.64	0.46
1:B:111:ASP:HB3	1:B:113:LYS:HZ3	1.80	0.46
1:B:403:LYS:HB3	1:B:403:LYS:HE2	1.67	0.46
1:B:553:LYS:O	1:B:554:SER:HB2	2.16	0.46
1:C:542:PHE:HE2	1:C:577:ASP:HA	1.80	0.46
1:C:1116:THR:HG22	1:C:1138:TYR:HD2	1.79	0.46
2:T:163:TRP:O	2:T:167:SER:N	2.48	0.46
2:T:264:ALA:HB3	2:T:490:PRO:CG	2.45	0.46
2:T:470:LYS:HA	2:T:473:TRP:CG	2.50	0.46
2:T:527:GLU:O	2:T:528:ALA:HB2	2.14	0.46
2:X:25:ALA:O	2:X:28:PHE:N	2.48	0.46
2:Z:264:ALA:HB3	2:Z:490:PRO:CG	2.45	0.46
1:A:24:THR:CA	1:A:80:ASP:HB3	2.44	0.46
1:A:107:GLY:H	1:A:234:ILE:HB	1.80	0.46
1:A:205:SER:OG	1:A:206:LYS:N	2.48	0.46
1:A:851:CYS:O	1:A:854:LYS:HB2	2.15	0.46
1:A:935:GLN:HE21	1:A:935:GLN:HB3	1.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:ILE:HG23	1:B:1000:ARG:HB2	1.97	0.46
1:C:352:ALA:O	1:C:354:ASN:N	2.47	0.46
1:C:359:SER:O	1:C:360:ASN:HB2	2.15	0.46
1:C:391:CYS:CB	1:C:524:CYS:HA	2.30	0.46
1:C:400:PHE:HE2	1:C:423:TYR:CE1	2.34	0.46
1:C:423:TYR:HE2	1:C:425:LEU:HD21	1.80	0.46
1:C:441:LEU:HG	1:C:442:ASP:N	2.29	0.46
1:C:479:PRO:O	1:C:480:CYS:HB2	2.15	0.46
1:C:483:LYS:HA	1:C:488:TYR:CD2	2.42	0.46
1:C:655:VAL:CG2	1:C:695:TYR:HB3	2.45	0.46
1:C:743:CYS:O	1:C:745:ASP:N	2.48	0.46
2:T:128:SER:C	2:T:130:GLY:H	2.23	0.46
2:T:276:THR:HB	2:T:445:THR:HG23	1.96	0.46
2:X:110:GLU:O	2:X:111:ASP:C	2.59	0.46
2:X:539:LEU:C	2:X:541:LYS:N	2.71	0.46
2:Z:508:ASN:O	2:Z:509:ASP:C	2.58	0.46
1:A:20:ASN:C	1:A:22:ILE:N	2.70	0.46
1:A:216:PRO:O	1:A:217:GLN:C	2.59	0.46
1:A:396:TYR:HD1	1:A:513:SER:O	1.97	0.46
1:A:855:PHE:CE1	1:C:588:PRO:HG2	2.51	0.46
1:B:543:ASN:OD1	1:B:543:ASN:N	2.47	0.46
1:C:56:LEU:O	1:C:57:PRO:C	2.57	0.46
1:C:400:PHE:HE2	1:C:423:TYR:CZ	2.33	0.46
1:C:850:ILE:O	1:C:852:ALA:N	2.48	0.46
1:C:974:SER:O	1:C:980:ILE:HD11	2.15	0.46
2:T:25:ALA:O	2:T:28:PHE:N	2.48	0.46
2:T:508:ASN:O	2:T:509:ASP:C	2.58	0.46
2:X:204:ARG:O	2:X:219:ARG:HG2	2.16	0.46
2:X:505:HIS:H	2:X:505:HIS:HD2	1.62	0.46
2:Z:25:ALA:O	2:Z:28:PHE:N	2.48	0.46
2:Z:68:LYS:O	2:Z:71:ALA:N	2.49	0.46
2:Z:472:GLN:NE2	2:Z:476:LYS:HG2	2.30	0.46
2:Z:505:HIS:HA	2:Z:510:TYR:HD2	1.81	0.46
1:A:128:ILE:HG12	1:A:170:TYR:HD2	1.80	0.46
1:B:112:SER:N	1:B:113:LYS:HZ2	2.14	0.46
1:B:353:TRP:HB3	1:B:423:TYR:HD2	1.81	0.46
1:B:471:GLU:O	1:B:472:ILE:C	2.58	0.46
1:B:521:ALA:O	1:B:522:THR:C	2.58	0.46
1:B:955:ASN:O	1:B:958:ALA:HB3	2.15	0.46
1:C:214:ASP:O	1:C:216:PRO:N	2.48	0.46
1:C:387:LEU:HD12	1:C:387:LEU:HA	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:68:LYS:O	2:T:71:ALA:N	2.49	0.46
2:T:402:GLU:O	2:T:403:ALA:C	2.59	0.46
2:X:455:MET:HB3	2:X:455:MET:HE3	1.54	0.46
2:Z:351:LEU:HD13	2:Z:355:ASP:HB3	1.98	0.46
2:Z:594:TRP:O	2:Z:598:GLN:HB2	2.14	0.46
1:A:64:TRP:HE1	1:A:214:ASP:CG	2.23	0.46
1:A:346:ARG:H	1:A:346:ARG:HG2	1.46	0.46
1:A:703:ASN:O	1:B:789:TYR:HA	2.16	0.46
1:B:54:LEU:HD23	1:B:272:PRO:HA	1.98	0.46
1:B:1057:PRO:O	1:B:1058:HIS:HB2	2.15	0.46
1:C:83:VAL:HG12	1:C:236:ARG:HB3	1.96	0.46
1:C:200:TYR:O	1:C:201:PHE:C	2.57	0.46
1:C:358:ILE:HG22	1:C:394:ASN:HB2	1.97	0.46
2:T:142:LEU:HD21	2:T:163:TRP:HH2	1.80	0.46
2:T:505:HIS:HA	2:T:510:TYR:HD2	1.81	0.46
2:X:142:LEU:HD21	2:X:163:TRP:HH2	1.80	0.46
2:X:594:TRP:O	2:X:598:GLN:HB2	2.14	0.46
2:Z:110:GLU:O	2:Z:111:ASP:C	2.59	0.46
2:Z:259:ILE:O	2:Z:607:SER:N	2.47	0.46
1:A:31:SER:N	1:A:60:SER:O	2.49	0.46
1:A:522:THR:HG23	1:A:523:VAL:N	2.27	0.46
1:A:653:GLU:HG3	1:A:693:ILE:HG22	1.97	0.46
1:B:108:THR:HA	1:B:235:THR:HG22	1.96	0.46
1:B:977:LEU:HD23	1:B:993:ILE:HG23	1.97	0.46
1:C:122:ASN:HB2	1:C:127:PHE:CD1	2.50	0.46
1:C:485:PRO:HD2	1:C:488:TYR:CE2	2.50	0.46
2:T:317:SER:C	2:T:319:GLY:N	2.74	0.46
2:T:560:LEU:O	2:T:561:GLY:C	2.56	0.46
2:X:205:GLY:O	2:X:206:ASP:C	2.58	0.46
2:X:288:LYS:HE2	2:X:433:GLU:HB2	1.97	0.46
2:X:470:LYS:HA	2:X:473:TRP:CG	2.50	0.46
2:Z:142:LEU:HD21	2:Z:163:TRP:HH2	1.80	0.46
2:Z:162:LEU:O	2:Z:166:GLU:N	2.44	0.46
2:Z:205:GLY:C	2:Z:207:TYR:N	2.72	0.46
1:A:353:TRP:HB3	1:A:423:TYR:HD2	1.81	0.46
1:A:391:CYS:C	1:A:521:ALA:HB1	2.40	0.46
1:A:395:VAL:HG22	1:A:514:PHE:HA	1.96	0.46
1:A:944:ALA:C	1:A:946:GLY:H	2.24	0.46
1:B:558:PHE:N	1:B:558:PHE:CD1	2.83	0.46
1:B:595:SER:OG	1:B:612:GLN:NE2	2.49	0.46
1:C:420:ASP:HA	1:C:460:LYS:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:ALA:O	1:C:522:THR:C	2.58	0.46
1:C:532:LEU:HG	1:C:536:LYS:HB2	1.97	0.46
2:T:250:ASN:C	2:T:252:TYR:H	2.23	0.46
2:T:379:ILE:O	2:T:383:MET:HG3	2.16	0.46
2:T:591:LEU:C	2:T:593:THR:N	2.72	0.46
2:T:593:THR:C	2:T:595:LEU:N	2.72	0.46
2:X:250:ASN:C	2:X:252:TYR:H	2.23	0.46
2:X:295:ASP:O	2:X:298:VAL:N	2.49	0.46
2:X:379:ILE:O	2:X:383:MET:HG3	2.15	0.46
2:X:402:GLU:O	2:X:403:ALA:C	2.59	0.46
2:Z:137:ASN:C	2:Z:139:GLN:H	2.24	0.46
2:Z:205:GLY:O	2:Z:206:ASP:C	2.58	0.46
2:Z:241:HIS:HB3	2:Z:606:TRP:CZ3	2.51	0.46
2:Z:537:GLY:O	2:Z:538:PRO:C	2.56	0.46
1:A:188:ASN:HB3	1:A:190:ARG:NH2	2.31	0.46
1:A:428:ASP:OD1	1:A:428:ASP:N	2.48	0.46
1:A:575:VAL:CG2	1:A:586:ILE:HD11	2.43	0.46
1:A:620:SER:O	1:A:620:SER:OG	2.30	0.46
1:A:753:LEU:HB2	1:A:997:ILE:HD11	1.98	0.46
1:A:877:LEU:O	1:A:881:THR:HG22	2.16	0.46
1:A:900:MET:HE3	1:A:900:MET:HB3	1.72	0.46
1:A:939:PHE:O	1:A:940:SER:C	2.59	0.46
1:A:969:LYS:HD2	1:A:974:SER:HA	1.98	0.46
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.98	0.46
1:B:110:LEU:HD22	1:B:135:PHE:CZ	2.50	0.46
1:B:1114:ILE:HG22	1:B:1116:THR:HG23	1.98	0.46
1:C:264:ASP:O	1:C:266:TYR:N	2.49	0.46
1:C:391:CYS:C	1:C:521:ALA:HB1	2.40	0.46
1:C:542:PHE:O	1:C:545:LEU:HG	2.16	0.46
1:C:987:PRO:HG2	1:C:988:GLU:CD	2.41	0.46
2:T:90:ASN:O	2:T:94:LYS:HG3	2.16	0.46
2:T:110:GLU:O	2:T:111:ASP:C	2.59	0.46
2:T:554:LEU:HD12	2:T:554:LEU:HA	1.76	0.46
2:X:112:LYS:NZ	2:X:189:GLU:HG2	2.29	0.46
2:X:431:ASP:OD1	2:X:434:THR:HB	2.16	0.46
2:Z:131:LYS:HB3	2:Z:131:LYS:HE2	1.43	0.46
2:Z:169:ARG:HH21	2:Z:169:ARG:HB2	1.79	0.46
1:A:102:ARG:HB2	1:A:141:LEU:HD13	1.98	0.46
1:A:707:TYR:HB2	1:B:883:THR:HG22	1.97	0.46
1:B:588:PRO:HG3	1:C:855:PHE:CD1	2.50	0.46
1:C:84:LEU:HD13	1:C:85:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:TYR:HA	1:C:493:SER:OG	2.16	0.46
1:C:483:LYS:CA	1:C:488:TYR:HD2	2.25	0.46
1:C:552:THR:OG1	1:C:553:LYS:N	2.48	0.46
2:T:136:ASP:O	2:T:137:ASN:HB2	2.16	0.46
2:T:204:ARG:O	2:T:219:ARG:HG2	2.16	0.46
2:T:295:ASP:O	2:T:298:VAL:N	2.49	0.46
2:T:304:ALA:C	2:T:306:ARG:H	2.24	0.46
2:T:476:LYS:O	2:T:480:MET:HG3	2.15	0.46
2:T:593:THR:C	2:T:595:LEU:H	2.24	0.46
2:X:131:LYS:HE2	2:X:131:LYS:HB3	1.43	0.46
2:X:351:LEU:HD13	2:X:355:ASP:HB3	1.98	0.46
2:X:584:LEU:C	2:X:586:ASN:H	2.23	0.46
2:Z:535:HIS:CG	2:Z:536:GLU:H	2.34	0.46
1:A:193:VAL:HG22	1:A:222:LEU:HD22	1.98	0.46
1:A:534:LYS:HE2	1:A:534:LYS:O	2.16	0.46
1:A:937:SER:O	1:A:938:LEU:C	2.59	0.46
1:B:65:PHE:CZ	1:B:84:LEU:HD11	2.51	0.46
1:B:131:CYS:HG	1:B:163:ALA:N	2.14	0.46
1:B:556:LYS:HZ2	1:C:847:ARG:NH1	2.13	0.46
1:B:1117:THR:H	1:B:1137:VAL:CG1	2.29	0.46
1:C:421:TYR:CD2	1:C:457:ARG:HB2	2.50	0.46
1:C:604:SER:OG	1:C:606:GLN:HG2	2.16	0.46
2:T:432:ASN:C	2:T:434:THR:H	2.24	0.46
2:T:468:ILE:HG21	2:T:476:LYS:HG3	1.98	0.46
2:T:594:TRP:NE1	2:T:598:GLN:HE21	2.14	0.46
2:X:338:ASN:C	2:X:340:GLN:N	2.74	0.46
2:Z:276:THR:O	2:Z:278:LEU:N	2.47	0.46
2:Z:304:ALA:C	2:Z:306:ARG:H	2.24	0.46
1:A:193:VAL:HG22	1:A:222:LEU:HD23	1.96	0.45
1:A:213:ARG:HH22	1:A:215:PHE:N	2.14	0.45
1:B:63:THR:O	1:B:64:TRP:C	2.59	0.45
1:B:393:THR:H	1:B:516:LEU:HA	1.81	0.45
1:B:977:LEU:O	1:B:978:ASN:C	2.59	0.45
1:C:623:ILE:HD12	1:C:623:ILE:HA	1.64	0.45
1:C:829:ALA:HB3	1:C:952:VAL:HG12	1.98	0.45
1:C:971:GLY:O	1:C:995:ARG:NE	2.49	0.45
2:T:27:THR:O	2:T:28:PHE:C	2.59	0.45
2:T:137:ASN:C	2:T:139:GLN:H	2.24	0.45
2:T:241:HIS:HB3	2:T:606:TRP:CZ3	2.51	0.45
2:T:265:HIS:ND1	2:T:266:LEU:HG	2.31	0.45
2:X:155:SER:OG	2:X:156:LEU:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:246:ALA:HA	2:X:249:MET:SD	2.56	0.45
2:X:304:ALA:C	2:X:306:ARG:H	2.24	0.45
2:Z:204:ARG:O	2:Z:219:ARG:HG2	2.16	0.45
2:Z:295:ASP:O	2:Z:298:VAL:N	2.49	0.45
2:Z:338:ASN:C	2:Z:340:GLN:N	2.74	0.45
2:Z:432:ASN:C	2:Z:434:THR:N	2.74	0.45
1:A:94:SER:O	1:A:190:ARG:HB2	2.16	0.45
1:A:106:PHE:CD2	1:A:234:ILE:CD1	2.99	0.45
1:B:200:TYR:N	1:B:200:TYR:CD1	2.81	0.45
1:B:417:ASN:HD22	1:B:417:ASN:HA	1.63	0.45
1:B:456:PHE:O	1:B:490:PRO:HB3	2.16	0.45
1:B:615:ASN:C	1:B:617:THR:H	2.24	0.45
1:B:831:ALA:HA	1:B:851:CYS:CA	2.45	0.45
1:C:346:ARG:H	1:C:346:ARG:HG2	1.46	0.45
1:C:402:ILE:HD11	1:C:407:VAL:HG12	1.98	0.45
1:C:492:GLN:HB3	2:Z:34:HIS:CE1	2.51	0.45
1:C:542:PHE:O	1:C:544:GLY:N	2.49	0.45
2:T:514:ARG:H	2:T:514:ARG:HG2	1.57	0.45
2:X:81:GLN:C	2:X:83:TYR:N	2.75	0.45
2:X:137:ASN:C	2:X:139:GLN:H	2.24	0.45
2:Z:414:THR:O	2:Z:415:PRO:C	2.57	0.45
2:Z:501:ALA:HA	2:Z:506:VAL:CB	2.46	0.45
2:Z:527:GLU:O	2:Z:528:ALA:HB2	2.14	0.45
2:Z:596:LYS:HB2	2:Z:596:LYS:HE2	1.72	0.45
1:A:85:PRO:HB2	1:A:87:ASN:ND2	2.31	0.45
1:A:201:PHE:CE1	1:A:234:ILE:HD13	2.47	0.45
1:A:403:LYS:HB3	1:A:403:LYS:HE2	1.67	0.45
1:A:534:LYS:HG2	1:A:535:ASN:CG	2.42	0.45
1:C:759:PHE:O	1:C:763:LEU:HG	2.16	0.45
1:C:914:ASN:O	1:C:918:GLU:HB2	2.17	0.45
2:T:278:LEU:C	2:T:280:SER:N	2.71	0.45
2:X:90:ASN:O	2:X:94:LYS:HG3	2.16	0.45
2:X:221:GLN:O	2:X:222:LEU:C	2.59	0.45
2:X:540:HIS:CD2	2:X:540:HIS:C	2.95	0.45
2:X:594:TRP:NE1	2:X:598:GLN:HE21	2.14	0.45
2:X:607:SER:O	2:X:608:THR:C	2.58	0.45
2:Z:239:HIS:HD2	2:Z:592:PHE:HE1	1.63	0.45
2:Z:295:ASP:O	2:Z:298:VAL:HG22	2.17	0.45
1:A:130:VAL:CG1	1:A:168:PHE:HD1	2.27	0.45
1:A:188:ASN:OD1	1:A:209:PRO:HG3	2.17	0.45
1:A:539:ASN:HD22	1:A:539:ASN:HA	1.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:CYS:O	1:B:362:VAL:C	2.58	0.45
1:B:724:THR:HG22	1:B:1063:LEU:HD23	1.98	0.45
1:B:745:ASP:O	1:B:747:THR:N	2.49	0.45
1:C:988:GLU:C	1:C:990:GLU:H	2.25	0.45
2:T:246:ALA:HA	2:T:249:MET:SD	2.57	0.45
2:X:68:LYS:O	2:X:71:ALA:N	2.49	0.45
2:X:95:LEU:C	2:X:97:LEU:N	2.74	0.45
2:X:293:VAL:O	2:X:294:THR:C	2.58	0.45
2:Z:90:ASN:O	2:Z:94:LYS:HG3	2.16	0.45
2:Z:379:ILE:O	2:Z:383:MET:HG3	2.15	0.45
2:Z:402:GLU:O	2:Z:403:ALA:C	2.59	0.45
1:A:208:THR:HB	1:A:210:ILE:HG13	1.98	0.45
1:A:358:ILE:O	1:A:394:ASN:HB2	2.16	0.45
1:A:522:THR:O	1:A:524:CYS:HB2	2.17	0.45
1:A:904:TYR:OH	1:C:1094:VAL:HG13	2.17	0.45
1:B:49:HIS:CD2	1:B:51:THR:HG23	2.51	0.45
1:B:323:THR:CG2	1:B:539:ASN:HB2	2.46	0.45
1:B:402:ILE:HD11	1:B:407:VAL:HG12	1.98	0.45
1:B:429:PHE:C	1:B:431:GLY:H	2.25	0.45
1:B:577:ASP:C	1:B:579:GLN:H	2.25	0.45
1:B:963:VAL:C	1:B:965:GLN:H	2.24	0.45
1:C:168:PHE:HE2	1:C:229:PRO:HG2	1.82	0.45
2:T:221:GLN:O	2:T:222:LEU:C	2.59	0.45
2:T:607:SER:O	2:T:608:THR:C	2.58	0.45
2:X:145:GLU:CB	2:X:146:PRO:HD3	2.28	0.45
2:Z:416:LYS:O	2:Z:419:LYS:N	2.49	0.45
2:Z:589:GLU:O	2:Z:590:PRO:C	2.60	0.45
2:Z:593:THR:C	2:Z:595:LEU:H	2.24	0.45
2:Z:594:TRP:NE1	2:Z:598:GLN:HE21	2.14	0.45
1:A:339:HIS:CD2	1:A:367:VAL:HB	2.52	0.45
1:A:471:GLU:OE2	1:A:472:ILE:N	2.48	0.45
1:A:850:ILE:O	1:A:851:CYS:C	2.60	0.45
1:B:351:TYR:CD2	1:B:491:LEU:HD11	2.51	0.45
1:B:417:ASN:O	1:B:418:ILE:C	2.60	0.45
1:C:121:ASN:HD22	1:C:122:ASN:N	2.15	0.45
1:C:393:THR:H	1:C:516:LEU:HA	1.81	0.45
1:C:740:MET:HA	1:C:745:ASP:HB3	1.99	0.45
1:C:781:VAL:O	1:C:1029:MET:HE3	2.17	0.45
2:T:332:MET:HE2	2:T:332:MET:HB3	1.71	0.45
2:X:241:HIS:HB3	2:X:606:TRP:CZ3	2.51	0.45
2:X:419:LYS:CG	2:X:426:PRO:HA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:494:ASP:OD1	2:X:496:THR:HG23	2.16	0.45
2:X:505:HIS:HA	2:X:510:TYR:HD2	1.81	0.45
2:X:593:THR:C	2:X:595:LEU:H	2.24	0.45
2:Z:136:ASP:O	2:Z:137:ASN:HB2	2.16	0.45
2:Z:477:TRP:CE3	2:Z:500:PRO:HG3	2.50	0.45
2:Z:505:HIS:H	2:Z:505:HIS:HD2	1.62	0.45
1:B:135:PHE:O	1:B:137:ASN:N	2.41	0.45
1:B:458:LYS:HE2	1:B:473:TYR:CE1	2.51	0.45
1:B:579:GLN:HE21	1:B:579:GLN:HB2	1.58	0.45
1:B:825:LYS:HD2	1:B:939:PHE:HA	1.99	0.45
1:C:209:PRO:O	1:C:210:ILE:HG23	2.17	0.45
1:C:819:GLU:O	1:C:823:PHE:HD1	1.99	0.45
2:T:227:GLU:H	2:T:227:GLU:HG2	1.51	0.45
2:X:51:ASN:HD22	2:X:349:TRP:HZ2	1.65	0.45
2:X:198:ASP:OD1	2:X:201:ASP:N	2.50	0.45
2:X:281:LEU:HD23	2:X:281:LEU:HA	1.75	0.45
2:X:332:MET:HE2	2:X:332:MET:HB3	1.71	0.45
2:Z:198:ASP:OD1	2:Z:201:ASP:N	2.50	0.45
2:Z:231:GLU:HA	2:Z:234:LYS:CD	2.47	0.45
2:Z:246:ALA:HA	2:Z:249:MET:SD	2.56	0.45
2:Z:402:GLU:O	2:Z:405:GLY:N	2.49	0.45
1:A:29:THR:HG23	1:A:62:VAL:HG23	1.99	0.45
1:A:43:PHE:HB2	1:C:562:GLN:HG2	1.99	0.45
1:A:104:TRP:HA	1:A:238:GLN:O	2.16	0.45
1:A:114:THR:HG23	1:A:115:GLN:H	1.82	0.45
1:A:422:ASN:O	1:A:423:TYR:HB2	2.17	0.45
1:B:96:GLU:HA	1:B:186:PHE:CD1	2.52	0.45
1:B:213:ARG:NH2	1:B:214:ASP:HB2	2.32	0.45
1:B:299:THR:O	1:B:303:LEU:HG	2.17	0.45
1:B:456:PHE:CE1	1:B:490:PRO:CA	2.96	0.45
1:C:776:LYS:HE3	1:C:776:LYS:HB3	1.64	0.45
2:T:562:LYS:HE3	2:T:562:LYS:HB3	1.65	0.45
2:X:65:ALA:HA	2:X:68:LYS:HB3	1.99	0.45
2:X:94:LYS:HE3	2:X:94:LYS:HB3	1.64	0.45
2:X:259:ILE:O	2:X:607:SER:N	2.47	0.45
2:X:419:LYS:C	2:X:421:ILE:H	2.25	0.45
2:X:421:ILE:HD12	2:X:421:ILE:HA	1.80	0.45
2:Z:56:GLU:O	2:Z:57:GLU:C	2.60	0.45
2:Z:200:GLY:O	2:Z:204:ARG:N	2.50	0.45
2:Z:243:TYR:HB3	2:Z:244:VAL:H	1.50	0.45
2:Z:494:ASP:OD1	2:Z:496:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PHE:CD1	1:A:171:VAL:HG13	2.52	0.45
1:A:440:LYS:HA	1:A:440:LYS:HD2	1.70	0.45
1:A:533:VAL:HG12	1:A:534:LYS:N	2.31	0.45
1:A:937:SER:OG	1:A:938:LEU:N	2.49	0.45
1:C:93:ALA:O	1:C:94:SER:HB2	2.17	0.45
1:C:200:TYR:HD1	1:C:229:PRO:HA	1.82	0.45
1:C:836:GLN:HG3	1:C:849:LEU:HD23	1.99	0.45
2:T:205:GLY:C	2:T:207:TYR:N	2.72	0.45
2:T:419:LYS:C	2:T:421:ILE:H	2.25	0.45
2:T:494:ASP:OD1	2:T:496:THR:HG23	2.16	0.45
2:X:383:MET:HE2	2:X:383:MET:HB3	1.73	0.45
2:X:395:GLY:O	2:X:396:ALA:C	2.60	0.45
2:X:408:MET:C	2:X:410:LEU:H	2.23	0.45
2:X:589:GLU:O	2:X:590:PRO:C	2.60	0.45
2:Z:419:LYS:C	2:Z:421:ILE:H	2.25	0.45
2:Z:468:ILE:HG21	2:Z:476:LYS:HG3	1.98	0.45
1:A:402:ILE:HD11	1:A:407:VAL:HG12	1.98	0.45
1:A:528:LYS:CE	1:A:529:SER:H	2.30	0.45
1:A:545:LEU:HB2	1:A:564:PHE:HE1	1.81	0.45
1:A:847:ARG:HH11	1:C:556:LYS:HA	1.81	0.45
1:B:209:PRO:C	1:B:211:ILE:N	2.75	0.45
1:B:358:ILE:O	1:B:394:ASN:HB2	2.16	0.45
1:B:1144:GLU:C	1:B:1146:ASP:N	2.75	0.45
1:C:522:THR:O	1:C:524:CYS:HB2	2.17	0.45
2:T:351:LEU:HD13	2:T:355:ASP:HB3	1.98	0.45
2:T:416:LYS:O	2:T:419:LYS:N	2.49	0.45
2:T:535:HIS:CG	2:T:536:GLU:H	2.34	0.45
2:X:416:LYS:O	2:X:419:LYS:N	2.50	0.45
2:X:562:LYS:HE3	2:X:562:LYS:HB3	1.65	0.45
2:X:586:ASN:O	2:X:589:GLU:HB2	2.17	0.45
2:Z:265:HIS:ND1	2:Z:266:LEU:HG	2.31	0.45
2:Z:460:ARG:C	2:Z:462:MET:N	2.75	0.45
2:Z:523:PHE:HD2	2:Z:584:LEU:HB2	1.82	0.45
2:Z:588:PHE:O	2:Z:589:GLU:C	2.60	0.45
1:B:110:LEU:N	1:B:110:LEU:HD23	2.32	0.44
1:B:339:HIS:CD2	1:B:367:VAL:HB	2.52	0.44
1:B:365:TYR:HA	1:B:368:LEU:HD22	1.98	0.44
1:B:960:ASN:O	1:B:961:THR:C	2.61	0.44
2:T:47:SER:HA	2:T:62:MET:CE	2.47	0.44
2:T:287:GLN:CG	2:T:288:LYS:HZ1	2.30	0.44
2:T:293:VAL:O	2:T:294:THR:C	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:304:ALA:C	2:T:306:ARG:N	2.75	0.44
2:X:231:GLU:HA	2:X:234:LYS:CD	2.47	0.44
2:X:304:ALA:C	2:X:306:ARG:N	2.75	0.44
2:X:402:GLU:O	2:X:405:GLY:N	2.49	0.44
2:X:503:LEU:O	2:X:506:VAL:HG23	2.18	0.44
2:X:535:HIS:CG	2:X:536:GLU:H	2.34	0.44
2:Z:261:CYS:O	2:Z:610:TRP:HZ3	2.00	0.44
2:Z:540:HIS:CD2	2:Z:540:HIS:C	2.94	0.44
1:A:420:ASP:HB3	1:A:421:TYR:CD2	2.52	0.44
1:A:492:GLN:HB3	2:T:34:HIS:CE1	2.51	0.44
1:A:534:LYS:HD3	1:A:553:LYS:HZ2	1.83	0.44
1:A:1144:GLU:C	1:A:1146:ASP:N	2.66	0.44
1:B:38:TYR:CE2	1:B:285:ILE:HG13	2.52	0.44
1:B:170:TYR:CD1	1:B:170:TYR:C	2.95	0.44
1:B:331:ASN:O	1:B:332:VAL:HB	2.17	0.44
1:C:365:TYR:HA	1:C:368:LEU:HD22	1.98	0.44
1:C:455:LEU:HB2	1:C:492:GLN:HG2	1.99	0.44
1:C:522:THR:HG23	1:C:523:VAL:N	2.27	0.44
1:C:853:GLN:C	1:C:855:PHE:N	2.72	0.44
2:T:276:THR:O	2:T:278:LEU:N	2.47	0.44
2:T:539:LEU:C	2:T:541:LYS:N	2.71	0.44
2:X:47:SER:HA	2:X:62:MET:CE	2.47	0.44
2:X:468:ILE:HG21	2:X:476:LYS:HG3	1.98	0.44
2:Z:65:ALA:HA	2:Z:68:LYS:HB3	1.99	0.44
2:Z:394:ASN:HB3	2:Z:395:GLY:H	1.61	0.44
1:A:111:ASP:HB2	1:A:113:LYS:CE	2.48	0.44
1:A:365:TYR:HA	1:A:368:LEU:HD22	1.98	0.44
1:A:480:CYS:SG	1:A:482:GLY:N	2.90	0.44
1:A:540:PHE:HE1	1:A:545:LEU:HD23	1.79	0.44
1:A:558:PHE:CE2	1:A:564:PHE:O	2.70	0.44
1:A:625:ALA:O	1:A:630:PRO:HD3	2.17	0.44
1:A:850:ILE:HD12	1:A:850:ILE:HA	1.72	0.44
1:A:869:MET:HB3	1:C:699:LEU:HD11	2.00	0.44
1:B:541:ASN:O	1:B:542:PHE:C	2.60	0.44
1:B:985:ASP:C	1:B:987:PRO:HD2	2.42	0.44
1:B:1138:TYR:CD1	1:B:1143:LEU:HD23	2.51	0.44
2:T:56:GLU:O	2:T:57:GLU:C	2.60	0.44
2:T:123:MET:C	2:T:125:THR:N	2.75	0.44
2:T:381:TYR:C	2:T:383:MET:H	2.25	0.44
2:T:395:GLY:O	2:T:396:ALA:C	2.60	0.44
2:T:535:HIS:O	2:T:536:GLU:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:156:LEU:HD11	2:X:281:LEU:HD11	1.99	0.44
2:X:265:HIS:ND1	2:X:266:LEU:HG	2.32	0.44
2:X:535:HIS:O	2:X:536:GLU:HB3	2.17	0.44
2:X:538:PRO:HG2	2:X:541:LYS:HZ3	1.83	0.44
1:A:429:PHE:C	1:A:431:GLY:H	2.25	0.44
1:A:1081:ILE:HD12	1:A:1115:ILE:HD13	2.00	0.44
1:B:128:ILE:H	1:B:128:ILE:HG12	1.61	0.44
1:B:130:VAL:HG21	1:B:230:ILE:HD12	1.98	0.44
1:B:422:ASN:O	1:B:423:TYR:HB2	2.17	0.44
1:B:569:VAL:O	1:B:570:ASP:HB3	2.16	0.44
1:C:316:SER:OG	1:C:317:ASN:N	2.50	0.44
1:C:339:HIS:CD2	1:C:367:VAL:HB	2.52	0.44
2:T:338:ASN:ND2	2:T:339:VAL:HG12	2.32	0.44
2:T:483:GLU:HB3	2:T:484:ILE:H	1.61	0.44
2:T:503:LEU:O	2:T:506:VAL:HG23	2.18	0.44
2:Z:47:SER:HA	2:Z:62:MET:HE1	2.00	0.44
2:Z:47:SER:HA	2:Z:62:MET:CE	2.47	0.44
2:Z:332:MET:HE2	2:Z:332:MET:HB3	1.71	0.44
2:Z:381:TYR:C	2:Z:383:MET:H	2.25	0.44
2:Z:418:LEU:C	2:Z:424:LEU:HB2	2.43	0.44
1:A:239:THR:O	1:A:240:LEU:HD23	2.17	0.44
1:A:372:ALA:O	1:A:374:PHE:N	2.47	0.44
1:B:230:ILE:HG22	1:B:231:GLY:H	1.81	0.44
1:B:533:VAL:O	1:B:534:LYS:HB2	2.17	0.44
1:B:966:LEU:HD12	1:B:966:LEU:HA	1.86	0.44
1:C:125:ASN:HD21	1:C:171:VAL:CG1	2.30	0.44
1:C:141:LEU:HD23	1:C:141:LEU:HA	1.72	0.44
1:C:417:ASN:HD22	1:C:417:ASN:HA	1.63	0.44
1:C:452:TRP:NE1	1:C:493:SER:HB2	2.32	0.44
1:C:458:LYS:HD3	1:C:458:LYS:HA	1.60	0.44
2:T:36:ALA:O	2:T:39:LEU:N	2.51	0.44
2:T:65:ALA:HA	2:T:68:LYS:HB3	1.99	0.44
2:T:95:LEU:C	2:T:97:LEU:N	2.74	0.44
2:T:150:GLU:O	2:T:152:MET:N	2.51	0.44
2:T:523:PHE:HD2	2:T:584:LEU:HB2	1.82	0.44
2:T:540:HIS:C	2:T:540:HIS:CD2	2.94	0.44
2:X:523:PHE:HD2	2:X:584:LEU:HB2	1.82	0.44
2:Z:51:ASN:HD22	2:Z:349:TRP:HZ2	1.65	0.44
2:Z:81:GLN:C	2:Z:83:TYR:N	2.75	0.44
1:A:106:PHE:HB3	1:A:234:ILE:HB	1.99	0.44
1:A:115:GLN:HA	1:A:132:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:THR:O	1:A:740:MET:C	2.61	0.44
1:B:558:PHE:N	1:B:558:PHE:HD1	2.16	0.44
1:B:635:TYR:C	1:B:635:TYR:CD1	2.96	0.44
1:B:849:LEU:HB2	1:B:850:ILE:H	1.57	0.44
1:C:236:ARG:O	1:C:237:PHE:HB3	2.17	0.44
1:C:353:TRP:HB3	1:C:423:TYR:HE1	1.82	0.44
1:C:481:LYS:HD3	1:C:481:LYS:HA	1.72	0.44
1:C:756:TYR:HB3	1:C:759:PHE:CD2	2.51	0.44
1:C:900:MET:HE3	1:C:900:MET:HB3	1.80	0.44
2:T:200:GLY:O	2:T:204:ARG:N	2.50	0.44
2:T:577:LYS:HB2	2:T:577:LYS:HE3	1.54	0.44
2:X:136:ASP:O	2:X:137:ASN:HB2	2.16	0.44
2:Z:503:LEU:O	2:Z:506:VAL:HG23	2.18	0.44
1:B:411:ALA:HB3	1:B:414:GLN:CD	2.43	0.44
1:B:443:SER:C	1:B:444:LYS:HG2	2.42	0.44
1:B:749:CYS:C	1:B:751:ASN:H	2.26	0.44
1:B:791:THR:OG1	1:B:795:LYS:HE3	2.17	0.44
2:T:261:CYS:O	2:T:610:TRP:HZ3	2.00	0.44
2:T:297:MET:HE3	2:T:297:MET:HB3	1.69	0.44
2:T:418:LEU:H	2:T:418:LEU:HG	1.57	0.44
2:X:381:TYR:C	2:X:383:MET:H	2.25	0.44
2:Z:150:GLU:O	2:Z:152:MET:N	2.51	0.44
2:Z:535:HIS:O	2:Z:536:GLU:HB3	2.17	0.44
1:A:348:ALA:HB1	1:A:352:ALA:O	2.18	0.44
1:B:335:LEU:HD23	1:B:336:CYS:O	2.18	0.44
1:B:357:ARG:HH21	1:B:394:ASN:CG	2.26	0.44
1:B:392:PHE:HA	1:B:516:LEU:HD22	2.00	0.44
1:B:460:LYS:HB2	1:B:460:LYS:HE3	1.38	0.44
2:T:295:ASP:O	2:T:298:VAL:HG22	2.16	0.44
2:X:36:ALA:O	2:X:39:LEU:N	2.51	0.44
2:X:123:MET:C	2:X:125:THR:N	2.75	0.44
2:X:150:GLU:O	2:X:152:MET:N	2.51	0.44
2:X:244:VAL:O	2:X:248:LEU:N	2.51	0.44
2:X:297:MET:HE3	2:X:297:MET:HB3	1.68	0.44
2:X:428:PHE:CD1	2:X:430:GLU:HG3	2.53	0.44
2:Z:36:ALA:O	2:Z:39:LEU:N	2.51	0.44
2:Z:221:GLN:O	2:Z:222:LEU:C	2.59	0.44
2:Z:288:LYS:H	2:Z:288:LYS:HG2	1.60	0.44
1:A:107:GLY:C	1:A:234:ILE:HA	2.42	0.44
1:A:140:PHE:CE1	1:A:241:LEU:HB2	2.52	0.44
1:A:364:ASP:C	1:A:366:SER:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:THR:H	1:A:516:LEU:HA	1.81	0.44
1:A:428:ASP:O	1:A:430:THR:N	2.51	0.44
1:A:978:ASN:O	1:A:981:LEU:N	2.51	0.44
1:B:478:LYS:NZ	1:B:485:PRO:HD3	2.33	0.44
1:B:831:ALA:CB	1:B:851:CYS:HA	2.48	0.44
1:B:914:ASN:H	1:B:914:ASN:ND2	2.16	0.44
1:B:959:LEU:O	1:B:963:VAL:HG23	2.18	0.44
1:C:274:THR:C	1:C:275:PHE:HD1	2.26	0.44
1:C:483:LYS:HD2	1:C:484:GLY:H	1.82	0.44
2:T:47:SER:HA	2:T:62:MET:HE1	2.00	0.44
2:T:51:ASN:HD22	2:T:349:TRP:HZ2	1.65	0.44
2:T:164:ALA:O	2:T:167:SER:N	2.51	0.44
2:T:244:VAL:O	2:T:248:LEU:N	2.51	0.44
2:X:591:LEU:C	2:X:593:THR:N	2.72	0.44
1:A:188:ASN:HD21	1:A:207:HIS:HB3	1.82	0.43
1:A:417:ASN:O	1:A:418:ILE:C	2.60	0.43
1:A:443:SER:C	1:A:444:LYS:HG2	2.42	0.43
1:A:474:GLN:HA	1:A:483:LYS:HB2	2.00	0.43
1:A:540:PHE:CD1	1:A:540:PHE:C	2.96	0.43
1:B:210:ILE:C	1:B:212:GLY:N	2.74	0.43
1:B:428:ASP:O	1:B:430:THR:N	2.51	0.43
1:B:558:PHE:HD2	1:B:563:GLN:O	2.00	0.43
1:B:976:VAL:HG12	1:B:978:ASN:OD1	2.18	0.43
1:C:303:LEU:O	1:C:304:LYS:C	2.60	0.43
1:C:417:ASN:O	1:C:418:ILE:C	2.60	0.43
2:T:470:LYS:O	2:T:472:GLN:N	2.45	0.43
2:T:545:SER:O	2:T:546:ASN:HB2	2.18	0.43
2:X:186:LEU:O	2:X:187:LYS:C	2.61	0.43
2:X:200:GLY:O	2:X:204:ARG:N	2.50	0.43
2:X:295:ASP:O	2:X:298:VAL:HG22	2.17	0.43
2:X:470:LYS:O	2:X:472:GLN:N	2.45	0.43
1:A:86:PHE:CB	1:A:235:THR:HA	2.48	0.43
1:A:337:PRO:O	1:A:340:GLU:HG2	2.19	0.43
1:A:372:ALA:C	1:A:374:PHE:N	2.75	0.43
1:A:420:ASP:O	1:A:460:LYS:HA	2.18	0.43
1:A:457:ARG:HH12	1:A:460:LYS:HA	1.83	0.43
1:A:753:LEU:C	1:A:755:GLN:H	2.26	0.43
1:B:372:ALA:C	1:B:374:PHE:N	2.75	0.43
1:B:414:GLN:HE21	1:B:414:GLN:HB3	1.58	0.43
1:B:492:GLN:HB3	2:X:34:HIS:CE1	2.53	0.43
1:B:522:THR:O	1:B:524:CYS:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:VAL:HG12	1:C:267:VAL:H	1.83	0.43
1:C:743:CYS:C	1:C:745:ASP:N	2.75	0.43
2:T:105:SER:O	2:T:107:VAL:HG13	2.18	0.43
2:T:165:TRP:HZ2	2:T:478:TRP:CZ2	2.37	0.43
2:T:264:ALA:O	2:T:266:LEU:N	2.51	0.43
2:X:27:THR:O	2:X:28:PHE:C	2.59	0.43
2:X:243:TYR:HB3	2:X:244:VAL:H	1.50	0.43
2:X:261:CYS:O	2:X:610:TRP:HZ3	2.00	0.43
2:X:338:ASN:ND2	2:X:339:VAL:HG12	2.32	0.43
2:Z:244:VAL:O	2:Z:248:LEU:N	2.51	0.43
2:Z:351:LEU:H	2:Z:351:LEU:CD1	2.25	0.43
2:Z:514:ARG:H	2:Z:514:ARG:HG2	1.57	0.43
1:A:90:VAL:HG22	1:A:92:PHE:N	2.33	0.43
1:A:106:PHE:CB	1:A:234:ILE:HB	2.47	0.43
1:A:328:ARG:HH21	1:A:579:GLN:HE21	1.66	0.43
1:A:335:LEU:HA	1:A:362:VAL:HB	2.00	0.43
1:A:461:LEU:HB3	1:A:465:GLU:HB3	2.00	0.43
1:A:474:GLN:O	1:A:474:GLN:HG2	2.18	0.43
1:A:478:LYS:H	1:A:484:GLY:H	1.66	0.43
1:A:979:ASP:C	1:A:983:ARG:HD2	2.43	0.43
1:B:36:VAL:HG21	1:B:219:PHE:CE2	2.53	0.43
1:B:85:PRO:HA	1:B:236:ARG:NH1	2.33	0.43
1:B:338:PHE:C	1:B:340:GLU:N	2.76	0.43
1:B:453:TYR:O	1:B:491:LEU:HA	2.18	0.43
2:T:123:MET:HE3	2:T:123:MET:HB2	1.77	0.43
2:T:156:LEU:HD11	2:T:281:LEU:HD11	1.99	0.43
2:X:116:LEU:HD13	2:X:186:LEU:HB2	2.00	0.43
2:X:165:TRP:HZ2	2:X:478:TRP:CZ2	2.37	0.43
2:X:188:ASN:HB3	2:X:192:ARG:NH1	2.33	0.43
2:X:285:PHE:HB3	2:X:287:GLN:CD	2.43	0.43
2:Z:402:GLU:HB3	2:Z:518:ARG:HD3	2.01	0.43
2:Z:470:LYS:HB2	2:Z:470:LYS:HE3	1.74	0.43
1:A:338:PHE:C	1:A:340:GLU:N	2.76	0.43
1:A:392:PHE:HA	1:A:516:LEU:HD22	1.99	0.43
1:A:457:ARG:HD2	1:A:467:ASP:OD2	2.18	0.43
1:A:577:ASP:CG	1:A:580:THR:HG23	2.43	0.43
1:A:978:ASN:O	1:A:979:ASP:C	2.62	0.43
1:B:312:ILE:HD12	1:B:597:ILE:CG1	2.48	0.43
1:B:348:ALA:HB1	1:B:352:ALA:O	2.18	0.43
1:B:420:ASP:HB3	1:B:421:TYR:CD2	2.52	0.43
1:B:558:PHE:HZ	1:B:574:ALA:CB	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:GLU:OE2	1:C:532:LEU:HD22	2.18	0.43
1:C:357:ARG:HH21	1:C:394:ASN:CG	2.26	0.43
1:C:392:PHE:HA	1:C:516:LEU:HD22	2.00	0.43
1:C:767:LEU:HD23	1:C:770:ILE:HD12	1.99	0.43
2:T:155:SER:OG	2:T:156:LEU:N	2.48	0.43
2:T:477:TRP:CH2	2:T:500:PRO:HB3	2.54	0.43
2:T:477:TRP:CZ3	2:T:500:PRO:HB3	2.53	0.43
2:X:247:LYS:HZ1	2:X:282:THR:HA	1.83	0.43
2:Z:105:SER:O	2:Z:107:VAL:HG13	2.18	0.43
2:Z:116:LEU:HD13	2:Z:186:LEU:HB2	2.00	0.43
2:Z:165:TRP:HZ2	2:Z:478:TRP:CZ2	2.37	0.43
2:Z:186:LEU:O	2:Z:187:LYS:C	2.61	0.43
2:Z:395:GLY:O	2:Z:396:ALA:C	2.60	0.43
1:A:558:PHE:CD2	1:A:576:ARG:HG3	2.53	0.43
1:B:111:ASP:C	1:B:113:LYS:H	2.25	0.43
1:B:969:LYS:O	1:B:970:PHE:C	2.59	0.43
1:C:372:ALA:C	1:C:374:PHE:N	2.75	0.43
2:T:132:VAL:C	2:T:141:CYS:HA	2.44	0.43
2:X:164:ALA:O	2:X:167:SER:N	2.51	0.43
2:X:279:TYR:HE2	2:X:290:ASN:HD21	1.65	0.43
2:Z:27:THR:O	2:Z:28:PHE:C	2.59	0.43
2:Z:123:MET:HE3	2:Z:123:MET:HB2	1.77	0.43
2:Z:348:ALA:HB1	2:Z:379:ILE:HD11	2.00	0.43
1:A:31:SER:O	1:A:32:PHE:HB2	2.19	0.43
1:B:319:ARG:NH2	1:B:537:CYS:SG	2.92	0.43
1:B:364:ASP:C	1:B:366:SER:H	2.26	0.43
1:B:813:SER:O	1:B:814:LYS:C	2.61	0.43
1:C:348:ALA:HB1	1:C:352:ALA:O	2.18	0.43
1:C:350:VAL:O	1:C:352:ALA:N	2.52	0.43
1:C:411:ALA:HB3	1:C:414:GLN:CD	2.43	0.43
1:C:714:ILE:HA	1:C:715:PRO:HD3	1.85	0.43
1:C:750:SER:O	1:C:751:ASN:C	2.60	0.43
1:C:833:PHE:CD1	1:C:836:GLN:HA	2.54	0.43
1:C:852:ALA:H	1:C:853:GLN:NE2	2.17	0.43
1:C:854:LYS:HA	1:C:858:LEU:O	2.19	0.43
2:T:351:LEU:CD1	2:T:355:ASP:HB3	2.48	0.43
2:T:419:LYS:O	2:T:421:ILE:N	2.52	0.43
2:T:596:LYS:HB2	2:T:596:LYS:HE2	1.72	0.43
2:X:56:GLU:O	2:X:57:GLU:C	2.60	0.43
2:X:247:LYS:NZ	2:X:247:LYS:HB3	2.34	0.43
2:X:264:ALA:O	2:X:266:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:474:MET:O	2:X:475:LYS:C	2.61	0.43
2:Z:304:ALA:C	2:Z:306:ARG:N	2.75	0.43
2:Z:317:SER:C	2:Z:319:GLY:N	2.74	0.43
2:Z:338:ASN:ND2	2:Z:339:VAL:HG12	2.32	0.43
1:A:39:PRO:O	1:A:40:ASP:C	2.62	0.43
1:A:357:ARG:HH21	1:A:394:ASN:CG	2.26	0.43
1:A:411:ALA:HB3	1:A:414:GLN:CD	2.43	0.43
1:A:422:ASN:HD21	1:A:454:ARG:N	2.05	0.43
1:A:980:ILE:HG23	1:A:984:LEU:HD13	2.00	0.43
1:A:998:THR:C	1:A:1000:ARG:H	2.27	0.43
1:C:20:ASN:O	1:C:21:LEU:HD13	2.19	0.43
1:C:120:VAL:HG22	1:C:122:ASN:OD1	2.19	0.43
1:C:190:ARG:HG2	1:C:207:HIS:CE1	2.53	0.43
1:C:438:SER:CB	1:C:508:ARG:HD2	2.47	0.43
2:T:180:TYR:C	2:T:182:GLU:N	2.77	0.43
2:T:247:LYS:NZ	2:T:247:LYS:HB3	2.34	0.43
2:T:475:LYS:HB3	2:T:479:GLU:OE1	2.19	0.43
2:X:134:ASN:HB3	2:X:137:ASN:O	2.19	0.43
2:X:247:LYS:HZ2	2:X:282:THR:HA	1.84	0.43
2:X:310:GLU:O	2:X:311:ALA:C	2.62	0.43
2:X:402:GLU:HB3	2:X:518:ARG:HD3	2.01	0.43
2:X:419:LYS:O	2:X:421:ILE:N	2.52	0.43
2:Z:188:ASN:HB3	2:Z:192:ARG:NH1	2.33	0.43
2:Z:499:ASP:HB2	2:Z:500:PRO:HD3	2.00	0.43
1:A:323:THR:HG23	1:A:537:CYS:O	2.18	0.43
1:A:350:VAL:O	1:A:352:ALA:N	2.52	0.43
1:A:644:THR:HG22	1:A:645:ARG:N	2.31	0.43
1:A:853:GLN:HG3	1:A:853:GLN:H	1.67	0.43
1:A:996:LEU:C	1:A:998:THR:N	2.74	0.43
1:A:1004:LEU:O	1:A:1008:VAL:HG23	2.19	0.43
1:B:281:GLU:C	1:B:283:GLY:N	2.77	0.43
1:B:319:ARG:NH1	1:B:621:VAL:HG11	2.33	0.43
1:B:321:GLN:C	1:B:323:THR:N	2.77	0.43
1:B:329:PHE:CD1	1:B:329:PHE:C	2.95	0.43
1:B:337:PRO:O	1:B:340:GLU:HG2	2.18	0.43
1:B:350:VAL:O	1:B:352:ALA:N	2.52	0.43
1:B:394:ASN:O	1:B:515:GLU:HG2	2.19	0.43
1:B:937:SER:OG	1:B:938:LEU:N	2.48	0.43
1:B:989:ALA:O	1:B:991:VAL:N	2.52	0.43
1:C:85:PRO:O	1:C:86:PHE:C	2.62	0.43
1:C:127:PHE:O	1:C:128:ILE:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:ILE:HG12	1:C:418:ILE:HG21	2.01	0.43
1:C:420:ASP:CG	1:C:460:LYS:HE2	2.44	0.43
1:C:831:ALA:HB1	1:C:833:PHE:CZ	2.54	0.43
1:C:984:LEU:HD22	1:C:985:ASP:H	1.84	0.43
2:T:169:ARG:HG3	2:T:499:ASP:HA	2.00	0.43
2:T:338:ASN:C	2:T:340:GLN:N	2.74	0.43
2:T:348:ALA:HB1	2:T:379:ILE:HD11	2.00	0.43
2:T:498:CYS:HB3	2:T:501:ALA:HB3	2.00	0.43
2:T:595:LEU:HD23	2:T:595:LEU:HA	1.84	0.43
2:X:122:THR:OG1	2:X:123:MET:N	2.52	0.43
2:X:132:VAL:C	2:X:141:CYS:HA	2.44	0.43
2:X:285:PHE:C	2:X:287:GLN:N	2.69	0.43
2:X:435:GLU:H	2:X:435:GLU:HG2	1.49	0.43
2:X:557:MET:HE3	2:X:557:MET:HB3	1.95	0.43
2:Z:97:LEU:HA	2:Z:97:LEU:HD23	1.71	0.43
2:Z:134:ASN:HB3	2:Z:137:ASN:O	2.19	0.43
2:Z:419:LYS:O	2:Z:421:ILE:N	2.52	0.43
1:A:33:THR:O	1:A:34:ARG:HG3	2.18	0.43
1:A:985:ASP:HB2	1:A:987:PRO:HD2	2.00	0.43
1:A:1029:MET:HG3	1:A:1029:MET:O	2.18	0.43
1:B:26:GLN:O	1:B:27:SER:CB	2.66	0.43
1:B:381:GLY:CA	1:B:429:PHE:HB3	2.48	0.43
1:B:420:ASP:HA	1:B:460:LYS:HD3	2.01	0.43
1:B:1072:GLU:CD	1:B:1072:GLU:H	2.26	0.43
1:C:424:LYS:HB2	1:C:461:LEU:HD12	2.01	0.43
1:C:614:VAL:O	1:C:643:GLN:NE2	2.52	0.43
1:C:834:ILE:HD12	1:C:834:ILE:HA	1.74	0.43
1:C:849:LEU:O	1:C:849:LEU:HG	2.18	0.43
1:C:1029:MET:HE2	1:C:1029:MET:HB2	1.83	0.43
2:T:134:ASN:HB3	2:T:137:ASN:O	2.19	0.43
2:T:280:SER:OG	2:T:281:LEU:N	2.51	0.43
2:T:374:HIS:HA	2:T:405:GLY:O	2.19	0.43
2:T:455:MET:HE3	2:T:455:MET:HB3	1.54	0.43
2:X:81:GLN:HG3	2:X:101:GLN:CG	2.46	0.43
2:X:105:SER:O	2:X:107:VAL:HG13	2.18	0.43
2:X:296:ALA:O	2:X:297:MET:C	2.61	0.43
2:X:317:SER:C	2:X:319:GLY:N	2.74	0.43
2:X:406:GLU:C	2:X:408:MET:N	2.73	0.43
2:X:514:ARG:O	2:X:518:ARG:HB2	2.19	0.43
2:Z:164:ALA:O	2:Z:167:SER:N	2.51	0.43
2:Z:247:LYS:NZ	2:Z:247:LYS:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:264:ALA:O	2:Z:266:LEU:N	2.51	0.43
2:Z:595:LEU:HD23	2:Z:595:LEU:HA	1.84	0.43
1:A:394:ASN:O	1:A:515:GLU:HG2	2.19	0.43
1:A:458:LYS:HD3	1:A:458:LYS:HA	1.60	0.43
1:A:485:PRO:HG3	1:A:488:TYR:HD2	1.84	0.43
1:A:598:THR:HG22	1:A:607:VAL:HG12	2.01	0.43
1:B:422:ASN:HD21	1:B:454:ARG:N	2.05	0.43
1:B:485:PRO:O	2:X:79:LEU:HD11	2.19	0.43
1:B:538:VAL:HG22	1:B:539:ASN:O	2.19	0.43
1:B:553:LYS:HE2	1:B:553:LYS:HB2	1.85	0.43
1:B:556:LYS:HZ2	1:C:847:ARG:HD3	1.84	0.43
1:B:563:GLN:H	1:B:563:GLN:HG2	1.47	0.43
1:B:586:ILE:H	1:B:586:ILE:HD12	1.83	0.43
1:B:621:VAL:HB	1:B:630:PRO:N	2.34	0.43
1:B:747:THR:HG21	1:B:977:LEU:HD22	2.01	0.43
1:C:364:ASP:C	1:C:366:SER:H	2.26	0.43
2:T:94:LYS:HB3	2:T:94:LYS:HE3	1.64	0.43
2:T:192:ARG:O	2:T:193:ALA:C	2.62	0.43
2:T:310:GLU:O	2:T:311:ALA:C	2.62	0.43
2:X:180:TYR:C	2:X:182:GLU:N	2.77	0.43
2:X:374:HIS:HA	2:X:405:GLY:O	2.19	0.43
2:X:596:LYS:HB2	2:X:596:LYS:HE2	1.72	0.43
2:Z:32:PHE:O	2:Z:34:HIS:N	2.52	0.43
2:Z:84:PRO:O	2:Z:85:LEU:C	2.61	0.43
2:Z:156:LEU:HD11	2:Z:281:LEU:HD11	1.99	0.43
2:Z:187:LYS:HD3	2:Z:187:LYS:HA	1.62	0.43
2:Z:192:ARG:O	2:Z:193:ALA:C	2.62	0.43
2:Z:474:MET:O	2:Z:475:LYS:C	2.61	0.43
1:A:485:PRO:O	1:A:486:ASN:C	2.60	0.42
1:A:745:ASP:O	1:A:746:SER:C	2.62	0.42
1:B:50:LEU:HG	1:B:276:LEU:CD1	2.49	0.42
1:B:130:VAL:HG11	1:B:230:ILE:CG2	2.48	0.42
1:C:411:ALA:HB3	1:C:414:GLN:HG3	2.01	0.42
1:C:539:ASN:HD22	1:C:539:ASN:HA	1.71	0.42
1:C:610:LEU:CD2	1:C:612:GLN:HG2	2.46	0.42
1:C:615:ASN:HA	1:C:643:GLN:NE2	2.34	0.42
2:T:265:HIS:CG	2:T:266:LEU:H	2.37	0.42
2:T:478:TRP:CE2	2:T:489:GLU:HB3	2.54	0.42
2:T:499:ASP:N	2:T:500:PRO:HD2	2.34	0.42
2:T:589:GLU:O	2:T:590:PRO:C	2.60	0.42
2:X:84:PRO:O	2:X:85:LEU:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:67:ASP:O	2:Z:70:SER:N	2.52	0.42
2:Z:95:LEU:C	2:Z:97:LEU:N	2.74	0.42
2:Z:351:LEU:CD1	2:Z:355:ASP:HB3	2.48	0.42
2:Z:360:MET:HE3	2:Z:360:MET:HB2	1.67	0.42
2:Z:538:PRO:HG2	2:Z:541:LYS:NZ	2.34	0.42
1:A:51:THR:OG1	1:A:277:LEU:HD12	2.17	0.42
1:A:128:ILE:HG12	1:A:170:TYR:CD2	2.55	0.42
1:A:215:PHE:CE2	1:A:266:TYR:HB3	2.54	0.42
1:A:329:PHE:CB	1:A:330:PRO:CD	2.97	0.42
1:A:534:LYS:HD3	1:A:553:LYS:NZ	2.33	0.42
1:A:588:PRO:HG2	1:B:855:PHE:CD1	2.54	0.42
1:B:281:GLU:O	1:B:283:GLY:N	2.52	0.42
1:B:297:SER:C	1:B:299:THR:N	2.77	0.42
1:B:329:PHE:CD2	1:B:330:PRO:CD	3.00	0.42
1:B:461:LEU:HB3	1:B:465:GLU:HB3	2.00	0.42
1:C:95:THR:HG21	1:C:210:ILE:HG21	2.00	0.42
1:C:190:ARG:C	1:C:190:ARG:HD3	2.43	0.42
1:C:372:ALA:O	1:C:374:PHE:N	2.47	0.42
1:C:483:LYS:HB3	1:C:488:TYR:H	1.84	0.42
1:C:486:ASN:H	2:Z:79:LEU:HD21	1.84	0.42
1:C:576:ARG:HA	1:C:582:GLU:O	2.18	0.42
2:T:62:MET:O	2:T:66:GLY:N	2.49	0.42
2:T:84:PRO:O	2:T:85:LEU:C	2.61	0.42
2:T:439:LEU:O	2:T:442:GLN:N	2.52	0.42
2:X:47:SER:HA	2:X:62:MET:HE1	2.00	0.42
2:X:215:TYR:HA	2:X:577:LYS:HZ3	1.84	0.42
2:X:246:ALA:C	2:X:248:LEU:H	2.27	0.42
2:X:351:LEU:CD1	2:X:355:ASP:HB3	2.48	0.42
2:X:450:LEU:O	2:X:451:PRO:C	2.62	0.42
2:Z:122:THR:OG1	2:Z:123:MET:N	2.52	0.42
2:Z:123:MET:C	2:Z:125:THR:N	2.75	0.42
2:Z:198:ASP:O	2:Z:201:ASP:N	2.52	0.42
2:Z:244:VAL:O	2:Z:245:ARG:C	2.62	0.42
2:Z:296:ALA:O	2:Z:297:MET:C	2.61	0.42
2:Z:374:HIS:HA	2:Z:405:GLY:O	2.19	0.42
1:A:138:ASP:O	1:A:140:PHE:N	2.50	0.42
1:A:825:LYS:HD2	1:A:945:LEU:HD22	2.01	0.42
1:B:457:ARG:HD2	1:B:467:ASP:OD2	2.18	0.42
1:B:462:LYS:O	1:B:463:PRO:C	2.62	0.42
1:B:770:ILE:HD11	1:B:1012:LEU:HG	2.01	0.42
1:C:138:ASP:C	1:C:140:PHE:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:PRO:O	1:C:340:GLU:HG2	2.19	0.42
1:C:358:ILE:HG21	1:C:523:VAL:CG1	2.46	0.42
1:C:982:SER:C	1:C:984:LEU:N	2.77	0.42
2:T:205:GLY:O	2:T:208:GLU:N	2.50	0.42
2:T:474:MET:O	2:T:475:LYS:C	2.61	0.42
2:T:552:GLN:O	2:T:553:LYS:C	2.62	0.42
2:X:32:PHE:O	2:X:34:HIS:N	2.52	0.42
2:Z:435:GLU:O	2:Z:436:ILE:C	2.63	0.42
2:Z:439:LEU:O	2:Z:442:GLN:N	2.52	0.42
2:Z:545:SER:O	2:Z:546:ASN:HB2	2.18	0.42
1:A:43:PHE:HD2	1:C:562:GLN:NE2	2.16	0.42
1:A:228:LEU:HA	1:A:229:PRO:HD2	1.92	0.42
1:A:386:LYS:C	1:A:389:ASP:H	2.27	0.42
1:A:862:PRO:HA	1:A:863:PRO:HD3	1.85	0.42
1:B:125:ASN:CB	1:B:171:VAL:HG12	2.49	0.42
1:C:91:TYR:HE2	1:C:215:PHE:HE1	1.67	0.42
1:C:382:VAL:CG2	1:C:431:GLY:HA2	2.45	0.42
1:C:536:LYS:NZ	1:C:538:VAL:HG11	2.34	0.42
1:C:902:MET:HG3	1:C:902:MET:O	2.18	0.42
1:C:966:LEU:HD12	1:C:966:LEU:HA	1.72	0.42
2:T:81:GLN:C	2:T:83:TYR:N	2.75	0.42
2:T:116:LEU:HD13	2:T:186:LEU:HB2	2.00	0.42
2:T:162:LEU:HD13	2:T:162:LEU:HA	1.92	0.42
2:T:246:ALA:C	2:T:248:LEU:H	2.27	0.42
2:T:248:LEU:HD22	2:T:248:LEU:HA	1.84	0.42
2:X:223:ILE:O	2:X:227:GLU:HG2	2.19	0.42
2:X:306:ARG:O	2:X:307:ILE:C	2.62	0.42
2:X:360:MET:HB2	2:X:360:MET:HE3	1.67	0.42
2:X:435:GLU:O	2:X:436:ILE:C	2.63	0.42
2:X:439:LEU:O	2:X:442:GLN:N	2.52	0.42
2:X:460:ARG:C	2:X:462:MET:N	2.75	0.42
2:Z:86:GLN:HG3	2:Z:87:GLU:OE2	2.19	0.42
2:Z:132:VAL:C	2:Z:141:CYS:HA	2.44	0.42
2:Z:278:LEU:O	2:Z:279:TYR:C	2.62	0.42
2:Z:361:CYS:O	2:Z:362:THR:C	2.62	0.42
2:Z:478:TRP:CE2	2:Z:489:GLU:HB3	2.54	0.42
2:Z:514:ARG:O	2:Z:518:ARG:HB2	2.19	0.42
1:A:319:ARG:CG	1:A:632:TRP:HE3	2.23	0.42
1:A:410:ILE:HG12	1:A:418:ILE:HG21	2.01	0.42
1:A:959:LEU:O	1:A:963:VAL:HG23	2.19	0.42
1:B:450:ASP:O	1:B:452:TRP:CD1	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:833:PHE:C	1:B:835:LYS:N	2.77	0.42
1:C:223:GLU:O	1:C:224:PRO:C	2.63	0.42
1:C:528:LYS:HB2	1:C:529:SER:H	1.75	0.42
2:X:187:LYS:HD3	2:X:187:LYS:HA	1.62	0.42
2:X:230:PHE:C	2:X:232:GLU:N	2.78	0.42
2:X:244:VAL:O	2:X:245:ARG:C	2.62	0.42
2:Z:162:LEU:O	2:Z:163:TRP:C	2.63	0.42
2:Z:230:PHE:C	2:Z:232:GLU:H	2.28	0.42
2:Z:369:PHE:CE2	2:Z:373:HIS:HE1	2.38	0.42
2:Z:382:ASP:HA	2:Z:385:TYR:CZ	2.55	0.42
2:Z:392:LEU:HD23	2:Z:392:LEU:HA	1.92	0.42
2:Z:435:GLU:O	2:Z:439:LEU:HD12	2.20	0.42
2:Z:471:ASP:OD1	2:Z:471:ASP:N	2.52	0.42
1:A:316:SER:HB2	1:A:317:ASN:H	1.61	0.42
1:A:381:GLY:CA	1:A:429:PHE:HB3	2.48	0.42
1:A:497:ARG:NH1	1:A:500:TYR:OH	2.53	0.42
1:A:829:ALA:HB1	1:A:850:ILE:CG2	2.49	0.42
1:B:560:PRO:O	1:B:561:PHE:HB3	2.20	0.42
1:B:1027:THR:HG22	1:B:1042:PHE:HZ	1.85	0.42
1:C:58:PHE:O	1:C:59:PHE:C	2.63	0.42
1:C:189:LEU:HD13	1:C:210:ILE:CG2	2.49	0.42
2:T:188:ASN:HB3	2:T:192:ARG:NH1	2.33	0.42
2:T:361:CYS:O	2:T:362:THR:C	2.62	0.42
2:T:406:GLU:C	2:T:408:MET:N	2.73	0.42
2:T:435:GLU:O	2:T:436:ILE:C	2.63	0.42
2:T:498:CYS:SG	2:T:501:ALA:HB3	2.60	0.42
2:T:514:ARG:O	2:T:518:ARG:HB2	2.19	0.42
2:X:174:LYS:O	2:X:175:GLN:C	2.63	0.42
2:X:278:LEU:O	2:X:279:TYR:C	2.62	0.42
2:X:475:LYS:HB3	2:X:479:GLU:OE1	2.19	0.42
2:X:545:SER:O	2:X:546:ASN:HB2	2.18	0.42
2:X:552:GLN:O	2:X:553:LYS:C	2.62	0.42
2:Z:148:LEU:HD13	2:Z:148:LEU:HA	1.77	0.42
2:Z:174:LYS:O	2:Z:175:GLN:C	2.63	0.42
2:Z:311:ALA:HA	2:Z:373:HIS:CD2	2.55	0.42
2:Z:472:GLN:O	2:Z:475:LYS:N	2.53	0.42
2:Z:552:GLN:O	2:Z:553:LYS:C	2.62	0.42
1:A:29:THR:OG1	1:A:30:ASN:N	2.52	0.42
1:A:450:ASP:O	1:A:452:TRP:CD1	2.71	0.42
1:A:577:ASP:CB	1:A:580:THR:HG23	2.49	0.42
1:A:834:ILE:HD12	1:A:834:ILE:HA	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:O	1:B:127:PHE:C	2.62	0.42
1:B:126:VAL:O	1:B:128:ILE:N	2.52	0.42
1:B:329:PHE:HB2	1:B:543:ASN:H	1.83	0.42
1:B:329:PHE:HB2	1:B:543:ASN:N	2.35	0.42
1:B:591:PHE:HZ	1:C:854:LYS:O	2.02	0.42
1:B:834:ILE:H	1:B:834:ILE:HG13	1.61	0.42
1:C:32:PHE:HB2	1:C:33:THR:H	1.63	0.42
1:C:324:GLU:O	1:C:325:SER:CB	2.65	0.42
1:C:435:ALA:HA	1:C:508:ARG:O	2.20	0.42
1:C:439:ASN:HA	1:C:506:PRO:HD2	2.00	0.42
2:T:198:ASP:O	2:T:201:ASP:N	2.52	0.42
2:T:244:VAL:O	2:T:245:ARG:C	2.62	0.42
2:T:296:ALA:O	2:T:297:MET:C	2.61	0.42
2:T:369:PHE:CE2	2:T:373:HIS:HE1	2.38	0.42
2:T:441:LYS:C	2:T:443:ALA:H	2.28	0.42
2:X:153:ALA:CB	2:X:277:ASN:HD22	2.33	0.42
2:X:186:LEU:O	2:X:189:GLU:HB2	2.20	0.42
2:X:234:LYS:O	2:X:235:PRO:C	2.62	0.42
2:X:302:TRP:CD2	2:X:306:ARG:HG2	2.55	0.42
2:X:478:TRP:CE2	2:X:489:GLU:HB3	2.54	0.42
2:Z:475:LYS:HB3	2:Z:479:GLU:OE1	2.19	0.42
2:Z:540:HIS:HA	2:Z:587:TYR:CE2	2.55	0.42
1:A:83:VAL:O	1:A:84:LEU:C	2.63	0.42
1:A:122:ASN:CG	1:A:123:ALA:H	2.28	0.42
1:A:484:GLY:C	1:A:486:ASN:H	2.25	0.42
1:A:663:ILE:HA	1:A:664:PRO:HD2	1.90	0.42
1:B:364:ASP:OD2	1:B:526:PRO:HG3	2.20	0.42
1:B:410:ILE:HG12	1:B:418:ILE:HG21	2.01	0.42
1:B:752:LEU:H	1:B:752:LEU:HG	1.69	0.42
1:C:115:GLN:HB2	1:C:232:ILE:HG22	2.02	0.42
1:C:310:LYS:HB3	1:C:310:LYS:HE3	1.76	0.42
1:C:417:ASN:HD22	1:C:421:TYR:HE1	1.68	0.42
1:C:801:ASN:OD1	1:C:803:SER:HB3	2.20	0.42
2:T:198:ASP:OD1	2:T:201:ASP:N	2.50	0.42
2:T:215:TYR:HA	2:T:577:LYS:HZ3	1.84	0.42
2:T:493:HIS:HD1	2:T:493:HIS:HA	1.77	0.42
2:X:86:GLN:HG3	2:X:87:GLU:OE2	2.19	0.42
2:X:288:LYS:HA	2:X:288:LYS:HD3	1.42	0.42
2:X:348:ALA:HB1	2:X:379:ILE:HD11	2.00	0.42
2:X:381:TYR:CE1	2:X:558:LEU:HA	2.55	0.42
2:X:382:ASP:HA	2:X:385:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:109:SER:HB3	2:Z:112:LYS:HB2	2.02	0.42
2:Z:223:ILE:O	2:Z:227:GLU:HG2	2.19	0.42
2:Z:246:ALA:C	2:Z:248:LEU:H	2.27	0.42
1:A:372:ALA:HB1	1:A:373:PRO:HD2	2.02	0.42
1:B:403:LYS:HG3	1:B:405:ASN:N	2.31	0.42
1:C:122:ASN:O	1:C:123:ALA:C	2.62	0.42
1:C:386:LYS:C	1:C:389:ASP:H	2.27	0.42
1:C:394:ASN:O	1:C:515:GLU:HG2	2.19	0.42
2:T:32:PHE:O	2:T:34:HIS:N	2.52	0.42
2:T:223:ILE:O	2:T:227:GLU:HG2	2.19	0.42
2:T:230:PHE:C	2:T:232:GLU:H	2.28	0.42
2:T:250:ASN:C	2:T:252:TYR:N	2.78	0.42
2:T:302:TRP:CD2	2:T:306:ARG:HG2	2.55	0.42
2:T:306:ARG:O	2:T:307:ILE:C	2.62	0.42
2:T:402:GLU:HB3	2:T:518:ARG:HD3	2.01	0.42
2:T:424:LEU:HD22	2:T:425:SER:N	2.34	0.42
2:T:462:MET:O	2:T:464:PHE:N	2.53	0.42
2:T:476:LYS:HA	2:T:479:GLU:CD	2.45	0.42
2:X:95:LEU:O	2:X:96:GLN:C	2.62	0.42
2:X:148:LEU:HD13	2:X:148:LEU:HA	1.78	0.42
2:X:198:ASP:O	2:X:201:ASP:N	2.52	0.42
2:X:311:ALA:HA	2:X:373:HIS:CD2	2.55	0.42
2:X:538:PRO:HG2	2:X:541:LYS:NZ	2.35	0.42
2:Z:70:SER:OG	2:Z:71:ALA:N	2.53	0.42
2:Z:288:LYS:HZ3	2:Z:433:GLU:CD	2.27	0.42
2:Z:483:GLU:O	2:Z:484:ILE:C	2.63	0.42
1:A:196:ASN:OD1	1:A:201:PHE:HD1	2.03	0.42
1:A:770:ILE:HD11	1:A:1012:LEU:HG	2.02	0.42
1:A:939:PHE:CD1	1:A:939:PHE:C	2.98	0.42
1:A:1001:LEU:HD23	1:A:1001:LEU:HA	1.75	0.42
1:B:316:SER:HB2	1:B:317:ASN:H	1.48	0.42
1:B:409:GLN:O	1:B:411:ALA:N	2.53	0.42
1:B:641:VAL:HG22	1:B:650:ILE:HG12	2.00	0.42
1:B:657:ASN:OD1	1:B:657:ASN:N	2.52	0.42
1:B:957:GLN:HE22	1:C:765:ARG:NE	2.18	0.42
1:C:127:PHE:HD1	1:C:127:PHE:H	1.68	0.42
1:C:215:PHE:O	1:C:217:GLN:N	2.53	0.42
1:C:329:PHE:HA	1:C:330:PRO:HD3	1.86	0.42
1:C:409:GLN:O	1:C:411:ALA:N	2.53	0.42
1:C:497:ARG:NH1	1:C:500:TYR:OH	2.53	0.42
1:C:833:PHE:CE2	1:C:851:CYS:SG	3.09	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:86:GLN:HG3	2:T:87:GLU:OE2	2.19	0.42
2:T:135:PRO:HB3	2:T:163:TRP:NE1	2.35	0.42
2:T:174:LYS:O	2:T:175:GLN:C	2.63	0.42
2:T:177:ARG:N	2:T:178:PRO:HD2	2.35	0.42
2:T:187:LYS:HA	2:T:187:LYS:HD3	1.62	0.42
2:T:230:PHE:C	2:T:232:GLU:N	2.78	0.42
2:T:234:LYS:O	2:T:235:PRO:C	2.62	0.42
2:T:281:LEU:HD23	2:T:281:LEU:HA	1.75	0.42
2:T:438:PHE:HZ	2:T:587:TYR:OH	2.03	0.42
2:X:70:SER:OG	2:X:71:ALA:N	2.53	0.42
2:X:177:ARG:N	2:X:178:PRO:HD2	2.35	0.42
2:X:441:LYS:C	2:X:443:ALA:H	2.28	0.42
2:Z:86:GLN:CD	2:Z:86:GLN:C	2.88	0.42
2:Z:135:PRO:HB3	2:Z:163:TRP:NE1	2.35	0.42
2:Z:186:LEU:O	2:Z:189:GLU:HB2	2.20	0.42
2:Z:310:GLU:O	2:Z:311:ALA:C	2.62	0.42
2:Z:441:LYS:C	2:Z:443:ALA:H	2.28	0.42
1:A:102:ARG:NH1	1:A:142:ASP:O	2.52	0.41
1:A:136:CYS:SG	1:A:139:PRO:HB3	2.60	0.41
1:A:749:CYS:HB2	1:A:977:LEU:CD2	2.50	0.41
1:B:411:ALA:HB3	1:B:414:GLN:HG3	2.01	0.41
1:B:439:ASN:O	1:B:441:LEU:N	2.53	0.41
1:B:489:PHE:O	1:B:492:GLN:NE2	2.53	0.41
1:C:957:GLN:O	1:C:961:THR:HG23	2.19	0.41
2:T:435:GLU:H	2:T:435:GLU:HG2	1.49	0.41
2:T:550:ALA:HA	2:T:553:LYS:HB2	2.02	0.41
2:T:586:ASN:N	2:T:586:ASN:HD22	2.16	0.41
2:X:78:THR:HG22	2:X:79:LEU:N	2.34	0.41
2:X:265:HIS:CG	2:X:266:LEU:H	2.37	0.41
2:X:333:LEU:HD23	2:X:333:LEU:HA	1.81	0.41
2:X:361:CYS:O	2:X:362:THR:C	2.62	0.41
2:X:369:PHE:CE2	2:X:373:HIS:HE1	2.38	0.41
2:X:394:ASN:HB3	2:X:395:GLY:H	1.61	0.41
2:X:472:GLN:O	2:X:475:LYS:N	2.53	0.41
2:X:501:ALA:HA	2:X:506:VAL:HB	2.02	0.41
2:Z:72:PHE:O	2:Z:73:LEU:C	2.63	0.41
2:Z:450:LEU:O	2:Z:451:PRO:C	2.62	0.41
1:A:22:ILE:HG22	1:A:23:THR:N	2.35	0.41
1:A:409:GLN:O	1:A:411:ALA:N	2.53	0.41
1:A:576:ARG:HG2	1:A:583:ILE:HA	2.02	0.41
1:B:201:PHE:CE2	1:B:203:ILE:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ASN:HA	1:B:522:THR:OG1	2.20	0.41
1:B:865:LEU:HD23	1:B:865:LEU:HA	1.90	0.41
1:C:50:LEU:HD23	1:C:275:PHE:O	2.19	0.41
1:C:198:ASP:O	1:C:200:TYR:N	2.53	0.41
1:C:472:ILE:HG13	1:C:473:TYR:H	1.85	0.41
1:C:1144:GLU:O	1:C:1146:ASP:N	2.52	0.41
2:T:186:LEU:O	2:T:189:GLU:HB2	2.20	0.41
2:T:231:GLU:HA	2:T:234:LYS:CD	2.47	0.41
2:T:460:ARG:C	2:T:462:MET:N	2.75	0.41
2:T:463:VAL:CG2	2:T:468:ILE:HD12	2.50	0.41
2:T:505:HIS:CD2	2:T:505:HIS:N	2.88	0.41
2:X:22:GLU:C	2:X:23:GLU:HG3	2.45	0.41
2:X:123:MET:HG2	2:X:179:LEU:HB3	2.02	0.41
2:X:156:LEU:O	2:X:157:ASP:C	2.64	0.41
2:X:566:TRP:O	2:X:567:THR:C	2.63	0.41
2:Z:177:ARG:N	2:Z:178:PRO:HD2	2.35	0.41
2:Z:263:PRO:CB	2:Z:265:HIS:HE1	2.28	0.41
2:Z:381:TYR:CE1	2:Z:558:LEU:HA	2.55	0.41
1:A:53:ASP:HB3	1:A:55:PHE:CE1	2.55	0.41
1:A:57:PRO:HB3	1:A:273:ARG:HE	1.85	0.41
1:A:411:ALA:HB3	1:A:414:GLN:HG3	2.02	0.41
1:A:555:ASN:HB3	1:B:847:ARG:NH1	2.35	0.41
1:B:118:LEU:C	1:B:119:ILE:HG12	2.45	0.41
1:B:284:THR:O	1:B:285:ILE:C	2.62	0.41
1:B:303:LEU:HG	1:B:303:LEU:H	1.74	0.41
1:B:319:ARG:HH12	1:B:621:VAL:HG11	1.85	0.41
1:B:483:LYS:HD2	1:B:486:ASN:HB2	2.02	0.41
1:B:530:THR:O	1:B:531:ASN:HB3	2.20	0.41
1:B:752:LEU:HD22	1:B:990:GLU:HG3	2.02	0.41
1:B:849:LEU:HD12	1:B:851:CYS:SG	2.60	0.41
1:C:478:LYS:HB2	1:C:484:GLY:CA	2.46	0.41
2:T:74:LYS:CE	2:T:75:GLU:HG2	2.50	0.41
2:T:95:LEU:O	2:T:96:GLN:C	2.62	0.41
2:T:142:LEU:H	2:T:142:LEU:HG	1.59	0.41
2:T:156:LEU:O	2:T:157:ASP:C	2.63	0.41
2:T:162:LEU:O	2:T:163:TRP:C	2.63	0.41
2:T:167:SER:HA	2:T:171:GLU:OE1	2.20	0.41
2:T:226:VAL:O	2:T:227:GLU:C	2.64	0.41
2:T:394:ASN:HB3	2:T:395:GLY:H	1.61	0.41
2:T:435:GLU:O	2:T:439:LEU:HD12	2.20	0.41
2:T:538:PRO:HG2	2:T:541:LYS:NZ	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:105:SER:O	2:Z:107:VAL:N	2.47	0.41
2:Z:205:GLY:O	2:Z:208:GLU:N	2.50	0.41
2:Z:462:MET:O	2:Z:464:PHE:N	2.53	0.41
2:Z:476:LYS:HA	2:Z:479:GLU:CD	2.45	0.41
2:Z:550:ALA:HA	2:Z:553:LYS:HB2	2.02	0.41
1:A:42:VAL:HG11	1:C:566:ARG:HG3	2.02	0.41
1:A:462:LYS:O	1:A:463:PRO:C	2.62	0.41
1:A:668:GLY:O	1:A:697:MET:HG2	2.20	0.41
1:A:989:ALA:C	1:A:991:VAL:N	2.78	0.41
1:B:310:LYS:HB3	1:B:310:LYS:HE2	1.64	0.41
1:B:497:ARG:NH1	1:B:500:TYR:OH	2.53	0.41
1:C:472:ILE:HG12	1:C:482:GLY:O	2.20	0.41
1:C:542:PHE:CE2	1:C:577:ASP:HA	2.54	0.41
1:C:688:ALA:O	1:C:689:SER:C	2.62	0.41
1:C:725:GLU:OE1	1:C:1028:LYS:HE2	2.20	0.41
2:T:122:THR:OG1	2:T:123:MET:N	2.52	0.41
2:T:123:MET:HG2	2:T:179:LEU:HB3	2.02	0.41
2:T:238:GLU:OE2	2:T:605:GLY:HA2	2.21	0.41
2:T:472:GLN:O	2:T:475:LYS:N	2.53	0.41
2:T:566:TRP:O	2:T:567:THR:C	2.63	0.41
2:X:167:SER:HA	2:X:171:GLU:OE1	2.21	0.41
2:X:226:VAL:O	2:X:227:GLU:C	2.64	0.41
2:X:285:PHE:HB2	2:X:288:LYS:HZ3	1.86	0.41
2:Z:230:PHE:C	2:Z:232:GLU:N	2.78	0.41
2:Z:234:LYS:O	2:Z:235:PRO:C	2.62	0.41
2:Z:250:ASN:C	2:Z:252:TYR:N	2.78	0.41
2:Z:374:HIS:HD2	2:Z:375:GLU:HG2	1.86	0.41
1:A:116:SER:CB	1:A:132:GLU:HB2	2.50	0.41
1:A:136:CYS:HB2	1:A:139:PRO:CD	2.50	0.41
1:A:435:ALA:HA	1:A:508:ARG:O	2.21	0.41
1:A:483:LYS:O	1:A:484:GLY:C	2.63	0.41
1:A:754:LEU:HD12	1:A:754:LEU:HA	1.92	0.41
1:B:112:SER:HB3	1:B:134:GLN:HG3	2.02	0.41
1:B:383:SER:O	1:B:384:PRO:C	2.64	0.41
1:B:449:TYR:CD1	1:B:495:GLY:HA3	2.56	0.41
1:B:632:TRP:O	1:B:634:VAL:HG23	2.20	0.41
1:B:632:TRP:C	1:B:634:VAL:N	2.77	0.41
1:B:1014:ARG:HE	1:B:1014:ARG:HB2	1.77	0.41
1:C:267:VAL:O	1:C:267:VAL:HG22	2.21	0.41
1:C:720:ILE:H	1:C:926:GLN:NE2	2.18	0.41
1:C:811:LYS:H	1:C:811:LYS:HG2	1.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1048:HIS:HE1	1:C:1051:SER:HB2	1.85	0.41
2:T:109:SER:HB3	2:T:112:LYS:HB2	2.02	0.41
2:T:481:LYS:HZ2	2:T:481:LYS:HG3	1.71	0.41
2:X:50:TYR:CZ	2:X:59:VAL:HG22	2.55	0.41
2:X:62:MET:O	2:X:66:GLY:N	2.49	0.41
2:X:462:MET:O	2:X:464:PHE:N	2.53	0.41
2:X:471:ASP:OD1	2:X:471:ASP:N	2.52	0.41
2:X:476:LYS:HA	2:X:479:GLU:CD	2.45	0.41
2:Z:74:LYS:CE	2:Z:75:GLU:HG2	2.51	0.41
2:Z:86:GLN:HG3	2:Z:87:GLU:CD	2.46	0.41
2:Z:265:HIS:CG	2:Z:266:LEU:H	2.37	0.41
1:A:360:ASN:HA	1:A:522:THR:OG1	2.20	0.41
1:A:480:CYS:SG	1:A:487:CYS:N	2.94	0.41
1:B:386:LYS:C	1:B:389:ASP:H	2.27	0.41
1:B:580:THR:HG22	1:B:582:GLU:OE2	2.20	0.41
1:C:310:LYS:HG2	1:C:663:ILE:HD11	2.02	0.41
1:C:377:PHE:HA	1:C:433:VAL:O	2.20	0.41
1:C:440:LYS:H	1:C:440:LYS:HG2	1.57	0.41
1:C:462:LYS:O	1:C:463:PRO:C	2.62	0.41
1:C:1105:THR:HG22	1:C:1106:GLN:N	2.36	0.41
1:C:1135:ASN:ND2	1:C:1136:THR:H	2.18	0.41
2:T:72:PHE:O	2:T:73:LEU:C	2.63	0.41
2:T:78:THR:HG22	2:T:79:LEU:N	2.34	0.41
2:T:97:LEU:HD23	2:T:97:LEU:HA	1.71	0.41
2:T:263:PRO:CB	2:T:265:HIS:HE1	2.28	0.41
2:T:382:ASP:HA	2:T:385:TYR:CZ	2.55	0.41
2:X:86:GLN:C	2:X:86:GLN:CD	2.88	0.41
2:X:246:ALA:C	2:X:248:LEU:N	2.78	0.41
2:X:336:PRO:HB3	2:X:342:ALA:HB2	2.01	0.41
2:Z:50:TYR:CZ	2:Z:59:VAL:HG22	2.55	0.41
2:Z:78:THR:HG22	2:Z:79:LEU:N	2.34	0.41
2:Z:167:SER:HA	2:Z:171:GLU:OE1	2.21	0.41
1:A:115:GLN:OE1	1:A:131:CYS:HA	2.21	0.41
1:A:130:VAL:CG1	1:A:168:PHE:H	2.34	0.41
1:A:225:LEU:C	1:A:226:VAL:HG22	2.45	0.41
1:A:829:ALA:HB1	1:A:850:ILE:HG22	2.03	0.41
1:A:935:GLN:H	1:A:935:GLN:HG2	1.71	0.41
1:B:619:VAL:C	1:B:621:VAL:N	2.78	0.41
1:C:553:LYS:HA	1:C:553:LYS:HE3	2.03	0.41
2:T:278:LEU:O	2:T:279:TYR:C	2.62	0.41
2:T:285:PHE:CE1	2:T:433:GLU:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:564:GLU:OE1	2:X:568:LEU:HD21	2.21	0.41
2:X:577:LYS:HE3	2:X:577:LYS:HB2	1.54	0.41
1:A:329:PHE:O	1:A:579:GLN:OE1	2.39	0.41
1:A:378:LYS:O	1:A:433:VAL:HG22	2.21	0.41
1:B:990:GLU:OE1	1:B:990:GLU:N	2.53	0.41
1:C:434:ILE:HB	1:C:436:TRP:CZ3	2.54	0.41
1:C:560:PRO:O	1:C:561:PHE:CD2	2.74	0.41
2:T:114:LYS:HB3	2:T:114:LYS:HE3	1.87	0.41
2:T:143:LEU:C	2:T:145:GLU:H	2.28	0.41
2:T:153:ALA:CB	2:T:277:ASN:HD22	2.33	0.41
2:T:157:ASP:O	2:T:161:ARG:HD2	2.21	0.41
2:T:325:GLN:HG3	2:T:329:GLU:OE2	2.21	0.41
2:T:418:LEU:C	2:T:424:LEU:HB2	2.46	0.41
2:T:483:GLU:O	2:T:484:ILE:C	2.63	0.41
2:X:238:GLU:OE2	2:X:605:GLY:HA2	2.21	0.41
2:X:325:GLN:HG3	2:X:329:GLU:OE2	2.21	0.41
2:X:352:GLY:O	2:X:353:LYS:HB2	2.21	0.41
2:X:455:MET:HB3	2:X:456:LEU:H	1.73	0.41
2:X:470:LYS:HB2	2:X:470:LYS:HE3	1.74	0.41
2:X:550:ALA:HA	2:X:553:LYS:HB2	2.02	0.41
2:X:603:PHE:CG	2:X:604:VAL:N	2.89	0.41
2:Z:171:GLU:O	2:Z:175:GLN:HG2	2.21	0.41
2:Z:180:TYR:C	2:Z:182:GLU:N	2.77	0.41
2:Z:306:ARG:O	2:Z:307:ILE:C	2.62	0.41
2:Z:459:TRP:O	2:Z:463:VAL:N	2.53	0.41
2:Z:555:PHE:C	2:Z:557:MET:H	2.29	0.41
1:A:39:PRO:O	1:A:40:ASP:O	2.38	0.41
1:A:115:GLN:HB3	1:A:130:VAL:CG2	2.50	0.41
1:A:130:VAL:HG12	1:A:168:PHE:CD1	2.44	0.41
1:A:138:ASP:C	1:A:140:PHE:N	2.71	0.41
1:A:364:ASP:C	1:A:366:SER:N	2.79	0.41
1:A:372:ALA:CB	1:A:373:PRO:CD	2.99	0.41
1:A:439:ASN:O	1:A:441:LEU:N	2.53	0.41
1:A:449:TYR:CD1	1:A:495:GLY:HA3	2.56	0.41
1:A:457:ARG:HH22	1:A:460:LYS:N	2.19	0.41
1:A:703:ASN:HB2	1:B:787:GLN:HG2	2.03	0.41
1:A:1010:GLN:O	1:A:1014:ARG:HG3	2.20	0.41
1:A:1105:THR:OG1	1:A:1106:GLN:N	2.52	0.41
1:B:50:LEU:HD12	1:B:304:LYS:HD3	2.03	0.41
1:B:362:VAL:HG13	1:B:526:PRO:CA	2.50	0.41
1:B:440:LYS:HA	1:B:440:LYS:HD2	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:LYS:HB3	1:B:444:LYS:HE3	1.71	0.41
1:B:779:GLN:HE21	1:B:779:GLN:HB3	1.58	0.41
1:B:1068:VAL:HA	1:B:1069:PRO:HD3	1.83	0.41
1:C:95:THR:C	1:C:96:GLU:HG3	2.46	0.41
1:C:118:LEU:O	1:C:120:VAL:N	2.54	0.41
1:C:169:GLU:CD	1:C:170:TYR:H	2.28	0.41
1:C:439:ASN:HA	1:C:506:PRO:HG2	2.02	0.41
1:C:531:ASN:ND2	1:C:532:LEU:H	2.18	0.41
1:C:545:LEU:CD1	1:C:575:VAL:HG21	2.47	0.41
1:C:564:PHE:N	1:C:564:PHE:CD1	2.85	0.41
1:C:736:VAL:HG22	1:C:858:LEU:CD2	2.51	0.41
1:C:752:LEU:HD23	1:C:993:ILE:CG2	2.51	0.41
2:T:67:ASP:O	2:T:70:SER:N	2.53	0.41
2:T:73:LEU:H	2:T:73:LEU:HG	1.75	0.41
2:T:86:GLN:HG3	2:T:87:GLU:CD	2.46	0.41
2:T:123:MET:H	2:T:123:MET:HG3	1.56	0.41
2:T:186:LEU:O	2:T:187:LYS:C	2.61	0.41
2:T:193:ALA:C	2:T:195:HIS:N	2.79	0.41
2:T:311:ALA:HA	2:T:373:HIS:CD2	2.55	0.41
2:T:316:VAL:O	2:T:317:SER:C	2.64	0.41
2:T:352:GLY:O	2:T:353:LYS:HB2	2.21	0.41
2:T:381:TYR:CE1	2:T:558:LEU:HA	2.55	0.41
2:T:555:PHE:C	2:T:557:MET:H	2.29	0.41
2:X:23:GLU:C	2:X:25:ALA:N	2.78	0.41
2:X:72:PHE:O	2:X:73:LEU:C	2.63	0.41
2:X:109:SER:HB3	2:X:112:LYS:HB2	2.02	0.41
2:X:135:PRO:HB3	2:X:163:TRP:NE1	2.35	0.41
2:X:157:ASP:O	2:X:161:ARG:HD2	2.21	0.41
2:X:162:LEU:O	2:X:163:TRP:C	2.63	0.41
2:X:435:GLU:O	2:X:439:LEU:HD12	2.20	0.41
2:X:555:PHE:C	2:X:557:MET:H	2.29	0.41
2:Z:22:GLU:C	2:Z:23:GLU:HG3	2.45	0.41
2:Z:302:TRP:CD2	2:Z:306:ARG:HG2	2.55	0.41
2:Z:325:GLN:HG3	2:Z:329:GLU:OE2	2.21	0.41
2:Z:406:GLU:C	2:Z:408:MET:N	2.73	0.41
2:Z:428:PHE:CD1	2:Z:429:GLN:N	2.89	0.41
2:Z:566:TRP:O	2:Z:567:THR:C	2.63	0.41
1:A:90:VAL:CG2	1:A:92:PHE:HB2	2.47	0.41
1:A:319:ARG:CG	1:A:632:TRP:CE3	3.02	0.41
1:A:576:ARG:O	1:A:577:ASP:C	2.64	0.41
1:A:855:PHE:O	1:A:856:ASN:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ASN:OD1	1:B:165:ASN:N	2.54	0.41
1:B:327:VAL:HG23	1:B:540:PHE:HB3	2.03	0.41
1:B:491:LEU:HA	1:B:491:LEU:HD22	1.78	0.41
1:B:898:PHE:N	1:B:899:PRO:HD2	2.36	0.41
1:B:1116:THR:O	1:B:1117:THR:C	2.64	0.41
1:C:81:ASN:HD22	1:C:238:GLN:HG2	1.86	0.41
1:C:338:PHE:C	1:C:340:GLU:N	2.76	0.41
1:C:362:VAL:O	1:C:362:VAL:HG12	2.20	0.41
1:C:437:ASN:ND2	1:C:506:PRO:O	2.54	0.41
1:C:688:ALA:O	1:C:690:GLN:HG2	2.20	0.41
2:T:50:TYR:CZ	2:T:59:VAL:HG22	2.55	0.41
2:T:171:GLU:O	2:T:175:GLN:HG2	2.21	0.41
2:T:603:PHE:CG	2:T:604:VAL:N	2.89	0.41
2:X:20:THR:O	2:X:20:THR:OG1	2.39	0.41
2:X:171:GLU:O	2:X:175:GLN:HG2	2.21	0.41
2:X:181:GLU:HB3	2:X:470:LYS:HZ1	1.85	0.41
2:X:192:ARG:O	2:X:193:ALA:C	2.62	0.41
2:X:217:TYR:OH	2:X:222:LEU:HA	2.21	0.41
2:X:483:GLU:O	2:X:484:ILE:C	2.63	0.41
2:Z:215:TYR:CE1	2:Z:568:LEU:HB2	2.56	0.41
2:Z:226:VAL:O	2:Z:227:GLU:C	2.64	0.41
2:Z:238:GLU:OE2	2:Z:605:GLY:HA2	2.21	0.41
2:Z:463:VAL:CG2	2:Z:468:ILE:HD12	2.50	0.41
2:Z:528:ALA:H	2:Z:530:CYS:H	1.69	0.41
2:Z:564:GLU:OE1	2:Z:568:LEU:HD21	2.21	0.41
1:A:232:ILE:H	1:A:232:ILE:HG13	1.61	0.40
1:A:633:ARG:NH1	1:A:635:TYR:CD2	2.89	0.40
1:A:731:MET:HG2	1:A:774:GLN:OE1	2.21	0.40
1:A:1141:LEU:O	1:A:1144:GLU:N	2.49	0.40
1:B:84:LEU:HD13	1:B:267:VAL:HG11	2.03	0.40
1:B:300:LYS:HB3	1:B:305:SER:O	2.20	0.40
1:B:328:ARG:N	1:B:530:THR:OG1	2.55	0.40
1:B:375:PHE:CE1	1:B:407:VAL:HG21	2.56	0.40
1:C:453:TYR:CZ	1:C:492:GLN:HB2	2.56	0.40
1:C:516:LEU:HD13	1:C:516:LEU:HA	1.95	0.40
1:C:983:ARG:HH21	1:C:983:ARG:CB	2.32	0.40
1:C:985:ASP:C	1:C:987:PRO:HD2	2.46	0.40
2:T:81:GLN:HG3	2:T:101:GLN:CG	2.46	0.40
2:T:246:ALA:C	2:T:248:LEU:N	2.78	0.40
2:T:333:LEU:HD23	2:T:333:LEU:HA	1.81	0.40
2:T:350:ASP:C	2:T:352:GLY:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:150:GLU:O	2:X:151:ILE:C	2.65	0.40
2:X:230:PHE:C	2:X:232:GLU:H	2.28	0.40
2:X:350:ASP:C	2:X:352:GLY:H	2.29	0.40
2:X:374:HIS:HD2	2:X:375:GLU:HG2	1.86	0.40
2:Z:178:PRO:HA	2:Z:181:GLU:CD	2.46	0.40
2:Z:316:VAL:O	2:Z:317:SER:C	2.64	0.40
1:A:447:GLY:HA2	1:A:496:PHE:O	2.22	0.40
1:A:871:ALA:O	1:A:875:SER:OG	2.38	0.40
1:B:470:THR:O	1:B:471:GLU:C	2.64	0.40
1:B:972:ALA:HB2	1:B:995:ARG:HG3	2.03	0.40
1:B:1029:MET:HG2	1:B:1062:PHE:CE1	2.56	0.40
1:C:116:SER:O	1:C:232:ILE:HD12	2.21	0.40
1:C:116:SER:HB3	1:C:117:LEU:H	1.71	0.40
1:C:189:LEU:HB2	1:C:209:PRO:O	2.22	0.40
1:C:204:TYR:N	1:C:204:TYR:CD1	2.88	0.40
1:C:391:CYS:CB	1:C:521:ALA:HB1	2.51	0.40
1:C:606:GLN:NE2	1:C:673:TYR:OH	2.55	0.40
1:C:862:PRO:HA	1:C:863:PRO:HD3	1.94	0.40
1:C:1141:LEU:O	1:C:1142:GLN:C	2.65	0.40
2:T:48:TRP:CH2	2:T:357:ARG:HB3	2.57	0.40
2:T:70:SER:OG	2:T:71:ALA:N	2.53	0.40
2:T:105:SER:O	2:T:107:VAL:N	2.47	0.40
2:T:143:LEU:O	2:T:145:GLU:N	2.54	0.40
2:T:215:TYR:CE1	2:T:568:LEU:HB2	2.56	0.40
2:T:260:GLY:HA3	2:T:610:TRP:CE3	2.56	0.40
2:X:123:MET:H	2:X:123:MET:HG3	1.56	0.40
2:X:133:CYS:HA	2:X:141:CYS:CB	2.51	0.40
2:X:599:ASN:O	2:X:601:ASN:N	2.55	0.40
2:X:613:TYR:CG	2:X:614:ALA:N	2.89	0.40
2:Z:153:ALA:CB	2:Z:277:ASN:HD22	2.33	0.40
2:Z:215:TYR:HA	2:Z:577:LYS:HZ1	1.86	0.40
2:Z:338:ASN:HD22	2:Z:339:VAL:HG12	1.87	0.40
2:Z:483:GLU:HB3	2:Z:484:ILE:H	1.61	0.40
2:Z:577:LYS:HB2	2:Z:577:LYS:HE3	1.54	0.40
1:A:186:PHE:CE1	1:A:187:LYS:NZ	2.55	0.40
1:A:457:ARG:HH12	1:A:460:LYS:CA	2.34	0.40
1:A:567:ASP:CG	1:A:568:ILE:H	2.30	0.40
1:B:339:HIS:C	1:B:341:VAL:N	2.80	0.40
1:C:284:THR:H	1:C:284:THR:HG1	1.58	0.40
1:C:339:HIS:C	1:C:341:VAL:N	2.80	0.40
1:C:426:PRO:CA	1:C:463:PRO:HB3	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:21:ILE:H	2:T:21:ILE:HG13	1.55	0.40
2:T:217:TYR:OH	2:T:222:LEU:HA	2.21	0.40
2:T:316:VAL:O	2:T:319:GLY:N	2.49	0.40
2:T:374:HIS:HD2	2:T:375:GLU:HG2	1.86	0.40
2:X:40:PHE:O	2:X:41:TYR:C	2.64	0.40
2:X:48:TRP:CH2	2:X:357:ARG:HB3	2.57	0.40
2:X:67:ASP:O	2:X:70:SER:N	2.52	0.40
2:X:74:LYS:CE	2:X:75:GLU:HG2	2.51	0.40
2:X:189:GLU:HA	2:X:192:ARG:NE	2.33	0.40
2:X:584:LEU:HG	2:X:585:LEU:N	2.35	0.40
2:Z:352:GLY:O	2:Z:353:LYS:HB2	2.21	0.40
2:Z:599:ASN:O	2:Z:601:ASN:N	2.55	0.40
1:A:200:TYR:HE1	1:A:202:LYS:HD3	1.87	0.40
1:A:391:CYS:CB	1:A:521:ALA:HB1	2.51	0.40
1:B:110:LEU:O	1:B:135:PHE:HB2	2.21	0.40
1:B:391:CYS:CB	1:B:521:ALA:HB1	2.51	0.40
1:B:424:LYS:O	1:B:463:PRO:HA	2.21	0.40
1:B:732:THR:HG22	1:B:860:VAL:HG13	2.03	0.40
1:B:833:PHE:HB2	1:B:835:LYS:HG3	2.02	0.40
1:C:188:ASN:H	1:C:210:ILE:HG12	1.86	0.40
1:C:205:SER:HB3	1:C:225:LEU:HD22	2.04	0.40
1:C:319:ARG:HE	1:C:321:GLN:CG	2.35	0.40
1:C:364:ASP:C	1:C:366:SER:N	2.79	0.40
1:C:398:ASP:O	1:C:510:VAL:HA	2.22	0.40
1:C:426:PRO:HA	1:C:463:PRO:HG3	2.04	0.40
1:C:456:PHE:CE1	1:C:473:TYR:CG	3.09	0.40
1:C:810:SER:OG	1:C:811:LYS:N	2.55	0.40
1:C:985:ASP:OD1	1:C:986:PRO:HD2	2.21	0.40
2:T:86:GLN:CD	2:T:86:GLN:C	2.88	0.40
2:T:116:LEU:O	2:T:120:LEU:HG	2.21	0.40
2:T:164:ALA:C	2:T:167:SER:H	2.30	0.40
2:T:428:PHE:CD1	2:T:429:GLN:N	2.89	0.40
2:X:207:TYR:HH	2:X:398:GLU:CD	2.29	0.40
2:Z:157:ASP:O	2:Z:161:ARG:HD2	2.21	0.40
2:Z:350:ASP:C	2:Z:352:GLY:H	2.29	0.40
2:Z:562:LYS:HE3	2:Z:562:LYS:HB3	1.65	0.40
1:A:57:PRO:HA	1:A:273:ARG:CD	2.52	0.40
1:A:115:GLN:HB3	1:A:130:VAL:HG22	2.03	0.40
1:A:615:ASN:HA	1:A:643:GLN:HE22	1.87	0.40
1:B:103:GLY:HA3	1:B:119:ILE:O	2.22	0.40
1:B:379:CYS:HA	1:B:432:CYS:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:LYS:C	1:B:557:LYS:HE2	2.46	0.40
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	2.03	0.40
1:B:1027:THR:HG22	1:B:1042:PHE:CZ	2.57	0.40
1:C:62:VAL:HG21	1:C:215:PHE:CE2	2.57	0.40
1:C:130:VAL:O	1:C:131:CYS:HB3	2.20	0.40
1:C:198:ASP:C	1:C:200:TYR:N	2.79	0.40
1:C:542:PHE:CD2	1:C:578:PRO:HD3	2.56	0.40
2:T:599:ASN:O	2:T:601:ASN:N	2.55	0.40
2:X:250:ASN:C	2:X:252:TYR:N	2.78	0.40
2:X:260:GLY:HA3	2:X:610:TRP:CE3	2.56	0.40
2:X:381:TYR:O	2:X:383:MET:N	2.55	0.40
2:X:484:ILE:H	2:X:484:ILE:HG12	1.49	0.40
2:X:582:ARG:HA	2:X:582:ARG:HD2	1.21	0.40
2:Z:381:TYR:O	2:Z:383:MET:N	2.55	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%)	697 (69%)	215 (21%)	100 (10%)	0	2
1	B	1009/1123 (90%)	690 (68%)	208 (21%)	111 (11%)	0	1
1	C	1012/1123 (90%)	689 (68%)	203 (20%)	120 (12%)	0	1
2	T	595/597 (100%)	318 (53%)	186 (31%)	91 (15%)	0	0
2	X	595/597 (100%)	318 (53%)	187 (31%)	90 (15%)	0	0
2	Z	595/597 (100%)	316 (53%)	187 (31%)	92 (16%)	0	0
All	All	4818/5160 (93%)	3028 (63%)	1186 (25%)	604 (12%)	1	1

All (604) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	40	ASP
1	A	65	PHE
1	A	90	VAL
1	A	92	PHE
1	A	227	ASP
1	A	350	VAL
1	A	362	VAL
1	A	377	PHE
1	A	423	TYR
1	A	429	PHE
1	A	483	LYS
1	A	522	THR
1	A	530	THR
1	A	533	VAL
1	A	568	ILE
1	A	632	TRP
1	A	854	LYS
1	A	937	SER
1	A	939	PHE
1	A	982	SER
1	A	983	ARG
1	A	1141	LEU
1	B	27	SER
1	B	121	ASN
1	B	140	PHE
1	B	226	VAL
1	B	265	TYR
1	B	322	PRO
1	B	329	PHE
1	B	332	VAL
1	B	350	VAL
1	B	362	VAL
1	B	377	PHE
1	B	423	TYR
1	B	429	PHE
1	B	485	PRO
1	B	522	THR
1	B	530	THR
1	B	561	PHE
1	B	564	PHE
1	B	603	THR
1	B	689	SER

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Mol	Chain	Res	Type
1	B	853	GLN
1	B	919	ASN
1	B	936	ASP
1	B	937	SER
1	B	943	SER
1	B	1117	THR
1	C	27	SER
1	C	32	PHE
1	C	88	ASP
1	C	92	PHE
1	C	94	SER
1	C	128	ILE
1	C	265	TYR
1	C	267	VAL
1	C	324	GLU
1	C	325	SER
1	C	350	VAL
1	C	361	CYS
1	C	377	PHE
1	C	382	VAL
1	C	420	ASP
1	C	427	ASP
1	C	429	PHE
1	C	439	ASN
1	C	475	ALA
1	C	480	CYS
1	C	481	LYS
1	C	483	LYS
1	C	522	THR
1	C	536	LYS
1	C	558	PHE
1	C	564	PHE
1	C	579	GLN
1	C	580	THR
1	C	632	TRP
1	C	831	ALA
1	C	835	LYS
1	C	850	ILE
2	T	73	LEU
2	T	99	ALA
2	T	100	LEU
2	T	119	ILE

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Mol	Chain	Res	Type
2	T	145	GLU
2	T	168	TRP
2	T	243	TYR
2	T	264	ALA
2	T	265	HIS
2	T	454	TYR
2	T	455	MET
2	T	472	GLN
2	T	536	GLU
2	T	574	VAL
2	T	577	LYS
2	X	73	LEU
2	X	99	ALA
2	X	100	LEU
2	X	119	ILE
2	X	168	TRP
2	X	243	TYR
2	X	264	ALA
2	X	265	HIS
2	X	454	TYR
2	X	455	MET
2	X	472	GLN
2	X	536	GLU
2	X	574	VAL
2	X	577	LYS
2	Z	73	LEU
2	Z	99	ALA
2	Z	100	LEU
2	Z	119	ILE
2	Z	168	TRP
2	Z	243	TYR
2	Z	264	ALA
2	Z	265	HIS
2	Z	454	TYR
2	Z	455	MET
2	Z	472	GLN
2	Z	536	GLU
2	Z	574	VAL
2	Z	577	LYS
1	A	21	LEU
1	A	87	ASN
1	A	88	ASP

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Mol	Chain	Res	Type
1	A	119	ILE
1	A	133	PHE
1	A	135	PHE
1	A	140	PHE
1	A	170	TYR
1	A	210	ILE
1	A	238	GLN
1	A	292	ALA
1	A	334	ASN
1	A	351	TYR
1	A	353	TRP
1	A	372	ALA
1	A	374	PHE
1	A	420	ASP
1	A	426	PRO
1	A	448	ASN
1	A	465	GLU
1	A	488	TYR
1	A	523	VAL
1	A	548	THR
1	A	569	VAL
1	A	618	GLU
1	A	623	ILE
1	A	851	CYS
1	A	990	GLU
1	A	991	VAL
1	B	95	THR
1	B	128	ILE
1	B	129	LYS
1	B	135	PHE
1	B	136	CYS
1	B	227	ASP
1	B	285	ILE
1	B	304	LYS
1	B	327	VAL
1	B	351	TYR
1	B	353	TRP
1	B	372	ALA
1	B	374	PHE
1	B	420	ASP
1	B	426	PRO
1	B	448	ASN

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Mol	Chain	Res	Type
1	B	465	GLU
1	B	481	LYS
1	B	523	VAL
1	B	535	ASN
1	B	553	LYS
1	B	568	ILE
1	B	569	VAL
1	B	585	ASP
1	B	744	GLY
1	B	831	ALA
1	B	855	PHE
1	B	983	ARG
1	B	990	GLU
1	B	1127	ASP
1	C	26	GLN
1	C	52	GLN
1	C	64	TRP
1	C	113	LYS
1	C	124	THR
1	C	129	LYS
1	C	131	CYS
1	C	133	PHE
1	C	171	VAL
1	C	210	ILE
1	C	230	ILE
1	C	323	THR
1	C	351	TYR
1	C	353	TRP
1	C	360	ASN
1	C	372	ALA
1	C	374	PHE
1	C	426	PRO
1	C	465	GLU
1	C	488	TYR
1	C	523	VAL
1	C	829	ALA
1	C	851	CYS
1	C	856	ASN
1	C	937	SER
2	T	71	ALA
2	T	102	GLN
2	T	120	LEU

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Mol	Chain	Res	Type
2	T	130	GLY
2	T	151	ILE
2	T	158	TYR
2	T	169	ARG
2	T	171	GLU
2	T	279	TYR
2	T	286	GLY
2	T	338	ASN
2	T	420	SER
2	T	436	ILE
2	T	463	VAL
2	T	483	GLU
2	T	504	PHE
2	T	509	ASP
2	T	528	ALA
2	T	573	VAL
2	T	592	PHE
2	T	600	LYS
2	T	608	THR
2	X	71	ALA
2	X	102	GLN
2	X	120	LEU
2	X	128	SER
2	X	130	GLY
2	X	146	PRO
2	X	151	ILE
2	X	158	TYR
2	X	169	ARG
2	X	171	GLU
2	X	279	TYR
2	X	286	GLY
2	X	338	ASN
2	X	420	SER
2	X	436	ILE
2	X	463	VAL
2	X	483	GLU
2	X	504	PHE
2	X	509	ASP
2	X	528	ALA
2	X	573	VAL
2	X	592	PHE
2	X	600	LYS

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Mol	Chain	Res	Type
2	X	608	THR
2	Z	71	ALA
2	Z	102	GLN
2	Z	120	LEU
2	Z	128	SER
2	Z	130	GLY
2	Z	146	PRO
2	Z	151	ILE
2	Z	158	TYR
2	Z	169	ARG
2	Z	171	GLU
2	Z	279	TYR
2	Z	286	GLY
2	Z	338	ASN
2	Z	420	SER
2	Z	436	ILE
2	Z	463	VAL
2	Z	483	GLU
2	Z	504	PHE
2	Z	509	ASP
2	Z	528	ALA
2	Z	573	VAL
2	Z	592	PHE
2	Z	600	LYS
2	Z	608	THR
1	A	59	PHE
1	A	321	GLN
1	A	324	GLU
1	A	329	PHE
1	A	375	PHE
1	A	440	LYS
1	A	459	SER
1	A	463	PRO
1	A	484	GLY
1	A	487	CYS
1	A	560	PRO
1	A	567	ASP
1	A	738	CYS
1	A	825	LYS
1	A	848	ASP
1	A	856	ASN
1	A	951	VAL

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Mol	Chain	Res	Type
1	A	1140	PRO
1	A	1145	LEU
1	B	21	LEU
1	B	127	PHE
1	B	131	CYS
1	B	168	PHE
1	B	198	ASP
1	B	282	ASN
1	B	331	ASN
1	B	375	PHE
1	B	440	LYS
1	B	463	PRO
1	B	471	GLU
1	B	475	ALA
1	B	560	PRO
1	B	738	CYS
1	B	745	ASP
1	B	746	SER
1	B	851	CYS
1	B	854	LYS
1	B	978	ASN
1	B	979	ASP
1	C	46	SER
1	C	81	ASN
1	C	112	SER
1	C	116	SER
1	C	188	ASN
1	C	192	PHE
1	C	216	PRO
1	C	227	ASP
1	C	282	ASN
1	C	375	PHE
1	C	442	ASP
1	C	463	PRO
1	C	537	CYS
1	C	542	PHE
1	C	543	ASN
1	C	633	ARG
1	C	1145	LEU
2	T	23	GLU
2	T	84	PRO
2	T	118	THR

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Mol	Chain	Res	Type
2	T	121	ASN
2	T	122	THR
2	T	126	ILE
2	T	146	PRO
2	T	147	GLY
2	T	194	ASN
2	T	197	GLU
2	T	236	LEU
2	T	255	TYR
2	T	280	SER
2	T	341	LYS
2	T	382	ASP
2	T	394	ASN
2	T	458	LYS
2	T	471	ASP
2	X	23	GLU
2	X	84	PRO
2	X	118	THR
2	X	121	ASN
2	X	122	THR
2	X	126	ILE
2	X	144	LEU
2	X	145	GLU
2	X	194	ASN
2	X	197	GLU
2	X	236	LEU
2	X	255	TYR
2	X	280	SER
2	X	341	LYS
2	X	382	ASP
2	X	394	ASN
2	X	427	ASP
2	X	458	LYS
2	X	471	ASP
2	Z	23	GLU
2	Z	84	PRO
2	Z	118	THR
2	Z	121	ASN
2	Z	122	THR
2	Z	126	ILE
2	Z	144	LEU
2	Z	145	GLU

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Mol	Chain	Res	Type
2	Z	194	ASN
2	Z	197	GLU
2	Z	236	LEU
2	Z	255	TYR
2	Z	280	SER
2	Z	341	LYS
2	Z	382	ASP
2	Z	394	ASN
2	Z	458	LYS
2	Z	471	ASP
1	A	23	THR
1	A	110	LEU
1	A	129	LYS
1	A	410	ILE
1	A	466	ARG
1	A	580	THR
1	A	810	SER
1	A	940	SER
1	B	59	PHE
1	B	120	VAL
1	B	123	ALA
1	B	165	ASN
1	B	187	LYS
1	B	410	ILE
1	B	466	ARG
1	B	524	CYS
1	B	555	ASN
1	B	558	PHE
1	B	639	SER
1	B	938	LEU
1	C	119	ILE
1	C	209	PRO
1	C	224	PRO
1	C	281	GLU
1	C	358	ILE
1	C	380	TYR
1	C	410	ILE
1	C	459	SER
1	C	466	ARG
1	C	486	ASN
1	C	487	CYS
1	C	489	PHE

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Mol	Chain	Res	Type
1	C	531	ASN
1	C	534	LYS
1	C	557	LYS
1	C	689	SER
1	C	854	LYS
1	C	982	SER
1	C	983	ARG
2	T	144	LEU
2	T	149	ASN
2	T	192	ARG
2	T	206	ASP
2	T	277	ASN
2	T	284	PRO
2	T	295	ASP
2	T	353	LYS
2	T	477	TRP
2	T	548	THR
2	X	149	ASN
2	X	192	ARG
2	X	206	ASP
2	X	277	ASN
2	X	284	PRO
2	X	295	ASP
2	X	353	LYS
2	X	477	TRP
2	X	548	THR
2	Z	149	ASN
2	Z	192	ARG
2	Z	206	ASP
2	Z	277	ASN
2	Z	284	PRO
2	Z	295	ASP
2	Z	353	LYS
2	Z	477	TRP
2	Z	548	THR
1	A	114	THR
1	A	207	HIS
1	A	226	VAL
1	A	333	THR
1	A	464	PHE
1	A	485	PRO
1	A	1084	ASP

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Mol	Chain	Res	Type
1	B	64	TRP
1	B	214	ASP
1	B	228	LEU
1	B	323	THR
1	B	464	PHE
1	B	474	GLN
1	B	835	LYS
1	B	993	ILE
1	B	1135	ASN
1	C	118	LEU
1	C	168	PHE
1	C	211	ILE
1	C	228	LEU
1	C	316	SER
1	C	331	ASN
1	C	454	ARG
1	C	464	PHE
1	C	744	GLY
1	C	832	GLY
1	C	973	ILE
1	C	979	ASP
2	T	24	GLN
2	T	25	ALA
2	T	33	ASN
2	T	137	ASN
2	T	155	SER
2	T	189	GLU
2	T	254	SER
2	T	269	ASP
2	T	403	ALA
2	T	433	GLU
2	T	456	LEU
2	T	470	LYS
2	T	575	GLY
2	X	24	GLN
2	X	25	ALA
2	X	33	ASN
2	X	137	ASN
2	X	155	SER
2	X	189	GLU
2	X	254	SER
2	X	269	ASP

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Mol	Chain	Res	Type
2	X	403	ALA
2	X	456	LEU
2	X	470	LYS
2	X	575	GLY
2	Z	24	GLN
2	Z	25	ALA
2	Z	33	ASN
2	Z	137	ASN
2	Z	155	SER
2	Z	189	GLU
2	Z	254	SER
2	Z	269	ASP
2	Z	291	ILE
2	Z	403	ALA
2	Z	433	GLU
2	Z	456	LEU
2	Z	470	LYS
2	Z	575	GLY
1	A	139	PRO
1	A	217	GLN
1	A	293	LEU
1	A	354	ASN
1	A	524	CYS
1	A	534	LYS
1	A	817	PRO
1	A	938	LEU
1	A	1123	SER
1	B	42	VAL
1	B	62	VAL
1	B	215	PHE
1	B	230	ILE
1	B	354	ASN
1	B	459	SER
1	B	1126	CYS
1	C	199	GLY
1	C	354	ASN
1	C	455	LEU
1	C	524	CYS
1	C	756	TYR
2	T	46	ALA
2	T	128	SER
2	T	212	VAL

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Mol	Chain	Res	Type
2	T	213	ASP
2	T	311	ALA
2	T	339	VAL
2	T	435	GLU
2	T	446	ILE
2	X	46	ALA
2	X	212	VAL
2	X	213	ASP
2	X	311	ALA
2	X	339	VAL
2	X	435	GLU
2	X	446	ILE
2	Z	46	ALA
2	Z	212	VAL
2	Z	213	ASP
2	Z	311	ALA
2	Z	339	VAL
2	Z	424	LEU
2	Z	435	GLU
2	Z	446	ILE
1	A	267	VAL
1	C	447	GLY
1	C	560	PRO
2	T	244	VAL
2	X	244	VAL
2	Z	244	VAL
1	A	987	PRO
2	T	447	VAL
2	X	211	GLY
2	X	447	VAL
2	Z	211	GLY
2	Z	447	VAL
1	A	367	VAL
1	A	621	VAL
1	B	289	VAL
1	B	326	ILE
1	B	367	VAL
1	B	634	VAL
1	B	785	VAL
1	C	105	ILE
1	C	231	GLY
1	C	367	VAL

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Mol	Chain	Res	Type
1	C	621	VAL
2	T	211	GLY
1	B	105	ILE
1	B	484	GLY
1	C	485	PRO
1	C	963	VAL
1	A	482	GLY
1	C	329	PHE
1	C	586	ILE
2	T	253	PRO
2	T	415	PRO
2	X	253	PRO
2	X	415	PRO
2	Z	253	PRO
2	Z	415	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	903/978 (92%)	599 (66%)	304 (34%)	0	1
1	B	902/978 (92%)	604 (67%)	298 (33%)	0	1
1	C	903/978 (92%)	592 (66%)	311 (34%)	0	1
2	T	527/527 (100%)	328 (62%)	199 (38%)	0	1
2	X	527/527 (100%)	329 (62%)	198 (38%)	0	1
2	Z	527/527 (100%)	331 (63%)	196 (37%)	0	1
All	All	4289/4515 (95%)	2783 (65%)	1506 (35%)	1	1

All (1506) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	24	THR
1	A	25	THR

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Mol	Chain	Res	Type
1	A	26	GLN
1	A	27	SER
1	A	29	THR
1	A	31	SER
1	A	34	ARG
1	A	36	VAL
1	A	41	LYS
1	A	46	SER
1	A	50	LEU
1	A	51	THR
1	A	52	GLN
1	A	54	LEU
1	A	55	PHE
1	A	56	LEU
1	A	62	VAL
1	A	66	HIS
1	A	83	VAL
1	A	84	LEU
1	A	88	ASP
1	A	94	SER
1	A	95	THR
1	A	96	GLU
1	A	102	ARG
1	A	105	ILE
1	A	108	THR
1	A	109	THR
1	A	112	SER
1	A	113	LYS
1	A	114	THR
1	A	118	LEU
1	A	127	PHE
1	A	128	ILE
1	A	129	LYS
1	A	130	VAL
1	A	132	GLU
1	A	133	PHE
1	A	134	GLN
1	A	135	PHE
1	A	137	ASN
1	A	141	LEU
1	A	166	CYS
1	A	167	THR

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Mol	Chain	Res	Type
1	A	168	PHE
1	A	169	GLU
1	A	171	VAL
1	A	187	LYS
1	A	188	ASN
1	A	189	LEU
1	A	190	ARG
1	A	193	VAL
1	A	195	LYS
1	A	198	ASP
1	A	202	LYS
1	A	205	SER
1	A	206	LYS
1	A	208	THR
1	A	210	ILE
1	A	211	ILE
1	A	213	ARG
1	A	214	ASP
1	A	217	GLN
1	A	223	GLU
1	A	225	LEU
1	A	226	VAL
1	A	228	LEU
1	A	230	ILE
1	A	234	ILE
1	A	236	ARG
1	A	239	THR
1	A	241	LEU
1	A	266	TYR
1	A	271	GLN
1	A	278	LYS
1	A	282	ASN
1	A	294	ASP
1	A	304	LYS
1	A	312	ILE
1	A	316	SER
1	A	317	ASN
1	A	319	ARG
1	A	323	THR
1	A	324	GLU
1	A	326	ILE
1	A	328	ARG

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Mol	Chain	Res	Type
1	A	329	PHE
1	A	332	VAL
1	A	335	LEU
1	A	340	GLU
1	A	341	VAL
1	A	345	THR
1	A	346	ARG
1	A	349	SER
1	A	350	VAL
1	A	353	TRP
1	A	354	ASN
1	A	355	ARG
1	A	356	THR
1	A	357	ARG
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	383	SER
1	A	386	LYS
1	A	387	LEU
1	A	388	ASN
1	A	390	LEU
1	A	392	PHE
1	A	393	THR
1	A	396	TYR
1	A	398	ASP
1	A	401	VAL
1	A	403	LYS
1	A	407	VAL
1	A	408	SER
1	A	410	ILE
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

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Mol	Chain	Res	Type
1	A	444	LYS
1	A	445	HIS
1	A	454	ARG
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	463	PRO
1	A	466	ARG
1	A	468	ILE
1	A	472	ILE
1	A	474	GLN
1	A	481	LYS
1	A	483	LYS
1	A	488	TYR
1	A	497	ARG
1	A	508	ARG
1	A	511	VAL
1	A	516	LEU
1	A	523	VAL
1	A	524	CYS
1	A	528	LYS
1	A	530	THR
1	A	531	ASN
1	A	534	LYS
1	A	538	VAL
1	A	539	ASN
1	A	540	PHE
1	A	545	LEU
1	A	546	THR
1	A	548	THR
1	A	552	THR
1	A	553	LYS
1	A	556	LYS
1	A	559	LEU
1	A	562	GLN
1	A	563	GLN
1	A	570	ASP
1	A	571	THR
1	A	572	THR

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Mol	Chain	Res	Type
1	A	575	VAL
1	A	576	ARG
1	A	577	ASP
1	A	579	GLN
1	A	580	THR
1	A	585	ASP
1	A	587	THR
1	A	588	PRO
1	A	590	SER
1	A	602	ASN
1	A	604	SER
1	A	606	GLN
1	A	612	GLN
1	A	614	VAL
1	A	619	VAL
1	A	631	THR
1	A	633	ARG
1	A	635	TYR
1	A	640	ASN
1	A	641	VAL
1	A	643	GLN
1	A	645	ARG
1	A	665	ILE
1	A	674	GLN
1	A	675	THR
1	A	676	GLN
1	A	692	ILE
1	A	702	GLU
1	A	705	VAL
1	A	711	SER
1	A	714	ILE
1	A	719	THR
1	A	721	SER
1	A	723	THR
1	A	727	LEU
1	A	733	LYS
1	A	738	CYS
1	A	739	THR
1	A	740	MET
1	A	745	ASP
1	A	750	SER
1	A	752	LEU

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Mol	Chain	Res	Type
1	A	754	LEU
1	A	755	GLN
1	A	759	PHE
1	A	761	THR
1	A	764	LYS
1	A	765	ARG
1	A	772	VAL
1	A	776	LYS
1	A	779	GLN
1	A	786	LYS
1	A	787	GLN
1	A	791	THR
1	A	794	ILE
1	A	804	GLN
1	A	810	SER
1	A	813	SER
1	A	817	PRO
1	A	818	ILE
1	A	821	LEU
1	A	824	ASN
1	A	825	LYS
1	A	828	LEU
1	A	834	ILE
1	A	835	LYS
1	A	847	ARG
1	A	849	LEU
1	A	850	ILE
1	A	851	CYS
1	A	853	GLN
1	A	854	LYS
1	A	855	PHE
1	A	868	GLU
1	A	874	THR
1	A	875	SER
1	A	878	LEU
1	A	884	SER
1	A	895	GLN
1	A	896	ILE
1	A	901	GLN
1	A	902	MET
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	931	ILE
1	A	935	GLN
1	A	936	ASP
1	A	942	PRO
1	A	945	LEU
1	A	947	LYS
1	A	960	ASN
1	A	964	LYS
1	A	965	GLN
1	A	967	SER
1	A	969	LYS
1	A	975	SER
1	A	977	LEU
1	A	978	ASN
1	A	985	ASP
1	A	990	GLU
1	A	991	VAL
1	A	993	ILE
1	A	995	ARG
1	A	1001	LEU
1	A	1002	GLN
1	A	1014	ARG
1	A	1017	GLU
1	A	1037	SER
1	A	1038	LYS
1	A	1045	LYS
1	A	1055	SER
1	A	1072	GLU
1	A	1076	THR
1	A	1081	ILE
1	A	1086	LYS
1	A	1092	GLU
1	A	1106	GLN
1	A	1108	ASN
1	A	1111	GLU
1	A	1113	GLN
1	A	1114	ILE
1	A	1119	ASN
1	A	1122	VAL
1	A	1125	ASN

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Mol	Chain	Res	Type
1	A	1127	ASP
1	A	1133	VAL
1	A	1136	THR
1	A	1141	LEU
1	A	1143	LEU
1	A	1144	GLU
1	A	1147	SER
1	B	21	LEU
1	B	24	THR
1	B	25	THR
1	B	26	GLN
1	B	31	SER
1	B	32	PHE
1	B	34	ARG
1	B	36	VAL
1	B	40	ASP
1	B	41	LYS
1	B	45	SER
1	B	47	VAL
1	B	48	LEU
1	B	51	THR
1	B	52	GLN
1	B	80	ASP
1	B	81	ASN
1	B	83	VAL
1	B	88	ASP
1	B	90	VAL
1	B	95	THR
1	B	96	GLU
1	B	105	ILE
1	B	109	THR
1	B	110	LEU
1	B	113	LYS
1	B	114	THR
1	B	115	GLN
1	B	116	SER
1	B	119	ILE
1	B	121	ASN
1	B	125	ASN
1	B	126	VAL
1	B	127	PHE
1	B	128	ILE

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Mol	Chain	Res	Type
1	B	129	LYS
1	B	132	GLU
1	B	134	GLN
1	B	142	ASP
1	B	165	ASN
1	B	167	THR
1	B	170	TYR
1	B	171	VAL
1	B	172	SER
1	B	187	LYS
1	B	190	ARG
1	B	195	LYS
1	B	197	ILE
1	B	198	ASP
1	B	200	TYR
1	B	202	LYS
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	215	PHE
1	B	217	GLN
1	B	223	GLU
1	B	225	LEU
1	B	230	ILE
1	B	232	ILE
1	B	236	ARG
1	B	237	PHE
1	B	271	GLN
1	B	273	ARG
1	B	278	LYS
1	B	281	GLU
1	B	284	THR
1	B	303	LEU
1	B	304	LYS
1	B	305	SER
1	B	307	THR
1	B	308	VAL
1	B	310	LYS
1	B	312	ILE

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Mol	Chain	Res	Type
1	B	314	GLN
1	B	316	SER
1	B	322	PRO
1	B	326	ILE
1	B	329	PHE
1	B	332	VAL
1	B	335	LEU
1	B	340	GLU
1	B	341	VAL
1	B	345	THR
1	B	346	ARG
1	B	349	SER
1	B	350	VAL
1	B	353	TRP
1	B	354	ASN
1	B	355	ARG
1	B	356	THR
1	B	357	ARG
1	B	366	SER
1	B	367	VAL
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	387	LEU
1	B	388	ASN
1	B	390	LEU
1	B	392	PHE
1	B	393	THR
1	B	396	TYR
1	B	398	ASP
1	B	401	VAL
1	B	403	LYS
1	B	407	VAL
1	B	408	SER
1	B	410	ILE
1	B	415	THR
1	B	417	ASN
1	B	418	ILE

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Mol	Chain	Res	Type
1	B	420	ASP
1	B	428	ASP
1	B	429	PHE
1	B	432	CYS
1	B	444	LYS
1	B	445	HIS
1	B	454	ARG
1	B	456	PHE
1	B	457	ARG
1	B	458	LYS
1	B	459	SER
1	B	460	LYS
1	B	461	LEU
1	B	462	LYS
1	B	463	PRO
1	B	466	ARG
1	B	468	ILE
1	B	470	THR
1	B	471	GLU
1	B	474	GLN
1	B	477	ASN
1	B	478	LYS
1	B	481	LYS
1	B	483	LYS
1	B	485	PRO
1	B	486	ASN
1	B	491	LEU
1	B	497	ARG
1	B	508	ARG
1	B	511	VAL
1	B	516	LEU
1	B	523	VAL
1	B	524	CYS
1	B	528	LYS
1	B	530	THR
1	B	532	LEU
1	B	534	LYS
1	B	541	ASN
1	B	543	ASN
1	B	545	LEU
1	B	548	THR
1	B	552	THR

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Mol	Chain	Res	Type
1	B	553	LYS
1	B	555	ASN
1	B	557	LYS
1	B	559	LEU
1	B	562	GLN
1	B	563	GLN
1	B	564	PHE
1	B	566	ARG
1	B	568	ILE
1	B	569	VAL
1	B	570	ASP
1	B	575	VAL
1	B	576	ARG
1	B	579	GLN
1	B	582	GLU
1	B	584	LEU
1	B	585	ASP
1	B	587	THR
1	B	590	SER
1	B	598	THR
1	B	602	ASN
1	B	604	SER
1	B	614	VAL
1	B	618	GLU
1	B	623	ILE
1	B	624	HIS
1	B	630	PRO
1	B	631	THR
1	B	633	ARG
1	B	637	THR
1	B	645	ARG
1	B	653	GLU
1	B	657	ASN
1	B	675	THR
1	B	689	SER
1	B	696	THR
1	B	697	MET
1	B	705	VAL
1	B	709	ASN
1	B	711	SER
1	B	712	ILE
1	B	714	ILE

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Mol	Chain	Res	Type
1	B	719	THR
1	B	723	THR
1	B	727	LEU
1	B	731	MET
1	B	732	THR
1	B	735	SER
1	B	738	CYS
1	B	739	THR
1	B	740	MET
1	B	742	ILE
1	B	746	SER
1	B	747	THR
1	B	748	GLU
1	B	749	CYS
1	B	750	SER
1	B	752	LEU
1	B	755	GLN
1	B	758	SER
1	B	764	LYS
1	B	776	LYS
1	B	779	GLN
1	B	785	VAL
1	B	786	LYS
1	B	787	GLN
1	B	791	THR
1	B	794	ILE
1	B	811	LYS
1	B	813	SER
1	B	814	LYS
1	B	818	ILE
1	B	821	LEU
1	B	825	LYS
1	B	828	LEU
1	B	833	PHE
1	B	834	ILE
1	B	836	GLN
1	B	848	ASP
1	B	849	LEU
1	B	850	ILE
1	B	854	LYS
1	B	855	PHE
1	B	859	THR

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Mol	Chain	Res	Type
1	B	868	GLU
1	B	874	THR
1	B	878	LEU
1	B	883	THR
1	B	895	GLN
1	B	900	MET
1	B	905	ARG
1	B	907	ASN
1	B	914	ASN
1	B	916	LEU
1	B	921	LYS
1	B	929	SER
1	B	931	ILE
1	B	933	LYS
1	B	935	GLN
1	B	936	ASP
1	B	939	PHE
1	B	968	SER
1	B	969	LYS
1	B	974	SER
1	B	975	SER
1	B	976	VAL
1	B	978	ASN
1	B	979	ASP
1	B	984	LEU
1	B	993	ILE
1	B	996	LEU
1	B	1001	LEU
1	B	1010	GLN
1	B	1018	ILE
1	B	1028	LYS
1	B	1029	MET
1	B	1037	SER
1	B	1045	LYS
1	B	1066	THR
1	B	1072	GLU
1	B	1073	LYS
1	B	1081	ILE
1	B	1086	LYS
1	B	1100	THR
1	B	1105	THR
1	B	1106	GLN

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Mol	Chain	Res	Type
1	B	1113	GLN
1	B	1114	ILE
1	B	1128	VAL
1	B	1134	ASN
1	B	1136	THR
1	B	1141	LEU
1	B	1142	GLN
1	B	1143	LEU
1	B	1144	GLU
1	B	1145	LEU
1	B	1146	ASP
1	C	21	LEU
1	C	23	THR
1	C	25	THR
1	C	28	TYR
1	C	31	SER
1	C	32	PHE
1	C	36	VAL
1	C	41	LYS
1	C	50	LEU
1	C	51	THR
1	C	52	GLN
1	C	55	PHE
1	C	60	SER
1	C	62	VAL
1	C	63	THR
1	C	66	HIS
1	C	83	VAL
1	C	84	LEU
1	C	86	PHE
1	C	87	ASN
1	C	96	GLU
1	C	102	ARG
1	C	105	ILE
1	C	110	LEU
1	C	112	SER
1	C	113	LYS
1	C	114	THR
1	C	118	LEU
1	C	125	ASN
1	C	128	ILE
1	C	129	LYS

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Mol	Chain	Res	Type
1	C	130	VAL
1	C	132	GLU
1	C	135	PHE
1	C	136	CYS
1	C	140	PHE
1	C	141	LEU
1	C	165	ASN
1	C	166	CYS
1	C	171	VAL
1	C	172	SER
1	C	187	LYS
1	C	188	ASN
1	C	190	ARG
1	C	191	GLU
1	C	192	PHE
1	C	193	VAL
1	C	195	LYS
1	C	196	ASN
1	C	202	LYS
1	C	203	ILE
1	C	206	LYS
1	C	207	HIS
1	C	208	THR
1	C	210	ILE
1	C	211	ILE
1	C	213	ARG
1	C	214	ASP
1	C	217	GLN
1	C	224	PRO
1	C	225	LEU
1	C	226	VAL
1	C	230	ILE
1	C	232	ILE
1	C	236	ARG
1	C	238	GLN
1	C	240	LEU
1	C	241	LEU
1	C	271	GLN
1	C	278	LYS
1	C	284	THR
1	C	289	VAL
1	C	300	LYS

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Mol	Chain	Res	Type
1	C	304	LYS
1	C	305	SER
1	C	307	THR
1	C	309	GLU
1	C	310	LYS
1	C	312	ILE
1	C	314	GLN
1	C	315	THR
1	C	317	ASN
1	C	319	ARG
1	C	324	GLU
1	C	326	ILE
1	C	327	VAL
1	C	328	ARG
1	C	332	VAL
1	C	335	LEU
1	C	340	GLU
1	C	341	VAL
1	C	345	THR
1	C	346	ARG
1	C	349	SER
1	C	350	VAL
1	C	353	TRP
1	C	354	ASN
1	C	355	ARG
1	C	356	THR
1	C	357	ARG
1	C	358	ILE
1	C	359	SER
1	C	360	ASN
1	C	362	VAL
1	C	366	SER
1	C	367	VAL
1	C	374	PHE
1	C	375	PHE
1	C	377	PHE
1	C	378	LYS
1	C	380	TYR
1	C	382	VAL
1	C	383	SER
1	C	386	LYS
1	C	387	LEU

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Mol	Chain	Res	Type
1	C	388	ASN
1	C	390	LEU
1	C	392	PHE
1	C	393	THR
1	C	396	TYR
1	C	398	ASP
1	C	401	VAL
1	C	403	LYS
1	C	407	VAL
1	C	408	SER
1	C	410	ILE
1	C	415	THR
1	C	417	ASN
1	C	418	ILE
1	C	420	ASP
1	C	421	TYR
1	C	424	LYS
1	C	428	ASP
1	C	429	PHE
1	C	432	CYS
1	C	433	VAL
1	C	434	ILE
1	C	440	LYS
1	C	441	LEU
1	C	442	ASP
1	C	443	SER
1	C	444	LYS
1	C	446	SER
1	C	450	ASP
1	C	454	ARG
1	C	457	ARG
1	C	458	LYS
1	C	459	SER
1	C	461	LEU
1	C	462	LYS
1	C	463	PRO
1	C	466	ARG
1	C	468	ILE
1	C	474	GLN
1	C	477	ASN
1	C	478	LYS
1	C	481	LYS

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Mol	Chain	Res	Type
1	C	483	LYS
1	C	488	TYR
1	C	497	ARG
1	C	508	ARG
1	C	511	VAL
1	C	516	LEU
1	C	523	VAL
1	C	524	CYS
1	C	527	LYS
1	C	528	LYS
1	C	534	LYS
1	C	535	ASN
1	C	536	LYS
1	C	537	CYS
1	C	538	VAL
1	C	545	LEU
1	C	552	THR
1	C	553	LYS
1	C	556	LYS
1	C	557	LYS
1	C	559	LEU
1	C	561	PHE
1	C	562	GLN
1	C	564	PHE
1	C	566	ARG
1	C	567	ASP
1	C	568	ILE
1	C	569	VAL
1	C	570	ASP
1	C	576	ARG
1	C	577	ASP
1	C	580	THR
1	C	582	GLU
1	C	583	ILE
1	C	584	LEU
1	C	587	THR
1	C	589	CYS
1	C	590	SER
1	C	598	THR
1	C	614	VAL
1	C	618	GLU
1	C	621	VAL

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Mol	Chain	Res	Type
1	C	623	ILE
1	C	632	TRP
1	C	633	ARG
1	C	634	VAL
1	C	637	THR
1	C	640	ASN
1	C	641	VAL
1	C	643	GLN
1	C	650	ILE
1	C	653	GLU
1	C	674	GLN
1	C	675	THR
1	C	676	GLN
1	C	690	GLN
1	C	691	SER
1	C	696	THR
1	C	697	MET
1	C	702	GLU
1	C	704	SER
1	C	705	VAL
1	C	708	SER
1	C	709	ASN
1	C	711	SER
1	C	714	ILE
1	C	719	THR
1	C	721	SER
1	C	723	THR
1	C	724	THR
1	C	727	LEU
1	C	730	SER
1	C	740	MET
1	C	743	CYS
1	C	745	ASP
1	C	746	SER
1	C	747	THR
1	C	750	SER
1	C	761	THR
1	C	764	LYS
1	C	776	LYS
1	C	779	GLN
1	C	785	VAL
1	C	786	LYS

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Mol	Chain	Res	Type
1	C	787	GLN
1	C	790	LYS
1	C	792	PRO
1	C	794	ILE
1	C	803	SER
1	C	810	SER
1	C	811	LYS
1	C	814	LYS
1	C	815	ARG
1	C	820	ASP
1	C	821	LEU
1	C	827	THR
1	C	830	ASP
1	C	833	PHE
1	C	835	LYS
1	C	847	ARG
1	C	848	ASP
1	C	849	LEU
1	C	851	CYS
1	C	853	GLN
1	C	854	LYS
1	C	855	PHE
1	C	859	THR
1	C	865	LEU
1	C	868	GLU
1	C	878	LEU
1	C	895	GLN
1	C	918	GLU
1	C	931	ILE
1	C	933	LYS
1	C	934	ILE
1	C	935	GLN
1	C	945	LEU
1	C	947	LYS
1	C	951	VAL
1	C	952	VAL
1	C	963	VAL
1	C	965	GLN
1	C	966	LEU
1	C	969	LYS
1	C	980	ILE
1	C	982	SER

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Mol	Chain	Res	Type
1	C	983	ARG
1	C	984	LEU
1	C	988	GLU
1	C	990	GLU
1	C	993	ILE
1	C	995	ARG
1	C	1011	GLN
1	C	1018	ILE
1	C	1037	SER
1	C	1038	LYS
1	C	1045	LYS
1	C	1081	ILE
1	C	1086	LYS
1	C	1092	GLU
1	C	1094	VAL
1	C	1100	THR
1	C	1104	VAL
1	C	1106	GLN
1	C	1111	GLU
1	C	1113	GLN
1	C	1114	ILE
1	C	1118	ASP
1	C	1128	VAL
1	C	1133	VAL
1	C	1136	THR
1	C	1138	TYR
1	C	1142	GLN
1	C	1143	LEU
2	T	20	THR
2	T	21	ILE
2	T	22	GLU
2	T	23	GLU
2	T	24	GLN
2	T	30	ASP
2	T	31	LYS
2	T	34	HIS
2	T	39	LEU
2	T	45	LEU
2	T	57	GLU
2	T	62	MET
2	T	64	ASN
2	T	67	ASP

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Mol	Chain	Res	Type
2	T	68	LYS
2	T	74	LYS
2	T	75	GLU
2	T	78	THR
2	T	79	LEU
2	T	82	MET
2	T	84	PRO
2	T	85	LEU
2	T	86	GLN
2	T	87	GLU
2	T	89	GLN
2	T	93	VAL
2	T	97	LEU
2	T	98	GLN
2	T	103	ASN
2	T	107	VAL
2	T	108	LEU
2	T	110	GLU
2	T	111	ASP
2	T	114	LYS
2	T	115	ARG
2	T	117	ASN
2	T	118	THR
2	T	120	LEU
2	T	123	MET
2	T	131	LYS
2	T	136	ASP
2	T	142	LEU
2	T	143	LEU
2	T	145	GLU
2	T	148	LEU
2	T	150	GLU
2	T	151	ILE
2	T	152	MET
2	T	154	ASN
2	T	156	LEU
2	T	159	ASN
2	T	161	ARG
2	T	162	LEU
2	T	166	GLU
2	T	169	ARG
2	T	172	VAL

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Mol	Chain	Res	Type
2	T	174	LYS
2	T	176	LEU
2	T	183	TYR
2	T	184	VAL
2	T	187	LYS
2	T	189	GLU
2	T	190	MET
2	T	197	GLU
2	T	212	VAL
2	T	213	ASP
2	T	216	ASP
2	T	219	ARG
2	T	223	ILE
2	T	227	GLU
2	T	232	GLU
2	T	233	ILE
2	T	234	LYS
2	T	236	LEU
2	T	245	ARG
2	T	247	LYS
2	T	248	LEU
2	T	255	TYR
2	T	265	HIS
2	T	266	LEU
2	T	267	LEU
2	T	269	ASP
2	T	271	TRP
2	T	273	ARG
2	T	277	ASN
2	T	282	THR
2	T	284	PRO
2	T	287	GLN
2	T	288	LYS
2	T	290	ASN
2	T	295	ASP
2	T	297	MET
2	T	298	VAL
2	T	300	GLN
2	T	305	GLN
2	T	306	ARG
2	T	307	ILE
2	T	313	LYS

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Mol	Chain	Res	Type
2	T	317	SER
2	T	324	THR
2	T	329	GLU
2	T	332	MET
2	T	334	THR
2	T	335	ASP
2	T	340	GLN
2	T	341	LYS
2	T	344	CYS
2	T	351	LEU
2	T	355	ASP
2	T	359	LEU
2	T	363	LYS
2	T	365	THR
2	T	366	MET
2	T	368	ASP
2	T	369	PHE
2	T	376	MET
2	T	379	ILE
2	T	385	TYR
2	T	394	ASN
2	T	397	ASN
2	T	398	GLU
2	T	410	LEU
2	T	414	THR
2	T	416	LYS
2	T	418	LEU
2	T	419	LYS
2	T	421	ILE
2	T	423	LEU
2	T	424	LEU
2	T	425	SER
2	T	427	ASP
2	T	429	GLN
2	T	430	GLU
2	T	431	ASP
2	T	432	ASN
2	T	434	THR
2	T	435	GLU
2	T	436	ILE
2	T	438	PHE
2	T	440	LEU

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Mol	Chain	Res	Type
2	T	442	GLN
2	T	445	THR
2	T	446	ILE
2	T	447	VAL
2	T	450	LEU
2	T	455	MET
2	T	456	LEU
2	T	465	LYS
2	T	470	LYS
2	T	472	GLN
2	T	474	MET
2	T	475	LYS
2	T	476	LYS
2	T	480	MET
2	T	481	LYS
2	T	483	GLU
2	T	484	ILE
2	T	485	VAL
2	T	488	VAL
2	T	491	VAL
2	T	493	HIS
2	T	494	ASP
2	T	495	GLU
2	T	496	THR
2	T	498	CYS
2	T	502	SER
2	T	503	LEU
2	T	506	VAL
2	T	509	ASP
2	T	511	SER
2	T	518	ARG
2	T	520	LEU
2	T	527	GLU
2	T	529	LEU
2	T	534	LYS
2	T	539	LEU
2	T	540	HIS
2	T	545	SER
2	T	553	LYS
2	T	554	LEU
2	T	559	ARG
2	T	560	LEU

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Mol	Chain	Res	Type
2	T	567	THR
2	T	568	LEU
2	T	571	GLU
2	T	577	LYS
2	T	582	ARG
2	T	584	LEU
2	T	585	LEU
2	T	589	GLU
2	T	590	PRO
2	T	595	LEU
2	T	596	LYS
2	T	597	ASP
2	T	600	LYS
2	T	601	ASN
2	T	606	TRP
2	T	609	ASP
2	T	611	SER
2	X	20	THR
2	X	21	ILE
2	X	22	GLU
2	X	23	GLU
2	X	24	GLN
2	X	30	ASP
2	X	31	LYS
2	X	34	HIS
2	X	39	LEU
2	X	45	LEU
2	X	57	GLU
2	X	62	MET
2	X	64	ASN
2	X	67	ASP
2	X	68	LYS
2	X	74	LYS
2	X	75	GLU
2	X	78	THR
2	X	79	LEU
2	X	82	MET
2	X	84	PRO
2	X	85	LEU
2	X	86	GLN
2	X	87	GLU
2	X	89	GLN

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Mol	Chain	Res	Type
2	X	93	VAL
2	X	97	LEU
2	X	98	GLN
2	X	103	ASN
2	X	107	VAL
2	X	108	LEU
2	X	110	GLU
2	X	111	ASP
2	X	114	LYS
2	X	115	ARG
2	X	117	ASN
2	X	118	THR
2	X	120	LEU
2	X	123	MET
2	X	129	THR
2	X	131	LYS
2	X	136	ASP
2	X	142	LEU
2	X	143	LEU
2	X	148	LEU
2	X	150	GLU
2	X	151	ILE
2	X	152	MET
2	X	154	ASN
2	X	156	LEU
2	X	159	ASN
2	X	161	ARG
2	X	162	LEU
2	X	166	GLU
2	X	169	ARG
2	X	172	VAL
2	X	174	LYS
2	X	176	LEU
2	X	183	TYR
2	X	184	VAL
2	X	187	LYS
2	X	189	GLU
2	X	190	MET
2	X	197	GLU
2	X	212	VAL
2	X	213	ASP
2	X	216	ASP

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Mol	Chain	Res	Type
2	X	219	ARG
2	X	223	ILE
2	X	227	GLU
2	X	232	GLU
2	X	233	ILE
2	X	234	LYS
2	X	236	LEU
2	X	245	ARG
2	X	247	LYS
2	X	248	LEU
2	X	255	TYR
2	X	265	HIS
2	X	266	LEU
2	X	267	LEU
2	X	269	ASP
2	X	271	TRP
2	X	273	ARG
2	X	277	ASN
2	X	282	THR
2	X	284	PRO
2	X	288	LYS
2	X	295	ASP
2	X	297	MET
2	X	298	VAL
2	X	300	GLN
2	X	305	GLN
2	X	306	ARG
2	X	307	ILE
2	X	313	LYS
2	X	317	SER
2	X	324	THR
2	X	329	GLU
2	X	332	MET
2	X	334	THR
2	X	335	ASP
2	X	340	GLN
2	X	341	LYS
2	X	344	CYS
2	X	351	LEU
2	X	355	ASP
2	X	359	LEU
2	X	363	LYS

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Mol	Chain	Res	Type
2	X	365	THR
2	X	366	MET
2	X	368	ASP
2	X	369	PHE
2	X	376	MET
2	X	379	ILE
2	X	385	TYR
2	X	394	ASN
2	X	397	ASN
2	X	398	GLU
2	X	408	MET
2	X	410	LEU
2	X	414	THR
2	X	416	LYS
2	X	418	LEU
2	X	419	LYS
2	X	421	ILE
2	X	423	LEU
2	X	424	LEU
2	X	425	SER
2	X	427	ASP
2	X	429	GLN
2	X	430	GLU
2	X	432	ASN
2	X	434	THR
2	X	435	GLU
2	X	436	ILE
2	X	438	PHE
2	X	440	LEU
2	X	442	GLN
2	X	445	THR
2	X	446	ILE
2	X	447	VAL
2	X	450	LEU
2	X	455	MET
2	X	456	LEU
2	X	465	LYS
2	X	470	LYS
2	X	472	GLN
2	X	474	MET
2	X	475	LYS
2	X	476	LYS

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Mol	Chain	Res	Type
2	X	480	MET
2	X	481	LYS
2	X	483	GLU
2	X	484	ILE
2	X	485	VAL
2	X	488	VAL
2	X	491	VAL
2	X	493	HIS
2	X	494	ASP
2	X	495	GLU
2	X	496	THR
2	X	498	CYS
2	X	499	ASP
2	X	502	SER
2	X	503	LEU
2	X	506	VAL
2	X	509	ASP
2	X	511	SER
2	X	518	ARG
2	X	520	LEU
2	X	527	GLU
2	X	529	LEU
2	X	534	LYS
2	X	539	LEU
2	X	540	HIS
2	X	545	SER
2	X	553	LYS
2	X	554	LEU
2	X	559	ARG
2	X	560	LEU
2	X	567	THR
2	X	568	LEU
2	X	571	GLU
2	X	577	LYS
2	X	582	ARG
2	X	584	LEU
2	X	585	LEU
2	X	589	GLU
2	X	590	PRO
2	X	595	LEU
2	X	596	LYS
2	X	597	ASP

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Mol	Chain	Res	Type
2	X	600	LYS
2	X	601	ASN
2	X	606	TRP
2	X	609	ASP
2	X	611	SER
2	Z	20	THR
2	Z	21	ILE
2	Z	22	GLU
2	Z	23	GLU
2	Z	24	GLN
2	Z	30	ASP
2	Z	31	LYS
2	Z	34	HIS
2	Z	39	LEU
2	Z	45	LEU
2	Z	57	GLU
2	Z	62	MET
2	Z	64	ASN
2	Z	67	ASP
2	Z	68	LYS
2	Z	74	LYS
2	Z	75	GLU
2	Z	78	THR
2	Z	79	LEU
2	Z	82	MET
2	Z	84	PRO
2	Z	85	LEU
2	Z	86	GLN
2	Z	87	GLU
2	Z	89	GLN
2	Z	93	VAL
2	Z	97	LEU
2	Z	98	GLN
2	Z	103	ASN
2	Z	107	VAL
2	Z	108	LEU
2	Z	110	GLU
2	Z	111	ASP
2	Z	114	LYS
2	Z	115	ARG
2	Z	117	ASN
2	Z	118	THR

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Mol	Chain	Res	Type
2	Z	120	LEU
2	Z	123	MET
2	Z	129	THR
2	Z	131	LYS
2	Z	136	ASP
2	Z	142	LEU
2	Z	143	LEU
2	Z	148	LEU
2	Z	150	GLU
2	Z	151	ILE
2	Z	152	MET
2	Z	154	ASN
2	Z	156	LEU
2	Z	159	ASN
2	Z	161	ARG
2	Z	162	LEU
2	Z	166	GLU
2	Z	169	ARG
2	Z	172	VAL
2	Z	174	LYS
2	Z	176	LEU
2	Z	183	TYR
2	Z	184	VAL
2	Z	187	LYS
2	Z	189	GLU
2	Z	190	MET
2	Z	197	GLU
2	Z	212	VAL
2	Z	213	ASP
2	Z	216	ASP
2	Z	219	ARG
2	Z	223	ILE
2	Z	227	GLU
2	Z	232	GLU
2	Z	233	ILE
2	Z	234	LYS
2	Z	236	LEU
2	Z	245	ARG
2	Z	247	LYS
2	Z	248	LEU
2	Z	255	TYR
2	Z	265	HIS

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Mol	Chain	Res	Type
2	Z	266	LEU
2	Z	267	LEU
2	Z	269	ASP
2	Z	271	TRP
2	Z	273	ARG
2	Z	277	ASN
2	Z	282	THR
2	Z	284	PRO
2	Z	287	GLN
2	Z	288	LYS
2	Z	295	ASP
2	Z	297	MET
2	Z	298	VAL
2	Z	300	GLN
2	Z	305	GLN
2	Z	306	ARG
2	Z	307	ILE
2	Z	313	LYS
2	Z	317	SER
2	Z	324	THR
2	Z	329	GLU
2	Z	332	MET
2	Z	334	THR
2	Z	335	ASP
2	Z	340	GLN
2	Z	341	LYS
2	Z	344	CYS
2	Z	351	LEU
2	Z	355	ASP
2	Z	359	LEU
2	Z	363	LYS
2	Z	365	THR
2	Z	366	MET
2	Z	368	ASP
2	Z	369	PHE
2	Z	376	MET
2	Z	379	ILE
2	Z	385	TYR
2	Z	394	ASN
2	Z	397	ASN
2	Z	398	GLU
2	Z	410	LEU

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Mol	Chain	Res	Type
2	Z	414	THR
2	Z	416	LYS
2	Z	418	LEU
2	Z	419	LYS
2	Z	421	ILE
2	Z	423	LEU
2	Z	424	LEU
2	Z	427	ASP
2	Z	429	GLN
2	Z	430	GLU
2	Z	431	ASP
2	Z	434	THR
2	Z	435	GLU
2	Z	436	ILE
2	Z	438	PHE
2	Z	440	LEU
2	Z	442	GLN
2	Z	445	THR
2	Z	446	ILE
2	Z	447	VAL
2	Z	450	LEU
2	Z	455	MET
2	Z	456	LEU
2	Z	465	LYS
2	Z	470	LYS
2	Z	472	GLN
2	Z	474	MET
2	Z	475	LYS
2	Z	476	LYS
2	Z	480	MET
2	Z	481	LYS
2	Z	483	GLU
2	Z	484	ILE
2	Z	485	VAL
2	Z	488	VAL
2	Z	491	VAL
2	Z	493	HIS
2	Z	494	ASP
2	Z	495	GLU
2	Z	496	THR
2	Z	498	CYS
2	Z	502	SER

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Mol	Chain	Res	Type
2	Z	503	LEU
2	Z	506	VAL
2	Z	509	ASP
2	Z	511	SER
2	Z	518	ARG
2	Z	520	LEU
2	Z	527	GLU
2	Z	529	LEU
2	Z	534	LYS
2	Z	539	LEU
2	Z	540	HIS
2	Z	545	SER
2	Z	553	LYS
2	Z	554	LEU
2	Z	559	ARG
2	Z	560	LEU
2	Z	567	THR
2	Z	568	LEU
2	Z	571	GLU
2	Z	577	LYS
2	Z	582	ARG
2	Z	584	LEU
2	Z	585	LEU
2	Z	589	GLU
2	Z	590	PRO
2	Z	595	LEU
2	Z	596	LYS
2	Z	597	ASP
2	Z	600	LYS
2	Z	601	ASN
2	Z	606	TRP
2	Z	609	ASP
2	Z	611	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	52	GLN
1	A	87	ASN
1	A	233	ASN
1	A	238	GLN

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Mol	Chain	Res	Type
1	A	271	GLN
1	A	317	ASN
1	A	354	ASN
1	A	370	ASN
1	A	414	GLN
1	A	417	ASN
1	A	422	ASN
1	A	486	ASN
1	A	539	ASN
1	A	602	ASN
1	A	612	GLN
1	A	640	ASN
1	A	643	GLN
1	A	751	ASN
1	A	779	GLN
1	A	804	GLN
1	A	856	ASN
1	A	872	GLN
1	A	901	GLN
1	A	907	ASN
1	A	955	ASN
1	A	965	GLN
1	A	1134	ASN
1	A	1135	ASN
1	B	30	ASN
1	B	52	GLN
1	B	115	GLN
1	B	314	GLN
1	B	354	ASN
1	B	370	ASN
1	B	414	GLN
1	B	417	ASN
1	B	422	ASN
1	B	474	GLN
1	B	535	ASN
1	B	579	GLN
1	B	602	ASN
1	B	605	ASN
1	B	612	GLN
1	B	640	ASN
1	B	774	GLN
1	B	779	GLN

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Mol	Chain	Res	Type
1	B	784	GLN
1	B	836	GLN
1	B	856	ASN
1	B	907	ASN
1	B	914	ASN
1	B	919	ASN
1	B	935	GLN
1	B	957	GLN
1	B	1113	GLN
1	B	1135	ASN
1	C	121	ASN
1	C	125	ASN
1	C	188	ASN
1	C	217	GLN
1	C	314	GLN
1	C	334	ASN
1	C	354	ASN
1	C	370	ASN
1	C	414	GLN
1	C	417	ASN
1	C	437	ASN
1	C	477	ASN
1	C	539	ASN
1	C	541	ASN
1	C	563	GLN
1	C	579	GLN
1	C	606	GLN
1	C	612	GLN
1	C	674	GLN
1	C	690	GLN
1	C	853	GLN
1	C	856	ASN
1	C	872	GLN
1	C	901	GLN
1	C	907	ASN
1	C	913	GLN
1	C	926	GLN
1	C	957	GLN
1	C	960	ASN
1	C	965	GLN
1	C	978	ASN
1	C	1005	GLN

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Mol	Chain	Res	Type
1	C	1023	ASN
1	C	1048	HIS
1	C	1054	GLN
1	C	1074	ASN
1	C	1083	HIS
1	C	1088	HIS
1	C	1135	ASN
2	T	34	HIS
2	T	58	ASN
2	T	64	ASN
2	T	76	GLN
2	T	81	GLN
2	T	96	GLN
2	T	149	ASN
2	T	154	ASN
2	T	175	GLN
2	T	194	ASN
2	T	239	HIS
2	T	250	ASN
2	T	330	ASN
2	T	340	GLN
2	T	373	HIS
2	T	374	HIS
2	T	429	GLN
2	T	505	HIS
2	T	522	GLN
2	T	572	ASN
2	T	586	ASN
2	T	598	GLN
2	X	34	HIS
2	X	58	ASN
2	X	64	ASN
2	X	76	GLN
2	X	81	GLN
2	X	96	GLN
2	X	149	ASN
2	X	154	ASN
2	X	194	ASN
2	X	239	HIS
2	X	250	ASN
2	X	300	GLN
2	X	330	ASN

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Mol	Chain	Res	Type
2	X	340	GLN
2	X	373	HIS
2	X	374	HIS
2	X	429	GLN
2	X	505	HIS
2	X	522	GLN
2	X	598	GLN
2	Z	34	HIS
2	Z	58	ASN
2	Z	64	ASN
2	Z	76	GLN
2	Z	81	GLN
2	Z	96	GLN
2	Z	149	ASN
2	Z	154	ASN
2	Z	194	ASN
2	Z	239	HIS
2	Z	250	ASN
2	Z	330	ASN
2	Z	340	GLN
2	Z	373	HIS
2	Z	374	HIS
2	Z	505	HIS
2	Z	522	GLN
2	Z	586	ASN
2	Z	598	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

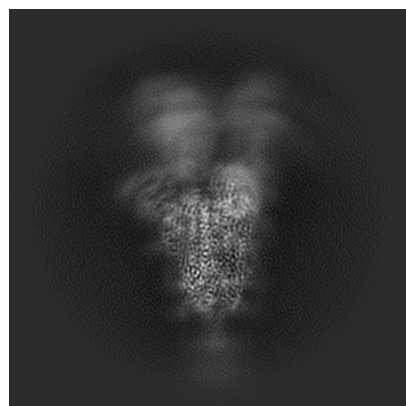
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37928. These allow visual inspection of the internal detail of the map and identification of artifacts.

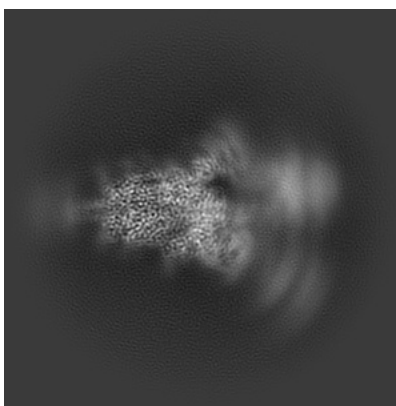
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

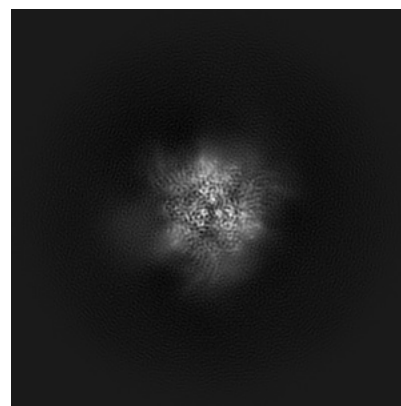
6.1.1 Primary map



X

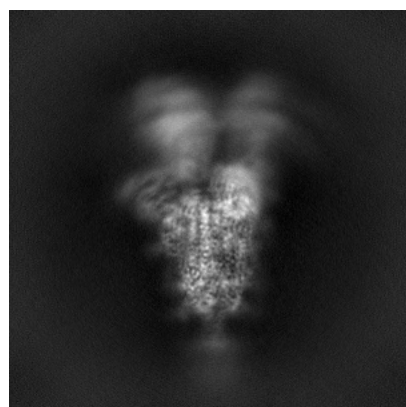


Y

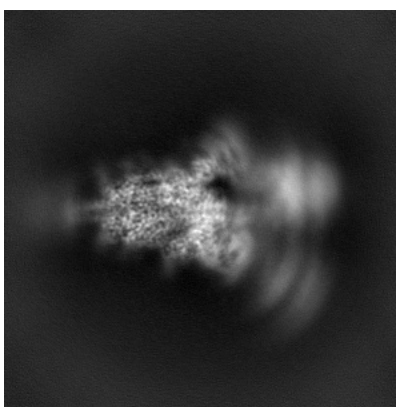


Z

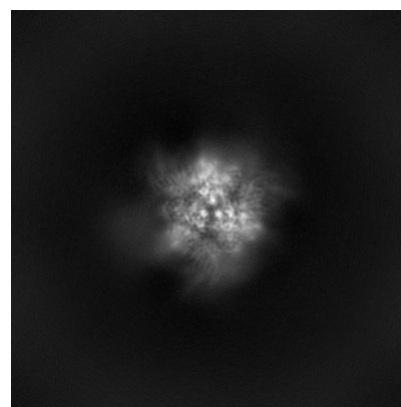
6.1.2 Raw map



X



Y

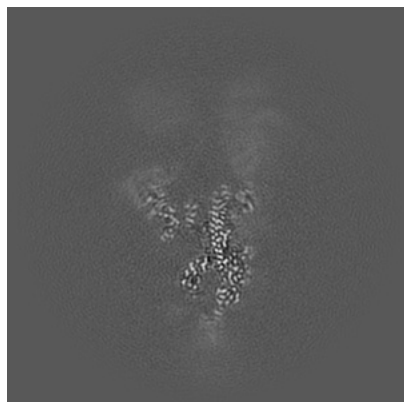


Z

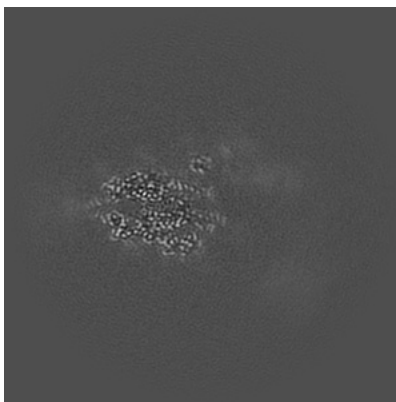
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

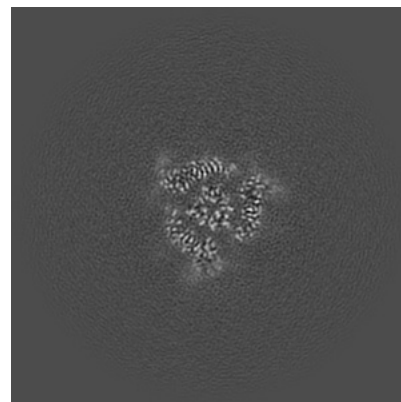
6.2.1 Primary map



X Index: 210

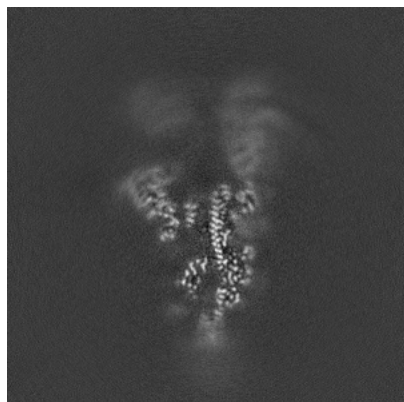


Y Index: 210

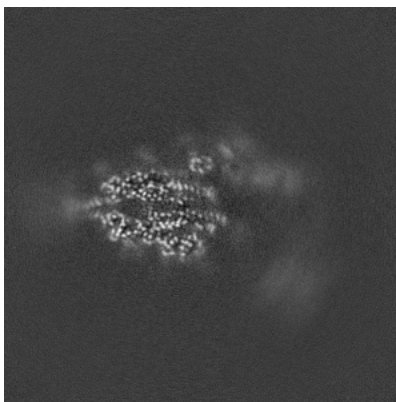


Z Index: 210

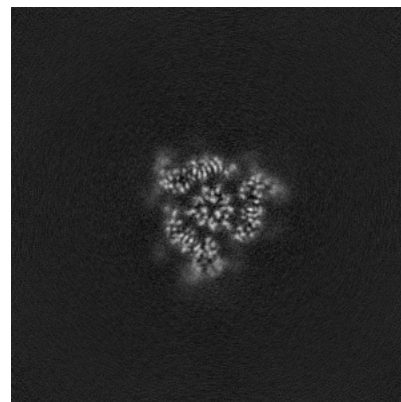
6.2.2 Raw map



X Index: 210



Y Index: 210

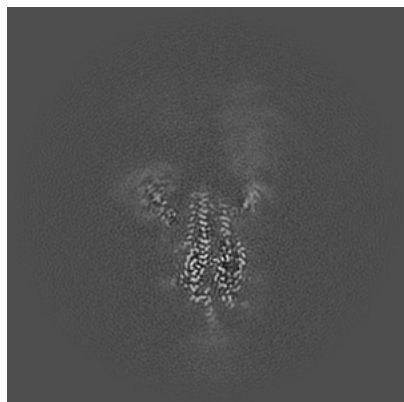


Z Index: 210

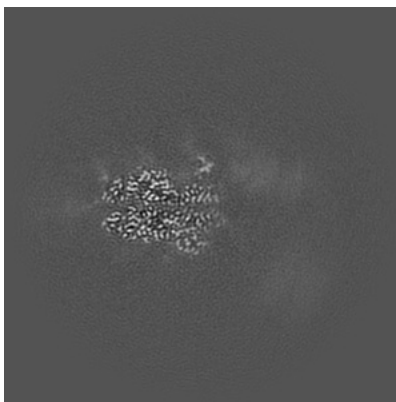
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

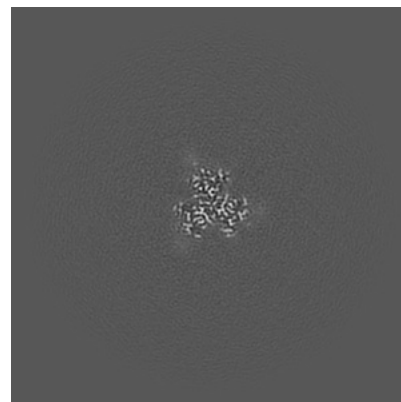
6.3.1 Primary map



X Index: 201

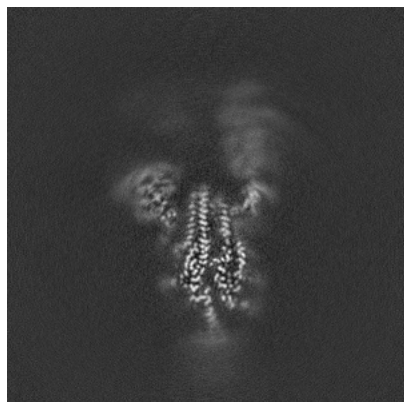


Y Index: 202

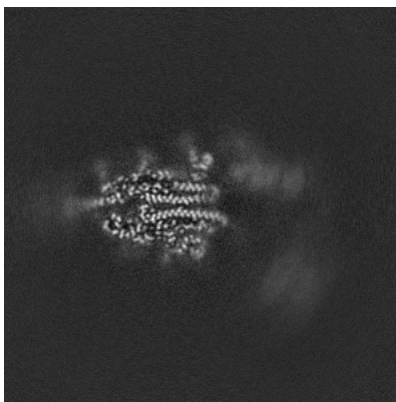


Z Index: 151

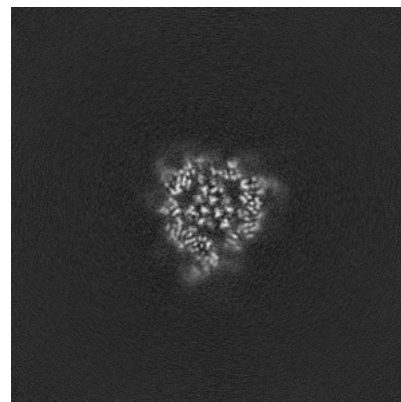
6.3.2 Raw map



X Index: 201



Y Index: 206

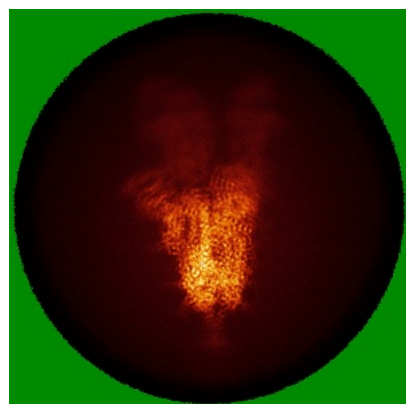


Z Index: 204

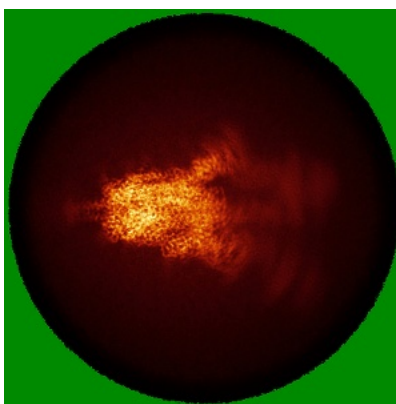
The images above show the largest variance slices of the map in three orthogonal directions.

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

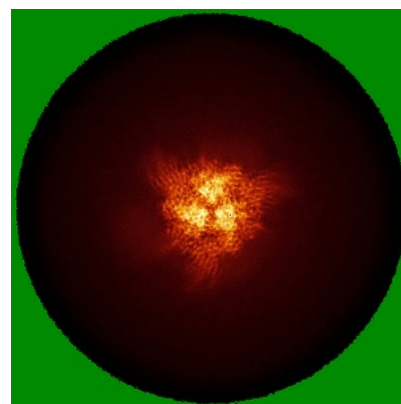
6.4.1 Primary map



X

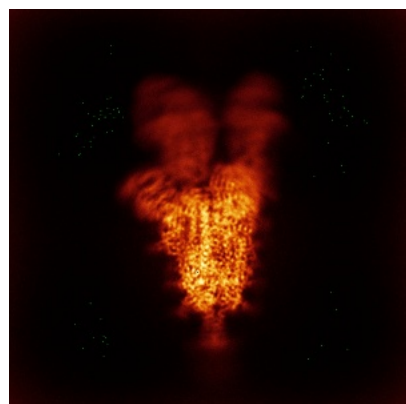


Y

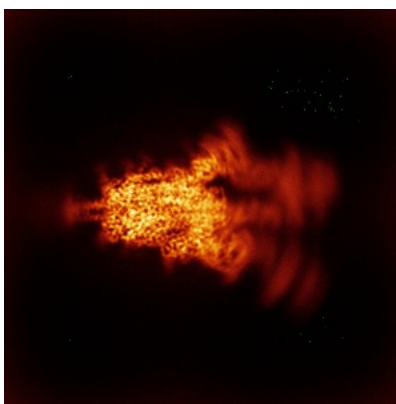


Z

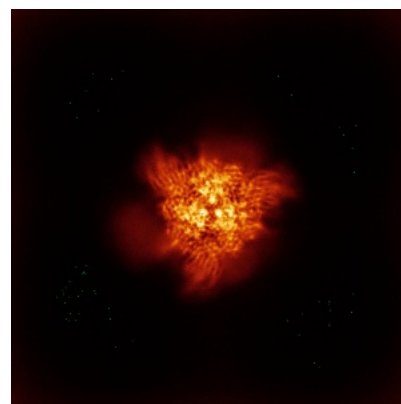
6.4.2 Raw map



X



Y

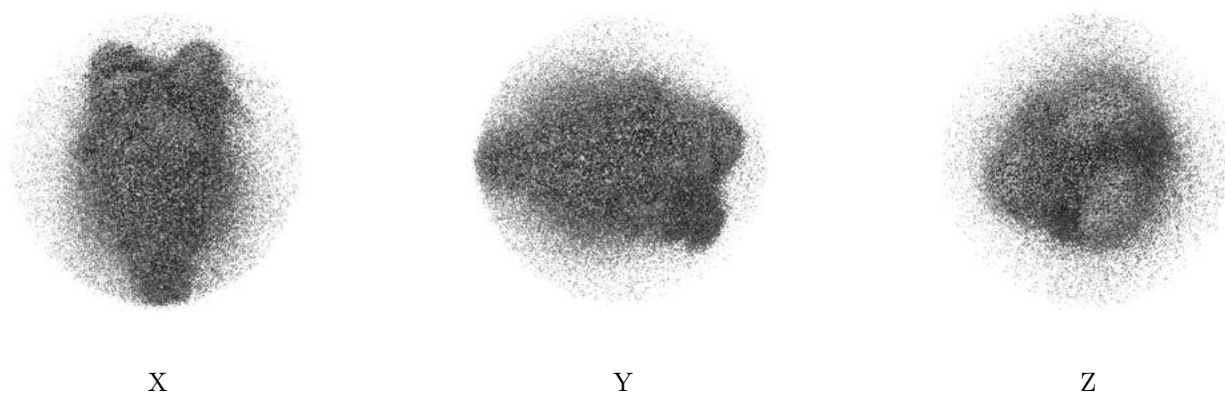


Z

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.

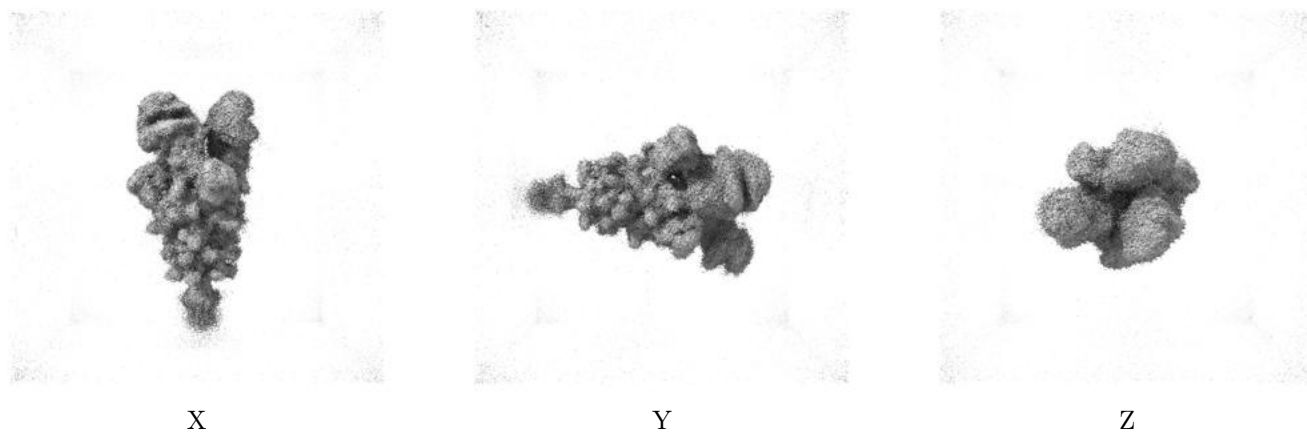
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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



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.

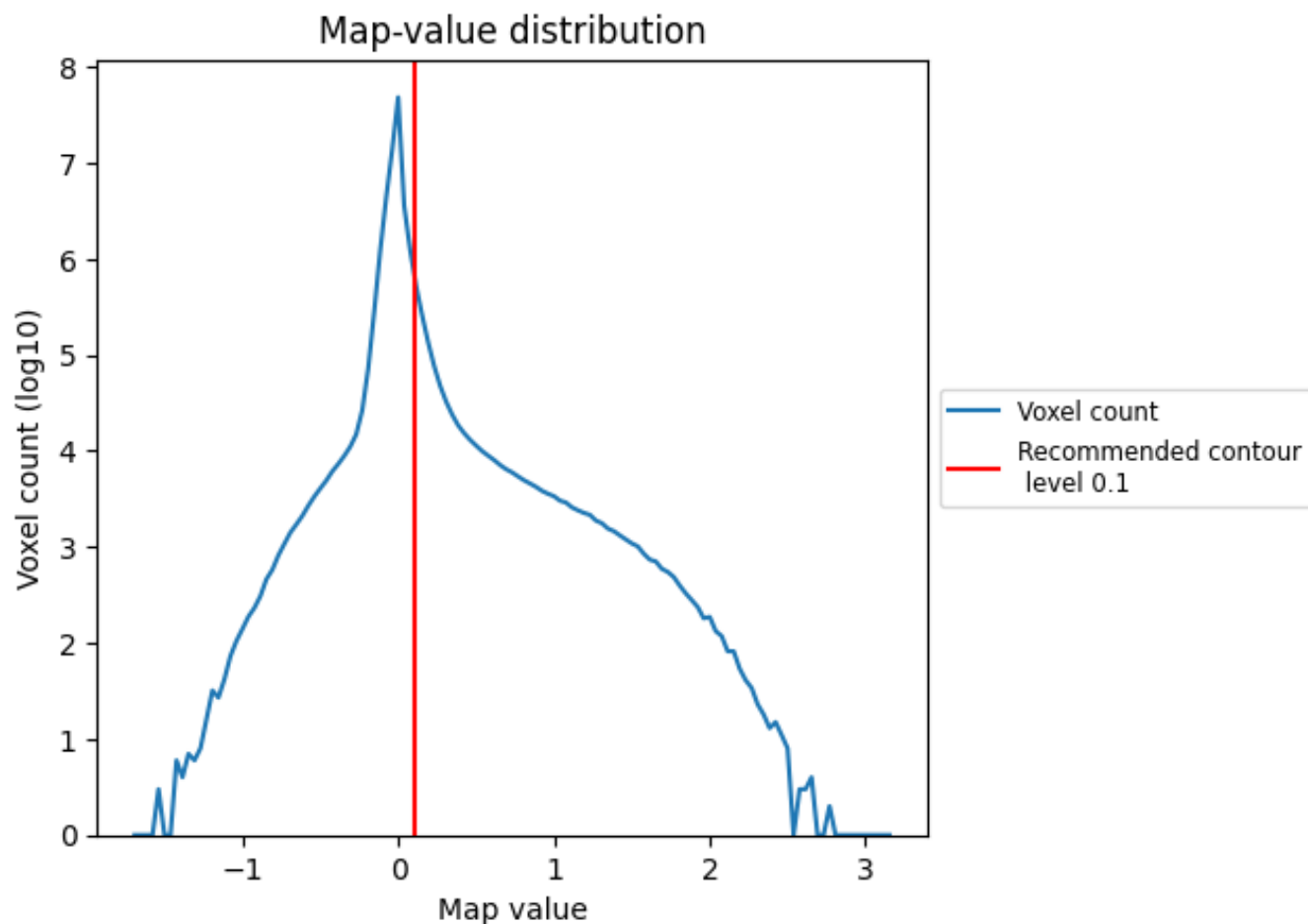
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

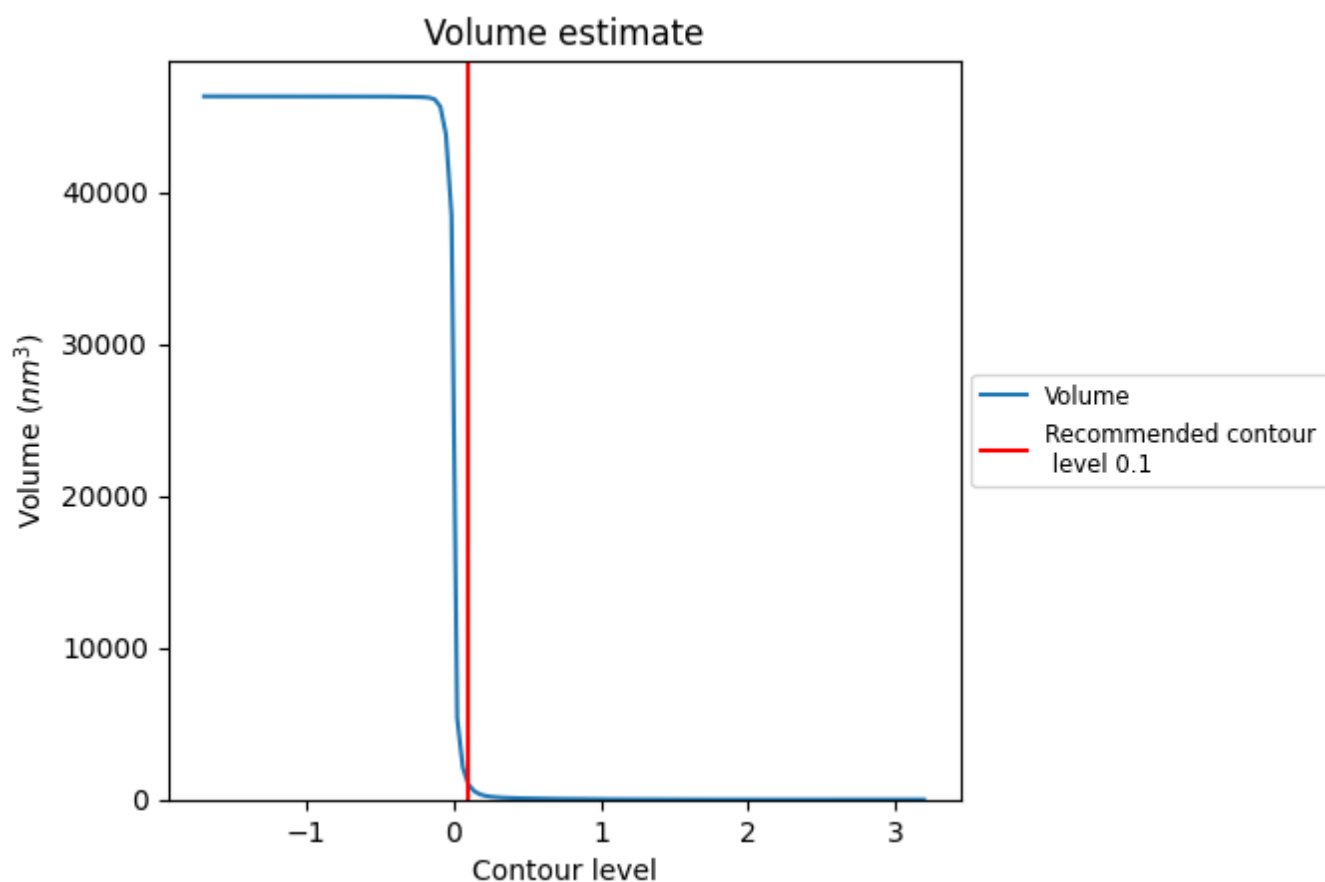
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

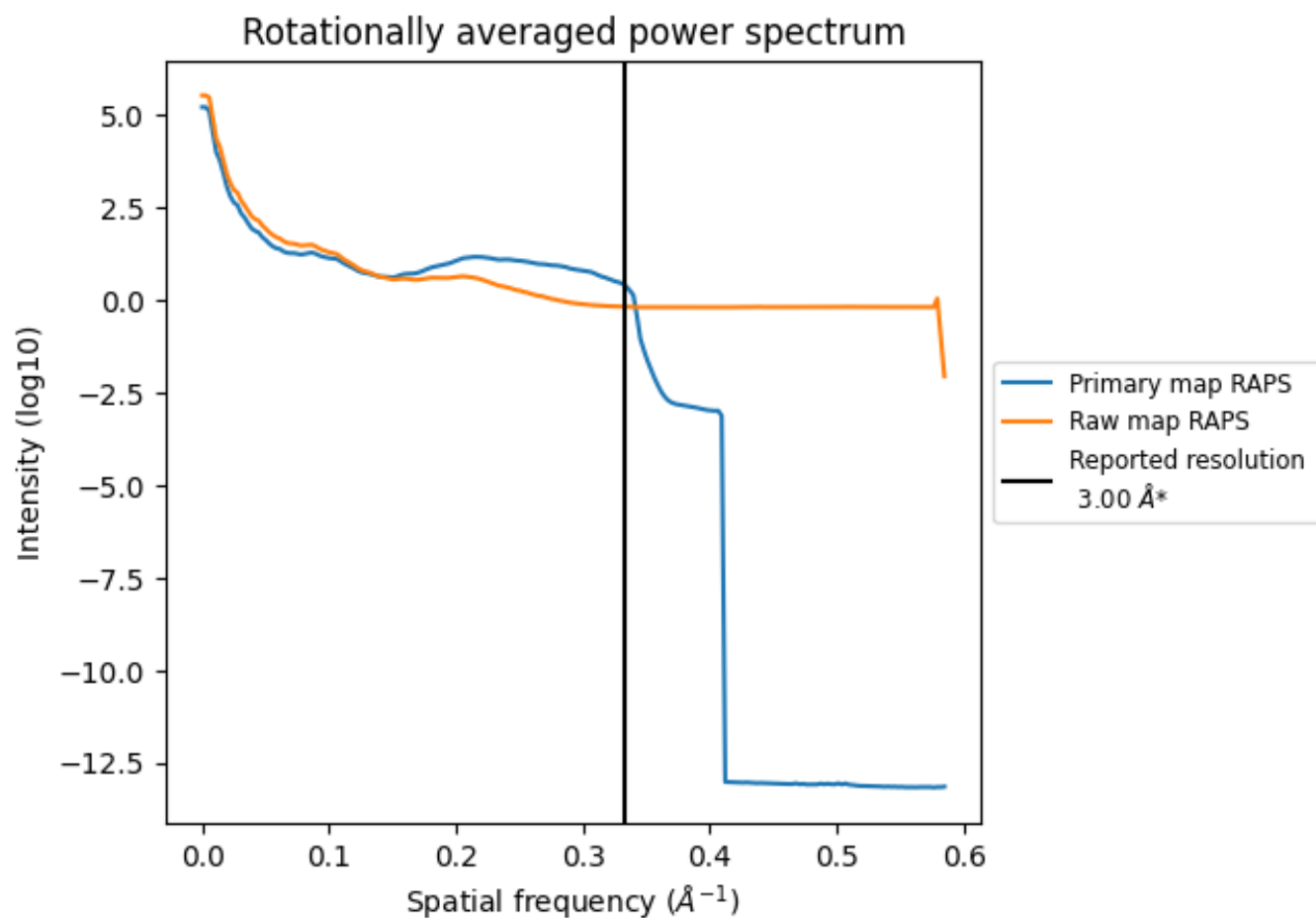
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1015 nm^3 ; this corresponds to an approximate mass of 917 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

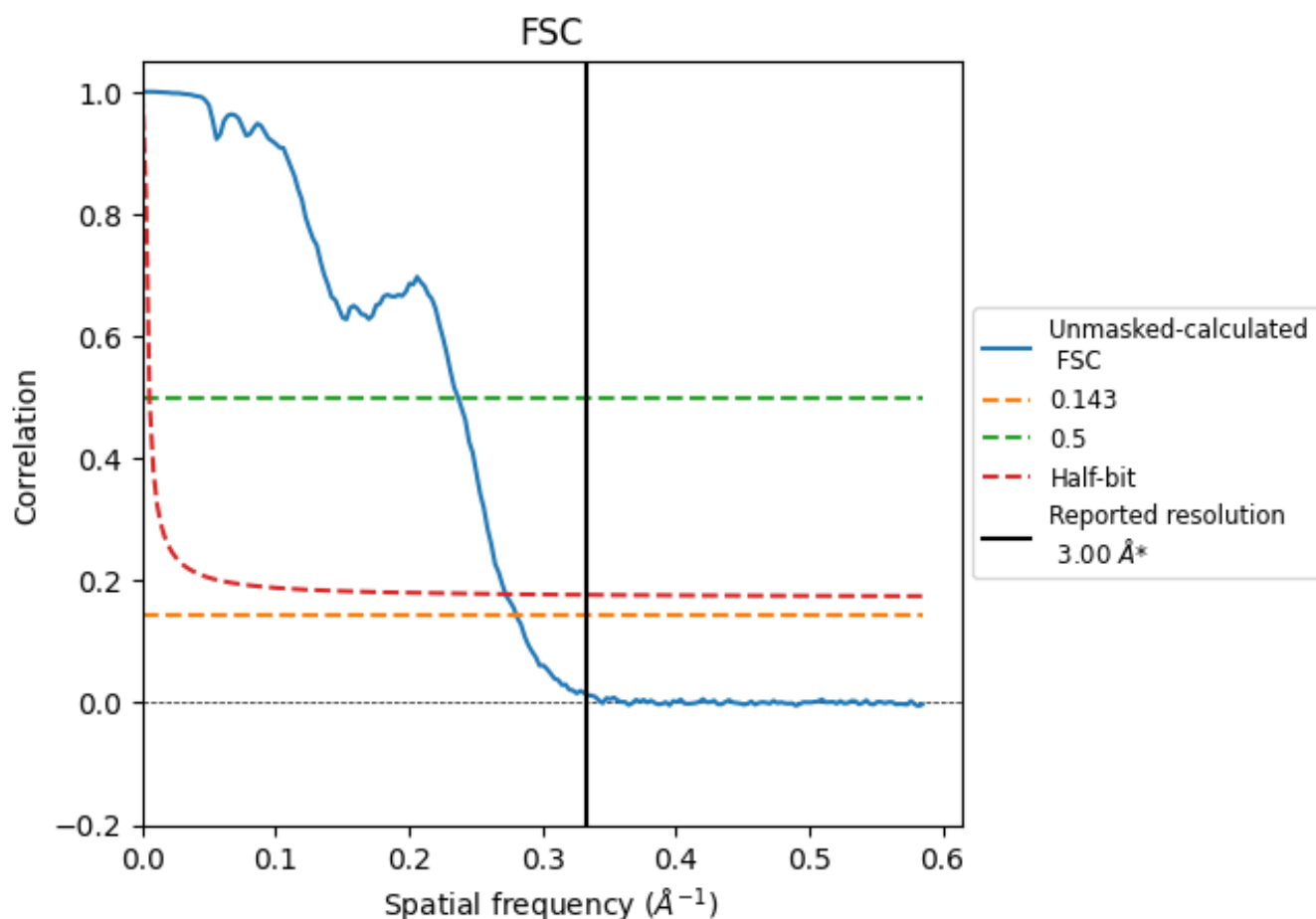


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

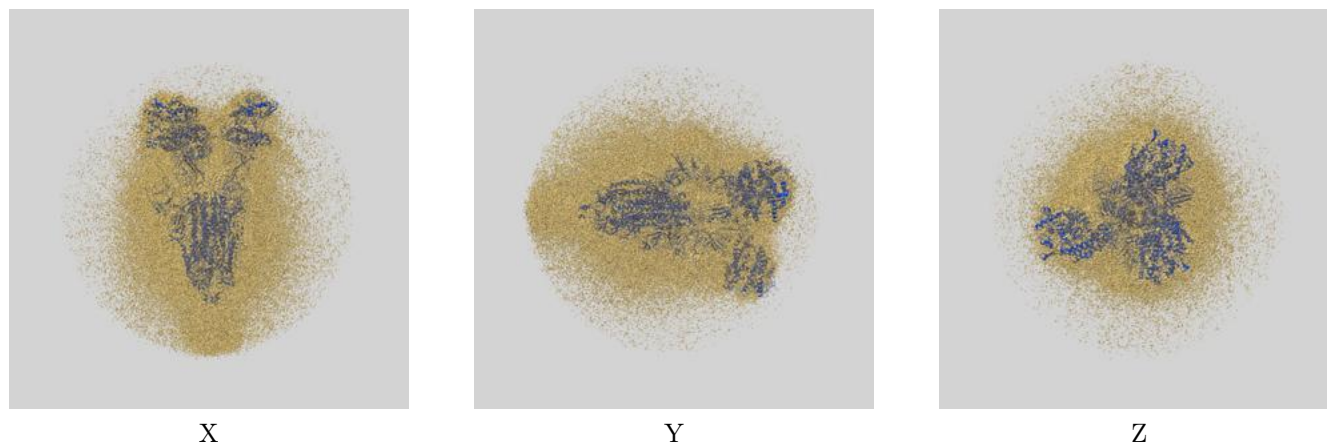
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.57	4.22	3.67

*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 3.57 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

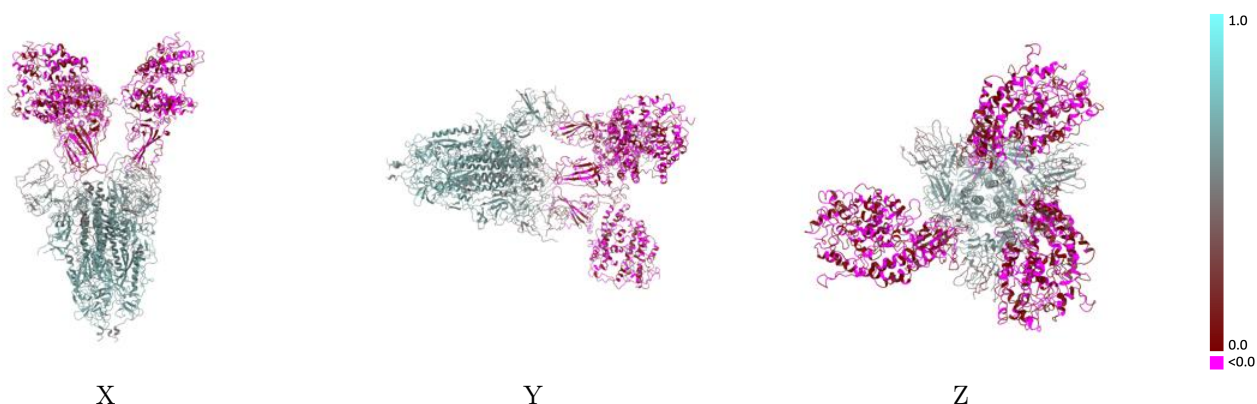
This section contains information regarding the fit between EMDB map EMD-37928 and PDB model 8WYH. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



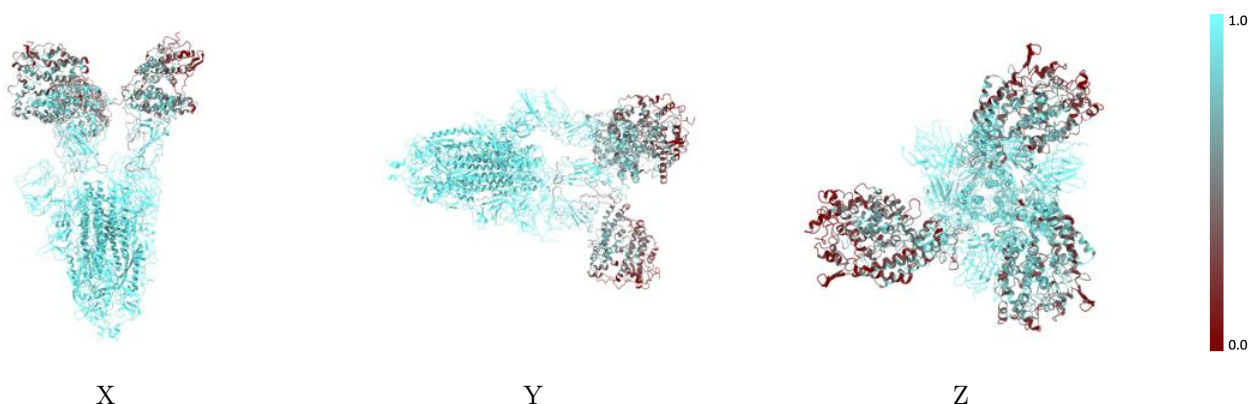
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



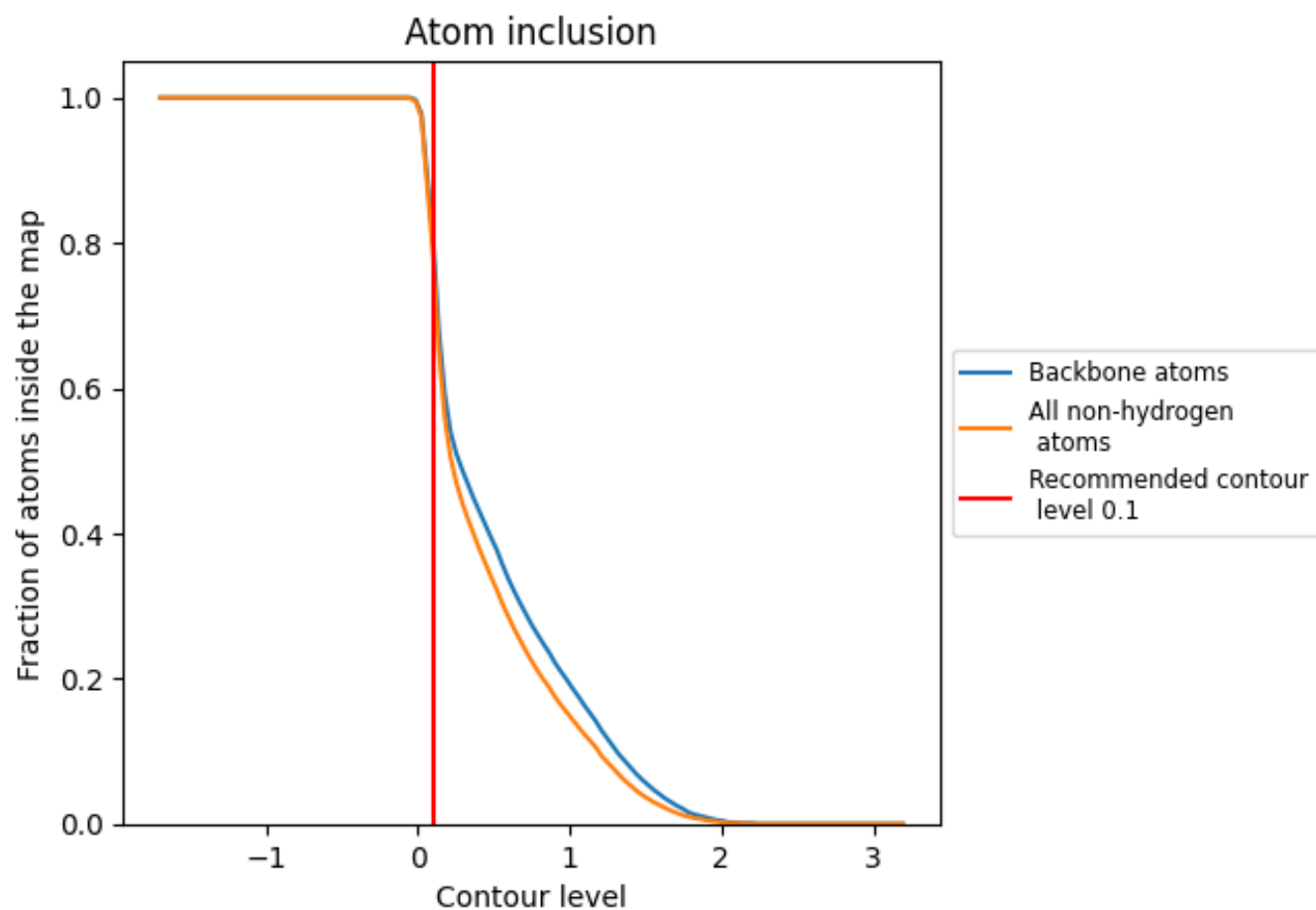
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 79% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7860	<div></div> 0.2970
A	<div></div> 0.9620	<div></div> 0.4630
B	<div></div> 0.9520	<div></div> 0.4640
C	<div></div> 0.9380	<div></div> 0.4590
T	<div></div> 0.6210	<div></div> 0.0340
X	<div></div> 0.5130	<div></div> 0.0170
Z	<div></div> 0.4000	<div></div> 0.0170

1.0
0.0
-0.0