



Full wwPDB EM Validation Report ⓘ

Feb 27, 2024 – 08:00 AM EST

PDB ID : 6UWT
EMDB ID : EMD-20927
Title : Clostridium difficile binary toxin translocase CDTb tetradecamer in symmetric conformation
Authors : Xu, X.; Pozharski, E.; des Georges, A.
Deposited on : 2019-11-05
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

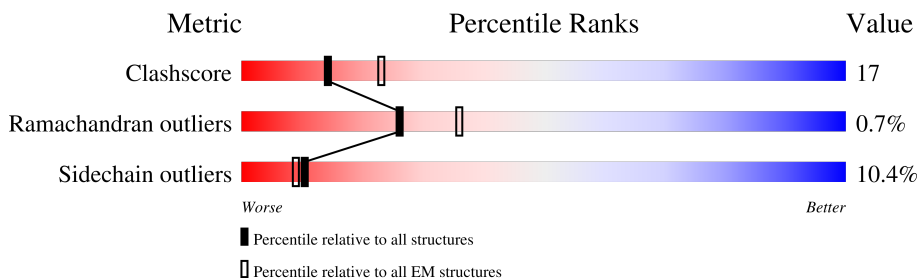
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	667	
1	B	667	
1	C	667	
1	D	667	
1	E	667	
1	F	667	
1	G	667	
1	H	667	

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Mol	Chain	Length	Quality of chain
1	I	667	
1	J	667	
1	K	667	
1	L	667	
1	M	667	
1	N	667	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 72744 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 ADP-ribosyltransferase binding component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	660	5194	3252	844	1088	10	0	0
1	I	660	5194	3252	844	1088	10	0	0
1	J	660	5194	3252	844	1088	10	0	0
1	K	660	5194	3252	844	1088	10	0	0
1	L	660	5194	3252	844	1088	10	0	0
1	M	660	5194	3252	844	1088	10	0	0
1	N	660	5194	3252	844	1088	10	0	0
1	A	660	5194	3252	844	1088	10	0	0
1	B	660	5194	3252	844	1088	10	0	0
1	C	660	5194	3252	844	1088	10	0	0
1	D	660	5194	3252	844	1088	10	0	0
1	E	660	5194	3252	844	1088	10	0	0
1	F	660	5194	3252	844	1088	10	0	0
1	G	660	5194	3252	844	1088	10	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
2	H	2	Total	Ca	0
			2	2	

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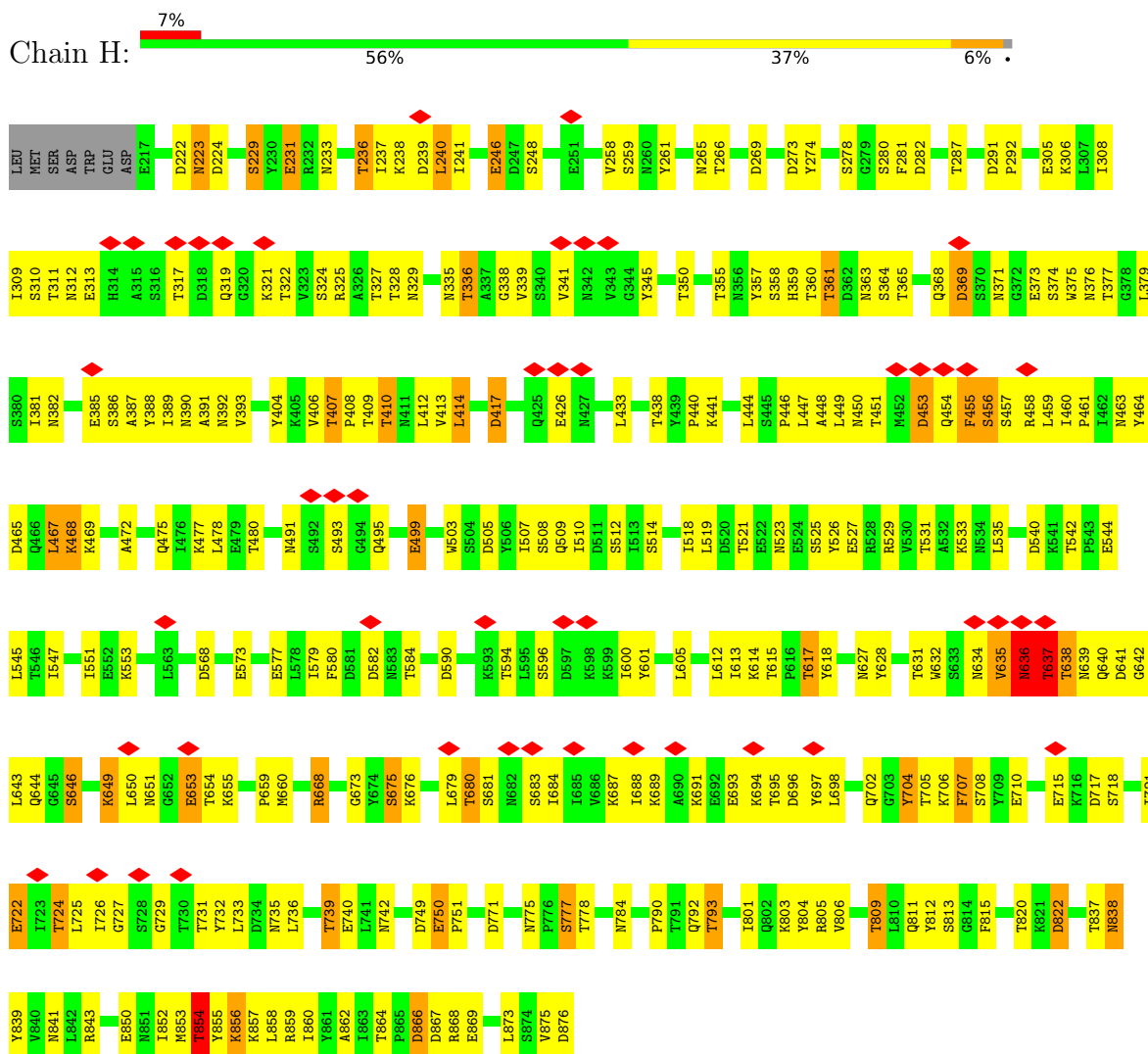
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Mol	Chain	Residues	Atoms		AltConf
2	I	2	Total 2	Ca 2	0
2	J	2	Total 2	Ca 2	0
2	K	2	Total 2	Ca 2	0
2	L	2	Total 2	Ca 2	0
2	M	2	Total 2	Ca 2	0
2	N	2	Total 2	Ca 2	0
2	A	2	Total 2	Ca 2	0
2	B	2	Total 2	Ca 2	0
2	C	2	Total 2	Ca 2	0
2	D	2	Total 2	Ca 2	0
2	E	2	Total 2	Ca 2	0
2	F	2	Total 2	Ca 2	0
2	G	2	Total 2	Ca 2	0

3 Residue-property plots

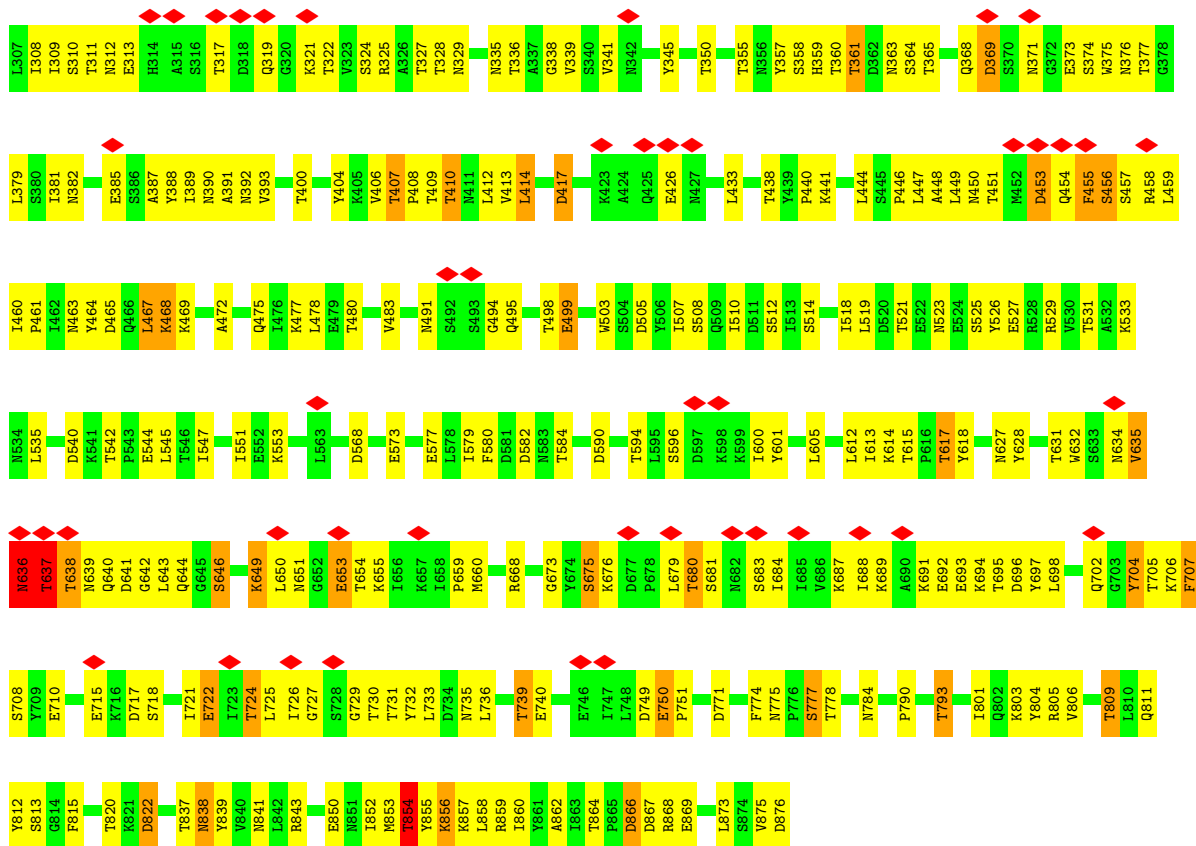
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: ADP-ribosyltransferase binding component

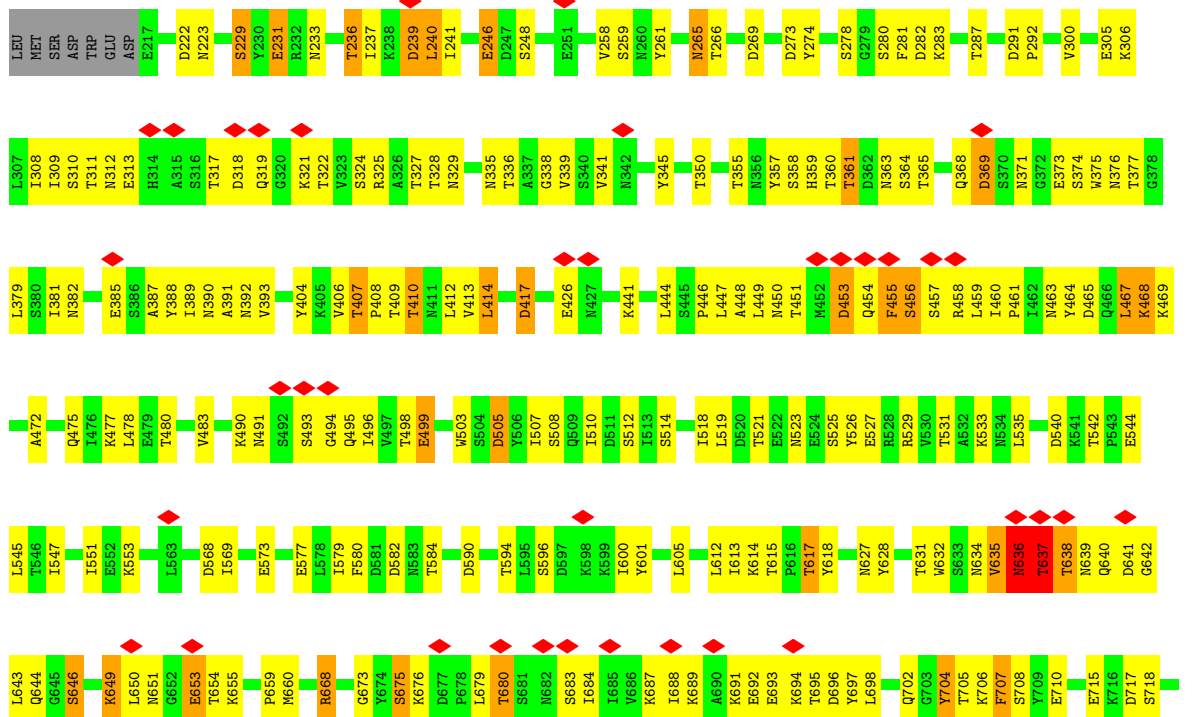


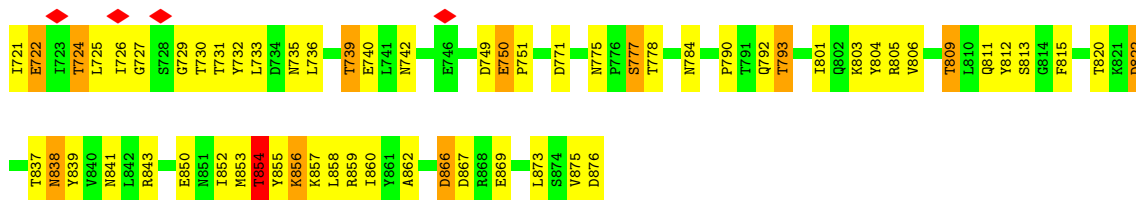
- Molecule 1: ADP-ribosyltransferase binding component



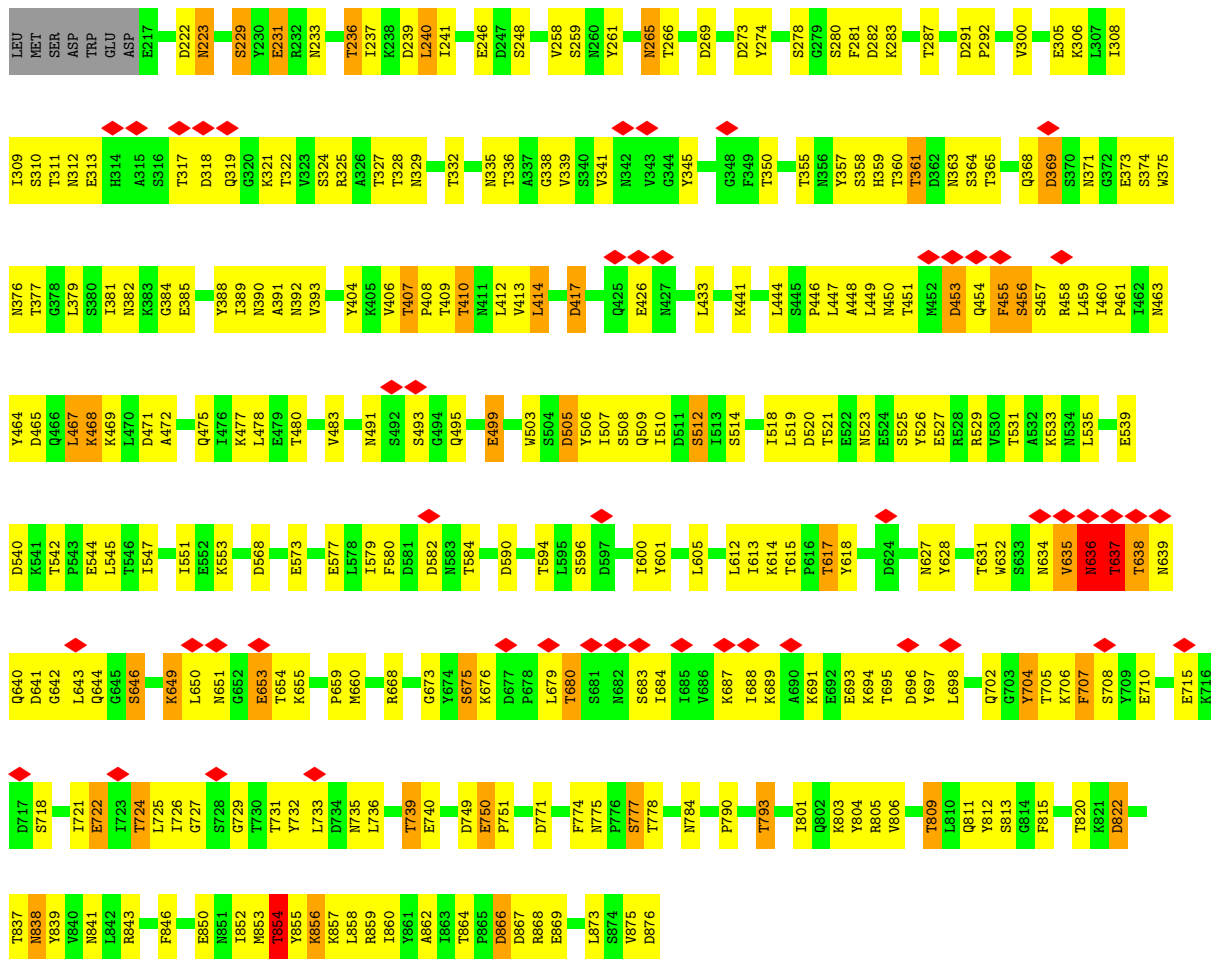


• Molecule 1: ADP-ribosyltransferase binding component

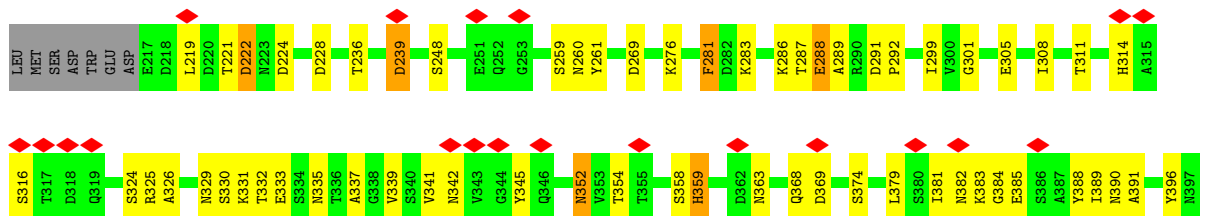


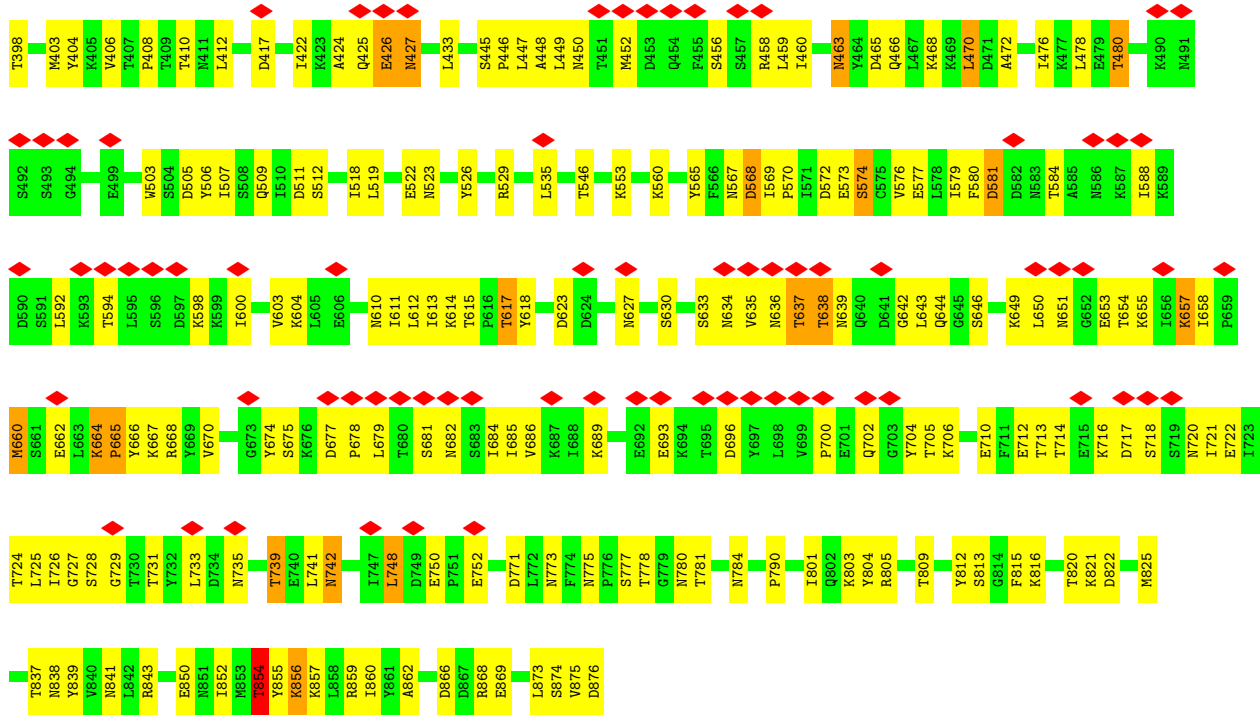


• Molecule 1: ADP-ribosyltransferase binding component

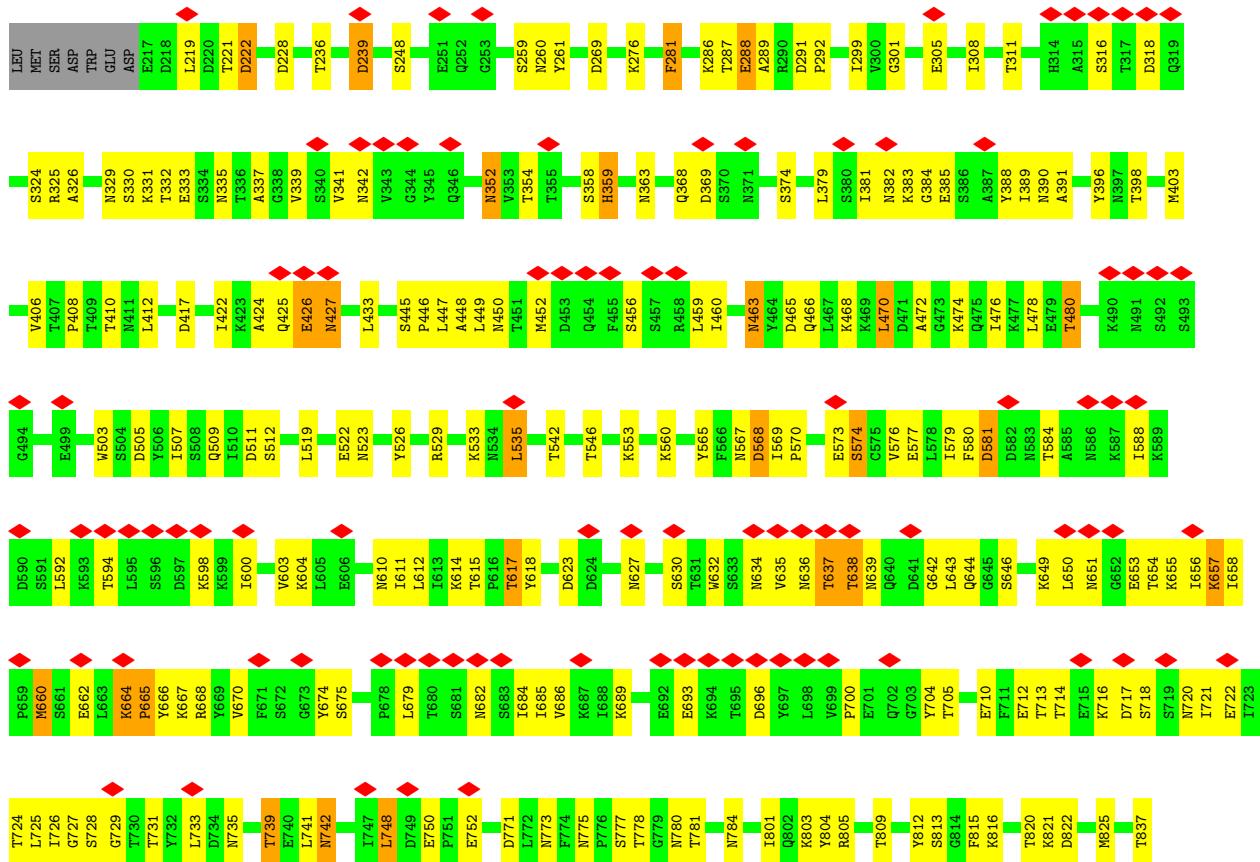


• Molecule 1: ADP-ribosyltransferase binding component



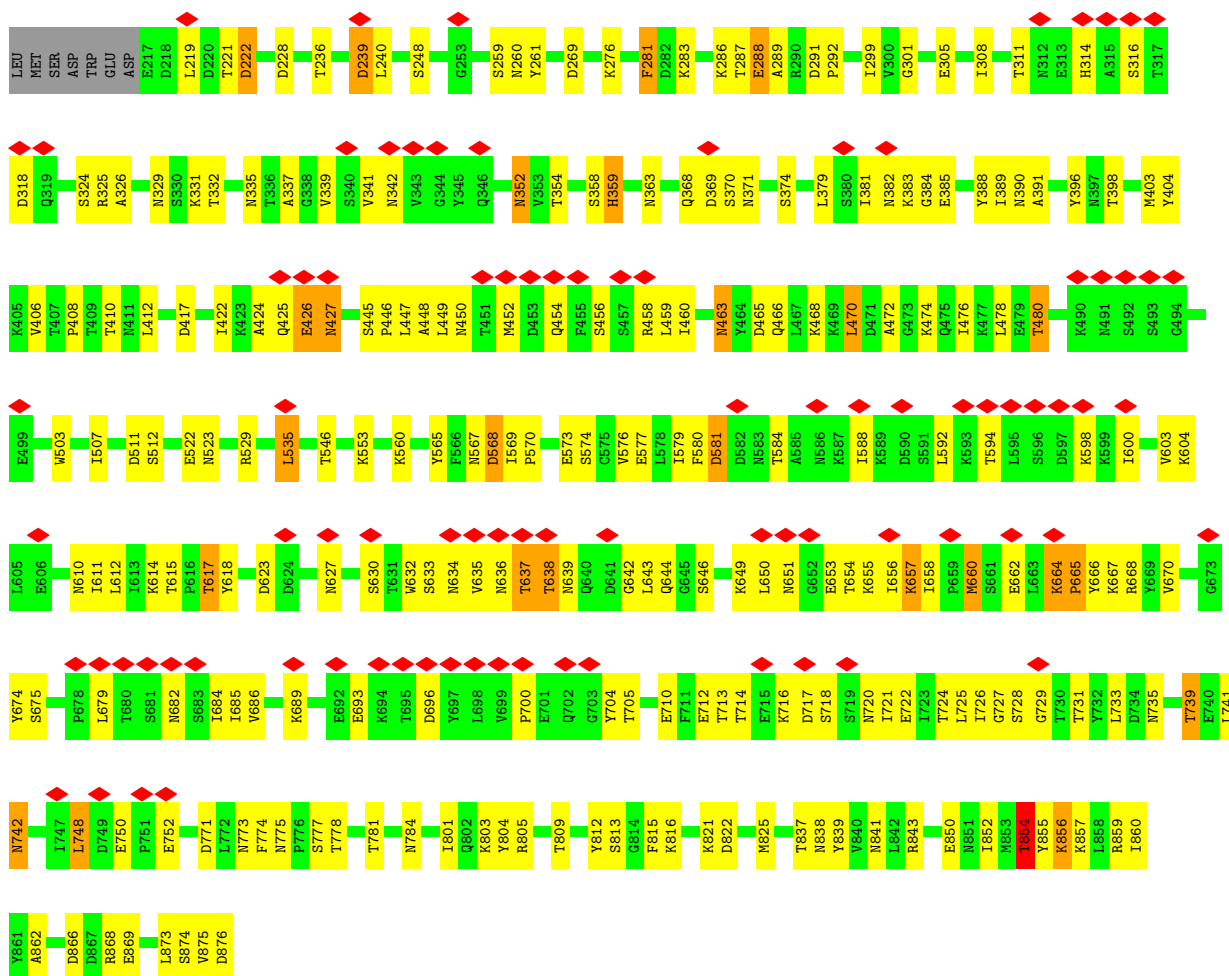


● Molecule 1: ADP-ribosyltransferase binding component

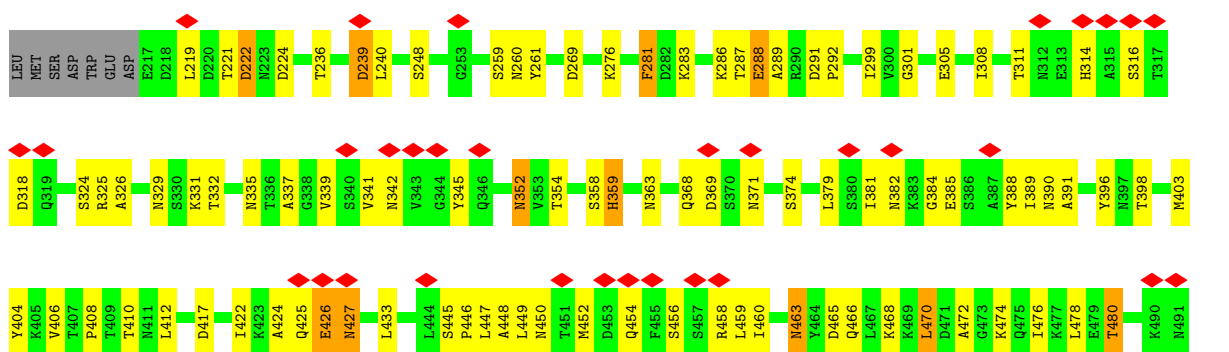


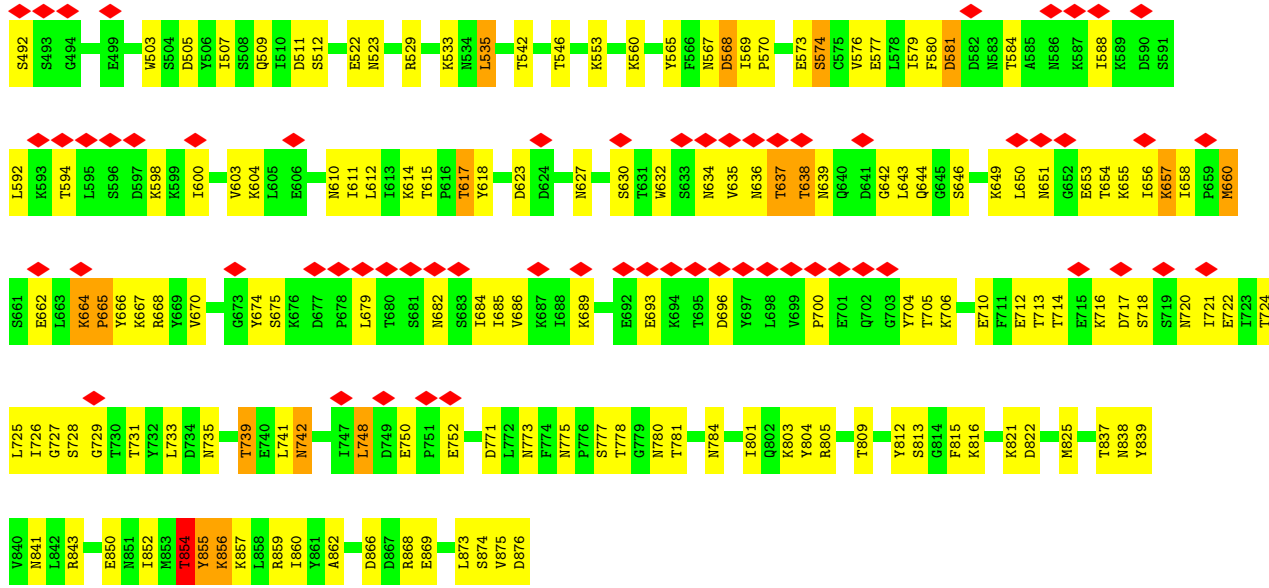


• Molecule 1: ADP-ribosyltransferase binding component

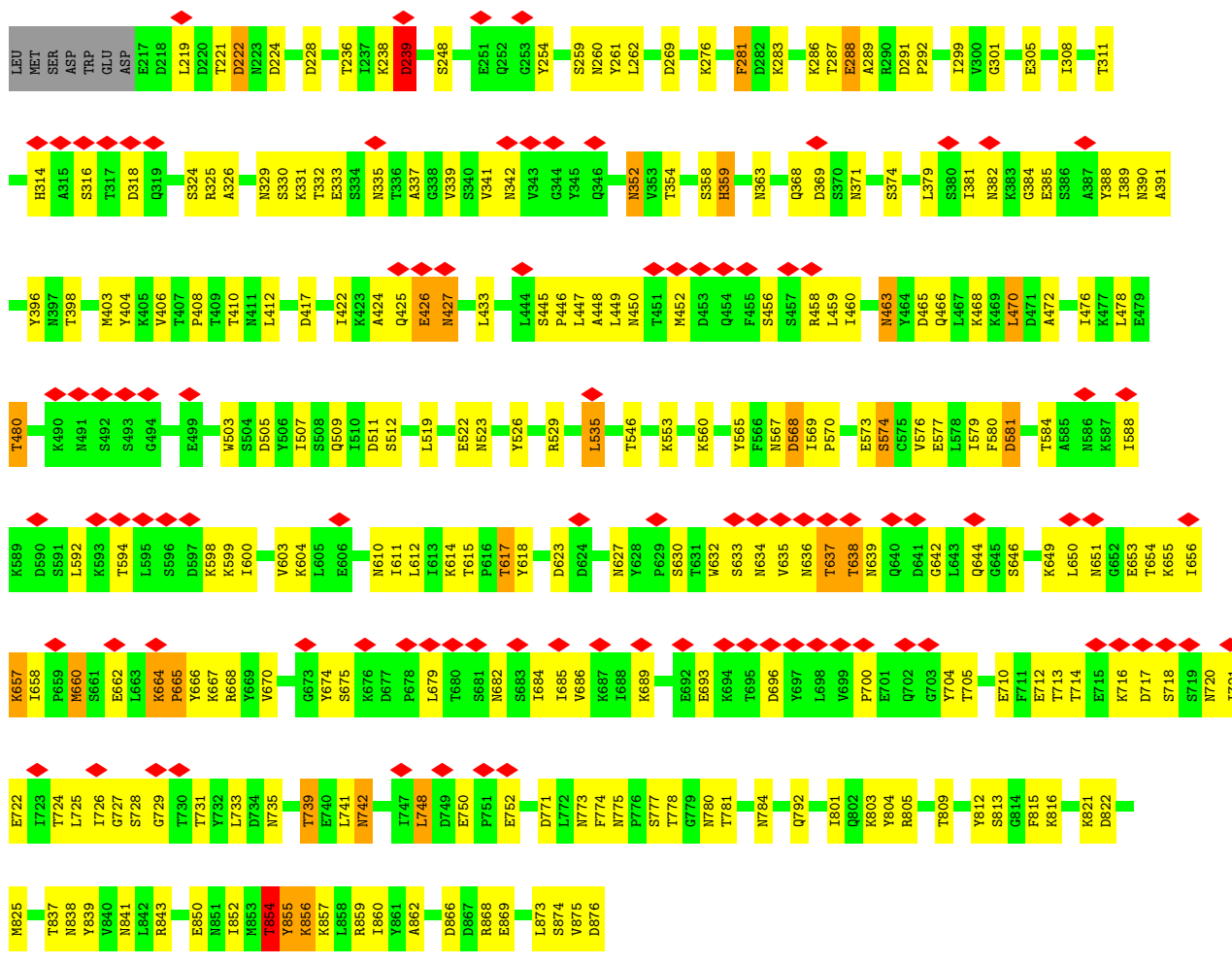


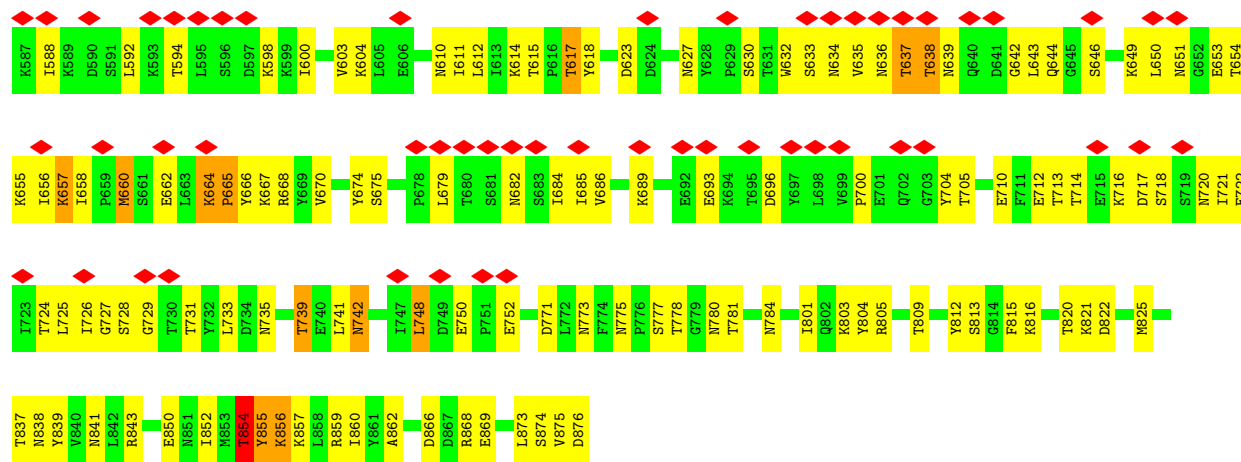
• Molecule 1: ADP-ribosyltransferase binding component





• Molecule 1: ADP-ribosyltransferase binding component





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	19944	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	0/5290	0.53	0/7181
1	B	0.45	0/5290	0.53	0/7181
1	C	0.45	0/5290	0.53	0/7181
1	D	0.45	0/5290	0.53	0/7181
1	E	0.45	0/5290	0.53	0/7181
1	F	0.45	0/5290	0.52	0/7181
1	G	0.45	0/5290	0.53	0/7181
1	H	0.46	0/5290	0.54	0/7181
1	I	0.46	0/5290	0.54	0/7181
1	J	0.46	0/5290	0.54	0/7181
1	K	0.46	0/5290	0.54	0/7181
1	L	0.46	0/5290	0.54	0/7181
1	M	0.46	0/5290	0.54	0/7181
1	N	0.46	0/5290	0.54	0/7181
All	All	0.45	0/74060	0.53	0/100534

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	4
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	4
1	G	0	4
1	H	0	5
1	I	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	5
1	K	0	5
1	L	0	5
1	M	0	5
1	N	0	5
All	All	0	63

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	ASP	Peptide
1	A	637	THR	Peptide
1	A	852	ILE	Peptide
1	A	854	THR	Peptide
1	B	239	ASP	Peptide
1	B	637	THR	Peptide
1	B	852	ILE	Peptide
1	B	854	THR	Peptide
1	C	239	ASP	Peptide
1	C	637	THR	Peptide
1	C	852	ILE	Peptide
1	C	854	THR	Peptide
1	D	239	ASP	Peptide
1	D	637	THR	Peptide
1	D	852	ILE	Peptide
1	D	854	THR	Peptide
1	E	239	ASP	Peptide
1	E	637	THR	Peptide
1	E	852	ILE	Peptide
1	E	854	THR	Peptide
1	F	239	ASP	Peptide
1	F	637	THR	Peptide
1	F	852	ILE	Peptide
1	F	854	THR	Peptide
1	G	239	ASP	Peptide
1	G	637	THR	Peptide
1	G	852	ILE	Peptide
1	G	854	THR	Peptide

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Mol	Chain	Res	Type	Group
1	H	239	ASP	Peptide
1	H	369	ASP	Peptide
1	H	636	ASN	Peptide
1	H	637	THR	Peptide
1	H	854	THR	Peptide
1	I	239	ASP	Peptide
1	I	369	ASP	Peptide
1	I	636	ASN	Peptide
1	I	637	THR	Peptide
1	I	854	THR	Peptide
1	J	239	ASP	Peptide
1	J	369	ASP	Peptide
1	J	636	ASN	Peptide
1	J	637	THR	Peptide
1	J	854	THR	Peptide
1	K	239	ASP	Peptide
1	K	369	ASP	Peptide
1	K	636	ASN	Peptide
1	K	637	THR	Peptide
1	K	854	THR	Peptide
1	L	239	ASP	Peptide
1	L	369	ASP	Peptide
1	L	636	ASN	Peptide
1	L	637	THR	Peptide
1	L	854	THR	Peptide
1	M	239	ASP	Peptide
1	M	369	ASP	Peptide
1	M	636	ASN	Peptide
1	M	637	THR	Peptide
1	M	854	THR	Peptide
1	N	239	ASP	Peptide
1	N	369	ASP	Peptide
1	N	636	ASN	Peptide
1	N	637	THR	Peptide
1	N	854	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5194	0	5037	173	0
1	B	5194	0	5037	164	0
1	C	5194	0	5037	167	0
1	D	5194	0	5037	172	0
1	E	5194	0	5037	179	0
1	F	5194	0	5037	173	0
1	G	5194	0	5037	168	0
1	H	5194	0	5037	188	0
1	I	5194	0	5037	178	0
1	J	5194	0	5037	196	0
1	K	5194	0	5037	189	0
1	L	5194	0	5037	184	0
1	M	5194	0	5037	198	0
1	N	5194	0	5037	198	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
All	All	72744	0	70518	2474	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 17.

All (2474) 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:M:494:GLY:HA3	1:N:265:ASN:HD21	1.10	1.05
1:M:239:ASP:N	1:N:539:GLU:OE2	2.03	0.92
1:J:494:GLY:HA3	1:K:265:ASN:HD21	1.37	0.90
1:J:859:ARG:NH1	1:J:876:ASP:OD1	2.08	0.87
1:H:859:ARG:NH1	1:H:876:ASP:OD1	2.08	0.87
1:N:859:ARG:NH1	1:N:876:ASP:OD1	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:859:ARG:NH1	1:K:876:ASP:OD1	2.08	0.85
1:L:859:ARG:NH1	1:L:876:ASP:OD1	2.08	0.85
1:M:859:ARG:NH1	1:M:876:ASP:OD1	2.08	0.85
1:I:859:ARG:NH1	1:I:876:ASP:OD1	2.08	0.85
1:M:498:THR:OG1	1:N:505:ASP:OD1	1.96	0.83
1:M:494:GLY:HA3	1:N:265:ASN:ND2	1.95	0.80
1:C:358:SER:O	1:C:359:HIS:ND1	2.16	0.79
1:D:358:SER:O	1:D:359:HIS:ND1	2.16	0.79
1:E:358:SER:O	1:E:359:HIS:ND1	2.16	0.79
1:G:358:SER:O	1:G:359:HIS:ND1	2.16	0.79
1:A:358:SER:O	1:A:359:HIS:ND1	2.16	0.78
1:B:358:SER:O	1:B:359:HIS:ND1	2.16	0.78
1:F:358:SER:O	1:F:359:HIS:ND1	2.16	0.78
1:H:453:ASP:H	1:H:456:SER:HB3	1.49	0.77
1:I:453:ASP:H	1:I:456:SER:HB3	1.49	0.77
1:J:310:SER:HB2	1:J:322:THR:HG23	1.66	0.77
1:I:310:SER:HB2	1:I:322:THR:HG23	1.66	0.76
1:M:453:ASP:H	1:M:456:SER:HB3	1.49	0.76
1:N:453:ASP:H	1:N:456:SER:HB3	1.49	0.76
1:H:310:SER:HB2	1:H:322:THR:HG23	1.66	0.76
1:J:453:ASP:H	1:J:456:SER:HB3	1.49	0.76
1:M:310:SER:HB2	1:M:322:THR:HG23	1.66	0.76
1:L:453:ASP:H	1:L:456:SER:HB3	1.49	0.76
1:K:310:SER:HB2	1:K:322:THR:HG23	1.66	0.76
1:L:310:SER:HB2	1:L:322:THR:HG23	1.66	0.76
1:H:509:GLN:HG3	1:N:283:LYS:HB2	1.65	0.76
1:K:453:ASP:H	1:K:456:SER:HB3	1.49	0.76
1:N:310:SER:HB2	1:N:322:THR:HG23	1.66	0.75
1:H:792:GLN:HG3	1:I:846:PHE:CD2	2.21	0.74
1:B:374:SER:HA	1:B:748:LEU:HD12	1.71	0.73
1:B:854:THR:O	1:B:856:LYS:N	2.21	0.73
1:E:283:LYS:HB2	1:F:509:GLN:HG3	1.68	0.73
1:G:854:THR:O	1:G:856:LYS:N	2.21	0.73
1:K:750:GLU:HB2	1:K:751:PRO:HD3	1.71	0.73
1:F:854:THR:O	1:F:856:LYS:N	2.21	0.73
1:A:374:SER:HA	1:A:748:LEU:HD12	1.71	0.73
1:C:854:THR:O	1:C:856:LYS:N	2.21	0.73
1:J:854:THR:O	1:J:856:LYS:N	2.22	0.73
1:C:374:SER:HA	1:C:748:LEU:HD12	1.71	0.73
1:K:854:THR:O	1:K:856:LYS:N	2.22	0.73
1:L:750:GLU:HB2	1:L:751:PRO:HD3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:854:THR:O	1:I:856:LYS:N	2.22	0.73
1:M:750:GLU:HB2	1:M:751:PRO:HD3	1.71	0.73
1:L:854:THR:O	1:L:856:LYS:N	2.22	0.73
1:J:750:GLU:HB2	1:J:751:PRO:HD3	1.71	0.73
1:A:854:THR:O	1:A:856:LYS:N	2.21	0.73
1:D:374:SER:HA	1:D:748:LEU:HD12	1.70	0.72
1:D:854:THR:O	1:D:856:LYS:N	2.21	0.72
1:G:374:SER:HA	1:G:748:LEU:HD12	1.70	0.72
1:M:283:LYS:O	1:N:512:SER:OG	2.06	0.72
1:L:229:SER:O	1:L:233:ASN:ND2	2.23	0.72
1:M:854:THR:O	1:M:856:LYS:N	2.22	0.72
1:N:750:GLU:HB2	1:N:751:PRO:HD3	1.71	0.72
1:E:617:THR:O	1:E:627:ASN:ND2	2.23	0.72
1:H:854:THR:O	1:H:856:LYS:N	2.22	0.72
1:K:229:SER:O	1:K:233:ASN:ND2	2.23	0.72
1:J:229:SER:O	1:J:233:ASN:ND2	2.23	0.72
1:F:374:SER:HA	1:F:748:LEU:HD12	1.70	0.72
1:G:617:THR:O	1:G:627:ASN:ND2	2.23	0.72
1:A:617:THR:O	1:A:627:ASN:ND2	2.23	0.71
1:C:617:THR:O	1:C:627:ASN:ND2	2.23	0.71
1:I:750:GLU:HB2	1:I:751:PRO:HD3	1.71	0.71
1:J:843:ARG:NH2	1:J:850:GLU:O	2.23	0.71
1:M:229:SER:O	1:M:233:ASN:ND2	2.23	0.71
1:N:843:ARG:NH2	1:N:850:GLU:O	2.23	0.71
1:E:374:SER:HA	1:E:748:LEU:HD12	1.71	0.71
1:E:854:THR:O	1:E:856:LYS:N	2.21	0.71
1:I:843:ARG:NH2	1:I:850:GLU:O	2.23	0.71
1:N:854:THR:O	1:N:856:LYS:N	2.22	0.71
1:M:843:ARG:NH2	1:M:850:GLU:O	2.23	0.71
1:H:750:GLU:HB2	1:H:751:PRO:HD3	1.71	0.71
1:H:843:ARG:NH2	1:H:850:GLU:O	2.23	0.71
1:B:617:THR:O	1:B:627:ASN:ND2	2.23	0.71
1:D:617:THR:O	1:D:627:ASN:ND2	2.23	0.71
1:L:843:ARG:NH2	1:L:850:GLU:O	2.23	0.71
1:N:229:SER:O	1:N:233:ASN:ND2	2.23	0.71
1:K:636:ASN:O	1:K:637:THR:HG23	1.91	0.71
1:M:636:ASN:O	1:M:637:THR:HG23	1.91	0.71
1:I:229:SER:O	1:I:233:ASN:ND2	2.23	0.71
1:A:801:ILE:HD13	1:A:862:ALA:HB1	1.73	0.71
1:B:422:ILE:HD13	1:B:449:LEU:HD11	1.73	0.71
1:G:801:ILE:HD13	1:G:862:ALA:HB1	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:422:ILE:HD13	1:G:449:LEU:HD11	1.73	0.71
1:K:843:ARG:NH2	1:K:850:GLU:O	2.23	0.70
1:C:801:ILE:HD13	1:C:862:ALA:HB1	1.73	0.70
1:H:229:SER:O	1:H:233:ASN:ND2	2.23	0.70
1:A:422:ILE:HD13	1:A:449:LEU:HD11	1.73	0.70
1:C:422:ILE:HD13	1:C:449:LEU:HD11	1.73	0.70
1:E:332:THR:HG23	1:E:335:ASN:HB3	1.73	0.70
1:B:801:ILE:HD13	1:B:862:ALA:HB1	1.73	0.70
1:F:801:ILE:HD13	1:F:862:ALA:HB1	1.73	0.70
1:D:801:ILE:HD13	1:D:862:ALA:HB1	1.73	0.70
1:F:422:ILE:HD13	1:F:449:LEU:HD11	1.73	0.70
1:I:636:ASN:O	1:I:637:THR:HG23	1.91	0.70
1:I:660:MET:HB2	1:I:721:ILE:HG12	1.74	0.70
1:A:332:THR:HG23	1:A:335:ASN:HB3	1.73	0.70
1:J:660:MET:HB2	1:J:721:ILE:HG12	1.74	0.70
1:K:510:ILE:O	1:K:514:SER:OG	2.10	0.70
1:M:660:MET:HB2	1:M:721:ILE:HG12	1.74	0.70
1:E:801:ILE:HD13	1:E:862:ALA:HB1	1.73	0.70
1:F:332:THR:HG23	1:F:335:ASN:HB3	1.73	0.70
1:H:510:ILE:O	1:H:514:SER:OG	2.10	0.70
1:H:636:ASN:O	1:H:637:THR:HG23	1.91	0.70
1:H:660:MET:HB2	1:H:721:ILE:HG12	1.74	0.70
1:J:636:ASN:O	1:J:637:THR:HG23	1.91	0.70
1:N:660:MET:HB2	1:N:721:ILE:HG12	1.74	0.70
1:B:332:THR:HG23	1:B:335:ASN:HB3	1.73	0.70
1:D:332:THR:HG23	1:D:335:ASN:HB3	1.73	0.70
1:F:617:THR:O	1:F:627:ASN:ND2	2.23	0.70
1:L:660:MET:HB2	1:L:721:ILE:HG12	1.74	0.70
1:K:660:MET:HB2	1:K:721:ILE:HG12	1.74	0.70
1:L:510:ILE:O	1:L:514:SER:OG	2.10	0.69
1:L:636:ASN:O	1:L:637:THR:HG23	1.91	0.69
1:A:674:TYR:HB3	1:A:704:TYR:HB3	1.74	0.69
1:G:308:ILE:HB	1:G:390:ASN:HB3	1.73	0.69
1:D:422:ILE:HD13	1:D:449:LEU:HD11	1.73	0.69
1:F:308:ILE:HB	1:F:390:ASN:HB3	1.74	0.69
1:G:674:TYR:HB3	1:G:704:TYR:HB3	1.74	0.69
1:N:510:ILE:O	1:N:514:SER:OG	2.10	0.69
1:N:636:ASN:O	1:N:637:THR:HG23	1.91	0.69
1:C:308:ILE:HB	1:C:390:ASN:HB3	1.74	0.69
1:H:509:GLN:CG	1:N:283:LYS:HB2	2.22	0.69
1:I:510:ILE:O	1:I:514:SER:OG	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:545:LEU:HD21	1:I:553:LYS:HD2	1.74	0.69
1:M:577:GLU:HG3	1:M:739:THR:HG21	1.74	0.69
1:E:422:ILE:HD13	1:E:449:LEU:HD11	1.73	0.69
1:G:332:THR:HG23	1:G:335:ASN:HB3	1.73	0.69
1:H:545:LEU:HD21	1:H:553:LYS:HD2	1.74	0.69
1:B:674:TYR:HB3	1:B:704:TYR:HB3	1.74	0.69
1:E:308:ILE:HB	1:E:390:ASN:HB3	1.73	0.69
1:F:674:TYR:HB3	1:F:704:TYR:HB3	1.74	0.69
1:J:545:LEU:HD21	1:J:553:LYS:HD2	1.74	0.69
1:N:545:LEU:HD21	1:N:553:LYS:HD2	1.74	0.69
1:A:308:ILE:HB	1:A:390:ASN:HB3	1.74	0.69
1:C:332:THR:HG23	1:C:335:ASN:HB3	1.73	0.69
1:D:843:ARG:NH2	1:D:850:GLU:O	2.26	0.69
1:H:417:ASP:N	1:H:417:ASP:OD1	2.26	0.69
1:I:577:GLU:HG3	1:I:739:THR:HG21	1.74	0.69
1:B:308:ILE:HB	1:B:390:ASN:HB3	1.74	0.69
1:C:843:ARG:NH2	1:C:850:GLU:O	2.26	0.69
1:G:644:GLN:OE1	1:G:735:ASN:ND2	2.22	0.68
1:N:577:GLU:HG3	1:N:739:THR:HG21	1.74	0.68
1:D:308:ILE:HB	1:D:390:ASN:HB3	1.74	0.68
1:J:417:ASP:OD1	1:J:417:ASP:N	2.26	0.68
1:A:843:ARG:NH2	1:A:850:GLU:O	2.26	0.68
1:G:843:ARG:NH2	1:G:850:GLU:O	2.26	0.68
1:H:577:GLU:HG3	1:H:739:THR:HG21	1.74	0.68
1:K:545:LEU:HD21	1:K:553:LYS:HD2	1.74	0.68
1:K:577:GLU:HG3	1:K:739:THR:HG21	1.74	0.68
1:M:545:LEU:HD21	1:M:553:LYS:HD2	1.74	0.68
1:K:417:ASP:N	1:K:417:ASP:OD1	2.26	0.68
1:L:545:LEU:HD21	1:L:553:LYS:HD2	1.74	0.68
1:J:577:GLU:HG3	1:J:739:THR:HG21	1.74	0.68
1:L:577:GLU:HG3	1:L:739:THR:HG21	1.74	0.68
1:M:510:ILE:O	1:M:514:SER:OG	2.10	0.68
1:B:843:ARG:NH2	1:B:850:GLU:O	2.26	0.68
1:J:441:LYS:HB2	1:J:444:LEU:HD12	1.76	0.67
1:K:641:ASP:OD1	1:K:704:TYR:OH	2.12	0.67
1:B:623:ASP:OD1	1:B:646:SER:N	2.27	0.67
1:C:674:TYR:HB3	1:C:704:TYR:HB3	1.74	0.67
1:E:674:TYR:HB3	1:E:704:TYR:HB3	1.74	0.67
1:F:623:ASP:OD1	1:F:646:SER:N	2.27	0.67
1:D:623:ASP:OD1	1:D:646:SER:N	2.27	0.67
1:E:843:ARG:NH2	1:E:850:GLU:O	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:843:ARG:NH2	1:F:850:GLU:O	2.26	0.67
1:C:369:ASP:O	1:C:716:LYS:NZ	2.28	0.67
1:J:381:ILE:HG23	1:J:385:GLU:HG2	1.77	0.67
1:K:441:LYS:HB2	1:K:444:LEU:HD12	1.76	0.67
1:L:494:GLY:HA3	1:M:265:ASN:HD21	1.59	0.67
1:B:369:ASP:O	1:B:716:LYS:NZ	2.28	0.67
1:D:369:ASP:O	1:D:716:LYS:NZ	2.28	0.67
1:F:369:ASP:O	1:F:716:LYS:NZ	2.28	0.67
1:J:510:ILE:O	1:J:514:SER:OG	2.10	0.67
1:L:417:ASP:OD1	1:L:417:ASP:N	2.26	0.67
1:K:381:ILE:HG23	1:K:385:GLU:HG2	1.77	0.67
1:N:441:LYS:HB2	1:N:444:LEU:HD12	1.76	0.67
1:N:641:ASP:OD1	1:N:704:TYR:OH	2.13	0.67
1:C:623:ASP:OD1	1:C:646:SER:N	2.27	0.67
1:I:381:ILE:HG23	1:I:385:GLU:HG2	1.77	0.67
1:J:382:ASN:N	1:J:385:GLU:OE2	2.24	0.67
1:J:641:ASP:OD1	1:J:704:TYR:OH	2.12	0.67
1:I:417:ASP:OD1	1:I:417:ASP:N	2.26	0.67
1:M:441:LYS:HB2	1:M:444:LEU:HD12	1.76	0.67
1:E:369:ASP:O	1:E:716:LYS:NZ	2.28	0.67
1:H:441:LYS:HB2	1:H:444:LEU:HD12	1.76	0.66
1:I:441:LYS:HB2	1:I:444:LEU:HD12	1.76	0.66
1:M:650:LEU:HD23	1:M:654:THR:HG22	1.77	0.66
1:A:369:ASP:O	1:A:716:LYS:NZ	2.28	0.66
1:H:382:ASN:N	1:H:385:GLU:OE2	2.24	0.66
1:D:644:GLN:OE1	1:D:735:ASN:ND2	2.22	0.66
1:D:674:TYR:HB3	1:D:704:TYR:HB3	1.74	0.66
1:M:417:ASP:N	1:M:417:ASP:OD1	2.26	0.66
1:B:805:ARG:NH2	1:B:869:GLU:OE2	2.28	0.66
1:A:644:GLN:OE1	1:A:735:ASN:ND2	2.22	0.66
1:D:522:GLU:O	1:D:523:ASN:ND2	2.29	0.66
1:E:522:GLU:O	1:E:523:ASN:ND2	2.29	0.66
1:G:369:ASP:O	1:G:716:LYS:NZ	2.28	0.66
1:L:381:ILE:HG23	1:L:385:GLU:HG2	1.77	0.66
1:G:623:ASP:OD1	1:G:646:SER:N	2.27	0.66
1:M:494:GLY:CA	1:N:265:ASN:HD21	1.99	0.66
1:B:860:ILE:HD12	1:B:873:LEU:HD23	1.78	0.66
1:G:468:LYS:NZ	1:G:750:GLU:OE1	2.29	0.66
1:I:650:LEU:HD23	1:I:654:THR:HG22	1.77	0.66
1:L:650:LEU:HD23	1:L:654:THR:HG22	1.77	0.66
1:A:468:LYS:NZ	1:A:750:GLU:OE1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:805:ARG:NH2	1:C:869:GLU:OE2	2.28	0.66
1:C:860:ILE:HD12	1:C:873:LEU:HD23	1.78	0.66
1:H:381:ILE:HG23	1:H:385:GLU:HG2	1.77	0.66
1:J:650:LEU:HD23	1:J:654:THR:HG22	1.77	0.66
1:N:650:LEU:HD23	1:N:654:THR:HG22	1.77	0.66
1:F:468:LYS:NZ	1:F:750:GLU:OE1	2.29	0.66
1:H:465:ASP:OD1	1:H:465:ASP:N	2.29	0.65
1:C:522:GLU:O	1:C:523:ASN:ND2	2.29	0.65
1:B:468:LYS:NZ	1:B:750:GLU:OE1	2.29	0.65
1:B:522:GLU:O	1:B:523:ASN:ND2	2.29	0.65
1:D:404:TYR:HE1	1:E:505:ASP:HA	1.62	0.65
1:E:468:LYS:NZ	1:E:750:GLU:OE1	2.29	0.65
1:N:381:ILE:HG23	1:N:385:GLU:HG2	1.77	0.65
1:N:417:ASP:N	1:N:417:ASP:OD1	2.26	0.65
1:B:581:ASP:N	1:B:581:ASP:OD1	2.28	0.65
1:D:468:LYS:NZ	1:D:750:GLU:OE1	2.29	0.65
1:F:644:GLN:OE1	1:F:735:ASN:ND2	2.22	0.65
1:M:381:ILE:HG23	1:M:385:GLU:HG2	1.77	0.65
1:M:641:ASP:OD1	1:M:704:TYR:OH	2.12	0.65
1:A:860:ILE:HD12	1:A:873:LEU:HD23	1.78	0.65
1:K:382:ASN:N	1:K:385:GLU:OE2	2.24	0.65
1:A:522:GLU:O	1:A:523:ASN:ND2	2.29	0.65
1:E:860:ILE:HD12	1:E:873:LEU:HD23	1.78	0.65
1:G:522:GLU:O	1:G:523:ASN:ND2	2.29	0.65
1:H:650:LEU:HD23	1:H:654:THR:HG22	1.77	0.65
1:L:382:ASN:N	1:L:385:GLU:OE2	2.24	0.65
1:A:805:ARG:NH2	1:A:869:GLU:OE2	2.28	0.65
1:C:468:LYS:NZ	1:C:750:GLU:OE1	2.29	0.65
1:I:641:ASP:OD1	1:I:704:TYR:OH	2.12	0.65
1:J:448:ALA:HB3	1:J:451:THR:HG22	1.79	0.65
1:L:441:LYS:HB2	1:L:444:LEU:HD12	1.76	0.65
1:D:581:ASP:OD1	1:D:581:ASP:N	2.28	0.65
1:I:448:ALA:HB3	1:I:451:THR:HG22	1.79	0.65
1:J:498:THR:OG1	1:K:505:ASP:OD1	2.14	0.65
1:C:581:ASP:OD1	1:C:581:ASP:N	2.28	0.65
1:E:623:ASP:OD1	1:E:646:SER:N	2.27	0.65
1:F:522:GLU:O	1:F:523:ASN:ND2	2.29	0.65
1:G:805:ARG:NH2	1:G:869:GLU:OE2	2.28	0.65
1:K:650:LEU:HD23	1:K:654:THR:HG22	1.77	0.65
1:D:860:ILE:HD12	1:D:873:LEU:HD23	1.78	0.65
1:K:448:ALA:HB3	1:K:451:THR:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:465:ASP:OD1	1:M:465:ASP:N	2.29	0.64
1:G:860:ILE:HD12	1:G:873:LEU:HD23	1.78	0.64
1:I:465:ASP:N	1:I:465:ASP:OD1	2.29	0.64
1:A:581:ASP:OD1	1:A:581:ASP:N	2.28	0.64
1:A:623:ASP:OD1	1:A:646:SER:N	2.27	0.64
1:H:801:ILE:HD13	1:H:862:ALA:HB1	1.80	0.64
1:I:801:ILE:HD13	1:I:862:ALA:HB1	1.80	0.64
1:C:412:LEU:HB3	1:C:476:ILE:HD11	1.80	0.64
1:I:450:ASN:ND2	1:I:457:SER:H	1.96	0.64
1:B:412:LEU:HB3	1:B:476:ILE:HD11	1.80	0.64
1:B:644:GLN:OE1	1:B:735:ASN:ND2	2.22	0.64
1:D:412:LEU:HB3	1:D:476:ILE:HD11	1.80	0.64
1:F:860:ILE:HD12	1:F:873:LEU:HD23	1.78	0.64
1:J:450:ASN:ND2	1:J:457:SER:H	1.96	0.64
1:D:283:LYS:HB2	1:E:509:GLN:HG3	1.77	0.64
1:H:448:ALA:HB3	1:H:451:THR:HG22	1.79	0.64
1:L:448:ALA:HB3	1:L:451:THR:HG22	1.79	0.64
1:M:448:ALA:HB3	1:M:451:THR:HG22	1.79	0.64
1:N:448:ALA:HB3	1:N:451:THR:HG22	1.79	0.64
1:A:417:ASP:OD1	1:A:417:ASP:N	2.31	0.64
1:E:417:ASP:N	1:E:417:ASP:OD1	2.31	0.64
1:F:412:LEU:HB3	1:F:476:ILE:HD11	1.80	0.64
1:F:417:ASP:N	1:F:417:ASP:OD1	2.31	0.64
1:M:450:ASN:ND2	1:M:457:SER:H	1.96	0.63
1:N:465:ASP:N	1:N:465:ASP:OD1	2.29	0.63
1:N:801:ILE:HD13	1:N:862:ALA:HB1	1.80	0.63
1:A:412:LEU:HB3	1:A:476:ILE:HD11	1.80	0.63
1:E:412:LEU:HB3	1:E:476:ILE:HD11	1.80	0.63
1:L:450:ASN:ND2	1:L:457:SER:OG	2.29	0.63
1:G:412:LEU:HB3	1:G:476:ILE:HD11	1.80	0.63
1:B:417:ASP:OD1	1:B:417:ASP:N	2.31	0.63
1:C:417:ASP:N	1:C:417:ASP:OD1	2.31	0.63
1:F:805:ARG:NH2	1:F:869:GLU:OE2	2.28	0.63
1:K:450:ASN:ND2	1:K:457:SER:OG	2.29	0.63
1:E:581:ASP:N	1:E:581:ASP:OD1	2.28	0.63
1:J:801:ILE:HD13	1:J:862:ALA:HB1	1.80	0.63
1:K:450:ASN:ND2	1:K:457:SER:H	1.96	0.63
1:K:694:LYS:NZ	1:K:696:ASP:OD1	2.31	0.63
1:L:335:ASN:OD1	1:L:358:SER:N	2.29	0.63
1:L:641:ASP:OD1	1:L:704:TYR:OH	2.12	0.63
1:N:450:ASN:ND2	1:N:457:SER:H	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:450:ASN:ND2	1:H:457:SER:H	1.96	0.63
1:D:813:SER:O	1:D:813:SER:OG	2.16	0.63
1:J:450:ASN:ND2	1:J:457:SER:OG	2.29	0.63
1:M:335:ASN:OD1	1:M:358:SER:N	2.29	0.63
1:D:805:ARG:NH2	1:D:869:GLU:OE2	2.28	0.63
1:H:694:LYS:NZ	1:H:696:ASP:OD1	2.31	0.62
1:L:801:ILE:HD13	1:L:862:ALA:HB1	1.80	0.62
1:E:805:ARG:NH2	1:E:869:GLU:OE2	2.28	0.62
1:H:450:ASN:ND2	1:H:457:SER:OG	2.29	0.62
1:F:283:LYS:HB2	1:G:509:GLN:HG3	1.81	0.62
1:K:805:ARG:NH1	1:K:869:GLU:OE2	2.33	0.62
1:M:406:VAL:HG12	1:M:408:PRO:HD3	1.82	0.62
1:M:450:ASN:ND2	1:M:457:SER:OG	2.29	0.62
1:M:801:ILE:HD13	1:M:862:ALA:HB1	1.80	0.62
1:I:450:ASN:ND2	1:I:457:SER:OG	2.29	0.62
1:K:406:VAL:HG12	1:K:408:PRO:HD3	1.82	0.62
1:M:382:ASN:N	1:M:385:GLU:OE2	2.24	0.62
1:I:805:ARG:NH1	1:I:869:GLU:OE2	2.33	0.62
1:K:465:ASP:OD1	1:K:465:ASP:N	2.29	0.62
1:G:339:VAL:HA	1:G:354:THR:HG22	1.82	0.62
1:K:801:ILE:HD13	1:K:862:ALA:HB1	1.80	0.62
1:C:813:SER:O	1:C:813:SER:OG	2.16	0.62
1:F:339:VAL:HA	1:F:354:THR:HG22	1.82	0.62
1:L:450:ASN:ND2	1:L:457:SER:H	1.96	0.62
1:L:793:THR:O	1:L:793:THR:OG1	2.18	0.62
1:J:406:VAL:HG12	1:J:408:PRO:HD3	1.82	0.62
1:L:694:LYS:NZ	1:L:696:ASP:OD1	2.31	0.62
1:L:805:ARG:NH1	1:L:869:GLU:OE2	2.33	0.62
1:N:406:VAL:HG12	1:N:408:PRO:HD3	1.82	0.62
1:F:581:ASP:OD1	1:F:581:ASP:N	2.28	0.62
1:G:417:ASP:OD1	1:G:417:ASP:N	2.31	0.62
1:G:581:ASP:N	1:G:581:ASP:OD1	2.28	0.62
1:H:805:ARG:NH1	1:H:869:GLU:OE2	2.33	0.62
1:N:805:ARG:NH1	1:N:869:GLU:OE2	2.33	0.62
1:H:641:ASP:OD1	1:H:704:TYR:OH	2.13	0.61
1:J:805:ARG:NH1	1:J:869:GLU:OE2	2.33	0.61
1:B:308:ILE:HG23	1:B:324:SER:HB3	1.82	0.61
1:F:665:PRO:HG3	1:F:716:LYS:HA	1.82	0.61
1:I:291:ASP:OD1	1:I:553:LYS:NZ	2.31	0.61
1:C:511:ASP:OD1	1:C:529:ARG:NH1	2.33	0.61
1:C:644:GLN:OE1	1:C:735:ASN:ND2	2.22	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:382:ASN:N	1:I:385:GLU:OE2	2.24	0.61
1:I:793:THR:O	1:I:793:THR:OG1	2.18	0.61
1:A:308:ILE:HG23	1:A:324:SER:HB3	1.83	0.61
1:E:339:VAL:HA	1:E:354:THR:HG22	1.82	0.61
1:J:465:ASP:OD1	1:J:465:ASP:N	2.29	0.61
1:M:805:ARG:NH1	1:M:869:GLU:OE2	2.33	0.61
1:B:511:ASP:OD1	1:B:529:ARG:NH1	2.34	0.61
1:C:308:ILE:HG23	1:C:324:SER:HB3	1.83	0.61
1:G:665:PRO:HG3	1:G:716:LYS:HA	1.82	0.61
1:M:291:ASP:OD1	1:M:553:LYS:NZ	2.31	0.61
1:D:308:ILE:HG23	1:D:324:SER:HB3	1.82	0.61
1:E:308:ILE:HG23	1:E:324:SER:HB3	1.83	0.61
1:E:665:PRO:HG3	1:E:716:LYS:HA	1.82	0.61
1:F:511:ASP:OD1	1:F:529:ARG:NH1	2.34	0.61
1:K:793:THR:O	1:K:793:THR:OG1	2.18	0.61
1:L:465:ASP:N	1:L:465:ASP:OD1	2.29	0.61
1:B:222:ASP:N	1:B:222:ASP:OD1	2.34	0.61
1:F:308:ILE:HG23	1:F:324:SER:HB3	1.83	0.61
1:F:781:THR:O	1:F:854:THR:OG1	2.15	0.61
1:K:335:ASN:OD1	1:K:358:SER:N	2.30	0.61
1:N:382:ASN:N	1:N:385:GLU:OE2	2.24	0.61
1:G:308:ILE:HG23	1:G:324:SER:HB3	1.82	0.61
1:A:339:VAL:HA	1:A:354:THR:HG22	1.82	0.61
1:D:417:ASP:OD1	1:D:417:ASP:N	2.31	0.61
1:M:308:ILE:HB	1:M:390:ASN:HB3	1.83	0.61
1:B:813:SER:O	1:B:813:SER:OG	2.16	0.61
1:E:511:ASP:OD1	1:E:529:ARG:NH1	2.34	0.61
1:G:511:ASP:OD1	1:G:529:ARG:NH1	2.34	0.61
1:N:335:ASN:OD1	1:N:358:SER:N	2.29	0.61
1:A:381:ILE:HG23	1:A:385:GLU:HG2	1.83	0.61
1:A:665:PRO:HB3	1:A:716:LYS:H	1.66	0.61
1:H:282:ASP:OD2	1:H:404:TYR:OH	2.19	0.60
1:H:617:THR:O	1:H:627:ASN:ND2	2.35	0.60
1:I:406:VAL:HG12	1:I:408:PRO:HD3	1.82	0.60
1:I:533:LYS:NZ	1:I:540:ASP:O	2.34	0.60
1:J:308:ILE:HB	1:J:390:ASN:HB3	1.83	0.60
1:M:617:THR:O	1:M:627:ASN:ND2	2.35	0.60
1:A:505:ASP:HA	1:G:404:TYR:HE1	1.66	0.60
1:B:219:LEU:HD21	1:B:221:THR:HG23	1.83	0.60
1:C:219:LEU:HD21	1:C:221:THR:HG23	1.83	0.60
1:G:665:PRO:HB3	1:G:716:LYS:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:406:VAL:HG12	1:L:408:PRO:HD3	1.82	0.60
1:L:533:LYS:NZ	1:L:540:ASP:O	2.34	0.60
1:N:450:ASN:ND2	1:N:457:SER:OG	2.29	0.60
1:E:381:ILE:HG23	1:E:385:GLU:HG2	1.83	0.60
1:F:813:SER:O	1:F:813:SER:OG	2.16	0.60
1:L:617:THR:O	1:L:627:ASN:ND2	2.34	0.60
1:M:282:ASP:OD2	1:M:404:TYR:OH	2.19	0.60
1:A:509:GLN:HG3	1:G:283:LYS:HB2	1.83	0.60
1:C:665:PRO:HG3	1:C:716:LYS:HA	1.82	0.60
1:D:381:ILE:HG23	1:D:385:GLU:HG2	1.83	0.60
1:E:813:SER:O	1:E:813:SER:OG	2.16	0.60
1:G:381:ILE:HG23	1:G:385:GLU:HG2	1.83	0.60
1:H:406:VAL:HG12	1:H:408:PRO:HD3	1.82	0.60
1:J:617:THR:O	1:J:627:ASN:ND2	2.35	0.60
1:A:511:ASP:OD1	1:A:529:ARG:NH1	2.34	0.60
1:H:653:GLU:HB3	1:H:726:ILE:HG23	1.84	0.60
1:I:653:GLU:HB3	1:I:726:ILE:HG23	1.84	0.60
1:K:308:ILE:HB	1:K:390:ASN:HB3	1.83	0.60
1:A:665:PRO:HG3	1:A:716:LYS:HA	1.83	0.60
1:B:665:PRO:HB3	1:B:716:LYS:H	1.66	0.60
1:D:511:ASP:OD1	1:D:529:ARG:NH1	2.33	0.60
1:E:665:PRO:HB3	1:E:716:LYS:H	1.66	0.60
1:G:445:SER:O	1:G:445:SER:OG	2.20	0.60
1:H:335:ASN:OD1	1:H:358:SER:N	2.29	0.60
1:H:793:THR:O	1:H:793:THR:OG1	2.18	0.60
1:I:694:LYS:NZ	1:I:696:ASP:OD1	2.31	0.60
1:N:308:ILE:HB	1:N:390:ASN:HB3	1.83	0.60
1:B:381:ILE:HG23	1:B:385:GLU:HG2	1.83	0.60
1:B:618:TYR:HA	1:B:627:ASN:HB3	1.84	0.60
1:D:665:PRO:HG3	1:D:716:LYS:HA	1.82	0.60
1:H:308:ILE:HB	1:H:390:ASN:HB3	1.83	0.60
1:M:496:ILE:HB	1:N:506:TYR:CE1	2.37	0.60
1:N:617:THR:O	1:N:627:ASN:ND2	2.34	0.60
1:B:665:PRO:HG3	1:B:716:LYS:HA	1.82	0.60
1:C:618:TYR:HA	1:C:627:ASN:HB3	1.84	0.60
1:D:219:LEU:HD21	1:D:221:THR:HG23	1.83	0.60
1:F:665:PRO:HB3	1:F:716:LYS:H	1.66	0.60
1:I:308:ILE:HB	1:I:390:ASN:HB3	1.83	0.60
1:L:308:ILE:HB	1:L:390:ASN:HB3	1.83	0.60
1:N:653:GLU:HB3	1:N:726:ILE:HG23	1.84	0.60
1:A:219:LEU:HD21	1:A:221:THR:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:VAL:HA	1:B:354:THR:HG22	1.82	0.60
1:C:665:PRO:HB3	1:C:716:LYS:H	1.66	0.60
1:D:339:VAL:HA	1:D:354:THR:HG22	1.82	0.60
1:E:644:GLN:OE1	1:E:735:ASN:ND2	2.22	0.60
1:F:381:ILE:HG23	1:F:385:GLU:HG2	1.83	0.60
1:J:839:TYR:CE2	1:J:841:ASN:HB3	2.36	0.60
1:K:617:THR:O	1:K:627:ASN:ND2	2.34	0.60
1:C:381:ILE:HG23	1:C:385:GLU:HG2	1.83	0.60
1:L:839:TYR:CE2	1:L:841:ASN:HB3	2.36	0.60
1:A:445:SER:O	1:A:445:SER:OG	2.19	0.60
1:G:222:ASP:N	1:G:222:ASP:OD1	2.34	0.60
1:J:653:GLU:HB3	1:J:726:ILE:HG23	1.84	0.59
1:N:533:LYS:NZ	1:N:540:ASP:O	2.34	0.59
1:I:617:THR:O	1:I:627:ASN:ND2	2.34	0.59
1:J:494:GLY:HA3	1:K:265:ASN:ND2	2.15	0.59
1:K:839:TYR:CE2	1:K:841:ASN:HB3	2.36	0.59
1:B:658:ILE:N	1:B:721:ILE:O	2.34	0.59
1:C:222:ASP:OD1	1:C:222:ASP:N	2.34	0.59
1:D:665:PRO:HB3	1:D:716:LYS:H	1.66	0.59
1:J:533:LYS:NZ	1:J:540:ASP:O	2.34	0.59
1:M:653:GLU:HB3	1:M:726:ILE:HG23	1.84	0.59
1:F:219:LEU:HD21	1:F:221:THR:HG23	1.83	0.59
1:I:839:TYR:CE2	1:I:841:ASN:HB3	2.36	0.59
1:M:839:TYR:CE2	1:M:841:ASN:HB3	2.36	0.59
1:N:291:ASP:OD1	1:N:553:LYS:NZ	2.31	0.59
1:E:781:THR:O	1:E:854:THR:OG1	2.15	0.59
1:G:592:LEU:O	1:G:598:LYS:NZ	2.29	0.59
1:J:282:ASP:OD2	1:J:404:TYR:OH	2.19	0.59
1:J:809:THR:O	1:J:809:THR:OG1	2.21	0.59
1:N:839:TYR:CE2	1:N:841:ASN:HB3	2.36	0.59
1:A:720:ASN:OD1	1:A:721:ILE:N	2.36	0.59
1:F:222:ASP:OD1	1:F:222:ASP:N	2.34	0.59
1:F:618:TYR:HA	1:F:627:ASN:HB3	1.84	0.59
1:H:291:ASP:OD1	1:H:553:LYS:NZ	2.31	0.59
1:A:618:TYR:HA	1:A:627:ASN:HB3	1.84	0.59
1:E:720:ASN:OD1	1:E:721:ILE:N	2.36	0.59
1:G:291:ASP:OD1	1:G:553:LYS:NZ	2.28	0.59
1:K:651:ASN:OD1	1:K:729:GLY:N	2.36	0.59
1:A:813:SER:OG	1:A:813:SER:O	2.16	0.59
1:C:339:VAL:HA	1:C:354:THR:HG22	1.82	0.59
1:D:618:TYR:HA	1:D:627:ASN:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:618:TYR:HA	1:G:627:ASN:HB3	1.84	0.59
1:H:839:TYR:CE2	1:H:841:ASN:HB3	2.36	0.59
1:K:282:ASP:OD2	1:K:404:TYR:OH	2.19	0.59
1:F:584:THR:HG21	1:F:610:ASN:H	1.68	0.59
1:G:720:ASN:OD1	1:G:721:ILE:N	2.36	0.59
1:L:653:GLU:HB3	1:L:726:ILE:HG23	1.84	0.59
1:N:282:ASP:OD2	1:N:404:TYR:OH	2.19	0.59
1:A:584:THR:HG21	1:A:610:ASN:H	1.68	0.59
1:A:658:ILE:N	1:A:721:ILE:O	2.34	0.59
1:B:720:ASN:OD1	1:B:721:ILE:N	2.36	0.59
1:D:720:ASN:OD1	1:D:721:ILE:N	2.36	0.59
1:E:222:ASP:N	1:E:222:ASP:OD1	2.34	0.59
1:G:658:ILE:N	1:G:721:ILE:O	2.34	0.59
1:K:653:GLU:HB3	1:K:726:ILE:HG23	1.84	0.59
1:M:694:LYS:NZ	1:M:696:ASP:OD1	2.31	0.59
1:I:282:ASP:OD2	1:I:404:TYR:OH	2.19	0.58
1:F:720:ASN:OD1	1:F:721:ILE:N	2.36	0.58
1:K:291:ASP:OD1	1:K:553:LYS:NZ	2.31	0.58
1:L:651:ASN:OD1	1:L:729:GLY:N	2.36	0.58
1:A:633:SER:OG	1:A:654:THR:OG1	2.09	0.58
1:E:618:TYR:HA	1:E:627:ASN:HB3	1.84	0.58
1:F:308:ILE:O	1:F:390:ASN:N	2.32	0.58
1:I:335:ASN:OD1	1:I:358:SER:N	2.30	0.58
1:G:781:THR:O	1:G:854:THR:OG1	2.15	0.58
1:C:341:VAL:HG23	1:C:342:ASN:H	1.69	0.58
1:E:219:LEU:HD21	1:E:221:THR:HG23	1.83	0.58
1:J:450:ASN:HD21	1:J:457:SER:HG	1.52	0.58
1:J:651:ASN:OD1	1:J:729:GLY:N	2.36	0.58
1:M:651:ASN:OD1	1:M:729:GLY:N	2.36	0.58
1:C:720:ASN:OD1	1:C:721:ILE:N	2.36	0.58
1:G:341:VAL:HG23	1:G:342:ASN:H	1.69	0.58
1:J:335:ASN:OD1	1:J:358:SER:N	2.29	0.58
1:J:361:THR:O	1:J:361:THR:OG1	2.22	0.58
1:J:793:THR:O	1:J:793:THR:OG1	2.18	0.58
1:N:651:ASN:OD1	1:N:729:GLY:N	2.36	0.58
1:B:584:THR:HG21	1:B:610:ASN:H	1.68	0.58
1:E:308:ILE:O	1:E:390:ASN:N	2.32	0.58
1:G:219:LEU:HD21	1:G:221:THR:HG23	1.83	0.58
1:H:533:LYS:NZ	1:H:540:ASP:O	2.34	0.58
1:C:308:ILE:O	1:C:390:ASN:N	2.32	0.58
1:C:445:SER:O	1:C:445:SER:OG	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:312:ASN:ND2	1:M:319:GLN:HB2	2.19	0.58
1:A:341:VAL:HG23	1:A:342:ASN:H	1.69	0.58
1:D:658:ILE:N	1:D:721:ILE:O	2.34	0.58
1:E:404:TYR:HE1	1:F:505:ASP:HA	1.68	0.58
1:F:341:VAL:HG23	1:F:342:ASN:H	1.69	0.58
1:H:312:ASN:ND2	1:H:319:GLN:HB2	2.19	0.58
1:L:282:ASP:OD2	1:L:404:TYR:OH	2.19	0.58
1:B:341:VAL:HG23	1:B:342:ASN:H	1.69	0.58
1:D:584:THR:HG21	1:D:610:ASN:H	1.68	0.58
1:E:584:THR:HG21	1:E:610:ASN:H	1.68	0.58
1:G:584:THR:HG21	1:G:610:ASN:H	1.68	0.58
1:H:651:ASN:OD1	1:H:729:GLY:N	2.36	0.58
1:L:312:ASN:ND2	1:L:319:GLN:HB2	2.19	0.57
1:A:634:ASN:HB2	1:A:650:LEU:HD22	1.86	0.57
1:G:634:ASN:HB2	1:G:650:LEU:HD22	1.86	0.57
1:G:813:SER:O	1:G:813:SER:OG	2.16	0.57
1:J:694:LYS:NZ	1:J:696:ASP:OD1	2.31	0.57
1:K:312:ASN:ND2	1:K:319:GLN:HB2	2.19	0.57
1:M:533:LYS:NZ	1:M:540:ASP:O	2.34	0.57
1:J:240:LEU:O	1:J:274:TYR:OH	2.17	0.57
1:I:651:ASN:OD1	1:I:729:GLY:N	2.36	0.57
1:J:456:SER:OG	1:J:457:SER:N	2.38	0.57
1:N:809:THR:O	1:N:809:THR:OG1	2.21	0.57
1:G:308:ILE:O	1:G:390:ASN:N	2.32	0.57
1:I:361:THR:O	1:I:361:THR:OG1	2.22	0.57
1:J:312:ASN:ND2	1:J:319:GLN:HB2	2.19	0.57
1:B:592:LEU:O	1:B:598:LYS:NZ	2.29	0.57
1:D:222:ASP:N	1:D:222:ASP:OD1	2.34	0.57
1:D:341:VAL:HG23	1:D:342:ASN:H	1.69	0.57
1:D:781:THR:O	1:D:854:THR:OG1	2.15	0.57
1:E:341:VAL:HG23	1:E:342:ASN:H	1.69	0.57
1:I:312:ASN:ND2	1:I:319:GLN:HB2	2.19	0.57
1:K:533:LYS:NZ	1:K:540:ASP:O	2.34	0.57
1:N:329:ASN:HB3	1:N:365:THR:HA	1.87	0.57
1:A:222:ASP:N	1:A:222:ASP:OD1	2.34	0.57
1:E:573:GLU:OE2	1:E:600:ILE:N	2.38	0.57
1:I:456:SER:OG	1:I:457:SER:N	2.38	0.57
1:J:329:ASN:HB3	1:J:365:THR:HA	1.87	0.57
1:K:329:ASN:HB3	1:K:365:THR:HA	1.87	0.57
1:C:465:ASP:N	1:C:465:ASP:OD1	2.37	0.57
1:I:329:ASN:HB3	1:I:365:THR:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:379:LEU:HD23	1:K:467:LEU:HD21	1.87	0.57
1:M:329:ASN:HB3	1:M:365:THR:HA	1.87	0.57
1:B:634:ASN:HB2	1:B:650:LEU:HD22	1.86	0.57
1:C:584:THR:HG21	1:C:610:ASN:H	1.68	0.57
1:D:634:ASN:HB2	1:D:650:LEU:HD22	1.86	0.57
1:E:465:ASP:OD1	1:E:465:ASP:N	2.37	0.57
1:F:465:ASP:N	1:F:465:ASP:OD1	2.37	0.57
1:F:634:ASN:HB2	1:F:650:LEU:HD22	1.86	0.57
1:L:379:LEU:HD23	1:L:467:LEU:HD21	1.87	0.57
1:L:634:ASN:HB2	1:L:650:LEU:HD22	1.87	0.57
1:A:573:GLU:OE2	1:A:600:ILE:N	2.38	0.57
1:H:329:ASN:HB3	1:H:365:THR:HA	1.87	0.57
1:L:329:ASN:HB3	1:L:365:THR:HA	1.87	0.57
1:N:361:THR:O	1:N:361:THR:OG1	2.22	0.57
1:N:860:ILE:HD12	1:N:873:LEU:HD23	1.87	0.57
1:A:283:LYS:HB2	1:B:509:GLN:HG3	1.85	0.57
1:E:634:ASN:HB2	1:E:650:LEU:HD22	1.86	0.57
1:E:658:ILE:N	1:E:721:ILE:O	2.34	0.57
1:H:379:LEU:HD23	1:H:467:LEU:HD21	1.87	0.56
1:I:259:SER:HB3	1:I:292:PRO:HB2	1.87	0.56
1:N:259:SER:HB3	1:N:292:PRO:HB2	1.87	0.56
1:N:312:ASN:ND2	1:N:319:GLN:HB2	2.19	0.56
1:F:573:GLU:OE2	1:F:600:ILE:N	2.38	0.56
1:M:450:ASN:O	1:M:451:THR:OG1	2.22	0.56
1:M:634:ASN:HB2	1:M:650:LEU:HD22	1.87	0.56
1:M:793:THR:O	1:M:793:THR:OG1	2.18	0.56
1:M:809:THR:O	1:M:809:THR:OG1	2.21	0.56
1:D:573:GLU:OE2	1:D:600:ILE:N	2.38	0.56
1:G:573:GLU:OE2	1:G:600:ILE:N	2.38	0.56
1:H:259:SER:HB3	1:H:292:PRO:HB2	1.87	0.56
1:I:240:LEU:O	1:I:274:TYR:OH	2.17	0.56
1:J:259:SER:HB3	1:J:292:PRO:HB2	1.88	0.56
1:J:291:ASP:OD1	1:J:553:LYS:NZ	2.31	0.56
1:K:634:ASN:HB2	1:K:650:LEU:HD22	1.87	0.56
1:L:374:SER:OG	1:L:375:TRP:N	2.39	0.56
1:C:301:GLY:HA2	1:C:480:THR:HG21	1.88	0.56
1:C:634:ASN:HB2	1:C:650:LEU:HD22	1.86	0.56
1:C:658:ILE:N	1:C:721:ILE:O	2.34	0.56
1:D:308:ILE:O	1:D:390:ASN:N	2.32	0.56
1:L:809:THR:OG1	1:L:809:THR:O	2.21	0.56
1:M:456:SER:OG	1:M:457:SER:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:860:ILE:HD12	1:M:873:LEU:HD23	1.87	0.56
1:G:301:GLY:HA2	1:G:480:THR:HG21	1.88	0.56
1:H:339:VAL:HG21	1:H:579:ILE:HD13	1.88	0.56
1:H:374:SER:OG	1:H:375:TRP:N	2.39	0.56
1:H:456:SER:OG	1:H:457:SER:N	2.38	0.56
1:H:689:LYS:HB2	1:H:722:GLU:HG3	1.88	0.56
1:I:379:LEU:HD23	1:I:467:LEU:HD21	1.87	0.56
1:I:689:LYS:HB2	1:I:722:GLU:HG3	1.87	0.56
1:J:379:LEU:HD23	1:J:467:LEU:HD21	1.87	0.56
1:M:259:SER:HB3	1:M:292:PRO:HB2	1.87	0.56
1:N:339:VAL:HG21	1:N:579:ILE:HD13	1.88	0.56
1:N:374:SER:OG	1:N:375:TRP:N	2.39	0.56
1:N:694:LYS:NZ	1:N:696:ASP:OD1	2.31	0.56
1:B:301:GLY:HA2	1:B:480:THR:HG21	1.88	0.56
1:B:308:ILE:O	1:B:390:ASN:N	2.32	0.56
1:B:573:GLU:OE2	1:B:600:ILE:N	2.38	0.56
1:G:465:ASP:N	1:G:465:ASP:OD1	2.37	0.56
1:H:860:ILE:HD12	1:H:873:LEU:HD23	1.87	0.56
1:J:374:SER:OG	1:J:375:TRP:N	2.39	0.56
1:M:496:ILE:HG22	1:N:505:ASP:HB3	1.87	0.56
1:N:379:LEU:HD23	1:N:467:LEU:HD21	1.87	0.56
1:A:301:GLY:HA2	1:A:480:THR:HG21	1.88	0.56
1:C:592:LEU:O	1:C:598:LYS:NZ	2.29	0.56
1:D:301:GLY:HA2	1:D:480:THR:HG21	1.88	0.56
1:I:450:ASN:O	1:I:451:THR:OG1	2.22	0.56
1:K:259:SER:HB3	1:K:292:PRO:HB2	1.88	0.56
1:K:361:THR:O	1:K:361:THR:OG1	2.22	0.56
1:M:379:LEU:HD23	1:M:467:LEU:HD21	1.87	0.56
1:F:301:GLY:HA2	1:F:480:THR:HG21	1.88	0.56
1:H:809:THR:O	1:H:809:THR:OG1	2.21	0.56
1:K:860:ILE:HD12	1:K:873:LEU:HD23	1.87	0.56
1:L:689:LYS:HB2	1:L:722:GLU:HG3	1.87	0.56
1:L:860:ILE:HD12	1:L:873:LEU:HD23	1.87	0.56
1:M:374:SER:OG	1:M:375:TRP:N	2.39	0.56
1:D:465:ASP:N	1:D:465:ASP:OD1	2.37	0.56
1:I:339:VAL:HG21	1:I:579:ILE:HD13	1.88	0.56
1:J:634:ASN:HB2	1:J:650:LEU:HD22	1.87	0.56
1:J:860:ILE:HD12	1:J:873:LEU:HD23	1.87	0.56
1:L:259:SER:HB3	1:L:292:PRO:HB2	1.87	0.56
1:H:509:GLN:HE21	1:N:283:LYS:HG2	1.71	0.56
1:I:374:SER:OG	1:I:375:TRP:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:860:ILE:HD12	1:I:873:LEU:HD23	1.87	0.56
1:B:465:ASP:OD1	1:B:465:ASP:N	2.37	0.56
1:D:426:GLU:OE2	1:D:426:GLU:N	2.39	0.56
1:F:592:LEU:O	1:F:598:LYS:NZ	2.29	0.56
1:I:222:ASP:OD1	1:I:222:ASP:N	2.40	0.55
1:K:689:LYS:HB2	1:K:722:GLU:HG3	1.87	0.55
1:N:456:SER:OG	1:N:457:SER:N	2.38	0.55
1:N:689:LYS:HB2	1:N:722:GLU:HG3	1.87	0.55
1:E:301:GLY:HA2	1:E:480:THR:HG21	1.88	0.55
1:E:426:GLU:N	1:E:426:GLU:OE2	2.39	0.55
1:J:283:LYS:HE3	1:K:263:GLU:OE2	2.06	0.55
1:K:456:SER:OG	1:K:457:SER:N	2.38	0.55
1:L:240:LEU:O	1:L:274:TYR:OH	2.17	0.55
1:M:239:ASP:H	1:N:539:GLU:CD	2.06	0.55
1:E:637:THR:HG22	1:E:649:LYS:HD2	1.88	0.55
1:G:426:GLU:N	1:G:426:GLU:OE2	2.39	0.55
1:I:733:LEU:HD22	1:I:736:LEU:HD21	1.89	0.55
1:L:291:ASP:OD1	1:L:553:LYS:NZ	2.31	0.55
1:M:339:VAL:HG21	1:M:579:ILE:HD13	1.88	0.55
1:C:781:THR:O	1:C:854:THR:OG1	2.15	0.55
1:D:581:ASP:OD2	1:D:610:ASN:ND2	2.32	0.55
1:F:637:THR:HG22	1:F:649:LYS:HD2	1.88	0.55
1:F:658:ILE:N	1:F:721:ILE:O	2.34	0.55
1:L:733:LEU:HD22	1:L:736:LEU:HD21	1.89	0.55
1:N:634:ASN:HB2	1:N:650:LEU:HD22	1.87	0.55
1:J:222:ASP:N	1:J:222:ASP:OD1	2.40	0.55
1:J:733:LEU:HD22	1:J:736:LEU:HD21	1.89	0.55
1:M:689:LYS:HB2	1:M:722:GLU:HG3	1.87	0.55
1:H:634:ASN:HB2	1:H:650:LEU:HD22	1.87	0.55
1:I:634:ASN:HB2	1:I:650:LEU:HD22	1.87	0.55
1:J:339:VAL:HG21	1:J:579:ILE:HD13	1.88	0.55
1:J:689:LYS:HB2	1:J:722:GLU:HG3	1.87	0.55
1:M:283:LYS:H	1:N:509:GLN:HG3	1.70	0.55
1:K:733:LEU:HD22	1:K:736:LEU:HD21	1.89	0.55
1:A:781:THR:O	1:A:854:THR:OG1	2.15	0.55
1:B:426:GLU:N	1:B:426:GLU:OE2	2.39	0.55
1:C:573:GLU:OE2	1:C:600:ILE:N	2.38	0.55
1:D:637:THR:HG22	1:D:649:LYS:HD2	1.88	0.55
1:F:426:GLU:N	1:F:426:GLU:OE2	2.39	0.55
1:H:733:LEU:HD22	1:H:736:LEU:HD21	1.89	0.55
1:K:311:THR:O	1:K:311:THR:OG1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:374:SER:OG	1:K:375:TRP:N	2.39	0.55
1:M:733:LEU:HD22	1:M:736:LEU:HD21	1.89	0.55
1:H:450:ASN:O	1:H:451:THR:OG1	2.22	0.55
1:C:291:ASP:OD1	1:C:553:LYS:NZ	2.28	0.55
1:C:426:GLU:N	1:C:426:GLU:OE2	2.39	0.55
1:H:464:TYR:CE1	1:H:468:LYS:HE2	2.42	0.55
1:H:733:LEU:HB3	1:H:736:LEU:HD11	1.89	0.55
1:I:809:THR:O	1:I:809:THR:OG1	2.21	0.55
1:H:306:LYS:HB3	1:H:392:ASN:HB2	1.88	0.54
1:L:464:TYR:CE1	1:L:468:LYS:HE2	2.43	0.54
1:M:464:TYR:CE1	1:M:468:LYS:HE2	2.43	0.54
1:N:464:TYR:CE1	1:N:468:LYS:HE2	2.43	0.54
1:N:733:LEU:HB3	1:N:736:LEU:HD11	1.89	0.54
1:G:637:THR:HG22	1:G:649:LYS:HD2	1.88	0.54
1:H:361:THR:O	1:H:361:THR:OG1	2.22	0.54
1:K:222:ASP:OD1	1:K:222:ASP:N	2.40	0.54
1:K:339:VAL:HG21	1:K:579:ILE:HD13	1.88	0.54
1:L:374:SER:HB3	1:L:750:GLU:HG3	1.89	0.54
1:L:456:SER:OG	1:L:457:SER:N	2.38	0.54
1:L:635:VAL:O	1:L:649:LYS:HB2	2.07	0.54
1:M:306:LYS:HB3	1:M:392:ASN:HB2	1.88	0.54
1:N:306:LYS:HB3	1:N:392:ASN:HB2	1.88	0.54
1:N:733:LEU:HD22	1:N:736:LEU:HD21	1.89	0.54
1:A:426:GLU:N	1:A:426:GLU:OE2	2.39	0.54
1:B:637:THR:HG22	1:B:649:LYS:HD2	1.88	0.54
1:C:658:ILE:O	1:C:721:ILE:N	2.40	0.54
1:I:464:TYR:CE1	1:I:468:LYS:HE2	2.42	0.54
1:K:374:SER:HB3	1:K:750:GLU:HG3	1.89	0.54
1:L:339:VAL:HG21	1:L:579:ILE:HD13	1.88	0.54
1:M:733:LEU:HB3	1:M:736:LEU:HD11	1.89	0.54
1:A:308:ILE:O	1:A:390:ASN:N	2.32	0.54
1:A:465:ASP:N	1:A:465:ASP:OD1	2.37	0.54
1:I:306:LYS:HB3	1:I:392:ASN:HB2	1.88	0.54
1:J:680:THR:O	1:J:680:THR:OG1	2.23	0.54
1:K:464:TYR:CE1	1:K:468:LYS:HE2	2.42	0.54
1:M:374:SER:HB3	1:M:750:GLU:HG3	1.89	0.54
1:M:618:TYR:HB3	1:M:628:TYR:CD1	2.43	0.54
1:H:222:ASP:OD1	1:H:222:ASP:N	2.39	0.54
1:I:733:LEU:HB3	1:I:736:LEU:HD11	1.89	0.54
1:J:618:TYR:HB3	1:J:628:TYR:CD1	2.43	0.54
1:K:635:VAL:O	1:K:649:LYS:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:306:LYS:HB3	1:J:392:ASN:HB2	1.88	0.54
1:J:527:GLU:OE2	1:J:529:ARG:NH2	2.41	0.54
1:N:527:GLU:OE2	1:N:529:ARG:NH2	2.41	0.54
1:C:637:THR:HG22	1:C:649:LYS:HD2	1.88	0.54
1:D:291:ASP:OD1	1:D:553:LYS:NZ	2.28	0.54
1:H:527:GLU:OE2	1:H:529:ARG:NH2	2.41	0.54
1:H:635:VAL:O	1:H:649:LYS:HB2	2.07	0.54
1:I:527:GLU:OE2	1:I:529:ARG:NH2	2.41	0.54
1:K:680:THR:O	1:K:680:THR:OG1	2.23	0.54
1:N:551:ILE:HD13	1:N:613:ILE:HD11	1.90	0.54
1:I:618:TYR:HB3	1:I:628:TYR:CD1	2.43	0.54
1:J:464:TYR:CE1	1:J:468:LYS:HE2	2.42	0.54
1:M:551:ILE:HD13	1:M:613:ILE:HD11	1.90	0.54
1:N:618:TYR:HB3	1:N:628:TYR:CD1	2.43	0.54
1:J:374:SER:HB3	1:J:750:GLU:HG3	1.89	0.54
1:L:222:ASP:N	1:L:222:ASP:OD1	2.40	0.54
1:L:540:ASP:OD2	1:L:542:THR:OG1	2.24	0.54
1:N:222:ASP:OD1	1:N:222:ASP:N	2.40	0.54
1:H:240:LEU:O	1:H:274:TYR:OH	2.17	0.54
1:H:551:ILE:HD13	1:H:613:ILE:HD11	1.90	0.54
1:K:527:GLU:OE2	1:K:529:ARG:NH2	2.41	0.54
1:K:733:LEU:HB3	1:K:736:LEU:HD11	1.89	0.54
1:L:551:ILE:HD13	1:L:613:ILE:HD11	1.90	0.54
1:N:374:SER:HB3	1:N:750:GLU:HG3	1.89	0.54
1:N:635:VAL:O	1:N:649:LYS:HB2	2.07	0.54
1:A:658:ILE:O	1:A:721:ILE:N	2.40	0.54
1:B:391:ALA:O	1:B:449:LEU:N	2.41	0.54
1:B:781:THR:O	1:B:854:THR:OG1	2.15	0.54
1:E:391:ALA:O	1:E:449:LEU:N	2.41	0.54
1:H:311:THR:OG1	1:H:311:THR:O	2.24	0.53
1:K:618:TYR:HB3	1:K:628:TYR:CD1	2.43	0.53
1:L:527:GLU:OE2	1:L:529:ARG:NH2	2.41	0.53
1:M:635:VAL:O	1:M:649:LYS:HB2	2.07	0.53
1:C:689:LYS:HD3	1:C:693:GLU:HB2	1.91	0.53
1:J:450:ASN:O	1:J:451:THR:OG1	2.22	0.53
1:J:635:VAL:O	1:J:649:LYS:HB2	2.07	0.53
1:J:733:LEU:HB3	1:J:736:LEU:HD11	1.89	0.53
1:L:618:TYR:HB3	1:L:628:TYR:CD1	2.43	0.53
1:M:222:ASP:N	1:M:222:ASP:OD1	2.40	0.53
1:M:527:GLU:OE2	1:M:529:ARG:NH2	2.41	0.53
1:B:581:ASP:OD2	1:B:610:ASN:ND2	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:306:LYS:HB3	1:K:392:ASN:HB2	1.89	0.53
1:K:809:THR:O	1:K:809:THR:OG1	2.21	0.53
1:A:637:THR:HG22	1:A:649:LYS:HD2	1.88	0.53
1:D:689:LYS:HD3	1:D:693:GLU:HB2	1.91	0.53
1:H:618:TYR:HB3	1:H:628:TYR:CD1	2.43	0.53
1:L:306:LYS:HB3	1:L:392:ASN:HB2	1.88	0.53
1:A:391:ALA:O	1:A:449:LEU:N	2.41	0.53
1:B:291:ASP:OD1	1:B:553:LYS:NZ	2.28	0.53
1:F:689:LYS:HD3	1:F:693:GLU:HB2	1.91	0.53
1:E:689:LYS:HD3	1:E:693:GLU:HB2	1.91	0.53
1:G:633:SER:OG	1:G:654:THR:OG1	2.09	0.53
1:I:374:SER:HB3	1:I:750:GLU:HG3	1.89	0.53
1:L:733:LEU:HB3	1:L:736:LEU:HD11	1.89	0.53
1:B:658:ILE:O	1:B:721:ILE:N	2.40	0.53
1:D:391:ALA:O	1:D:449:LEU:N	2.41	0.53
1:B:689:LYS:HD3	1:B:693:GLU:HB2	1.91	0.53
1:C:391:ALA:O	1:C:449:LEU:N	2.41	0.53
1:G:689:LYS:HD3	1:G:693:GLU:HB2	1.91	0.53
1:H:491:ASN:HB2	1:H:495:GLN:HB2	1.91	0.53
1:H:540:ASP:OD2	1:H:542:THR:OG1	2.24	0.53
1:I:635:VAL:O	1:I:649:LYS:HB2	2.07	0.53
1:M:311:THR:O	1:M:311:THR:OG1	2.25	0.53
1:A:291:ASP:OD1	1:A:553:LYS:NZ	2.28	0.53
1:H:308:ILE:HG12	1:H:324:SER:HB2	1.91	0.53
1:I:308:ILE:HG12	1:I:324:SER:HB2	1.91	0.53
1:K:551:ILE:HD13	1:K:613:ILE:HD11	1.90	0.53
1:L:308:ILE:HG12	1:L:324:SER:HB2	1.91	0.53
1:N:491:ASN:HB2	1:N:495:GLN:HB2	1.91	0.53
1:C:503:TRP:O	1:C:507:ILE:HG12	2.09	0.53
1:K:308:ILE:HG12	1:K:324:SER:HB2	1.91	0.52
1:L:361:THR:O	1:L:361:THR:OG1	2.22	0.52
1:A:689:LYS:HD3	1:A:693:GLU:HB2	1.91	0.52
1:B:503:TRP:O	1:B:507:ILE:HG12	2.09	0.52
1:D:503:TRP:O	1:D:507:ILE:HG12	2.09	0.52
1:F:503:TRP:O	1:F:507:ILE:HG12	2.09	0.52
1:H:374:SER:HB3	1:H:750:GLU:HG3	1.89	0.52
1:I:491:ASN:HB2	1:I:495:GLN:HB2	1.91	0.52
1:J:308:ILE:HG12	1:J:324:SER:HB2	1.91	0.52
1:K:240:LEU:O	1:K:274:TYR:OH	2.17	0.52
1:L:573:GLU:HB3	1:L:600:ILE:HD12	1.91	0.52
1:A:503:TRP:O	1:A:507:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:308:ILE:HG12	1:N:324:SER:HB2	1.91	0.52
1:D:815:PHE:CE1	1:D:857:LYS:HD2	2.45	0.52
1:F:658:ILE:O	1:F:721:ILE:N	2.40	0.52
1:G:815:PHE:CE1	1:G:857:LYS:HD2	2.45	0.52
1:K:341:VAL:HG11	1:K:710:GLU:HG2	1.92	0.52
1:M:308:ILE:HG12	1:M:324:SER:HB2	1.91	0.52
1:M:806:VAL:HG22	1:M:860:ILE:HG12	1.91	0.52
1:N:341:VAL:HG11	1:N:710:GLU:HG2	1.92	0.52
1:A:358:SER:OG	1:A:359:HIS:N	2.42	0.52
1:A:592:LEU:O	1:A:598:LYS:NZ	2.29	0.52
1:C:581:ASP:OD2	1:C:610:ASN:ND2	2.32	0.52
1:G:358:SER:OG	1:G:359:HIS:N	2.42	0.52
1:M:341:VAL:HG11	1:M:710:GLU:HG2	1.92	0.52
1:B:358:SER:OG	1:B:359:HIS:N	2.42	0.52
1:C:358:SER:OG	1:C:359:HIS:N	2.43	0.52
1:E:581:ASP:OD2	1:E:610:ASN:ND2	2.32	0.52
1:E:592:LEU:O	1:E:598:LYS:NZ	2.29	0.52
1:E:815:PHE:CE1	1:E:857:LYS:HD2	2.45	0.52
1:F:815:PHE:CE1	1:F:857:LYS:HD2	2.45	0.52
1:I:551:ILE:HD13	1:I:613:ILE:HD11	1.90	0.52
1:I:573:GLU:HB3	1:I:600:ILE:HD12	1.91	0.52
1:K:521:THR:H	1:K:615:THR:HG23	1.75	0.52
1:L:341:VAL:HG11	1:L:710:GLU:HG2	1.92	0.52
1:C:299:ILE:O	1:C:398:THR:OG1	2.28	0.52
1:D:299:ILE:O	1:D:398:THR:OG1	2.28	0.52
1:D:358:SER:OG	1:D:359:HIS:N	2.42	0.52
1:E:503:TRP:O	1:E:507:ILE:HG12	2.09	0.52
1:H:573:GLU:HB3	1:H:600:ILE:HD12	1.91	0.52
1:J:341:VAL:HG11	1:J:710:GLU:HG2	1.92	0.52
1:L:812:TYR:O	1:L:813:SER:OG	2.28	0.52
1:M:573:GLU:HB3	1:M:600:ILE:HD12	1.91	0.52
1:A:581:ASP:OD2	1:A:610:ASN:ND2	2.32	0.52
1:D:565:TYR:HD1	1:D:570:PRO:HA	1.75	0.52
1:G:658:ILE:O	1:G:721:ILE:N	2.40	0.52
1:E:658:ILE:O	1:E:721:ILE:N	2.40	0.52
1:G:329:ASN:HD22	1:G:363:ASN:HB3	1.75	0.52
1:I:806:VAL:HG22	1:I:860:ILE:HG12	1.92	0.52
1:K:540:ASP:OD2	1:K:542:THR:OG1	2.24	0.52
1:M:540:ASP:OD2	1:M:542:THR:OG1	2.24	0.52
1:B:815:PHE:CE1	1:B:857:LYS:HD2	2.45	0.52
1:H:413:VAL:HG22	1:H:414:LEU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:341:VAL:HG11	1:I:710:GLU:HG2	1.92	0.52
1:I:413:VAL:HG22	1:I:414:LEU:O	2.10	0.52
1:J:551:ILE:HD13	1:J:613:ILE:HD11	1.90	0.52
1:J:806:VAL:HG22	1:J:860:ILE:HG12	1.92	0.52
1:K:413:VAL:HG22	1:K:414:LEU:O	2.10	0.52
1:L:715:GLU:HB2	1:L:718:SER:HB3	1.92	0.52
1:A:565:TYR:HD1	1:A:570:PRO:HA	1.75	0.52
1:C:329:ASN:HD22	1:C:363:ASN:HB3	1.75	0.52
1:E:299:ILE:O	1:E:398:THR:OG1	2.28	0.52
1:E:875:VAL:O	1:E:875:VAL:HG12	2.10	0.52
1:H:341:VAL:HG11	1:H:710:GLU:HG2	1.92	0.51
1:J:413:VAL:HG22	1:J:414:LEU:O	2.10	0.51
1:J:491:ASN:HB2	1:J:495:GLN:HB2	1.91	0.51
1:L:413:VAL:HG22	1:L:414:LEU:O	2.10	0.51
1:M:715:GLU:HB2	1:M:718:SER:HB3	1.93	0.51
1:A:657:LYS:HE2	1:A:722:GLU:HG2	1.93	0.51
1:A:815:PHE:CE1	1:A:857:LYS:HD2	2.45	0.51
1:B:299:ILE:O	1:B:398:THR:OG1	2.28	0.51
1:B:329:ASN:HD22	1:B:363:ASN:HB3	1.75	0.51
1:E:329:ASN:HD22	1:E:363:ASN:HB3	1.75	0.51
1:H:521:THR:H	1:H:615:THR:HG23	1.75	0.51
1:I:805:ARG:HG3	1:I:820:THR:OG1	2.10	0.51
1:J:573:GLU:HB3	1:J:600:ILE:HD12	1.91	0.51
1:K:573:GLU:HB3	1:K:600:ILE:HD12	1.91	0.51
1:N:680:THR:O	1:N:680:THR:OG1	2.23	0.51
1:A:875:VAL:O	1:A:875:VAL:HG12	2.10	0.51
1:B:875:VAL:O	1:B:875:VAL:HG12	2.11	0.51
1:E:657:LYS:HE2	1:E:722:GLU:HG2	1.92	0.51
1:G:503:TRP:O	1:G:507:ILE:HG12	2.09	0.51
1:H:454:GLN:HG3	1:H:455:PHE:CD1	2.46	0.51
1:J:805:ARG:HG3	1:J:820:THR:OG1	2.10	0.51
1:L:806:VAL:HG22	1:L:860:ILE:HG12	1.92	0.51
1:M:454:GLN:HG3	1:M:455:PHE:CD1	2.46	0.51
1:M:491:ASN:HB2	1:M:495:GLN:HB2	1.91	0.51
1:N:573:GLU:HB3	1:N:600:ILE:HD12	1.91	0.51
1:N:715:GLU:HB2	1:N:718:SER:HB3	1.93	0.51
1:B:657:LYS:HE2	1:B:722:GLU:HG2	1.93	0.51
1:D:657:LYS:HE2	1:D:722:GLU:HG2	1.93	0.51
1:I:521:THR:H	1:I:615:THR:HG23	1.75	0.51
1:K:577:GLU:HB2	1:K:614:LYS:HB3	1.93	0.51
1:K:822:ASP:OD1	1:K:822:ASP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:805:ARG:HG3	1:M:820:THR:OG1	2.10	0.51
1:C:565:TYR:HD1	1:C:570:PRO:HA	1.75	0.51
1:D:875:VAL:HG12	1:D:875:VAL:O	2.11	0.51
1:E:468:LYS:O	1:E:472:ALA:N	2.44	0.51
1:F:565:TYR:HD1	1:F:570:PRO:HA	1.75	0.51
1:L:491:ASN:HB2	1:L:495:GLN:HB2	1.91	0.51
1:L:577:GLU:HB2	1:L:614:LYS:HB3	1.93	0.51
1:N:413:VAL:HG22	1:N:414:LEU:O	2.10	0.51
1:N:806:VAL:HG22	1:N:860:ILE:HG12	1.92	0.51
1:C:657:LYS:HE2	1:C:722:GLU:HG2	1.93	0.51
1:C:875:VAL:O	1:C:875:VAL:HG12	2.10	0.51
1:D:329:ASN:HD22	1:D:363:ASN:HB3	1.75	0.51
1:E:291:ASP:OD1	1:E:553:LYS:NZ	2.28	0.51
1:F:875:VAL:O	1:F:875:VAL:HG12	2.11	0.51
1:G:468:LYS:O	1:G:472:ALA:N	2.44	0.51
1:G:565:TYR:HD1	1:G:570:PRO:HA	1.75	0.51
1:G:657:LYS:HE2	1:G:722:GLU:HG2	1.93	0.51
1:H:715:GLU:HB2	1:H:718:SER:HB3	1.93	0.51
1:I:577:GLU:HB2	1:I:614:LYS:HB3	1.93	0.51
1:J:521:THR:H	1:J:615:THR:HG23	1.75	0.51
1:J:822:ASP:OD1	1:J:822:ASP:N	2.43	0.51
1:K:407:THR:O	1:K:407:THR:OG1	2.29	0.51
1:K:805:ARG:HG3	1:K:820:THR:OG1	2.10	0.51
1:M:521:THR:H	1:M:615:THR:HG23	1.75	0.51
1:N:805:ARG:HG3	1:N:820:THR:OG1	2.10	0.51
1:A:329:ASN:HD22	1:A:363:ASN:HB3	1.75	0.51
1:C:815:PHE:CE1	1:C:857:LYS:HD2	2.45	0.51
1:D:592:LEU:O	1:D:598:LYS:NZ	2.29	0.51
1:F:657:LYS:HE2	1:F:722:GLU:HG2	1.93	0.51
1:G:875:VAL:O	1:G:875:VAL:HG12	2.11	0.51
1:H:806:VAL:HG22	1:H:860:ILE:HG12	1.92	0.51
1:L:454:GLN:HG3	1:L:455:PHE:CD1	2.46	0.51
1:N:540:ASP:OD2	1:N:542:THR:OG1	2.24	0.51
1:A:468:LYS:O	1:A:472:ALA:N	2.44	0.51
1:J:540:ASP:OD2	1:J:542:THR:OG1	2.24	0.51
1:J:577:GLU:HB2	1:J:614:LYS:HB3	1.93	0.51
1:K:715:GLU:HB2	1:K:718:SER:HB3	1.93	0.51
1:K:806:VAL:HG22	1:K:860:ILE:HG12	1.91	0.51
1:K:812:TYR:O	1:K:813:SER:OG	2.28	0.51
1:L:407:THR:O	1:L:407:THR:OG1	2.29	0.51
1:B:468:LYS:O	1:B:472:ALA:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:TYR:HD1	1:B:570:PRO:HA	1.75	0.51
1:E:565:TYR:HD1	1:E:570:PRO:HA	1.75	0.51
1:H:805:ARG:HG3	1:H:820:THR:OG1	2.10	0.51
1:K:491:ASN:HB2	1:K:495:GLN:HB2	1.91	0.51
1:L:822:ASP:OD1	1:L:822:ASP:N	2.43	0.51
1:F:299:ILE:O	1:F:398:THR:OG1	2.28	0.51
1:F:633:SER:OG	1:F:654:THR:OG1	2.09	0.51
1:I:311:THR:O	1:I:311:THR:OG1	2.24	0.51
1:I:407:THR:O	1:I:407:THR:OG1	2.29	0.51
1:K:345:TYR:CD2	1:K:706:LYS:HB3	2.46	0.51
1:K:454:GLN:HG3	1:K:455:PHE:CD1	2.46	0.51
1:L:805:ARG:HG3	1:L:820:THR:OG1	2.10	0.51
1:D:468:LYS:O	1:D:472:ALA:N	2.44	0.51
1:F:269:ASP:OD2	1:F:269:ASP:N	2.44	0.51
1:F:664:LYS:HB3	1:F:667:LYS:HD3	1.93	0.51
1:H:577:GLU:HB2	1:H:614:LYS:HB3	1.93	0.50
1:H:822:ASP:OD1	1:H:822:ASP:N	2.43	0.50
1:I:454:GLN:HG3	1:I:455:PHE:CD1	2.46	0.50
1:I:822:ASP:OD1	1:I:822:ASP:N	2.43	0.50
1:L:345:TYR:CD2	1:L:706:LYS:HB3	2.46	0.50
1:L:521:THR:H	1:L:615:THR:HG23	1.75	0.50
1:M:490:LYS:HE2	1:N:509:GLN:HE22	1.76	0.50
1:N:345:TYR:CD2	1:N:706:LYS:HB3	2.46	0.50
1:N:822:ASP:OD1	1:N:822:ASP:N	2.43	0.50
1:A:639:ASN:O	1:A:646:SER:HA	2.12	0.50
1:B:639:ASN:O	1:B:646:SER:HA	2.12	0.50
1:C:468:LYS:O	1:C:472:ALA:N	2.44	0.50
1:F:329:ASN:HD22	1:F:363:ASN:HB3	1.75	0.50
1:M:413:VAL:HG22	1:M:414:LEU:O	2.10	0.50
1:M:651:ASN:OD1	1:M:730:THR:N	2.25	0.50
1:N:454:GLN:HG3	1:N:455:PHE:CD1	2.46	0.50
1:E:664:LYS:HB3	1:E:667:LYS:HD3	1.94	0.50
1:F:639:ASN:O	1:F:646:SER:HA	2.12	0.50
1:J:454:GLN:HG3	1:J:455:PHE:CD1	2.46	0.50
1:L:311:THR:O	1:L:311:THR:OG1	2.24	0.50
1:M:345:TYR:CD2	1:M:706:LYS:HB3	2.46	0.50
1:N:793:THR:O	1:N:793:THR:OG1	2.18	0.50
1:B:636:ASN:O	1:B:637:THR:HB	2.12	0.50
1:D:658:ILE:O	1:D:721:ILE:N	2.40	0.50
1:D:664:LYS:HB3	1:D:667:LYS:HD3	1.94	0.50
1:E:358:SER:OG	1:E:359:HIS:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:637:THR:O	1:E:639:ASN:N	2.45	0.50
1:F:468:LYS:O	1:F:472:ALA:N	2.44	0.50
1:F:637:THR:O	1:F:639:ASN:N	2.45	0.50
1:G:391:ALA:O	1:G:449:LEU:N	2.41	0.50
1:H:345:TYR:CD2	1:H:706:LYS:HB3	2.46	0.50
1:H:638:THR:HG22	1:H:638:THR:O	2.12	0.50
1:I:680:THR:O	1:I:680:THR:OG1	2.23	0.50
1:J:499:GLU:OE1	1:J:499:GLU:HA	2.12	0.50
1:K:499:GLU:OE1	1:K:499:GLU:HA	2.12	0.50
1:N:577:GLU:HB2	1:N:614:LYS:HB3	1.93	0.50
1:A:642:GLY:C	1:A:644:GLN:H	2.14	0.50
1:D:533:LYS:NZ	1:D:542:THR:O	2.32	0.50
1:G:466:GLN:O	1:G:470:LEU:HD12	2.12	0.50
1:G:636:ASN:O	1:G:637:THR:HB	2.12	0.50
1:I:638:THR:O	1:I:638:THR:HG22	2.12	0.50
1:M:361:THR:O	1:M:361:THR:OG1	2.22	0.50
1:N:311:THR:O	1:N:311:THR:OG1	2.24	0.50
1:A:276:LYS:NZ	1:A:289:ALA:O	2.43	0.50
1:A:466:GLN:O	1:A:470:LEU:HD12	2.12	0.50
1:B:269:ASP:OD2	1:B:269:ASP:N	2.44	0.50
1:B:466:GLN:O	1:B:470:LEU:HD12	2.12	0.50
1:B:655:LYS:HG2	1:B:724:THR:HA	1.93	0.50
1:C:637:THR:O	1:C:639:ASN:N	2.45	0.50
1:C:664:LYS:HB3	1:C:667:LYS:HD3	1.94	0.50
1:G:269:ASP:OD2	1:G:269:ASP:N	2.44	0.50
1:I:410:THR:HA	1:I:480:THR:HA	1.94	0.50
1:K:410:THR:HA	1:K:480:THR:HA	1.94	0.50
1:M:577:GLU:HB2	1:M:614:LYS:HB3	1.93	0.50
1:A:666:TYR:CD1	1:A:714:THR:HG22	2.47	0.50
1:B:637:THR:O	1:B:639:ASN:N	2.45	0.50
1:C:670:VAL:HG23	1:C:741:LEU:HD13	1.94	0.50
1:F:358:SER:OG	1:F:359:HIS:N	2.42	0.50
1:F:466:GLN:O	1:F:470:LEU:HD12	2.12	0.50
1:G:639:ASN:O	1:G:646:SER:HA	2.11	0.50
1:G:664:LYS:HB3	1:G:667:LYS:HD3	1.94	0.50
1:I:499:GLU:OE1	1:I:499:GLU:HA	2.12	0.50
1:J:345:TYR:CD2	1:J:706:LYS:HB3	2.46	0.50
1:J:410:THR:HA	1:J:480:THR:HA	1.94	0.50
1:L:809:THR:HG22	1:L:815:PHE:HD1	1.77	0.50
1:N:638:THR:HG22	1:N:638:THR:O	2.12	0.50
1:A:269:ASP:OD2	1:A:269:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LYS:NZ	1:B:289:ALA:O	2.43	0.50
1:B:389:ILE:O	1:B:459:LEU:HD22	2.12	0.50
1:B:445:SER:O	1:B:445:SER:OG	2.20	0.50
1:B:670:VAL:HG23	1:B:741:LEU:HD13	1.94	0.50
1:C:389:ILE:O	1:C:459:LEU:HD22	2.12	0.50
1:C:636:ASN:O	1:C:637:THR:HB	2.12	0.50
1:F:445:SER:O	1:F:445:SER:OG	2.20	0.50
1:G:642:GLY:C	1:G:644:GLN:H	2.14	0.50
1:H:407:THR:O	1:H:407:THR:OG1	2.29	0.50
1:H:809:THR:HG22	1:H:815:PHE:HD1	1.77	0.50
1:I:358:SER:O	1:I:359:HIS:CG	2.65	0.50
1:N:521:THR:H	1:N:615:THR:HG23	1.75	0.50
1:B:666:TYR:CD1	1:B:714:THR:HG22	2.47	0.50
1:C:639:ASN:O	1:C:646:SER:HA	2.11	0.50
1:G:666:TYR:CD1	1:G:714:THR:HG22	2.47	0.50
1:I:345:TYR:CD2	1:I:706:LYS:HB3	2.46	0.50
1:K:450:ASN:O	1:K:451:THR:OG1	2.22	0.50
1:L:358:SER:O	1:L:359:HIS:CG	2.65	0.50
1:L:651:ASN:OD1	1:L:730:THR:N	2.25	0.50
1:A:655:LYS:HG2	1:A:724:THR:HA	1.93	0.50
1:B:533:LYS:NZ	1:B:542:THR:O	2.32	0.50
1:D:389:ILE:O	1:D:459:LEU:HD22	2.12	0.50
1:E:389:ILE:O	1:E:459:LEU:HD22	2.12	0.50
1:E:639:ASN:O	1:E:646:SER:HA	2.11	0.50
1:F:391:ALA:O	1:F:449:LEU:N	2.41	0.50
1:H:325:ARG:HD3	1:H:369:ASP:HB2	1.94	0.49
1:H:358:SER:O	1:H:359:HIS:CG	2.65	0.49
1:J:638:THR:O	1:J:638:THR:HG22	2.12	0.49
1:L:410:THR:HA	1:L:480:THR:HA	1.94	0.49
1:A:637:THR:O	1:A:639:ASN:N	2.45	0.49
1:B:642:GLY:C	1:B:644:GLN:H	2.14	0.49
1:B:778:THR:OG1	1:B:778:THR:O	2.30	0.49
1:C:655:LYS:HG2	1:C:724:THR:HA	1.93	0.49
1:D:637:THR:O	1:D:639:ASN:N	2.45	0.49
1:D:642:GLY:C	1:D:644:GLN:H	2.14	0.49
1:E:466:GLN:O	1:E:470:LEU:HD12	2.12	0.49
1:F:636:ASN:O	1:F:637:THR:HB	2.12	0.49
1:F:666:TYR:CD1	1:F:714:THR:HG22	2.47	0.49
1:G:581:ASP:OD2	1:G:610:ASN:ND2	2.32	0.49
1:H:775:ASN:O	1:H:777:SER:N	2.41	0.49
1:I:325:ARG:HD3	1:I:369:ASP:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:715:GLU:HB2	1:I:718:SER:HB3	1.93	0.49
1:J:325:ARG:HD3	1:J:369:ASP:HB2	1.94	0.49
1:J:715:GLU:HB2	1:J:718:SER:HB3	1.93	0.49
1:M:638:THR:O	1:M:638:THR:HG22	2.12	0.49
1:N:358:SER:O	1:N:359:HIS:CG	2.65	0.49
1:N:812:TYR:O	1:N:813:SER:OG	2.28	0.49
1:C:276:LYS:NZ	1:C:289:ALA:O	2.43	0.49
1:D:639:ASN:O	1:D:646:SER:HA	2.11	0.49
1:F:581:ASP:OD2	1:F:610:ASN:ND2	2.32	0.49
1:F:655:LYS:HG2	1:F:724:THR:HA	1.93	0.49
1:G:668:ARG:HB3	1:G:712:GLU:HG2	1.95	0.49
1:K:638:THR:HG22	1:K:638:THR:O	2.12	0.49
1:M:407:THR:O	1:M:407:THR:OG1	2.29	0.49
1:N:809:THR:HG22	1:N:815:PHE:HD1	1.77	0.49
1:A:778:THR:O	1:A:778:THR:OG1	2.30	0.49
1:B:664:LYS:HB3	1:B:667:LYS:HD3	1.93	0.49
1:D:260:ASN:OD1	1:D:261:TYR:N	2.45	0.49
1:D:670:VAL:HG23	1:D:741:LEU:HD13	1.94	0.49
1:G:778:THR:OG1	1:G:778:THR:O	2.30	0.49
1:J:809:THR:HG22	1:J:815:PHE:HD1	1.77	0.49
1:M:410:THR:HA	1:M:480:THR:HA	1.94	0.49
1:M:809:THR:HG22	1:M:815:PHE:HD1	1.77	0.49
1:A:668:ARG:HB3	1:A:712:GLU:HG2	1.94	0.49
1:C:466:GLN:O	1:C:470:LEU:HD12	2.12	0.49
1:D:276:LYS:NZ	1:D:289:ALA:O	2.43	0.49
1:E:655:LYS:HG2	1:E:724:THR:HA	1.93	0.49
1:E:839:TYR:CE2	1:E:841:ASN:HB3	2.48	0.49
1:F:581:ASP:OD1	1:F:584:THR:OG1	2.27	0.49
1:F:668:ARG:HB3	1:F:712:GLU:HG2	1.94	0.49
1:J:358:SER:O	1:J:359:HIS:CG	2.65	0.49
1:J:812:TYR:O	1:J:813:SER:OG	2.28	0.49
1:M:269:ASP:N	1:M:269:ASP:OD1	2.46	0.49
1:M:358:SER:O	1:M:359:HIS:CG	2.65	0.49
1:A:389:ILE:O	1:A:459:LEU:HD22	2.12	0.49
1:A:664:LYS:HB3	1:A:667:LYS:HD3	1.93	0.49
1:D:839:TYR:CE2	1:D:841:ASN:HB3	2.48	0.49
1:F:642:GLY:C	1:F:644:GLN:H	2.14	0.49
1:F:839:TYR:CE2	1:F:841:ASN:HB3	2.48	0.49
1:H:410:THR:HA	1:H:480:THR:HA	1.94	0.49
1:J:775:ASN:O	1:J:777:SER:N	2.41	0.49
1:K:325:ARG:HD3	1:K:369:ASP:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:358:SER:O	1:K:359:HIS:CG	2.65	0.49
1:N:325:ARG:HD3	1:N:369:ASP:HB2	1.94	0.49
1:A:636:ASN:O	1:A:637:THR:HB	2.12	0.49
1:A:670:VAL:HG23	1:A:741:LEU:HD13	1.94	0.49
1:C:668:ARG:HB3	1:C:712:GLU:HG2	1.94	0.49
1:D:666:TYR:CD1	1:D:714:THR:HG22	2.47	0.49
1:E:260:ASN:OD1	1:E:261:TYR:N	2.45	0.49
1:E:269:ASP:N	1:E:269:ASP:OD2	2.44	0.49
1:G:260:ASN:OD1	1:G:261:TYR:N	2.45	0.49
1:G:660:MET:HG3	1:G:717:ASP:HA	1.95	0.49
1:H:509:GLN:HE21	1:N:283:LYS:CG	2.26	0.49
1:I:809:THR:HG22	1:I:815:PHE:HD1	1.77	0.49
1:L:774:PHE:HB2	1:E:774:PHE:CG	2.48	0.49
1:N:499:GLU:OE1	1:N:499:GLU:HA	2.12	0.49
1:C:269:ASP:OD2	1:C:269:ASP:N	2.44	0.49
1:E:666:TYR:CD1	1:E:714:THR:HG22	2.47	0.49
1:E:670:VAL:HG23	1:E:741:LEU:HD13	1.94	0.49
1:F:576:VAL:HG12	1:F:615:THR:HA	1.95	0.49
1:G:389:ILE:O	1:G:459:LEU:HD22	2.12	0.49
1:G:576:VAL:HG12	1:G:615:THR:HA	1.95	0.49
1:G:637:THR:O	1:G:639:ASN:N	2.45	0.49
1:H:493:SER:O	1:H:493:SER:OG	2.31	0.49
1:I:655:LYS:HG3	1:I:724:THR:HG22	1.95	0.49
1:I:866:ASP:N	1:I:866:ASP:OD1	2.46	0.49
1:J:655:LYS:HG3	1:J:724:THR:HG22	1.95	0.49
1:N:240:LEU:O	1:N:274:TYR:OH	2.17	0.49
1:N:410:THR:HA	1:N:480:THR:HA	1.94	0.49
1:B:576:VAL:HG12	1:B:615:THR:HA	1.95	0.49
1:B:581:ASP:OD1	1:B:584:THR:OG1	2.27	0.49
1:C:260:ASN:OD1	1:C:261:TYR:N	2.45	0.49
1:D:636:ASN:O	1:D:637:THR:HB	2.12	0.49
1:F:260:ASN:OD1	1:F:261:TYR:N	2.45	0.49
1:H:866:ASP:OD1	1:H:866:ASP:N	2.46	0.49
1:J:376:ASN:HB3	1:J:750:GLU:HG2	1.95	0.49
1:K:357:TYR:HE1	1:K:612:LEU:HB2	1.78	0.49
1:K:376:ASN:HB3	1:K:750:GLU:HG2	1.95	0.49
1:K:643:LEU:O	1:K:644:GLN:HG3	2.13	0.49
1:K:809:THR:HG22	1:K:815:PHE:HD1	1.77	0.49
1:L:357:TYR:HE1	1:L:612:LEU:HB2	1.78	0.49
1:L:638:THR:O	1:L:638:THR:HG22	2.12	0.49
1:A:260:ASN:OD1	1:A:261:TYR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:839:TYR:CE2	1:B:841:ASN:HB3	2.48	0.49
1:C:666:TYR:CD1	1:C:714:THR:HG22	2.47	0.49
1:C:839:TYR:CE2	1:C:841:ASN:HB3	2.48	0.49
1:E:636:ASN:O	1:E:637:THR:HB	2.12	0.49
1:E:778:THR:OG1	1:E:778:THR:O	2.30	0.49
1:F:660:MET:HG3	1:F:717:ASP:HA	1.95	0.49
1:L:499:GLU:OE1	1:L:499:GLU:HA	2.12	0.49
1:L:675:SER:HB2	1:L:707:PHE:HE1	1.78	0.49
1:M:822:ASP:OD1	1:M:822:ASP:N	2.43	0.49
1:N:269:ASP:OD1	1:N:269:ASP:N	2.46	0.49
1:N:637:THR:O	1:N:639:ASN:N	2.46	0.49
1:B:260:ASN:OD1	1:B:261:TYR:N	2.45	0.49
1:D:454:GLN:HE21	1:E:458:ARG:HG3	1.76	0.49
1:D:466:GLN:O	1:D:470:LEU:HD12	2.12	0.49
1:F:389:ILE:O	1:F:459:LEU:HD22	2.12	0.49
1:G:655:LYS:HG2	1:G:724:THR:HA	1.93	0.49
1:I:376:ASN:HB3	1:I:750:GLU:HG2	1.95	0.48
1:J:866:ASP:OD1	1:J:866:ASP:N	2.46	0.48
1:K:391:ALA:HB3	1:K:449:LEU:HD12	1.96	0.48
1:L:521:THR:O	1:L:521:THR:HG23	2.13	0.48
1:L:637:THR:O	1:L:639:ASN:N	2.46	0.48
1:M:637:THR:O	1:M:639:ASN:N	2.46	0.48
1:A:576:VAL:HG12	1:A:615:THR:HA	1.95	0.48
1:A:660:MET:HG3	1:A:717:ASP:HA	1.95	0.48
1:D:576:VAL:HG12	1:D:615:THR:HA	1.95	0.48
1:D:667:LYS:HG3	1:D:742:ASN:O	2.13	0.48
1:D:668:ARG:HB3	1:D:712:GLU:HG2	1.94	0.48
1:E:668:ARG:HB3	1:E:712:GLU:HG2	1.94	0.48
1:F:778:THR:O	1:F:778:THR:OG1	2.30	0.48
1:H:643:LEU:O	1:H:644:GLN:HG3	2.13	0.48
1:H:812:TYR:O	1:H:813:SER:OG	2.28	0.48
1:I:540:ASP:OD2	1:I:542:THR:OG1	2.24	0.48
1:K:655:LYS:HG3	1:K:724:THR:HG22	1.95	0.48
1:N:521:THR:HG23	1:N:521:THR:O	2.13	0.48
1:N:643:LEU:O	1:N:644:GLN:HG3	2.13	0.48
1:N:864:THR:OG1	1:N:868:ARG:O	2.25	0.48
1:N:866:ASP:N	1:N:866:ASP:OD1	2.46	0.48
1:A:286:LYS:HB3	1:A:288:GLU:HG2	1.96	0.48
1:A:839:TYR:CE2	1:A:841:ASN:HB3	2.48	0.48
1:C:576:VAL:HG12	1:C:615:THR:HA	1.95	0.48
1:E:667:LYS:HG3	1:E:742:ASN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:LYS:HB3	1:F:288:GLU:HG2	1.96	0.48
1:G:286:LYS:HB3	1:G:288:GLU:HG2	1.96	0.48
1:H:391:ALA:HB3	1:H:449:LEU:HD12	1.96	0.48
1:H:637:THR:O	1:H:639:ASN:N	2.46	0.48
1:I:813:SER:OG	1:I:813:SER:O	2.31	0.48
1:L:643:LEU:O	1:L:644:GLN:HG3	2.13	0.48
1:M:499:GLU:HA	1:M:499:GLU:OE1	2.12	0.48
1:M:675:SER:HB2	1:M:707:PHE:HE1	1.78	0.48
1:N:407:THR:O	1:N:407:THR:OG1	2.29	0.48
1:A:658:ILE:HB	1:A:721:ILE:HB	1.96	0.48
1:B:286:LYS:HB3	1:B:288:GLU:HG2	1.95	0.48
1:C:642:GLY:C	1:C:644:GLN:H	2.14	0.48
1:D:655:LYS:HG2	1:D:724:THR:HA	1.93	0.48
1:E:567:ASN:OD1	1:E:569:ILE:HG12	2.14	0.48
1:F:408:PRO:HD2	1:F:424:ALA:HB2	1.95	0.48
1:G:299:ILE:O	1:G:398:THR:OG1	2.28	0.48
1:G:658:ILE:HB	1:G:721:ILE:HB	1.96	0.48
1:K:345:TYR:CD1	1:K:350:THR:HA	2.49	0.48
1:K:521:THR:HG23	1:K:521:THR:O	2.13	0.48
1:M:325:ARG:HD3	1:M:369:ASP:HB2	1.94	0.48
1:N:357:TYR:HE1	1:N:612:LEU:HB2	1.78	0.48
1:N:391:ALA:HB3	1:N:449:LEU:HD12	1.96	0.48
1:N:775:ASN:O	1:N:777:SER:N	2.41	0.48
1:B:658:ILE:HB	1:B:721:ILE:HB	1.96	0.48
1:D:581:ASP:OD1	1:D:584:THR:OG1	2.27	0.48
1:E:286:LYS:HB3	1:E:288:GLU:HG2	1.96	0.48
1:E:576:VAL:HG12	1:E:615:THR:HA	1.95	0.48
1:F:567:ASN:OD1	1:F:569:ILE:HG12	2.14	0.48
1:F:670:VAL:HG23	1:F:741:LEU:HD13	1.94	0.48
1:G:670:VAL:HG23	1:G:741:LEU:HD13	1.94	0.48
1:G:839:TYR:CE2	1:G:841:ASN:HB3	2.48	0.48
1:H:499:GLU:OE1	1:H:499:GLU:HA	2.12	0.48
1:J:494:GLY:CA	1:K:265:ASN:HD21	2.20	0.48
1:J:643:LEU:O	1:J:644:GLN:HG3	2.13	0.48
1:K:269:ASP:OD1	1:K:269:ASP:N	2.46	0.48
1:K:637:THR:O	1:K:639:ASN:N	2.46	0.48
1:L:325:ARG:HD3	1:L:369:ASP:HB2	1.94	0.48
1:M:643:LEU:O	1:M:644:GLN:HG3	2.13	0.48
1:M:812:TYR:O	1:M:813:SER:OG	2.28	0.48
1:N:675:SER:HB2	1:N:707:PHE:HE1	1.78	0.48
1:A:667:LYS:HG3	1:A:742:ASN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:667:LYS:HG3	1:B:742:ASN:O	2.13	0.48
1:D:240:LEU:HD23	1:D:240:LEU:HA	1.75	0.48
1:E:408:PRO:HD2	1:E:424:ALA:HB2	1.95	0.48
1:F:450:ASN:HD22	1:F:456:SER:HB2	1.79	0.48
1:H:675:SER:HB2	1:H:707:PHE:HE1	1.78	0.48
1:I:675:SER:HB2	1:I:707:PHE:HE1	1.78	0.48
1:J:391:ALA:HB3	1:J:449:LEU:HD12	1.96	0.48
1:K:675:SER:HB2	1:K:707:PHE:HE1	1.78	0.48
1:L:391:ALA:HB3	1:L:449:LEU:HD12	1.96	0.48
1:A:567:ASN:OD1	1:A:569:ILE:HG12	2.14	0.48
1:E:642:GLY:C	1:E:644:GLN:H	2.14	0.48
1:G:408:PRO:HD2	1:G:424:ALA:HB2	1.95	0.48
1:H:345:TYR:CD1	1:H:350:THR:HA	2.49	0.48
1:I:345:TYR:CD1	1:I:350:THR:HA	2.49	0.48
1:I:391:ALA:HB3	1:I:449:LEU:HD12	1.96	0.48
1:L:345:TYR:CD1	1:L:350:THR:HA	2.49	0.48
1:N:345:TYR:CD1	1:N:350:THR:HA	2.49	0.48
1:N:655:LYS:HG3	1:N:724:THR:HG22	1.95	0.48
1:B:660:MET:HG3	1:B:717:ASP:HA	1.95	0.48
1:C:403:MET:HG2	1:C:406:VAL:HG22	1.96	0.48
1:D:403:MET:HG2	1:D:406:VAL:HG22	1.96	0.48
1:E:403:MET:HG2	1:E:406:VAL:HG22	1.96	0.48
1:F:403:MET:HG2	1:F:406:VAL:HG22	1.96	0.48
1:H:363:ASN:O	1:H:478:LEU:N	2.47	0.48
1:I:812:TYR:O	1:I:813:SER:OG	2.28	0.48
1:J:357:TYR:HE1	1:J:612:LEU:HB2	1.78	0.48
1:J:637:THR:O	1:J:639:ASN:N	2.46	0.48
1:L:376:ASN:HB3	1:L:750:GLU:HG2	1.95	0.48
1:M:357:TYR:HE1	1:M:612:LEU:HB2	1.78	0.48
1:C:667:LYS:HG3	1:C:742:ASN:O	2.13	0.48
1:E:433:LEU:HD23	1:E:433:LEU:HA	1.74	0.48
1:E:450:ASN:HD22	1:E:456:SER:HB2	1.79	0.48
1:G:567:ASN:OD1	1:G:569:ILE:HG12	2.14	0.48
1:H:655:LYS:HG3	1:H:724:THR:HG22	1.95	0.48
1:I:441:LYS:HB3	1:I:441:LYS:HE2	1.73	0.48
1:I:643:LEU:O	1:I:644:GLN:HG3	2.13	0.48
1:J:675:SER:HB2	1:J:707:PHE:HE1	1.78	0.48
1:M:345:TYR:CD1	1:M:350:THR:HA	2.49	0.48
1:M:655:LYS:HG3	1:M:724:THR:HG22	1.95	0.48
1:A:305:GLU:CD	1:A:446:PRO:HG3	2.35	0.48
1:C:286:LYS:HB3	1:C:288:GLU:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:LYS:HB3	1:D:288:GLU:HG2	1.96	0.48
1:D:352:ASN:OD1	1:D:352:ASN:N	2.47	0.48
1:F:533:LYS:NZ	1:F:542:THR:O	2.32	0.48
1:H:357:TYR:HE1	1:H:612:LEU:HB2	1.78	0.48
1:H:521:THR:HG23	1:H:521:THR:O	2.13	0.48
1:J:521:THR:HG23	1:J:521:THR:O	2.13	0.48
1:K:866:ASP:N	1:K:866:ASP:OD1	2.46	0.48
1:M:521:THR:HG23	1:M:521:THR:O	2.13	0.48
1:B:668:ARG:HB3	1:B:712:GLU:HG2	1.94	0.48
1:C:352:ASN:N	1:C:352:ASN:OD1	2.47	0.48
1:F:668:ARG:NH2	1:F:710:GLU:OE1	2.47	0.48
1:G:352:ASN:OD1	1:G:352:ASN:N	2.47	0.48
1:G:780:ASN:O	1:G:781:THR:OG1	2.31	0.48
1:H:376:ASN:HB3	1:H:750:GLU:HG2	1.95	0.47
1:H:771:ASP:O	1:H:784:ASN:HB2	2.15	0.47
1:L:363:ASN:O	1:L:478:LEU:N	2.47	0.47
1:L:655:LYS:HG3	1:L:724:THR:HG22	1.95	0.47
1:L:866:ASP:OD1	1:L:866:ASP:N	2.46	0.47
1:M:778:THR:OG1	1:M:778:THR:O	2.32	0.47
1:A:775:ASN:O	1:A:777:SER:N	2.42	0.47
1:B:567:ASN:OD1	1:B:569:ILE:HG12	2.14	0.47
1:C:408:PRO:HD2	1:C:424:ALA:HB2	1.95	0.47
1:D:567:ASN:OD1	1:D:569:ILE:HG12	2.14	0.47
1:D:658:ILE:HB	1:D:721:ILE:HB	1.96	0.47
1:E:660:MET:HG3	1:E:717:ASP:HA	1.95	0.47
1:F:276:LYS:NZ	1:F:289:ALA:O	2.43	0.47
1:F:667:LYS:HG3	1:F:742:ASN:O	2.13	0.47
1:G:403:MET:HG2	1:G:406:VAL:HG22	1.96	0.47
1:I:637:THR:O	1:I:639:ASN:N	2.46	0.47
1:K:771:ASP:O	1:K:784:ASN:HB2	2.14	0.47
1:M:389:ILE:HB	1:M:460:ILE:HB	1.96	0.47
1:M:391:ALA:HB3	1:M:449:LEU:HD12	1.96	0.47
1:M:680:THR:O	1:M:680:THR:OG1	2.23	0.47
1:M:775:ASN:O	1:M:777:SER:N	2.41	0.47
1:N:363:ASN:O	1:N:478:LEU:N	2.47	0.47
1:N:389:ILE:HB	1:N:460:ILE:HB	1.96	0.47
1:A:685:ILE:HG23	1:A:696:ASP:O	2.15	0.47
1:B:403:MET:HG2	1:B:406:VAL:HG22	1.96	0.47
1:C:660:MET:HG3	1:C:717:ASP:HA	1.95	0.47
1:D:269:ASP:OD2	1:D:269:ASP:N	2.44	0.47
1:D:660:MET:HG3	1:D:717:ASP:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:305:GLU:CD	1:G:446:PRO:HG3	2.35	0.47
1:G:450:ASN:HD22	1:G:456:SER:HB2	1.79	0.47
1:H:813:SER:OG	1:H:813:SER:O	2.31	0.47
1:I:357:TYR:HE1	1:I:612:LEU:HB2	1.78	0.47
1:I:363:ASN:O	1:I:478:LEU:N	2.47	0.47
1:L:811:GLN:HA	1:L:853:MET:HE3	1.96	0.47
1:M:771:ASP:O	1:M:784:ASN:HB2	2.15	0.47
1:M:866:ASP:OD1	1:M:866:ASP:N	2.46	0.47
1:A:408:PRO:HD2	1:A:424:ALA:HB2	1.95	0.47
1:A:450:ASN:HD22	1:A:456:SER:HB2	1.79	0.47
1:B:670:VAL:HG22	1:B:710:GLU:HB3	1.97	0.47
1:C:305:GLU:CD	1:C:446:PRO:HG3	2.35	0.47
1:E:305:GLU:CD	1:E:446:PRO:HG3	2.35	0.47
1:E:658:ILE:HB	1:E:721:ILE:HB	1.96	0.47
1:G:668:ARG:NH2	1:G:710:GLU:OE1	2.47	0.47
1:H:642:GLY:C	1:H:644:GLN:H	2.18	0.47
1:I:345:TYR:CE2	1:I:706:LYS:HB3	2.50	0.47
1:I:521:THR:O	1:I:521:THR:HG23	2.13	0.47
1:K:231:GLU:HB3	1:K:261:TYR:HB3	1.97	0.47
1:K:329:ASN:HD22	1:K:363:ASN:HD21	1.62	0.47
1:K:363:ASN:O	1:K:478:LEU:N	2.47	0.47
1:K:381:ILE:O	1:K:382:ASN:ND2	2.47	0.47
1:M:813:SER:OG	1:M:813:SER:O	2.31	0.47
1:N:231:GLU:HB3	1:N:261:TYR:HB3	1.97	0.47
1:N:813:SER:OG	1:N:813:SER:O	2.31	0.47
1:A:299:ILE:O	1:A:398:THR:OG1	2.28	0.47
1:C:404:TYR:HE1	1:D:505:ASP:HA	1.79	0.47
1:C:816:LYS:HE2	1:C:816:LYS:HB3	1.66	0.47
1:D:408:PRO:HD2	1:D:424:ALA:HB2	1.95	0.47
1:D:866:ASP:OD2	1:D:868:ARG:NH1	2.48	0.47
1:E:816:LYS:HE2	1:E:816:LYS:HB3	1.66	0.47
1:F:224:ASP:OD1	1:F:224:ASP:N	2.41	0.47
1:F:305:GLU:CD	1:F:446:PRO:HG3	2.35	0.47
1:G:685:ILE:HG23	1:G:696:ASP:O	2.15	0.47
1:H:269:ASP:HA	1:H:510:ILE:HD11	1.97	0.47
1:I:269:ASP:HA	1:I:510:ILE:HD11	1.97	0.47
1:I:381:ILE:O	1:I:382:ASN:ND2	2.47	0.47
1:J:329:ASN:HD22	1:J:363:ASN:ND2	2.13	0.47
1:J:345:TYR:CD1	1:J:350:THR:HA	2.49	0.47
1:J:363:ASN:O	1:J:478:LEU:N	2.47	0.47
1:L:778:THR:O	1:L:778:THR:OG1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:269:ASP:HA	1:M:510:ILE:HD11	1.97	0.47
1:M:363:ASN:O	1:M:478:LEU:N	2.47	0.47
1:N:269:ASP:HA	1:N:510:ILE:HD11	1.97	0.47
1:N:376:ASN:HB3	1:N:750:GLU:HG2	1.95	0.47
1:N:778:THR:O	1:N:778:THR:OG1	2.32	0.47
1:A:670:VAL:HG22	1:A:710:GLU:HB3	1.97	0.47
1:B:305:GLU:CD	1:B:446:PRO:HG3	2.35	0.47
1:B:450:ASN:HD22	1:B:456:SER:HB2	1.79	0.47
1:D:450:ASN:HD22	1:D:456:SER:HB2	1.79	0.47
1:D:684:ILE:HD11	1:D:700:PRO:HG3	1.96	0.47
1:E:389:ILE:HB	1:E:460:ILE:HB	1.96	0.47
1:E:684:ILE:HD11	1:E:700:PRO:HG3	1.96	0.47
1:F:658:ILE:HB	1:F:721:ILE:HB	1.96	0.47
1:F:775:ASN:O	1:F:777:SER:N	2.42	0.47
1:G:866:ASP:OD2	1:G:868:ARG:NH1	2.48	0.47
1:H:269:ASP:N	1:H:269:ASP:OD1	2.46	0.47
1:H:389:ILE:HB	1:H:460:ILE:HB	1.97	0.47
1:J:852:ILE:O	1:J:852:ILE:HG22	2.15	0.47
1:L:269:ASP:HA	1:L:510:ILE:HD11	1.97	0.47
1:L:389:ILE:HB	1:L:460:ILE:HB	1.97	0.47
1:M:345:TYR:CE2	1:M:706:LYS:HB3	2.50	0.47
1:M:376:ASN:HB3	1:M:750:GLU:HG2	1.95	0.47
1:A:403:MET:HG2	1:A:406:VAL:HG22	1.96	0.47
1:B:866:ASP:OD2	1:B:868:ARG:NH1	2.48	0.47
1:C:685:ILE:HG23	1:C:696:ASP:O	2.15	0.47
1:D:685:ILE:HG23	1:D:696:ASP:O	2.15	0.47
1:E:670:VAL:HG22	1:E:710:GLU:HB3	1.97	0.47
1:E:866:ASP:OD2	1:E:868:ARG:NH1	2.48	0.47
1:H:231:GLU:HB3	1:H:261:TYR:HB3	1.97	0.47
1:H:345:TYR:HD1	1:H:350:THR:HA	1.79	0.47
1:I:503:TRP:O	1:I:507:ILE:HG12	2.15	0.47
1:I:790:PRO:HD3	1:I:837:THR:HG21	1.96	0.47
1:J:345:TYR:CE2	1:J:706:LYS:HB3	2.50	0.47
1:J:345:TYR:HD1	1:J:350:THR:HA	1.79	0.47
1:J:496:ILE:HB	1:K:506:TYR:CE1	2.50	0.47
1:J:503:TRP:O	1:J:507:ILE:HG12	2.15	0.47
1:J:642:GLY:C	1:J:644:GLN:H	2.18	0.47
1:K:329:ASN:HD22	1:K:363:ASN:ND2	2.13	0.47
1:K:345:TYR:HD1	1:K:350:THR:HA	1.79	0.47
1:K:389:ILE:HB	1:K:460:ILE:HB	1.96	0.47
1:K:503:TRP:O	1:K:507:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:642:GLY:C	1:K:644:GLN:H	2.18	0.47
1:K:790:PRO:HD3	1:K:837:THR:HG21	1.96	0.47
1:K:852:ILE:HG22	1:K:852:ILE:O	2.15	0.47
1:L:231:GLU:HB3	1:L:261:TYR:HB3	1.97	0.47
1:L:329:ASN:HD22	1:L:363:ASN:ND2	2.13	0.47
1:L:345:TYR:CE2	1:L:706:LYS:HB3	2.50	0.47
1:L:573:GLU:OE2	1:L:601:TYR:N	2.41	0.47
1:L:642:GLY:C	1:L:644:GLN:H	2.18	0.47
1:L:771:ASP:O	1:L:784:ASN:HB2	2.15	0.47
1:L:775:ASN:O	1:L:777:SER:N	2.41	0.47
1:L:790:PRO:HD3	1:L:837:THR:HG21	1.96	0.47
1:N:345:TYR:CE2	1:N:706:LYS:HB3	2.50	0.47
1:N:573:GLU:OE2	1:N:601:TYR:N	2.40	0.47
1:A:352:ASN:OD1	1:A:352:ASN:N	2.47	0.47
1:B:352:ASN:N	1:B:352:ASN:OD1	2.47	0.47
1:B:685:ILE:HG23	1:B:696:ASP:O	2.15	0.47
1:C:658:ILE:HB	1:C:721:ILE:HB	1.96	0.47
1:C:670:VAL:HG22	1:C:710:GLU:HB3	1.97	0.47
1:C:866:ASP:OD2	1:C:868:ARG:NH1	2.48	0.47
1:D:670:VAL:HG22	1:D:710:GLU:HB3	1.97	0.47
1:H:329:ASN:HD22	1:H:363:ASN:ND2	2.13	0.47
1:I:345:TYR:HD1	1:I:350:THR:HA	1.79	0.47
1:J:231:GLU:HB3	1:J:261:TYR:HB3	1.97	0.47
1:J:811:GLN:HA	1:J:853:MET:HE3	1.96	0.47
1:M:231:GLU:HB3	1:M:261:TYR:HB3	1.97	0.47
1:M:329:ASN:HD22	1:M:363:ASN:ND2	2.13	0.47
1:N:329:ASN:HD22	1:N:363:ASN:ND2	2.13	0.47
1:A:866:ASP:OD2	1:A:868:ARG:NH1	2.47	0.47
1:C:684:ILE:HD11	1:C:700:PRO:HG3	1.97	0.47
1:D:389:ILE:HB	1:D:460:ILE:HB	1.96	0.47
1:D:816:LYS:HE2	1:D:816:LYS:HB3	1.66	0.47
1:F:389:ILE:HB	1:F:460:ILE:HB	1.96	0.47
1:G:670:VAL:HG22	1:G:710:GLU:HB3	1.97	0.47
1:H:345:TYR:CE2	1:H:706:LYS:HB3	2.50	0.47
1:H:778:THR:O	1:H:778:THR:OG1	2.32	0.47
1:J:283:LYS:HB3	1:K:513:ILE:HG21	1.97	0.47
1:J:389:ILE:HB	1:J:460:ILE:HB	1.96	0.47
1:K:775:ASN:O	1:K:777:SER:N	2.41	0.47
1:L:503:TRP:O	1:L:507:ILE:HG12	2.15	0.47
1:M:329:ASN:HD22	1:M:363:ASN:HD21	1.63	0.47
1:M:503:TRP:O	1:M:507:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:792:GLN:HG3	1:N:846:PHE:CD2	2.50	0.47
1:B:389:ILE:HB	1:B:460:ILE:HB	1.96	0.47
1:C:450:ASN:HD22	1:C:456:SER:HB2	1.79	0.47
1:D:778:THR:OG1	1:D:778:THR:O	2.30	0.47
1:E:668:ARG:NH2	1:E:710:GLU:OE1	2.47	0.47
1:E:685:ILE:HG23	1:E:696:ASP:O	2.15	0.47
1:F:670:VAL:HG22	1:F:710:GLU:HB3	1.97	0.47
1:F:866:ASP:OD2	1:F:868:ARG:NH1	2.48	0.47
1:G:667:LYS:HG3	1:G:742:ASN:O	2.13	0.47
1:H:695:THR:O	1:H:695:THR:OG1	2.33	0.47
1:H:790:PRO:HD3	1:H:837:THR:HG21	1.96	0.47
1:I:389:ILE:HB	1:I:460:ILE:HB	1.97	0.47
1:I:771:ASP:O	1:I:784:ASN:HB2	2.14	0.47
1:J:269:ASP:HA	1:J:510:ILE:HD11	1.97	0.47
1:J:695:THR:O	1:J:695:THR:OG1	2.33	0.47
1:K:750:GLU:HB2	1:K:751:PRO:CD	2.43	0.47
1:K:778:THR:O	1:K:778:THR:OG1	2.32	0.47
1:K:811:GLN:HA	1:K:853:MET:HE3	1.96	0.47
1:C:567:ASN:OD1	1:C:569:ILE:HG12	2.14	0.47
1:H:503:TRP:O	1:H:507:ILE:HG12	2.15	0.46
1:I:231:GLU:HB3	1:I:261:TYR:HB3	1.97	0.46
1:I:269:ASP:OD1	1:I:269:ASP:N	2.46	0.46
1:I:329:ASN:HD22	1:I:363:ASN:HD21	1.63	0.46
1:L:269:ASP:OD1	1:L:269:ASP:N	2.46	0.46
1:L:329:ASN:HD22	1:L:363:ASN:HD21	1.63	0.46
1:L:345:TYR:HD1	1:L:350:THR:HA	1.79	0.46
1:A:389:ILE:HB	1:A:460:ILE:HB	1.96	0.46
1:A:780:ASN:O	1:A:781:THR:OG1	2.31	0.46
1:B:816:LYS:HB3	1:B:816:LYS:HE2	1.66	0.46
1:F:685:ILE:HG23	1:F:696:ASP:O	2.15	0.46
1:I:811:GLN:HA	1:I:853:MET:HE3	1.97	0.46
1:J:269:ASP:N	1:J:269:ASP:OD1	2.46	0.46
1:J:414:LEU:HD13	1:J:414:LEU:HA	1.80	0.46
1:N:852:ILE:HG22	1:N:852:ILE:O	2.15	0.46
1:A:684:ILE:HD11	1:A:700:PRO:HG3	1.97	0.46
1:B:408:PRO:HD2	1:B:424:ALA:HB2	1.95	0.46
1:B:780:ASN:O	1:B:781:THR:OG1	2.31	0.46
1:I:775:ASN:O	1:I:777:SER:N	2.41	0.46
1:K:345:TYR:CE2	1:K:706:LYS:HB3	2.50	0.46
1:L:813:SER:OG	1:L:813:SER:O	2.31	0.46
1:N:771:ASP:O	1:N:784:ASN:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:LYS:HE2	1:C:383:LYS:HB3	1.85	0.46
1:D:305:GLU:CD	1:D:446:PRO:HG3	2.35	0.46
1:F:684:ILE:HD11	1:F:700:PRO:HG3	1.96	0.46
1:G:389:ILE:HB	1:G:460:ILE:HB	1.96	0.46
1:I:778:THR:O	1:I:778:THR:OG1	2.32	0.46
1:J:329:ASN:HD22	1:J:363:ASN:HD21	1.62	0.46
1:L:365:THR:O	1:L:475:GLN:NE2	2.48	0.46
1:M:459:LEU:HD23	1:M:459:LEU:HA	1.74	0.46
1:N:345:TYR:HD1	1:N:350:THR:HA	1.79	0.46
1:N:642:GLY:C	1:N:644:GLN:H	2.18	0.46
1:B:684:ILE:HD11	1:B:700:PRO:HG3	1.96	0.46
1:D:780:ASN:O	1:D:781:THR:OG1	2.31	0.46
1:F:816:LYS:HB3	1:F:816:LYS:HE2	1.66	0.46
1:H:852:ILE:HG22	1:H:852:ILE:O	2.15	0.46
1:J:778:THR:OG1	1:J:778:THR:O	2.32	0.46
1:K:269:ASP:HA	1:K:510:ILE:HD11	1.97	0.46
1:K:365:THR:O	1:K:475:GLN:NE2	2.49	0.46
1:M:414:LEU:HD13	1:M:414:LEU:HA	1.79	0.46
1:N:493:SER:O	1:N:493:SER:OG	2.31	0.46
1:B:689:LYS:HA	1:B:689:LYS:HD2	1.74	0.46
1:C:689:LYS:HA	1:C:689:LYS:HD2	1.74	0.46
1:G:371:ASN:OD1	1:G:371:ASN:N	2.46	0.46
1:H:750:GLU:HB2	1:H:751:PRO:CD	2.43	0.46
1:H:815:PHE:CE1	1:H:857:LYS:HD2	2.51	0.46
1:I:642:GLY:C	1:I:644:GLN:H	2.18	0.46
1:J:224:ASP:OD1	1:J:224:ASP:N	2.45	0.46
1:J:771:ASP:O	1:J:784:ASN:HB2	2.15	0.46
1:J:790:PRO:HD3	1:J:837:THR:HG21	1.96	0.46
1:L:695:THR:O	1:L:695:THR:OG1	2.33	0.46
1:N:790:PRO:HD3	1:N:837:THR:HG21	1.96	0.46
1:B:568:ASP:N	1:B:568:ASP:OD1	2.49	0.46
1:B:838:ASN:HD22	1:B:838:ASN:N	2.14	0.46
1:C:331:LYS:HG2	1:C:396:TYR:CZ	2.51	0.46
1:G:568:ASP:N	1:G:568:ASP:OD1	2.49	0.46
1:G:684:ILE:HD11	1:G:700:PRO:HG3	1.96	0.46
1:M:852:ILE:O	1:M:852:ILE:HG22	2.15	0.46
1:B:588:ILE:HG23	1:B:603:VAL:HG21	1.97	0.46
1:D:331:LYS:HG2	1:D:396:TYR:CZ	2.51	0.46
1:D:445:SER:O	1:D:445:SER:OG	2.20	0.46
1:D:588:ILE:HG23	1:D:603:VAL:HG21	1.97	0.46
1:E:445:SER:O	1:E:445:SER:OG	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:276:LYS:NZ	1:G:289:ALA:O	2.43	0.46
1:H:223:ASN:HD22	1:H:223:ASN:HA	1.54	0.46
1:I:365:THR:O	1:I:475:GLN:NE2	2.48	0.46
1:L:815:PHE:CE1	1:L:857:LYS:HD2	2.51	0.46
1:L:852:ILE:O	1:L:852:ILE:HG22	2.15	0.46
1:M:790:PRO:HD3	1:M:837:THR:HG21	1.96	0.46
1:A:283:LYS:HD3	1:A:283:LYS:HA	1.74	0.46
1:C:389:ILE:HB	1:C:460:ILE:HB	1.96	0.46
1:I:852:ILE:O	1:I:852:ILE:HG22	2.15	0.46
1:J:815:PHE:CE1	1:J:857:LYS:HD2	2.51	0.46
1:M:642:GLY:C	1:M:644:GLN:H	2.18	0.46
1:N:329:ASN:HD22	1:N:363:ASN:HD21	1.63	0.46
1:N:503:TRP:O	1:N:507:ILE:HG12	2.15	0.46
1:A:581:ASP:OD1	1:A:584:THR:OG1	2.27	0.46
1:D:635:VAL:O	1:D:649:LYS:HB2	2.16	0.46
1:E:588:ILE:HG23	1:E:603:VAL:HG21	1.97	0.46
1:I:329:ASN:HD22	1:I:363:ASN:ND2	2.13	0.46
1:K:815:PHE:CE1	1:K:857:LYS:HD2	2.51	0.46
1:M:345:TYR:HD1	1:M:350:THR:HA	1.79	0.46
1:M:365:THR:O	1:M:475:GLN:NE2	2.49	0.46
1:N:815:PHE:CE1	1:N:857:LYS:HD2	2.51	0.46
1:B:331:LYS:HG2	1:B:396:TYR:CZ	2.51	0.46
1:D:568:ASP:N	1:D:568:ASP:OD1	2.49	0.46
1:D:668:ARG:NH2	1:D:710:GLU:OE1	2.47	0.46
1:E:283:LYS:HB2	1:F:509:GLN:CG	2.42	0.46
1:G:588:ILE:HG23	1:G:603:VAL:HG21	1.97	0.46
1:H:573:GLU:OE2	1:H:601:TYR:N	2.41	0.45
1:K:651:ASN:OD1	1:K:730:THR:N	2.25	0.45
1:L:381:ILE:O	1:L:382:ASN:ND2	2.47	0.45
1:A:331:LYS:HG2	1:A:396:TYR:CZ	2.51	0.45
1:A:588:ILE:HG23	1:A:603:VAL:HG21	1.97	0.45
1:A:668:ARG:NH2	1:A:710:GLU:OE1	2.47	0.45
1:C:635:VAL:O	1:C:649:LYS:HB2	2.16	0.45
1:C:838:ASN:HD22	1:C:838:ASN:N	2.14	0.45
1:E:331:LYS:HG2	1:E:396:TYR:CZ	2.51	0.45
1:E:568:ASP:OD1	1:E:568:ASP:N	2.49	0.45
1:F:588:ILE:HG23	1:F:603:VAL:HG21	1.97	0.45
1:G:600:ILE:O	1:G:603:VAL:HG22	2.16	0.45
1:I:815:PHE:CE1	1:I:857:LYS:HD2	2.51	0.45
1:J:365:THR:O	1:J:475:GLN:NE2	2.48	0.45
1:J:392:ASN:HA	1:J:447:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:573:GLU:OE2	1:M:601:TYR:N	2.41	0.45
1:A:404:TYR:HE1	1:B:505:ASP:HA	1.82	0.45
1:C:581:ASP:OD1	1:C:584:THR:OG1	2.27	0.45
1:C:588:ILE:HG23	1:C:603:VAL:HG21	1.97	0.45
1:E:838:ASN:HD22	1:E:838:ASN:N	2.14	0.45
1:F:568:ASP:OD1	1:F:568:ASP:N	2.49	0.45
1:G:474:LYS:HD3	1:G:474:LYS:HA	1.76	0.45
1:G:838:ASN:HD22	1:G:838:ASN:N	2.14	0.45
1:I:695:THR:O	1:I:695:THR:OG1	2.33	0.45
1:J:750:GLU:HB2	1:J:751:PRO:CD	2.43	0.45
1:L:441:LYS:HE2	1:L:441:LYS:HB3	1.73	0.45
1:N:459:LEU:HD23	1:N:459:LEU:HA	1.74	0.45
1:N:811:GLN:HA	1:N:853:MET:HE3	1.97	0.45
1:C:600:ILE:O	1:C:603:VAL:HG22	2.17	0.45
1:C:668:ARG:NH2	1:C:710:GLU:OE1	2.47	0.45
1:D:838:ASN:HD22	1:D:838:ASN:N	2.14	0.45
1:H:365:THR:O	1:H:475:GLN:NE2	2.49	0.45
1:J:875:VAL:O	1:J:875:VAL:HG12	2.17	0.45
1:K:459:LEU:HD23	1:K:459:LEU:HA	1.74	0.45
1:L:750:GLU:HB2	1:L:751:PRO:CD	2.43	0.45
1:N:365:THR:O	1:N:475:GLN:NE2	2.49	0.45
1:A:568:ASP:OD1	1:A:568:ASP:N	2.49	0.45
1:B:635:VAL:O	1:B:649:LYS:HB2	2.16	0.45
1:B:668:ARG:NH2	1:B:710:GLU:OE1	2.47	0.45
1:C:568:ASP:OD1	1:C:568:ASP:N	2.49	0.45
1:C:684:ILE:HG12	1:C:731:THR:HG21	1.99	0.45
1:D:775:ASN:O	1:D:777:SER:N	2.42	0.45
1:E:352:ASN:N	1:E:352:ASN:OD1	2.47	0.45
1:F:635:VAL:O	1:F:649:LYS:HB2	2.16	0.45
1:H:811:GLN:HA	1:H:853:MET:HE3	1.98	0.45
1:J:223:ASN:HD22	1:J:223:ASN:HA	1.55	0.45
1:M:750:GLU:HB2	1:M:751:PRO:CD	2.43	0.45
1:A:463:ASN:HB2	1:A:465:ASP:OD1	2.16	0.45
1:A:600:ILE:O	1:A:603:VAL:HG22	2.17	0.45
1:A:713:THR:O	1:A:714:THR:HG23	2.17	0.45
1:B:684:ILE:HG12	1:B:731:THR:HG21	1.99	0.45
1:C:666:TYR:HD1	1:C:714:THR:HG22	1.82	0.45
1:D:433:LEU:HD23	1:D:433:LEU:HA	1.74	0.45
1:D:600:ILE:O	1:D:603:VAL:HG22	2.17	0.45
1:H:392:ASN:HA	1:H:447:LEU:O	2.16	0.45
1:H:469:LYS:HA	1:H:472:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:498:THR:OG1	1:M:505:ASP:OD1	2.29	0.45
1:L:875:VAL:HG12	1:L:875:VAL:O	2.17	0.45
1:M:490:LYS:CE	1:N:509:GLN:HE22	2.30	0.45
1:M:875:VAL:O	1:M:875:VAL:HG12	2.17	0.45
1:N:312:ASN:OD1	1:N:313:GLU:N	2.50	0.45
1:N:695:THR:O	1:N:695:THR:OG1	2.33	0.45
1:A:635:VAL:O	1:A:649:LYS:HB2	2.16	0.45
1:B:713:THR:O	1:B:714:THR:HG23	2.17	0.45
1:D:684:ILE:HG12	1:D:731:THR:HG21	1.99	0.45
1:F:463:ASN:HB2	1:F:465:ASP:OD1	2.16	0.45
1:F:651:ASN:OD1	1:F:729:GLY:N	2.48	0.45
1:F:803:LYS:O	1:F:804:TYR:C	2.55	0.45
1:H:680:THR:O	1:H:680:THR:OG1	2.23	0.45
1:J:312:ASN:OD1	1:J:313:GLU:N	2.50	0.45
1:J:350:THR:O	1:J:350:THR:OG1	2.34	0.45
1:J:684:ILE:HG23	1:J:727:GLY:HA3	1.99	0.45
1:K:875:VAL:O	1:K:875:VAL:HG12	2.17	0.45
1:L:710:GLU:N	1:L:710:GLU:OE2	2.50	0.45
1:M:710:GLU:N	1:M:710:GLU:OE2	2.50	0.45
1:M:815:PHE:CE1	1:M:857:LYS:HD2	2.51	0.45
1:B:859:ARG:HH22	1:B:876:ASP:HB2	1.82	0.45
1:C:577:GLU:HG2	1:C:739:THR:HG21	1.99	0.45
1:E:463:ASN:HB2	1:E:465:ASP:OD1	2.16	0.45
1:F:331:LYS:HG2	1:F:396:TYR:CZ	2.51	0.45
1:F:352:ASN:OD1	1:F:352:ASN:N	2.47	0.45
1:G:463:ASN:HB2	1:G:465:ASP:OD1	2.16	0.45
1:G:635:VAL:O	1:G:649:LYS:HB2	2.16	0.45
1:H:329:ASN:HD22	1:H:363:ASN:HD21	1.63	0.45
1:I:392:ASN:HA	1:I:447:LEU:O	2.16	0.45
1:I:684:ILE:HG23	1:I:727:GLY:HA3	1.99	0.45
1:I:710:GLU:N	1:I:710:GLU:OE2	2.50	0.45
1:I:864:THR:OG1	1:I:868:ARG:O	2.25	0.45
1:L:392:ASN:HA	1:L:447:LEU:O	2.16	0.45
1:L:469:LYS:HA	1:L:472:ALA:HB3	1.99	0.45
1:B:463:ASN:HB2	1:B:465:ASP:OD1	2.16	0.45
1:B:577:GLU:HG2	1:B:739:THR:HG21	1.99	0.45
1:C:259:SER:HB3	1:C:292:PRO:HB2	1.99	0.45
1:C:682:ASN:HB2	1:C:728:SER:O	2.17	0.45
1:C:859:ARG:HH22	1:C:876:ASP:HB2	1.82	0.45
1:E:259:SER:HB3	1:E:292:PRO:HB2	1.99	0.45
1:E:581:ASP:OD1	1:E:584:THR:OG1	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:635:VAL:O	1:E:649:LYS:HB2	2.16	0.45
1:E:666:TYR:HD1	1:E:714:THR:HG22	1.82	0.45
1:E:684:ILE:HG12	1:E:731:THR:HG21	1.99	0.45
1:F:404:TYR:HE1	1:G:505:ASP:HA	1.82	0.45
1:F:577:GLU:HG2	1:F:739:THR:HG21	1.99	0.45
1:G:331:LYS:HG2	1:G:396:TYR:CZ	2.51	0.45
1:G:713:THR:O	1:G:714:THR:HG23	2.17	0.45
1:I:875:VAL:O	1:I:875:VAL:HG12	2.17	0.45
1:K:392:ASN:HA	1:K:447:LEU:O	2.16	0.45
1:M:469:LYS:HA	1:M:472:ALA:HB3	1.99	0.45
1:N:392:ASN:HA	1:N:447:LEU:O	2.16	0.45
1:N:433:LEU:HD12	1:N:433:LEU:HA	1.83	0.45
1:B:584:THR:CG2	1:B:610:ASN:H	2.30	0.45
1:B:600:ILE:O	1:B:603:VAL:HG22	2.17	0.45
1:C:463:ASN:HB2	1:C:465:ASP:OD1	2.16	0.45
1:D:259:SER:HB3	1:D:292:PRO:HB2	1.99	0.45
1:D:371:ASN:OD1	1:D:371:ASN:N	2.46	0.45
1:D:577:GLU:HG2	1:D:739:THR:HG21	1.99	0.45
1:E:600:ILE:O	1:E:603:VAL:HG22	2.17	0.45
1:E:651:ASN:OD1	1:E:729:GLY:N	2.48	0.45
1:F:682:ASN:HB2	1:F:728:SER:O	2.17	0.45
1:H:618:TYR:HA	1:H:627:ASN:HB3	1.99	0.45
1:I:469:LYS:HA	1:I:472:ALA:HB3	1.99	0.45
1:K:684:ILE:HG23	1:K:727:GLY:HA3	1.99	0.45
1:K:710:GLU:OE2	1:K:710:GLU:N	2.50	0.45
1:K:813:SER:OG	1:K:813:SER:O	2.31	0.45
1:M:547:ILE:O	1:M:551:ILE:HG13	2.17	0.45
1:M:811:GLN:HA	1:M:853:MET:HE3	1.97	0.45
1:N:618:TYR:HA	1:N:627:ASN:HB3	1.99	0.45
1:N:875:VAL:O	1:N:875:VAL:HG12	2.17	0.45
1:A:617:THR:HG23	1:A:618:TYR:H	1.82	0.45
1:A:684:ILE:HG12	1:A:731:THR:HG21	1.99	0.45
1:A:859:ARG:HH22	1:A:876:ASP:HB2	1.82	0.45
1:B:259:SER:HB3	1:B:292:PRO:HB2	1.99	0.45
1:C:713:THR:O	1:C:714:THR:HG23	2.17	0.45
1:E:577:GLU:HG2	1:E:739:THR:HG21	1.99	0.45
1:F:600:ILE:O	1:F:603:VAL:HG22	2.17	0.45
1:F:859:ARG:HH22	1:F:876:ASP:HB2	1.82	0.45
1:G:577:GLU:HG2	1:G:739:THR:HG21	1.99	0.45
1:G:651:ASN:OD1	1:G:729:GLY:N	2.48	0.45
1:G:859:ARG:HH22	1:G:876:ASP:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:433:LEU:HD12	1:H:433:LEU:HA	1.83	0.44
1:I:494:GLY:HA3	1:J:265:ASN:HD21	1.81	0.44
1:K:493:SER:O	1:K:493:SER:OG	2.31	0.44
1:M:338:GLY:O	1:M:355:THR:HG23	2.17	0.44
1:M:376:ASN:OD1	1:M:381:ILE:HB	2.18	0.44
1:N:469:LYS:HA	1:N:472:ALA:HB3	1.99	0.44
1:E:713:THR:O	1:E:714:THR:HG23	2.17	0.44
1:F:838:ASN:HD22	1:F:838:ASN:N	2.14	0.44
1:H:580:PHE:HD1	1:H:584:THR:HG21	1.82	0.44
1:H:864:THR:OG1	1:H:868:ARG:O	2.25	0.44
1:H:875:VAL:O	1:H:875:VAL:HG12	2.17	0.44
1:I:688:ILE:HA	1:I:722:GLU:O	2.18	0.44
1:J:547:ILE:O	1:J:551:ILE:HG13	2.17	0.44
1:J:688:ILE:HA	1:J:722:GLU:O	2.18	0.44
1:K:312:ASN:OD1	1:K:313:GLU:N	2.50	0.44
1:K:350:THR:O	1:K:350:THR:OG1	2.34	0.44
1:K:441:LYS:HB3	1:K:441:LYS:HE2	1.73	0.44
1:N:376:ASN:OD1	1:N:381:ILE:HB	2.18	0.44
1:D:463:ASN:HB2	1:D:465:ASP:OD1	2.16	0.44
1:D:809:THR:HG22	1:D:815:PHE:HD1	1.83	0.44
1:H:659:PRO:O	1:H:660:MET:HB3	2.18	0.44
1:I:618:TYR:HA	1:I:627:ASN:HB3	1.99	0.44
1:I:659:PRO:O	1:I:660:MET:HB3	2.18	0.44
1:J:493:SER:O	1:J:493:SER:OG	2.31	0.44
1:L:312:ASN:OD1	1:L:313:GLU:N	2.50	0.44
1:L:547:ILE:O	1:L:551:ILE:HG13	2.17	0.44
1:L:684:ILE:HG23	1:L:727:GLY:HA3	1.99	0.44
1:M:392:ASN:HA	1:M:447:LEU:O	2.16	0.44
1:N:547:ILE:O	1:N:551:ILE:HG13	2.17	0.44
1:E:224:ASP:OD1	1:E:224:ASP:N	2.41	0.44
1:E:809:THR:HG22	1:E:815:PHE:HD1	1.83	0.44
1:F:259:SER:HB3	1:F:292:PRO:HB2	1.99	0.44
1:F:584:THR:CG2	1:F:610:ASN:H	2.31	0.44
1:G:664:LYS:HA	1:G:664:LYS:HD2	1.40	0.44
1:G:809:THR:HG22	1:G:815:PHE:HD1	1.83	0.44
1:H:688:ILE:HA	1:H:722:GLU:O	2.18	0.44
1:I:338:GLY:O	1:I:355:THR:HG23	2.17	0.44
1:J:469:LYS:HA	1:J:472:ALA:HB3	1.99	0.44
1:J:580:PHE:HD1	1:J:584:THR:HG21	1.82	0.44
1:L:338:GLY:O	1:L:355:THR:HG23	2.17	0.44
1:L:580:PHE:HD1	1:L:584:THR:HG21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:580:PHE:HD1	1:M:584:THR:HG21	1.83	0.44
1:A:259:SER:HB3	1:A:292:PRO:HB2	1.99	0.44
1:A:773:ASN:O	1:A:781:THR:HA	2.18	0.44
1:A:803:LYS:O	1:A:804:TYR:C	2.55	0.44
1:B:276:LYS:HA	1:B:281:PHE:CE1	2.53	0.44
1:B:617:THR:HG23	1:B:618:TYR:H	1.82	0.44
1:B:803:LYS:O	1:B:804:TYR:C	2.55	0.44
1:B:825:MET:HA	1:B:837:THR:O	2.18	0.44
1:C:325:ARG:HG2	1:C:369:ASP:HB3	2.00	0.44
1:C:454:GLN:HE21	1:D:458:ARG:HG3	1.82	0.44
1:C:655:LYS:HE3	1:C:657:LYS:HE3	2.00	0.44
1:C:773:ASN:O	1:C:781:THR:HA	2.18	0.44
1:C:825:MET:HA	1:C:837:THR:O	2.18	0.44
1:D:584:THR:CG2	1:D:610:ASN:H	2.31	0.44
1:D:666:TYR:HD1	1:D:714:THR:HG22	1.82	0.44
1:D:825:MET:HA	1:D:837:THR:O	2.18	0.44
1:E:854:THR:HB	1:E:855:TYR:H	1.74	0.44
1:F:580:PHE:HE1	1:F:611:ILE:HG12	1.83	0.44
1:F:684:ILE:HG12	1:F:731:THR:HG21	1.99	0.44
1:F:713:THR:O	1:F:714:THR:HG23	2.17	0.44
1:G:584:THR:CG2	1:G:610:ASN:H	2.31	0.44
1:G:666:TYR:HD1	1:G:714:THR:HG22	1.82	0.44
1:G:682:ASN:HB2	1:G:728:SER:O	2.17	0.44
1:H:547:ILE:O	1:H:551:ILE:HG13	2.17	0.44
1:H:684:ILE:HG23	1:H:727:GLY:HA3	1.99	0.44
1:J:266:THR:OG1	1:J:273:ASP:OD2	2.36	0.44
1:J:407:THR:O	1:J:407:THR:OG1	2.29	0.44
1:K:688:ILE:HA	1:K:722:GLU:O	2.18	0.44
1:M:312:ASN:OD1	1:M:313:GLU:N	2.50	0.44
1:M:493:SER:O	1:M:493:SER:OG	2.31	0.44
1:N:688:ILE:HA	1:N:722:GLU:O	2.18	0.44
1:N:710:GLU:N	1:N:710:GLU:OE2	2.50	0.44
1:A:577:GLU:HG2	1:A:739:THR:HG21	1.99	0.44
1:A:825:MET:HA	1:A:837:THR:O	2.18	0.44
1:A:838:ASN:HD22	1:A:838:ASN:N	2.14	0.44
1:B:383:LYS:HE2	1:B:383:LYS:HB3	1.85	0.44
1:D:682:ASN:HB2	1:D:728:SER:O	2.17	0.44
1:E:773:ASN:O	1:E:781:THR:HA	2.18	0.44
1:E:803:LYS:O	1:E:804:TYR:C	2.55	0.44
1:J:659:PRO:O	1:J:660:MET:HB3	2.18	0.44
1:J:710:GLU:N	1:J:710:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:450:ASN:O	1:N:451:THR:OG1	2.22	0.44
1:A:816:LYS:HE2	1:A:816:LYS:HB3	1.66	0.44
1:B:666:TYR:HD1	1:B:714:THR:HG22	1.82	0.44
1:D:325:ARG:HG2	1:D:369:ASP:HB3	1.99	0.44
1:D:655:LYS:HE3	1:D:657:LYS:HE3	2.00	0.44
1:D:713:THR:O	1:D:714:THR:HG23	2.17	0.44
1:E:276:LYS:NZ	1:E:289:ALA:O	2.43	0.44
1:E:371:ASN:OD1	1:E:371:ASN:N	2.46	0.44
1:E:775:ASN:O	1:E:777:SER:N	2.42	0.44
1:F:276:LYS:HA	1:F:281:PHE:CE1	2.53	0.44
1:G:617:THR:HG23	1:G:618:TYR:H	1.82	0.44
1:H:312:ASN:OD1	1:H:313:GLU:N	2.50	0.44
1:H:376:ASN:OD1	1:H:381:ILE:HB	2.17	0.44
1:I:547:ILE:O	1:I:551:ILE:HG13	2.17	0.44
1:J:381:ILE:O	1:J:382:ASN:ND2	2.47	0.44
1:K:266:THR:OG1	1:K:273:ASP:OD2	2.36	0.44
1:K:469:LYS:HA	1:K:472:ALA:HB3	1.99	0.44
1:K:573:GLU:OE2	1:K:601:TYR:N	2.41	0.44
1:L:371:ASN:OD1	1:L:371:ASN:N	2.51	0.44
1:L:376:ASN:OD1	1:L:381:ILE:HB	2.18	0.44
1:M:618:TYR:HA	1:M:627:ASN:HB3	1.99	0.44
1:N:338:GLY:O	1:N:355:THR:HG23	2.17	0.44
1:A:651:ASN:OD1	1:A:729:GLY:N	2.48	0.44
1:A:655:LYS:HE3	1:A:657:LYS:HE3	2.00	0.44
1:A:666:TYR:HD1	1:A:714:THR:HG22	1.82	0.44
1:B:682:ASN:HB2	1:B:728:SER:O	2.17	0.44
1:E:859:ARG:HH22	1:E:876:ASP:HB2	1.82	0.44
1:F:291:ASP:OD1	1:F:553:LYS:NZ	2.28	0.44
1:H:338:GLY:O	1:H:355:THR:HG23	2.17	0.44
1:K:371:ASN:OD1	1:K:371:ASN:N	2.51	0.44
1:N:684:ILE:HG23	1:N:727:GLY:HA3	1.99	0.44
1:A:276:LYS:HA	1:A:281:PHE:CE1	2.53	0.44
1:A:689:LYS:HD2	1:A:689:LYS:HA	1.74	0.44
1:B:773:ASN:O	1:B:781:THR:HA	2.18	0.44
1:C:684:ILE:HG23	1:C:727:GLY:HA3	2.00	0.44
1:C:809:THR:HG22	1:C:815:PHE:HD1	1.83	0.44
1:D:651:ASN:OD1	1:D:729:GLY:N	2.48	0.44
1:E:580:PHE:HE1	1:E:611:ILE:HG12	1.82	0.44
1:E:617:THR:HG23	1:E:618:TYR:H	1.82	0.44
1:H:386:SER:OG	1:N:318:ASP:OD1	2.35	0.44
1:H:389:ILE:O	1:H:459:LEU:HD22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:750:GLU:HB2	1:I:751:PRO:CD	2.43	0.44
1:J:441:LYS:HE2	1:J:441:LYS:HB3	1.73	0.44
1:M:381:ILE:O	1:M:382:ASN:ND2	2.47	0.44
1:M:684:ILE:HG23	1:M:727:GLY:HA3	1.99	0.44
1:N:332:THR:OG1	1:N:520:ASP:OD1	2.30	0.44
1:A:580:PHE:HE1	1:A:611:ILE:HG12	1.82	0.44
1:A:584:THR:CG2	1:A:610:ASN:H	2.31	0.44
1:A:809:THR:HG22	1:A:815:PHE:HD1	1.83	0.44
1:B:325:ARG:HG2	1:B:369:ASP:HB3	2.00	0.44
1:B:684:ILE:HG23	1:B:727:GLY:HA3	2.00	0.44
1:C:579:ILE:HB	1:C:612:LEU:HD23	2.00	0.44
1:C:778:THR:O	1:C:778:THR:OG1	2.30	0.44
1:C:803:LYS:O	1:C:804:TYR:C	2.55	0.44
1:D:579:ILE:HB	1:D:612:LEU:HD23	2.00	0.44
1:D:617:THR:HG23	1:D:618:TYR:H	1.82	0.44
1:G:283:LYS:HD3	1:G:283:LYS:HA	1.74	0.44
1:G:825:MET:HA	1:G:837:THR:O	2.18	0.44
1:H:710:GLU:N	1:H:710:GLU:OE2	2.50	0.43
1:J:246:GLU:H	1:J:246:GLU:HG3	1.70	0.43
1:J:618:TYR:HA	1:J:627:ASN:HB3	1.99	0.43
1:J:673:GLY:HA2	1:J:735:ASN:O	2.18	0.43
1:K:659:PRO:O	1:K:660:MET:HB3	2.18	0.43
1:L:618:TYR:HA	1:L:627:ASN:HB3	1.99	0.43
1:M:371:ASN:N	1:M:371:ASN:OD1	2.51	0.43
1:A:682:ASN:HB2	1:A:728:SER:O	2.17	0.43
1:B:655:LYS:HE3	1:B:657:LYS:HE3	2.00	0.43
1:C:276:LYS:HA	1:C:281:PHE:CE1	2.53	0.43
1:C:617:THR:HG23	1:C:618:TYR:H	1.82	0.43
1:E:682:ASN:HB2	1:E:728:SER:O	2.17	0.43
1:G:259:SER:HB3	1:G:292:PRO:HB2	1.99	0.43
1:G:276:LYS:HA	1:G:281:PHE:CE1	2.53	0.43
1:G:684:ILE:HG12	1:G:731:THR:HG21	1.99	0.43
1:I:312:ASN:OD1	1:I:313:GLU:N	2.50	0.43
1:I:673:GLY:HA2	1:I:735:ASN:O	2.18	0.43
1:M:688:ILE:HA	1:M:722:GLU:O	2.18	0.43
1:E:825:MET:HA	1:E:837:THR:O	2.18	0.43
1:F:341:VAL:HG11	1:F:668:ARG:HH22	1.83	0.43
1:F:664:LYS:HD2	1:F:664:LYS:HA	1.41	0.43
1:F:825:MET:HA	1:F:837:THR:O	2.18	0.43
1:G:580:PHE:HE1	1:G:611:ILE:HG12	1.83	0.43
1:J:338:GLY:O	1:J:355:THR:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:649:LYS:HE3	1:K:649:LYS:HB3	1.88	0.43
1:L:412:LEU:HD12	1:L:478:LEU:HG	2.01	0.43
1:L:659:PRO:O	1:L:660:MET:HB3	2.18	0.43
1:M:412:LEU:HD12	1:M:478:LEU:HG	2.01	0.43
1:N:360:THR:HG23	1:N:518:ILE:HD13	2.00	0.43
1:N:389:ILE:O	1:N:459:LEU:HD22	2.18	0.43
1:A:684:ILE:HG23	1:A:727:GLY:HA3	2.00	0.43
1:B:854:THR:HB	1:B:855:TYR:H	1.73	0.43
1:C:341:VAL:HG11	1:C:668:ARG:HH22	1.84	0.43
1:D:341:VAL:HG11	1:D:668:ARG:HH22	1.83	0.43
1:D:859:ARG:HH22	1:D:876:ASP:HB2	1.82	0.43
1:G:325:ARG:HG2	1:G:369:ASP:HB3	2.00	0.43
1:G:655:LYS:HE3	1:G:657:LYS:HE3	2.00	0.43
1:H:673:GLY:HA2	1:H:735:ASN:O	2.18	0.43
1:J:376:ASN:OD1	1:J:381:ILE:HB	2.18	0.43
1:J:409:THR:O	1:J:409:THR:OG1	2.35	0.43
1:K:547:ILE:O	1:K:551:ILE:HG13	2.17	0.43
1:K:618:TYR:HA	1:K:627:ASN:HB3	1.99	0.43
1:L:688:ILE:HA	1:L:722:GLU:O	2.18	0.43
1:M:266:THR:OG1	1:M:273:ASP:OD2	2.36	0.43
1:M:360:THR:HG23	1:M:518:ILE:HD13	2.00	0.43
1:A:341:VAL:HG11	1:A:668:ARG:HH22	1.83	0.43
1:A:560:LYS:HB2	1:A:565:TYR:CD2	2.54	0.43
1:B:560:LYS:HB2	1:B:565:TYR:CD2	2.54	0.43
1:B:809:THR:HG22	1:B:815:PHE:HD1	1.83	0.43
1:C:371:ASN:OD1	1:C:371:ASN:N	2.46	0.43
1:D:684:ILE:HG23	1:D:727:GLY:HA3	2.00	0.43
1:G:579:ILE:HB	1:G:612:LEU:HD23	2.00	0.43
1:G:773:ASN:O	1:G:781:THR:HA	2.18	0.43
1:G:803:LYS:O	1:G:804:TYR:C	2.55	0.43
1:H:360:THR:HG23	1:H:518:ILE:HD13	2.00	0.43
1:I:376:ASN:OD1	1:I:381:ILE:HB	2.17	0.43
1:I:580:PHE:HD1	1:I:584:THR:HG21	1.82	0.43
1:K:389:ILE:O	1:K:459:LEU:HD22	2.18	0.43
1:N:381:ILE:O	1:N:382:ASN:ND2	2.47	0.43
1:D:773:ASN:O	1:D:781:THR:HA	2.18	0.43
1:F:773:ASN:O	1:F:781:THR:HA	2.18	0.43
1:J:332:THR:OG1	1:J:520:ASP:OD1	2.30	0.43
1:J:687:LYS:HB3	1:J:687:LYS:HE3	1.70	0.43
1:N:673:GLY:HA2	1:N:735:ASN:O	2.18	0.43
1:N:774:PHE:CD2	1:C:774:PHE:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ILE:HB	1:A:612:LEU:HD23	2.00	0.43
1:C:777:SER:O	1:C:778:THR:OG1	2.37	0.43
1:E:535:LEU:HD13	1:E:535:LEU:HA	1.91	0.43
1:E:655:LYS:HE3	1:E:657:LYS:HE3	2.00	0.43
1:F:325:ARG:HG2	1:F:369:ASP:HB3	2.00	0.43
1:I:389:ILE:O	1:I:459:LEU:HD22	2.18	0.43
1:K:338:GLY:O	1:K:355:THR:HG23	2.17	0.43
1:K:376:ASN:OD1	1:K:381:ILE:HB	2.18	0.43
1:K:580:PHE:HD1	1:K:584:THR:HG21	1.82	0.43
1:L:266:THR:OG1	1:L:273:ASP:OD2	2.36	0.43
1:M:659:PRO:O	1:M:660:MET:HB3	2.18	0.43
1:M:695:THR:O	1:M:695:THR:OG1	2.33	0.43
1:M:777:SER:O	1:M:778:THR:OG1	2.36	0.43
1:N:223:ASN:HD22	1:N:223:ASN:HA	1.55	0.43
1:N:580:PHE:HD1	1:N:584:THR:HG21	1.83	0.43
1:A:664:LYS:HD2	1:A:664:LYS:HA	1.41	0.43
1:B:433:LEU:HA	1:B:433:LEU:HD23	1.74	0.43
1:C:584:THR:CG2	1:C:610:ASN:H	2.30	0.43
1:D:276:LYS:HA	1:D:281:PHE:CE1	2.53	0.43
1:D:580:PHE:HE1	1:D:611:ILE:HG12	1.82	0.43
1:F:433:LEU:HD23	1:F:433:LEU:HA	1.74	0.43
1:F:666:TYR:HD1	1:F:714:THR:HG22	1.82	0.43
1:I:350:THR:O	1:I:350:THR:OG1	2.34	0.43
1:N:659:PRO:O	1:N:660:MET:HB3	2.18	0.43
1:E:579:ILE:HB	1:E:612:LEU:HD23	2.00	0.43
1:F:579:ILE:HB	1:F:612:LEU:HD23	2.00	0.43
1:F:617:THR:HG23	1:F:618:TYR:H	1.82	0.43
1:F:655:LYS:HE3	1:F:657:LYS:HE3	2.00	0.43
1:G:560:LYS:HB2	1:G:565:TYR:CD2	2.54	0.43
1:H:350:THR:O	1:H:350:THR:OG1	2.34	0.43
1:I:266:THR:HG1	1:I:273:ASP:CG	2.22	0.43
1:K:673:GLY:HA2	1:K:735:ASN:O	2.18	0.43
1:M:673:GLY:HA2	1:M:735:ASN:O	2.18	0.43
1:N:266:THR:OG1	1:N:273:ASP:OD2	2.36	0.43
1:N:310:SER:O	1:N:388:TYR:N	2.49	0.43
1:N:441:LYS:HB3	1:N:441:LYS:HE2	1.73	0.43
1:N:859:ARG:NH2	1:N:876:ASP:OD2	2.49	0.43
1:A:325:ARG:HG2	1:A:369:ASP:HB3	2.00	0.43
1:B:228:ASP:OD1	1:B:228:ASP:N	2.52	0.43
1:B:580:PHE:HE1	1:B:611:ILE:HG12	1.83	0.43
1:D:535:LEU:HD13	1:D:535:LEU:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:LYS:HD2	1:E:238:LYS:HA	1.95	0.43
1:E:325:ARG:HG2	1:E:369:ASP:HB3	2.00	0.43
1:E:341:VAL:HG11	1:E:668:ARG:HH22	1.84	0.43
1:E:546:THR:HG22	1:E:604:LYS:HD3	2.01	0.43
1:F:780:ASN:O	1:F:781:THR:OG1	2.31	0.43
1:H:266:THR:OG1	1:H:273:ASP:OD2	2.36	0.43
1:H:414:LEU:HD13	1:H:414:LEU:HA	1.79	0.43
1:I:371:ASN:OD1	1:I:371:ASN:N	2.51	0.43
1:N:412:LEU:HD12	1:N:478:LEU:HG	2.01	0.43
1:C:240:LEU:HD23	1:C:240:LEU:HA	1.75	0.43
1:C:560:LYS:HB2	1:C:565:TYR:CD2	2.54	0.43
1:C:633:SER:OG	1:C:654:THR:OG1	2.09	0.43
1:C:803:LYS:HA	1:C:821:LYS:O	2.19	0.43
1:E:228:ASP:N	1:E:228:ASP:OD1	2.52	0.43
1:E:803:LYS:HA	1:E:821:LYS:O	2.19	0.43
1:H:409:THR:O	1:H:409:THR:OG1	2.35	0.42
1:I:360:THR:HG23	1:I:518:ILE:HD13	2.00	0.42
1:I:519:LEU:HD23	1:I:526:TYR:HD2	1.85	0.42
1:J:305:GLU:OE2	1:J:446:PRO:HG3	2.19	0.42
1:J:573:GLU:OE2	1:J:601:TYR:N	2.40	0.42
1:J:777:SER:O	1:J:778:THR:OG1	2.36	0.42
1:K:859:ARG:NH2	1:K:876:ASP:OD2	2.49	0.42
1:M:246:GLU:H	1:M:246:GLU:HG3	1.70	0.42
1:M:389:ILE:O	1:M:459:LEU:HD22	2.18	0.42
1:N:858:LEU:HD23	1:N:875:VAL:HG21	2.01	0.42
1:A:809:THR:HG23	1:A:857:LYS:O	2.19	0.42
1:B:579:ILE:HB	1:B:612:LEU:HD23	2.00	0.42
1:B:653:GLU:CB	1:B:726:ILE:HD13	2.49	0.42
1:B:809:THR:HG23	1:B:857:LYS:O	2.19	0.42
1:C:337:ALA:HA	1:C:742:ASN:ND2	2.34	0.42
1:C:653:GLU:CB	1:C:726:ILE:HD13	2.49	0.42
1:C:664:LYS:HD2	1:C:664:LYS:HA	1.40	0.42
1:D:546:THR:HG22	1:D:604:LYS:HD3	2.01	0.42
1:D:854:THR:HB	1:D:855:TYR:H	1.74	0.42
1:E:771:ASP:O	1:E:784:ASN:HB2	2.19	0.42
1:F:450:ASN:C	1:F:452:MET:H	2.22	0.42
1:F:684:ILE:HG23	1:F:727:GLY:HA3	2.00	0.42
1:F:809:THR:HG22	1:F:815:PHE:HD1	1.83	0.42
1:I:450:ASN:O	1:I:456:SER:HB2	2.20	0.42
1:J:389:ILE:O	1:J:459:LEU:HD22	2.18	0.42
1:J:639:ASN:OD1	1:J:640:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:412:LEU:HD12	1:K:478:LEU:HG	2.01	0.42
1:K:639:ASN:OD1	1:K:640:GLN:N	2.52	0.42
1:L:360:THR:HG23	1:L:518:ILE:HD13	2.00	0.42
1:L:680:THR:O	1:L:680:THR:OG1	2.23	0.42
1:M:240:LEU:O	1:M:274:TYR:OH	2.17	0.42
1:N:660:MET:SD	1:N:721:ILE:HD11	2.60	0.42
1:A:228:ASP:OD1	1:A:228:ASP:N	2.52	0.42
1:A:653:GLU:CB	1:A:726:ILE:HD13	2.50	0.42
1:B:341:VAL:HG11	1:B:668:ARG:HH22	1.84	0.42
1:B:803:LYS:HA	1:B:821:LYS:O	2.19	0.42
1:C:580:PHE:HE1	1:C:611:ILE:HG12	1.82	0.42
1:C:651:ASN:OD1	1:C:729:GLY:N	2.48	0.42
1:C:809:THR:HG23	1:C:857:LYS:O	2.19	0.42
1:D:560:LYS:HB2	1:D:565:TYR:CD2	2.54	0.42
1:E:276:LYS:HA	1:E:281:PHE:CE1	2.53	0.42
1:F:546:THR:HG22	1:F:604:LYS:HD3	2.01	0.42
1:F:560:LYS:HB2	1:F:565:TYR:CD2	2.54	0.42
1:G:771:ASP:O	1:G:784:ASN:HB2	2.19	0.42
1:H:412:LEU:HD12	1:H:478:LEU:HG	2.01	0.42
1:I:803:LYS:O	1:I:804:TYR:C	2.58	0.42
1:J:388:TYR:CE1	1:J:461:PRO:HB3	2.55	0.42
1:J:803:LYS:O	1:J:804:TYR:C	2.58	0.42
1:L:519:LEU:HD23	1:L:526:TYR:HD2	1.85	0.42
1:L:774:PHE:CG	1:E:774:PHE:HB2	2.54	0.42
1:L:864:THR:OG1	1:L:868:ARG:O	2.25	0.42
1:N:388:TYR:CE1	1:N:461:PRO:HB3	2.55	0.42
1:N:750:GLU:HB2	1:N:751:PRO:CD	2.43	0.42
1:A:565:TYR:CD1	1:A:570:PRO:HA	2.55	0.42
1:B:771:ASP:O	1:B:784:ASN:HB2	2.19	0.42
1:D:316:SER:H	1:D:452:MET:CE	2.32	0.42
1:D:803:LYS:O	1:D:804:TYR:C	2.55	0.42
1:F:653:GLU:CB	1:F:726:ILE:HD13	2.49	0.42
1:G:410:THR:CG2	1:G:478:LEU:HB3	2.50	0.42
1:G:684:ILE:HG23	1:G:727:GLY:HA3	2.00	0.42
1:H:459:LEU:HA	1:H:459:LEU:HD23	1.74	0.42
1:H:639:ASN:OD1	1:H:640:GLN:N	2.52	0.42
1:J:529:ARG:HD3	1:J:529:ARG:HA	1.79	0.42
1:K:310:SER:O	1:K:388:TYR:N	2.49	0.42
1:K:374:SER:CB	1:K:750:GLU:HG3	2.50	0.42
1:K:414:LEU:HD13	1:K:414:LEU:HA	1.79	0.42
1:L:529:ARG:HD3	1:L:529:ARG:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:858:LEU:HD23	1:M:875:VAL:HG21	2.02	0.42
1:N:350:THR:O	1:N:350:THR:OG1	2.34	0.42
1:N:371:ASN:OD1	1:N:371:ASN:N	2.51	0.42
1:N:374:SER:CB	1:N:750:GLU:HG3	2.50	0.42
1:N:687:LYS:HA	1:N:694:LYS:O	2.20	0.42
1:A:383:LYS:HE2	1:A:383:LYS:HB3	1.84	0.42
1:A:803:LYS:HA	1:A:821:LYS:O	2.19	0.42
1:C:450:ASN:C	1:C:452:MET:H	2.22	0.42
1:C:565:TYR:CD1	1:C:570:PRO:HA	2.55	0.42
1:E:684:ILE:HG23	1:E:727:GLY:HA3	2.00	0.42
1:F:535:LEU:HD13	1:F:535:LEU:HA	1.91	0.42
1:G:450:ASN:C	1:G:452:MET:H	2.22	0.42
1:G:803:LYS:HA	1:G:821:LYS:O	2.19	0.42
1:H:438:THR:OG1	1:H:440:PRO:O	2.29	0.42
1:H:594:THR:O	1:H:594:THR:HG22	2.20	0.42
1:I:529:ARG:HA	1:I:529:ARG:HD3	1.80	0.42
1:I:687:LYS:HB3	1:I:687:LYS:HE3	1.70	0.42
1:I:777:SER:O	1:I:778:THR:OG1	2.36	0.42
1:J:813:SER:OG	1:J:813:SER:O	2.31	0.42
1:K:519:LEU:HD23	1:K:526:TYR:HD2	1.85	0.42
1:K:803:LYS:O	1:K:804:TYR:C	2.58	0.42
1:L:673:GLY:HA2	1:L:735:ASN:O	2.18	0.42
1:M:450:ASN:O	1:M:456:SER:HB2	2.20	0.42
1:A:316:SER:H	1:A:452:MET:CE	2.32	0.42
1:A:506:TYR:CE1	1:G:496:ILE:HB	2.55	0.42
1:C:283:LYS:HD3	1:C:283:LYS:HA	1.74	0.42
1:D:410:THR:CG2	1:D:478:LEU:HB3	2.50	0.42
1:E:560:LYS:HB2	1:E:565:TYR:CD2	2.54	0.42
1:H:687:LYS:HA	1:H:694:LYS:O	2.20	0.42
1:H:858:LEU:HD23	1:H:875:VAL:HG21	2.01	0.42
1:I:493:SER:O	1:I:493:SER:OG	2.31	0.42
1:I:594:THR:HG22	1:I:594:THR:O	2.20	0.42
1:I:639:ASN:OD1	1:I:640:GLN:N	2.52	0.42
1:J:360:THR:HG23	1:J:518:ILE:HD13	2.00	0.42
1:J:453:ASP:N	1:J:456:SER:HB3	2.27	0.42
1:J:459:LEU:HD23	1:J:459:LEU:HA	1.74	0.42
1:J:628:TYR:HE2	1:J:632:TRP:HE1	1.67	0.42
1:K:450:ASN:O	1:K:456:SER:HB2	2.19	0.42
1:K:838:ASN:HD22	1:K:838:ASN:N	2.17	0.42
1:L:450:ASN:O	1:L:456:SER:HB2	2.19	0.42
1:M:859:ARG:NH2	1:M:876:ASP:OD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:519:LEU:HD23	1:N:526:TYR:HD2	1.85	0.42
1:B:316:SER:H	1:B:452:MET:CE	2.32	0.42
1:D:771:ASP:O	1:D:784:ASN:HB2	2.19	0.42
1:D:803:LYS:HA	1:D:821:LYS:O	2.19	0.42
1:E:410:THR:CG2	1:E:478:LEU:HB3	2.50	0.42
1:E:584:THR:CG2	1:E:610:ASN:H	2.30	0.42
1:F:228:ASP:N	1:F:228:ASP:OD1	2.52	0.42
1:F:427:ASN:OD1	1:F:427:ASN:N	2.53	0.42
1:F:565:TYR:CD1	1:F:570:PRO:HA	2.55	0.42
1:G:809:THR:HG23	1:G:857:LYS:O	2.19	0.42
1:H:374:SER:CB	1:H:750:GLU:HG3	2.50	0.42
1:I:388:TYR:CE1	1:I:461:PRO:HB3	2.54	0.42
1:I:687:LYS:HA	1:I:694:LYS:O	2.20	0.42
1:K:223:ASN:HD22	1:K:223:ASN:HA	1.55	0.42
1:K:305:GLU:OE2	1:K:446:PRO:HG3	2.20	0.42
1:L:350:THR:O	1:L:350:THR:OG1	2.34	0.42
1:L:374:SER:CB	1:L:750:GLU:HG3	2.50	0.42
1:L:389:ILE:O	1:L:459:LEU:HD22	2.18	0.42
1:L:838:ASN:HD22	1:L:838:ASN:N	2.18	0.42
1:M:310:SER:O	1:M:388:TYR:N	2.49	0.42
1:N:450:ASN:O	1:N:456:SER:HB2	2.19	0.42
1:A:771:ASP:O	1:A:784:ASN:HB2	2.19	0.42
1:B:337:ALA:HA	1:B:742:ASN:ND2	2.34	0.42
1:B:450:ASN:C	1:B:452:MET:H	2.22	0.42
1:C:546:THR:HG22	1:C:604:LYS:HD3	2.02	0.42
1:C:654:THR:HG22	1:C:725:LEU:HB3	2.01	0.42
1:C:771:ASP:O	1:C:784:ASN:HB2	2.19	0.42
1:D:654:THR:HG22	1:D:725:LEU:HB3	2.02	0.42
1:E:653:GLU:CB	1:E:726:ILE:HD13	2.49	0.42
1:E:654:THR:HG22	1:E:725:LEU:HB3	2.01	0.42
1:F:809:THR:HG23	1:F:857:LYS:O	2.19	0.42
1:G:653:GLU:CB	1:G:726:ILE:HD13	2.49	0.42
1:G:775:ASN:O	1:G:777:SER:N	2.42	0.42
1:H:310:SER:O	1:H:388:TYR:N	2.49	0.42
1:H:660:MET:SD	1:H:721:ILE:HD11	2.60	0.42
1:J:328:THR:HG23	1:J:368:GLN:HG3	2.02	0.42
1:J:373:GLU:HB3	1:J:377:THR:HG21	2.02	0.42
1:J:412:LEU:HD12	1:J:478:LEU:HG	2.01	0.42
1:J:687:LYS:HA	1:J:694:LYS:O	2.20	0.42
1:K:373:GLU:HB3	1:K:377:THR:HG21	2.02	0.42
1:L:310:SER:O	1:L:388:TYR:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:639:ASN:OD1	1:L:640:GLN:N	2.52	0.42
1:M:318:ASP:CG	1:N:384:GLY:O	2.58	0.42
1:M:388:TYR:CE1	1:M:461:PRO:HB3	2.54	0.42
1:M:660:MET:SD	1:M:721:ILE:HD11	2.60	0.42
1:N:594:THR:HG22	1:N:594:THR:O	2.20	0.42
1:B:535:LEU:HD13	1:B:535:LEU:HA	1.91	0.42
1:B:546:THR:HG22	1:B:604:LYS:HD3	2.01	0.42
1:C:228:ASP:OD1	1:C:228:ASP:N	2.52	0.42
1:C:316:SER:H	1:C:452:MET:CE	2.32	0.42
1:C:535:LEU:HD13	1:C:535:LEU:HA	1.91	0.42
1:F:316:SER:H	1:F:452:MET:CE	2.32	0.42
1:G:316:SER:H	1:G:452:MET:CE	2.32	0.42
1:G:427:ASN:OD1	1:G:427:ASN:N	2.53	0.42
1:G:546:THR:HG22	1:G:604:LYS:HD3	2.01	0.42
1:H:388:TYR:CE1	1:H:461:PRO:HB3	2.54	0.42
1:I:305:GLU:OE2	1:I:446:PRO:HG3	2.20	0.42
1:I:412:LEU:HD12	1:I:478:LEU:HG	2.00	0.42
1:K:328:THR:HG23	1:K:368:GLN:HG3	2.02	0.42
1:K:433:LEU:HD12	1:K:433:LEU:HA	1.83	0.42
1:K:858:LEU:HD23	1:K:875:VAL:HG21	2.01	0.42
1:M:639:ASN:OD1	1:M:640:GLN:N	2.53	0.42
1:M:687:LYS:HA	1:M:694:LYS:O	2.20	0.42
1:A:410:THR:CG2	1:A:478:LEU:HB3	2.50	0.42
1:A:546:THR:HG22	1:A:604:LYS:HD3	2.01	0.42
1:B:410:THR:CG2	1:B:478:LEU:HB3	2.50	0.42
1:B:651:ASN:OD1	1:B:729:GLY:N	2.48	0.42
1:C:388:TYR:HA	1:C:460:ILE:O	2.20	0.42
1:C:410:THR:CG2	1:C:478:LEU:HB3	2.49	0.42
1:C:580:PHE:CE1	1:C:611:ILE:HG12	2.55	0.42
1:D:337:ALA:HA	1:D:742:ASN:ND2	2.34	0.42
1:E:283:LYS:HA	1:E:283:LYS:HD3	1.74	0.42
1:E:581:ASP:H	1:E:584:THR:HG1	1.68	0.42
1:F:388:TYR:HA	1:F:460:ILE:O	2.20	0.42
1:F:771:ASP:O	1:F:784:ASN:HB2	2.19	0.42
1:G:341:VAL:HG11	1:G:668:ARG:HH22	1.84	0.42
1:G:388:TYR:HA	1:G:460:ILE:O	2.20	0.42
1:G:580:PHE:CE1	1:G:611:ILE:HG12	2.55	0.42
1:J:450:ASN:O	1:J:456:SER:HB2	2.20	0.42
1:J:858:LEU:HD23	1:J:875:VAL:HG21	2.01	0.42
1:K:676:LYS:HD2	1:K:702:GLN:O	2.20	0.42
1:N:309:ILE:HD12	1:N:375:TRP:CE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:639:ASN:OD1	1:N:640:GLN:N	2.52	0.42
1:C:305:GLU:OE2	1:C:446:PRO:HG3	2.20	0.42
1:D:450:ASN:C	1:D:452:MET:H	2.22	0.42
1:F:654:THR:HG22	1:F:725:LEU:HB3	2.01	0.42
1:F:803:LYS:HA	1:F:821:LYS:O	2.19	0.42
1:G:337:ALA:HA	1:G:742:ASN:ND2	2.34	0.42
1:I:328:THR:HG23	1:I:368:GLN:HG3	2.02	0.41
1:I:374:SER:CB	1:I:750:GLU:HG3	2.50	0.41
1:I:660:MET:SD	1:I:721:ILE:HD11	2.60	0.41
1:J:374:SER:CB	1:J:750:GLU:HG3	2.50	0.41
1:K:360:THR:HG23	1:K:518:ILE:HD13	2.00	0.41
1:K:463:ASN:HB2	1:K:465:ASP:OD1	2.21	0.41
1:L:409:THR:O	1:L:409:THR:OG1	2.35	0.41
1:L:649:LYS:NZ	1:L:732:TYR:HE1	2.18	0.41
1:L:859:ARG:NH2	1:L:876:ASP:OD2	2.49	0.41
1:M:364:SER:HA	1:M:477:LYS:HA	2.02	0.41
1:M:628:TYR:HE2	1:M:632:TRP:HE1	1.67	0.41
1:N:305:GLU:OE2	1:N:446:PRO:HG3	2.19	0.41
1:N:409:THR:O	1:N:409:THR:OG1	2.35	0.41
1:B:654:THR:HG22	1:B:725:LEU:HB3	2.01	0.41
1:D:427:ASN:N	1:D:427:ASN:OD1	2.53	0.41
1:H:381:ILE:O	1:H:382:ASN:ND2	2.47	0.41
1:I:858:LEU:HD23	1:I:875:VAL:HG21	2.02	0.41
1:J:463:ASN:HB2	1:J:465:ASP:OD1	2.21	0.41
1:L:717:ASP:N	1:L:717:ASP:OD2	2.53	0.41
1:M:594:THR:O	1:M:594:THR:HG22	2.20	0.41
1:M:803:LYS:O	1:M:804:TYR:C	2.58	0.41
1:N:529:ARG:HD3	1:N:529:ARG:HA	1.79	0.41
1:B:305:GLU:OE2	1:B:446:PRO:HG3	2.20	0.41
1:B:642:GLY:O	1:B:643:LEU:HB2	2.21	0.41
1:C:427:ASN:OD1	1:C:427:ASN:N	2.53	0.41
1:C:675:SER:HA	1:C:733:LEU:HD23	2.02	0.41
1:E:337:ALA:HA	1:E:742:ASN:ND2	2.34	0.41
1:E:427:ASN:OD1	1:E:427:ASN:N	2.53	0.41
1:E:664:LYS:HD2	1:E:664:LYS:HA	1.41	0.41
1:E:780:ASN:O	1:E:781:THR:OG1	2.31	0.41
1:F:642:GLY:O	1:F:643:LEU:HB2	2.21	0.41
1:F:675:SER:HA	1:F:733:LEU:HD23	2.02	0.41
1:G:581:ASP:OD1	1:G:584:THR:OG1	2.27	0.41
1:H:450:ASN:O	1:H:456:SER:HB2	2.20	0.41
1:I:309:ILE:HG22	1:I:387:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:309:ILE:HG22	1:J:387:ALA:HB1	2.02	0.41
1:J:594:THR:HG22	1:J:594:THR:O	2.20	0.41
1:L:328:THR:HG23	1:L:368:GLN:HG3	2.02	0.41
1:L:388:TYR:CE1	1:L:461:PRO:HB3	2.54	0.41
1:M:373:GLU:HB3	1:M:377:THR:HG21	2.02	0.41
1:N:628:TYR:HE2	1:N:632:TRP:HE1	1.67	0.41
1:A:337:ALA:HA	1:A:742:ASN:ND2	2.34	0.41
1:B:427:ASN:N	1:B:427:ASN:OD1	2.53	0.41
1:E:239:ASP:OD2	1:F:262:LEU:HD11	2.21	0.41
1:E:675:SER:HA	1:E:733:LEU:HD23	2.03	0.41
1:G:228:ASP:OD1	1:G:228:ASP:N	2.52	0.41
1:G:577:GLU:O	1:G:614:LYS:HB3	2.21	0.41
1:H:309:ILE:HD12	1:H:375:TRP:CE3	2.55	0.41
1:H:328:THR:HG23	1:H:368:GLN:HG3	2.02	0.41
1:H:676:LYS:HD2	1:H:702:GLN:O	2.20	0.41
1:I:309:ILE:HD12	1:I:375:TRP:CE3	2.55	0.41
1:I:777:SER:O	1:I:777:SER:OG	2.39	0.41
1:J:438:THR:OG1	1:J:440:PRO:O	2.29	0.41
1:J:838:ASN:HD22	1:J:838:ASN:N	2.18	0.41
1:K:236:THR:OG1	1:K:237:ILE:N	2.54	0.41
1:K:594:THR:HG22	1:K:594:THR:O	2.20	0.41
1:L:300:VAL:HB	1:L:483:VAL:HG21	2.03	0.41
1:L:364:SER:HA	1:L:477:LYS:HA	2.02	0.41
1:L:463:ASN:HB2	1:L:465:ASP:OD1	2.20	0.41
1:L:676:LYS:HD2	1:L:702:GLN:O	2.20	0.41
1:L:858:LEU:HD23	1:L:875:VAL:HG21	2.01	0.41
1:M:300:VAL:HB	1:M:483:VAL:HG21	2.03	0.41
1:M:309:ILE:HD12	1:M:375:TRP:CE3	2.55	0.41
1:M:838:ASN:N	1:M:838:ASN:HD22	2.18	0.41
1:N:364:SER:HA	1:N:477:LYS:HA	2.02	0.41
1:A:330:SER:HB3	1:A:333:GLU:HB2	2.03	0.41
1:B:474:LYS:HD3	1:B:474:LYS:HA	1.76	0.41
1:B:577:GLU:O	1:B:614:LYS:HB3	2.21	0.41
1:C:657:LYS:HG3	1:C:722:GLU:HG3	2.03	0.41
1:D:305:GLU:OE2	1:D:446:PRO:HG3	2.20	0.41
1:D:474:LYS:HA	1:D:474:LYS:HD3	1.76	0.41
1:D:577:GLU:O	1:D:614:LYS:HB3	2.21	0.41
1:D:675:SER:HA	1:D:733:LEU:HD23	2.02	0.41
1:E:238:LYS:HZ3	1:E:254:TYR:HH	1.60	0.41
1:G:675:SER:HA	1:G:733:LEU:HD23	2.02	0.41
1:I:463:ASN:HB2	1:I:465:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:676:LYS:HD2	1:I:702:GLN:O	2.20	0.41
1:J:653:GLU:H	1:J:653:GLU:HG3	1.43	0.41
1:K:660:MET:SD	1:K:721:ILE:HD11	2.60	0.41
1:K:687:LYS:HA	1:K:694:LYS:O	2.20	0.41
1:K:717:ASP:N	1:K:717:ASP:OD2	2.53	0.41
1:L:309:ILE:HD12	1:L:375:TRP:CE3	2.55	0.41
1:M:305:GLU:OE2	1:M:446:PRO:HG3	2.20	0.41
1:M:453:ASP:N	1:M:456:SER:HB3	2.27	0.41
1:N:236:THR:OG1	1:N:237:ILE:N	2.54	0.41
1:A:580:PHE:CE1	1:A:611:ILE:HG12	2.55	0.41
1:B:447:LEU:HD12	1:B:448:ALA:O	2.21	0.41
1:C:447:LEU:HD12	1:C:448:ALA:O	2.21	0.41
1:D:447:LEU:HD12	1:D:448:ALA:O	2.21	0.41
1:D:580:PHE:CE1	1:D:611:ILE:HG12	2.55	0.41
1:E:447:LEU:HD12	1:E:448:ALA:O	2.21	0.41
1:E:580:PHE:CE1	1:E:611:ILE:HG12	2.55	0.41
1:F:337:ALA:HA	1:F:742:ASN:ND2	2.34	0.41
1:F:410:THR:CG2	1:F:478:LEU:HB3	2.50	0.41
1:F:599:LYS:HD3	1:F:599:LYS:HA	1.95	0.41
1:G:657:LYS:HG3	1:G:722:GLU:HG3	2.03	0.41
1:H:305:GLU:OE2	1:H:446:PRO:HG3	2.20	0.41
1:H:376:ASN:CB	1:H:750:GLU:HG2	2.51	0.41
1:I:236:THR:OG1	1:I:237:ILE:N	2.54	0.41
1:J:660:MET:SD	1:J:721:ILE:HD11	2.60	0.41
1:K:388:TYR:CE1	1:K:461:PRO:HB3	2.55	0.41
1:L:313:GLU:OE1	1:L:458:ARG:HB3	2.21	0.41
1:L:438:THR:OG1	1:L:440:PRO:O	2.29	0.41
1:M:676:LYS:HD2	1:M:702:GLN:O	2.20	0.41
1:N:376:ASN:CB	1:N:750:GLU:HG2	2.51	0.41
1:N:649:LYS:NZ	1:N:732:TYR:HE1	2.18	0.41
1:N:803:LYS:O	1:N:804:TYR:C	2.58	0.41
1:A:388:TYR:HA	1:A:460:ILE:O	2.20	0.41
1:A:642:GLY:HA2	1:A:704:TYR:OH	2.21	0.41
1:A:803:LYS:HE2	1:A:820:THR:HG22	2.03	0.41
1:B:580:PHE:CE1	1:B:611:ILE:HG12	2.55	0.41
1:B:675:SER:HA	1:B:733:LEU:HD23	2.03	0.41
1:C:642:GLY:O	1:C:643:LEU:HB2	2.21	0.41
1:D:642:GLY:O	1:D:643:LEU:HB2	2.21	0.41
1:D:653:GLU:CB	1:D:726:ILE:HD13	2.50	0.41
1:D:657:LYS:HG3	1:D:722:GLU:HG3	2.03	0.41
1:E:305:GLU:OE2	1:E:446:PRO:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:450:ASN:C	1:E:452:MET:H	2.22	0.41
1:F:657:LYS:HG3	1:F:722:GLU:HG3	2.03	0.41
1:H:236:THR:OG1	1:H:237:ILE:N	2.54	0.41
1:H:238:LYS:HE2	1:H:238:LYS:HB3	1.85	0.41
1:H:364:SER:HA	1:H:477:LYS:HA	2.02	0.41
1:H:455:PHE:CD1	1:H:455:PHE:N	2.89	0.41
1:J:519:LEU:HD23	1:J:526:TYR:HD2	1.85	0.41
1:K:364:SER:HA	1:K:477:LYS:HA	2.02	0.41
1:K:649:LYS:NZ	1:K:732:TYR:HE1	2.18	0.41
1:K:777:SER:O	1:K:777:SER:OG	2.39	0.41
1:L:236:THR:OG1	1:L:237:ILE:N	2.54	0.41
1:M:668:ARG:HG2	1:M:742:ASN:H	1.86	0.41
1:N:385:GLU:OE1	1:N:385:GLU:N	2.54	0.41
1:N:838:ASN:HD22	1:N:838:ASN:N	2.18	0.41
1:A:305:GLU:OE2	1:A:446:PRO:HG3	2.20	0.41
1:A:574:SER:HB2	1:A:644:GLN:HE22	1.86	0.41
1:A:654:THR:HG22	1:A:725:LEU:HB3	2.01	0.41
1:A:657:LYS:HG3	1:A:722:GLU:HG3	2.03	0.41
1:A:675:SER:HA	1:A:733:LEU:HD23	2.02	0.41
1:B:574:SER:HB2	1:B:644:GLN:HE22	1.86	0.41
1:D:224:ASP:OD1	1:D:224:ASP:N	2.41	0.41
1:D:492:SER:O	1:D:492:SER:OG	2.38	0.41
1:D:574:SER:HB2	1:D:644:GLN:HE22	1.86	0.41
1:D:809:THR:HG23	1:D:857:LYS:O	2.19	0.41
1:E:577:GLU:O	1:E:614:LYS:HB3	2.21	0.41
1:E:657:LYS:HG3	1:E:722:GLU:HG3	2.03	0.41
1:F:238:LYS:HZ3	1:F:254:TYR:HH	1.60	0.41
1:F:330:SER:HB3	1:F:333:GLU:HB2	2.03	0.41
1:F:580:PHE:CE1	1:F:611:ILE:HG12	2.55	0.41
1:G:330:SER:HB3	1:G:333:GLU:HB2	2.03	0.41
1:G:642:GLY:HA2	1:G:704:TYR:OH	2.21	0.41
1:G:859:ARG:NH1	1:G:874:SER:HB3	2.36	0.41
1:H:309:ILE:HG22	1:H:387:ALA:HB1	2.02	0.41
1:H:668:ARG:HG2	1:H:742:ASN:H	1.86	0.41
1:I:373:GLU:HB3	1:I:377:THR:HG21	2.02	0.41
1:I:838:ASN:N	1:I:838:ASN:HD22	2.18	0.41
1:J:310:SER:O	1:J:388:TYR:N	2.49	0.41
1:J:349:PHE:HB2	1:J:592:LEU:HD12	2.03	0.41
1:K:300:VAL:HB	1:K:483:VAL:HG21	2.03	0.41
1:L:373:GLU:HB3	1:L:377:THR:HG21	2.02	0.41
1:L:660:MET:SD	1:L:721:ILE:HD11	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:803:LYS:O	1:L:804:TYR:C	2.58	0.41
1:M:309:ILE:HG22	1:M:387:ALA:HB1	2.02	0.41
1:M:374:SER:CB	1:M:750:GLU:HG3	2.50	0.41
1:N:328:THR:HG23	1:N:368:GLN:HG3	2.02	0.41
1:N:777:SER:O	1:N:777:SER:OG	2.39	0.41
1:A:326:ALA:O	1:A:368:GLN:HB2	2.21	0.41
1:A:450:ASN:C	1:A:452:MET:H	2.22	0.41
1:B:326:ALA:O	1:B:368:GLN:HB2	2.21	0.41
1:C:314:HIS:CE1	1:C:458:ARG:HE	2.39	0.41
1:C:577:GLU:O	1:C:614:LYS:HB3	2.21	0.41
1:D:326:ALA:O	1:D:368:GLN:HB2	2.21	0.41
1:D:598:LYS:HA	1:D:598:LYS:HD3	1.79	0.41
1:E:388:TYR:HA	1:E:460:ILE:O	2.20	0.41
1:E:599:LYS:HD3	1:E:599:LYS:HA	1.94	0.41
1:E:792:GLN:HG3	1:F:846:PHE:CD2	2.56	0.41
1:E:809:THR:HG23	1:E:857:LYS:O	2.19	0.41
1:G:305:GLU:OE2	1:G:446:PRO:HG3	2.21	0.41
1:G:574:SER:HB2	1:G:644:GLN:HE22	1.86	0.41
1:G:632:TRP:CD1	1:G:656:ILE:HD13	2.56	0.41
1:G:803:LYS:HE2	1:G:820:THR:HG22	2.03	0.41
1:G:854:THR:HB	1:G:855:TYR:H	1.73	0.41
1:H:519:LEU:HD23	1:H:526:TYR:HD2	1.85	0.41
1:H:628:TYR:HE2	1:H:632:TRP:HE1	1.67	0.41
1:H:717:ASP:N	1:H:717:ASP:OD2	2.53	0.41
1:H:803:LYS:O	1:H:804:TYR:C	2.58	0.41
1:H:838:ASN:N	1:H:838:ASN:HD22	2.18	0.41
1:I:310:SER:O	1:I:388:TYR:N	2.49	0.41
1:I:376:ASN:CB	1:I:750:GLU:HG2	2.51	0.41
1:I:385:GLU:OE1	1:I:385:GLU:N	2.54	0.41
1:I:455:PHE:CD1	1:I:455:PHE:N	2.89	0.41
1:I:639:ASN:O	1:I:646:SER:HA	2.21	0.41
1:I:649:LYS:NZ	1:I:732:TYR:HE1	2.18	0.41
1:J:309:ILE:HD12	1:J:375:TRP:CE3	2.55	0.41
1:J:311:THR:O	1:J:311:THR:OG1	2.24	0.41
1:J:433:LEU:HD12	1:J:433:LEU:HA	1.83	0.41
1:K:309:ILE:HD12	1:K:375:TRP:CE3	2.55	0.41
1:K:309:ILE:HG22	1:K:387:ALA:HB1	2.02	0.41
1:K:628:TYR:HE2	1:K:632:TRP:HE1	1.67	0.41
1:K:639:ASN:O	1:K:646:SER:HA	2.21	0.41
1:L:305:GLU:OE2	1:L:446:PRO:HG3	2.20	0.41
1:L:777:SER:O	1:L:778:THR:OG1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:376:ASN:CB	1:M:750:GLU:HG2	2.51	0.41
1:M:519:LEU:HD23	1:M:526:TYR:HD2	1.85	0.41
1:M:529:ARG:HD3	1:M:529:ARG:HA	1.80	0.41
1:M:649:LYS:NZ	1:M:732:TYR:HE1	2.18	0.41
1:N:313:GLU:OE1	1:N:458:ARG:HB3	2.21	0.41
1:N:373:GLU:HB3	1:N:377:THR:HG21	2.02	0.41
1:A:427:ASN:OD1	1:A:427:ASN:N	2.53	0.41
1:A:447:LEU:HD12	1:A:448:ALA:O	2.21	0.41
1:A:519:LEU:HD23	1:A:526:TYR:CD2	2.56	0.41
1:A:577:GLU:O	1:A:614:LYS:HB3	2.21	0.41
1:A:642:GLY:O	1:A:643:LEU:HB2	2.21	0.41
1:A:859:ARG:NH1	1:A:874:SER:HB3	2.36	0.41
1:B:330:SER:HB3	1:B:333:GLU:HB2	2.03	0.41
1:B:388:TYR:HA	1:B:460:ILE:O	2.20	0.41
1:B:775:ASN:O	1:B:777:SER:N	2.42	0.41
1:B:803:LYS:HE2	1:B:820:THR:HG22	2.03	0.41
1:B:859:ARG:NH1	1:B:874:SER:HB3	2.36	0.41
1:C:326:ALA:O	1:C:368:GLN:HB2	2.21	0.41
1:C:632:TRP:CD1	1:C:656:ILE:HD13	2.56	0.41
1:C:775:ASN:O	1:C:777:SER:N	2.42	0.41
1:D:314:HIS:CE1	1:D:458:ARG:HE	2.39	0.41
1:D:382:ASN:O	1:D:384:GLY:N	2.54	0.41
1:D:388:TYR:HA	1:D:460:ILE:O	2.20	0.41
1:D:777:SER:O	1:D:778:THR:OG1	2.37	0.41
1:E:314:HIS:CE1	1:E:458:ARG:HE	2.39	0.41
1:E:316:SER:H	1:E:452:MET:CE	2.32	0.41
1:E:382:ASN:O	1:E:384:GLY:N	2.54	0.41
1:E:633:SER:OG	1:E:654:THR:OG1	2.09	0.41
1:F:305:GLU:OE2	1:F:446:PRO:HG3	2.21	0.41
1:F:642:GLY:HA2	1:F:704:TYR:OH	2.21	0.41
1:G:240:LEU:HD23	1:G:240:LEU:HA	1.75	0.41
1:G:433:LEU:HA	1:G:433:LEU:HD23	1.74	0.41
1:G:565:TYR:CD1	1:G:570:PRO:HA	2.54	0.41
1:G:642:GLY:O	1:G:643:LEU:HB2	2.21	0.41
1:H:453:ASP:N	1:H:456:SER:HB3	2.27	0.41
1:I:313:GLU:OE1	1:I:458:ARG:HB3	2.21	0.41
1:J:308:ILE:N	1:J:390:ASN:O	2.44	0.41
1:J:385:GLU:N	1:J:385:GLU:OE1	2.54	0.41
1:J:649:LYS:NZ	1:J:732:TYR:HE1	2.18	0.41
1:J:676:LYS:HD2	1:J:702:GLN:O	2.20	0.41
1:K:349:PHE:HB2	1:K:592:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:309:ILE:HG22	1:L:387:ALA:HB1	2.02	0.41
1:L:594:THR:O	1:L:594:THR:HG22	2.20	0.41
1:L:687:LYS:HA	1:L:694:LYS:O	2.20	0.41
1:M:409:THR:O	1:M:409:THR:OG1	2.35	0.41
1:M:569:ILE:H	1:M:569:ILE:HG13	1.74	0.41
1:B:519:LEU:HD23	1:B:526:TYR:CD2	2.56	0.41
1:B:632:TRP:CD1	1:B:656:ILE:HD13	2.56	0.41
1:B:657:LYS:HG3	1:B:722:GLU:HG3	2.03	0.41
1:C:859:ARG:NH1	1:C:874:SER:HB3	2.36	0.41
1:D:341:VAL:HG23	1:D:342:ASN:N	2.35	0.41
1:D:565:TYR:CD1	1:D:570:PRO:HA	2.55	0.41
1:E:318:ASP:O	1:E:318:ASP:OD2	2.39	0.41
1:E:341:VAL:HG23	1:E:342:ASN:N	2.35	0.41
1:E:574:SER:HB2	1:E:644:GLN:HE22	1.86	0.41
1:F:632:TRP:CD1	1:F:656:ILE:HD13	2.56	0.41
1:F:859:ARG:NH1	1:F:874:SER:HB3	2.36	0.41
1:G:382:ASN:O	1:G:384:GLY:N	2.54	0.41
1:G:519:LEU:HD23	1:G:526:TYR:CD2	2.56	0.41
1:H:336:THR:O	1:H:336:THR:OG1	2.39	0.40
1:H:371:ASN:OD1	1:H:371:ASN:N	2.51	0.40
1:H:373:GLU:HB3	1:H:377:THR:HG21	2.02	0.40
1:I:459:LEU:HD23	1:I:459:LEU:HA	1.74	0.40
1:J:236:THR:OG1	1:J:237:ILE:N	2.54	0.40
1:J:859:ARG:NH2	1:J:876:ASP:OD2	2.49	0.40
1:K:313:GLU:OE1	1:K:458:ARG:HB3	2.21	0.40
1:K:385:GLU:N	1:K:385:GLU:OE1	2.54	0.40
1:K:809:THR:HA	1:K:815:PHE:HA	2.03	0.40
1:L:628:TYR:HE2	1:L:632:TRP:HE1	1.68	0.40
1:M:313:GLU:OE1	1:M:458:ARG:HB3	2.21	0.40
1:M:639:ASN:O	1:M:646:SER:HA	2.21	0.40
1:N:300:VAL:HB	1:N:483:VAL:HG21	2.03	0.40
1:N:639:ASN:O	1:N:646:SER:HA	2.21	0.40
1:B:642:GLY:HA2	1:B:704:TYR:OH	2.21	0.40
1:C:283:LYS:HB2	1:D:509:GLN:HG3	2.02	0.40
1:D:283:LYS:HB2	1:E:509:GLN:CG	2.47	0.40
1:D:859:ARG:NH1	1:D:874:SER:HB3	2.36	0.40
1:F:382:ASN:O	1:F:384:GLY:N	2.54	0.40
1:F:447:LEU:HD12	1:F:448:ALA:O	2.21	0.40
1:F:519:LEU:HD23	1:F:526:TYR:CD2	2.56	0.40
1:F:577:GLU:O	1:F:614:LYS:HB3	2.21	0.40
1:G:816:LYS:HB3	1:G:816:LYS:HE2	1.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:364:SER:HA	1:I:477:LYS:HA	2.02	0.40
1:I:374:SER:OG	1:I:471:ASP:OD2	2.36	0.40
1:J:376:ASN:CB	1:J:750:GLU:HG2	2.51	0.40
1:J:809:THR:HA	1:J:815:PHE:HA	2.03	0.40
1:L:455:PHE:CD1	1:L:455:PHE:N	2.89	0.40
1:L:689:LYS:HA	1:L:692:GLU:O	2.22	0.40
1:L:809:THR:HA	1:L:815:PHE:HA	2.04	0.40
1:M:717:ASP:N	1:M:717:ASP:OD2	2.53	0.40
1:A:224:ASP:OD1	1:A:224:ASP:N	2.41	0.40
1:A:518:ILE:O	1:A:613:ILE:N	2.46	0.40
1:C:325:ARG:HD3	1:C:370:SER:H	1.87	0.40
1:F:318:ASP:O	1:F:318:ASP:OD2	2.39	0.40
1:F:574:SER:HB2	1:F:644:GLN:HE22	1.86	0.40
1:F:677:ASP:OD1	1:F:681:SER:HB2	2.22	0.40
1:G:326:ALA:O	1:G:368:GLN:HB2	2.21	0.40
1:G:654:THR:HG22	1:G:725:LEU:HB3	2.02	0.40
1:H:313:GLU:OE1	1:H:458:ARG:HB3	2.21	0.40
1:H:649:LYS:NZ	1:H:732:TYR:HE1	2.18	0.40
1:J:296:ALA:HA	1:J:400:THR:OG1	2.22	0.40
1:J:364:SER:HA	1:J:477:LYS:HA	2.02	0.40
1:K:668:ARG:HG2	1:K:742:ASN:H	1.86	0.40
1:K:687:LYS:HB3	1:K:687:LYS:HE3	1.70	0.40
1:K:689:LYS:HA	1:K:692:GLU:O	2.22	0.40
1:K:774:PHE:HB2	1:F:774:PHE:CG	2.56	0.40
1:L:224:ASP:OD1	1:L:224:ASP:N	2.45	0.40
1:L:376:ASN:CB	1:L:750:GLU:HG2	2.51	0.40
1:M:455:PHE:CD1	1:M:455:PHE:N	2.89	0.40
1:N:676:LYS:HD2	1:N:702:GLN:O	2.20	0.40
1:A:677:ASP:OD1	1:A:681:SER:HB2	2.22	0.40
1:B:318:ASP:O	1:B:318:ASP:OD2	2.39	0.40
1:B:565:TYR:CD1	1:B:570:PRO:HA	2.55	0.40
1:C:318:ASP:O	1:C:318:ASP:OD2	2.39	0.40
1:C:382:ASN:O	1:C:384:GLY:N	2.54	0.40
1:C:474:LYS:HD3	1:C:474:LYS:HA	1.76	0.40
1:D:345:TYR:CE2	1:D:706:LYS:HB3	2.57	0.40
1:D:632:TRP:CD1	1:D:656:ILE:HD13	2.56	0.40
1:E:326:ALA:O	1:E:368:GLN:HB2	2.21	0.40
1:E:519:LEU:HD23	1:E:526:TYR:CD2	2.56	0.40
1:E:859:ARG:NH1	1:E:874:SER:HB3	2.35	0.40
1:F:238:LYS:HD2	1:F:238:LYS:HA	1.95	0.40
1:F:314:HIS:CE1	1:F:458:ARG:HE	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:463:ASN:HB2	1:H:465:ASP:OD1	2.21	0.40
1:H:579:ILE:HB	1:H:612:LEU:HD23	2.04	0.40
1:I:689:LYS:HA	1:I:692:GLU:O	2.22	0.40
1:J:300:VAL:HB	1:J:483:VAL:HG21	2.03	0.40
1:J:345:TYR:CZ	1:J:706:LYS:HD3	2.57	0.40
1:L:246:GLU:H	1:L:246:GLU:HG3	1.70	0.40
1:L:296:ALA:HA	1:L:400:THR:OG1	2.22	0.40
1:L:639:ASN:O	1:L:646:SER:HA	2.21	0.40
1:M:328:THR:HG23	1:M:368:GLN:HG3	2.02	0.40
1:M:385:GLU:N	1:M:385:GLU:OE1	2.54	0.40
1:M:579:ILE:HB	1:M:612:LEU:HD23	2.04	0.40
1:M:689:LYS:HA	1:M:692:GLU:O	2.22	0.40
1:M:809:THR:HA	1:M:815:PHE:HA	2.03	0.40
1:N:463:ASN:HB2	1:N:465:ASP:OD1	2.21	0.40
1:N:579:ILE:HB	1:N:612:LEU:HD23	2.04	0.40
1:A:382:ASN:O	1:A:384:GLY:N	2.54	0.40
1:A:433:LEU:HD23	1:A:433:LEU:HA	1.74	0.40
1:A:777:SER:O	1:A:778:THR:OG1	2.37	0.40
1:A:790:PRO:HD3	1:A:837:THR:HG21	2.04	0.40
1:D:809:THR:HA	1:D:815:PHE:HA	2.04	0.40
1:E:330:SER:HB3	1:E:333:GLU:HB2	2.03	0.40
1:E:642:GLY:HA2	1:E:704:TYR:OH	2.21	0.40
1:G:572:ASP:O	1:G:576:VAL:HG22	2.21	0.40
1:H:224:ASP:OD1	1:H:224:ASP:N	2.45	0.40
1:H:246:GLU:H	1:H:246:GLU:HG3	1.70	0.40
1:H:345:TYR:CZ	1:H:706:LYS:HD3	2.57	0.40
1:H:639:ASN:O	1:H:646:SER:HA	2.21	0.40
1:I:653:GLU:H	1:I:653:GLU:HG3	1.43	0.40
1:I:809:THR:HA	1:I:815:PHE:HA	2.03	0.40
1:J:313:GLU:OE1	1:J:458:ARG:HB3	2.21	0.40
1:J:371:ASN:OD1	1:J:371:ASN:N	2.51	0.40
1:K:376:ASN:CB	1:K:750:GLU:HG2	2.51	0.40
1:L:433:LEU:HD12	1:L:433:LEU:HA	1.83	0.40
1:M:236:THR:OG1	1:M:237:ILE:N	2.54	0.40
1:M:463:ASN:HB2	1:M:465:ASP:OD1	2.21	0.40
1:N:374:SER:OG	1:N:471:ASP:OD2	2.36	0.40
1:A:314:HIS:CE1	1:A:458:ARG:HE	2.39	0.40
1:A:345:TYR:CE2	1:A:706:LYS:HB3	2.57	0.40
1:A:572:ASP:O	1:A:576:VAL:HG22	2.21	0.40
1:A:678:PRO:C	1:A:702:GLN:HE22	2.25	0.40
1:B:382:ASN:O	1:B:384:GLY:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:GLY:HA2	1:C:704:TYR:OH	2.21	0.40
1:C:809:THR:HA	1:C:815:PHE:HA	2.04	0.40
1:D:318:ASP:O	1:D:318:ASP:OD2	2.39	0.40
1:E:260:ASN:OD1	1:E:262:LEU:N	2.29	0.40
1:E:565:TYR:CD1	1:E:570:PRO:HA	2.55	0.40
1:E:632:TRP:CD1	1:E:656:ILE:HD13	2.56	0.40
1:F:572:ASP:O	1:F:576:VAL:HG22	2.21	0.40
1:G:777:SER:O	1:G:778:THR:OG1	2.37	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	658/667 (99%)	545 (83%)	109 (17%)	4 (1%)	25	59
1	B	658/667 (99%)	545 (83%)	109 (17%)	4 (1%)	25	59
1	C	658/667 (99%)	546 (83%)	108 (16%)	4 (1%)	25	59
1	D	658/667 (99%)	545 (83%)	109 (17%)	4 (1%)	25	59
1	E	658/667 (99%)	545 (83%)	109 (17%)	4 (1%)	25	59
1	F	658/667 (99%)	546 (83%)	108 (16%)	4 (1%)	25	59
1	G	658/667 (99%)	545 (83%)	109 (17%)	4 (1%)	25	59
1	H	658/667 (99%)	550 (84%)	103 (16%)	5 (1%)	19	54
1	I	658/667 (99%)	549 (83%)	104 (16%)	5 (1%)	19	54
1	J	658/667 (99%)	547 (83%)	106 (16%)	5 (1%)	19	54
1	K	658/667 (99%)	550 (84%)	103 (16%)	5 (1%)	19	54
1	L	658/667 (99%)	549 (83%)	104 (16%)	5 (1%)	19	54
1	M	658/667 (99%)	548 (83%)	105 (16%)	5 (1%)	19	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	658/667 (99%)	550 (84%)	103 (16%)	5 (1%)	19	54
All	All	9212/9338 (99%)	7660 (83%)	1489 (16%)	63 (1%)	26	57

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	854	THR
1	H	855	TYR
1	I	854	THR
1	I	855	TYR
1	J	854	THR
1	J	855	TYR
1	K	854	THR
1	K	855	TYR
1	L	854	THR
1	L	855	TYR
1	M	854	THR
1	M	855	TYR
1	N	854	THR
1	N	855	TYR
1	A	854	THR
1	A	855	TYR
1	B	854	THR
1	B	855	TYR
1	C	854	THR
1	C	855	TYR
1	D	854	THR
1	D	855	TYR
1	E	854	THR
1	E	855	TYR
1	F	854	THR
1	F	855	TYR
1	G	854	THR
1	G	855	TYR
1	A	638	THR
1	B	638	THR
1	C	638	THR
1	D	638	THR
1	E	638	THR
1	F	638	THR
1	G	638	THR
1	H	240	LEU

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Mol	Chain	Res	Type
1	H	638	THR
1	I	240	LEU
1	I	638	THR
1	J	240	LEU
1	J	638	THR
1	K	240	LEU
1	K	638	THR
1	L	240	LEU
1	L	638	THR
1	M	240	LEU
1	M	638	THR
1	N	240	LEU
1	N	638	THR
1	H	637	THR
1	I	637	THR
1	J	637	THR
1	K	637	THR
1	L	637	THR
1	M	637	THR
1	N	637	THR
1	A	665	PRO
1	B	665	PRO
1	C	665	PRO
1	D	665	PRO
1	E	665	PRO
1	F	665	PRO
1	G	665	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	586/593 (99%)	544 (93%)	42 (7%)	14	44
1	B	586/593 (99%)	544 (93%)	42 (7%)	14	44
1	C	586/593 (99%)	544 (93%)	42 (7%)	14	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	586/593 (99%)	544 (93%)	42 (7%)	14	44
1	E	586/593 (99%)	544 (93%)	42 (7%)	14	44
1	F	586/593 (99%)	544 (93%)	42 (7%)	14	44
1	G	586/593 (99%)	544 (93%)	42 (7%)	14	44
1	H	586/593 (99%)	505 (86%)	81 (14%)	3	16
1	I	586/593 (99%)	506 (86%)	80 (14%)	3	16
1	J	586/593 (99%)	506 (86%)	80 (14%)	3	16
1	K	586/593 (99%)	506 (86%)	80 (14%)	3	16
1	L	586/593 (99%)	505 (86%)	81 (14%)	3	16
1	M	586/593 (99%)	506 (86%)	80 (14%)	3	16
1	N	586/593 (99%)	506 (86%)	80 (14%)	3	16
All	All	8204/8302 (99%)	7348 (90%)	856 (10%)	10	27

All (856) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	223	ASN
1	H	229	SER
1	H	231	GLU
1	H	236	THR
1	H	241	ILE
1	H	246	GLU
1	H	248	SER
1	H	258	VAL
1	H	265	ASN
1	H	278	SER
1	H	280	SER
1	H	281	PHE
1	H	287	THR
1	H	317	THR
1	H	321	LYS
1	H	327	THR
1	H	336	THR
1	H	361	THR
1	H	393	VAL
1	H	407	THR
1	H	410	THR
1	H	414	LEU

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Mol	Chain	Res	Type
1	H	417	ASP
1	H	426	GLU
1	H	453	ASP
1	H	455	PHE
1	H	456	SER
1	H	467	LEU
1	H	468	LYS
1	H	499	GLU
1	H	505	ASP
1	H	508	SER
1	H	512	SER
1	H	523	ASN
1	H	525	SER
1	H	531	THR
1	H	535	LEU
1	H	544	GLU
1	H	568	ASP
1	H	582	ASP
1	H	590	ASP
1	H	596	SER
1	H	605	LEU
1	H	617	THR
1	H	631	THR
1	H	635	VAL
1	H	636	ASN
1	H	646	SER
1	H	649	LYS
1	H	653	GLU
1	H	668	ARG
1	H	675	SER
1	H	679	LEU
1	H	680	THR
1	H	681	SER
1	H	683	SER
1	H	691	LYS
1	H	693	GLU
1	H	697	TYR
1	H	698	LEU
1	H	704	TYR
1	H	705	THR
1	H	707	PHE
1	H	708	SER

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Mol	Chain	Res	Type
1	H	722	GLU
1	H	724	THR
1	H	725	LEU
1	H	731	THR
1	H	739	THR
1	H	740	GLU
1	H	749	ASP
1	H	750	GLU
1	H	777	SER
1	H	793	THR
1	H	809	THR
1	H	822	ASP
1	H	838	ASN
1	H	854	THR
1	H	856	LYS
1	H	866	ASP
1	H	867	ASP
1	I	223	ASN
1	I	229	SER
1	I	231	GLU
1	I	236	THR
1	I	241	ILE
1	I	246	GLU
1	I	248	SER
1	I	258	VAL
1	I	265	ASN
1	I	278	SER
1	I	280	SER
1	I	281	PHE
1	I	287	THR
1	I	317	THR
1	I	321	LYS
1	I	327	THR
1	I	336	THR
1	I	361	THR
1	I	393	VAL
1	I	407	THR
1	I	410	THR
1	I	414	LEU
1	I	417	ASP
1	I	426	GLU
1	I	453	ASP

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Mol	Chain	Res	Type
1	I	455	PHE
1	I	456	SER
1	I	467	LEU
1	I	468	LYS
1	I	499	GLU
1	I	505	ASP
1	I	508	SER
1	I	512	SER
1	I	523	ASN
1	I	525	SER
1	I	531	THR
1	I	535	LEU
1	I	544	GLU
1	I	568	ASP
1	I	582	ASP
1	I	590	ASP
1	I	596	SER
1	I	605	LEU
1	I	617	THR
1	I	631	THR
1	I	635	VAL
1	I	636	ASN
1	I	646	SER
1	I	649	LYS
1	I	653	GLU
1	I	668	ARG
1	I	675	SER
1	I	679	LEU
1	I	680	THR
1	I	683	SER
1	I	691	LYS
1	I	693	GLU
1	I	697	TYR
1	I	698	LEU
1	I	704	TYR
1	I	705	THR
1	I	707	PHE
1	I	708	SER
1	I	722	GLU
1	I	724	THR
1	I	725	LEU
1	I	731	THR

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Mol	Chain	Res	Type
1	I	739	THR
1	I	740	GLU
1	I	749	ASP
1	I	750	GLU
1	I	777	SER
1	I	793	THR
1	I	809	THR
1	I	822	ASP
1	I	838	ASN
1	I	854	THR
1	I	856	LYS
1	I	866	ASP
1	I	867	ASP
1	J	223	ASN
1	J	229	SER
1	J	231	GLU
1	J	236	THR
1	J	241	ILE
1	J	246	GLU
1	J	248	SER
1	J	258	VAL
1	J	265	ASN
1	J	278	SER
1	J	280	SER
1	J	281	PHE
1	J	287	THR
1	J	317	THR
1	J	321	LYS
1	J	327	THR
1	J	336	THR
1	J	361	THR
1	J	393	VAL
1	J	407	THR
1	J	410	THR
1	J	414	LEU
1	J	417	ASP
1	J	426	GLU
1	J	453	ASP
1	J	455	PHE
1	J	456	SER
1	J	467	LEU
1	J	468	LYS

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Mol	Chain	Res	Type
1	J	499	GLU
1	J	505	ASP
1	J	508	SER
1	J	512	SER
1	J	523	ASN
1	J	525	SER
1	J	531	THR
1	J	535	LEU
1	J	544	GLU
1	J	568	ASP
1	J	582	ASP
1	J	590	ASP
1	J	596	SER
1	J	605	LEU
1	J	617	THR
1	J	631	THR
1	J	635	VAL
1	J	636	ASN
1	J	646	SER
1	J	649	LYS
1	J	653	GLU
1	J	668	ARG
1	J	675	SER
1	J	679	LEU
1	J	680	THR
1	J	683	SER
1	J	691	LYS
1	J	693	GLU
1	J	697	TYR
1	J	698	LEU
1	J	704	TYR
1	J	705	THR
1	J	707	PHE
1	J	708	SER
1	J	722	GLU
1	J	724	THR
1	J	725	LEU
1	J	731	THR
1	J	739	THR
1	J	740	GLU
1	J	749	ASP
1	J	750	GLU

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Mol	Chain	Res	Type
1	J	777	SER
1	J	793	THR
1	J	809	THR
1	J	822	ASP
1	J	838	ASN
1	J	854	THR
1	J	856	LYS
1	J	866	ASP
1	J	867	ASP
1	K	223	ASN
1	K	229	SER
1	K	231	GLU
1	K	236	THR
1	K	241	ILE
1	K	246	GLU
1	K	248	SER
1	K	258	VAL
1	K	265	ASN
1	K	278	SER
1	K	280	SER
1	K	281	PHE
1	K	287	THR
1	K	317	THR
1	K	321	LYS
1	K	327	THR
1	K	336	THR
1	K	361	THR
1	K	393	VAL
1	K	407	THR
1	K	410	THR
1	K	414	LEU
1	K	417	ASP
1	K	426	GLU
1	K	453	ASP
1	K	455	PHE
1	K	456	SER
1	K	467	LEU
1	K	468	LYS
1	K	499	GLU
1	K	505	ASP
1	K	508	SER
1	K	512	SER

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Mol	Chain	Res	Type
1	K	523	ASN
1	K	525	SER
1	K	531	THR
1	K	535	LEU
1	K	544	GLU
1	K	568	ASP
1	K	582	ASP
1	K	590	ASP
1	K	596	SER
1	K	605	LEU
1	K	617	THR
1	K	631	THR
1	K	635	VAL
1	K	636	ASN
1	K	646	SER
1	K	649	LYS
1	K	653	GLU
1	K	668	ARG
1	K	675	SER
1	K	679	LEU
1	K	680	THR
1	K	683	SER
1	K	691	LYS
1	K	693	GLU
1	K	697	TYR
1	K	698	LEU
1	K	704	TYR
1	K	705	THR
1	K	707	PHE
1	K	708	SER
1	K	722	GLU
1	K	724	THR
1	K	725	LEU
1	K	731	THR
1	K	739	THR
1	K	740	GLU
1	K	749	ASP
1	K	750	GLU
1	K	777	SER
1	K	793	THR
1	K	809	THR
1	K	822	ASP

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Mol	Chain	Res	Type
1	K	838	ASN
1	K	854	THR
1	K	856	LYS
1	K	866	ASP
1	K	867	ASP
1	L	223	ASN
1	L	229	SER
1	L	231	GLU
1	L	236	THR
1	L	241	ILE
1	L	246	GLU
1	L	248	SER
1	L	258	VAL
1	L	265	ASN
1	L	278	SER
1	L	280	SER
1	L	281	PHE
1	L	287	THR
1	L	317	THR
1	L	321	LYS
1	L	327	THR
1	L	336	THR
1	L	361	THR
1	L	393	VAL
1	L	407	THR
1	L	410	THR
1	L	414	LEU
1	L	417	ASP
1	L	426	GLU
1	L	453	ASP
1	L	455	PHE
1	L	456	SER
1	L	467	LEU
1	L	468	LYS
1	L	499	GLU
1	L	505	ASP
1	L	508	SER
1	L	512	SER
1	L	523	ASN
1	L	525	SER
1	L	531	THR
1	L	535	LEU

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Mol	Chain	Res	Type
1	L	544	GLU
1	L	568	ASP
1	L	582	ASP
1	L	590	ASP
1	L	596	SER
1	L	605	LEU
1	L	617	THR
1	L	631	THR
1	L	635	VAL
1	L	636	ASN
1	L	646	SER
1	L	649	LYS
1	L	653	GLU
1	L	668	ARG
1	L	675	SER
1	L	679	LEU
1	L	680	THR
1	L	681	SER
1	L	683	SER
1	L	691	LYS
1	L	693	GLU
1	L	697	TYR
1	L	698	LEU
1	L	704	TYR
1	L	705	THR
1	L	707	PHE
1	L	708	SER
1	L	722	GLU
1	L	724	THR
1	L	725	LEU
1	L	731	THR
1	L	739	THR
1	L	740	GLU
1	L	749	ASP
1	L	750	GLU
1	L	777	SER
1	L	793	THR
1	L	809	THR
1	L	822	ASP
1	L	838	ASN
1	L	854	THR
1	L	856	LYS

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Mol	Chain	Res	Type
1	L	866	ASP
1	L	867	ASP
1	M	223	ASN
1	M	229	SER
1	M	231	GLU
1	M	236	THR
1	M	241	ILE
1	M	246	GLU
1	M	248	SER
1	M	258	VAL
1	M	265	ASN
1	M	278	SER
1	M	280	SER
1	M	281	PHE
1	M	287	THR
1	M	317	THR
1	M	321	LYS
1	M	327	THR
1	M	336	THR
1	M	361	THR
1	M	393	VAL
1	M	407	THR
1	M	410	THR
1	M	414	LEU
1	M	417	ASP
1	M	426	GLU
1	M	453	ASP
1	M	455	PHE
1	M	456	SER
1	M	467	LEU
1	M	468	LYS
1	M	499	GLU
1	M	505	ASP
1	M	508	SER
1	M	512	SER
1	M	523	ASN
1	M	525	SER
1	M	531	THR
1	M	535	LEU
1	M	544	GLU
1	M	568	ASP
1	M	582	ASP

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Mol	Chain	Res	Type
1	M	590	ASP
1	M	596	SER
1	M	605	LEU
1	M	617	THR
1	M	631	THR
1	M	635	VAL
1	M	636	ASN
1	M	646	SER
1	M	649	LYS
1	M	653	GLU
1	M	668	ARG
1	M	675	SER
1	M	679	LEU
1	M	680	THR
1	M	683	SER
1	M	691	LYS
1	M	693	GLU
1	M	697	TYR
1	M	698	LEU
1	M	704	TYR
1	M	705	THR
1	M	707	PHE
1	M	708	SER
1	M	722	GLU
1	M	724	THR
1	M	725	LEU
1	M	731	THR
1	M	739	THR
1	M	740	GLU
1	M	749	ASP
1	M	750	GLU
1	M	777	SER
1	M	793	THR
1	M	809	THR
1	M	822	ASP
1	M	838	ASN
1	M	854	THR
1	M	856	LYS
1	M	866	ASP
1	M	867	ASP
1	N	223	ASN
1	N	229	SER

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Mol	Chain	Res	Type
1	N	231	GLU
1	N	236	THR
1	N	241	ILE
1	N	246	GLU
1	N	248	SER
1	N	258	VAL
1	N	265	ASN
1	N	278	SER
1	N	280	SER
1	N	281	PHE
1	N	287	THR
1	N	317	THR
1	N	321	LYS
1	N	327	THR
1	N	336	THR
1	N	361	THR
1	N	393	VAL
1	N	407	THR
1	N	410	THR
1	N	414	LEU
1	N	417	ASP
1	N	426	GLU
1	N	453	ASP
1	N	455	PHE
1	N	456	SER
1	N	467	LEU
1	N	468	LYS
1	N	499	GLU
1	N	505	ASP
1	N	508	SER
1	N	512	SER
1	N	523	ASN
1	N	525	SER
1	N	531	THR
1	N	535	LEU
1	N	544	GLU
1	N	568	ASP
1	N	582	ASP
1	N	590	ASP
1	N	596	SER
1	N	605	LEU
1	N	617	THR

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Mol	Chain	Res	Type
1	N	631	THR
1	N	635	VAL
1	N	636	ASN
1	N	646	SER
1	N	649	LYS
1	N	653	GLU
1	N	668	ARG
1	N	675	SER
1	N	679	LEU
1	N	680	THR
1	N	683	SER
1	N	691	LYS
1	N	693	GLU
1	N	697	TYR
1	N	698	LEU
1	N	704	TYR
1	N	705	THR
1	N	707	PHE
1	N	708	SER
1	N	722	GLU
1	N	724	THR
1	N	725	LEU
1	N	731	THR
1	N	739	THR
1	N	740	GLU
1	N	749	ASP
1	N	750	GLU
1	N	777	SER
1	N	793	THR
1	N	809	THR
1	N	822	ASP
1	N	838	ASN
1	N	854	THR
1	N	856	LYS
1	N	866	ASP
1	N	867	ASP
1	A	222	ASP
1	A	236	THR
1	A	239	ASP
1	A	248	SER
1	A	281	PHE
1	A	287	THR

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Mol	Chain	Res	Type
1	A	288	GLU
1	A	311	THR
1	A	352	ASN
1	A	359	HIS
1	A	379	LEU
1	A	425	GLN
1	A	426	GLU
1	A	427	ASN
1	A	463	ASN
1	A	470	LEU
1	A	480	THR
1	A	512	SER
1	A	535	LEU
1	A	568	ASP
1	A	574	SER
1	A	581	ASP
1	A	594	THR
1	A	617	THR
1	A	630	SER
1	A	638	THR
1	A	657	LYS
1	A	660	MET
1	A	662	GLU
1	A	664	LYS
1	A	679	LEU
1	A	686	VAL
1	A	705	THR
1	A	718	SER
1	A	739	THR
1	A	742	ASN
1	A	748	LEU
1	A	752	GLU
1	A	812	TYR
1	A	822	ASP
1	A	854	THR
1	A	856	LYS
1	B	222	ASP
1	B	236	THR
1	B	239	ASP
1	B	248	SER
1	B	281	PHE
1	B	287	THR

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Mol	Chain	Res	Type
1	B	288	GLU
1	B	311	THR
1	B	352	ASN
1	B	359	HIS
1	B	379	LEU
1	B	425	GLN
1	B	426	GLU
1	B	427	ASN
1	B	463	ASN
1	B	470	LEU
1	B	480	THR
1	B	512	SER
1	B	535	LEU
1	B	568	ASP
1	B	574	SER
1	B	581	ASP
1	B	594	THR
1	B	617	THR
1	B	630	SER
1	B	638	THR
1	B	657	LYS
1	B	660	MET
1	B	662	GLU
1	B	664	LYS
1	B	679	LEU
1	B	686	VAL
1	B	705	THR
1	B	718	SER
1	B	739	THR
1	B	742	ASN
1	B	748	LEU
1	B	752	GLU
1	B	812	TYR
1	B	822	ASP
1	B	854	THR
1	B	856	LYS
1	C	222	ASP
1	C	236	THR
1	C	239	ASP
1	C	248	SER
1	C	281	PHE
1	C	287	THR

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Mol	Chain	Res	Type
1	C	288	GLU
1	C	311	THR
1	C	352	ASN
1	C	359	HIS
1	C	379	LEU
1	C	425	GLN
1	C	426	GLU
1	C	427	ASN
1	C	463	ASN
1	C	470	LEU
1	C	480	THR
1	C	512	SER
1	C	535	LEU
1	C	568	ASP
1	C	574	SER
1	C	581	ASP
1	C	594	THR
1	C	617	THR
1	C	630	SER
1	C	638	THR
1	C	657	LYS
1	C	660	MET
1	C	662	GLU
1	C	664	LYS
1	C	679	LEU
1	C	686	VAL
1	C	705	THR
1	C	718	SER
1	C	739	THR
1	C	742	ASN
1	C	748	LEU
1	C	752	GLU
1	C	812	TYR
1	C	822	ASP
1	C	854	THR
1	C	856	LYS
1	D	222	ASP
1	D	236	THR
1	D	239	ASP
1	D	248	SER
1	D	281	PHE
1	D	287	THR

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Mol	Chain	Res	Type
1	D	288	GLU
1	D	311	THR
1	D	352	ASN
1	D	359	HIS
1	D	379	LEU
1	D	425	GLN
1	D	426	GLU
1	D	427	ASN
1	D	463	ASN
1	D	470	LEU
1	D	480	THR
1	D	512	SER
1	D	535	LEU
1	D	568	ASP
1	D	574	SER
1	D	581	ASP
1	D	594	THR
1	D	617	THR
1	D	630	SER
1	D	638	THR
1	D	657	LYS
1	D	660	MET
1	D	662	GLU
1	D	664	LYS
1	D	679	LEU
1	D	686	VAL
1	D	705	THR
1	D	718	SER
1	D	739	THR
1	D	742	ASN
1	D	748	LEU
1	D	752	GLU
1	D	812	TYR
1	D	822	ASP
1	D	854	THR
1	D	856	LYS
1	E	222	ASP
1	E	236	THR
1	E	239	ASP
1	E	248	SER
1	E	281	PHE
1	E	287	THR

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Mol	Chain	Res	Type
1	E	288	GLU
1	E	311	THR
1	E	352	ASN
1	E	359	HIS
1	E	379	LEU
1	E	425	GLN
1	E	426	GLU
1	E	427	ASN
1	E	463	ASN
1	E	470	LEU
1	E	480	THR
1	E	512	SER
1	E	535	LEU
1	E	568	ASP
1	E	574	SER
1	E	581	ASP
1	E	594	THR
1	E	617	THR
1	E	630	SER
1	E	638	THR
1	E	657	LYS
1	E	660	MET
1	E	662	GLU
1	E	664	LYS
1	E	679	LEU
1	E	686	VAL
1	E	705	THR
1	E	718	SER
1	E	739	THR
1	E	742	ASN
1	E	748	LEU
1	E	752	GLU
1	E	812	TYR
1	E	822	ASP
1	E	854	THR
1	E	856	LYS
1	F	222	ASP
1	F	236	THR
1	F	239	ASP
1	F	248	SER
1	F	281	PHE
1	F	287	THR

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Mol	Chain	Res	Type
1	F	288	GLU
1	F	311	THR
1	F	352	ASN
1	F	359	HIS
1	F	379	LEU
1	F	425	GLN
1	F	426	GLU
1	F	427	ASN
1	F	463	ASN
1	F	470	LEU
1	F	480	THR
1	F	512	SER
1	F	535	LEU
1	F	568	ASP
1	F	574	SER
1	F	581	ASP
1	F	594	THR
1	F	617	THR
1	F	630	SER
1	F	638	THR
1	F	657	LYS
1	F	660	MET
1	F	662	GLU
1	F	664	LYS
1	F	679	LEU
1	F	686	VAL
1	F	705	THR
1	F	718	SER
1	F	739	THR
1	F	742	ASN
1	F	748	LEU
1	F	752	GLU
1	F	812	TYR
1	F	822	ASP
1	F	854	THR
1	F	856	LYS
1	G	222	ASP
1	G	236	THR
1	G	239	ASP
1	G	248	SER
1	G	281	PHE
1	G	287	THR

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Mol	Chain	Res	Type
1	G	288	GLU
1	G	311	THR
1	G	352	ASN
1	G	359	HIS
1	G	379	LEU
1	G	425	GLN
1	G	426	GLU
1	G	427	ASN
1	G	463	ASN
1	G	470	LEU
1	G	480	THR
1	G	512	SER
1	G	535	LEU
1	G	568	ASP
1	G	574	SER
1	G	581	ASP
1	G	594	THR
1	G	617	THR
1	G	630	SER
1	G	638	THR
1	G	657	LYS
1	G	660	MET
1	G	662	GLU
1	G	664	LYS
1	G	679	LEU
1	G	686	VAL
1	G	705	THR
1	G	718	SER
1	G	739	THR
1	G	742	ASN
1	G	748	LEU
1	G	752	GLU
1	G	812	TYR
1	G	822	ASP
1	G	854	THR
1	G	856	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	223	ASN
1	H	329	ASN

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Mol	Chain	Res	Type
1	H	382	ASN
1	H	450	ASN
1	H	475	GLN
1	H	501	ASN
1	H	509	GLN
1	H	586	ASN
1	H	827	ASN
1	H	838	ASN
1	I	223	ASN
1	I	329	ASN
1	I	382	ASN
1	I	450	ASN
1	I	475	GLN
1	I	501	ASN
1	I	586	ASN
1	I	827	ASN
1	I	838	ASN
1	J	223	ASN
1	J	329	ASN
1	J	382	ASN
1	J	450	ASN
1	J	475	GLN
1	J	501	ASN
1	J	586	ASN
1	J	827	ASN
1	J	838	ASN
1	K	223	ASN
1	K	265	ASN
1	K	329	ASN
1	K	382	ASN
1	K	450	ASN
1	K	475	GLN
1	K	501	ASN
1	K	586	ASN
1	K	827	ASN
1	K	838	ASN
1	L	223	ASN
1	L	329	ASN
1	L	450	ASN
1	L	475	GLN
1	L	501	ASN
1	L	586	ASN

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Mol	Chain	Res	Type
1	L	827	ASN
1	L	838	ASN
1	M	223	ASN
1	M	329	ASN
1	M	382	ASN
1	M	431	ASN
1	M	450	ASN
1	M	475	GLN
1	M	501	ASN
1	M	827	ASN
1	M	838	ASN
1	N	223	ASN
1	N	265	ASN
1	N	329	ASN
1	N	382	ASN
1	N	450	ASN
1	N	475	GLN
1	N	501	ASN
1	N	509	GLN
1	N	586	ASN
1	N	827	ASN
1	N	838	ASN
1	A	225	ASN
1	A	329	ASN
1	A	363	ASN
1	A	382	ASN
1	A	425	GLN
1	A	450	ASN
1	A	536	GLN
1	A	626	ASN
1	A	702	GLN
1	A	775	ASN
1	A	838	ASN
1	B	225	ASN
1	B	329	ASN
1	B	363	ASN
1	B	382	ASN
1	B	425	GLN
1	B	450	ASN
1	B	536	GLN
1	B	626	ASN
1	B	702	GLN

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Mol	Chain	Res	Type
1	B	775	ASN
1	B	838	ASN
1	C	225	ASN
1	C	329	ASN
1	C	363	ASN
1	C	382	ASN
1	C	425	GLN
1	C	450	ASN
1	C	454	GLN
1	C	536	GLN
1	C	626	ASN
1	C	702	GLN
1	C	775	ASN
1	C	838	ASN
1	D	225	ASN
1	D	329	ASN
1	D	363	ASN
1	D	382	ASN
1	D	425	GLN
1	D	450	ASN
1	D	454	GLN
1	D	536	GLN
1	D	626	ASN
1	D	702	GLN
1	D	775	ASN
1	D	838	ASN
1	E	225	ASN
1	E	329	ASN
1	E	363	ASN
1	E	382	ASN
1	E	425	GLN
1	E	450	ASN
1	E	536	GLN
1	E	626	ASN
1	E	702	GLN
1	E	775	ASN
1	E	838	ASN
1	F	225	ASN
1	F	329	ASN
1	F	363	ASN
1	F	382	ASN
1	F	425	GLN

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Mol	Chain	Res	Type
1	F	450	ASN
1	F	536	GLN
1	F	626	ASN
1	F	702	GLN
1	F	775	ASN
1	F	838	ASN
1	G	225	ASN
1	G	329	ASN
1	G	363	ASN
1	G	382	ASN
1	G	425	GLN
1	G	450	ASN
1	G	536	GLN
1	G	626	ASN
1	G	702	GLN
1	G	775	ASN
1	G	838	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 28 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

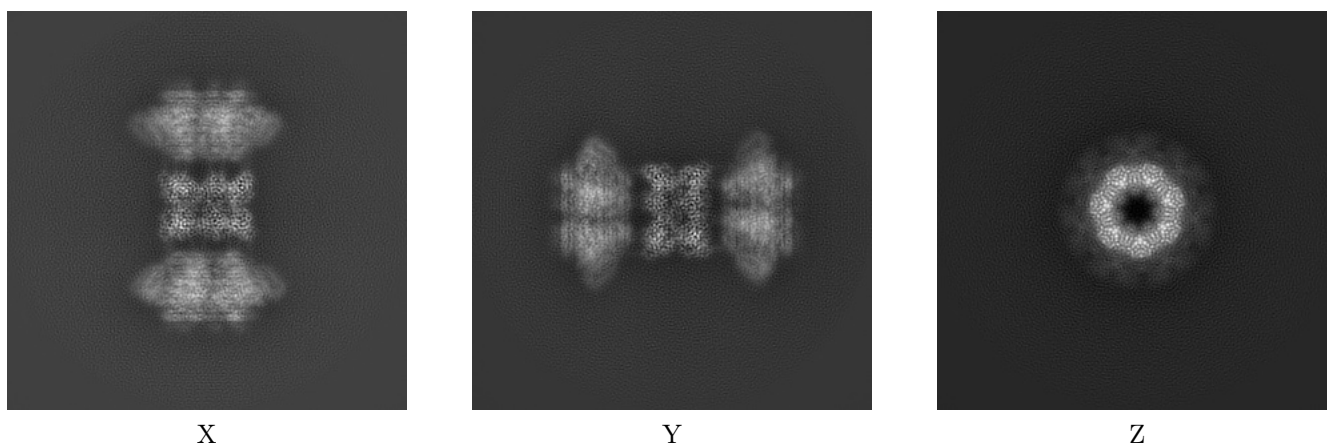
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20927. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

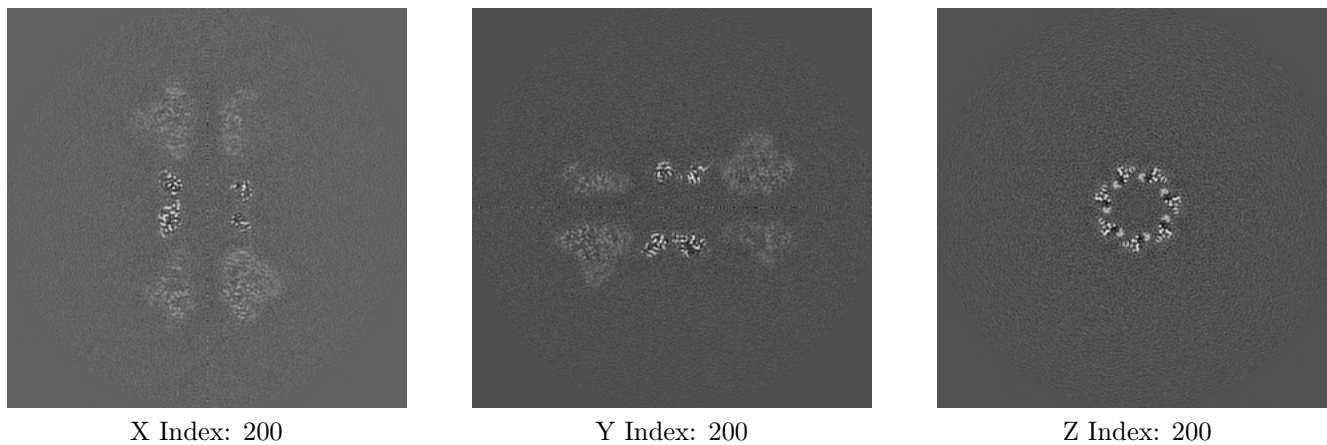
6.1.1 Primary map



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

6.2 Central slices [i](#)

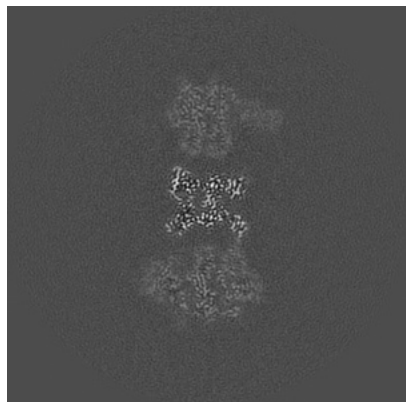
6.2.1 Primary map



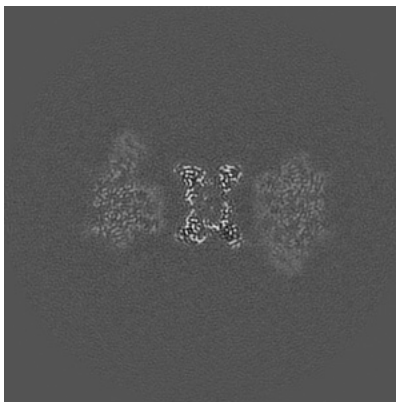
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

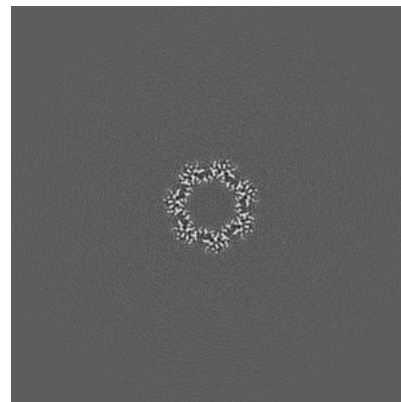
6.3.1 Primary map



X Index: 171



Y Index: 174

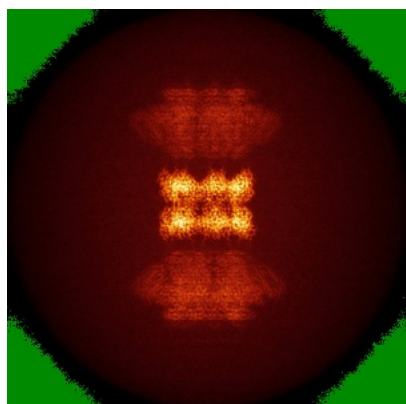


Z Index: 222

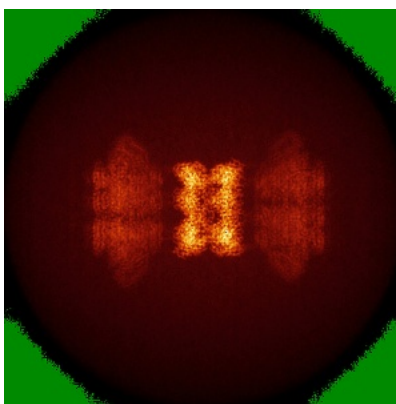
The images above show the largest variance slices of the map in three orthogonal directions.

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

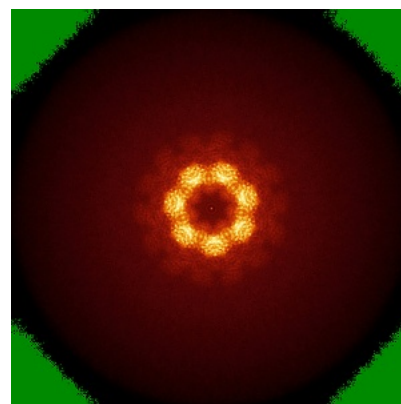
6.4.1 Primary map



X



Y

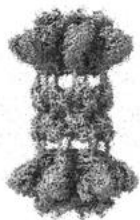


Z

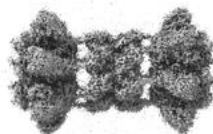
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

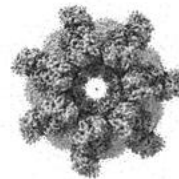
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

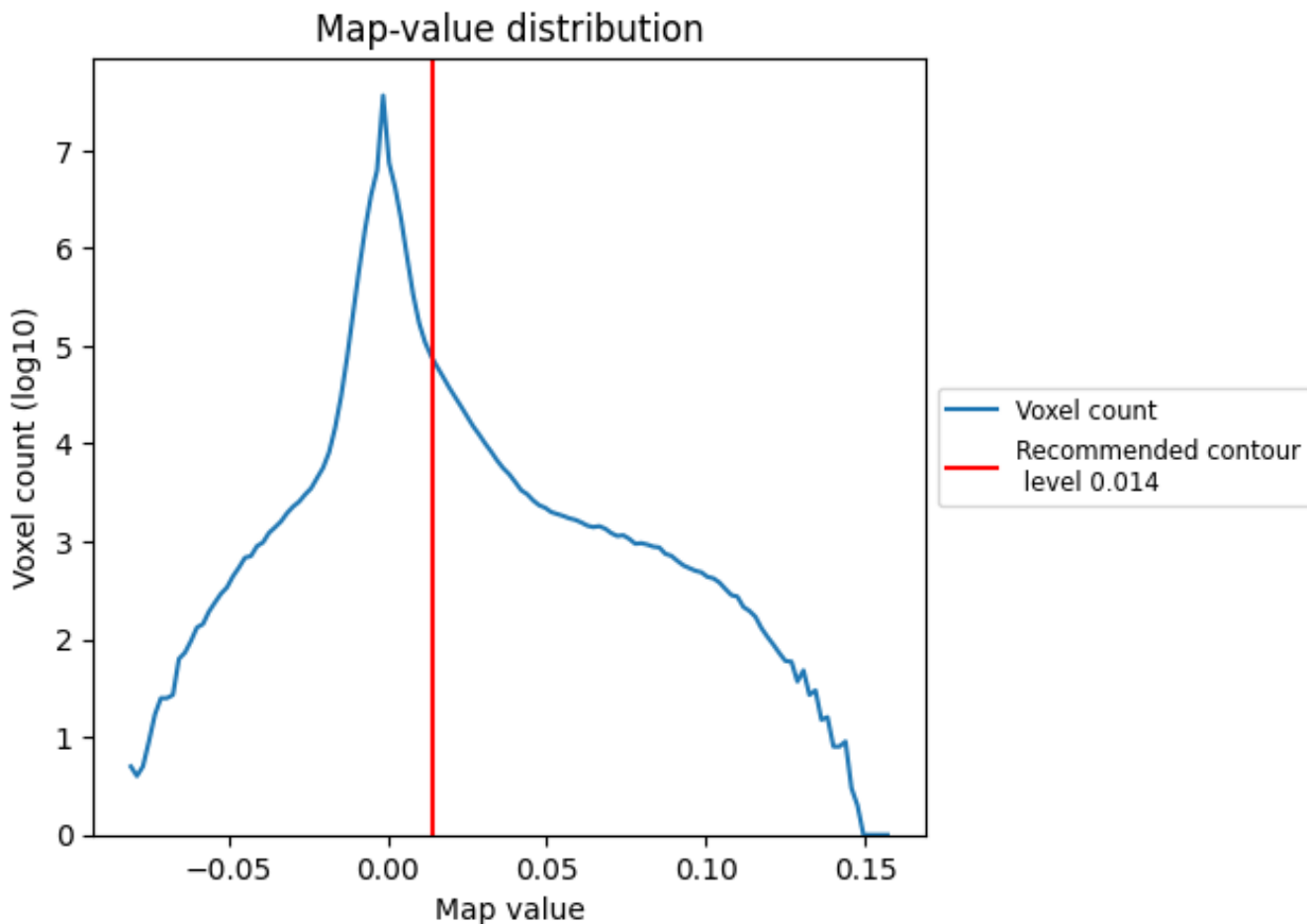
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

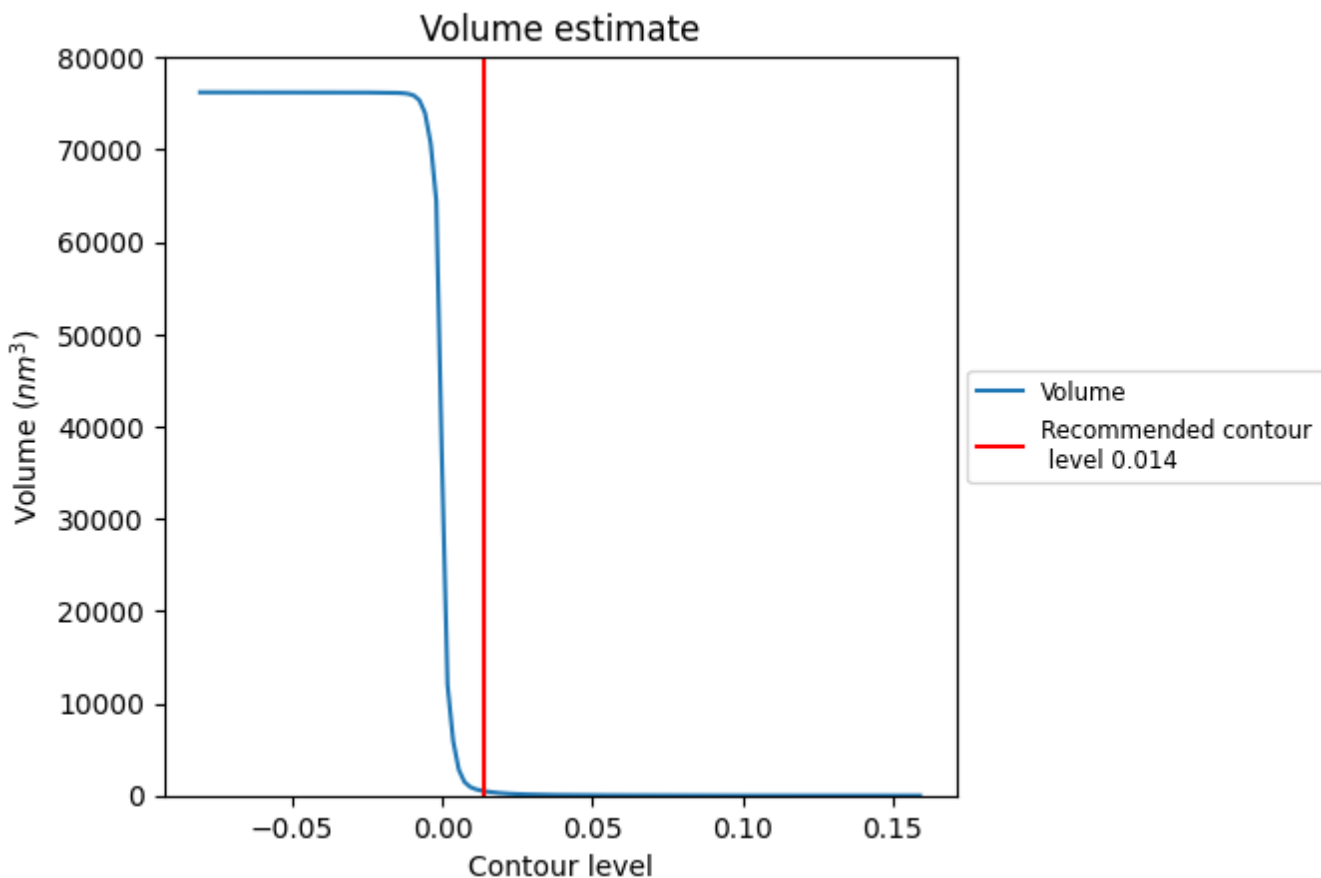
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

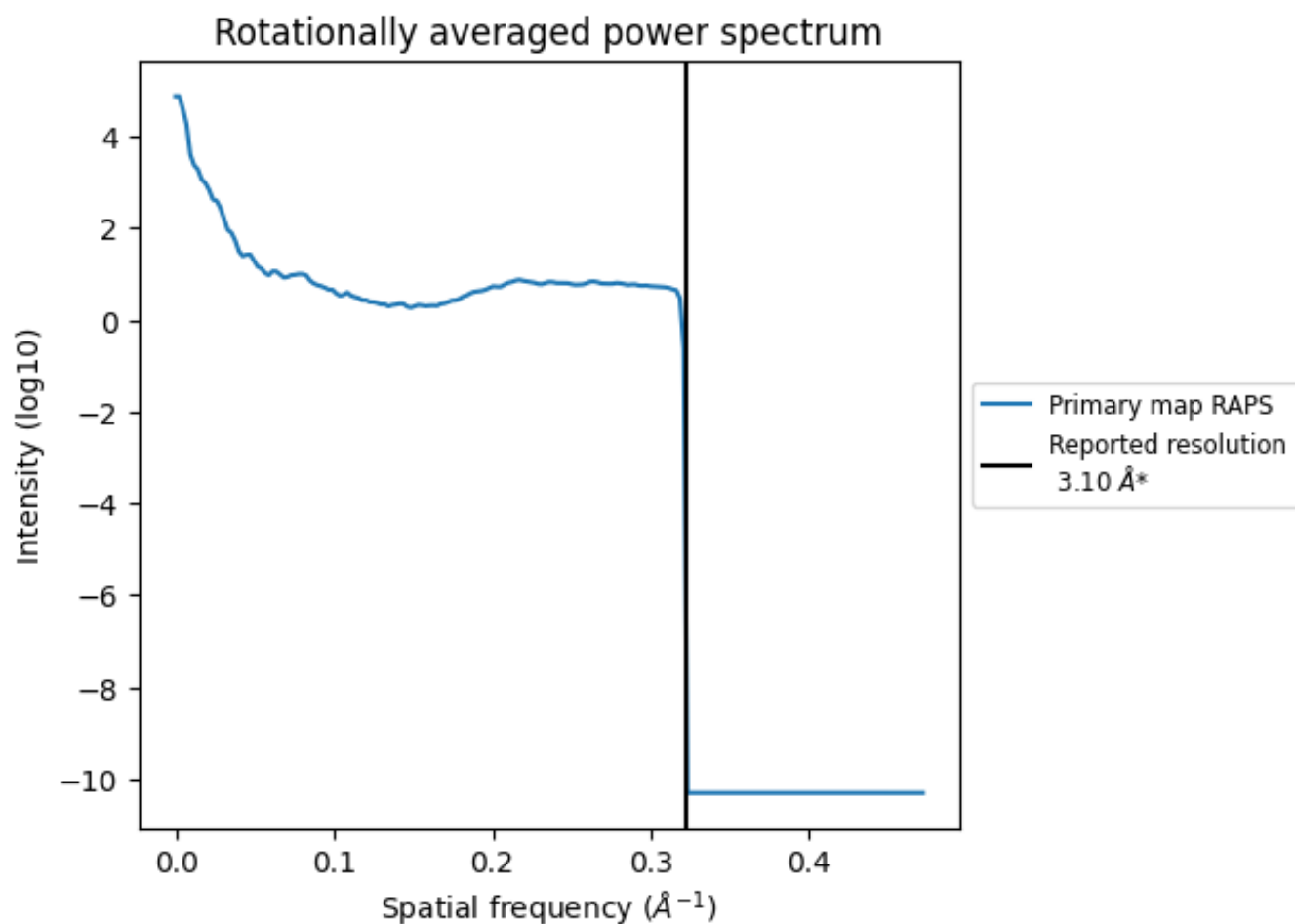
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 479 nm³; this corresponds to an approximate mass of 433 kDa.

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

7.3 Rotationally averaged power spectrum [\(i\)](#)

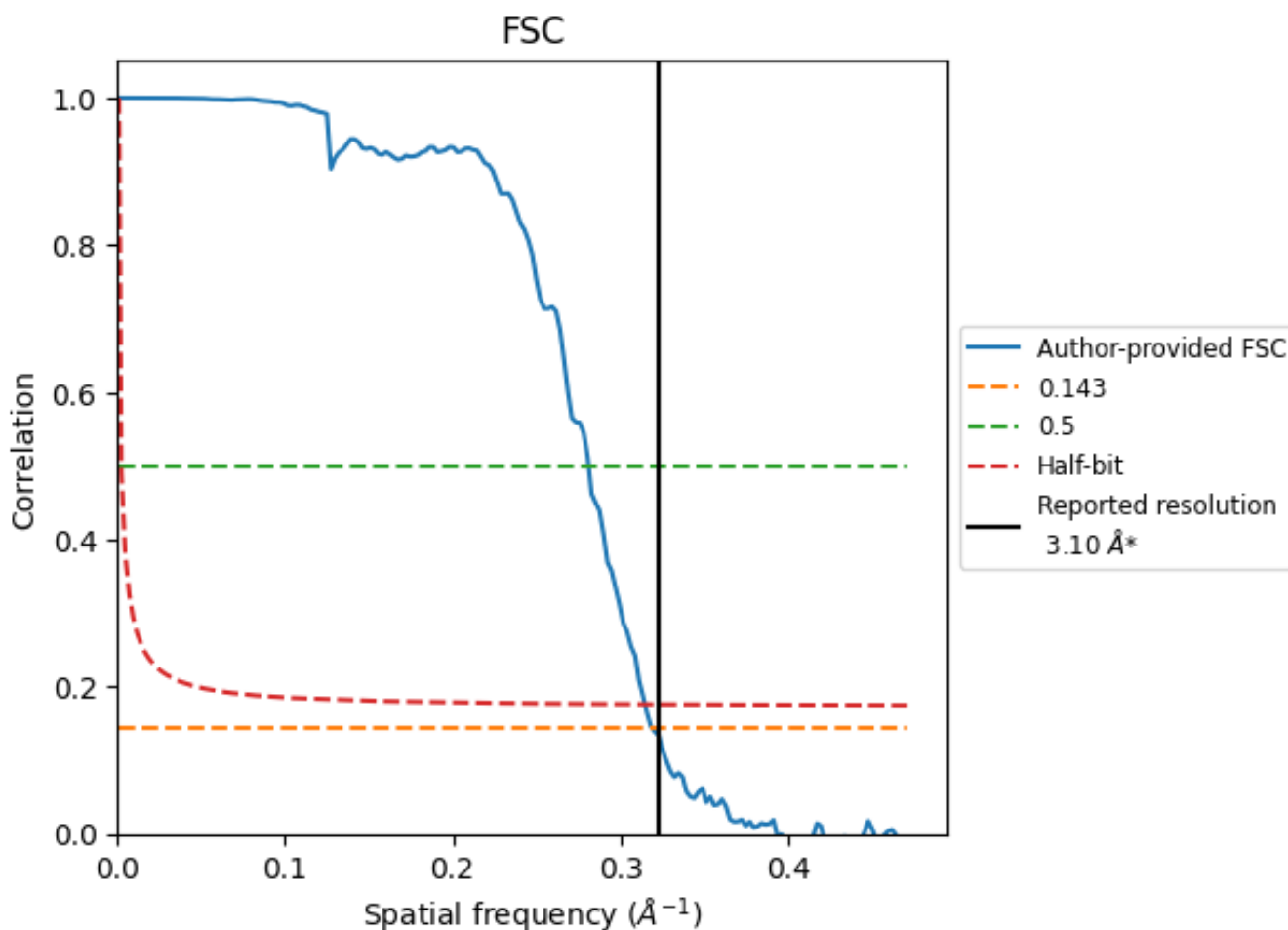


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [\(i\)](#)

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

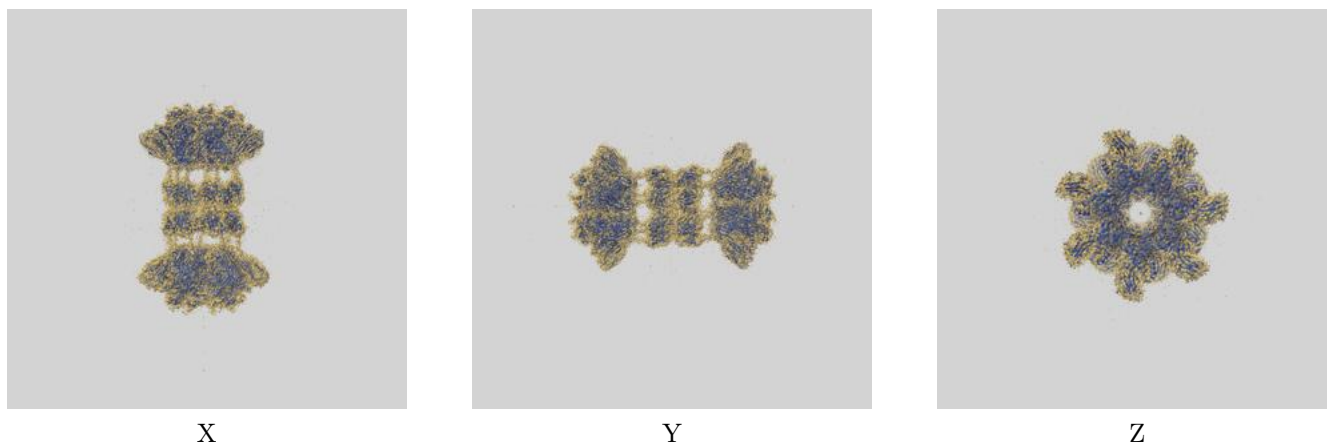
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.56	3.18
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

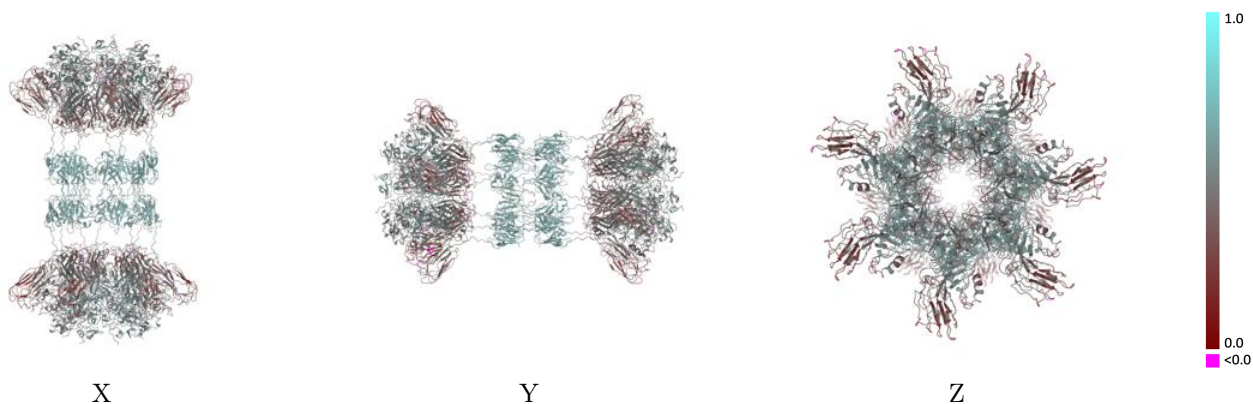
This section contains information regarding the fit between EMDB map EMD-20927 and PDB model 6UWT. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



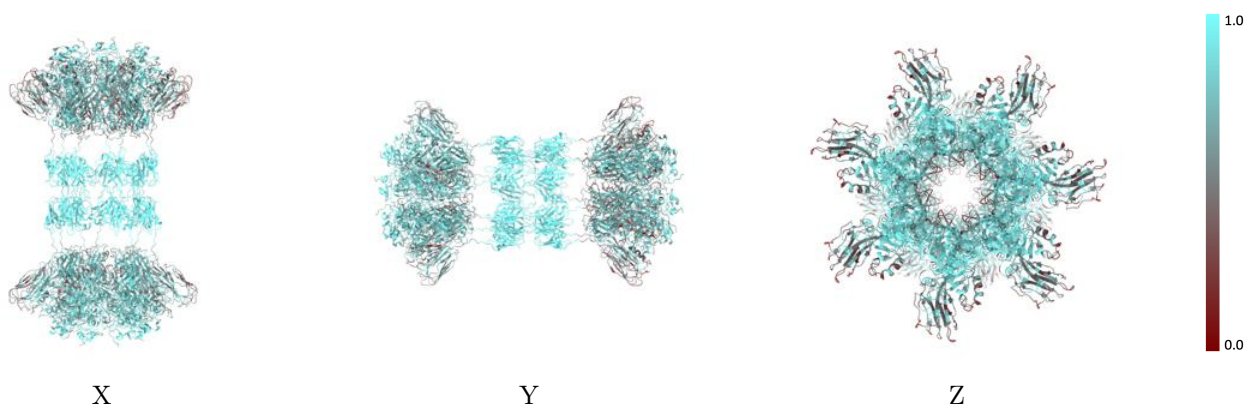
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



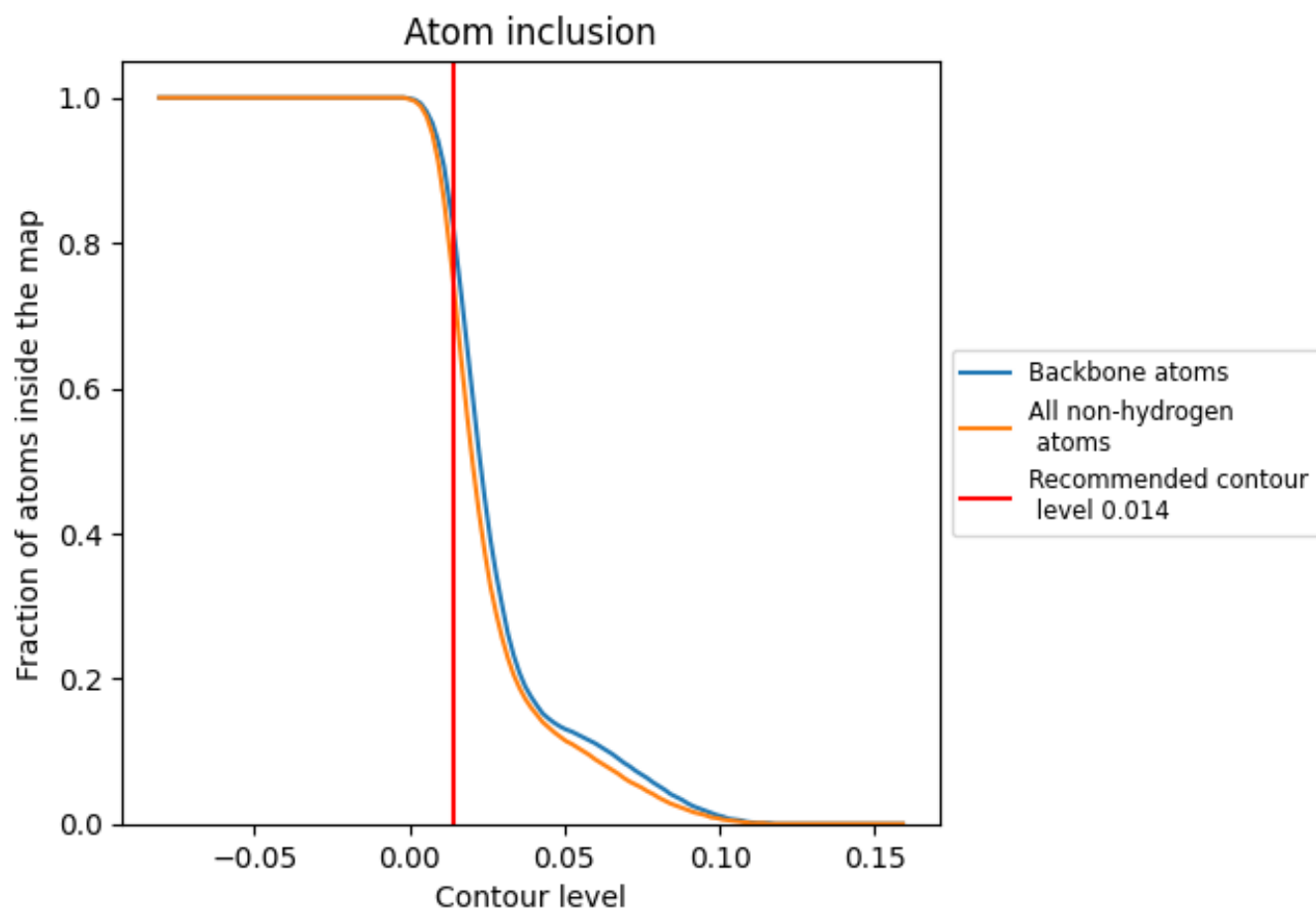
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 75% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7520	 0.4720
A	 0.7210	 0.4680
B	 0.7230	 0.4690
C	 0.7210	 0.4680
D	 0.7190	 0.4670
E	 0.7200	 0.4670
F	 0.7170	 0.4660
G	 0.7160	 0.4650
H	 0.7860	 0.4810
I	 0.7970	 0.4890
J	 0.7900	 0.4810
K	 0.7620	 0.4520
L	 0.7930	 0.4880
M	 0.7910	 0.4870
N	 0.7660	 0.4550

