



wwPDB EM Map/Model Validation Report ⓘ

Oct 18, 2016 – 12:02 PM EDT

PDB ID : 5HX2
EMDB ID: : EMD-8064
Title : In vitro assembled star-shaped hubless T4 baseplate
Authors : Yap, M.L.; Klose, T.; Fokine, A.; Rossmann, M.G.
Deposited on : 2016-01-29
Resolution : 3.80 Å(reported)
Based on PDB ID : 1N80, 3H2T, 2FKK

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

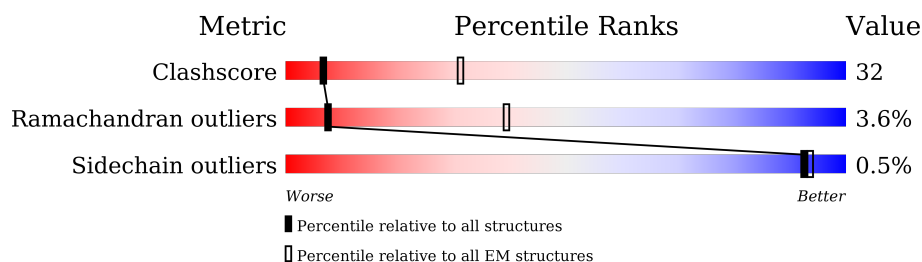
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	1032	55% 42% .
2	B	334	46% 47% 6% .
2	C	334	52% 47% ..
3	D	660	54% 41% ..
3	E	660	63% 30% . .
4	F	196	50% 46% ..
5	G	602	39% 16% . 44%
5	H	602	41% 14% . 44%
5	I	602	40% 15% . 44%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28612 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 Baseplate wedge protein gp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1030	Total	C	N	O	S	0	0
			7511	4844	1265	1383	19		

- Molecule 2 is a protein called Baseplate wedge protein gp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	334	Total	C	N	O	S	0	0
			2521	1598	423	485	15		
2	C	332	Total	C	N	O	S	0	0
			2585	1650	428	491	16		

- Molecule 3 is a protein called Baseplate wedge protein gp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	647	Total	C	N	O	S	0	0
			4845	3072	811	953	9		
3	E	634	Total	C	N	O	S	0	0
			4660	2966	784	902	8		

- Molecule 4 is a protein called Baseplate wedge protein gp53.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	192	Total	C	N	O	S	0	0
			1495	972	239	278	6		

- Molecule 5 is a protein called Baseplate wedge protein gp10.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	340	Total	C	N	O	0	0
			1665	985	340	340		
5	H	340	Total	C	N	O	0	0
			1665	985	340	340		

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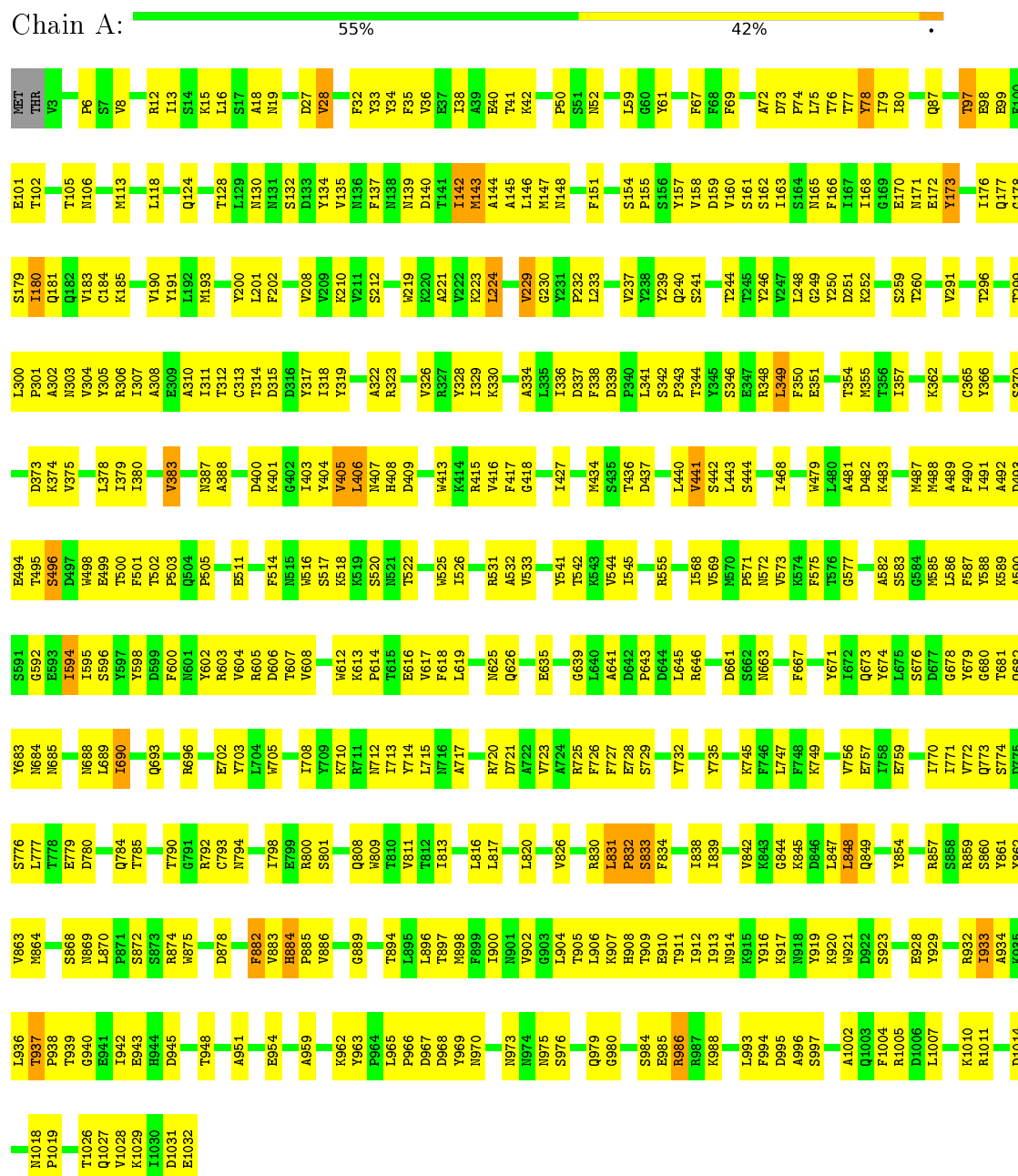
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Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	340	Total	C	N	O	0	0
			1665	985	340	340		

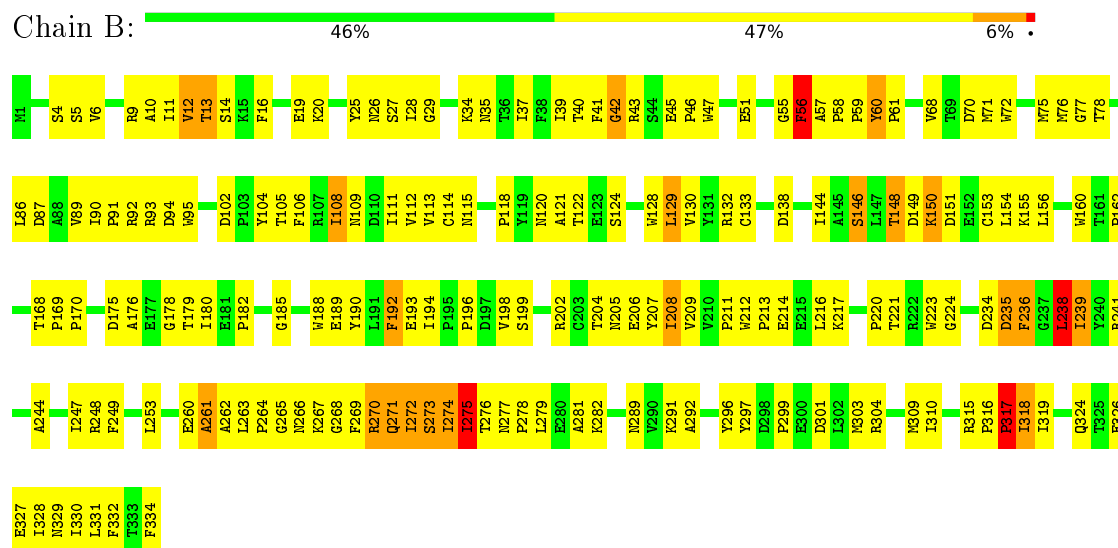
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

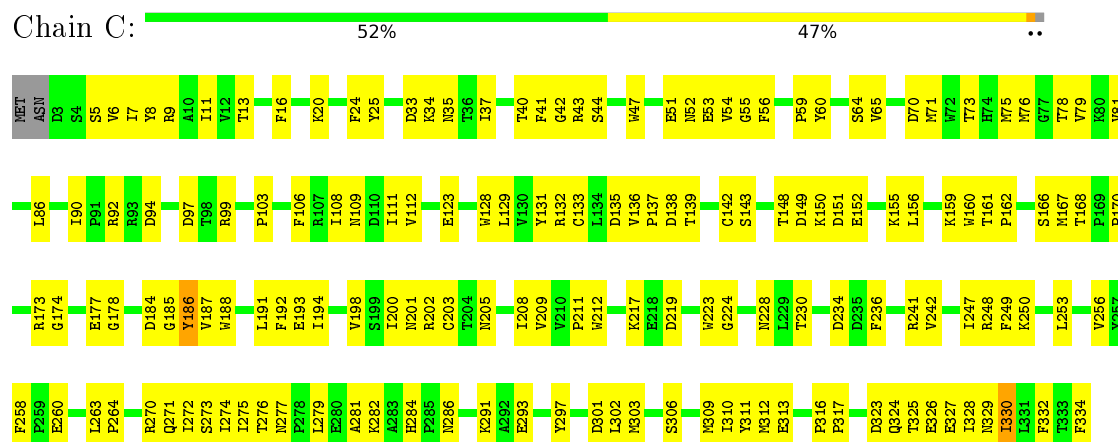
- Molecule 1: Baseplate wedge protein gp7



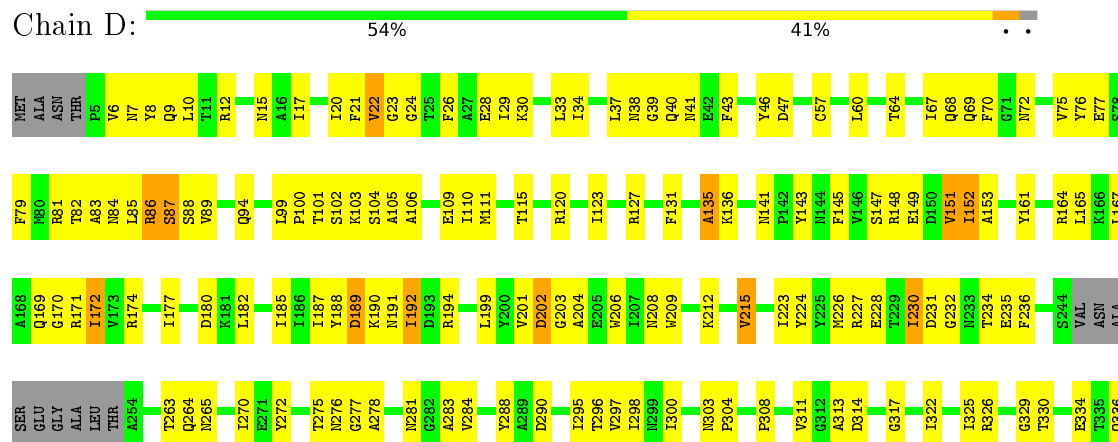
- Molecule 2: Baseplate wedge protein gp8

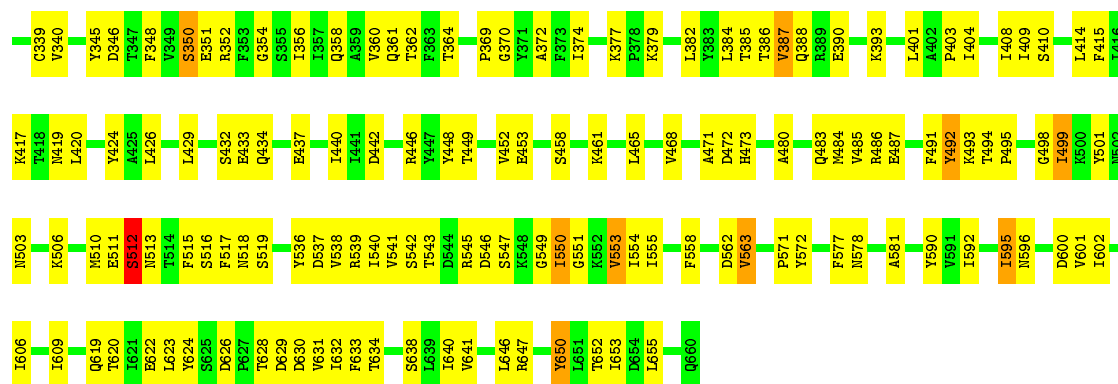


- Molecule 2: Baseplate wedge protein gp8

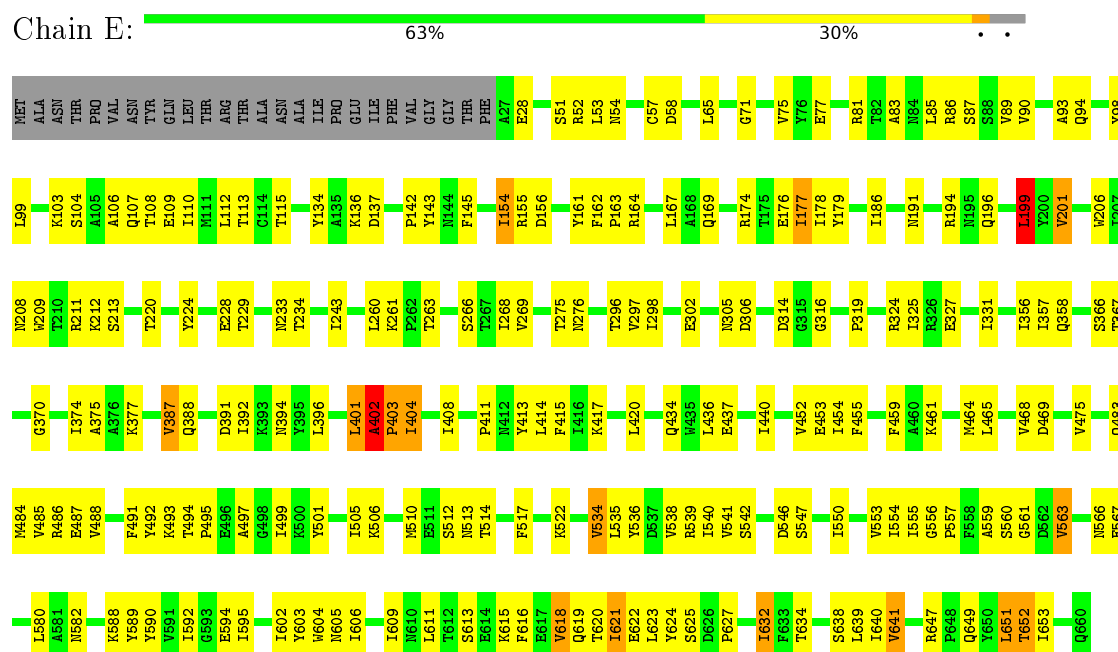


- Molecule 3: Baseplate wedge protein gp6

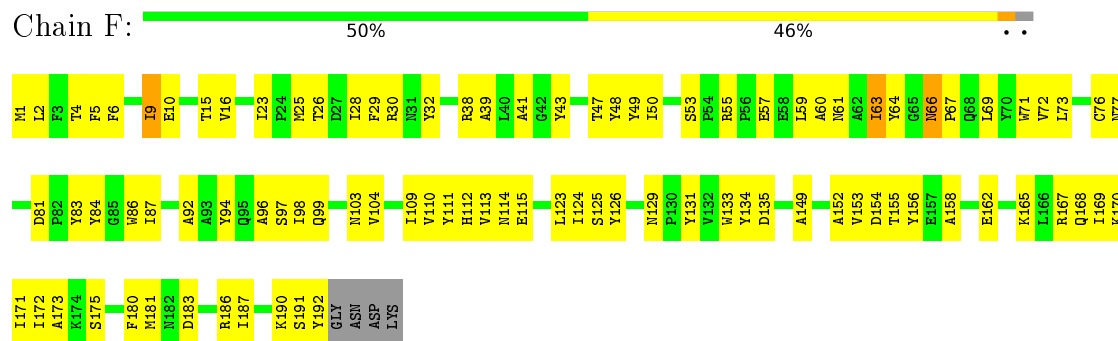




• Molecule 3: Baseplate wedge protein gp6



• Molecule 4: Baseplate wedge protein gp53



• Molecule 5: Baseplate wedge protein gp10



W478	W479	L480	V486	L487	V488	G489	W490	A516	G517	G518	G521	S522	T523	E528	N531	T537	I543	G554	G555	Q556	Y557	D560	E561	S562	G563	P564	Y569	A572	P583	T584	N588	P591	F592	I593	T594	V595	W598	I599	R600	I601	A602				
GLU	HIS	GLY	ASP	ILE	ASN	THR	TRP	PHE	ASN	ASN	GLY	THR	LEU	LEU	LYS	GLU	ILE	ASP	ASP	ASN	L406	Y407	G418	D419	V420	G429	W430	P431	N432	V433	E434	A435	V436	S447	D451	T452	I456	G457	T458	Y460	A463	W469			
ILE	LEU	GLN	GLU	ALA	GLY	ILE	VAL	MET	PRO	PHE	CYS	VAL	GLY	ALA	THR	ASP	ASP	GLY	ILE	GLY	THR	THR	TRP	GLU	GLN	SER	HIS	SER	ASP	THR	ASP	GLU	ASN	GLY	ILE	PRO	ILE	LEU	HIS	PHE	ASP	SER	VAL	THR	
SER	SER	TYR	THR	ARG	GLN	ILE	ARG	LEU	ASP	SER	THR	SER	LYS	THR	GLY	SER	GLY	GLU	LEU	SER	GLY	THR	LYS	SER	ILE	PRO	PHE	ALA	ASP	THR	GLY	LEU	ILE	PRO	ILE	ASN	PRO	THR	LEU	GLU	VAL	ARG	ASN	GLY	
ARG	GLY	GLU	LEU	TYR	TYR	GLY	ASP	VAL	PHE	VAL	ASP	GLY	SER	THR	ASP	GLY	GLU	ASP	GLY	GLY	ASP	PHE	ASN	VAL	GLY	ARG	GLY	THR	ASN	GLY	THR	GLY	ASP	THR	GLY	ASP	THR	GLY	ASP	THR	GLY	VAL	THR	ASP	THR
V128	I7	D12	D13	G16	D17	Y18	L19	R20	K21	G22	G23	I24	K25	I26	I27	E28	P43	A46	G47	K50	T51	Y52	N53	L60	T61	A62	E63	N64	G65	R66	S67	V68	T72	S73	S74	G75	R76	V77	G84	N87	I93	V104	I117	E125	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C	Depositor
Number of particles used	45607	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	22500	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.37	0/7697	0.62	2/10550 (0.0%)
2	B	0.51	0/2591	0.72	2/3546 (0.1%)
2	C	0.55	0/2662	0.65	0/3640
3	D	0.30	0/4935	0.61	0/6735
3	E	0.28	0/4750	0.56	0/6485
4	F	0.52	0/1536	0.64	0/2095
5	G	0.33	0/1663	0.68	0/2304
5	H	0.34	0/1663	0.72	0/2304
5	I	0.35	0/1663	0.68	0/2304
All	All	0.39	0/29160	0.64	4/39963 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
2	B	0	3
2	C	0	2
3	D	0	9
3	E	0	5
4	F	0	1
5	G	0	9
5	H	0	10
5	I	0	11
All	All	0	55

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	848	LEU	CA-CB-CG	5.42	127.77	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	274	ILE	N-CA-C	-5.34	96.59	111.00
2	B	42	GLY	N-CA-C	5.29	126.31	113.10
1	A	349	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	496	SER	Peptide
1	A	831	LEU	Peptide
1	A	832	PRO	Peptide
1	A	917	LYS	Peptide
1	A	97	THR	Peptide
2	B	124	SER	Peptide
2	B	129	LEU	Peptide
2	B	317	PRO	Peptide
2	C	186	TYR	Peptide
2	C	316	PRO	Peptide
3	D	135	ALA	Peptide
3	D	136	LYS	Peptide
3	D	149	GLU	Peptide
3	D	189	ASP	Peptide
3	D	43	PHE	Peptide
3	D	512	SER	Peptide
3	D	572	TYR	Peptide
3	D	577	PHE	Peptide
3	D	650	TYR	Peptide
3	E	199	LEU	Peptide
3	E	401	LEU	Peptide
3	E	402	ALA	Peptide
3	E	588	LYS	Peptide
3	E	651	LEU	Peptide
4	F	66	ASN	Peptide
5	G	112	ALA	Peptide
5	G	125	GLU	Peptide
5	G	137	TYR	Peptide
5	G	431	PRO	Peptide
5	G	524	SER	Peptide
5	G	566	TYR	Peptide
5	G	567	THR	Peptide
5	G	580	HIS	Peptide
5	G	66	LYS	Peptide

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Mol	Chain	Res	Type	Group
5	H	120	SER	Peptide
5	H	17	ASP	Peptide
5	H	408	VAL	Peptide
5	H	429	GLY	Peptide
5	H	49	TRP	Peptide
5	H	496	ASP	Peptide
5	H	583	PRO	Peptide
5	H	592	TYR	Peptide
5	H	76	ARG	Peptide
5	H	97	ASP	Peptide
5	I	125	GLU	Peptide
5	I	18	TYR	Peptide
5	I	50	LYS	Peptide
5	I	556	GLN	Peptide
5	I	557	TYR	Peptide
5	I	60	LEU	Peptide
5	I	62	ALA	Peptide
5	I	66	LYS	Peptide
5	I	68	TYR	Peptide
5	I	7	ILE	Peptide
5	I	84	GLY	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	7511	0	6716	677	0
2	B	2521	0	2282	345	0
2	C	2585	0	2410	232	0
3	D	4845	0	4477	346	0
3	E	4660	0	4258	182	0
4	F	1495	0	1361	121	0
5	G	1665	0	764	81	0
5	H	1665	0	764	81	0
5	I	1665	0	764	86	0
All	All	28612	0	23796	1674	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 32.

All (1674) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:TRP:CZ2	2:B:59:PRO:HD2	1.18	1.67
1:A:902:VAL:HG21	2:B:16:PHE:CE2	1.20	1.67
1:A:685:ASN:ND2	3:D:21:PHE:CE1	1.68	1.58
1:A:663:ASN:CB	3:D:46:TYR:HA	1.11	1.57
1:A:898:MET:HE3	2:C:272:ILE:CD1	1.33	1.56
1:A:667:PHE:HE1	3:D:37:LEU:CD2	1.19	1.52
1:A:1032:GLU:CB	2:B:60:TYR:CD2	1.95	1.50
1:A:720:ARG:NH1	3:D:12:ARG:HD3	1.17	1.47
1:A:667:PHE:CE1	3:D:37:LEU:HD23	1.46	1.47
1:A:679:TYR:CE2	3:D:20:ILE:CD1	1.97	1.46
1:A:898:MET:CE	2:C:272:ILE:HD13	1.46	1.45
1:A:679:TYR:CZ	3:D:20:ILE:HD13	1.48	1.43
1:A:667:PHE:CE1	3:D:37:LEU:CD2	1.97	1.43
1:A:663:ASN:CB	3:D:46:TYR:CA	1.97	1.43
1:A:911:THR:CG2	2:B:315:ARG:HH22	1.27	1.43
1:A:679:TYR:CZ	3:D:20:ILE:CD1	1.98	1.42
1:A:911:THR:HG23	2:B:315:ARG:NH2	1.32	1.42
2:B:47:TRP:CZ2	2:B:59:PRO:CD	2.01	1.42
1:A:161:SER:OG	3:E:156:ASP:CB	1.64	1.41
1:A:886:VAL:HG11	3:D:345:TYR:CE2	1.56	1.41
1:A:902:VAL:CG2	2:B:16:PHE:HE2	1.29	1.40
1:A:685:ASN:ND2	3:D:21:PHE:CD1	1.90	1.40
2:B:239:ILE:HD11	2:B:244:ALA:CB	1.53	1.39
1:A:1002:ALA:HB3	5:G:10:VAL:CB	1.49	1.39
1:A:679:TYR:OH	3:D:20:ILE:CD1	1.64	1.39
1:A:689:LEU:CD1	3:D:75:VAL:HG12	1.52	1.38
1:A:923:SER:HB2	5:I:20:ARG:CB	1.54	1.35
1:A:898:MET:CE	2:C:272:ILE:CD1	2.01	1.33
3:D:288:TYR:CB	3:D:297:VAL:HG11	1.58	1.31
1:A:679:TYR:CE2	3:D:20:ILE:HD11	1.61	1.29
1:A:911:THR:OG1	2:B:330:ILE:HG22	1.14	1.29
1:A:1032:GLU:CB	2:B:60:TYR:HD2	1.37	1.26
2:B:275:ILE:HD12	2:B:276:THR:N	1.47	1.25
2:B:60:TYR:OH	2:C:11:ILE:HG21	1.31	1.25
3:D:86:ARG:HG3	3:D:322:ILE:CD1	1.68	1.24
1:A:898:MET:CB	2:C:330:ILE:CD1	2.17	1.23
1:A:661:ASP:CB	3:D:47:ASP:CB	2.17	1.22
4:F:57:GLU:O	4:F:86:TRP:CZ3	1.92	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:VAL:CG2	2:B:16:PHE:CE2	2.11	1.22
1:A:1032:GLU:CB	2:B:60:TYR:CE2	2.22	1.21
1:A:911:THR:OG1	2:B:330:ILE:CG2	1.87	1.21
3:D:70:PHE:CE1	4:F:26:THR:CG2	2.25	1.20
1:A:908:HIS:HB2	2:B:332:PHE:CE1	1.78	1.19
1:A:1028:VAL:CG2	2:C:7:ILE:HG22	1.74	1.18
1:A:720:ARG:NH1	3:D:12:ARG:CD	2.07	1.17
1:A:995:ASP:O	5:I:12:ASP:O	1.61	1.17
2:B:47:TRP:HZ2	2:B:59:PRO:CD	1.44	1.17
1:A:898:MET:CG	2:C:330:ILE:HD13	1.73	1.17
1:A:913:ILE:HG21	2:B:328:ILE:CD1	1.52	1.17
3:D:115:THR:HG22	3:D:298:ILE:HD11	1.26	1.17
3:D:70:PHE:HE1	4:F:26:THR:CG2	1.56	1.17
1:A:912:ILE:N	2:B:329:ASN:O	1.79	1.16
1:A:679:TYR:CE2	3:D:20:ILE:HD13	1.69	1.16
1:A:685:ASN:CG	3:D:21:PHE:CE1	2.17	1.16
1:A:161:SER:O	3:E:154:ILE:HD12	1.45	1.15
1:A:913:ILE:CG2	2:B:328:ILE:HD13	1.76	1.14
3:D:70:PHE:HE1	4:F:26:THR:HG23	1.09	1.14
1:A:898:MET:CB	2:C:330:ILE:HD12	1.74	1.14
1:A:1018:ASN:CB	2:B:91:PRO:HB3	1.79	1.13
2:B:239:ILE:CD1	2:B:244:ALA:CB	2.25	1.13
2:B:239:ILE:CD1	2:B:244:ALA:HB2	1.79	1.13
1:A:886:VAL:CG1	3:D:345:TYR:HE2	1.61	1.13
1:A:997:SER:O	5:G:19:LEU:HA	1.44	1.12
1:A:689:LEU:HD12	3:D:75:VAL:HG12	1.31	1.12
2:B:239:ILE:HD11	2:B:244:ALA:HB3	1.15	1.11
1:A:886:VAL:O	3:D:364:THR:HB	1.48	1.11
1:A:33:TYR:HE2	2:B:155:LYS:NZ	1.48	1.11
1:A:912:ILE:O	2:B:329:ASN:HB2	1.52	1.10
3:D:86:ARG:HD2	3:D:322:ILE:HD11	1.22	1.10
3:D:86:ARG:CD	3:D:322:ILE:HD11	1.80	1.10
3:D:82:THR:O	4:F:15:THR:HG21	1.49	1.10
1:A:679:TYR:OH	3:D:20:ILE:HD12	1.47	1.10
1:A:874:ARG:NH2	2:C:54:VAL:HA	1.66	1.10
1:A:912:ILE:HG23	2:B:329:ASN:HB2	1.34	1.09
1:A:902:VAL:HG21	2:B:16:PHE:CD2	1.87	1.09
1:A:874:ARG:HH22	2:C:54:VAL:CA	1.65	1.09
1:A:898:MET:HB2	2:C:330:ILE:HD12	1.11	1.09
1:A:161:SER:O	3:E:154:ILE:CD1	1.99	1.08
1:A:913:ILE:HG21	2:B:328:ILE:HD13	1.19	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:MET:HG3	2:C:330:ILE:HD13	1.21	1.08
1:A:861:TYR:HE2	3:D:369:PRO:HG3	1.01	1.08
3:D:115:THR:CG2	3:D:298:ILE:HD11	1.84	1.08
1:A:645:LEU:HD11	4:F:83:TYR:CD2	1.89	1.08
1:A:689:LEU:HD13	3:D:75:VAL:HG12	1.37	1.07
1:A:667:PHE:CZ	3:D:60:LEU:HD21	1.89	1.07
1:A:906:LEU:CD2	2:B:334:PHE:CB	2.32	1.07
1:A:33:TYR:CE2	2:B:155:LYS:NZ	2.23	1.06
1:A:861:TYR:CE2	3:D:369:PRO:HG3	1.88	1.06
3:D:77:GLU:OE2	4:F:29:PHE:CZ	2.08	1.06
1:A:898:MET:SD	2:C:272:ILE:HD11	1.96	1.06
1:A:923:SER:CB	5:I:20:ARG:CB	2.34	1.05
1:A:912:ILE:O	2:B:329:ASN:N	1.89	1.05
1:A:1002:ALA:CB	5:G:10:VAL:CB	2.35	1.05
1:A:645:LEU:HD11	4:F:83:TYR:CE2	1.91	1.05
1:A:898:MET:HB2	2:C:330:ILE:CD1	1.82	1.04
1:A:645:LEU:CD1	4:F:83:TYR:CD2	2.41	1.04
1:A:162:SER:OG	3:E:162:PHE:CD2	2.08	1.04
1:A:667:PHE:CE1	3:D:37:LEU:HD21	1.86	1.03
1:A:161:SER:CB	3:E:156:ASP:CB	2.36	1.03
2:B:47:TRP:CH2	2:B:59:PRO:HD2	1.92	1.03
1:A:1028:VAL:HG22	2:C:7:ILE:HG22	1.36	1.02
1:A:847:LEU:CD2	2:C:325:THR:CG2	2.38	1.02
3:D:86:ARG:HG3	3:D:322:ILE:HD12	1.42	1.01
1:A:6:PRO:HG2	2:B:9:ARG:NH1	1.75	1.01
1:A:847:LEU:CD2	2:C:325:THR:HG22	1.91	1.01
1:A:745:LYS:HE2	2:C:99:ARG:HH22	1.24	1.01
1:A:845:LYS:HD2	2:C:201:ASN:ND2	1.72	1.01
3:D:69:GLN:HG2	4:F:25:MET:CE	1.90	1.00
1:A:912:ILE:O	2:B:329:ASN:CB	2.09	1.00
1:A:720:ARG:HH11	3:D:12:ARG:HD3	1.20	1.00
3:D:69:GLN:HG2	4:F:25:MET:HE2	1.43	1.00
1:A:844:GLY:O	2:C:200:ILE:HG21	1.61	0.99
1:A:685:ASN:OD1	3:D:21:PHE:CZ	2.14	0.99
1:A:745:LYS:CE	2:C:99:ARG:HH22	1.75	0.99
1:A:908:HIS:HA	2:B:332:PHE:HD1	1.24	0.99
1:A:306:ARG:CZ	5:H:561:GLU:CB	2.41	0.99
1:A:912:ILE:CG2	2:B:329:ASN:HB2	1.93	0.98
1:A:720:ARG:HH12	3:D:12:ARG:CD	1.70	0.98
3:D:86:ARG:CG	3:D:322:ILE:HD11	1.94	0.97
1:A:898:MET:CB	2:C:330:ILE:HD13	1.85	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:70:PHE:CE1	4:F:26:THR:HG23	1.92	0.97
1:A:874:ARG:HH22	2:C:54:VAL:N	1.61	0.96
3:D:85:LEU:CD2	4:F:29:PHE:HD2	1.79	0.96
1:A:685:ASN:OD1	3:D:21:PHE:CE1	2.18	0.96
3:D:70:PHE:CE1	4:F:26:THR:HG21	2.01	0.96
1:A:908:HIS:HB2	2:B:332:PHE:HE1	1.23	0.96
1:A:913:ILE:CB	2:B:328:ILE:HD13	1.95	0.96
3:D:182:LEU:CD2	4:F:41:ALA:HB1	1.94	0.96
3:D:288:TYR:CB	3:D:297:VAL:CG1	2.43	0.95
2:B:60:TYR:CZ	2:C:11:ILE:HG21	2.01	0.95
2:B:275:ILE:CD1	2:B:276:THR:N	2.29	0.95
1:A:845:LYS:HA	2:C:201:ASN:HD21	1.29	0.95
1:A:667:PHE:CZ	3:D:37:LEU:HD21	2.02	0.95
1:A:602:TYR:OH	3:E:391:ASP:OD2	1.83	0.95
1:A:1014:ASP:OD2	2:B:206:GLU:OE1	1.84	0.95
1:A:33:TYR:HE2	2:B:155:LYS:HZ2	1.01	0.95
3:D:290:ASP:HB2	3:D:297:VAL:HG21	1.46	0.94
1:A:909:THR:CG2	2:B:331:LEU:HB3	1.97	0.94
3:D:86:ARG:CG	3:D:322:ILE:CD1	2.44	0.94
2:B:60:TYR:OH	2:C:11:ILE:CG2	2.16	0.93
1:A:908:HIS:HA	2:B:332:PHE:CD1	2.03	0.93
5:G:464:VAL:HA	5:I:429:GLY:HA3	1.48	0.93
1:A:919:TYR:O	5:H:19:LEU:O	1.73	0.93
5:I:478:TRP:HA	5:I:601:ILE:H	1.31	0.92
1:A:909:THR:HG23	2:B:331:LEU:HB2	1.49	0.92
2:B:275:ILE:HD12	2:B:276:THR:CA	1.99	0.92
1:A:1004:PHE:O	5:G:13:ASP:HA	1.68	0.92
1:A:997:SER:O	5:G:19:LEU:CA	2.18	0.92
1:A:1028:VAL:HG23	2:C:7:ILE:HG22	1.52	0.92
1:A:912:ILE:HG23	2:B:329:ASN:CB	2.00	0.92
1:A:685:ASN:ND2	3:D:21:PHE:HE1	1.58	0.91
2:B:275:ILE:HD11	2:B:278:PRO:HG3	1.53	0.91
1:A:602:TYR:HB2	3:E:356:ILE:HG21	1.52	0.91
3:D:86:ARG:HG3	3:D:322:ILE:HD11	1.51	0.91
1:A:898:MET:HG3	2:C:330:ILE:CD1	2.00	0.90
1:A:913:ILE:CB	2:B:327:GLU:O	2.20	0.90
3:D:512:SER:HB2	3:D:539:ARG:HB2	1.49	0.90
2:B:260:GLU:O	2:B:261:ALA:HB3	1.70	0.90
1:A:844:GLY:O	2:C:200:ILE:CG2	2.19	0.90
3:D:553:VAL:HG13	3:D:592:ILE:HG23	1.53	0.90
4:F:63:ILE:HG22	4:F:64:TYR:H	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:57:GLU:O	4:F:86:TRP:CH2	2.26	0.89
1:A:909:THR:CG2	2:B:331:LEU:CB	2.51	0.89
5:H:486:VAL:H	5:I:592:TYR:HA	1.37	0.89
1:A:679:TYR:HE2	3:D:20:ILE:CD1	1.62	0.89
1:A:900:ILE:HG22	2:C:311:TYR:CE1	2.07	0.89
2:B:274:ILE:O	2:B:275:ILE:HG22	1.73	0.88
1:A:306:ARG:NE	5:H:561:GLU:CB	2.36	0.88
1:A:667:PHE:HZ	3:D:60:LEU:HD21	1.29	0.88
1:A:436:THR:HG23	1:A:441:VAL:H	1.38	0.88
2:B:263:LEU:H	2:B:266:ASN:HD22	1.20	0.88
5:I:480:LEU:HA	5:I:598:TRP:HA	1.53	0.88
1:A:847:LEU:HD21	2:C:325:THR:CG2	2.02	0.88
2:B:262:ALA:C	2:B:263:LEU:HD23	1.94	0.88
1:A:847:LEU:HD21	2:C:325:THR:HG21	1.56	0.88
1:A:732:TYR:HD1	3:D:336:GLN:HE22	1.18	0.87
1:A:906:LEU:HD22	2:B:334:PHE:CB	2.04	0.87
1:A:911:THR:CG2	2:B:315:ARG:NH2	2.08	0.87
1:A:847:LEU:HD22	2:C:325:THR:CG2	2.03	0.87
3:D:182:LEU:HD21	4:F:41:ALA:CB	2.05	0.87
1:A:861:TYR:HE2	3:D:369:PRO:CG	1.87	0.87
1:A:885:PRO:HA	3:D:340:VAL:O	1.75	0.86
5:G:569:TYR:N	5:I:543:ILE:O	2.06	0.86
1:A:945:ASP:O	2:B:118:PRO:CB	2.23	0.86
1:A:874:ARG:NH2	2:C:54:VAL:CA	2.31	0.86
1:A:911:THR:HG23	2:B:315:ARG:HH22	0.69	0.86
4:F:63:ILE:O	4:F:66:ASN:ND2	2.08	0.86
1:A:679:TYR:CZ	3:D:20:ILE:HD11	1.86	0.85
1:A:886:VAL:O	3:D:364:THR:CB	2.24	0.85
5:I:430:TRP:O	5:I:432:ASN:N	2.10	0.85
1:A:667:PHE:CZ	3:D:37:LEU:CD2	2.59	0.85
2:B:57:ALA:HB2	2:C:7:ILE:CD1	2.07	0.85
1:A:679:TYR:HE2	3:D:20:ILE:HD11	1.15	0.85
1:A:874:ARG:NH2	2:C:53:GLU:O	2.10	0.84
1:A:1028:VAL:CG2	2:C:7:ILE:CG2	2.56	0.84
1:A:6:PRO:HG2	2:B:9:ARG:HH12	1.37	0.84
1:A:898:MET:HB3	2:C:330:ILE:CD1	2.05	0.84
2:B:282:LYS:NZ	2:B:303:MET:SD	2.51	0.84
1:A:911:THR:CB	2:B:330:ILE:HG22	2.08	0.84
1:A:1002:ALA:HA	5:H:20:ARG:O	1.77	0.84
1:A:643:PRO:HB2	4:F:84:TYR:CZ	2.12	0.84
2:B:47:TRP:CZ2	2:B:59:PRO:HD3	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:430:TRP:C	5:I:432:ASN:H	1.81	0.84
1:A:921:TRP:H	5:H:17:ASP:CB	1.90	0.83
2:B:263:LEU:H	2:B:266:ASN:ND2	1.77	0.83
4:F:126:TYR:HB3	4:F:129:ASN:HD22	1.44	0.83
2:B:262:ALA:O	2:B:263:LEU:HD23	1.78	0.83
2:B:275:ILE:CD1	2:B:276:THR:O	2.26	0.83
3:D:85:LEU:CD2	4:F:29:PHE:CD2	2.61	0.83
1:A:909:THR:HG22	2:B:331:LEU:O	1.77	0.83
1:A:1018:ASN:CB	2:B:91:PRO:CB	2.56	0.82
3:D:115:THR:HG22	3:D:298:ILE:CD1	2.07	0.82
1:A:874:ARG:HH22	2:C:53:GLU:C	1.83	0.82
1:A:908:HIS:HB2	2:B:332:PHE:CD1	2.13	0.82
1:A:907:LYS:O	1:A:908:HIS:ND1	2.12	0.82
2:C:234:ASP:HB3	2:C:236:PHE:HB2	1.61	0.82
1:A:909:THR:HG23	2:B:331:LEU:CB	2.08	0.82
1:A:913:ILE:CG2	2:B:328:ILE:CD1	2.39	0.81
1:A:909:THR:HG21	2:B:331:LEU:HB3	1.62	0.81
1:A:845:LYS:HD2	2:C:201:ASN:HD22	1.45	0.81
1:A:443:LEU:HD23	1:A:444:SER:H	1.44	0.81
1:A:913:ILE:HB	2:B:327:GLU:O	1.80	0.81
1:A:902:VAL:HG11	2:B:16:PHE:CZ	2.15	0.81
1:A:898:MET:HB2	2:C:330:ILE:HA	1.60	0.81
4:F:57:GLU:C	4:F:86:TRP:CZ3	2.54	0.81
5:G:34:TYR:O	5:G:38:GLY:N	2.13	0.81
1:A:1002:ALA:CA	5:H:20:ARG:O	2.29	0.81
1:A:908:HIS:CA	2:B:332:PHE:HD1	1.94	0.81
1:A:663:ASN:CB	3:D:46:TYR:N	2.43	0.81
1:A:162:SER:C	3:E:154:ILE:HD11	2.00	0.81
5:I:23:GLY:O	5:I:27:ASN:N	2.14	0.81
1:A:874:ARG:NH2	2:C:53:GLU:C	2.34	0.80
5:G:463:ALA:N	5:I:457:GLY:O	2.12	0.80
1:A:912:ILE:O	2:B:329:ASN:CA	2.29	0.80
2:B:60:TYR:CE1	2:C:11:ILE:HD13	2.17	0.80
3:D:182:LEU:HD21	4:F:41:ALA:HB1	1.62	0.80
2:C:135:ASP:OD1	2:C:150:LYS:NZ	2.11	0.80
1:A:908:HIS:CB	2:B:332:PHE:CE1	2.65	0.80
5:I:22:GLY:O	5:I:25:LYS:N	2.14	0.80
1:A:886:VAL:CG1	3:D:345:TYR:CE2	2.48	0.79
4:F:171:ILE:HG22	4:F:173:ALA:H	1.47	0.79
2:B:57:ALA:HB2	2:C:7:ILE:HD11	1.64	0.79
1:A:176:ILE:HG13	1:A:177:GLN:H	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:912:ILE:CG2	2:B:329:ASN:CB	2.60	0.79
1:A:179:SER:H	1:A:531:ARG:HA	1.48	0.79
1:A:671:TYR:CD1	3:D:60:LEU:HD13	2.17	0.79
1:A:124:GLN:HA	1:A:128:THR:HG22	1.65	0.78
1:A:568:ILE:HG13	1:A:618:PHE:HB3	1.65	0.78
1:A:689:LEU:HD12	3:D:75:VAL:CG1	2.12	0.78
1:A:161:SER:O	3:E:154:ILE:HD11	1.83	0.78
3:D:199:LEU:HD13	3:D:270:ILE:HG13	1.65	0.78
3:E:513:ASN:ND2	3:E:622:GLU:OE1	2.17	0.78
1:A:404:TYR:HA	1:A:415:ARG:HA	1.64	0.78
1:A:162:SER:OG	3:E:162:PHE:HD2	1.65	0.78
2:B:263:LEU:HB3	2:B:264:PRO:HD2	1.65	0.78
2:B:274:ILE:O	2:B:275:ILE:CG2	2.32	0.78
1:A:900:ILE:HG23	2:C:330:ILE:HD11	1.65	0.78
1:A:682:GLN:HE22	3:D:72:ASN:HB2	1.47	0.78
1:A:847:LEU:HD22	2:C:325:THR:HG22	1.61	0.77
3:D:358:GLN:OE1	3:D:453:GLU:OE2	2.01	0.77
2:B:60:TYR:CE1	2:C:11:ILE:HG21	2.18	0.77
3:D:212:LYS:HG2	3:D:215:VAL:HA	1.66	0.77
3:D:86:ARG:HD2	3:D:322:ILE:CD1	2.11	0.77
3:D:182:LEU:HD23	4:F:41:ALA:HB1	1.65	0.77
1:A:928:GLU:HG3	1:A:929:TYR:H	1.48	0.77
2:B:239:ILE:HD12	2:B:244:ALA:HB2	1.66	0.77
4:F:60:ALA:O	4:F:66:ASN:ND2	2.17	0.77
1:A:312:THR:HB	1:A:319:TYR:HB2	1.67	0.77
2:B:55:GLY:O	2:B:56:PHE:HD1	1.68	0.77
1:A:19:ASN:HD22	1:A:130:ASN:HB3	1.50	0.77
1:A:641:ALA:HB3	4:F:99:GLN:O	1.85	0.77
1:A:776:SER:OG	1:A:833:SER:O	2.03	0.77
1:A:337:ASP:O	1:A:344:THR:OG1	2.03	0.76
1:A:1027:GLN:HA	2:C:6:VAL:O	1.86	0.76
1:A:902:VAL:CB	2:B:16:PHE:HE2	1.98	0.76
1:A:995:ASP:O	5:I:12:ASP:C	2.23	0.76
1:A:667:PHE:HE1	3:D:37:LEU:HD23	0.61	0.76
1:A:745:LYS:CE	2:C:99:ARG:NH2	2.48	0.76
1:A:745:LYS:HE2	2:C:99:ARG:NH2	2.00	0.76
1:A:832:PRO:O	1:A:834:PHE:N	2.18	0.76
2:B:260:GLU:O	2:B:261:ALA:CB	2.33	0.76
1:A:902:VAL:CB	2:B:16:PHE:CE2	2.68	0.76
3:D:182:LEU:CD2	4:F:41:ALA:CB	2.61	0.76
1:A:674:TYR:CD2	3:D:33:LEU:HD21	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:LEU:HD12	4:F:83:TYR:CD2	2.19	0.76
2:B:60:TYR:CE1	2:C:11:ILE:CG2	2.69	0.76
4:F:9:ILE:HG22	4:F:10:GLU:H	1.51	0.76
5:G:516:ALA:HB1	5:H:595:VAL:HA	1.67	0.76
2:B:239:ILE:CD1	2:B:244:ALA:HB3	2.02	0.75
1:A:882:PHE:HE1	3:D:334:GLU:OE2	1.68	0.75
1:A:240:GLN:NE2	1:A:517:SER:OG	2.19	0.75
5:H:28:GLU:O	5:H:32:GLU:N	2.19	0.75
1:A:898:MET:HE1	2:C:272:ILE:HG12	1.69	0.75
3:D:87:SER:HB3	3:D:230:ILE:HG23	1.68	0.75
1:A:1032:GLU:CB	2:B:60:TYR:HE2	1.95	0.75
1:A:143:MET:HA	1:A:544:VAL:HA	1.68	0.75
1:A:897:THR:HG22	2:C:329:ASN:CG	2.07	0.75
1:A:898:MET:CE	2:C:272:ILE:CG1	2.65	0.75
2:B:239:ILE:O	2:B:239:ILE:HD12	1.86	0.75
1:A:897:THR:HG22	2:C:329:ASN:ND2	2.01	0.75
3:D:230:ILE:HG22	3:D:231:ASP:H	1.52	0.75
4:F:124:ILE:N	4:F:134:TYR:O	2.18	0.74
3:D:185:ILE:HD11	3:D:270:ILE:HD11	1.69	0.74
5:I:18:TYR:O	5:I:20:ARG:N	2.20	0.74
2:C:137:PRO:HD3	2:C:186:TYR:CD2	2.21	0.74
2:B:92:ARG:HD2	2:B:207:TYR:O	1.87	0.74
1:A:913:ILE:CA	2:B:327:GLU:O	2.35	0.74
3:E:452:VAL:HG12	3:E:640:ILE:HG21	1.67	0.74
2:B:114:CYS:HB2	2:B:120:ASN:HB2	1.69	0.74
1:A:142:ILE:HG22	1:A:143:MET:H	1.52	0.74
2:B:273:SER:OG	2:B:274:ILE:N	2.19	0.74
3:D:70:PHE:CD1	4:F:26:THR:CG2	2.71	0.74
3:E:539:ARG:HH21	3:E:580:LEU:HB2	1.52	0.73
5:G:43:PRO:O	5:G:47:GLY:N	2.21	0.73
1:A:639:GLY:O	4:F:103:ASN:ND2	2.21	0.73
1:A:902:VAL:HG11	2:B:16:PHE:CE2	2.22	0.73
2:B:275:ILE:HD12	2:B:276:THR:C	2.08	0.73
3:D:208:ASN:HA	3:D:224:TYR:H	1.52	0.73
1:A:898:MET:CG	2:C:330:ILE:CD1	2.49	0.73
1:A:720:ARG:HH12	3:D:12:ARG:HD3	0.90	0.73
3:D:151:VAL:HG12	3:D:152:ILE:H	1.53	0.73
2:C:108:ILE:HD11	2:C:160:TRP:H	1.54	0.73
3:E:370:GLY:HA2	3:E:404:ILE:HG22	1.70	0.73
5:G:107:VAL:O	5:G:110:VAL:N	2.17	0.73
2:B:19:GLU:OE2	2:C:35:ASN:ND2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:HIS:HA	2:B:332:PHE:HA	1.70	0.73
1:A:1026:THR:O	2:C:5:SER:CB	2.36	0.73
1:A:908:HIS:CB	2:B:332:PHE:CD1	2.72	0.72
1:A:898:MET:SD	2:C:272:ILE:CD1	2.69	0.72
3:D:401:LEU:HD13	3:D:403:PRO:HD2	1.69	0.72
4:F:57:GLU:HA	4:F:86:TRP:CE3	2.24	0.72
1:A:831:LEU:O	1:A:833:SER:OG	2.08	0.72
3:E:465:LEU:HA	3:E:468:VAL:HG12	1.71	0.72
3:E:536:TYR:HE2	3:E:557:PRO:HG2	1.53	0.72
1:A:913:ILE:HG21	2:B:328:ILE:HD12	1.67	0.72
1:A:208:VAL:HG23	5:H:555:CYS:CB	2.19	0.72
3:D:86:ARG:CD	3:D:322:ILE:CD1	2.63	0.72
5:G:481:PHE:N	5:G:597:ARG:O	2.23	0.72
1:A:1014:ASP:OD2	2:B:206:GLU:CD	2.27	0.72
3:D:511:GLU:OE2	3:D:539:ARG:NH1	2.23	0.72
1:A:997:SER:O	5:G:19:LEU:CB	2.35	0.72
2:B:265:GLY:O	2:B:267:LYS:NZ	2.20	0.72
1:A:896:LEU:HD12	2:C:328:ILE:O	1.90	0.72
1:A:682:GLN:NE2	3:D:72:ASN:HB2	2.04	0.72
1:A:27:ASP:O	1:A:34:TYR:OH	2.07	0.72
1:A:685:ASN:CG	3:D:21:PHE:HE1	1.81	0.72
2:C:123:GLU:OE1	2:C:173:ARG:NH2	2.22	0.72
1:A:671:TYR:CE1	3:D:60:LEU:HD13	2.25	0.72
3:D:85:LEU:HD21	4:F:29:PHE:HD2	1.54	0.71
3:D:512:SER:HA	3:D:540:ILE:HG13	1.70	0.71
2:B:25:TYR:CD1	2:B:86:LEU:HD11	2.24	0.71
4:F:77:ASN:HD21	4:F:169:ILE:HG22	1.55	0.71
5:G:574:ALA:HB3	5:I:537:THR:H	1.55	0.71
3:E:209:TRP:CH2	3:E:212:LYS:HD2	2.25	0.71
2:B:51:GLU:HG2	2:B:269:PHE:CE1	2.26	0.71
2:B:275:ILE:HD11	2:B:278:PRO:CG	2.19	0.71
1:A:908:HIS:CA	2:B:332:PHE:CD1	2.72	0.71
5:H:63:GLU:HA	5:H:89:TYR:HA	1.73	0.71
1:A:913:ILE:HA	2:B:327:GLU:O	1.91	0.70
2:B:47:TRP:HE1	2:B:58:PRO:HA	1.56	0.70
2:C:303:MET:HB3	2:C:306:SER:HB2	1.72	0.70
1:A:679:TYR:OH	3:D:20:ILE:HD11	1.73	0.70
5:G:462:ASN:N	5:G:596:TYR:O	2.23	0.70
1:A:355:MET:SD	1:A:413:TRP:NE1	2.64	0.70
5:H:494:ILE:O	5:H:500:ALA:HB1	1.92	0.70
2:B:144:ILE:HG22	2:B:160:TRP:HA	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:GLN:NE2	2:C:8:TYR:CE2	2.59	0.70
1:A:906:LEU:HD21	2:B:334:PHE:CB	2.19	0.70
3:E:403:PRO:O	3:E:404:ILE:HG13	1.91	0.70
5:H:22:GLY:O	5:H:26:ILE:N	2.20	0.69
1:A:1027:GLN:CD	2:C:8:TYR:CE2	2.66	0.69
1:A:233:LEU:HD11	1:A:366:TYR:HA	1.75	0.69
4:F:81:ASP:OD2	4:F:84:TYR:N	2.24	0.69
1:A:15:LYS:HA	1:A:625:ASN:HB3	1.73	0.69
2:C:327:GLU:OE1	2:C:329:ASN:ND2	2.24	0.69
4:F:47:THR:HG23	4:F:171:ILE:HD12	1.74	0.69
5:H:415:ASP:HA	5:H:440:GLN:HA	1.74	0.69
5:G:486:VAL:HA	5:I:488:VAL:HA	1.74	0.69
1:A:645:LEU:CD1	4:F:83:TYR:CE2	2.70	0.69
3:E:220:THR:HG21	3:E:243:ILE:HD13	1.73	0.69
1:A:667:PHE:CE1	3:D:37:LEU:CG	2.75	0.68
2:B:11:ILE:O	2:B:12:VAL:HG12	1.93	0.68
2:B:115:ASN:HA	2:B:121:ALA:HA	1.75	0.68
1:A:678:GLY:O	1:A:684:ASN:ND2	2.27	0.68
2:B:179:THR:OG1	2:B:189:GLU:HA	1.94	0.68
1:A:936:LEU:HG	1:A:937:THR:H	1.58	0.68
2:B:273:SER:C	2:B:274:ILE:HG13	2.14	0.68
1:A:162:SER:O	3:E:154:ILE:CG1	2.42	0.68
3:E:563:VAL:HG12	3:E:611:LEU:HD21	1.76	0.68
1:A:162:SER:O	3:E:154:ILE:HD11	1.91	0.68
1:A:180:ILE:HG22	1:A:181:GLN:H	1.58	0.68
1:A:715:LEU:O	3:D:9:GLN:CB	2.41	0.68
4:F:15:THR:HG23	4:F:16:VAL:HG23	1.75	0.68
5:G:595:VAL:O	5:I:490:TRP:N	2.27	0.68
5:G:31:ASP:O	5:G:34:TYR:N	2.24	0.68
5:G:460:TYR:O	5:G:598:TRP:N	2.26	0.68
2:B:277:ASN:HA	2:B:291:LYS:HE3	1.75	0.68
5:I:19:LEU:C	5:I:21:LYS:H	1.96	0.68
1:A:170:GLU:OE2	1:A:541:TYR:OH	2.07	0.67
1:A:896:LEU:O	2:C:328:ILE:O	2.12	0.67
1:A:911:THR:HA	2:B:330:ILE:HA	1.75	0.67
1:A:714:TYR:OH	1:A:749:LYS:O	2.09	0.67
1:A:494:GLU:O	1:A:496:SER:N	2.28	0.67
2:C:135:ASP:HB3	2:C:187:VAL:HG11	1.76	0.67
1:A:720:ARG:HH12	3:D:12:ARG:HH11	1.42	0.67
5:G:22:GLY:O	5:G:26:ILE:N	2.27	0.67
2:B:115:ASN:OD1	2:B:122:THR:N	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:PHE:O	2:B:270:ARG:O	2.13	0.67
3:E:459:PHE:HD2	3:E:632:ILE:HD11	1.59	0.67
4:F:103:ASN:OD1	4:F:104:VAL:N	2.27	0.67
1:A:643:PRO:HB2	4:F:84:TYR:CE2	2.30	0.67
4:F:109:ILE:HA	4:F:154:ASP:HA	1.77	0.67
1:A:13:ILE:HD13	1:A:16:LEU:HD23	1.77	0.67
1:A:735:TYR:CE1	3:D:334:GLU:HA	2.30	0.67
3:D:623:LEU:HD12	3:D:624:TYR:H	1.60	0.67
4:F:49:TYR:HB2	4:F:171:ILE:HD11	1.77	0.67
1:A:1002:ALA:HA	5:H:20:ARG:C	2.15	0.67
5:H:530:ALA:O	5:I:584:THR:N	2.28	0.67
2:B:179:THR:HG21	2:B:190:TYR:H	1.59	0.66
2:B:281:ALA:HB2	2:B:301:ASP:HA	1.75	0.66
2:C:143:SER:OG	2:C:159:LYS:O	2.10	0.66
3:D:17:ILE:HD13	4:F:16:VAL:HG22	1.76	0.66
2:C:217:LYS:HB2	2:C:236:PHE:CZ	2.30	0.66
2:C:92:ARG:NH2	2:C:94:ASP:OD2	2.29	0.66
3:D:543:THR:OG1	3:D:551:GLY:O	2.13	0.66
1:A:720:ARG:HH11	3:D:12:ARG:CD	1.90	0.66
1:A:334:ALA:HB3	1:A:348:ARG:HD3	1.78	0.66
2:C:275:ILE:HG22	2:C:309:MET:HB3	1.77	0.66
5:G:594:THR:H	5:I:518:GLY:HA3	1.60	0.66
2:B:144:ILE:HG21	2:B:160:TRP:CD1	2.30	0.66
1:A:667:PHE:CE2	3:D:60:LEU:HD21	2.29	0.66
1:A:1028:VAL:HG23	2:C:7:ILE:CG2	2.21	0.66
1:A:667:PHE:HE1	3:D:37:LEU:CG	2.05	0.66
3:D:433:GLU:HG3	3:D:655:LEU:HD22	1.77	0.66
5:H:517:GLY:N	5:I:594:THR:O	2.28	0.66
2:B:132:ARG:HB3	2:B:190:TYR:HA	1.77	0.66
2:C:44:SER:O	2:C:270:ARG:NH1	2.29	0.66
1:A:1027:GLN:HB3	2:C:6:VAL:HG13	1.78	0.66
1:A:370:SER:HB2	1:A:375:VAL:HG12	1.78	0.66
1:A:689:LEU:CD1	3:D:75:VAL:CG1	2.49	0.66
2:B:122:THR:HG21	2:B:170:PRO:HG3	1.77	0.66
1:A:996:ALA:N	5:G:20:ARG:CB	2.59	0.65
2:B:275:ILE:HD13	2:B:276:THR:O	1.94	0.65
1:A:387:ASN:OD1	1:A:388:ALA:N	2.29	0.65
3:E:85:LEU:HG	3:E:86:ARG:H	1.61	0.65
1:A:1002:ALA:N	5:H:20:ARG:O	2.29	0.65
2:C:132:ARG:NH1	2:C:241:ARG:O	2.29	0.65
1:A:792:ARG:HD2	1:A:859:ARG:HH22	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:GLU:HG2	2:B:224:GLY:HA3	1.79	0.65
1:A:330:LYS:HB2	1:A:334:ALA:HB2	1.79	0.65
1:A:845:LYS:HA	2:C:201:ASN:ND2	2.07	0.65
1:A:913:ILE:HB	2:B:328:ILE:HD13	1.76	0.65
3:E:417:LYS:HB3	3:E:483:GLN:HB2	1.79	0.65
5:H:469:PRO:O	5:H:474:GLY:N	2.29	0.65
1:A:911:THR:OG1	2:B:329:ASN:O	2.14	0.65
3:D:433:GLU:HG2	3:D:434:GLN:H	1.62	0.65
3:E:420:LEU:HG	3:E:653:ILE:HG22	1.79	0.65
5:G:593:ILE:N	5:I:486:VAL:O	2.30	0.65
1:A:514:PHE:HA	1:A:525:TRP:HB2	1.79	0.65
2:B:275:ILE:CD1	2:B:276:THR:C	2.65	0.65
2:B:238:LEU:HD23	2:B:238:LEU:C	2.17	0.65
2:B:292:ALA:HB1	2:B:297:TYR:CE2	2.32	0.65
5:I:419:ASP:O	5:I:436:VAL:N	2.30	0.65
1:A:900:ILE:CG2	2:C:330:ILE:HD11	2.26	0.64
3:D:350:SER:O	3:D:354:GLY:N	2.30	0.64
3:E:319:PRO:HG2	3:E:324:ARG:HH21	1.62	0.64
5:G:34:TYR:O	5:G:37:LEU:N	2.29	0.64
1:A:712:ASN:HD21	1:A:720:ARG:HB2	1.62	0.64
3:D:86:ARG:NH1	3:D:86:ARG:HG2	2.12	0.64
5:I:479:LYS:N	5:I:599:ILE:O	2.30	0.64
5:H:520:GLY:O	5:I:592:TYR:N	2.30	0.64
3:D:429:LEU:HD13	3:D:432:SER:HA	1.80	0.64
3:E:413:TYR:CD1	3:E:641:VAL:HG11	2.33	0.64
3:E:413:TYR:HD1	3:E:641:VAL:HG11	1.61	0.64
5:G:589:ILE:O	5:I:521:GLY:HA3	1.97	0.64
1:A:717:ALA:H	3:D:9:GLN:HE21	1.43	0.64
1:A:408:HIS:CG	1:A:409:ASP:H	2.15	0.64
2:B:90:ILE:O	2:B:207:TYR:HA	1.98	0.64
2:B:16:PHE:HB2	2:C:310:ILE:HB	1.80	0.64
2:C:51:GLU:HA	2:C:56:PHE:CZ	2.33	0.64
5:I:430:TRP:C	5:I:432:ASN:N	2.49	0.64
2:B:108:ILE:HG23	2:B:109:ASN:H	1.62	0.63
1:A:886:VAL:HG11	3:D:345:TYR:HE2	0.66	0.63
1:A:911:THR:CB	2:B:330:ILE:HA	2.28	0.63
3:D:208:ASN:HB3	3:D:224:TYR:CE2	2.33	0.63
1:A:975:ASN:HA	1:A:980:GLY:HA2	1.80	0.63
2:B:175:ASP:OD1	2:B:176:ALA:N	2.31	0.63
2:B:87:ASP:HA	2:B:212:TRP:CH2	2.34	0.63
2:B:60:TYR:HE1	2:C:11:ILE:CG2	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:LEU:HD11	2:C:247:ILE:HG12	1.79	0.63
1:A:720:ARG:NH1	3:D:12:ARG:HB3	2.13	0.63
1:A:176:ILE:HG22	1:A:533:VAL:HG12	1.80	0.63
1:A:845:LYS:HD2	2:C:201:ASN:HD21	1.63	0.63
3:D:483:GLN:HG2	3:D:626:ASP:HB3	1.81	0.63
1:A:984:SER:C	1:A:986:ARG:H	2.00	0.63
2:B:275:ILE:HD12	2:B:275:ILE:C	2.14	0.63
2:B:60:TYR:CZ	2:C:11:ILE:CG2	2.78	0.63
3:D:562:ASP:O	3:D:563:VAL:HG13	1.98	0.63
4:F:57:GLU:C	4:F:86:TRP:HZ3	1.99	0.63
1:A:911:THR:HG21	2:B:315:ARG:HH22	1.53	0.63
4:F:76:CYS:SG	4:F:170:LYS:N	2.59	0.63
1:A:702:GLU:CB	3:D:79:PHE:CE1	2.82	0.63
1:A:605:ARG:CB	3:E:387:VAL:CB	2.77	0.63
4:F:57:GLU:O	4:F:86:TRP:HZ3	1.73	0.63
5:I:447:SER:O	5:I:451:ASP:N	2.25	0.63
1:A:717:ALA:CB	3:D:9:GLN:NE2	2.62	0.63
3:E:436:LEU:O	3:E:440:ILE:N	2.26	0.63
2:C:42:GLY:HA2	2:C:76:MET:H	1.64	0.62
3:D:278:ALA:O	3:D:281:ASN:ND2	2.32	0.62
3:D:491:PHE:CG	3:D:492:TYR:N	2.67	0.62
4:F:167:ARG:O	4:F:168:GLN:HG3	1.99	0.62
1:A:939:THR:HG21	5:G:16:GLY:HA2	1.81	0.62
1:A:171:ASN:O	1:A:172:GLU:HG2	1.98	0.62
2:B:4:SER:OG	2:B:6:VAL:O	2.17	0.62
5:G:414:VAL:O	5:G:441:ARG:N	2.31	0.62
5:G:507:ASP:N	5:G:511:ASN:O	2.24	0.62
1:A:499:GLU:O	1:A:500:THR:OG1	2.17	0.62
5:I:43:PRO:O	5:I:47:GLY:N	2.32	0.62
1:A:771:ILE:HD11	1:A:839:ILE:HD11	1.79	0.62
3:D:77:GLU:OE2	4:F:29:PHE:CE1	2.51	0.62
5:G:535:THR:O	5:H:576:THR:N	2.21	0.62
2:C:274:ILE:HG12	2:C:311:TYR:HB3	1.80	0.62
3:D:296:THR:OG1	3:D:298:ILE:HG13	1.99	0.62
1:A:902:VAL:CG1	2:B:16:PHE:CE2	2.83	0.62
1:A:306:ARG:CD	5:H:561:GLU:CB	2.77	0.62
1:A:1018:ASN:CB	2:B:91:PRO:CA	2.78	0.62
3:D:81:ARG:HD3	3:D:330:THR:HG21	1.82	0.62
3:E:534:VAL:HG22	3:E:535:LEU:H	1.64	0.62
3:E:566:ASN:OD1	3:E:567:GLU:N	2.33	0.62
1:A:306:ARG:HD3	5:H:561:GLU:CB	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:PHE:CE2	3:D:60:LEU:CD2	2.83	0.62
2:B:263:LEU:CB	2:B:264:PRO:HD2	2.29	0.62
2:C:279:LEU:N	2:C:306:SER:OG	2.19	0.62
2:B:238:LEU:HD12	2:B:241:ARG:NH2	2.14	0.62
2:B:95:TRP:CE3	2:B:169:PRO:HG2	2.35	0.61
2:B:43:ARG:HG2	2:B:45:GLU:H	1.65	0.61
3:D:30:LYS:HE3	3:D:34:ILE:HD11	1.81	0.61
3:D:501:TYR:OH	3:D:510:MET:SD	2.58	0.61
4:F:61:ASN:HA	4:F:66:ASN:HA	1.81	0.61
1:A:137:PHE:O	1:A:555:ARG:NH2	2.34	0.61
3:D:543:THR:HG22	3:D:578:ASN:HB2	1.80	0.61
1:A:1014:ASP:OD2	2:B:206:GLU:OE2	2.19	0.61
1:A:679:TYR:CE2	3:D:20:ILE:CG1	2.81	0.61
3:D:77:GLU:HA	3:D:83:ALA:HB2	1.81	0.61
5:G:482:GLY:O	5:I:489:GLY:HA3	2.01	0.61
1:A:373:ASP:O	1:A:374:LYS:HG3	2.00	0.61
3:D:110:ILE:HG22	3:D:303:ASN:HA	1.83	0.61
1:A:703:TYR:OH	1:A:725:ARG:NH2	2.34	0.61
1:A:863:VAL:HG12	1:A:889:GLY:HA3	1.82	0.61
1:A:713:ILE:CD1	2:B:5:SER:HB2	2.31	0.61
1:A:1027:GLN:CD	2:C:8:TYR:HE2	2.04	0.61
3:D:595:ILE:HG13	3:D:602:ILE:HA	1.81	0.61
3:D:87:SER:HB3	3:D:230:ILE:CG2	2.31	0.61
5:G:409:SER:N	5:H:444:ASN:O	2.32	0.61
1:A:897:THR:HA	2:C:329:ASN:HB2	1.83	0.60
3:D:297:VAL:O	3:D:297:VAL:HG12	2.01	0.60
1:A:326:VAL:HG12	1:A:354:THR:HG23	1.83	0.60
2:B:28:ILE:HD12	2:B:37:ILE:HD11	1.83	0.60
5:G:430:TRP:O	5:G:432:ASN:N	2.34	0.60
1:A:720:ARG:NH2	3:D:10:LEU:HA	2.16	0.60
1:A:904:LEU:O	1:A:905:THR:OG1	2.16	0.60
5:G:523:THR:O	5:G:588:ASN:N	2.35	0.60
5:G:76:ARG:N	5:G:102:TRP:O	2.34	0.60
1:A:511:GLU:HA	1:A:514:PHE:CD2	2.36	0.60
1:A:747:LEU:HD22	1:A:883:VAL:HG21	1.83	0.60
1:A:75:LEU:N	1:A:102:THR:OG1	2.34	0.60
5:G:421:ASN:N	5:G:434:GLU:O	2.34	0.60
3:E:106:ALA:H	3:E:169:GLN:HG2	1.66	0.60
1:A:772:VAL:HG12	1:A:838:ILE:HG12	1.82	0.60
3:E:107:GLN:HE21	3:E:196:GLN:HE21	1.48	0.60
3:E:98:TYR:HE2	3:E:327:GLU:HB3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:ASP:CB	5:I:16:GLY:O	2.50	0.60
2:B:148:THR:OG1	2:B:153:CYS:SG	2.47	0.60
2:C:203:CYS:SG	2:C:209:VAL:HG12	2.42	0.60
1:A:161:SER:C	3:E:156:ASP:CB	2.70	0.60
5:H:541:VAL:O	5:I:572:ALA:N	2.31	0.60
1:A:1028:VAL:HG22	2:C:7:ILE:CG2	2.22	0.60
1:A:948:THR:CA	2:B:118:PRO:CB	2.79	0.60
2:C:54:VAL:HG11	3:D:10:LEU:HD21	1.83	0.60
3:D:86:ARG:O	3:D:89:VAL:N	2.35	0.60
3:E:415:PHE:HB2	3:E:485:VAL:HG13	1.84	0.60
1:A:689:LEU:HD13	3:D:75:VAL:CG1	2.23	0.60
2:C:92:ARG:HH21	2:C:94:ASP:CG	2.05	0.60
3:E:209:TRP:NE1	3:E:213:SER:O	2.35	0.60
1:A:882:PHE:HE1	3:D:334:GLU:CD	2.04	0.59
2:B:316:PRO:HG2	2:B:317:PRO:HD3	1.82	0.59
1:A:1032:GLU:HA	2:C:9:ARG:HH21	1.66	0.59
5:H:518:GLY:O	5:I:594:THR:N	2.35	0.59
1:A:844:GLY:O	2:C:200:ILE:HG23	2.02	0.59
2:B:194:ILE:HA	2:B:223:TRP:CZ3	2.38	0.59
2:B:35:ASN:HA	2:B:291:LYS:HZ1	1.68	0.59
2:B:89:VAL:HB	2:B:207:TYR:HB3	1.83	0.59
1:A:336:ILE:HG12	1:A:346:SER:HA	1.83	0.59
1:A:674:TYR:CE2	3:D:33:LEU:HD21	2.36	0.59
3:D:415:PHE:HB2	3:D:485:VAL:CG2	2.32	0.59
1:A:442:SER:HA	1:A:491:ILE:HG12	1.84	0.59
3:D:208:ASN:HB3	3:D:224:TYR:CZ	2.38	0.59
3:D:77:GLU:HA	3:D:83:ALA:CB	2.32	0.59
1:A:248:LEU:HD13	1:A:311:ILE:HG13	1.85	0.59
3:D:192:ILE:O	3:D:192:ILE:HG13	2.03	0.59
3:E:169:GLN:NE2	3:E:275:THR:OG1	2.35	0.59
3:E:595:ILE:HG12	3:E:602:ILE:HG23	1.83	0.59
4:F:154:ASP:OD1	4:F:155:THR:N	2.35	0.59
2:B:275:ILE:CD1	2:B:276:THR:H	2.15	0.59
1:A:720:ARG:NH1	3:D:12:ARG:CG	2.66	0.59
3:E:401:LEU:HG	3:E:402:ALA:HB2	1.83	0.59
1:A:641:ALA:CB	4:F:99:GLN:O	2.50	0.59
5:H:528:GLU:O	5:H:531:ASN:N	2.21	0.59
1:A:921:TRP:N	5:H:17:ASP:CB	2.63	0.59
1:A:583:SER:OG	1:A:604:VAL:N	2.36	0.58
2:C:90:ILE:HD12	2:C:111:ILE:HD12	1.84	0.58
5:H:532:LEU:H	5:I:583:PRO:CB	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:69:ALA:O	5:H:71:ASN:N	2.36	0.58
1:A:1031:ASP:OD1	1:A:1032:GLU:N	2.37	0.58
1:A:405:VAL:HG12	1:A:407:ASN:H	1.68	0.58
3:D:358:GLN:NE2	3:D:379:LYS:HA	2.19	0.58
5:H:541:VAL:HA	5:I:543:ILE:HA	1.85	0.58
2:C:167:MET:O	2:C:168:THR:HG22	2.03	0.58
3:E:199:LEU:HD11	3:E:206:TRP:HB2	1.83	0.58
5:H:414:VAL:O	5:H:441:ARG:N	2.36	0.58
1:A:900:ILE:HG23	2:C:330:ILE:CD1	2.31	0.58
1:A:945:ASP:C	2:B:118:PRO:CB	2.71	0.58
3:E:358:GLN:NE2	3:E:453:GLU:OE2	2.36	0.58
5:G:473:MET:HA	5:I:452:THR:O	2.04	0.58
5:G:463:ALA:HB3	5:I:457:GLY:HA2	1.85	0.58
3:D:24:GLY:HA3	3:D:29:ILE:HD11	1.85	0.58
1:A:679:TYR:HE2	3:D:20:ILE:CG1	2.15	0.58
1:A:684:ASN:OD1	1:A:688:ASN:ND2	2.37	0.58
1:A:6:PRO:HD2	1:A:32:PHE:CE2	2.39	0.58
4:F:71:TRP:C	4:F:73:LEU:H	2.06	0.58
1:A:717:ALA:HB2	3:D:9:GLN:NE2	2.18	0.58
1:A:165:ASN:H	3:E:154:ILE:HD13	1.68	0.58
2:B:275:ILE:CD1	2:B:278:PRO:HG3	2.29	0.58
5:H:502:ASN:HA	5:H:518:GLY:HA3	1.86	0.57
1:A:968:ASP:OD1	1:A:969:TYR:N	2.32	0.57
2:B:60:TYR:CE1	2:C:11:ILE:HG23	2.37	0.57
3:E:501:TYR:OH	3:E:510:MET:SD	2.60	0.57
1:A:161:SER:HB2	3:E:156:ASP:CB	2.30	0.57
2:B:144:ILE:O	2:B:146:SER:N	2.31	0.57
1:A:898:MET:HE1	2:C:272:ILE:CG1	2.27	0.57
3:D:440:ILE:HD11	3:D:468:VAL:HG13	1.87	0.57
3:D:503:ASN:HD21	3:D:632:ILE:HG23	1.70	0.57
2:C:202:ARG:HD3	2:C:209:VAL:HG21	1.85	0.57
5:G:70:ILE:HA	5:G:97:ASP:CB	2.35	0.57
1:A:403:ILE:HD12	1:A:405:VAL:H	1.70	0.57
3:D:415:PHE:HB2	3:D:485:VAL:HG22	1.87	0.57
4:F:87:ILE:HG21	4:F:167:ARG:HB3	1.87	0.57
1:A:301:PRO:HD2	1:A:304:VAL:HG22	1.85	0.57
3:E:536:TYR:CE2	3:E:557:PRO:HG2	2.38	0.57
1:A:914:ASN:HB3	1:A:1011:ARG:HG3	1.87	0.57
1:A:200:TYR:OH	1:A:259:SER:O	2.20	0.57
3:D:127:ARG:NH1	3:D:148:ARG:O	2.38	0.57
4:F:6:PHE:HE2	4:F:32:TYR:HE1	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HB3	1:A:168:ILE:HD12	1.86	0.57
1:A:162:SER:O	3:E:154:ILE:CD1	2.53	0.57
1:A:909:THR:HG22	2:B:331:LEU:C	2.24	0.57
1:A:6:PRO:CG	2:B:9:ARG:NH1	2.61	0.57
3:D:69:GLN:HE22	4:F:23:ILE:HB	1.70	0.57
3:E:553:VAL:HG13	3:E:592:ILE:HB	1.85	0.57
5:I:19:LEU:C	5:I:21:LYS:N	2.58	0.57
1:A:732:TYR:HD1	3:D:336:GLN:NE2	1.95	0.57
1:A:910:GLU:O	2:B:331:LEU:HD13	2.04	0.57
1:A:715:LEU:O	3:D:9:GLN:HB3	2.03	0.57
3:E:540:ILE:HG22	3:E:555:ILE:HD12	1.87	0.57
5:H:33:LEU:O	5:H:36:GLU:N	2.34	0.57
1:A:163:ILE:HD11	1:A:587:PHE:CZ	2.39	0.56
3:D:170:GLY:HA3	3:D:275:THR:H	1.70	0.56
3:E:374:ILE:HD11	3:E:408:ILE:HG12	1.87	0.56
3:E:220:THR:HG23	3:E:260:LEU:HD13	1.87	0.56
1:A:689:LEU:O	1:A:690:ILE:HG22	2.05	0.56
2:C:178:GLY:HA3	2:C:187:VAL:H	1.68	0.56
3:D:263:THR:O	3:D:265:ASN:N	2.28	0.56
3:D:634:THR:OG1	3:D:638:SER:O	2.22	0.56
3:D:85:LEU:HD23	4:F:29:PHE:CD2	2.39	0.56
1:A:144:ALA:O	1:A:542:THR:HA	2.06	0.56
1:A:886:VAL:HG13	3:D:372:ALA:HB2	1.86	0.56
1:A:902:VAL:CG2	2:B:16:PHE:CD2	2.68	0.56
3:D:506:LYS:HE3	3:D:628:THR:HA	1.88	0.56
1:A:602:TYR:CB	3:E:356:ILE:HG21	2.31	0.56
1:A:919:TYR:OH	1:A:1005:ARG:HD2	2.05	0.56
1:A:898:MET:CG	2:C:330:ILE:HB	2.35	0.56
2:C:136:VAL:O	2:C:150:LYS:NZ	2.35	0.56
2:C:275:ILE:HA	2:C:309:MET:HA	1.87	0.56
1:A:201:LEU:HD11	1:A:210:LYS:HB2	1.88	0.56
1:A:401:LYS:O	1:A:415:ARG:NH2	2.38	0.56
2:B:26:ASN:ND2	2:C:33:ASP:O	2.38	0.56
3:D:298:ILE:O	3:D:298:ILE:HG22	2.04	0.56
1:A:911:THR:C	2:B:329:ASN:O	2.41	0.56
1:A:162:SER:N	3:E:156:ASP:CB	2.69	0.56
1:A:400:ASP:O	1:A:415:ARG:NE	2.36	0.56
1:A:735:TYR:CD1	3:D:334:GLU:HA	2.41	0.56
2:C:135:ASP:OD1	2:C:136:VAL:N	2.33	0.56
1:A:680:GLY:HA2	3:D:20:ILE:HG23	1.88	0.56
3:D:360:VAL:HG23	3:D:361:GLN:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:SER:OG	1:A:374:LYS:O	2.12	0.56
1:A:643:PRO:CB	4:F:84:TYR:CZ	2.89	0.56
2:B:144:ILE:HG13	2:B:144:ILE:O	2.05	0.56
2:C:217:LYS:N	2:C:236:PHE:HZ	2.03	0.56
3:D:325:ILE:O	3:D:329:GLY:N	2.38	0.56
3:E:536:TYR:OH	3:E:582:ASN:ND2	2.39	0.56
1:A:379:ILE:HD11	1:A:401:LYS:HA	1.88	0.55
3:D:630:ASP:OD1	3:D:631:VAL:N	2.39	0.55
1:A:911:THR:CA	2:B:329:ASN:O	2.55	0.55
1:A:916:TYR:O	2:B:324:GLN:HA	2.06	0.55
2:B:292:ALA:HB1	2:B:297:TYR:HE2	1.71	0.55
3:D:382:LEU:HD23	3:D:646:LEU:HD23	1.87	0.55
4:F:114:ASN:OD1	4:F:115:GLU:N	2.39	0.55
2:C:170:PRO:HG3	2:C:188:TRP:CD2	2.41	0.55
2:C:42:GLY:HA3	2:C:75:MET:HA	1.88	0.55
3:D:424:TYR:HE2	3:D:655:LEU:HB3	1.71	0.55
3:D:86:ARG:CG	3:D:86:ARG:HH11	2.18	0.55
3:E:263:THR:OG1	3:E:266:SER:OG	2.24	0.55
5:I:43:PRO:O	5:I:46:ALA:N	2.38	0.55
1:A:909:THR:CG2	2:B:331:LEU:O	2.51	0.55
2:B:72:TRP:HA	2:B:75:MET:HG2	1.88	0.55
3:D:39:GLY:O	3:D:41:ASN:N	2.40	0.55
4:F:112:HIS:HA	4:F:152:ALA:HA	1.87	0.55
2:B:318:ILE:HG12	2:B:319:ILE:H	1.71	0.55
5:H:421:ASN:O	5:H:434:GLU:N	2.36	0.55
1:A:8:VAL:HA	1:A:28:VAL:HG21	1.89	0.55
1:A:913:ILE:CG2	2:B:327:GLU:O	2.47	0.55
3:E:177:ILE:HG13	3:E:178:ILE:H	1.71	0.55
1:A:708:ILE:HD12	1:A:727:PHE:CE2	2.42	0.55
2:C:81:VAL:HG23	2:C:249:PHE:HE1	1.71	0.55
2:C:281:ALA:HB2	2:C:301:ASP:HA	1.88	0.55
3:D:290:ASP:HB2	3:D:297:VAL:CG2	2.29	0.55
3:D:495:PRO:HG2	3:D:498:GLY:HA3	1.89	0.55
3:E:554:ILE:HD13	3:E:589:TYR:CG	2.41	0.55
1:A:798:ILE:HD12	1:A:811:VAL:HG12	1.89	0.55
2:B:273:SER:O	2:B:274:ILE:HG13	2.07	0.55
2:B:273:SER:OG	2:B:274:ILE:O	2.25	0.55
2:B:94:ASP:HB3	2:B:113:VAL:CG2	2.36	0.55
5:I:528:GLU:O	5:I:531:ASN:N	2.36	0.55
2:C:41:PHE:HD1	2:C:272:ILE:HG22	1.72	0.55
3:E:554:ILE:HB	3:E:589:TYR:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:461:GLU:HA	5:G:598:TRP:H	1.70	0.55
5:H:516:ALA:HB1	5:I:595:VAL:HA	1.87	0.55
1:A:934:ALA:HB2	1:A:954:GLU:H	1.72	0.54
5:G:518:GLY:N	5:H:594:THR:O	2.22	0.54
1:A:13:ILE:HG23	1:A:97:THR:HG21	1.88	0.54
1:A:676:SER:HA	1:A:683:TYR:HB3	1.89	0.54
2:B:253:LEU:HB2	2:B:326:GLU:HB2	1.90	0.54
3:D:499:ILE:HG23	3:D:602:ILE:HB	1.89	0.54
2:B:169:PRO:N	2:B:170:PRO:HD2	2.23	0.54
2:C:228:ASN:HB3	2:C:230:THR:HG23	1.88	0.54
3:E:136:LYS:HG2	3:E:137:ASP:H	1.72	0.54
5:H:531:ASN:HA	5:I:584:THR:H	1.72	0.54
1:A:545:ILE:HG12	1:A:573:VAL:HG22	1.90	0.54
2:C:148:THR:HG23	2:C:149:ASP:H	1.73	0.54
2:C:37:ILE:O	2:C:81:VAL:HG12	2.07	0.54
3:D:501:TYR:N	3:D:600:ASP:OD2	2.27	0.54
1:A:909:THR:O	1:A:1029:LYS:NZ	2.40	0.54
1:A:976:SER:N	1:A:979:GLN:O	2.38	0.54
1:A:683:TYR:CE1	4:F:83:TYR:HD2	2.26	0.54
1:A:614:PRO:HB2	1:A:617:VAL:CG1	2.37	0.54
5:G:461:GLU:HA	5:G:597:ARG:HA	1.89	0.54
1:A:494:GLU:C	1:A:496:SER:H	2.10	0.54
1:A:600:PHE:CE1	1:A:608:VAL:HG21	2.42	0.54
1:A:78:TYR:CD1	1:A:101:GLU:HA	2.42	0.54
3:D:571:PRO:HB3	3:D:590:TYR:CD1	2.43	0.54
2:B:46:PRO:O	2:B:269:PHE:CZ	2.59	0.54
3:E:208:ASN:HA	3:E:224:TYR:CE2	2.43	0.54
1:A:176:ILE:HG13	1:A:177:GLN:N	2.20	0.54
1:A:511:GLU:HA	1:A:514:PHE:HD2	1.72	0.54
1:A:845:LYS:CA	2:C:201:ASN:HD21	2.11	0.54
3:E:366:SER:O	3:E:367:THR:OG1	2.25	0.54
1:A:160:VAL:HG21	1:A:589:LYS:HE3	1.89	0.54
1:A:774:SER:O	1:A:809:TRP:HZ3	1.90	0.54
2:B:248:ARG:HB3	2:B:331:LEU:HG	1.90	0.54
3:D:103:LYS:HE2	3:D:277:GLY:HA2	1.88	0.54
3:D:70:PHE:CD1	4:F:26:THR:HG22	2.43	0.54
5:H:470:VAL:O	5:H:474:GLY:HA2	2.07	0.54
1:A:41:THR:OG1	1:A:42:LYS:N	2.41	0.53
2:B:92:ARG:HG3	2:B:92:ARG:O	2.08	0.53
3:E:89:VAL:O	3:E:93:ALA:N	2.39	0.53
4:F:28:ILE:HG23	4:F:29:PHE:CE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:SER:O	1:A:522:THR:HG23	2.08	0.53
1:A:38:ILE:HD13	1:A:80:ILE:HG22	1.91	0.53
1:A:820:LEU:HD13	1:A:838:ILE:HD13	1.89	0.53
2:C:142:CYS:SG	2:C:161:THR:N	2.75	0.53
2:C:40:THR:HG22	2:C:78:THR:HG22	1.90	0.53
3:D:230:ILE:O	3:D:232:GLY:N	2.40	0.53
5:H:421:ASN:N	5:H:434:GLU:O	2.33	0.53
5:I:25:LYS:O	5:I:28:GLU:N	2.39	0.53
1:A:314:THR:HG22	1:A:315:ASP:H	1.72	0.53
1:A:911:THR:CA	2:B:330:ILE:HA	2.39	0.53
3:D:192:ILE:HG22	3:D:272:TYR:CD1	2.43	0.53
4:F:48:TYR:HE1	4:F:170:LYS:HE3	1.73	0.53
1:A:146:LEU:HD11	1:A:575:PHE:CZ	2.43	0.53
2:B:144:ILE:HD11	2:B:153:CYS:HB3	1.90	0.53
2:C:151:ASP:OD1	2:C:152:GLU:N	2.42	0.53
3:D:151:VAL:O	3:D:152:ILE:HG12	2.08	0.53
2:B:204:THR:HG22	2:B:205:ASN:H	1.74	0.53
1:A:1018:ASN:CB	2:B:91:PRO:HA	2.39	0.53
2:C:42:GLY:CA	2:C:76:MET:H	2.21	0.53
3:D:26:PHE:O	3:D:29:ILE:N	2.33	0.53
5:G:477:SER:O	5:G:601:ILE:N	2.39	0.53
5:H:80:ASN:CB	5:H:111:ALA:HA	2.38	0.53
1:A:437:ASP:CB	1:A:440:LEU:HD12	2.39	0.53
1:A:490:PHE:O	1:A:501:PHE:HB3	2.08	0.53
1:A:945:ASP:HA	2:B:118:PRO:CB	2.38	0.53
2:B:154:LEU:HB3	2:B:160:TRP:NE1	2.24	0.53
2:B:20:LYS:HD2	2:C:20:LYS:HD3	1.89	0.53
3:D:563:VAL:HG11	3:D:590:TYR:CZ	2.43	0.53
3:E:112:LEU:HB3	3:E:163:PRO:HG2	1.90	0.53
3:E:375:ALA:HB1	3:E:411:PRO:HG3	1.88	0.53
1:A:710:LYS:O	3:D:12:ARG:NH2	2.42	0.53
2:C:184:ASP:OD1	2:C:185:GLY:N	2.40	0.53
2:C:51:GLU:O	2:C:52:ASN:HB2	2.09	0.53
3:E:512:SER:CB	3:E:624:TYR:H	2.21	0.53
1:A:777:LEU:HD22	1:A:809:TRP:CD2	2.44	0.53
2:C:70:ASP:OD1	2:C:71:MET:N	2.42	0.53
1:A:155:PRO:HG3	3:E:306:ASP:CB	2.39	0.53
1:A:326:VAL:HG11	1:A:355:MET:HG2	1.91	0.53
1:A:569:VAL:HG23	1:A:616:GLU:O	2.09	0.53
2:C:178:GLY:H	2:C:187:VAL:HA	1.74	0.53
2:C:198:VAL:HG22	2:C:202:ARG:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:53:LEU:O	3:E:57:CYS:N	2.42	0.53
3:E:54:ASN:O	3:E:58:ASP:N	2.41	0.53
1:A:479:TRP:CD1	1:A:505:PRO:HG3	2.43	0.52
2:B:93:ARG:NH2	2:B:102:ASP:O	2.42	0.52
3:D:517:PHE:CE2	3:D:538:VAL:HB	2.43	0.52
4:F:59:LEU:HD13	4:F:63:ILE:HD13	1.90	0.52
1:A:210:LYS:HG2	1:A:221:ALA:HA	1.90	0.52
3:D:131:PHE:HB2	3:D:145:PHE:HB2	1.91	0.52
3:D:83:ALA:O	3:D:326:ARG:NH2	2.42	0.52
5:H:35:TYR:HA	5:H:38:GLY:HA3	1.91	0.52
5:H:485:LYS:HA	5:I:591:PRO:O	2.09	0.52
5:I:478:TRP:HA	5:I:601:ILE:N	2.13	0.52
1:A:714:TYR:HE2	1:A:723:VAL:HG21	1.74	0.52
1:A:770:ILE:HD12	1:A:813:ILE:HG21	1.91	0.52
1:A:869:ASN:OD1	1:A:870:LEU:N	2.39	0.52
2:B:180:ILE:CD1	2:B:182:PRO:HD3	2.38	0.52
2:C:53:GLU:N	2:C:53:GLU:OE1	2.43	0.52
1:A:912:ILE:H	2:B:329:ASN:C	2.01	0.52
2:C:79:VAL:HB	2:C:256:VAL:HA	1.91	0.52
3:D:414:LEU:HD11	3:D:484:MET:HB3	1.92	0.52
3:D:492:TYR:HA	3:D:606:ILE:HD13	1.90	0.52
4:F:63:ILE:HG22	4:F:64:TYR:N	2.16	0.52
2:B:132:ARG:CB	2:B:190:TYR:HA	2.40	0.52
1:A:912:ILE:C	2:B:329:ASN:HB2	2.25	0.52
2:B:56:PHE:CD1	2:B:56:PHE:C	2.82	0.52
1:A:717:ALA:H	3:D:9:GLN:NE2	2.07	0.52
1:A:906:LEU:HD23	2:B:334:PHE:CB	2.35	0.52
2:C:138:ASP:O	2:C:139:THR:OG1	2.26	0.52
3:D:227:ARG:HG3	3:D:228:GLU:H	1.75	0.52
1:A:436:THR:HG23	1:A:441:VAL:N	2.18	0.52
1:A:872:SER:HA	1:A:875:TRP:NE1	2.25	0.52
3:E:388:GLN:O	3:E:392:ILE:HG12	2.09	0.52
1:A:36:VAL:HG11	1:A:67:PHE:CZ	2.45	0.52
1:A:160:VAL:HG11	1:A:589:LYS:NZ	2.25	0.52
2:C:211:PRO:HG3	2:C:223:TRP:CE3	2.45	0.52
2:C:70:ASP:O	2:C:73:THR:OG1	2.18	0.52
3:D:171:ARG:O	3:D:172:ILE:HG23	2.10	0.52
3:D:553:VAL:HB	3:D:595:ILE:HD13	1.92	0.52
3:E:459:PHE:CD2	3:E:632:ILE:HD11	2.44	0.52
3:E:81:ARG:HD2	3:E:325:ILE:CG2	2.39	0.52
1:A:415:ARG:NH1	1:A:418:GLY:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:VAL:H	1:A:592:GLY:HA2	1.74	0.52
2:B:238:LEU:O	2:B:238:LEU:HD23	2.10	0.52
2:B:318:ILE:HG23	2:B:319:ILE:N	2.24	0.52
4:F:94:TYR:O	4:F:97:SER:OG	2.17	0.52
1:A:408:HIS:CG	1:A:409:ASP:N	2.78	0.52
2:B:138:ASP:HA	2:B:185:GLY:HA3	1.91	0.52
2:B:128:TRP:O	2:B:194:ILE:HG23	2.10	0.52
3:D:386:THR:O	3:D:387:VAL:HG22	2.09	0.52
3:D:555:ILE:HG22	3:D:590:TYR:HB2	1.92	0.52
1:A:178:GLY:HA3	1:A:532:ALA:H	1.74	0.51
1:A:585:MET:CB	1:A:598:TYR:H	2.23	0.51
1:A:943:GLU:H	1:A:951:ALA:HA	1.74	0.51
2:B:29:GLY:N	2:B:34:LYS:HB3	2.25	0.51
2:C:270:ARG:HG2	2:C:317:PRO:HA	1.92	0.51
1:A:705:TRP:CZ2	3:D:15:ASN:C	2.84	0.51
1:A:984:SER:C	1:A:986:ARG:N	2.63	0.51
2:B:51:GLU:HG2	2:B:269:PHE:HE1	1.73	0.51
2:C:149:ASP:OD1	2:C:152:GLU:HB3	2.10	0.51
2:C:40:THR:OG1	2:C:273:SER:O	2.15	0.51
2:C:79:VAL:HB	2:C:256:VAL:HG12	1.92	0.51
3:D:358:GLN:HG2	3:D:379:LYS:HG2	1.92	0.51
3:D:539:ARG:HH21	3:D:581:ALA:HA	1.75	0.51
5:G:595:VAL:O	5:I:489:GLY:HA2	2.11	0.51
1:A:168:ILE:HG22	1:A:541:TYR:CE2	2.45	0.51
2:B:204:THR:HG22	2:B:205:ASN:N	2.26	0.51
1:A:913:ILE:CG1	2:B:328:ILE:HD13	2.40	0.51
3:D:512:SER:CB	3:D:539:ARG:HB2	2.31	0.51
1:A:221:ALA:HB3	5:I:562:SER:O	2.10	0.51
1:A:777:LEU:O	1:A:777:LEU:HD23	2.10	0.51
1:A:934:ALA:HB2	1:A:954:GLU:N	2.25	0.51
1:A:61:TYR:CG	2:B:156:LEU:HD22	2.45	0.51
2:B:57:ALA:HB2	2:C:7:ILE:CG1	2.39	0.51
3:D:86:ARG:HH11	3:D:86:ARG:HG2	1.73	0.51
1:A:770:ILE:HD13	1:A:820:LEU:HD11	1.92	0.51
1:A:87:GLN:HA	2:B:155:LYS:O	2.09	0.51
2:B:95:TRP:CZ3	2:B:169:PRO:HG2	2.45	0.51
4:F:38:ARG:HD2	4:F:187:ILE:HG21	1.93	0.51
4:F:53:SER:C	4:F:55:ARG:H	2.13	0.51
1:A:696:ARG:HG3	1:A:729:SER:HB2	1.92	0.51
4:F:53:SER:O	4:F:55:ARG:N	2.35	0.51
5:G:106:PRO:O	5:G:111:ALA:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:LYS:HE3	2:C:99:ARG:NH2	2.25	0.51
1:A:942:ILE:HA	1:A:951:ALA:HB2	1.92	0.51
2:B:89:VAL:HA	2:B:208:ILE:O	2.11	0.51
2:C:92:ARG:HD3	2:C:205:ASN:O	2.11	0.51
2:C:37:ILE:HD12	2:C:276:THR:HG22	1.92	0.51
1:A:882:PHE:CE1	3:D:334:GLU:OE2	2.57	0.51
3:E:155:ARG:HB2	3:E:161:TYR:HE1	1.75	0.51
1:A:492:ALA:HB2	1:A:501:PHE:HA	1.92	0.51
2:B:130:VAL:O	2:B:132:ARG:N	2.44	0.51
2:C:97:ASP:O	2:C:103:PRO:HB3	2.10	0.51
3:E:174:ARG:NH2	3:E:269:VAL:HG21	2.26	0.51
3:D:298:ILE:HG22	3:D:300:ILE:CD1	2.40	0.51
3:D:518:ASN:OD1	3:D:519:SER:N	2.35	0.51
3:E:602:ILE:HG22	3:E:603:TYR:H	1.76	0.51
1:A:906:LEU:CD2	2:B:334:PHE:CA	2.88	0.51
1:A:912:ILE:HG22	2:B:329:ASN:CB	2.40	0.50
2:B:93:ARG:O	2:B:112:VAL:HA	2.11	0.50
2:C:135:ASP:HB3	2:C:187:VAL:CG1	2.41	0.50
2:B:271:GLN:O	2:B:272:ILE:HG13	2.11	0.50
2:C:297:TYR:HB3	2:C:302:LEU:HD11	1.93	0.50
3:D:105:ALA:HB1	3:D:169:GLN:HB3	1.92	0.50
3:D:350:SER:O	3:D:352:ARG:N	2.45	0.50
3:E:602:ILE:HG22	3:E:603:TYR:N	2.26	0.50
1:A:165:ASN:N	3:E:154:ILE:HD13	2.26	0.50
1:A:571:PRO:O	1:A:572:ASN:HB2	2.11	0.50
1:A:817:LEU:HA	1:A:845:LYS:HB3	1.94	0.50
2:B:111:ILE:HD13	2:B:133:CYS:HB3	1.92	0.50
2:B:180:ILE:HD12	2:B:182:PRO:HD3	1.93	0.50
2:B:211:PRO:HG2	2:B:216:LEU:HD11	1.92	0.50
3:D:503:ASN:ND2	3:D:632:ILE:HG23	2.27	0.50
3:E:113:THR:HG22	3:E:298:ILE:HD13	1.93	0.50
3:E:541:VAL:O	3:E:554:ILE:HG13	2.10	0.50
3:D:188:TYR:CE1	4:F:190:LYS:HG3	2.47	0.50
1:A:310:ALA:O	1:A:311:ILE:HG13	2.12	0.50
2:C:131:TYR:HB3	2:C:188:TRP:HB3	1.92	0.50
3:D:151:VAL:HG12	3:D:152:ILE:N	2.24	0.50
3:D:194:ARG:HH21	3:D:234:THR:HG22	1.77	0.50
3:E:143:TYR:HE1	3:E:276:ASN:HD22	1.60	0.50
1:A:996:ALA:H	5:G:20:ARG:CB	2.24	0.50
1:A:932:ARG:O	1:A:933:ILE:HB	2.12	0.50
2:B:220:PRO:O	2:B:221:THR:OG1	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:491:PHE:O	3:D:493:LYS:N	2.44	0.50
3:D:540:ILE:HG22	3:D:555:ILE:HA	1.94	0.50
3:E:90:VAL:HA	3:E:93:ALA:HB3	1.94	0.50
4:F:135:ASP:OD1	4:F:135:ASP:N	2.43	0.50
5:G:409:SER:O	5:H:445:ALA:HA	2.10	0.50
5:H:51:THR:C	5:H:69:ALA:HA	2.31	0.50
1:A:643:PRO:HB2	4:F:84:TYR:OH	2.11	0.50
1:A:770:ILE:HD11	1:A:842:VAL:HG12	1.93	0.50
2:B:113:VAL:HA	2:B:130:VAL:HB	1.94	0.50
2:B:87:ASP:HA	2:B:212:TRP:HH2	1.74	0.50
3:D:226:MET:HG2	3:D:236:PHE:CE1	2.46	0.50
3:D:386:THR:C	3:D:388:GLN:H	2.14	0.50
3:D:461:LYS:NZ	3:D:480:ALA:O	2.36	0.50
3:D:623:LEU:HD12	3:D:624:TYR:N	2.26	0.50
5:G:410:GLN:N	5:I:407:TYR:HA	2.26	0.50
1:A:679:TYR:HA	1:A:684:ASN:HD22	1.76	0.50
2:B:275:ILE:HD11	2:B:278:PRO:CD	2.42	0.50
3:D:135:ALA:HA	3:D:283:ALA:N	2.27	0.50
4:F:63:ILE:CG2	4:F:64:TYR:H	2.18	0.50
1:A:251:ASP:O	1:A:299:THR:OG1	2.27	0.50
2:B:263:LEU:N	2:B:266:ASN:ND2	2.55	0.50
2:C:253:LEU:O	2:C:256:VAL:HG22	2.11	0.50
3:E:493:LYS:O	3:E:494:THR:OG1	2.23	0.50
4:F:109:ILE:HG23	4:F:152:ALA:HB1	1.94	0.50
5:H:25:LYS:O	5:H:28:GLU:N	2.45	0.50
2:C:281:ALA:N	2:C:301:ASP:O	2.45	0.50
1:A:898:MET:HB3	2:C:330:ILE:HD13	1.74	0.50
2:C:247:ILE:HG22	2:C:332:PHE:HB2	1.94	0.50
3:D:370:GLY:HA2	3:D:404:ILE:HG22	1.94	0.50
3:D:442:ASP:O	3:D:446:ARG:N	2.37	0.50
5:G:430:TRP:C	5:G:432:ASN:H	2.15	0.50
5:I:87:ASN:HA	5:I:136:VAL:N	2.27	0.50
1:A:339:ASP:O	1:A:341:LEU:N	2.39	0.49
1:A:341:LEU:O	1:A:342:SER:OG	2.23	0.49
1:A:911:THR:OG1	2:B:330:ILE:HA	2.12	0.49
3:D:34:ILE:O	3:D:38:ASN:N	2.45	0.49
1:A:626:GLN:N	1:A:626:GLN:OE1	2.44	0.49
1:A:306:ARG:NH2	5:H:561:GLU:CB	2.75	0.49
1:A:139:ASN:C	1:A:555:ARG:HH12	2.14	0.49
1:A:708:ILE:HD12	1:A:727:PHE:CZ	2.47	0.49
2:B:193:GLU:HB2	2:B:223:TRP:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:ILE:HD12	2:B:276:THR:H	1.60	0.49
2:B:45:GLU:CD	2:B:46:PRO:HD2	2.32	0.49
3:D:298:ILE:HG22	3:D:300:ILE:HD12	1.93	0.49
3:E:469:ASP:HA	3:E:475:VAL:HG21	1.94	0.49
3:E:71:GLY:O	3:E:75:VAL:HG23	2.11	0.49
4:F:87:ILE:HD13	4:F:167:ARG:HB3	1.93	0.49
4:F:167:ARG:O	4:F:167:ARG:HG3	2.12	0.49
5:G:410:GLN:H	5:I:407:TYR:HA	1.77	0.49
5:G:464:VAL:CA	5:I:429:GLY:HA3	2.29	0.49
1:A:69:PHE:HE2	1:A:72:ALA:HB2	1.76	0.49
3:E:134:TYR:HE1	3:E:142:PRO:HG3	1.77	0.49
4:F:2:LEU:HB3	4:F:181:MET:HE1	1.95	0.49
5:I:51:THR:O	5:I:53:ASN:N	2.45	0.49
1:A:1027:GLN:NE2	2:C:8:TYR:HE2	2.06	0.49
1:A:937:THR:O	1:A:939:THR:N	2.45	0.49
2:B:249:PHE:CE1	2:B:330:ILE:HD11	2.46	0.49
2:B:70:ASP:OD1	2:B:71:MET:N	2.45	0.49
2:C:329:ASN:O	2:C:330:ILE:HG22	2.13	0.49
3:D:145:PHE:CG	3:D:167:LEU:HD13	2.46	0.49
3:E:179:TYR:HB2	3:E:268:ILE:CD1	2.41	0.49
5:I:19:LEU:O	5:I:21:LYS:N	2.45	0.49
1:A:404:TYR:HA	1:A:415:ARG:CA	2.40	0.49
2:C:152:GLU:HA	2:C:155:LYS:HG2	1.94	0.49
3:E:377:LYS:HD2	3:E:639:LEU:HD13	1.95	0.49
3:E:459:PHE:HZ	3:E:464:MET:SD	2.36	0.49
3:E:640:ILE:HG23	3:E:641:VAL:H	1.76	0.49
1:A:1007:LEU:HD23	1:A:1010:LYS:H	1.78	0.49
1:A:646:ARG:HD3	1:A:673:GLN:OE1	2.13	0.49
2:C:284:HIS:C	2:C:286:ASN:H	2.15	0.49
2:C:323:ASP:OD1	2:C:324:GLN:N	2.46	0.49
3:D:424:TYR:HE1	3:D:426:LEU:HD23	1.78	0.49
3:D:491:PHE:C	3:D:493:LYS:H	2.16	0.49
3:D:549:GLY:HA3	3:D:596:ASN:OD1	2.13	0.49
3:E:417:LYS:NZ	3:E:649:GLN:O	2.45	0.49
3:E:546:ASP:O	3:E:547:SER:OG	2.28	0.49
5:H:554:GLY:HA2	5:I:564:PRO:O	2.13	0.49
1:A:443:LEU:CD2	1:A:444:SER:H	2.21	0.49
3:D:513:ASN:HB2	3:D:622:GLU:O	2.13	0.49
3:E:106:ALA:HA	3:E:314:ASP:HA	1.94	0.49
3:E:517:PHE:HB3	3:E:536:TYR:HB3	1.93	0.49
4:F:162:GLU:O	4:F:165:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:548:GLY:HA3	5:I:569:TYR:HA	1.95	0.49
1:A:229:VAL:O	1:A:250:TYR:N	2.46	0.49
2:B:221:THR:HA	2:B:224:GLY:HA2	1.95	0.49
2:B:41:PHE:CG	2:B:42:GLY:N	2.80	0.49
3:E:606:ILE:O	3:E:609:ILE:HG22	2.13	0.49
5:I:61:THR:O	5:I:63:GLU:N	2.46	0.49
1:A:869:ASN:CG	1:A:870:LEU:H	2.17	0.49
2:B:196:PRO:O	2:B:199:SER:OG	2.14	0.49
2:B:57:ALA:HB2	2:C:7:ILE:HG13	1.95	0.49
1:A:717:ALA:N	3:D:9:GLN:HE21	2.10	0.49
3:E:229:THR:OG1	3:E:233:ASN:N	2.45	0.49
3:E:495:PRO:C	3:E:497:ALA:H	2.17	0.49
1:A:405:VAL:HG21	1:A:416:VAL:HG13	1.95	0.48
1:A:674:TYR:O	1:A:681:THR:OG1	2.18	0.48
1:A:712:ASN:HD21	1:A:720:ARG:CB	2.25	0.48
1:A:713:ILE:HD12	2:B:5:SER:HB2	1.95	0.48
1:A:936:LEU:HG	1:A:937:THR:N	2.28	0.48
5:G:488:VAL:HA	5:H:486:VAL:HA	1.95	0.48
1:A:303:ASN:OD1	1:A:304:VAL:HG13	2.12	0.48
1:A:326:VAL:HG21	1:A:355:MET:HE3	1.95	0.48
1:A:342:SER:HB2	1:A:343:PRO:HD2	1.94	0.48
3:D:189:ASP:O	3:D:191:ASN:N	2.45	0.48
3:E:485:VAL:HB	3:E:624:TYR:HD1	1.79	0.48
4:F:43:TYR:CE2	4:F:180:PHE:HA	2.48	0.48
1:A:379:ILE:HG12	1:A:404:TYR:CE2	2.48	0.48
1:A:440:LEU:HD23	1:A:493:ASP:OD2	2.12	0.48
2:B:93:ARG:NH2	2:B:102:ASP:HB3	2.28	0.48
2:C:106:PHE:CE1	2:C:112:VAL:HG11	2.48	0.48
2:B:60:TYR:HE1	2:C:11:ILE:HD13	1.77	0.48
2:C:247:ILE:CG2	2:C:332:PHE:HB2	2.43	0.48
1:A:898:MET:HG3	2:C:330:ILE:HB	1.94	0.48
3:D:135:ALA:HB3	3:D:143:TYR:CE2	2.48	0.48
3:D:472:ASP:CG	3:D:473:HIS:H	2.17	0.48
4:F:73:LEU:O	4:F:76:CYS:HB3	2.12	0.48
5:G:414:VAL:N	5:G:441:ARG:O	2.46	0.48
1:A:105:THR:O	1:A:106:ASN:HB2	2.12	0.48
1:A:230:GLY:HA3	1:A:249:GLY:HA2	1.95	0.48
1:A:586:LEU:HD23	1:A:588:TYR:OH	2.13	0.48
1:A:36:VAL:HG13	1:A:59:LEU:HB2	1.95	0.48
1:A:848:LEU:HD12	1:A:849:GLN:HG2	1.95	0.48
1:A:97:THR:O	1:A:99:GLU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:90:ILE:HD12	2:C:111:ILE:CD1	2.43	0.48
3:D:339:CYS:HB3	3:D:348:PHE:CD2	2.49	0.48
3:D:434:GLN:O	3:D:437:GLU:N	2.46	0.48
3:D:69:GLN:CG	4:F:25:MET:CE	2.79	0.48
5:I:43:PRO:CB	5:I:65:GLY:HA3	2.43	0.48
1:A:241:SER:HA	1:A:518:LYS:HD3	1.95	0.48
1:A:252:LYS:HA	1:A:299:THR:OG1	2.13	0.48
1:A:577:GLY:H	1:A:607:THR:HG22	1.79	0.48
1:A:575:PHE:HE2	1:A:586:LEU:HD11	1.78	0.48
2:B:275:ILE:HD11	2:B:278:PRO:HD3	1.96	0.48
2:B:43:ARG:HB3	2:B:269:PHE:O	2.14	0.48
2:C:92:ARG:HB3	2:C:208:ILE:HG23	1.94	0.48
3:D:554:ILE:HG21	3:D:578:ASN:ND2	2.28	0.48
4:F:110:VAL:HG13	4:F:111:TYR:CD2	2.49	0.48
4:F:112:HIS:ND1	4:F:152:ALA:HB2	2.28	0.48
4:F:131:TYR:CE2	4:F:149:ALA:HB2	2.48	0.48
5:G:103:ASN:CB	5:G:123:PRO:HA	2.43	0.48
5:I:60:LEU:O	5:I:64:TRP:N	2.46	0.48
1:A:184:CYS:SG	1:A:185:LYS:N	2.86	0.48
1:A:362:LYS:O	1:A:383:VAL:HA	2.14	0.48
1:A:403:ILE:HD11	1:A:416:VAL:HG22	1.94	0.48
1:A:488:MET:HG2	1:A:489:ALA:N	2.29	0.48
1:A:771:ILE:HD11	1:A:839:ILE:CD1	2.44	0.48
1:A:757:GLU:HA	1:A:868:SER:CB	2.44	0.48
3:D:487:GLU:OE2	3:D:647:ARG:NH2	2.26	0.48
5:G:478:TRP:HA	5:G:601:ILE:H	1.78	0.48
5:H:86:VAL:C	5:H:88:ASP:H	2.17	0.48
1:A:317:TYR:HB3	1:A:330:LYS:HA	1.95	0.48
1:A:437:ASP:HA	1:A:516:TRP:CE3	2.49	0.48
4:F:57:GLU:HA	4:F:86:TRP:CZ3	2.48	0.48
5:I:22:GLY:O	5:I:23:GLY:C	2.51	0.48
3:D:143:TYR:HD1	3:D:276:ASN:HD22	1.60	0.48
3:D:485:VAL:HG21	3:D:650:TYR:CZ	2.49	0.48
3:D:420:LEU:O	3:D:653:ILE:HA	2.14	0.48
3:E:108:THR:HG22	3:E:109:GLU:N	2.29	0.48
3:E:556:GLY:O	3:E:589:TYR:HD1	1.97	0.48
2:B:279:LEU:HD23	2:B:289:ASN:HB2	1.96	0.48
3:E:112:LEU:HD21	3:E:297:VAL:HG22	1.94	0.48
5:G:101:THR:H	5:G:124:VAL:CB	2.27	0.48
1:A:1018:ASN:CA	2:B:91:PRO:HB3	2.41	0.48
2:C:260:GLU:CD	2:C:263:LEU:HB3	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:277:ASN:OD1	2:C:291:LYS:HE3	2.14	0.48
5:I:50:LYS:O	5:I:52:TYR:N	2.46	0.48
1:A:191:TYR:CD2	1:A:237:VAL:HG21	2.49	0.47
1:A:296:THR:HG22	1:A:348:ARG:HD2	1.95	0.47
1:A:404:TYR:O	1:A:413:TRP:HB3	2.14	0.47
2:B:129:LEU:H	2:B:130:VAL:HG23	1.79	0.47
2:C:155:LYS:HG3	2:C:156:LEU:HD13	1.96	0.47
3:E:110:ILE:HG22	3:E:302:GLU:HA	1.95	0.47
2:B:144:ILE:CG2	2:B:160:TRP:HA	2.43	0.47
2:C:37:ILE:HB	2:C:81:VAL:HG11	1.95	0.47
3:D:510:MET:SD	3:D:623:LEU:HD13	2.54	0.47
3:E:211:ARG:HG3	3:E:211:ARG:O	2.14	0.47
1:A:113:MET:HE3	1:A:613:LYS:H	1.78	0.47
1:A:140:ASP:O	1:A:555:ARG:NH2	2.47	0.47
1:A:146:LEU:HD21	1:A:575:PHE:CE1	2.49	0.47
1:A:635:GLU:CB	1:A:679:TYR:H	2.27	0.47
1:A:900:ILE:HG22	2:C:311:TYR:CD1	2.47	0.47
2:B:282:LYS:HE3	2:B:289:ASN:HB3	1.96	0.47
2:C:132:ARG:O	2:C:133:CYS:HB3	2.14	0.47
3:D:590:TYR:HB3	3:D:609:ILE:HG21	1.96	0.47
3:E:522:LYS:HB2	3:E:534:VAL:HG11	1.96	0.47
5:G:594:THR:O	5:I:516:ALA:HA	2.15	0.47
1:A:777:LEU:HD21	1:A:798:ILE:HD11	1.96	0.47
1:A:1027:GLN:CB	2:C:6:VAL:HG13	2.44	0.47
3:E:103:LYS:NZ	3:E:191:ASN:OD1	2.45	0.47
1:A:894:THR:O	2:C:326:GLU:CB	2.61	0.47
1:A:911:THR:OG1	2:B:330:ILE:CA	2.63	0.47
2:B:130:VAL:HG12	2:B:130:VAL:O	2.14	0.47
2:B:277:ASN:CA	2:B:291:LYS:HE3	2.44	0.47
2:C:193:GLU:HB3	2:C:224:GLY:HA3	1.96	0.47
3:E:51:SER:O	3:E:53:LEU:N	2.45	0.47
4:F:111:TYR:O	4:F:153:VAL:HG22	2.14	0.47
3:D:115:THR:O	3:D:296:THR:HG23	2.14	0.47
3:D:298:ILE:CG2	3:D:298:ILE:O	2.62	0.47
5:G:30:PHE:O	5:G:34:TYR:N	2.47	0.47
5:G:83:LYS:HA	5:G:137:TYR:CB	2.45	0.47
1:A:69:PHE:CE2	1:A:72:ALA:HB2	2.50	0.47
1:A:720:ARG:NH1	3:D:12:ARG:CB	2.77	0.47
2:B:274:ILE:C	2:B:275:ILE:CG2	2.79	0.47
2:C:43:ARG:HH21	2:C:47:TRP:HB3	1.79	0.47
3:E:550:ILE:HB	3:E:594:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:87:SER:HA	3:E:90:VAL:HG12	1.95	0.47
5:H:95:ALA:HA	5:H:126:ILE:HA	1.95	0.47
1:A:241:SER:O	1:A:244:THR:OG1	2.33	0.47
1:A:158:VAL:O	1:A:594:ILE:HG22	2.15	0.47
1:A:720:ARG:HG3	1:A:721:ASP:N	2.29	0.47
2:B:151:ASP:HA	2:B:160:TRP:CH2	2.50	0.47
1:A:33:TYR:CZ	2:B:155:LYS:NZ	2.80	0.47
2:B:263:LEU:HD23	2:B:263:LEU:N	2.27	0.47
3:D:102:SER:H	3:D:194:ARG:NH1	2.13	0.47
3:E:356:ILE:HD12	3:E:357:ILE:HG12	1.96	0.47
3:E:651:LEU:O	3:E:652:THR:OG1	2.28	0.47
1:A:883:VAL:HG12	1:A:884:HIS:N	2.29	0.47
2:B:42:GLY:O	2:B:76:MET:HE2	2.13	0.47
4:F:77:ASN:ND2	4:F:169:ILE:HG22	2.25	0.47
4:F:173:ALA:C	4:F:175:SER:H	2.17	0.47
5:H:503:ASN:H	5:H:519:THR:H	1.63	0.47
1:A:329:ILE:HG12	1:A:350:PHE:CD1	2.50	0.47
1:A:404:TYR:CE1	1:A:415:ARG:HD2	2.49	0.47
2:B:95:TRP:CE2	2:B:169:PRO:HB2	2.50	0.47
3:E:486:ARG:CD	3:E:501:TYR:HB3	2.44	0.47
1:A:720:ARG:HH22	3:D:10:LEU:HA	1.80	0.47
3:D:493:LYS:O	3:D:494:THR:OG1	2.26	0.47
3:E:179:TYR:OH	3:E:261:LYS:NZ	2.42	0.47
5:H:576:THR:HA	5:I:537:THR:HA	1.96	0.47
1:A:191:TYR:HB2	1:A:202:PHE:HB2	1.97	0.46
1:A:350:PHE:N	1:A:350:PHE:CD1	2.83	0.46
1:A:784:GLN:NE2	1:A:830:ARG:HB2	2.30	0.46
2:B:108:ILE:HG23	2:B:109:ASN:N	2.29	0.46
1:A:896:LEU:O	2:C:329:ASN:HB2	2.15	0.46
2:C:37:ILE:HB	2:C:81:VAL:CG1	2.45	0.46
3:D:546:ASP:HB3	3:D:550:ILE:CB	2.45	0.46
3:D:592:ILE:HD12	3:D:606:ILE:HG13	1.96	0.46
1:A:900:ILE:HG13	2:C:332:PHE:HA	1.96	0.46
1:A:993:LEU:HB3	5:I:17:ASP:CB	2.44	0.46
2:C:202:ARG:O	2:C:248:ARG:NH2	2.45	0.46
2:B:315:ARG:HG2	2:C:8:TYR:HB3	1.96	0.46
5:G:540:GLU:HA	5:H:572:ALA:O	2.15	0.46
1:A:417:PHE:HE2	1:A:427:ILE:HD11	1.80	0.46
1:A:482:ASP:CG	1:A:483:LYS:H	2.19	0.46
1:A:496:SER:OG	1:A:498:TRP:N	2.49	0.46
2:B:234:ASP:O	2:B:235:ASP:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:LEU:HB3	2:B:249:PHE:HB3	1.96	0.46
2:B:278:PRO:O	2:B:279:LEU:HD12	2.15	0.46
2:C:137:PRO:HD3	2:C:186:TYR:CE2	2.50	0.46
3:E:179:TYR:HB2	3:E:268:ILE:HD12	1.96	0.46
3:E:394:ASN:C	3:E:396:LEU:H	2.19	0.46
3:E:559:ALA:C	3:E:561:GLY:H	2.18	0.46
5:H:80:ASN:N	5:H:110:VAL:O	2.47	0.46
5:H:518:GLY:O	5:I:593:ILE:HA	2.16	0.46
1:A:403:ILE:HG12	1:A:417:PHE:HB2	1.96	0.46
2:C:56:PHE:CB	3:D:6:VAL:HG11	2.46	0.46
2:C:64:SER:OG	2:C:65:VAL:N	2.49	0.46
3:E:493:LYS:HG3	3:E:494:THR:O	2.14	0.46
2:B:263:LEU:O	2:B:264:PRO:C	2.52	0.46
2:C:166:SER:HB3	2:C:186:TYR:CE2	2.51	0.46
2:C:170:PRO:HG3	2:C:188:TRP:CG	2.51	0.46
2:C:42:GLY:HA2	2:C:76:MET:N	2.30	0.46
3:E:620:THR:O	3:E:621:ILE:HB	2.16	0.46
5:G:593:ILE:O	5:I:488:VAL:N	2.29	0.46
5:G:536:GLU:HA	5:H:574:ALA:O	2.15	0.46
1:A:113:MET:HE3	1:A:612:TRP:HA	1.98	0.46
1:A:906:LEU:HD23	2:B:334:PHE:CA	2.45	0.46
2:B:309:MET:HE3	2:C:13:THR:HG21	1.98	0.46
2:C:184:ASP:CG	2:C:185:GLY:H	2.18	0.46
3:D:374:ILE:HB	3:D:408:ILE:HD13	1.98	0.46
3:D:94:GLN:NE2	3:D:228:GLU:HB2	2.30	0.46
3:E:491:PHE:O	3:E:492:TYR:HB3	2.16	0.46
5:G:23:GLY:O	5:G:26:ILE:N	2.48	0.46
5:G:592:TYR:HA	5:I:486:VAL:H	1.81	0.46
1:A:260:THR:HB	1:A:291:VAL:HG12	1.97	0.46
5:G:467:ASN:CB	5:I:418:GLY:HA2	2.45	0.46
5:I:420:VAL:HA	5:I:435:ALA:HA	1.98	0.46
1:A:132:SER:C	1:A:134:TYR:H	2.19	0.46
1:A:481:ALA:HB3	1:A:487:MET:H	1.81	0.46
2:B:168:THR:N	2:B:169:PRO:HD3	2.30	0.46
1:A:713:ILE:HD12	2:B:5:SER:CB	2.45	0.46
3:D:542:SER:HA	3:D:553:VAL:HG23	1.97	0.46
1:A:357:ILE:HG13	1:A:413:TRP:CE3	2.50	0.46
1:A:793:CYS:CB	1:A:813:ILE:HD11	2.46	0.46
1:A:860:SER:HB2	1:A:863:VAL:HG22	1.98	0.46
2:B:92:ARG:NH2	2:B:205:ASN:O	2.49	0.46
2:B:238:LEU:HD12	2:B:241:ARG:HH21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:ALA:N	2:B:301:ASP:O	2.49	0.46
1:A:1019:PRO:HD2	2:B:91:PRO:CB	2.46	0.46
2:C:55:GLY:O	2:C:56:PHE:CD2	2.69	0.46
1:A:965:LEU:O	1:A:967:ASP:N	2.38	0.46
2:B:86:LEU:CB	2:B:249:PHE:HB3	2.46	0.46
1:A:679:TYR:OH	3:D:20:ILE:HD13	1.61	0.46
2:C:56:PHE:HB3	3:D:6:VAL:HG11	1.98	0.46
3:E:28:GLU:HG2	3:E:65:LEU:CD1	2.46	0.46
5:G:123:PRO:O	5:G:125:GLU:N	2.49	0.46
1:A:326:VAL:CG1	1:A:355:MET:HG2	2.46	0.45
1:A:667:PHE:CE1	3:D:37:LEU:HG	2.51	0.45
2:B:281:ALA:O	2:B:282:LYS:HB2	2.16	0.45
2:B:55:GLY:O	2:B:56:PHE:CD1	2.58	0.45
2:B:47:TRP:NE1	2:B:58:PRO:HA	2.27	0.45
2:C:250:LYS:HE2	2:C:327:GLU:HG3	1.98	0.45
2:C:258:PHE:CD2	2:C:264:PRO:HG3	2.52	0.45
2:B:13:THR:HG22	2:C:310:ILE:O	2.16	0.45
3:D:449:THR:HA	3:D:453:GLU:HB2	1.98	0.45
3:E:104:SER:OG	3:E:316:GLY:O	2.28	0.45
3:E:514:THR:HA	3:E:539:ARG:HB2	1.98	0.45
1:A:50:PRO:C	1:A:52:ASN:H	2.19	0.45
1:A:800:ARG:HG2	1:A:801:SER:O	2.16	0.45
2:C:137:PRO:HD2	2:C:162:PRO:HB3	1.98	0.45
3:E:228:GLU:HG3	3:E:229:THR:H	1.81	0.45
5:G:139:ALA:HB1	5:G:142:ARG:H	1.81	0.45
1:A:246:TYR:OH	1:A:318:ILE:HG12	2.16	0.45
1:A:32:PHE:CZ	2:C:60:TYR:CB	2.99	0.45
1:A:405:VAL:HG12	1:A:407:ASN:N	2.29	0.45
2:B:192:PHE:HD1	2:B:193:GLU:H	1.65	0.45
3:D:204:ALA:O	3:D:206:TRP:HD1	2.00	0.45
3:E:539:ARG:HE	3:E:580:LEU:HD22	1.81	0.45
1:A:223:LYS:O	1:A:224:LEU:HG	2.17	0.45
1:A:365:CYS:HA	1:A:379:ILE:HA	1.98	0.45
3:D:101:THR:HG21	3:D:351:GLU:O	2.16	0.45
3:E:595:ILE:HG23	3:E:602:ILE:HG13	1.98	0.45
5:G:518:GLY:HA3	5:H:594:THR:CB	2.46	0.45
1:A:161:SER:OG	3:E:156:ASP:CA	2.57	0.45
2:B:303:MET:O	2:B:304:ARG:C	2.55	0.45
2:B:55:GLY:O	2:B:56:PHE:O	2.35	0.45
3:D:516:SER:HA	3:D:537:ASP:HA	1.97	0.45
3:D:536:TYR:OH	3:D:558:PHE:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:64:THR:HA	3:D:67:ILE:HG22	1.99	0.45
4:F:187:ILE:O	4:F:190:LYS:HB3	2.16	0.45
4:F:92:ALA:O	4:F:96:ALA:N	2.44	0.45
5:G:100:ALA:C	5:G:102:TRP:H	2.19	0.45
5:I:478:TRP:CB	5:I:600:ARG:HA	2.47	0.45
1:A:502:THR:OG1	1:A:503:PRO:HD2	2.16	0.45
1:A:923:SER:HA	1:A:988:LYS:NZ	2.31	0.45
2:B:217:LYS:HZ3	2:B:236:PHE:H	1.64	0.45
3:D:104:SER:HB2	3:D:317:GLY:HA3	1.99	0.45
3:D:448:TYR:HA	3:D:452:VAL:HG12	1.98	0.45
1:A:337:ASP:OD1	1:A:338:PHE:N	2.48	0.45
1:A:854:TYR:O	1:A:857:ARG:HG2	2.16	0.45
1:A:948:THR:N	2:B:118:PRO:CB	2.80	0.45
2:B:60:TYR:HD1	2:B:61:PRO:CD	2.29	0.45
2:C:271:GLN:HB2	2:C:313:GLU:O	2.16	0.45
3:D:453:GLU:HA	3:D:641:VAL:HG22	1.99	0.45
3:E:107:GLN:O	3:E:108:THR:OG1	2.34	0.45
3:E:108:THR:HG22	3:E:109:GLU:H	1.81	0.45
4:F:6:PHE:HE2	4:F:32:TYR:CE1	2.33	0.45
5:G:47:GLY:HA2	5:G:66:LYS:HA	1.98	0.45
1:A:726:PHE:O	1:A:728:GLU:N	2.43	0.45
1:A:785:THR:HG22	1:A:794:ASN:OD1	2.16	0.45
1:A:913:ILE:HG22	2:B:327:GLU:O	1.98	0.45
3:D:23:GLY:HA2	3:D:68:GLN:HE21	1.82	0.45
3:E:634:THR:HB	3:E:638:SER:OG	2.17	0.45
4:F:125:SER:HB2	4:F:133:TRP:NE1	2.32	0.45
5:G:78:THR:O	5:G:109:LEU:N	2.38	0.45
5:H:86:VAL:C	5:H:88:ASP:N	2.70	0.45
1:A:212:SER:OG	1:A:219:TRP:HA	2.17	0.45
1:A:910:GLU:O	2:B:331:LEU:HB2	2.16	0.45
2:B:202:ARG:NH1	2:B:209:VAL:HG21	2.32	0.45
2:C:138:ASP:HB3	2:C:150:LYS:HD2	1.98	0.45
2:C:81:VAL:HG23	2:C:249:PHE:CE1	2.51	0.45
3:D:440:ILE:HD11	3:D:468:VAL:HA	1.99	0.45
3:E:177:ILE:HG13	3:E:178:ILE:N	2.32	0.45
3:E:484:MET:SD	3:E:627:PRO:HB3	2.57	0.45
3:E:651:LEU:HB3	3:E:653:ILE:HG23	1.98	0.45
5:H:18:TYR:O	5:H:21:LYS:N	2.34	0.45
1:A:875:TRP:O	1:A:878:ASP:N	2.47	0.45
1:A:928:GLU:HG2	1:A:959:ALA:HA	1.98	0.45
2:C:148:THR:HG23	2:C:149:ASP:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:105:ALA:HB2	3:D:275:THR:HG22	1.98	0.45
3:D:420:LEU:HB3	3:D:480:ALA:HB2	1.99	0.45
4:F:103:ASN:OD1	4:F:104:VAL:HG12	2.17	0.45
1:A:323:ARG:NH1	1:A:388:ALA:HA	2.32	0.44
1:A:525:TRP:CG	1:A:526:ILE:N	2.85	0.44
1:A:793:CYS:SG	1:A:813:ILE:HD11	2.57	0.44
1:A:834:PHE:O	1:A:834:PHE:CG	2.70	0.44
2:B:78:THR:O	2:B:296:TYR:HA	2.16	0.44
3:E:486:ARG:HD3	3:E:501:TYR:HB3	1.99	0.44
5:H:415:ASP:HA	5:H:441:ARG:H	1.81	0.44
1:A:1014:ASP:OD1	1:A:1014:ASP:N	2.49	0.44
1:A:366:TYR:CD1	1:A:380:ILE:HD11	2.53	0.44
1:A:595:ILE:HG13	1:A:596:SER:N	2.32	0.44
1:A:73:ASP:O	1:A:76:THR:OG1	2.33	0.44
1:A:920:LYS:CB	5:H:17:ASP:CB	2.95	0.44
2:B:60:TYR:HE1	2:C:11:ILE:HG23	1.79	0.44
2:B:94:ASP:HB3	2:B:113:VAL:HG22	1.98	0.44
2:B:95:TRP:CD2	2:B:169:PRO:HG2	2.52	0.44
2:B:310:ILE:HD11	2:C:16:PHE:HD1	1.82	0.44
3:D:177:ILE:HG21	3:D:185:ILE:HD12	2.00	0.44
3:E:640:ILE:HG23	3:E:641:VAL:N	2.33	0.44
5:H:480:LEU:HA	5:H:597:ARG:O	2.17	0.44
1:A:923:SER:HB3	5:I:20:ARG:CB	2.38	0.44
1:A:304:VAL:HG12	1:A:322:ALA:HB3	2.00	0.44
1:A:378:LEU:HB2	1:A:434:MET:HE3	1.99	0.44
3:D:123:ILE:HD11	3:D:295:ILE:HD11	1.98	0.44
3:D:127:ARG:O	3:D:147:SER:OG	2.35	0.44
3:D:187:ILE:HD12	3:D:189:ASP:H	1.81	0.44
5:H:519:THR:HA	5:I:592:TYR:O	2.17	0.44
1:A:790:THR:HG1	1:A:820:LEU:HA	1.83	0.44
1:A:884:HIS:ND1	1:A:885:PRO:HD2	2.32	0.44
3:D:180:ASP:C	3:D:182:LEU:H	2.20	0.44
3:E:370:GLY:C	3:E:404:ILE:HA	2.38	0.44
3:E:604:TRP:HZ2	3:E:623:LEU:HD21	1.83	0.44
4:F:2:LEU:HB2	4:F:71:TRP:HZ2	1.83	0.44
5:I:22:GLY:O	5:I:24:ILE:N	2.51	0.44
1:A:336:ILE:HD13	1:A:348:ARG:HA	2.00	0.44
2:B:132:ARG:NH2	2:B:169:PRO:O	2.47	0.44
2:B:95:TRP:CE3	2:B:104:TYR:HE1	2.35	0.44
2:B:10:ALA:HA	2:C:312:MET:O	2.18	0.44
3:D:458:SER:OG	3:D:633:PHE:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:517:PHE:HE2	3:D:538:VAL:HB	1.81	0.44
3:D:571:PRO:HB3	3:D:590:TYR:CE1	2.53	0.44
3:E:51:SER:C	3:E:53:LEU:H	2.21	0.44
3:E:589:TYR:O	3:E:590:TYR:CG	2.70	0.44
5:H:87:ASN:H	5:H:136:VAL:CB	2.30	0.44
1:A:713:ILE:HD12	2:B:5:SER:OG	2.16	0.44
1:A:779:GLU:CD	1:A:780:ASP:H	2.21	0.44
1:A:921:TRP:N	5:H:19:LEU:HA	2.31	0.44
2:B:68:VAL:HG22	2:B:309:MET:CE	2.48	0.44
3:D:102:SER:H	3:D:194:ARG:HH12	1.64	0.44
3:D:311:VAL:HG22	3:D:646:LEU:HD13	1.99	0.44
3:E:555:ILE:HG23	3:E:555:ILE:O	2.18	0.44
3:E:559:ALA:O	3:E:560:SER:OG	2.29	0.44
3:E:592:ILE:HG21	3:E:606:ILE:HG22	1.99	0.44
4:F:4:THR:HG23	4:F:5:PHE:H	1.82	0.44
5:H:457:GLY:O	5:I:463:ALA:HB3	2.18	0.44
1:A:682:GLN:HE22	3:D:72:ASN:CB	2.23	0.44
2:B:92:ARG:HD3	2:B:205:ASN:O	2.18	0.44
2:B:213:PRO:HD3	2:B:239:ILE:HG22	2.00	0.44
3:E:81:ARG:HD2	3:E:325:ILE:HG21	2.00	0.44
4:F:191:SER:O	4:F:192:TYR:CD2	2.71	0.44
4:F:53:SER:C	4:F:55:ARG:N	2.71	0.44
1:A:18:ALA:HB1	1:A:74:PRO:HB3	1.99	0.44
1:A:488:MET:HG2	1:A:489:ALA:H	1.83	0.44
2:B:175:ASP:HB3	2:B:178:GLY:O	2.18	0.44
2:C:202:ARG:CD	2:C:209:VAL:HG21	2.47	0.44
2:C:25:TYR:CD1	2:C:212:TRP:CZ2	3.06	0.44
2:C:263:LEU:N	2:C:264:PRO:HD2	2.33	0.44
3:D:419:ASN:HA	3:D:652:THR:O	2.18	0.44
3:E:414:LEU:HD21	3:E:484:MET:HE3	2.00	0.44
3:E:510:MET:HB3	3:E:542:SER:OG	2.18	0.44
1:A:436:THR:OG1	1:A:441:VAL:HA	2.18	0.43
1:A:690:ILE:HA	1:A:693:GLN:HG2	2.00	0.43
2:B:179:THR:OG1	2:B:188:TRP:O	2.26	0.43
2:B:28:ILE:HD12	2:B:37:ILE:CD1	2.46	0.43
3:D:209:TRP:HB2	3:D:223:ILE:HB	2.00	0.43
5:H:86:VAL:CB	5:H:88:ASP:H	2.31	0.43
1:A:679:TYR:HA	1:A:684:ASN:ND2	2.33	0.43
1:A:777:LEU:HG	1:A:834:PHE:HE1	1.83	0.43
1:A:898:MET:HG3	2:C:330:ILE:CG1	2.47	0.43
1:A:913:ILE:HG12	2:B:328:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:TYR:C	2:B:105:THR:HG1	2.21	0.43
3:D:485:VAL:HG12	3:D:624:TYR:CB	2.49	0.43
3:E:488:VAL:HG11	3:E:499:ILE:HG13	2.00	0.43
5:H:125:GLU:CB	5:H:127:ASN:H	2.31	0.43
1:A:18:ALA:HB3	1:A:105:THR:O	2.18	0.43
1:A:35:PHE:HB3	1:A:61:TYR:HB3	1.99	0.43
1:A:898:MET:HE3	2:C:272:ILE:HD13	0.52	0.43
2:B:151:ASP:CG	2:B:160:TRP:HH2	2.21	0.43
2:B:310:ILE:CG1	2:C:16:PHE:HD1	2.31	0.43
2:B:317:PRO:O	2:B:318:ILE:HG22	2.17	0.43
2:C:43:ARG:HB2	2:C:271:GLN:HG2	2.00	0.43
3:E:176:GLU:HA	3:E:269:VAL:HA	1.99	0.43
3:E:465:LEU:HA	3:E:468:VAL:CG1	2.45	0.43
5:G:461:GLU:O	5:I:458:THR:HA	2.17	0.43
5:H:17:ASP:CB	5:H:19:LEU:H	2.30	0.43
5:I:76:ARG:O	5:I:104:VAL:HA	2.18	0.43
5:I:456:ILE:CB	5:I:602:ALA:HA	2.49	0.43
1:A:441:VAL:HG11	1:A:498:TRP:HD1	1.83	0.43
1:A:443:LEU:HD23	1:A:444:SER:O	2.18	0.43
3:E:134:TYR:CE1	3:E:142:PRO:HG3	2.53	0.43
4:F:112:HIS:NE2	4:F:123:LEU:O	2.52	0.43
5:G:564:PRO:CB	5:I:554:GLY:HA3	2.49	0.43
1:A:606:ASP:OD2	1:A:607:THR:HG23	2.19	0.43
3:E:194:ARG:HH21	3:E:234:THR:HG22	1.81	0.43
5:I:560:ASP:C	5:I:562:SER:H	2.21	0.43
3:D:120:ARG:O	3:D:161:TYR:OH	2.32	0.43
3:D:17:ILE:CD1	4:F:16:VAL:HG22	2.47	0.43
1:A:201:LEU:HG	1:A:210:LYS:O	2.18	0.43
1:A:626:GLN:O	1:A:626:GLN:HG2	2.18	0.43
1:A:685:ASN:OD1	3:D:21:PHE:HZ	1.91	0.43
1:A:773:GLN:HB3	1:A:808:GLN:HG2	2.00	0.43
3:D:106:ALA:HB1	3:D:313:ALA:HB1	2.00	0.43
3:D:199:LEU:HD23	3:D:224:TYR:CZ	2.54	0.43
3:D:546:ASP:CG	3:D:547:SER:H	2.22	0.43
3:D:417:LYS:HG3	3:D:650:TYR:HB2	2.00	0.43
1:A:145:ALA:O	1:A:587:PHE:HB3	2.19	0.43
1:A:317:TYR:CB	1:A:330:LYS:HA	2.48	0.43
1:A:492:ALA:CB	1:A:501:PHE:HA	2.48	0.43
2:C:47:TRP:CE2	2:C:59:PRO:HD2	2.53	0.43
3:D:202:ASP:OD1	3:D:203:GLY:N	2.52	0.43
3:E:542:SER:HA	3:E:553:VAL:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:47:THR:CG2	4:F:171:ILE:HD12	2.47	0.43
4:F:43:TYR:HD2	4:F:180:PHE:HD1	1.67	0.43
4:F:2:LEU:HD22	4:F:181:MET:CE	2.49	0.43
4:F:69:LEU:O	4:F:71:TRP:CD1	2.71	0.43
1:A:303:ASN:OD1	1:A:304:VAL:N	2.52	0.43
1:A:517:SER:HB3	1:A:522:THR:O	2.19	0.43
1:A:970:ASN:HB2	1:A:973:ASN:HA	2.01	0.43
1:A:984:SER:O	1:A:986:ARG:N	2.52	0.43
2:C:25:TYR:CE1	2:C:212:TRP:CZ3	3.07	0.43
2:C:217:LYS:HB2	2:C:236:PHE:HZ	1.78	0.43
2:C:34:LYS:O	2:C:291:LYS:NZ	2.45	0.43
3:D:109:GLU:HG3	3:D:165:LEU:O	2.19	0.43
3:E:109:GLU:OE2	3:E:164:ARG:NE	2.51	0.43
3:E:319:PRO:HG2	3:E:324:ARG:NH2	2.32	0.43
4:F:110:VAL:HG12	4:F:154:ASP:O	2.19	0.43
4:F:169:ILE:HD12	4:F:170:LYS:O	2.19	0.43
5:I:460:TYR:CB	5:I:600:ARG:H	2.32	0.43
1:A:239:TYR:HE2	1:A:313:CYS:H	1.66	0.43
1:A:326:VAL:HG11	1:A:355:MET:HE2	2.00	0.43
1:A:726:PHE:C	1:A:728:GLU:H	2.23	0.43
1:A:830:ARG:HH22	1:A:861:TYR:HE1	1.67	0.43
2:B:114:CYS:H	2:B:130:VAL:HG21	1.84	0.43
2:B:202:ARG:HH12	2:B:209:VAL:HG21	1.84	0.43
3:D:512:SER:O	3:D:623:LEU:HA	2.19	0.43
3:E:115:THR:O	3:E:296:THR:N	2.48	0.43
3:E:513:ASN:ND2	3:E:621:ILE:HA	2.33	0.43
1:A:305:TYR:O	1:A:307:ILE:HG22	2.19	0.42
2:B:270:ARG:O	2:B:271:GLN:O	2.37	0.42
2:B:71:MET:O	2:B:75:MET:N	2.52	0.42
3:D:629:ASP:OD1	3:D:630:ASP:N	2.52	0.42
3:E:201:VAL:CB	3:E:268:ILE:HA	2.49	0.42
4:F:158:ALA:O	4:F:162:GLU:N	2.49	0.42
5:H:520:GLY:N	5:I:592:TYR:O	2.50	0.42
1:A:962:LYS:O	1:A:963:TYR:CG	2.72	0.42
2:B:213:PRO:O	2:B:214:GLU:HB3	2.18	0.42
2:C:37:ILE:CD1	2:C:276:THR:HG22	2.49	0.42
5:G:54:ALA:C	5:G:56:SER:H	2.23	0.42
1:A:943:GLU:N	1:A:951:ALA:HA	2.34	0.42
2:C:128:TRP:HB2	2:C:194:ILE:HB	2.01	0.42
2:B:26:ASN:HD21	2:C:33:ASP:HB3	1.83	0.42
3:D:619:GLN:O	3:D:620:THR:OG1	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:377:LYS:HE3	3:D:641:VAL:HG11	2.00	0.42
5:H:111:ALA:O	5:H:114:GLY:N	2.44	0.42
1:A:180:ILE:HG22	1:A:181:GLN:N	2.29	0.42
1:A:300:LEU:CB	1:A:302:ALA:H	2.32	0.42
1:A:36:VAL:HG11	1:A:67:PHE:CE2	2.54	0.42
2:B:68:VAL:HG22	2:B:309:MET:HE2	2.01	0.42
2:B:94:ASP:N	2:B:94:ASP:OD1	2.51	0.42
3:D:434:GLN:O	3:D:437:GLU:HB3	2.19	0.42
3:D:538:VAL:HG22	3:D:539:ARG:H	1.84	0.42
1:A:162:SER:O	3:E:154:ILE:HG12	2.16	0.42
3:E:613:SER:C	3:E:615:LYS:H	2.22	0.42
1:A:193:MET:O	1:A:200:TYR:N	2.48	0.42
1:A:568:ILE:HD11	1:A:618:PHE:HD2	1.84	0.42
1:A:146:LEU:HD21	1:A:575:PHE:HE1	1.85	0.42
1:A:936:LEU:N	1:A:940:GLY:HA3	2.34	0.42
2:B:263:LEU:CB	2:B:264:PRO:CD	2.97	0.42
2:B:77:GLY:H	2:B:299:PRO:HD3	1.84	0.42
3:E:461:LYS:O	3:E:465:LEU:HD13	2.19	0.42
3:E:28:GLU:HA	3:E:65:LEU:HD11	2.02	0.42
1:A:148:ASN:HA	1:A:582:ALA:HB1	2.00	0.42
1:A:583:SER:OG	1:A:604:VAL:HG22	2.20	0.42
1:A:713:ILE:HD11	2:B:5:SER:HB2	2.02	0.42
2:C:71:MET:O	2:C:75:MET:HG3	2.20	0.42
3:D:123:ILE:HG22	3:D:153:ALA:HB3	2.02	0.42
3:D:39:GLY:C	3:D:41:ASN:H	2.22	0.42
3:D:515:PHE:HB2	3:D:538:VAL:O	2.19	0.42
3:D:554:ILE:HG12	3:D:578:ASN:ND2	2.35	0.42
3:E:495:PRO:O	3:E:497:ALA:N	2.43	0.42
4:F:28:ILE:HG23	4:F:29:PHE:CD1	2.54	0.42
1:A:172:GLU:O	1:A:173:TYR:HB3	2.19	0.42
1:A:406:LEU:HA	1:A:413:TRP:HA	2.01	0.42
2:B:106:PHE:CE1	2:B:188:TRP:CZ2	3.08	0.42
3:D:486:ARG:O	3:D:623:LEU:HG	2.19	0.42
3:D:84:ASN:O	3:D:85:LEU:CB	2.67	0.42
5:H:27:ASN:O	5:H:31:ASP:N	2.29	0.42
1:A:36:VAL:CG1	1:A:59:LEU:HB2	2.50	0.42
1:A:118:LEU:HD11	1:A:619:LEU:HD22	2.02	0.42
1:A:898:MET:HG3	2:C:330:ILE:CB	2.50	0.42
2:B:27:SER:OG	2:B:34:LYS:HA	2.19	0.42
1:A:898:MET:HG2	2:C:330:ILE:HB	2.01	0.42
3:D:346:ASP:HA	3:D:360:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:77:GLU:HB2	3:D:88:SER:OG	2.19	0.42
3:E:616:PHE:HB3	3:E:618:VAL:HG23	2.01	0.42
3:E:99:LEU:O	3:E:99:LEU:HD12	2.19	0.42
1:A:158:VAL:HG13	1:A:159:ASP:H	1.84	0.42
1:A:181:GLN:HG2	1:A:210:LYS:NZ	2.35	0.42
3:D:111:MET:HA	3:D:164:ARG:HA	2.02	0.42
3:D:541:VAL:HG12	3:D:543:THR:H	1.85	0.42
3:D:595:ILE:HA	3:D:601:VAL:O	2.19	0.42
1:A:40:GLU:HA	1:A:77:THR:O	2.19	0.42
1:A:966:PRO:C	1:A:968:ASP:H	2.24	0.42
3:D:420:LEU:HG	3:D:653:ILE:HG22	2.01	0.42
3:E:71:GLY:O	3:E:75:VAL:N	2.53	0.42
1:A:232:PRO:HG3	1:A:237:VAL:HG22	2.01	0.41
1:A:583:SER:HB2	1:A:603:ARG:HA	2.02	0.41
1:A:860:SER:HB2	1:A:863:VAL:CG2	2.50	0.41
2:B:114:CYS:N	2:B:130:VAL:HG11	2.34	0.41
2:B:198:VAL:HG21	2:B:223:TRP:CH2	2.55	0.41
2:B:275:ILE:C	2:B:275:ILE:CD1	2.84	0.41
1:A:913:ILE:CG1	2:B:328:ILE:CD1	2.98	0.41
2:C:90:ILE:HD13	2:C:242:VAL:HG11	2.01	0.41
3:D:414:LEU:O	3:D:640:ILE:HA	2.19	0.41
3:E:505:ILE:HG21	3:E:625:SER:HB2	2.02	0.41
3:E:77:GLU:HA	3:E:83:ALA:HB1	2.02	0.41
1:A:328:TYR:HB2	1:A:351:GLU:CB	2.50	0.41
1:A:366:TYR:HB2	1:A:380:ILE:HG13	2.01	0.41
1:A:792:ARG:O	1:A:816:LEU:HD12	2.20	0.41
2:B:270:ARG:HA	2:B:315:ARG:O	2.19	0.41
2:B:51:GLU:HG2	2:B:269:PHE:CZ	2.54	0.41
2:C:24:PHE:CG	2:C:334:PHE:CZ	3.09	0.41
3:D:187:ILE:HD12	3:D:188:TYR:N	2.35	0.41
3:D:201:VAL:O	3:D:203:GLY:N	2.39	0.41
3:D:390:GLU:O	3:D:393:LYS:HB3	2.20	0.41
3:E:94:GLN:HE22	3:E:228:GLU:H	1.67	0.41
4:F:39:ALA:HB2	4:F:187:ILE:HD13	2.02	0.41
5:H:18:TYR:O	5:H:19:LEU:C	2.58	0.41
5:H:558:ASP:O	5:H:560:ASP:N	2.53	0.41
2:B:169:PRO:HD2	2:B:170:PRO:HD2	2.02	0.41
2:B:169:PRO:CD	2:B:170:PRO:HD2	2.51	0.41
2:B:39:ILE:HG12	2:B:40:THR:H	1.85	0.41
2:C:282:LYS:HE2	2:C:303:MET:SD	2.60	0.41
3:D:174:ARG:HA	3:D:270:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:384:LEU:O	3:D:385:THR:OG1	2.36	0.41
3:D:448:TYR:O	3:D:453:GLU:N	2.53	0.41
3:D:414:LEU:HD12	3:D:485:VAL:O	2.20	0.41
3:D:22:VAL:O	3:D:76:TYR:OH	2.38	0.41
3:E:356:ILE:CD1	3:E:357:ILE:HG12	2.50	0.41
3:E:464:MET:HG3	3:E:465:LEU:N	2.35	0.41
5:G:537:THR:CB	5:H:574:ALA:HB3	2.49	0.41
1:A:338:PHE:O	1:A:338:PHE:CG	2.73	0.41
1:A:41:THR:HG1	1:A:78:TYR:HD2	1.66	0.41
1:A:798:ILE:O	1:A:798:ILE:HG13	2.20	0.41
1:A:968:ASP:C	1:A:970:ASN:H	2.24	0.41
2:B:47:TRP:CH2	2:B:59:PRO:CD	2.75	0.41
3:D:354:GLY:C	3:D:356:ILE:H	2.23	0.41
3:E:434:GLN:HA	3:E:437:GLU:HB3	2.03	0.41
3:E:652:THR:HG22	3:E:652:THR:O	2.21	0.41
4:F:2:LEU:HB2	4:F:71:TRP:CZ2	2.55	0.41
4:F:94:TYR:O	4:F:98:ILE:HD12	2.19	0.41
1:A:134:TYR:HD2	1:A:135:VAL:HG22	1.84	0.41
1:A:248:LEU:HD21	1:A:308:ALA:HB1	2.02	0.41
2:B:234:ASP:C	2:B:235:ASP:O	2.58	0.41
2:C:135:ASP:CB	2:C:187:VAL:HG11	2.49	0.41
4:F:1:MET:O	4:F:1:MET:HG2	2.19	0.41
5:H:494:ILE:C	5:H:500:ALA:HB1	2.41	0.41
1:A:157:TYR:CD2	1:A:163:ILE:HG21	2.56	0.41
1:A:229:VAL:HG22	1:A:230:GLY:H	1.85	0.41
1:A:749:LYS:NZ	1:A:756:VAL:HG12	2.36	0.41
1:A:897:THR:HG22	2:C:329:ASN:CB	2.50	0.41
2:B:144:ILE:HD11	2:B:153:CYS:CB	2.49	0.41
1:A:61:TYR:CD1	2:B:156:LEU:HD22	2.56	0.41
2:B:43:ARG:O	2:B:269:PHE:HB2	2.21	0.41
2:C:293:GLU:N	2:C:297:TYR:OH	2.52	0.41
4:F:94:TYR:HD1	4:F:156:TYR:CD1	2.38	0.41
5:G:23:GLY:O	5:G:27:ASN:N	2.41	0.41
5:I:523:THR:C	5:I:588:ASN:H	2.23	0.41
5:I:72:THR:C	5:I:74:SER:N	2.74	0.41
1:A:489:ALA:HB1	1:A:491:ILE:HG13	2.03	0.41
1:A:779:GLU:HG3	1:A:798:ILE:HG21	2.02	0.41
2:C:129:LEU:HB3	2:C:131:TYR:CE2	2.56	0.41
2:C:174:GLY:O	2:C:177:GLU:HG3	2.21	0.41
2:C:41:PHE:CD1	2:C:272:ILE:HG22	2.55	0.41
3:D:201:VAL:HB	3:D:206:TRP:NE1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:55:GLY:HA3	3:D:7:ASN:OD1	2.21	0.41
3:E:493:LYS:HA	3:E:605:ASN:HA	2.02	0.41
5:H:486:VAL:N	5:I:591:PRO:O	2.54	0.41
2:B:86:LEU:HD13	2:B:247:ILE:HD11	2.01	0.41
2:C:129:LEU:HD23	2:C:131:TYR:OH	2.21	0.41
3:D:106:ALA:HA	3:D:314:ASP:O	2.21	0.41
3:D:545:ARG:HG2	3:D:546:ASP:H	1.86	0.41
3:D:487:GLU:CD	3:D:647:ARG:HH22	2.18	0.41
5:G:446:VAL:O	5:G:450:PHE:N	2.54	0.41
5:I:431:PRO:O	5:I:432:ASN:CB	2.68	0.41
1:A:1019:PRO:HD2	2:B:91:PRO:HB2	2.02	0.41
1:A:142:ILE:HG22	1:A:143:MET:N	2.28	0.41
1:A:317:TYR:HB2	1:A:329:ILE:O	2.21	0.41
1:A:861:TYR:CE2	1:A:862:TYR:HD2	2.38	0.41
1:A:928:GLU:HG3	1:A:929:TYR:N	2.26	0.41
3:D:187:ILE:HG12	3:D:234:THR:OG1	2.20	0.41
3:D:230:ILE:C	3:D:232:GLY:H	2.24	0.41
3:D:26:PHE:O	3:D:28:GLU:N	2.53	0.41
1:A:667:PHE:HE2	3:D:60:LEU:CD2	2.33	0.41
3:E:541:VAL:HG12	3:E:542:SER:N	2.36	0.41
3:E:555:ILE:HG21	3:E:592:ILE:HD11	2.03	0.41
2:B:87:ASP:HA	2:B:212:TRP:CZ2	2.56	0.41
2:C:191:LEU:HD12	2:C:191:LEU:O	2.21	0.41
3:D:362:THR:HG22	3:D:374:ILE:HG12	2.02	0.41
3:D:362:THR:HG22	3:D:374:ILE:HG23	2.03	0.41
3:D:546:ASP:OD1	3:D:547:SER:N	2.54	0.41
3:E:592:ILE:HD12	3:E:606:ILE:HA	2.02	0.41
3:E:592:ILE:O	3:E:592:ILE:HG22	2.21	0.41
4:F:30:ARG:HD3	4:F:30:ARG:HA	1.80	0.41
1:A:154:SER:OG	3:E:305:ASN:N	2.47	0.41
1:A:897:THR:HA	2:C:329:ASN:CB	2.51	0.41
1:A:945:ASP:CA	2:B:118:PRO:CB	2.98	0.41
2:B:60:TYR:HD1	2:B:61:PRO:HD2	1.86	0.41
2:C:109:ASN:N	2:C:109:ASN:OD1	2.53	0.41
4:F:183:ASP:O	4:F:186:ARG:N	2.53	0.41
5:G:531:ASN:HA	5:H:584:THR:N	2.36	0.41
1:A:142:ILE:HD12	1:A:142:ILE:HG23	1.83	0.40
1:A:183:VAL:HG22	1:A:190:VAL:HG12	2.03	0.40
1:A:864:MET:HE1	1:A:884:HIS:ND1	2.36	0.40
2:B:13:THR:OG1	2:B:14:SER:N	2.53	0.40
2:B:160:TRP:O	2:B:162:PRO:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:GLU:OE1	2:B:223:TRP:O	2.39	0.40
3:E:505:ILE:HD12	3:E:506:LYS:O	2.20	0.40
4:F:30:ARG:HB2	4:F:32:TYR:CE1	2.56	0.40
5:G:76:ARG:O	5:G:104:VAL:HA	2.20	0.40
5:H:459:ILE:N	5:I:463:ALA:HB2	2.36	0.40
1:A:759:GLU:N	1:A:759:GLU:OE1	2.54	0.40
1:A:793:CYS:HB3	1:A:816:LEU:HD13	2.03	0.40
1:A:993:LEU:O	1:A:994:PHE:HB2	2.21	0.40
2:B:149:ASP:O	2:B:150:LYS:CB	2.68	0.40
3:D:227:ARG:HG3	3:D:235:GLU:HB3	2.03	0.40
3:D:30:LYS:NZ	3:D:57:CYS:HB2	2.37	0.40
3:E:454:ILE:HD12	3:E:455:PHE:O	2.21	0.40
5:G:100:ALA:HA	5:G:124:VAL:CB	2.50	0.40
1:A:12:ARG:NH1	3:D:8:TYR:HB2	2.37	0.40
1:A:140:ASP:OD2	1:A:590:ALA:HB1	2.22	0.40
1:A:151:PHE:HB2	1:A:166:PHE:CG	2.57	0.40
1:A:794:ASN:O	1:A:813:ILE:HG13	2.21	0.40
3:D:21:PHE:CD1	3:D:75:VAL:HG21	2.56	0.40
3:D:409:ILE:O	3:D:410:SER:OG	2.29	0.40
3:E:145:PHE:HB3	3:E:167:LEU:HD11	2.03	0.40
3:E:327:GLU:O	3:E:331:ILE:HG12	2.21	0.40
3:E:505:ILE:HG13	3:E:505:ILE:H	1.75	0.40
4:F:71:TRP:C	4:F:73:LEU:N	2.71	0.40
5:G:55:SER:N	5:G:74:SER:O	2.54	0.40
1:A:913:ILE:CB	2:B:328:ILE:CD1	2.84	0.40
1:A:913:ILE:HG12	2:B:328:ILE:HD12	2.03	0.40
2:B:20:LYS:CD	2:C:20:LYS:HD3	2.52	0.40
3:D:104:SER:HB2	3:D:317:GLY:CA	2.52	0.40
3:D:187:ILE:HD12	3:D:189:ASP:N	2.37	0.40
3:D:465:LEU:HA	3:D:468:VAL:HB	2.04	0.40
3:E:136:LYS:HG2	3:E:137:ASP:N	2.36	0.40
4:F:125:SER:HB2	4:F:133:TRP:CD1	2.56	0.40
4:F:155:THR:HG23	4:F:156:TYR:N	2.36	0.40
1:A:404:TYR:CZ	1:A:415:ARG:HD2	2.55	0.40
2:B:249:PHE:CZ	2:B:330:ILE:HD11	2.57	0.40
2:B:248:ARG:HB2	2:B:330:ILE:O	2.22	0.40
3:E:487:GLU:CD	3:E:647:ARG:HH12	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1028/1032 (100%)	803 (78%)	198 (19%)	27 (3%)	7	48
2	B	332/334 (99%)	266 (80%)	47 (14%)	19 (6%)	2	28
2	C	330/334 (99%)	286 (87%)	41 (12%)	3 (1%)	21	68
3	D	643/660 (97%)	454 (71%)	162 (25%)	27 (4%)	3	36
3	E	632/660 (96%)	483 (76%)	131 (21%)	18 (3%)	6	47
4	F	190/196 (97%)	151 (80%)	32 (17%)	7 (4%)	4	40
5	G	336/602 (56%)	250 (74%)	69 (20%)	17 (5%)	2	31
5	H	336/602 (56%)	253 (75%)	71 (21%)	12 (4%)	4	41
5	I	336/602 (56%)	254 (76%)	64 (19%)	18 (5%)	2	30
All	All	4163/5022 (83%)	3200 (77%)	815 (20%)	148 (4%)	7	41

All (148) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	383	VAL
1	A	468	ILE
1	A	690	ILE
1	A	833	SER
1	A	937	THR
1	A	938	PRO
1	A	986	ARG
2	B	12	VAL
2	B	56	PHE
2	B	270	ARG
2	B	271	GLN
3	D	190	LYS
3	D	215	VAL
3	D	387	VAL
3	E	201	VAL

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Mol	Chain	Res	Type
3	E	652	THR
4	F	50	ILE
4	F	72	VAL
4	F	172	ILE
5	G	70	ILE
5	H	117	ILE
5	H	126	ILE
5	H	433	VAL
5	I	19	LEU
5	I	117	ILE
5	I	432	ASN
1	A	142	ILE
2	B	150	LYS
2	B	208	ILE
2	B	238	LEU
2	B	268	GLY
2	B	275	ILE
2	B	318	ILE
3	D	22	VAL
3	D	151	VAL
3	D	172	ILE
3	D	230	ILE
3	D	553	VAL
3	D	563	VAL
3	E	177	ILE
3	E	534	VAL
3	E	621	ILE
4	F	9	ILE
5	G	93	ILE
5	H	93	ILE
5	H	136	VAL
5	I	13	ASP
5	I	104	VAL
5	I	431	PRO
5	I	433	VAL
1	A	79	ILE
1	A	98	GLU
1	A	180	ILE
1	A	229	VAL
1	A	405	VAL
1	A	495	THR
2	B	13	THR

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Mol	Chain	Res	Type
2	B	192	PHE
2	B	235	ASP
2	B	236	PHE
2	B	261	ALA
2	B	317	PRO
3	D	40	GLN
3	D	100	PRO
3	D	202	ASP
3	D	264	GLN
3	D	492	TYR
3	D	512	SER
3	E	403	PRO
3	E	538	VAL
3	E	563	VAL
5	G	123	PRO
5	G	136	VAL
5	G	433	VAL
5	H	120	SER
5	H	128	VAL
5	I	20	ARG
5	I	128	VAL
1	A	406	LEU
1	A	882	PHE
1	A	985	GLU
2	B	108	ILE
2	B	148	THR
2	C	192	PHE
3	D	152	ILE
3	D	284	VAL
3	D	471	ALA
3	D	550	ILE
3	E	52	ARG
3	E	402	ALA
4	F	67	PRO
5	G	55	SER
5	G	128	VAL
5	H	583	PRO
5	I	93	ILE
5	I	136	VAL
5	I	447	SER
1	A	143	MET
1	A	147	MET

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Mol	Chain	Res	Type
1	A	173	TYR
1	A	224	LEU
1	A	933	ILE
2	C	219	ASP
3	D	308	PRO
3	D	350	SER
3	E	154	ILE
3	E	619	GLN
5	G	31	ASP
5	G	124	VAL
5	G	503	ASN
5	H	86	VAL
3	E	632	ILE
5	G	104	VAL
1	A	826	VAL
4	F	113	VAL
5	G	110	VAL
5	I	77	VAL
5	I	140	PRO
5	I	141	GLY
1	A	441	VAL
1	A	594	ILE
2	C	330	ILE
3	D	99	LEU
3	D	192	ILE
3	D	499	ILE
3	E	186	ILE
3	E	404	ILE
3	E	618	VAL
4	F	63	ILE
5	G	7	ILE
5	H	70	ILE
5	I	7	ILE
5	I	430	TRP
3	D	304	PRO
3	D	595	ILE
3	E	387	VAL
3	E	641	VAL
5	G	81	LEU
5	G	126	ILE
5	I	468	ASN
1	A	884	HIS

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Mol	Chain	Res	Type
3	D	141	ASN
5	G	117	ILE
5	G	581	THR
5	H	104	VAL
2	B	272	ILE
5	H	430	TRP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	683/921 (74%)	681 (100%)	2 (0%)	94	98
2	B	252/295 (85%)	245 (97%)	7 (3%)	51	81
2	C	272/295 (92%)	272 (100%)	0	100	100
3	D	479/578 (83%)	477 (100%)	2 (0%)	93	97
3	E	440/578 (76%)	439 (100%)	1 (0%)	95	98
4	F	140/169 (83%)	140 (100%)	0	100	100
All	All	2266/2836 (80%)	2254 (100%)	12 (0%)	92	97

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	TYR
1	A	349	LEU
2	B	56	PHE
2	B	60	TYR
2	B	146	SER
2	B	238	LEU
2	B	239	ILE
2	B	273	SER
2	B	275	ILE
3	D	86	ARG
3	D	87	SER
3	E	199	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	111	GLN
1	A	130	ASN
1	A	174	HIS
1	A	240	GLN
1	A	447	ASN
1	A	504	GLN
1	A	682	GLN
1	A	684	ASN
1	A	688	ASN
1	A	712	ASN
1	A	784	GLN
1	A	944	HIS
2	B	23	ASN
2	B	26	ASN
2	B	205	ASN
2	B	233	GLN
2	B	266	ASN
2	B	305	HIS
2	C	35	ASN
2	C	52	ASN
2	C	74	HIS
2	C	201	ASN
2	C	329	ASN
3	D	9	GLN
3	D	69	GLN
3	D	119	ASN
3	D	281	ASN
3	D	578	ASN
3	E	107	GLN
3	E	582	ASN
4	F	77	ASN
4	F	129	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.