



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 2, 2017 – 03:25 AM EDT

PDB ID : 5UOW  
EMDB ID: : EMD-8579  
Title : Triheteromeric NMDA receptor GluN1/GluN2A/GluN2B in complex with  
glycine, glutamate, MK-801 and a GluN2B-specific Fab, at pH 6.5  
Authors : Lu, W.; Du, J.; Goehring, A.; Gouaux, E.  
Deposited on : unknown  
Resolution : 4.50 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

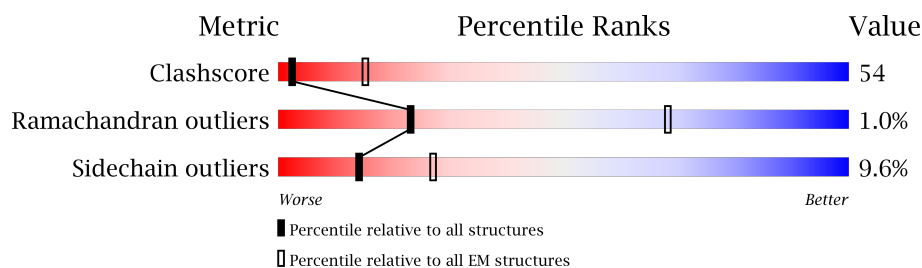
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 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.



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  $\geq 3$ , 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	814	51% 42% . .
1	C	814	59% 34% 5% .
2	B	832	46% 44% 6% .
3	D	837	62% 30% . 5%
4	F	216	91% 8% .
4	G	216	91% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GLU	B	1101	-	-	X	-
7	BMK	B	1102	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24347 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 N-methyl-D-aspartate receptor subunit NR1-8a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	797	Total	C	N	O	S	0	0
			5758	3713	971	1046	28		
1	C	798	Total	C	N	O	S	0	0
			5484	3492	946	1020	26		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	GLN	ASN	conflict	UNP C0KD18
A	350	GLN	ASN	conflict	UNP C0KD18
A	368	ASP	ASN	conflict	UNP C0KD18
A	440	ASP	ASN	conflict	UNP C0KD18
A	469	ASP	ASN	conflict	UNP C0KD18
A	493	ALA	LYS	conflict	UNP C0KD18
A	494	ALA	LYS	conflict	UNP C0KD18
A	495	ALA	GLU	conflict	UNP C0KD18
A	592	ALA	GLU	conflict	UNP C0KD18
A	593	ALA	GLU	conflict	UNP C0KD18
A	594	ALA	GLU	conflict	UNP C0KD18
A	610	ARG	GLY	conflict	UNP C0KD18
A	617	LEU	ILE	conflict	UNP C0KD18
A	636	LEU	GLY	conflict	UNP C0KD18
A	656	ARG	ASP	conflict	UNP C0KD18
A	741	ASP	LYS	conflict	UNP C0KD18
A	769	GLU	ASN	conflict	UNP C0KD18
A	816	TYR	MET	conflict	UNP C0KD18
C	300	GLN	ASN	conflict	UNP C0KD18
C	350	GLN	ASN	conflict	UNP C0KD18
C	368	ASP	ASN	conflict	UNP C0KD18
C	440	ASP	ASN	conflict	UNP C0KD18
C	469	ASP	ASN	conflict	UNP C0KD18
C	493	ALA	LYS	conflict	UNP C0KD18
C	494	ALA	LYS	conflict	UNP C0KD18
C	495	ALA	GLU	conflict	UNP C0KD18

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Chain	Residue	Modelled	Actual	Comment	Reference
C	592	ALA	GLU	conflict	UNP C0KD18
C	593	ALA	GLU	conflict	UNP C0KD18
C	594	ALA	GLU	conflict	UNP C0KD18
C	610	ARG	GLY	conflict	UNP C0KD18
C	617	LEU	ILE	conflict	UNP C0KD18
C	636	LEU	GLY	conflict	UNP C0KD18
C	656	ARG	ASP	conflict	UNP C0KD18
C	741	ASP	LYS	conflict	UNP C0KD18
C	769	GLU	ASN	conflict	UNP C0KD18
C	816	TYR	MET	conflict	UNP C0KD18

- Molecule 2 is a protein called N-methyl-D-aspartate receptor subunit NR2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	795	Total	C	N	O	S	0	0
			5582	3605	926	1020	31		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	GLN	ASN	conflict	UNP B7ZSK1
B	372	ALA	ASN	conflict	UNP B7ZSK1
B	?	-	THR	deletion	UNP B7ZSK1
B	?	-	ALA	deletion	UNP B7ZSK1
B	?	-	SER	deletion	UNP B7ZSK1
B	?	-	LEU	deletion	UNP B7ZSK1
B	431	ALA	ASN	conflict	UNP B7ZSK1
B	529	ALA	ASN	conflict	UNP B7ZSK1
B	605	LEU	VAL	conflict	UNP B7ZSK1
B	644	ARG	GLU	conflict	UNP B7ZSK1
B	645	ARG	GLU	conflict	UNP B7ZSK1
B	675	GLN	ASN	conflict	UNP B7ZSK1
B	831	LYS	-	expression tag	UNP B7ZSK1
B	832	GLU	-	expression tag	UNP B7ZSK1

- Molecule 3 is a protein called Ionotropic glutamate receptor subunit NR2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	795	Total	C	N	O	S	0	0
			5127	3279	868	955	25		

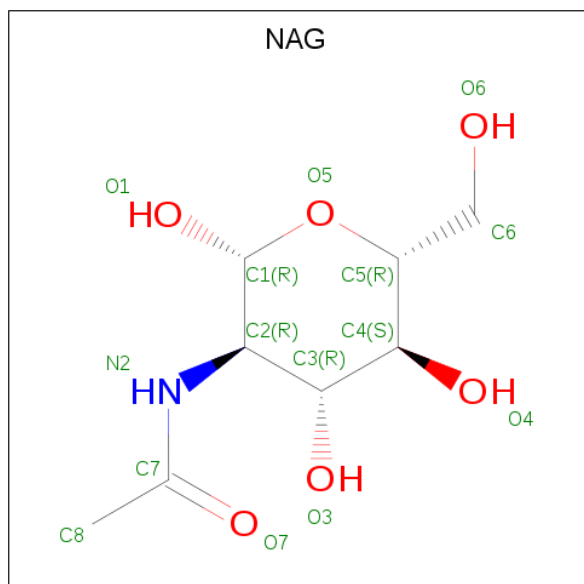
There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	20	SER	MET	conflict	UNP A7XY94
D	21	ARG	GLY	conflict	UNP A7XY94
D	22	ALA	CYS	conflict	UNP A7XY94
D	64	GLU	ALA	conflict	UNP A7XY94
D	69	GLN	ASN	conflict	UNP A7XY94
D	343	ASP	ASN	conflict	UNP A7XY94
D	?	-	LYS	deletion	UNP A7XY94
D	?	-	TYR	deletion	UNP A7XY94
D	?	-	TYR	deletion	UNP A7XY94
D	?	-	VAL	deletion	UNP A7XY94
D	486	VAL	THR	conflict	UNP A7XY94
D	581	ALA	CYS	conflict	UNP A7XY94
D	611	LEU	VAL	conflict	UNP A7XY94
D	650	ARG	GLU	conflict	UNP A7XY94
D	651	ARG	GLU	conflict	UNP A7XY94
D	836	TYR	PHE	conflict	UNP A7XY94
D	837	LYS	-	expression tag	UNP A7XY94

- Molecule 4 is a protein called GluN2B-specific Fab, termed 11D1.

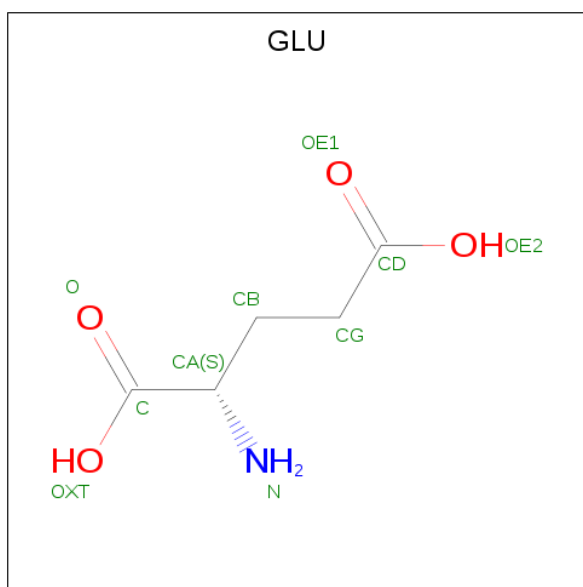
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	214	Total	C	N	O	0	0
			1070	642	214	214		
4	G	215	Total	C	N	O	0	0
			1075	645	215	215		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



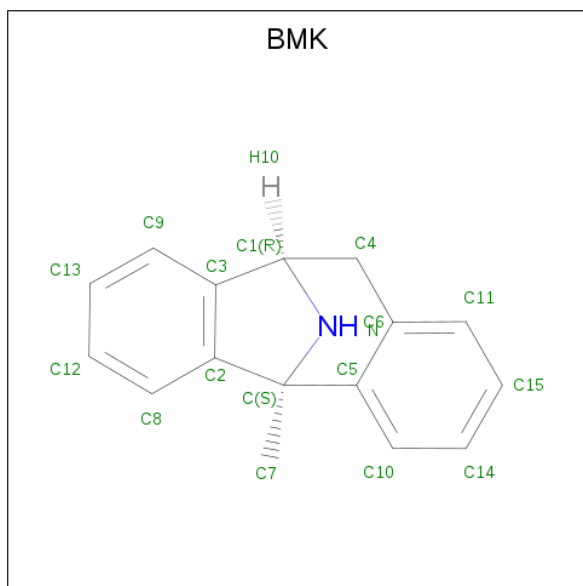
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			84	48	6	30	
5	A	1	Total	C	N	O	0
			84	48	6	30	
5	A	1	Total	C	N	O	0
			84	48	6	30	
5	A	1	Total	C	N	O	0
			84	48	6	30	
5	A	1	Total	C	N	O	0
			84	48	6	30	
5	A	1	Total	C	N	O	0
			84	48	6	30	
5	C	1	Total	C	N	O	0
			84	48	6	30	
5	C	1	Total	C	N	O	0
			84	48	6	30	
5	C	1	Total	C	N	O	0
			84	48	6	30	
5	C	1	Total	C	N	O	0
			84	48	6	30	
5	C	1	Total	C	N	O	0
			84	48	6	30	
5	C	1	Total	C	N	O	0
			84	48	6	30	
5	D	1	Total	C	N	O	0
			56	32	4	20	
5	D	1	Total	C	N	O	0
			56	32	4	20	
5	D	1	Total	C	N	O	0
			56	32	4	20	
5	D	1	Total	C	N	O	0
			56	32	4	20	

- Molecule 6 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			10	5	1	4	

- Molecule 7 is (5S,10R)-5-methyl-10,11-dihydro-5H-5,10-epiminodibenzo[a,d][7]annulene (three-letter code: BMK) (formula: C<sub>16</sub>H<sub>15</sub>N).



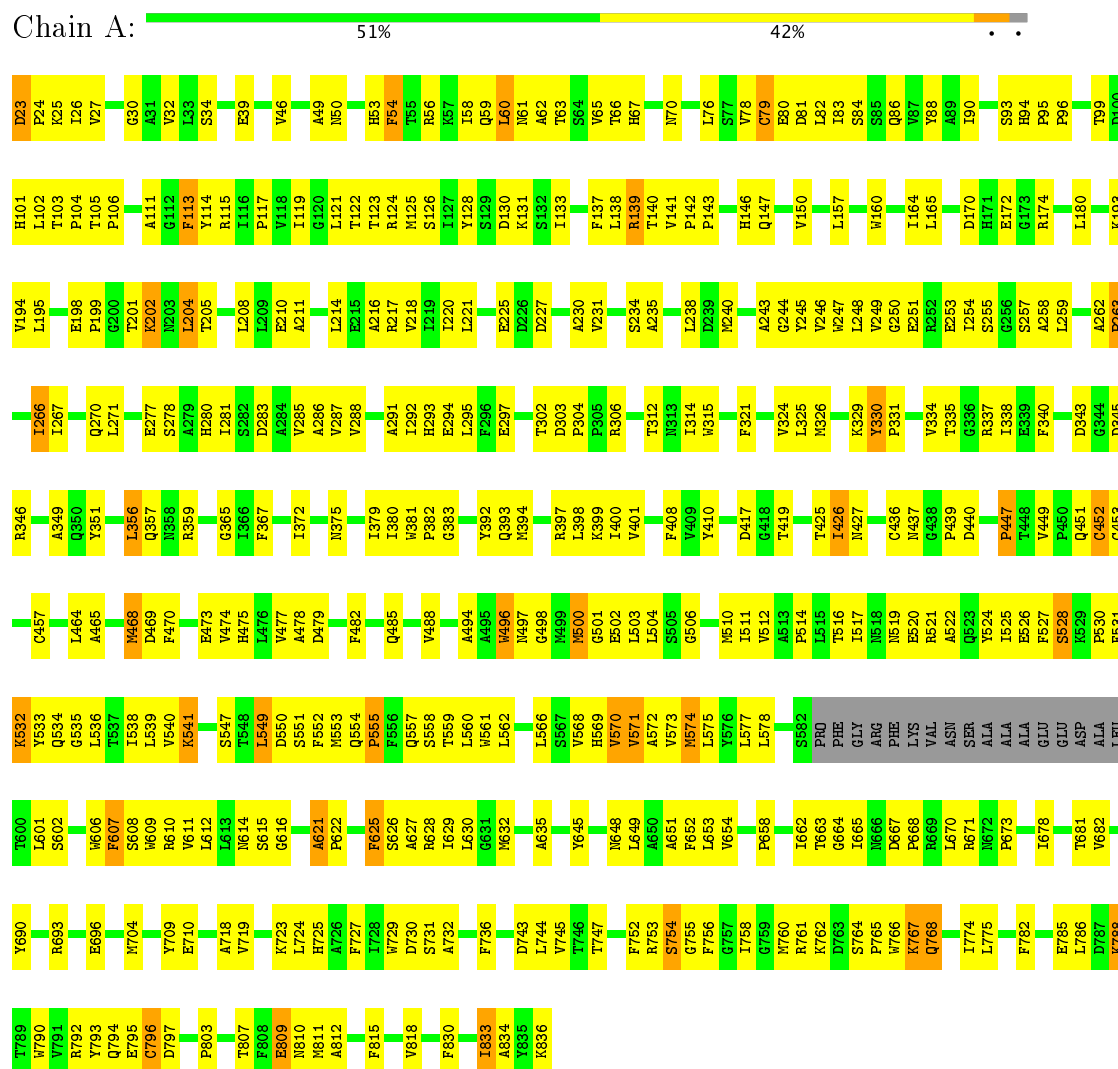
Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N		0
			17	16	1		



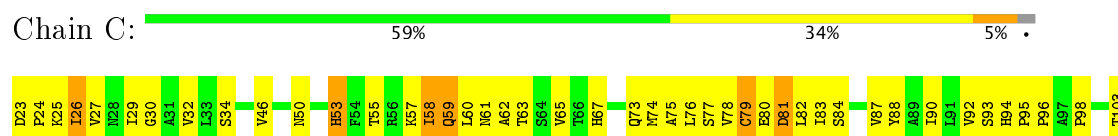
### 3 Residue-property plots

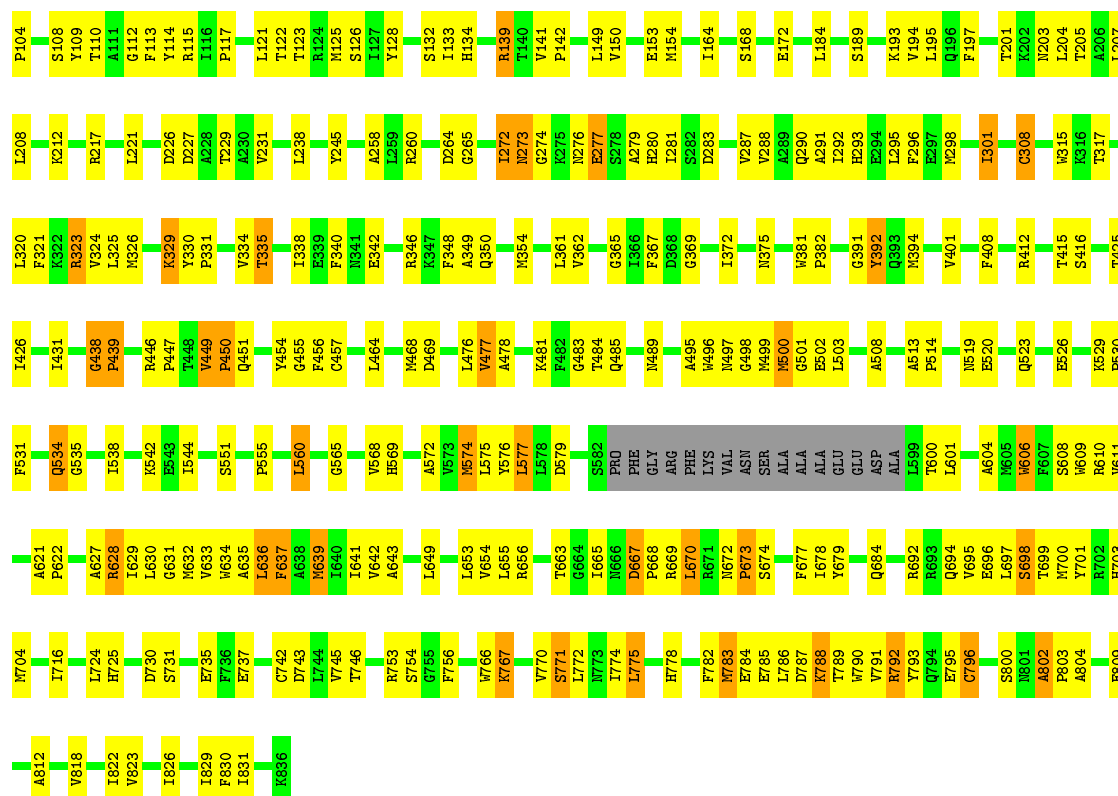
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: N-methyl-D-aspartate receptor subunit NR1-8a

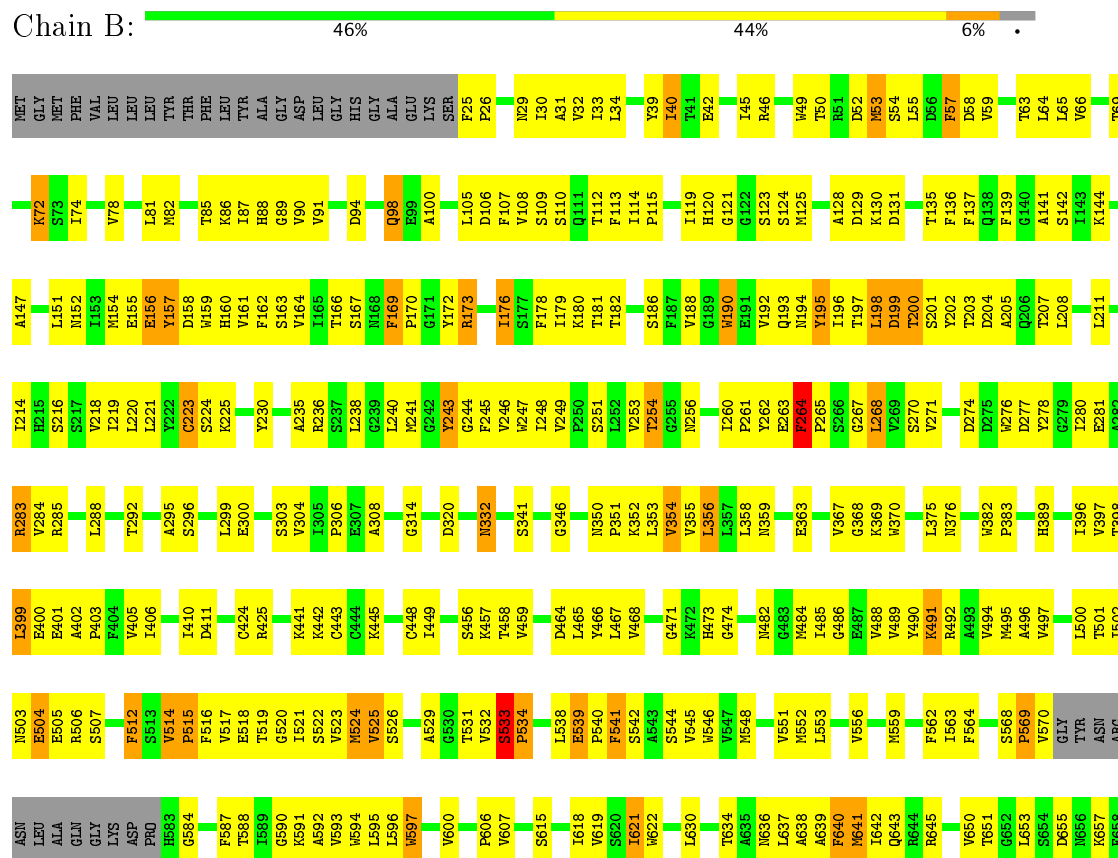


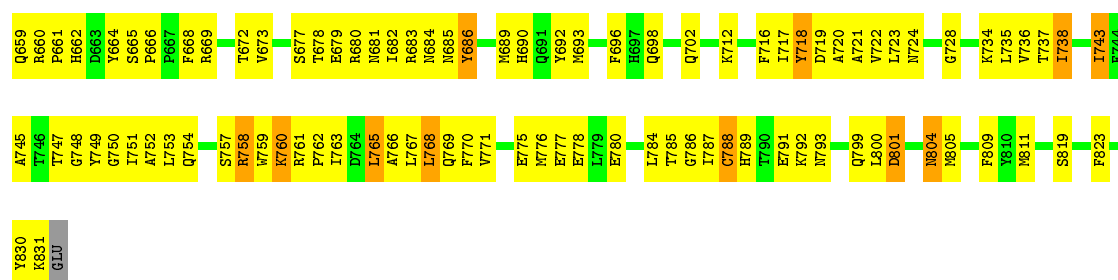
- Molecule 1: N-methyl-D-aspartate receptor subunit NR1-8a





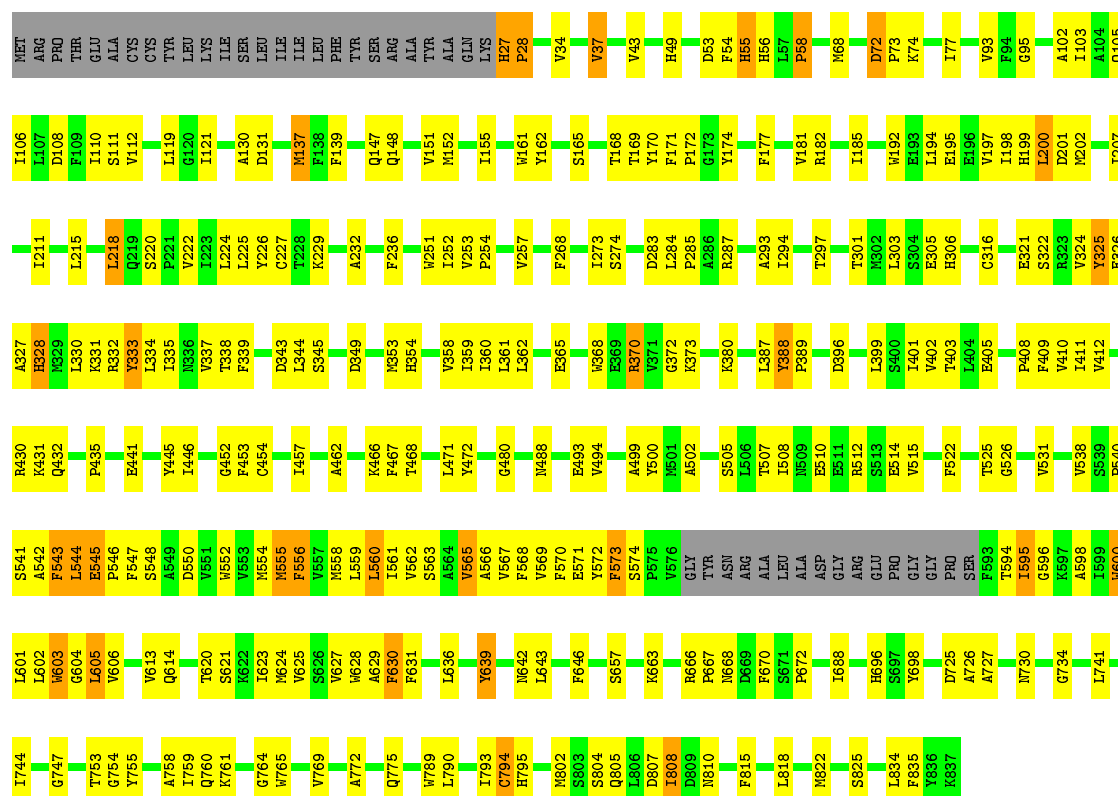
• Molecule 2: N-methyl-D-aspartate receptor subunit NR2A





• Molecule 3: Ionotropic glutamate receptor subunit NR2B

Chain D: 62% 30% 5%



• Molecule 4: GluN2B-specific Fab, termed 11D1

Chain F: 91% 8%



• Molecule 4: GluN2B-specific Fab, termed 11D1

Chain G: 91% 8%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	302052	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 ( $e^-/\text{\AA}^2$ )	0.84	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.49	1/5893 (0.0%)	0.75	4/8065 (0.0%)
1	C	0.34	0/5594	0.68	6/7670 (0.1%)
2	B	0.54	0/5708	0.79	11/7831 (0.1%)
3	D	0.38	0/5230	0.67	1/7225 (0.0%)
All	All	0.45	1/22425 (0.0%)	0.72	22/30791 (0.1%)

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	1
1	C	0	1
4	F	0	1
4	G	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	PRO	CA-C	7.98	1.68	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	533	SER	C-N-CD	-14.68	88.31	120.60
1	A	23	ASP	C-N-CD	-10.97	96.47	120.60
1	C	438	GLY	C-N-CD	-10.61	97.26	120.60
1	C	544	ILE	C-N-CD	-10.33	97.88	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	621	ALA	C-N-CD	-9.78	99.08	120.60
2	B	514	VAL	C-N-CD	-9.64	99.39	120.60
3	D	27	HIS	C-N-CD	-8.32	102.29	120.60
1	C	449	VAL	C-N-CD	-8.29	102.36	120.60
1	A	263	PRO	N-CA-C	7.04	130.41	112.10
2	B	758	ARG	C-N-CA	-6.54	105.34	121.70
2	B	230	TYR	CB-CG-CD1	-6.31	117.21	121.00
2	B	471	GLY	N-CA-C	6.26	128.74	113.10
1	C	673	PRO	N-CA-C	-6.18	96.02	112.10
2	B	200	THR	N-CA-C	5.82	126.70	111.00
1	A	754	SER	C-N-CA	5.55	133.95	122.30
1	C	489	ASN	N-CA-C	-5.51	96.12	111.00
2	B	464	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	469	ASP	CB-CG-OD2	5.18	122.97	118.30
2	B	129	ASP	CB-CG-OD2	5.17	122.95	118.30
2	B	131	ASP	CB-CG-OD2	5.16	122.95	118.30
2	B	106	ASP	CB-CG-OD2	5.16	122.94	118.30
2	B	39	TYR	N-CA-C	5.03	124.58	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	570	VAL	Mainchain
1	C	792	ARG	Mainchain
4	F	67	UNK	Mainchain
4	G	148	UNK	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	5758	0	5302	722	0
1	C	5484	0	4834	530	0
2	B	5582	0	4962	854	0
3	D	5127	0	4093	444	0
4	F	1070	0	235	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	1075	0	234	11	0
5	A	84	0	75	11	0
5	C	84	0	75	9	0
5	D	56	0	50	6	0
6	B	10	0	5	7	0
7	B	17	0	0	8	0
All	All	24347	0	19865	2370	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 54.

All (2370) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:PHE:CE2	3:D:554:MET:HG3	1.24	1.69
1:A:117:PRO:HG2	1:A:321:PHE:CD2	1.33	1.60
1:A:682:VAL:HG21	1:A:729:TRP:CH2	1.17	1.59
1:A:506:GLY:CA	1:A:761:ARG:NH2	1.68	1.57
1:A:86:GLN:HE21	1:A:306:ARG:CB	1.16	1.57
1:A:34:SER:CB	1:A:96:PRO:HG3	1.10	1.57
1:A:34:SER:HB2	1:A:96:PRO:CG	1.34	1.53
1:A:124:ARG:HD2	1:A:271:LEU:CD2	1.36	1.52
1:C:673:PRO:HB3	1:C:703:HIS:CG	1.44	1.51
1:A:815:PHE:CE2	3:D:554:MET:CG	1.90	1.51
2:B:164:VAL:CG2	2:B:220:LEU:HD12	1.44	1.47
1:C:53:HIS:CD2	1:C:293:HIS:CG	1.99	1.47
2:B:523:VAL:HG22	2:B:717:ILE:CG1	1.45	1.46
2:B:182:THR:HG22	2:B:190:TRP:CZ3	1.52	1.44
1:A:26:ILE:CG2	1:A:61:ASN:HB2	1.47	1.44
1:A:205:THR:CG2	1:A:238:LEU:HD11	1.44	1.43
1:A:578:LEU:CD1	1:A:627:ALA:CB	1.95	1.42
1:C:295:LEU:HD22	1:C:321:PHE:CD1	1.53	1.42
2:B:768:LEU:HD23	1:C:519:ASN:CA	1.50	1.40
2:B:135:THR:OG1	2:B:137:PHE:CE2	1.75	1.40
2:B:562:PHE:CE1	1:C:826:ILE:HD13	1.57	1.39
1:A:578:LEU:CD1	1:A:627:ALA:HA	1.51	1.39
1:A:86:GLN:NE2	1:A:306:ARG:CB	1.84	1.39
2:B:64:LEU:HD12	2:B:81:LEU:CD1	1.52	1.39
2:B:169:PHE:CE2	2:B:224:SER:HB3	1.56	1.38
1:C:53:HIS:CD2	1:C:293:HIS:CD2	2.12	1.38
1:C:477:VAL:HG21	1:C:499:MET:CA	1.53	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:PRO:CG	2:B:722:VAL:HG22	1.52	1.37
1:C:673:PRO:CB	1:C:703:HIS:CD2	2.05	1.37
2:B:64:LEU:CD1	2:B:81:LEU:HD21	1.53	1.37
1:C:301:ILE:CG2	1:C:317:THR:CG2	2.02	1.37
2:B:164:VAL:HG23	2:B:220:LEU:CD1	1.54	1.37
2:B:765:LEU:HD11	1:C:523:GLN:CG	1.52	1.37
1:A:578:LEU:CD1	1:A:627:ALA:CA	2.02	1.36
1:A:205:THR:HG23	1:A:238:LEU:CD1	1.56	1.34
1:A:682:VAL:CG2	1:A:729:TRP:CH2	2.09	1.34
1:A:578:LEU:HD13	1:A:627:ALA:CA	1.58	1.34
2:B:768:LEU:CD2	1:C:519:ASN:HA	1.55	1.34
2:B:562:PHE:CZ	1:C:826:ILE:HD11	1.63	1.32
1:A:117:PRO:CG	1:A:321:PHE:HD2	1.42	1.32
1:A:810:ASN:CB	3:D:631:PHE:HZ	1.44	1.31
1:A:682:VAL:CG2	1:A:729:TRP:CZ3	2.13	1.31
1:C:673:PRO:HB3	1:C:703:HIS:CD2	1.61	1.31
1:C:575:LEU:HB2	1:C:634:TRP:CH2	1.65	1.31
2:B:192:VAL:HG21	2:B:195:TYR:CE2	1.66	1.30
1:A:34:SER:CB	1:A:96:PRO:CG	1.94	1.30
1:A:606:TRP:HE1	3:D:623:ILE:CD1	1.42	1.30
1:A:810:ASN:HB2	3:D:631:PHE:CZ	1.66	1.30
1:C:301:ILE:CG2	1:C:317:THR:HG21	1.59	1.30
2:B:179:ILE:HG21	2:B:195:TYR:OH	1.20	1.29
1:C:477:VAL:CG2	1:C:499:MET:HA	1.62	1.29
1:A:709:TYR:OH	1:A:724:LEU:HD11	1.20	1.29
3:D:605:LEU:HD12	3:D:629:ALA:CB	1.62	1.29
2:B:562:PHE:CE1	1:C:826:ILE:CD1	2.15	1.29
2:B:651:THR:OG1	2:B:655:ASP:CB	1.80	1.29
2:B:34:LEU:O	2:B:65:LEU:HG	1.21	1.28
1:A:106:PRO:HB3	2:B:107:PHE:CZ	1.68	1.28
1:A:810:ASN:CB	3:D:631:PHE:CZ	2.17	1.28
2:B:192:VAL:HG21	2:B:195:TYR:CD2	1.68	1.28
2:B:182:THR:CG2	2:B:190:TRP:CZ3	2.17	1.27
2:B:673:VAL:CG2	2:B:718:TYR:HE1	1.47	1.27
1:A:578:LEU:HD12	1:A:627:ALA:CB	1.56	1.27
2:B:179:ILE:CG2	2:B:195:TYR:OH	1.83	1.26
1:C:438:GLY:HA3	1:C:451:GLN:NE2	1.50	1.25
1:C:133:ILE:CD1	3:D:130:ALA:HB1	1.64	1.25
1:A:815:PHE:CD2	3:D:554:MET:CG	2.17	1.25
1:A:568:VAL:O	1:A:571:VAL:HG12	1.35	1.25
1:C:245:TYR:O	1:C:382:PRO:HG3	1.35	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:VAL:HG23	2:B:466:TYR:O	1.13	1.24
1:A:606:TRP:NE1	3:D:623:ILE:HD11	1.50	1.24
3:D:562:VAL:HG22	3:D:621:SER:CB	1.68	1.24
1:A:119:ILE:CD1	1:A:288:VAL:HG21	1.68	1.23
2:B:57:PHE:CD2	2:B:292:THR:HG23	1.73	1.23
2:B:64:LEU:HD11	2:B:81:LEU:CD2	1.69	1.22
1:A:534:GLN:CG	1:A:732:ALA:HB2	1.68	1.22
2:B:42:GLU:CB	2:B:63:THR:HG21	1.69	1.22
1:C:342:GLU:OE2	3:D:170:TYR:CD2	1.91	1.22
2:B:519:THR:HG22	2:B:721:ALA:CB	1.70	1.22
3:D:562:VAL:CG2	3:D:621:SER:HB2	1.67	1.22
1:A:682:VAL:HG21	1:A:729:TRP:CZ3	1.72	1.22
1:A:815:PHE:CZ	3:D:554:MET:HG3	1.76	1.22
1:A:119:ILE:CD1	1:A:288:VAL:CG2	2.18	1.21
3:D:27:HIS:CB	3:D:28:PRO:CD	2.16	1.21
2:B:399:LEU:CD2	2:B:400:GLU:H	1.54	1.21
1:A:818:VAL:CG2	3:D:558:MET:HE1	1.70	1.20
1:C:575:LEU:HB2	1:C:634:TRP:CZ3	1.75	1.20
1:A:26:ILE:HG22	1:A:61:ASN:HB2	1.21	1.20
1:A:663:THR:O	1:A:667:ASP:HB2	1.05	1.20
2:B:720:ALA:HB2	2:B:743:ILE:CG2	1.69	1.19
1:C:673:PRO:CB	1:C:703:HIS:CG	2.21	1.19
1:A:578:LEU:CD1	1:A:627:ALA:HB2	1.69	1.19
1:A:815:PHE:CD2	3:D:554:MET:HG3	1.77	1.19
1:A:124:ARG:CD	1:A:271:LEU:CD2	2.21	1.19
1:C:673:PRO:HB2	1:C:703:HIS:CD2	1.77	1.19
2:B:120:HIS:CE1	2:B:280:ILE:HD11	1.77	1.19
1:C:132:SER:HB3	3:D:172:PRO:CB	1.73	1.18
1:A:506:GLY:HA2	1:A:761:ARG:NH2	0.87	1.18
1:A:568:VAL:O	1:A:571:VAL:CG1	1.91	1.18
2:B:403:PRO:HG2	2:B:722:VAL:CG2	1.73	1.18
2:B:752:ALA:O	2:B:753:LEU:HD12	1.42	1.18
1:A:247:TRP:CB	1:A:266:ILE:HG13	1.71	1.18
1:C:342:GLU:OE2	3:D:170:TYR:CE2	1.96	1.18
2:B:194:ASN:CG	2:B:214:ILE:HG13	1.65	1.17
2:B:523:VAL:CG2	2:B:717:ILE:HG12	1.74	1.17
2:B:169:PHE:HB3	2:B:170:PRO:CD	1.74	1.16
2:B:57:PHE:HB2	2:B:292:THR:HG21	1.22	1.16
1:A:663:THR:O	1:A:667:ASP:CB	1.91	1.16
3:D:561:ILE:O	3:D:565:VAL:HG22	1.44	1.16
1:A:709:TYR:OH	1:A:724:LEU:CD1	1.92	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:468:VAL:HG21	2:B:484:MET:HG2	1.22	1.16
2:B:151:LEU:HD23	2:B:190:TRP:CH2	1.79	1.16
1:A:818:VAL:HG22	3:D:558:MET:HE1	1.19	1.15
2:B:64:LEU:CD1	2:B:81:LEU:CD2	2.25	1.15
1:A:113:PHE:CE1	2:B:100:ALA:HB3	1.82	1.15
2:B:768:LEU:CB	1:C:519:ASN:HB2	1.76	1.15
2:B:162:PHE:HA	2:B:216:SER:CB	1.77	1.14
2:B:468:VAL:HG21	2:B:484:MET:CG	1.77	1.14
1:A:122:THR:HG23	1:A:277:GLU:CG	1.76	1.14
2:B:114:ILE:HD11	2:B:308:ALA:CB	1.78	1.14
2:B:57:PHE:HB2	2:B:292:THR:CG2	1.78	1.14
3:D:639:TYR:HE1	3:D:643:LEU:HD11	1.08	1.14
2:B:169:PHE:CE2	2:B:224:SER:CB	2.30	1.13
2:B:247:TRP:HB2	2:B:268:LEU:CB	1.78	1.13
2:B:179:ILE:CG2	2:B:195:TYR:HH	1.56	1.13
1:A:124:ARG:NH1	1:A:271:LEU:HB2	1.64	1.13
1:A:578:LEU:HD13	1:A:627:ALA:CB	1.63	1.13
2:B:659:GLN:NE2	2:B:686:TYR:OH	1.79	1.13
2:B:522:SER:O	2:B:717:ILE:HA	1.43	1.13
2:B:673:VAL:HG22	2:B:718:TYR:HE1	1.13	1.13
3:D:542:ALA:HB1	3:D:642:ASN:CB	1.79	1.13
3:D:332:ARG:O	3:D:335:ILE:HG13	1.45	1.12
1:C:272:ILE:HG22	1:C:350:GLN:O	1.46	1.12
1:C:53:HIS:CG	1:C:293:HIS:CD2	2.37	1.12
3:D:396:ASP:CB	3:D:468:THR:H	1.63	1.12
1:C:133:ILE:HD13	3:D:130:ALA:HB1	1.29	1.12
2:B:651:THR:OG1	2:B:655:ASP:HB2	0.97	1.12
1:C:354:MET:HE1	1:C:361:LEU:CB	1.80	1.12
2:B:541:PHE:O	2:B:545:VAL:N	1.83	1.11
1:A:815:PHE:CE2	3:D:554:MET:HG2	1.85	1.11
3:D:294:ILE:HD11	3:D:344:LEU:CB	1.78	1.11
2:B:247:TRP:CE3	2:B:268:LEU:HB3	1.83	1.11
1:A:551:SER:OG	1:A:649:LEU:HD13	1.48	1.11
1:C:354:MET:CE	1:C:361:LEU:CB	2.29	1.11
1:A:578:LEU:HD11	1:A:627:ALA:HA	1.31	1.11
2:B:32:VAL:HG22	2:B:91:VAL:HG22	1.22	1.11
1:A:53:HIS:HB3	1:A:293:HIS:CD2	1.85	1.11
1:A:578:LEU:HD12	1:A:627:ALA:HB1	1.23	1.10
2:B:514:VAL:CG2	2:B:767:LEU:HD13	1.81	1.10
1:A:247:TRP:HB2	1:A:266:ILE:HG13	1.13	1.10
2:B:523:VAL:HB	2:B:738:ILE:HD11	1.20	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:LEU:HD21	2:B:182:THR:HG21	1.30	1.10
1:C:53:HIS:CD2	1:C:293:HIS:ND1	2.19	1.10
2:B:468:VAL:CG2	2:B:484:MET:HG2	1.80	1.10
1:A:496:TRP:HD1	1:A:500:MET:HB3	1.01	1.10
2:B:247:TRP:HB2	2:B:268:LEU:HB2	1.16	1.09
3:D:131:ASP:HA	3:D:349:ASP:OD1	1.52	1.09
1:A:124:ARG:HD2	1:A:271:LEU:HD22	1.13	1.09
1:C:132:SER:CB	3:D:172:PRO:HB3	1.82	1.09
1:C:132:SER:HB3	3:D:172:PRO:HB3	1.11	1.09
1:A:124:ARG:CD	1:A:271:LEU:HD22	1.80	1.09
2:B:164:VAL:CG2	2:B:220:LEU:CD1	2.20	1.09
2:B:514:VAL:HG22	2:B:767:LEU:HD13	1.22	1.09
1:C:301:ILE:HG21	1:C:317:THR:HG21	1.29	1.09
1:A:551:SER:OG	1:A:649:LEU:CD1	2.01	1.09
2:B:768:LEU:HB2	1:C:519:ASN:CB	1.83	1.08
1:C:637:PHE:CD1	3:D:818:LEU:HD22	1.89	1.08
1:A:122:THR:HG23	1:A:277:GLU:HG2	1.12	1.08
5:A:1002:NAG:H83	5:A:1002:NAG:H3	1.36	1.08
2:B:502:ILE:HG23	2:B:512:PHE:CZ	1.89	1.08
2:B:42:GLU:CB	2:B:63:THR:CG2	2.32	1.08
1:C:53:HIS:NE2	1:C:293:HIS:CG	2.22	1.08
2:B:673:VAL:CG2	2:B:718:TYR:CE1	2.36	1.08
1:C:673:PRO:CG	1:C:703:HIS:HB2	1.82	1.08
3:D:605:LEU:CD1	3:D:629:ALA:HB2	1.84	1.08
5:C:1002:NAG:H83	5:C:1002:NAG:H3	1.33	1.07
1:A:690:TYR:CD2	1:A:752:PHE:CE2	2.41	1.07
2:B:194:ASN:HB2	2:B:214:ILE:HG21	1.30	1.07
1:C:575:LEU:CD1	1:C:627:ALA:HB1	1.84	1.07
2:B:592:ALA:O	2:B:596:LEU:N	1.88	1.07
1:C:673:PRO:HG2	1:C:703:HIS:HB2	1.33	1.07
1:A:124:ARG:HD2	1:A:271:LEU:HD23	1.37	1.07
1:C:53:HIS:CD2	1:C:293:HIS:CE1	2.42	1.07
1:C:133:ILE:HG12	3:D:130:ALA:HB2	1.34	1.07
1:A:525:ILE:CA	1:A:762:LYS:HE2	1.85	1.07
3:D:639:TYR:CE1	3:D:643:LEU:CD1	2.38	1.06
2:B:669:ARG:HD2	2:B:696:PHE:CD2	1.89	1.06
1:A:534:GLN:HG3	1:A:732:ALA:HB2	1.08	1.06
2:B:114:ILE:HD11	2:B:308:ALA:HB2	1.32	1.06
2:B:765:LEU:HD11	1:C:523:GLN:CD	1.75	1.06
1:A:610:ARG:CB	1:A:615:SER:CB	2.33	1.06
1:A:818:VAL:HG21	3:D:558:MET:SD	1.96	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LEU:CD1	2:B:81:LEU:HD11	1.84	1.06
2:B:765:LEU:HD11	1:C:523:GLN:HG3	1.26	1.06
1:A:500:MET:HE1	1:A:521:ARG:HB3	1.14	1.06
2:B:659:GLN:NE2	2:B:686:TYR:CZ	2.23	1.06
1:A:115:ARG:O	1:A:315:TRP:HE3	1.38	1.05
5:C:1006:NAG:H3	5:C:1006:NAG:H83	1.34	1.05
1:A:26:ILE:HG21	1:A:61:ASN:HB2	1.30	1.05
1:A:568:VAL:HG12	1:A:608:SER:HB3	1.37	1.05
1:A:575:LEU:HD13	1:A:622:PRO:HB3	1.39	1.05
1:A:131:LYS:NZ	1:A:343:ASP:HA	1.71	1.05
1:A:122:THR:CG2	1:A:277:GLU:CG	2.35	1.05
2:B:34:LEU:O	2:B:65:LEU:CG	2.02	1.05
1:A:496:TRP:CD1	1:A:500:MET:HB3	1.90	1.05
3:D:388:TYR:N	3:D:389:PRO:HD2	1.69	1.05
1:A:34:SER:HB3	1:A:96:PRO:HG3	1.38	1.05
2:B:135:THR:OG1	2:B:137:PHE:CZ	2.03	1.05
1:C:53:HIS:HD2	1:C:293:HIS:ND1	1.53	1.05
2:B:562:PHE:CZ	1:C:826:ILE:CD1	2.32	1.05
1:A:531:PHE:CZ	1:A:774:ILE:HG21	1.90	1.05
1:C:301:ILE:HG21	1:C:317:THR:CG2	1.79	1.04
2:B:399:LEU:HD23	2:B:400:GLU:H	1.11	1.04
2:B:397:VAL:CG2	2:B:466:TYR:O	2.05	1.04
5:A:1006:NAG:H3	5:A:1006:NAG:H83	1.34	1.04
2:B:351:PRO:HG2	2:B:370:TRP:HZ3	1.18	1.04
2:B:82:MET:HE2	2:B:114:ILE:HD13	1.38	1.04
2:B:552:MET:CE	2:B:622:TRP:CE3	2.40	1.04
2:B:486:GLY:O	2:B:490:TYR:HD2	1.39	1.04
1:C:697:LEU:O	1:C:699:THR:N	1.89	1.04
2:B:801:ASP:O	2:B:805:MET:HG3	1.56	1.04
2:B:621:ILE:HG21	1:C:818:VAL:HG13	1.38	1.04
3:D:600:TRP:CE3	3:D:613:VAL:CB	2.40	1.04
1:A:511:ILE:O	1:A:758:ILE:CD1	2.06	1.04
3:D:332:ARG:HA	3:D:335:ILE:CD1	1.88	1.03
3:D:58:PRO:HG2	3:D:303:LEU:CD1	1.87	1.03
3:D:200:LEU:HD22	3:D:201:ASP:H	1.17	1.03
1:A:534:GLN:HG3	1:A:732:ALA:CB	1.87	1.03
1:C:78:VAL:HA	1:C:82:LEU:HB2	1.40	1.03
1:A:621:ALA:HB1	1:A:622:PRO:HD2	1.37	1.03
2:B:519:THR:HG22	2:B:721:ALA:HB2	1.07	1.03
2:B:753:LEU:HD22	2:B:760:LYS:HG2	1.38	1.03
3:D:388:TYR:N	3:D:389:PRO:CD	2.20	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:ASN:HB3	3:D:631:PHE:CZ	1.90	1.03
1:C:425:THR:HG22	1:C:431:ILE:HG12	1.38	1.03
3:D:305:GLU:CB	3:D:333:TYR:HE2	1.71	1.03
3:D:27:HIS:CB	3:D:28:PRO:HD2	1.85	1.02
1:C:301:ILE:CG2	1:C:317:THR:HG23	1.86	1.02
3:D:639:TYR:HE1	3:D:643:LEU:CD1	1.73	1.02
3:D:27:HIS:CB	3:D:28:PRO:HD3	1.87	1.02
2:B:151:LEU:CD2	2:B:182:THR:HG21	1.90	1.02
2:B:541:PHE:C	2:B:545:VAL:HB	1.80	1.01
3:D:332:ARG:HA	3:D:335:ILE:HD11	1.39	1.01
3:D:305:GLU:CB	3:D:333:TYR:CE2	2.43	1.01
2:B:40:ILE:HD13	2:B:281:GLU:OE2	1.60	1.01
2:B:720:ALA:HB2	2:B:743:ILE:HG23	1.35	1.01
3:D:542:ALA:HB1	3:D:642:ASN:HB3	1.03	1.01
1:C:301:ILE:HG22	1:C:317:THR:HG21	1.39	1.01
2:B:64:LEU:HD11	2:B:81:LEU:HD21	1.02	1.01
1:A:531:PHE:N	1:A:756:PHE:O	1.94	1.00
2:B:621:ILE:CG2	1:C:818:VAL:HG13	1.90	1.00
1:A:119:ILE:HD11	1:A:288:VAL:CG2	1.90	1.00
3:D:58:PRO:HG2	3:D:303:LEU:HD11	1.39	1.00
3:D:765:TRP:HB3	3:D:769:VAL:HG23	1.43	1.00
1:C:575:LEU:CB	1:C:634:TRP:CH2	2.43	1.00
2:B:151:LEU:HD23	2:B:190:TRP:HH2	1.21	1.00
2:B:552:MET:CE	2:B:622:TRP:HE3	1.73	1.00
1:C:575:LEU:HD11	1:C:627:ALA:HB1	1.02	1.00
1:A:810:ASN:HB2	3:D:631:PHE:HZ	0.83	1.00
1:C:109:TYR:CD1	3:D:105:GLN:HG2	1.96	1.00
1:A:208:LEU:HD23	1:A:240:MET:SD	2.02	1.00
2:B:49:TRP:O	2:B:53:MET:HB2	1.61	1.00
1:A:125:MET:O	1:A:139:ARG:NH1	1.95	1.00
2:B:74:ILE:HG21	2:B:105:LEU:HD21	1.44	1.00
2:B:120:HIS:CE1	2:B:280:ILE:CD1	2.44	1.00
1:C:673:PRO:HB2	1:C:703:HIS:HD2	1.22	1.00
2:B:399:LEU:CD2	2:B:400:GLU:N	2.25	0.99
1:C:133:ILE:HG12	3:D:130:ALA:CB	1.92	0.99
1:C:477:VAL:HG21	1:C:499:MET:CB	1.92	0.99
2:B:765:LEU:CD1	1:C:523:GLN:CG	2.39	0.99
3:D:639:TYR:CE1	3:D:643:LEU:HD11	1.95	0.99
1:C:643:ALA:HB1	3:D:639:TYR:HE2	1.27	0.99
1:C:295:LEU:CD2	1:C:321:PHE:CD1	2.45	0.99
1:A:122:THR:CG2	1:A:277:GLU:HG2	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:MET:CE	2:B:248:ILE:HD11	1.93	0.99
2:B:169:PHE:HE2	2:B:224:SER:HG	1.02	0.99
1:C:438:GLY:HA3	1:C:451:GLN:HE21	1.17	0.99
3:D:332:ARG:HA	3:D:335:ILE:CG1	1.91	0.99
2:B:720:ALA:CB	2:B:743:ILE:HG23	1.90	0.99
1:C:627:ALA:O	1:C:631:GLY:N	1.95	0.99
1:A:818:VAL:CG2	3:D:558:MET:CE	2.41	0.99
1:A:113:PHE:CE1	2:B:100:ALA:CB	2.46	0.99
2:B:753:LEU:HD22	2:B:760:LYS:CG	1.92	0.99
2:B:541:PHE:O	2:B:545:VAL:HB	1.61	0.98
1:C:628:ARG:O	1:C:632:MET:N	1.96	0.98
2:B:523:VAL:CB	2:B:738:ILE:HD11	1.92	0.98
1:A:621:ALA:HB1	1:A:622:PRO:CD	1.92	0.98
2:B:720:ALA:CB	2:B:743:ILE:CG2	2.41	0.98
1:C:315:TRP:CE3	1:C:317:THR:O	2.16	0.98
2:B:765:LEU:HD21	1:C:523:GLN:HG2	1.45	0.98
2:B:474:GLY:HA2	2:B:482:ASN:O	1.64	0.98
1:A:498:GLY:O	1:A:502:GLU:HG2	1.61	0.98
2:B:167:SER:CB	2:B:223:CYS:SG	2.51	0.98
1:A:500:MET:CE	1:A:521:ARG:HB3	1.94	0.98
1:A:578:LEU:HD13	1:A:627:ALA:HB2	1.29	0.98
2:B:57:PHE:CG	2:B:292:THR:HG23	1.97	0.98
1:A:258:ALA:O	1:A:262:ALA:HB2	1.63	0.97
1:A:119:ILE:HD13	1:A:288:VAL:CG2	1.91	0.97
1:A:312:THR:OG1	2:B:98:GLN:NE2	1.96	0.97
1:A:736:PHE:HE1	1:A:794:GLN:CD	1.67	0.97
2:B:522:SER:OG	2:B:723:LEU:HD12	1.63	0.97
2:B:673:VAL:HG21	2:B:718:TYR:CE1	1.99	0.97
5:D:1002:NAG:H83	5:D:1002:NAG:H3	1.43	0.97
1:A:606:TRP:NE1	3:D:623:ILE:CD1	2.13	0.97
2:B:673:VAL:HG22	2:B:718:TYR:CE1	1.95	0.97
2:B:765:LEU:HD11	1:C:523:GLN:NE2	1.77	0.97
3:D:200:LEU:HD22	3:D:201:ASP:N	1.80	0.97
2:B:351:PRO:CG	2:B:370:TRP:HZ3	1.76	0.97
1:C:109:TYR:HE1	3:D:105:GLN:HE21	1.00	0.96
2:B:673:VAL:HG21	2:B:718:TYR:HE1	1.28	0.96
1:A:511:ILE:O	1:A:758:ILE:HD11	1.65	0.96
2:B:520:GLY:HA3	2:B:743:ILE:HG13	1.45	0.96
3:D:555:MET:SD	3:D:628:TRP:CZ2	2.59	0.96
2:B:169:PHE:HB3	2:B:170:PRO:HD2	1.42	0.96
1:A:394:MET:HE2	1:A:765:PRO:HG3	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:ASN:OD1	2:B:214:ILE:HG13	1.66	0.95
2:B:351:PRO:HG2	2:B:370:TRP:CZ3	2.00	0.95
1:A:815:PHE:CD2	3:D:554:MET:HG2	1.98	0.95
1:A:663:THR:C	1:A:667:ASP:HB2	1.85	0.95
2:B:82:MET:CE	2:B:114:ILE:HD13	1.95	0.95
2:B:520:GLY:O	2:B:743:ILE:HG21	1.65	0.95
2:B:57:PHE:CB	2:B:292:THR:CG2	2.44	0.95
5:C:1004:NAG:H3	5:C:1004:NAG:H83	1.48	0.95
1:C:245:TYR:O	1:C:382:PRO:CG	2.14	0.95
1:A:464:LEU:O	1:A:468:MET:N	1.98	0.94
1:A:25:LYS:C	1:A:59:GLN:HB3	1.87	0.94
1:C:391:GLY:O	1:C:392:TYR:HB2	1.63	0.94
2:B:57:PHE:CB	2:B:292:THR:HG23	1.97	0.94
1:C:274:GLY:HA2	1:C:280:HIS:CE1	2.02	0.94
1:A:119:ILE:HD11	1:A:288:VAL:HG22	1.48	0.94
1:C:194:VAL:O	1:C:195:LEU:HD23	1.65	0.94
1:C:673:PRO:CB	1:C:703:HIS:CB	2.45	0.94
1:C:53:HIS:CG	1:C:293:HIS:NE2	2.36	0.94
3:D:605:LEU:HG	3:D:625:VAL:HG12	1.48	0.94
1:C:568:VAL:CG1	1:C:608:SER:OG	2.15	0.94
3:D:605:LEU:HG	3:D:625:VAL:CG1	1.98	0.94
1:A:26:ILE:HG22	1:A:61:ASN:CB	1.97	0.94
1:A:283:ASP:OD2	1:A:335:THR:N	2.00	0.94
2:B:277:ASP:OD2	2:B:354:VAL:HG11	1.67	0.94
2:B:514:VAL:N	2:B:515:PRO:HD2	1.80	0.94
1:A:26:ILE:CG2	1:A:61:ASN:CB	2.43	0.94
1:A:503:LEU:HD11	1:A:761:ARG:N	1.82	0.94
2:B:64:LEU:HD12	2:B:81:LEU:HD11	0.96	0.94
2:B:512:PHE:O	1:C:529:LYS:NZ	2.00	0.93
3:D:284:LEU:N	3:D:285:PRO:CD	2.31	0.93
1:A:115:ARG:O	1:A:315:TRP:CE3	2.20	0.93
1:A:525:ILE:HA	1:A:762:LYS:HE2	1.47	0.93
1:A:610:ARG:O	1:A:614:ASN:N	2.00	0.93
1:A:678:ILE:HG22	1:A:724:LEU:HD22	1.51	0.93
2:B:169:PHE:HE2	2:B:224:SER:CB	1.76	0.93
2:B:669:ARG:HD2	2:B:696:PHE:CG	2.04	0.93
2:B:486:GLY:O	2:B:490:TYR:CD2	2.21	0.93
1:C:673:PRO:CG	1:C:703:HIS:CB	2.47	0.93
1:A:606:TRP:CE2	3:D:623:ILE:HD11	2.03	0.93
1:A:517:ILE:HG12	1:A:755:GLY:O	1.69	0.93
2:B:194:ASN:CB	2:B:214:ILE:HG13	1.97	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ILE:HG12	1:A:321:PHE:CZ	2.04	0.93
1:A:93:SER:HB2	1:A:277:GLU:OE2	1.67	0.93
1:C:575:LEU:CB	1:C:634:TRP:CZ3	2.51	0.93
1:A:34:SER:CA	1:A:96:PRO:CG	2.47	0.92
2:B:769:GLN:NE2	1:C:520:GLU:OE2	2.01	0.92
2:B:669:ARG:CD	2:B:696:PHE:CD2	2.52	0.92
2:B:523:VAL:CG2	2:B:717:ILE:CG1	2.40	0.92
1:C:575:LEU:HD11	1:C:627:ALA:CB	1.96	0.92
3:D:605:LEU:HD12	3:D:629:ALA:HB2	0.95	0.92
1:A:124:ARG:NH1	1:A:271:LEU:CB	2.32	0.92
1:A:27:VAL:N	1:A:59:GLN:O	2.03	0.92
2:B:523:VAL:HB	2:B:738:ILE:CD1	2.00	0.92
1:A:531:PHE:CE1	1:A:774:ILE:HG21	2.05	0.92
2:B:198:LEU:HB2	2:B:207:THR:CG2	1.99	0.92
2:B:57:PHE:HD2	2:B:292:THR:HG23	1.35	0.92
1:C:277:GLU:O	1:C:281:ILE:HG13	1.70	0.92
2:B:241:MET:HA	2:B:247:TRP:CZ2	2.05	0.92
1:C:53:HIS:CD2	1:C:293:HIS:NE2	2.38	0.92
1:C:109:TYR:HE1	3:D:105:GLN:NE2	1.68	0.91
1:A:245:TYR:O	1:A:382:PRO:HG3	1.70	0.91
2:B:552:MET:HE3	2:B:622:TRP:CE3	2.06	0.91
1:C:109:TYR:CE1	3:D:105:GLN:NE2	2.38	0.91
2:B:247:TRP:HE3	2:B:268:LEU:HB3	1.22	0.91
3:D:639:TYR:CE1	3:D:643:LEU:HD12	2.04	0.91
1:A:27:VAL:HG13	1:A:88:TYR:CD1	2.05	0.91
2:B:198:LEU:HB2	2:B:207:THR:HG21	1.52	0.91
3:D:345:SER:O	3:D:353:MET:N	2.03	0.91
1:A:115:ARG:HB2	1:A:315:TRP:HB3	1.53	0.91
2:B:651:THR:CG2	2:B:655:ASP:OD2	2.19	0.91
1:A:682:VAL:HG21	1:A:729:TRP:CZ2	2.04	0.91
2:B:801:ASP:O	2:B:805:MET:CG	2.18	0.91
1:C:477:VAL:HG21	1:C:499:MET:HA	0.91	0.91
1:C:630:LEU:HD13	1:C:634:TRP:CH2	2.06	0.91
1:C:643:ALA:HB1	3:D:639:TYR:CE2	2.04	0.91
1:A:552:PHE:O	1:A:555:PRO:HD2	1.71	0.90
2:B:588:THR:O	2:B:592:ALA:N	2.05	0.90
1:C:342:GLU:OE2	3:D:170:TYR:HD2	1.48	0.90
1:A:709:TYR:HH	1:A:724:LEU:HD11	0.99	0.90
2:B:651:THR:HG23	2:B:655:ASP:OD2	1.71	0.90
2:B:399:LEU:HD23	2:B:400:GLU:N	1.86	0.90
2:B:247:TRP:CB	2:B:268:LEU:HB2	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:PRO:CB	1:A:755:GLY:HA3	2.02	0.90
2:B:403:PRO:HG2	2:B:722:VAL:HG22	0.91	0.90
2:B:192:VAL:CG2	2:B:195:TYR:CD2	2.55	0.89
1:C:568:VAL:HG11	1:C:608:SER:OG	1.72	0.89
1:C:534:GLN:OE1	1:C:730:ASP:HB3	1.72	0.89
1:A:292:ILE:HG12	1:A:321:PHE:CE1	2.08	0.89
1:A:506:GLY:HA3	1:A:761:ARG:NH2	1.85	0.89
1:C:315:TRP:CE2	1:C:317:THR:HB	2.08	0.89
1:A:606:TRP:HE1	3:D:623:ILE:HD13	1.35	0.89
2:B:584:GLY:O	2:B:587:PHE:HD1	1.55	0.89
1:A:500:MET:HE1	1:A:521:ARG:CB	2.03	0.89
1:A:312:THR:CB	2:B:98:GLN:NE2	2.35	0.89
1:A:106:PRO:HB3	2:B:107:PHE:HZ	1.30	0.89
2:B:382:TRP:CE3	2:B:383:PRO:HD2	2.08	0.89
2:B:765:LEU:CD1	1:C:523:GLN:NE2	2.35	0.89
1:A:205:THR:HG23	1:A:238:LEU:HD11	0.91	0.89
1:C:425:THR:CG2	1:C:431:ILE:HG12	2.03	0.89
1:C:53:HIS:HB3	1:C:293:HIS:NE2	1.88	0.89
1:A:682:VAL:HG23	1:A:729:TRP:CZ3	2.07	0.88
2:B:541:PHE:HE1	2:B:636:ASN:HD22	1.13	0.88
1:C:205:THR:HG23	1:C:238:LEU:HD11	1.53	0.88
1:C:634:TRP:O	1:C:637:PHE:CD2	2.27	0.88
1:C:565:GLY:O	1:C:569:HIS:CE1	2.25	0.88
2:B:502:ILE:HG23	2:B:512:PHE:CE1	2.08	0.88
2:B:791:GLU:O	2:B:792:LYS:C	2.09	0.88
2:B:765:LEU:HD21	1:C:523:GLN:CG	2.04	0.88
5:D:1004:NAG:H83	5:D:1004:NAG:H3	1.56	0.88
1:A:140:THR:O	1:A:346:ARG:HB2	1.74	0.88
1:A:574:MET:SD	1:A:630:LEU:HD11	2.14	0.87
3:D:542:ALA:CB	3:D:642:ASN:HB3	2.00	0.87
1:A:286:ALA:HB3	1:A:330:TYR:CE2	2.09	0.87
1:A:292:ILE:CG1	1:A:321:PHE:CZ	2.57	0.87
2:B:194:ASN:HD21	2:B:211:LEU:HD23	1.38	0.87
2:B:514:VAL:HG22	2:B:767:LEU:CD1	2.04	0.87
2:B:768:LEU:HB2	1:C:519:ASN:HB2	0.92	0.87
1:C:673:PRO:HB3	1:C:703:HIS:CB	2.03	0.87
2:B:123:SER:O	2:B:139:PHE:CB	2.23	0.87
1:C:673:PRO:CB	1:C:703:HIS:HB2	2.04	0.87
3:D:409:PHE:CD2	3:D:755:TYR:HE2	1.91	0.87
3:D:430:ARG:O	3:D:472:TYR:HB2	1.74	0.87
3:D:734:GLY:O	3:D:793:ILE:CB	2.23	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:ILE:CD1	3:D:130:ALA:CB	2.52	0.87
1:A:286:ALA:HB3	1:A:330:TYR:HE2	1.38	0.87
1:A:609:TRP:CE3	1:A:612:LEU:CD1	2.58	0.87
1:C:301:ILE:HG23	1:C:317:THR:CG2	2.03	0.87
2:B:182:THR:CG2	2:B:190:TRP:CH2	2.58	0.87
1:C:301:ILE:HG23	1:C:317:THR:HG23	1.55	0.87
1:A:525:ILE:N	1:A:762:LYS:HE2	1.89	0.87
2:B:192:VAL:CG2	2:B:195:TYR:CE2	2.56	0.87
2:B:541:PHE:O	2:B:545:VAL:CB	2.22	0.87
4:G:121:UNK:O	4:G:148:UNK:CB	2.23	0.87
1:A:124:ARG:CD	1:A:271:LEU:HD23	1.94	0.86
2:B:169:PHE:HE2	2:B:224:SER:OG	1.56	0.86
2:B:240:LEU:HA	2:B:245:PHE:HD2	1.40	0.86
1:A:259:LEU:O	1:A:262:ALA:HB3	1.76	0.86
2:B:154:MET:HE1	2:B:248:ILE:HD11	1.56	0.86
2:B:403:PRO:HG3	2:B:722:VAL:HG22	1.55	0.86
1:C:133:ILE:CG1	3:D:130:ALA:CB	2.53	0.86
2:B:194:ASN:HD21	2:B:211:LEU:CD2	1.87	0.86
2:B:665:SER:N	2:B:666:PRO:HD2	1.90	0.86
1:C:778:HIS:CE1	1:C:783:MET:HG2	2.11	0.86
1:A:818:VAL:HG21	3:D:558:MET:CE	2.02	0.86
1:A:26:ILE:CG1	1:A:59:GLN:HG2	2.06	0.85
2:B:541:PHE:CZ	1:C:803:PRO:HB3	2.11	0.85
1:C:283:ASP:OD2	1:C:335:THR:N	2.08	0.85
1:A:394:MET:CE	1:A:765:PRO:HG3	2.06	0.85
1:C:665:ILE:HA	1:C:670:LEU:HD22	1.56	0.85
3:D:321:GLU:O	3:D:324:VAL:HG12	1.75	0.85
2:B:399:LEU:HD22	2:B:400:GLU:N	1.89	0.85
1:C:283:ASP:OD2	1:C:335:THR:HG22	1.77	0.85
1:C:315:TRP:CD2	1:C:317:THR:O	2.30	0.85
2:B:398:THR:HA	2:B:497:VAL:O	1.77	0.85
2:B:522:SER:O	2:B:717:ILE:CA	2.24	0.85
3:D:600:TRP:HE3	3:D:613:VAL:CB	1.86	0.85
1:A:117:PRO:CG	1:A:321:PHE:CD2	2.29	0.85
2:B:398:THR:HG22	2:B:497:VAL:HB	1.59	0.85
1:A:625:PHE:HZ	2:B:590:GLY:HA3	1.42	0.85
3:D:559:LEU:HD21	3:D:598:ALA:HB1	1.58	0.85
3:D:765:TRP:HB3	3:D:769:VAL:CG2	2.05	0.85
1:A:286:ALA:CB	1:A:330:TYR:CE2	2.60	0.85
1:C:637:PHE:CD1	3:D:818:LEU:CD2	2.59	0.85
2:B:154:MET:HA	2:B:158:ASP:CB	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:399:LEU:HD22	2:B:400:GLU:H	1.42	0.85
2:B:541:PHE:O	2:B:545:VAL:CA	2.25	0.84
1:C:273:ASN:OD1	1:C:335:THR:HA	1.77	0.84
2:B:182:THR:HG22	2:B:190:TRP:CE3	2.11	0.84
1:C:575:LEU:CA	1:C:634:TRP:HH2	1.90	0.84
2:B:600:VAL:CB	2:B:622:TRP:HZ2	1.90	0.84
1:C:53:HIS:NE2	1:C:293:HIS:CB	2.38	0.84
1:C:606:TRP:CZ3	1:C:609:TRP:HE3	1.95	0.84
1:A:106:PRO:CB	2:B:107:PHE:CZ	2.58	0.84
1:C:53:HIS:HD2	1:C:293:HIS:CE1	1.85	0.84
1:A:93:SER:HB2	1:A:277:GLU:CD	1.96	0.84
2:B:120:HIS:HB2	2:B:280:ILE:HG23	1.57	0.84
3:D:294:ILE:HG23	3:D:337:VAL:CB	2.07	0.84
3:D:543:PHE:O	3:D:546:PRO:HG2	1.77	0.84
1:A:157:LEU:HD22	1:A:372:ILE:HD11	1.59	0.84
2:B:765:LEU:CD1	1:C:523:GLN:HG3	2.05	0.84
1:A:811:MET:N	3:D:631:PHE:CE2	2.45	0.84
2:B:765:LEU:CD2	1:C:523:GLN:HG2	2.07	0.84
3:D:297:THR:HG21	3:D:338:THR:O	1.76	0.84
1:A:131:LYS:HZ1	1:A:343:ASP:HA	1.39	0.84
1:A:131:LYS:HZ3	1:A:343:ASP:HA	1.42	0.84
2:B:758:ARG:O	2:B:762:PRO:HD2	1.78	0.84
1:A:662:ILE:CB	1:A:747:THR:CB	2.55	0.84
1:A:287:VAL:HG23	1:A:330:TYR:HD2	1.43	0.83
2:B:64:LEU:CD1	2:B:81:LEU:CD1	2.47	0.83
1:A:575:LEU:CD1	1:A:622:PRO:HB3	2.07	0.83
1:A:690:TYR:CD2	1:A:752:PHE:CZ	2.66	0.83
1:A:632:MET:CB	2:B:597:TRP:CZ3	2.61	0.83
1:A:736:PHE:CE1	1:A:794:GLN:CD	2.50	0.83
2:B:114:ILE:CD1	2:B:308:ALA:HB2	2.07	0.83
1:C:295:LEU:HD22	1:C:321:PHE:HD1	1.01	0.83
2:B:130:LYS:CB	2:B:137:PHE:CZ	2.62	0.83
2:B:552:MET:HE2	2:B:622:TRP:CE3	2.13	0.83
2:B:32:VAL:HG22	2:B:91:VAL:CG2	2.08	0.83
1:A:286:ALA:HB1	1:A:330:TYR:CZ	2.14	0.83
2:B:125:MET:HE1	2:B:251:SER:O	1.79	0.83
1:C:342:GLU:OE2	3:D:170:TYR:HE2	1.60	0.83
2:B:501:THR:HG1	6:B:1101:GLU:N	1.75	0.83
1:A:394:MET:SD	1:A:766:TRP:CZ2	2.71	0.83
2:B:520:GLY:O	2:B:743:ILE:CG2	2.27	0.83
2:B:765:LEU:O	1:C:519:ASN:OD1	1.97	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:TRP:CZ2	1:C:317:THR:HB	2.14	0.83
2:B:458:THR:HG21	2:B:766:ALA:HB1	1.59	0.82
3:D:58:PRO:CG	3:D:303:LEU:CD1	2.56	0.82
1:C:627:ALA:O	1:C:630:LEU:HB2	1.79	0.82
1:A:105:THR:HA	1:A:128:TYR:HE2	1.44	0.82
1:C:301:ILE:HG22	1:C:317:THR:CG2	1.97	0.82
3:D:388:TYR:H	3:D:389:PRO:HD2	1.42	0.82
1:C:678:ILE:H	1:C:725:HIS:HD2	1.23	0.82
2:B:53:MET:HA	2:B:53:MET:CE	2.09	0.82
1:A:102:LEU:O	1:A:128:TYR:OH	1.98	0.82
1:A:53:HIS:HB3	1:A:293:HIS:NE2	1.94	0.82
1:A:682:VAL:HG21	1:A:729:TRP:HH2	1.35	0.82
2:B:154:MET:CE	2:B:218:VAL:HG11	2.08	0.82
2:B:169:PHE:CB	2:B:170:PRO:CD	2.57	0.82
1:C:481:LYS:HB2	1:C:498:GLY:HA3	1.61	0.82
2:B:169:PHE:HB3	2:B:170:PRO:HD3	1.59	0.82
2:B:268:LEU:O	2:B:268:LEU:HD13	1.78	0.82
2:B:568:SER:O	2:B:570:VAL:N	2.13	0.82
1:C:425:THR:HG22	1:C:431:ILE:CG1	2.09	0.82
1:C:575:LEU:CB	1:C:634:TRP:HH2	1.93	0.82
1:C:694:GLN:HB2	1:C:697:LEU:HD12	1.60	0.82
3:D:119:LEU:HA	3:D:139:PHE:O	1.80	0.82
1:A:26:ILE:N	1:A:59:GLN:HB3	1.93	0.82
1:A:381:TRP:HB3	1:A:382:PRO:HD2	1.62	0.82
1:A:530:PRO:HA	1:A:756:PHE:O	1.80	0.82
3:D:338:THR:HG22	3:D:343:ASP:HA	1.62	0.82
1:A:247:TRP:HB3	1:A:266:ILE:HG13	1.62	0.82
1:A:690:TYR:CE2	1:A:752:PHE:CD1	2.68	0.82
1:C:142:PRO:HD3	1:C:349:ALA:HB2	1.60	0.81
2:B:424:CYS:HB2	2:B:442:LYS:O	1.80	0.81
2:B:522:SER:HB3	2:B:743:ILE:HG22	1.59	0.81
1:C:576:TYR:HE2	1:C:604:ALA:HB2	1.45	0.81
1:A:602:SER:HB3	1:A:606:TRP:CZ3	2.15	0.81
1:C:217:ARG:CB	1:C:392:TYR:N	2.44	0.81
1:C:109:TYR:CD1	3:D:105:GLN:CG	2.63	0.81
1:A:678:ILE:CG2	1:A:724:LEU:HD22	2.09	0.81
1:C:674:SER:HB3	1:C:677:PHE:HB3	1.63	0.81
3:D:332:ARG:HA	3:D:335:ILE:HG12	1.61	0.81
3:D:294:ILE:CD1	3:D:344:LEU:CB	2.57	0.81
3:D:594:THR:HG23	3:D:598:ALA:HB2	1.63	0.81
1:A:547:SER:CB	1:A:550:ASP:HB2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:THR:HB	2:B:98:GLN:NE2	1.96	0.81
2:B:562:PHE:CD1	1:C:826:ILE:HD13	2.16	0.81
1:C:637:PHE:CG	3:D:818:LEU:HD22	2.15	0.81
1:A:574:MET:SD	2:B:819:SER:OG	2.39	0.81
1:A:621:ALA:CB	1:A:622:PRO:HD2	2.11	0.81
2:B:591:LYS:O	2:B:595:LEU:N	2.13	0.81
1:C:782:PHE:CE2	1:C:786:LEU:HD11	2.16	0.81
1:A:541:LYS:CB	1:A:745:VAL:HG23	2.11	0.80
3:D:325:TYR:CD1	3:D:326:GLU:N	2.50	0.80
2:B:114:ILE:HD11	2:B:308:ALA:HB1	1.61	0.80
1:C:298:MET:SD	1:C:320:LEU:HD21	2.21	0.80
1:C:133:ILE:CG1	3:D:130:ALA:HB1	2.11	0.80
2:B:765:LEU:HD13	1:C:519:ASN:OD1	1.81	0.80
3:D:283:ASP:C	3:D:285:PRO:HD2	2.02	0.80
1:A:26:ILE:CA	1:A:59:GLN:HB3	2.11	0.80
2:B:194:ASN:OD1	2:B:214:ILE:CG1	2.30	0.80
2:B:240:LEU:HA	2:B:245:PHE:CD2	2.17	0.80
1:C:142:PRO:CD	1:C:349:ALA:HB2	2.12	0.80
1:C:485:GLN:HA	1:C:495:ALA:HA	1.62	0.80
3:D:562:VAL:HA	3:D:565:VAL:CG2	2.12	0.80
2:B:523:VAL:HG22	2:B:717:ILE:HG12	0.81	0.80
1:A:122:THR:HG21	1:A:277:GLU:OE2	1.81	0.80
2:B:162:PHE:CD2	2:B:219:ILE:HG12	2.17	0.80
3:D:396:ASP:CB	3:D:467:PHE:HA	2.12	0.80
1:C:503:LEU:HD12	1:C:508:ALA:O	1.81	0.80
3:D:500:TYR:HE2	3:D:765:TRP:CD1	1.99	0.80
3:D:284:LEU:N	3:D:285:PRO:HD2	1.95	0.79
2:B:151:LEU:CD2	2:B:190:TRP:CH2	2.61	0.79
3:D:152:MET:HE2	3:D:224:LEU:HD22	1.64	0.79
3:D:396:ASP:CB	3:D:468:THR:N	2.43	0.79
1:A:530:PRO:HB3	1:A:755:GLY:HA3	1.64	0.79
1:A:119:ILE:HD12	1:A:288:VAL:HG21	1.60	0.79
1:A:512:VAL:HA	1:A:758:ILE:HD11	1.64	0.79
2:B:521:ILE:HD11	2:B:653:LEU:HD11	1.62	0.79
1:C:291:ALA:CB	1:C:325:LEU:HD13	2.12	0.79
2:B:157:TYR:OH	2:B:246:VAL:HG11	1.82	0.79
2:B:541:PHE:HB3	2:B:545:VAL:CB	2.12	0.79
2:B:559:MET:HG3	2:B:563:ILE:HD11	1.62	0.79
1:C:132:SER:CB	3:D:172:PRO:CB	2.48	0.79
2:B:765:LEU:CD1	1:C:523:GLN:HE21	1.96	0.79
2:B:157:TYR:OH	2:B:246:VAL:HG21	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:559:MET:O	2:B:563:ILE:HD12	1.82	0.79
1:C:391:GLY:O	1:C:392:TYR:CB	2.30	0.79
1:A:531:PHE:HE1	1:A:774:ILE:HG12	1.46	0.79
1:C:634:TRP:O	1:C:637:PHE:HD2	1.65	0.79
3:D:343:ASP:OD2	3:D:354:HIS:HB2	1.83	0.79
3:D:409:PHE:CE2	3:D:755:TYR:HE2	1.99	0.79
3:D:794:CYS:SG	3:D:794:CYS:O	2.41	0.79
1:C:287:VAL:HG21	1:C:338:ILE:HD13	1.65	0.78
2:B:801:ASP:O	2:B:805:MET:SD	2.41	0.78
1:A:552:PHE:CD1	1:A:553:MET:N	2.51	0.78
2:B:136:PHE:O	2:B:137:PHE:CG	2.36	0.78
3:D:605:LEU:CD1	3:D:629:ALA:CB	2.54	0.78
1:A:568:VAL:CG1	1:A:608:SER:HB3	2.14	0.78
2:B:541:PHE:HE1	2:B:636:ASN:ND2	1.81	0.78
1:C:142:PRO:CD	1:C:349:ALA:CB	2.61	0.78
1:C:274:GLY:HA2	1:C:280:HIS:NE2	1.99	0.78
1:A:609:TRP:HE3	1:A:612:LEU:HD12	1.49	0.78
1:A:690:TYR:HD2	1:A:752:PHE:CE2	2.00	0.78
1:A:536:LEU:HA	1:A:730:ASP:HA	1.66	0.78
1:A:26:ILE:HA	1:A:59:GLN:HB3	1.66	0.78
2:B:194:ASN:HB2	2:B:214:ILE:CG2	2.10	0.78
1:C:630:LEU:HD13	1:C:634:TRP:CZ2	2.18	0.78
1:A:496:TRP:CD1	1:A:500:MET:SD	2.77	0.77
3:D:600:TRP:CZ3	3:D:613:VAL:CB	2.66	0.77
1:C:133:ILE:HD13	3:D:130:ALA:CB	2.10	0.77
2:B:397:VAL:HG23	2:B:466:TYR:C	2.02	0.77
1:A:123:THR:O	1:A:139:ARG:HD2	1.85	0.77
2:B:765:LEU:CG	1:C:523:GLN:HG2	2.15	0.77
2:B:468:VAL:HG21	2:B:484:MET:HG3	1.64	0.77
2:B:502:ILE:CG2	2:B:512:PHE:CE1	2.68	0.77
2:B:520:GLY:C	2:B:743:ILE:HG21	2.04	0.77
1:A:312:THR:HB	2:B:98:GLN:HE22	1.49	0.77
3:D:49:HIS:O	3:D:53:ASP:N	2.17	0.77
3:D:566:ALA:O	3:D:570:PHE:CB	2.33	0.77
2:B:520:GLY:HA3	2:B:743:ILE:CG1	2.14	0.77
2:B:600:VAL:CB	2:B:622:TRP:CZ2	2.68	0.77
1:C:113:PHE:CD1	3:D:102:ALA:HB3	2.20	0.77
3:D:545:GLU:N	3:D:546:PRO:HD2	1.98	0.77
2:B:240:LEU:O	2:B:245:PHE:HB2	1.85	0.77
1:A:690:TYR:CD2	1:A:752:PHE:CD2	2.72	0.77
2:B:541:PHE:CA	2:B:545:VAL:HB	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:THR:O	2:B:198:LEU:HD12	1.85	0.76
1:A:124:ARG:HG2	1:A:141:VAL:CG2	2.15	0.76
2:B:615:SER:O	2:B:619:VAL:HG23	1.85	0.76
1:C:425:THR:CG2	1:C:431:ILE:CG1	2.63	0.76
1:C:53:HIS:CB	1:C:293:HIS:NE2	2.48	0.76
2:B:169:PHE:CD2	2:B:224:SER:HB3	2.19	0.76
2:B:525:VAL:HG21	2:B:650:VAL:HG21	1.67	0.76
1:C:627:ALA:HA	1:C:630:LEU:HB2	1.66	0.76
1:C:133:ILE:CG1	3:D:130:ALA:HB2	2.14	0.76
1:A:122:THR:CG2	1:A:277:GLU:OE2	2.32	0.76
2:B:519:THR:CG2	2:B:721:ALA:HB2	2.03	0.76
3:D:555:MET:SD	3:D:628:TRP:CE2	2.79	0.76
1:C:93:SER:HB3	1:C:121:LEU:HD12	1.67	0.76
3:D:560:LEU:O	3:D:560:LEU:HD22	1.84	0.76
3:D:627:VAL:O	3:D:630:PHE:CD2	2.38	0.76
1:A:292:ILE:CG1	1:A:321:PHE:CE1	2.67	0.76
2:B:502:ILE:HG12	2:B:512:PHE:CZ	2.21	0.76
2:B:591:LYS:O	2:B:595:LEU:CB	2.33	0.76
1:C:802:ALA:H	1:C:803:PRO:CD	1.99	0.76
2:B:82:MET:O	2:B:85:THR:O	2.04	0.75
2:B:182:THR:CG2	2:B:190:TRP:HZ3	1.96	0.75
2:B:752:ALA:C	2:B:753:LEU:HD12	2.05	0.75
2:B:164:VAL:HG21	2:B:179:ILE:CD1	2.17	0.75
2:B:64:LEU:HD12	2:B:81:LEU:CG	2.15	0.75
2:B:519:THR:CG2	2:B:721:ALA:CB	2.59	0.75
2:B:74:ILE:CG2	2:B:105:LEU:HD21	2.16	0.75
3:D:332:ARG:CA	3:D:335:ILE:HD11	2.16	0.75
2:B:651:THR:HG1	2:B:655:ASP:HB2	0.92	0.75
2:B:402:ALA:HB3	2:B:403:PRO:HD3	1.69	0.75
2:B:669:ARG:NH2	2:B:712:LYS:O	2.20	0.75
2:B:522:SER:HG	2:B:723:LEU:HD12	1.50	0.75
1:A:34:SER:CB	1:A:96:PRO:CD	2.65	0.75
1:A:488:VAL:CB	1:A:494:ALA:HB2	2.17	0.75
1:A:510:MET:HG3	1:A:760:MET:CG	2.17	0.75
2:B:120:HIS:ND1	2:B:280:ILE:HG12	2.01	0.75
1:A:312:THR:CB	2:B:98:GLN:HE21	1.97	0.75
2:B:525:VAL:HG21	2:B:650:VAL:CG2	2.16	0.75
1:A:26:ILE:HA	1:A:59:GLN:CB	2.17	0.75
1:C:34:SER:HB2	1:C:96:PRO:HG3	1.69	0.75
3:D:172:PRO:O	3:D:226:TYR:OH	2.02	0.75
1:C:291:ALA:CB	1:C:325:LEU:CD1	2.65	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:552:MET:HE2	2:B:622:TRP:CZ3	2.22	0.74
2:B:541:PHE:CE1	2:B:636:ASN:ND2	2.54	0.74
1:C:637:PHE:CE1	1:C:641:ILE:HD12	2.21	0.74
1:A:690:TYR:CE2	1:A:752:PHE:CG	2.75	0.74
1:A:94:HIS:H	1:A:122:THR:HG1	1.33	0.74
3:D:600:TRP:O	3:D:604:GLY:N	2.20	0.74
3:D:331:LYS:O	3:D:335:ILE:HG12	1.87	0.74
1:C:530:PRO:HA	1:C:756:PHE:O	1.88	0.74
2:B:120:HIS:CD2	2:B:280:ILE:HD13	2.22	0.74
2:B:49:TRP:O	2:B:53:MET:N	2.20	0.74
3:D:332:ARG:CA	3:D:335:ILE:CG1	2.66	0.74
1:A:690:TYR:HD2	1:A:752:PHE:CZ	2.04	0.74
2:B:154:MET:CE	2:B:248:ILE:CD1	2.65	0.74
1:C:298:MET:SD	1:C:320:LEU:HD11	2.28	0.74
1:A:512:VAL:HA	1:A:758:ILE:CD1	2.17	0.74
3:D:559:LEU:O	3:D:559:LEU:HD23	1.88	0.74
1:A:510:MET:SD	1:A:760:MET:SD	2.86	0.73
2:B:405:VAL:HG22	2:B:449:ILE:HG12	1.70	0.73
1:A:538:ILE:HG23	1:A:727:PHE:O	1.88	0.73
1:C:109:TYR:CE1	3:D:105:GLN:CG	2.71	0.73
3:D:373:LYS:O	3:D:380:LYS:CB	2.35	0.73
1:A:247:TRP:HB2	1:A:266:ILE:CG1	2.07	0.73
1:A:552:PHE:O	1:A:555:PRO:CD	2.35	0.73
5:D:1004:NAG:C8	5:D:1004:NAG:H3	2.17	0.73
3:D:161:TRP:HB3	3:D:222:VAL:HG21	1.69	0.73
1:A:525:ILE:CA	1:A:762:LYS:CE	2.66	0.73
2:B:162:PHE:HD1	2:B:216:SER:H	1.34	0.73
1:A:124:ARG:HH11	1:A:271:LEU:CB	2.02	0.73
2:B:485:ILE:HD11	2:B:506:ARG:HE	1.51	0.73
1:A:117:PRO:HG2	1:A:321:PHE:CE2	2.16	0.73
1:A:53:HIS:CB	1:A:293:HIS:CD2	2.68	0.73
2:B:25:PHE:CB	2:B:26:PRO:CD	2.66	0.73
2:B:40:ILE:CD1	2:B:281:GLU:OE2	2.36	0.73
2:B:753:LEU:HD22	2:B:760:LYS:CB	2.18	0.73
3:D:538:VAL:HA	3:D:646:PHE:CZ	2.24	0.73
1:A:286:ALA:HB1	1:A:330:TYR:OH	1.89	0.73
2:B:241:MET:HA	2:B:247:TRP:HZ2	1.49	0.73
2:B:552:MET:CE	2:B:622:TRP:CZ3	2.71	0.73
2:B:541:PHE:CE1	1:C:803:PRO:HB3	2.24	0.73
2:B:521:ILE:HG12	2:B:745:ALA:HB2	1.71	0.73
2:B:636:ASN:HA	1:C:803:PRO:HG3	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:766:TRP:O	1:C:770:VAL:HG23	1.89	0.72
1:C:526:GLU:OE2	1:C:767:LYS:HG3	1.89	0.72
1:A:525:ILE:C	1:A:762:LYS:NZ	2.43	0.72
2:B:403:PRO:CG	2:B:722:VAL:CG2	2.47	0.72
1:C:274:GLY:CA	1:C:280:HIS:NE2	2.52	0.72
3:D:345:SER:OG	3:D:353:MET:HB3	1.89	0.72
3:D:565:VAL:O	3:D:569:VAL:HG23	1.87	0.72
2:B:32:VAL:HG13	2:B:91:VAL:HG23	1.70	0.72
1:C:636:LEU:O	1:C:636:LEU:HD22	1.89	0.72
1:A:26:ILE:HG12	1:A:59:GLN:HG2	1.70	0.72
2:B:154:MET:O	2:B:158:ASP:N	2.21	0.72
1:C:354:MET:HE3	1:C:361:LEU:CB	2.19	0.72
1:A:510:MET:HG3	1:A:760:MET:HG2	1.70	0.72
1:A:530:PRO:HB2	1:A:755:GLY:CA	2.19	0.72
1:A:625:PHE:HZ	2:B:590:GLY:CA	2.03	0.72
2:B:665:SER:N	2:B:666:PRO:CD	2.53	0.72
1:C:565:GLY:O	1:C:569:HIS:ND1	2.21	0.72
1:C:637:PHE:CE1	1:C:641:ILE:CD1	2.72	0.72
1:A:496:TRP:CH2	1:A:524:TYR:CD2	2.77	0.72
1:A:53:HIS:CD2	1:A:293:HIS:CG	2.77	0.72
1:A:54:PHE:CE1	1:A:293:HIS:CD2	2.77	0.72
1:A:105:THR:HA	1:A:128:TYR:CE2	2.23	0.72
3:D:283:ASP:CB	3:D:285:PRO:HD2	2.20	0.72
3:D:332:ARG:O	3:D:335:ILE:CG1	2.34	0.72
1:A:663:THR:O	1:A:667:ASP:N	2.22	0.72
1:A:833:ILE:O	1:A:836:LYS:CB	2.37	0.72
1:A:815:PHE:HE2	3:D:554:MET:CG	1.96	0.72
2:B:241:MET:HA	2:B:247:TRP:CH2	2.25	0.71
2:B:125:MET:CE	2:B:251:SER:HB2	2.20	0.71
2:B:753:LEU:CD2	2:B:760:LYS:CG	2.68	0.71
1:A:609:TRP:HA	1:A:612:LEU:HD12	1.72	0.71
1:C:287:VAL:HG21	1:C:338:ILE:CD1	2.21	0.71
1:C:606:TRP:CZ3	1:C:609:TRP:CE3	2.76	0.71
3:D:388:TYR:H	3:D:389:PRO:CD	1.98	0.71
1:A:609:TRP:CE3	1:A:612:LEU:HD12	2.24	0.71
2:B:520:GLY:C	2:B:743:ILE:CG2	2.58	0.71
2:B:523:VAL:HG22	2:B:717:ILE:HG13	1.68	0.71
1:A:281:ILE:O	1:A:285:VAL:HG23	1.91	0.71
1:A:632:MET:CB	2:B:597:TRP:HZ3	2.03	0.71
1:A:764:SER:O	1:A:767:LYS:HG3	1.91	0.71
2:B:539:GLU:O	2:B:542:SER:HB3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:VAL:CG2	2:B:91:VAL:HG22	2.12	0.71
1:C:654:VAL:O	1:C:656:ARG:N	2.22	0.71
1:A:54:PHE:CE1	1:A:293:HIS:HD2	2.07	0.71
1:A:531:PHE:HE1	1:A:774:ILE:CG1	2.03	0.71
1:A:626:SER:HA	1:A:629:ILE:CD1	2.20	0.71
1:A:690:TYR:CE2	1:A:752:PHE:CE1	2.78	0.71
2:B:182:THR:HG23	2:B:190:TRP:CZ3	2.26	0.71
3:D:103:ILE:O	3:D:106:ILE:HG22	1.90	0.71
1:A:530:PRO:CB	1:A:755:GLY:CA	2.68	0.71
2:B:523:VAL:HG22	2:B:717:ILE:CD1	2.19	0.71
2:B:544:SER:O	2:B:548:MET:HG2	1.91	0.71
1:A:34:SER:CA	1:A:96:PRO:HG2	2.20	0.71
2:B:791:GLU:O	2:B:793:ASN:N	2.24	0.71
2:B:31:ALA:HB3	2:B:90:VAL:HG12	1.72	0.71
5:D:1004:NAG:C1	5:D:1004:NAG:H82	2.21	0.71
2:B:502:ILE:HG23	2:B:512:PHE:HZ	1.51	0.70
1:C:784:GLU:O	1:C:788:LYS:HB3	1.91	0.70
3:D:305:GLU:C	3:D:306:HIS:HD2	1.94	0.70
1:C:802:ALA:H	1:C:803:PRO:HD2	1.56	0.70
3:D:121:ILE:CB	3:D:287:ARG:CB	2.68	0.70
2:B:192:VAL:HG21	2:B:195:TYR:HE2	1.46	0.70
2:B:192:VAL:HG21	2:B:195:TYR:HD2	1.48	0.70
3:D:741:LEU:HD12	3:D:741:LEU:H	1.56	0.70
1:A:27:VAL:HG13	1:A:88:TYR:CE1	2.26	0.70
2:B:636:ASN:ND2	1:C:803:PRO:CB	2.55	0.70
2:B:768:LEU:O	2:B:771:VAL:N	2.23	0.70
1:C:217:ARG:CB	1:C:392:TYR:H	2.05	0.70
1:A:292:ILE:CG1	1:A:321:PHE:HZ	2.02	0.70
2:B:194:ASN:HB2	2:B:214:ILE:HG13	1.73	0.70
2:B:552:MET:HE3	2:B:622:TRP:HE3	1.44	0.70
2:B:630:LEU:HB3	7:B:1102:BMK:C14	2.22	0.70
1:A:121:LEU:HD13	1:A:281:ILE:HG12	1.74	0.70
2:B:197:THR:O	2:B:198:LEU:HB2	1.92	0.70
2:B:541:PHE:CB	2:B:545:VAL:HB	2.22	0.70
2:B:57:PHE:CD2	2:B:292:THR:CG2	2.66	0.70
2:B:765:LEU:HD11	1:C:523:GLN:HE21	1.52	0.70
1:A:140:THR:O	1:A:346:ARG:CB	2.40	0.69
1:A:625:PHE:CZ	2:B:590:GLY:HA3	2.27	0.69
2:B:621:ILE:HG23	1:C:818:VAL:HG13	1.74	0.69
1:C:568:VAL:HG13	1:C:608:SER:HB2	1.74	0.69
1:A:524:TYR:C	1:A:762:LYS:HE2	2.12	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:MET:O	2:B:139:PHE:CB	2.41	0.69
2:B:396:ILE:O	2:B:465:LEU:HA	1.93	0.69
2:B:268:LEU:HD12	2:B:268:LEU:H	1.57	0.69
1:C:273:ASN:CG	1:C:335:THR:HA	2.12	0.69
1:A:626:SER:HA	1:A:629:ILE:HD12	1.74	0.69
1:A:121:LEU:CD1	1:A:281:ILE:HG12	2.23	0.69
2:B:514:VAL:CG2	2:B:767:LEU:CD1	2.67	0.69
2:B:630:LEU:HB3	7:B:1102:BMK:C15	2.22	0.69
3:D:541:SER:HA	3:D:544:LEU:HG	1.75	0.69
3:D:594:THR:HG23	3:D:598:ALA:CB	2.21	0.69
3:D:741:LEU:HD12	3:D:741:LEU:N	2.08	0.69
1:A:496:TRP:HD1	1:A:500:MET:CB	1.93	0.69
1:A:525:ILE:HA	1:A:762:LYS:CE	2.21	0.69
2:B:162:PHE:CA	2:B:216:SER:CB	2.66	0.69
1:C:112:GLY:O	1:C:115:ARG:NH1	2.24	0.69
3:D:358:VAL:CG1	3:D:370:ARG:HB3	2.23	0.69
3:D:435:PRO:HD2	3:D:441:GLU:HA	1.74	0.69
1:A:34:SER:HB3	1:A:96:PRO:CD	2.23	0.69
2:B:524:MET:HE3	2:B:723:LEU:O	1.92	0.69
2:B:534:PRO:HG3	2:B:804:ASN:OD1	1.93	0.69
1:C:272:ILE:CG2	1:C:350:GLN:O	2.35	0.69
3:D:765:TRP:CB	3:D:769:VAL:CG2	2.71	0.69
3:D:411:ILE:HD12	3:D:789:TRP:CZ3	2.28	0.69
2:B:410:ILE:HG23	2:B:441:LYS:O	1.92	0.69
2:B:541:PHE:CE1	1:C:803:PRO:CB	2.75	0.69
1:A:262:ALA:O	1:A:359:ARG:CZ	2.41	0.69
3:D:358:VAL:HG11	3:D:370:ARG:HB3	1.74	0.69
1:A:126:SER:HB2	1:A:172:GLU:OE1	1.92	0.69
1:A:690:TYR:HE2	1:A:752:PHE:CE1	2.10	0.69
2:B:524:MET:CE	2:B:723:LEU:O	2.41	0.69
1:C:34:SER:CB	1:C:96:PRO:HD3	2.23	0.69
3:D:522:PHE:CE2	3:D:755:TYR:HD2	2.11	0.69
1:A:818:VAL:CG2	3:D:558:MET:SD	2.77	0.68
3:D:358:VAL:HG13	3:D:372:GLY:O	1.92	0.68
1:A:811:MET:HE1	3:D:631:PHE:HB3	1.74	0.68
1:A:34:SER:HB3	1:A:96:PRO:HD3	1.75	0.68
1:A:503:LEU:HD11	1:A:761:ARG:H	1.58	0.68
2:B:651:THR:OG1	2:B:655:ASP:CG	2.30	0.68
1:C:534:GLN:O	1:C:754:SER:O	2.11	0.68
1:A:818:VAL:HG11	3:D:558:MET:HE3	1.75	0.68
1:A:578:LEU:HD13	1:A:627:ALA:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:PHE:CB	2:B:292:THR:HG21	2.11	0.68
2:B:164:VAL:CG2	2:B:220:LEU:HD13	2.23	0.68
2:B:559:MET:C	2:B:563:ILE:HD12	2.14	0.68
1:A:247:TRP:CB	1:A:266:ILE:CG1	2.62	0.68
1:A:121:LEU:HD13	1:A:281:ILE:CG1	2.23	0.68
1:A:568:VAL:C	1:A:571:VAL:HG12	2.14	0.68
1:A:133:ILE:HG22	2:B:128:ALA:CB	2.23	0.68
1:A:218:VAL:HG13	1:A:246:VAL:HB	1.76	0.68
2:B:180:LYS:NZ	2:B:195:TYR:CE1	2.62	0.68
2:B:636:ASN:HD22	1:C:803:PRO:CB	2.06	0.68
2:B:514:VAL:HG21	2:B:767:LEU:HD13	1.76	0.68
1:C:221:LEU:HD22	1:C:231:VAL:HG11	1.75	0.68
1:A:729:TRP:HD1	1:A:730:ASP:H	1.41	0.68
1:A:124:ARG:CG	1:A:141:VAL:HG21	2.24	0.68
1:A:439:PRO:HG3	1:A:478:ALA:HA	1.75	0.68
2:B:534:PRO:HD3	2:B:804:ASN:OD1	1.94	0.68
1:C:342:GLU:CD	3:D:170:TYR:CE2	2.66	0.68
1:A:465:ALA:O	1:A:468:MET:O	2.11	0.68
1:A:609:TRP:HE3	1:A:612:LEU:CD1	2.03	0.68
2:B:636:ASN:HD22	1:C:803:PRO:HB3	1.58	0.68
2:B:736:VAL:HG12	2:B:737:THR:N	2.08	0.68
1:C:109:TYR:CD1	3:D:105:GLN:CD	2.68	0.68
3:D:500:TYR:CE2	3:D:765:TRP:NE1	2.62	0.68
1:C:575:LEU:N	1:C:634:TRP:HH2	1.92	0.67
3:D:734:GLY:O	3:D:793:ILE:N	2.26	0.67
1:A:124:ARG:HG3	1:A:141:VAL:HG21	1.75	0.67
1:A:534:GLN:CD	1:A:732:ALA:HB2	2.14	0.67
2:B:638:ALA:O	2:B:641:MET:HG3	1.95	0.67
2:B:753:LEU:HD22	2:B:760:LYS:HB3	1.76	0.67
3:D:37:VAL:HG13	3:D:68:MET:O	1.94	0.67
2:B:247:TRP:HB2	2:B:268:LEU:CG	2.25	0.67
1:C:639:MET:HA	1:C:639:MET:CE	2.23	0.67
3:D:606:VAL:CB	3:D:628:TRP:HH2	2.07	0.67
3:D:522:PHE:CE1	3:D:755:TYR:HB2	2.29	0.67
1:A:62:ALA:O	5:A:1001:NAG:H62	1.95	0.67
1:A:621:ALA:CB	1:A:622:PRO:CD	2.59	0.67
1:A:782:PHE:CE2	1:A:786:LEU:HD11	2.30	0.67
2:B:765:LEU:CD1	1:C:523:GLN:CD	2.58	0.67
1:C:53:HIS:NE2	1:C:293:HIS:HB2	2.09	0.67
1:C:629:ILE:O	1:C:633:VAL:HG23	1.94	0.67
3:D:594:THR:CG2	3:D:598:ALA:CB	2.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:HIS:N	1:A:122:THR:OG1	2.16	0.67
2:B:351:PRO:CG	2:B:370:TRP:CZ3	2.69	0.67
4:G:122:UNK:HA	4:G:148:UNK:O	1.95	0.67
1:A:201:THR:O	1:A:204:LEU:HD22	1.95	0.67
1:A:214:LEU:N	1:A:214:LEU:HD23	2.10	0.67
1:A:426:ILE:HD12	1:A:426:ILE:O	1.95	0.67
1:A:23:ASP:O	1:A:56:ARG:O	2.12	0.67
2:B:82:MET:HE2	2:B:114:ILE:CD1	2.19	0.67
1:A:122:THR:CG2	1:A:277:GLU:HG3	2.22	0.67
1:A:124:ARG:NE	1:A:271:LEU:HD22	2.09	0.67
1:A:53:HIS:CB	1:A:293:HIS:NE2	2.57	0.67
1:A:690:TYR:HE2	1:A:752:PHE:CD1	2.12	0.67
2:B:524:MET:HG3	2:B:736:VAL:O	1.95	0.67
1:C:637:PHE:HB3	3:D:818:LEU:HD13	1.76	0.67
3:D:453:PHE:O	3:D:457:ILE:HG12	1.95	0.67
1:A:439:PRO:CG	1:A:478:ALA:HA	2.24	0.67
2:B:765:LEU:HD11	1:C:523:GLN:HG2	1.70	0.67
2:B:31:ALA:HB3	2:B:90:VAL:CG1	2.24	0.67
1:C:576:TYR:CE2	1:C:604:ALA:HB2	2.28	0.67
1:C:673:PRO:HA	1:C:679:TYR:CE2	2.30	0.67
3:D:28:PRO:HB3	4:G:55:UNK:CB	2.25	0.67
2:B:369:LYS:O	2:B:376:ASN:HB2	1.94	0.66
2:B:559:MET:CG	2:B:563:ILE:HD11	2.25	0.66
3:D:305:GLU:C	3:D:306:HIS:CD2	2.69	0.66
1:C:132:SER:HB3	3:D:172:PRO:HB2	1.72	0.66
1:A:815:PHE:CD2	3:D:554:MET:SD	2.89	0.66
1:C:438:GLY:CA	1:C:451:GLN:NE2	2.44	0.66
1:C:484:THR:O	1:C:497:ASN:CB	2.43	0.66
3:D:327:ALA:O	3:D:330:LEU:HB3	1.95	0.66
3:D:543:PHE:CE1	3:D:643:LEU:HD11	2.30	0.66
1:C:301:ILE:CG2	1:C:317:THR:CB	2.74	0.66
1:C:74:MET:O	1:C:78:VAL:HG23	1.96	0.66
3:D:562:VAL:HA	3:D:565:VAL:HG23	1.74	0.66
1:A:330:TYR:N	1:A:331:PRO:HD3	2.10	0.66
2:B:402:ALA:HA	2:B:406:ILE:HD11	1.77	0.66
2:B:519:THR:HG22	2:B:721:ALA:HB3	1.74	0.66
1:A:286:ALA:HB1	1:A:330:TYR:CE2	2.30	0.66
2:B:405:VAL:O	2:B:406:ILE:HD13	1.96	0.66
1:A:294:GLU:O	1:A:297:GLU:HB2	1.95	0.66
1:A:525:ILE:HD11	1:A:527:PHE:CE1	2.30	0.66
1:A:124:ARG:CG	1:A:141:VAL:CG2	2.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:GLN:HB3	2:B:800:LEU:HD13	1.78	0.66
2:B:154:MET:HE3	2:B:218:VAL:HG11	1.77	0.66
1:C:673:PRO:HA	1:C:679:TYR:HE2	1.60	0.66
1:C:535:GLY:O	1:C:731:SER:HB3	1.96	0.66
3:D:171:PHE:O	3:D:174:TYR:HD2	1.79	0.66
3:D:409:PHE:CE2	3:D:755:TYR:CE2	2.83	0.66
1:A:26:ILE:HG21	1:A:61:ASN:CB	2.15	0.66
1:A:663:THR:O	1:A:667:ASP:CA	2.44	0.66
1:A:818:VAL:HG22	3:D:558:MET:CE	2.09	0.66
2:B:651:THR:HG1	2:B:655:ASP:CB	1.86	0.66
1:C:142:PRO:CG	1:C:349:ALA:HB3	2.26	0.66
1:C:627:ALA:CA	1:C:630:LEU:HB2	2.26	0.66
1:C:109:TYR:CE1	3:D:105:GLN:HG2	2.30	0.66
1:A:113:PHE:CD1	2:B:100:ALA:CB	2.80	0.65
1:A:574:MET:SD	1:A:630:LEU:CD1	2.84	0.65
1:A:150:VAL:HG21	1:A:351:TYR:HD2	1.61	0.65
1:A:609:TRP:CZ3	1:A:612:LEU:HD13	2.30	0.65
2:B:767:LEU:O	2:B:770:PHE:HB2	1.96	0.65
1:C:513:ALA:HB1	1:C:514:PRO:HD2	1.78	0.65
3:D:332:ARG:CA	3:D:335:ILE:HG12	2.26	0.65
1:A:204:LEU:HD23	1:A:204:LEU:N	2.11	0.65
1:A:287:VAL:CG2	1:A:330:TYR:HD2	2.09	0.65
1:A:400:ILE:HB	1:A:474:VAL:HG22	1.77	0.65
1:A:578:LEU:CB	1:A:627:ALA:HB2	2.26	0.65
2:B:253:VAL:O	2:B:256:ASN:OD1	2.13	0.65
2:B:304:VAL:O	2:B:306:PRO:HD3	1.96	0.65
1:C:301:ILE:CG2	1:C:317:THR:OG1	2.45	0.65
3:D:620:THR:O	3:D:624:MET:HG2	1.96	0.65
1:A:204:LEU:HD21	1:A:230:ALA:HB1	1.76	0.65
2:B:197:THR:O	2:B:207:THR:CG2	2.45	0.65
1:C:575:LEU:CD1	1:C:627:ALA:CB	2.66	0.65
1:A:25:LYS:O	1:A:59:GLN:HB3	1.96	0.65
2:B:634:THR:O	2:B:638:ALA:N	2.29	0.65
2:B:495:MET:CE	2:B:753:LEU:HD11	2.26	0.65
3:D:253:VAL:HB	3:D:274:SER:HB2	1.79	0.65
3:D:522:PHE:CZ	3:D:755:TYR:HD2	2.14	0.65
1:C:291:ALA:HB2	1:C:325:LEU:HD12	1.77	0.65
1:C:634:TRP:HA	1:C:637:PHE:HD2	1.60	0.65
1:A:287:VAL:HG23	1:A:330:TYR:CD2	2.31	0.65
1:A:440:ASP:CB	1:A:449:VAL:HG21	2.26	0.65
2:B:651:THR:OG1	2:B:655:ASP:OD2	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:TYR:OH	1:C:308:CYS:SG	2.54	0.65
2:B:541:PHE:HB3	2:B:545:VAL:HB	1.76	0.65
1:C:23:ASP:N	1:C:24:PRO:HD3	2.12	0.65
2:B:109:SER:OG	2:B:135:THR:HA	1.98	0.64
2:B:720:ALA:HB2	2:B:743:ILE:HG22	1.73	0.64
3:D:332:ARG:C	3:D:335:ILE:HG13	2.18	0.64
1:A:811:MET:HE2	3:D:631:PHE:HD2	1.62	0.64
1:A:202:LYS:O	1:A:204:LEU:HD23	1.97	0.64
1:A:621:ALA:HB1	1:A:622:PRO:HD3	1.77	0.64
1:C:301:ILE:HG22	1:C:317:THR:OG1	1.97	0.64
3:D:301:THR:HB	3:D:333:TYR:CD2	2.32	0.64
1:A:667:ASP:OD1	1:A:668:PRO:HD2	1.97	0.64
2:B:524:MET:HG2	2:B:735:LEU:HB3	1.80	0.64
1:A:205:THR:CG2	1:A:238:LEU:CD1	2.34	0.64
2:B:568:SER:O	2:B:569:PRO:C	2.34	0.64
1:A:102:LEU:CB	1:A:128:TYR:HE1	2.10	0.64
1:A:54:PHE:HE1	1:A:293:HIS:CD2	2.16	0.64
2:B:520:GLY:HA3	2:B:743:ILE:CB	2.28	0.64
2:B:64:LEU:HD13	2:B:81:LEU:HD21	1.74	0.64
2:B:459:VAL:HG12	2:B:459:VAL:O	1.97	0.64
3:D:200:LEU:CD2	3:D:201:ASP:H	2.03	0.64
1:A:540:VAL:HG21	1:A:725:HIS:O	1.97	0.64
1:C:477:VAL:CG2	1:C:499:MET:HG3	2.28	0.64
1:C:622:PRO:HG3	3:D:600:TRP:CH2	2.32	0.64
1:C:113:PHE:CD1	3:D:102:ALA:CB	2.81	0.64
3:D:500:TYR:CE2	3:D:765:TRP:CD1	2.85	0.64
3:D:765:TRP:CB	3:D:769:VAL:HG21	2.28	0.64
1:A:119:ILE:HD13	1:A:288:VAL:HG23	1.78	0.64
1:A:379:ILE:HG21	1:A:381:TRP:CZ2	2.33	0.64
1:A:811:MET:HB2	3:D:631:PHE:CD2	2.33	0.64
1:C:415:THR:HG22	1:C:416:SER:H	1.63	0.64
1:C:50:ASN:OD1	1:C:60:LEU:HB2	1.97	0.64
3:D:293:ALA:HB1	3:D:339:PHE:CB	2.27	0.64
1:A:124:ARG:HG2	1:A:141:VAL:HB	1.78	0.64
1:A:531:PHE:CE1	1:A:774:ILE:CG2	2.80	0.64
2:B:161:VAL:HG21	2:B:220:LEU:HD11	1.78	0.64
2:B:523:VAL:HA	2:B:716:PHE:O	1.97	0.64
3:D:480:GLY:HA2	3:D:488:ASN:O	1.98	0.64
3:D:569:VAL:O	3:D:573:PHE:N	2.31	0.64
1:A:115:ARG:HG3	1:A:314:ILE:HB	1.79	0.63
1:A:205:THR:HG22	1:A:238:LEU:HD11	1.72	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:559:MET:HB2	2:B:618:ILE:HG21	1.79	0.63
2:B:524:MET:HA	2:B:736:VAL:O	1.97	0.63
1:C:276:ASN:HB3	1:C:279:ALA:HB3	1.80	0.63
3:D:734:GLY:C	3:D:793:ILE:H	2.01	0.63
1:A:204:LEU:HD11	1:A:230:ALA:C	2.19	0.63
2:B:768:LEU:HD13	2:B:768:LEU:N	2.11	0.63
3:D:603:TRP:HA	3:D:603:TRP:CE3	2.32	0.63
1:A:262:ALA:O	1:A:359:ARG:NH1	2.32	0.63
2:B:121:GLY:O	2:B:124:SER:OG	2.14	0.63
2:B:64:LEU:HD11	2:B:81:LEU:HD22	1.75	0.63
1:C:637:PHE:CB	3:D:818:LEU:HD13	2.28	0.63
1:A:198:GLU:HG3	1:A:199:PRO:HD2	1.80	0.63
1:C:34:SER:CA	1:C:96:PRO:HD3	2.29	0.63
1:C:439:PRO:HD2	1:C:476:LEU:HB2	1.79	0.63
2:B:521:ILE:O	2:B:743:ILE:O	2.15	0.63
2:B:539:GLU:N	2:B:540:PRO:CD	2.61	0.63
1:C:654:VAL:CB	3:D:802:MET:CB	2.76	0.63
2:B:743:ILE:H	2:B:743:ILE:HD13	1.62	0.63
3:D:305:GLU:CB	3:D:333:TYR:OH	2.47	0.63
1:A:147:GLN:HE22	1:A:250:GLY:HA2	1.63	0.63
1:A:609:TRP:CE3	1:A:612:LEU:HD13	2.33	0.63
1:A:664:GLY:O	1:A:670:LEU:HD22	1.99	0.63
2:B:192:VAL:CG2	2:B:195:TYR:HD2	2.08	0.63
1:C:125:MET:O	1:C:139:ARG:NH1	2.20	0.63
2:B:214:ILE:N	2:B:214:ILE:HD13	2.13	0.63
2:B:669:ARG:CD	2:B:696:PHE:CE2	2.81	0.63
1:C:449:VAL:HG12	1:C:450:PRO:N	2.12	0.63
1:C:485:GLN:CA	1:C:495:ALA:HA	2.29	0.63
1:A:124:ARG:HD3	1:A:271:LEU:HD23	1.78	0.62
1:A:568:VAL:O	1:A:571:VAL:HG13	1.92	0.62
2:B:154:MET:O	2:B:158:ASP:O	2.17	0.62
1:A:736:PHE:CE1	1:A:794:GLN:OE1	2.52	0.62
7:B:1102:BMK:C14	1:C:649:LEU:HD11	2.30	0.62
2:B:151:LEU:O	2:B:155:GLU:N	2.31	0.62
1:C:568:VAL:HG13	1:C:608:SER:CB	2.28	0.62
1:A:782:PHE:CZ	1:A:786:LEU:HD11	2.32	0.62
2:B:225:LYS:HD2	2:B:256:ASN:ND2	2.14	0.62
2:B:474:GLY:CA	2:B:482:ASN:O	2.45	0.62
1:C:446:ARG:N	1:C:447:PRO:HD3	2.15	0.62
1:C:575:LEU:CB	1:C:634:TRP:HZ3	2.09	0.62
1:C:78:VAL:HG11	1:C:110:THR:CG2	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLU:N	1:A:253:GLU:OE1	2.28	0.62
1:A:39:GLU:OE1	1:A:66:THR:OG1	2.15	0.62
2:B:678:THR:O	2:B:681:ASN:N	2.33	0.62
1:A:811:MET:CE	3:D:631:PHE:HB3	2.28	0.62
2:B:512:PHE:HB3	2:B:751:ILE:N	2.14	0.62
1:C:283:ASP:OD1	1:C:334:VAL:HG23	1.99	0.62
1:C:425:THR:HG23	1:C:431:ILE:HG13	1.81	0.62
1:C:535:GLY:O	1:C:731:SER:CB	2.47	0.62
1:C:627:ALA:C	1:C:630:LEU:HB2	2.20	0.62
3:D:301:THR:HB	3:D:333:TYR:CG	2.35	0.62
3:D:305:GLU:CB	3:D:333:TYR:CZ	2.82	0.62
1:A:34:SER:HA	1:A:96:PRO:CG	2.30	0.62
1:A:568:VAL:HG12	1:A:608:SER:CB	2.23	0.62
1:A:632:MET:CB	2:B:597:TRP:CE3	2.82	0.62
1:A:616:GLY:HA2	2:B:606:PRO:HG3	1.81	0.62
3:D:253:VAL:HG11	3:D:257:VAL:HB	1.80	0.62
3:D:493:GLU:O	3:D:499:ALA:N	2.31	0.62
1:C:308:CYS:O	3:D:72:ASP:OD2	2.18	0.62
3:D:522:PHE:CZ	3:D:755:TYR:CD2	2.87	0.62
1:A:578:LEU:HB3	1:A:627:ALA:HB2	1.82	0.62
2:B:120:HIS:NE2	2:B:280:ILE:CD1	2.62	0.62
1:C:329:LYS:C	1:C:331:PRO:HD3	2.20	0.62
1:C:477:VAL:HB	1:C:499:MET:HG3	1.81	0.62
3:D:667:PRO:HG2	3:D:668:ASN:HD22	1.65	0.62
1:A:124:ARG:HD2	1:A:271:LEU:HD21	1.66	0.62
2:B:753:LEU:CD2	2:B:760:LYS:HB3	2.29	0.62
1:C:301:ILE:HG22	1:C:317:THR:CB	2.30	0.62
3:D:772:ALA:O	3:D:775:GLN:HB2	2.00	0.62
2:B:502:ILE:CG2	2:B:512:PHE:CZ	2.74	0.61
1:C:287:VAL:CG2	1:C:338:ILE:HD12	2.30	0.61
1:C:287:VAL:CG2	1:C:338:ILE:CD1	2.78	0.61
1:C:673:PRO:HD3	1:C:699:THR:HG22	1.82	0.61
1:C:679:TYR:H	1:C:703:HIS:HE1	1.48	0.61
1:A:551:SER:OG	1:A:649:LEU:HD11	1.99	0.61
2:B:396:ILE:HG23	2:B:495:MET:O	1.98	0.61
2:B:541:PHE:HD1	2:B:541:PHE:H	1.47	0.61
2:B:34:LEU:O	2:B:65:LEU:CD1	2.48	0.61
1:A:648:ASN:CB	2:B:800:LEU:HD11	2.30	0.61
1:A:394:MET:CE	1:A:765:PRO:CG	2.77	0.61
2:B:677:SER:H	6:B:1101:GLU:CB	2.13	0.61
1:C:477:VAL:HG21	1:C:499:MET:CG	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:PHE:CZ	1:C:756:PHE:HB3	2.36	0.61
1:C:631:GLY:O	1:C:635:ALA:CB	2.48	0.61
1:A:204:LEU:CD1	1:A:231:VAL:HA	2.31	0.61
1:A:512:VAL:CA	1:A:758:ILE:HD11	2.30	0.61
1:A:525:ILE:CD1	1:A:527:PHE:CE1	2.84	0.61
1:A:818:VAL:CG1	3:D:558:MET:CE	2.79	0.61
2:B:179:ILE:CB	2:B:195:TYR:OH	2.48	0.61
2:B:94:ASP:O	2:B:120:HIS:HD2	1.82	0.61
1:C:301:ILE:HG21	1:C:317:THR:HG23	1.64	0.61
1:A:26:ILE:HD13	5:A:1001:NAG:H82	1.82	0.61
1:A:204:LEU:HG	1:A:234:SER:OG	2.00	0.61
1:C:133:ILE:HD11	3:D:130:ALA:HB1	1.72	0.61
1:A:102:LEU:CB	1:A:128:TYR:CE1	2.83	0.61
1:A:26:ILE:HA	1:A:59:GLN:CG	2.31	0.61
1:A:511:ILE:O	1:A:758:ILE:HD12	1.98	0.61
2:B:64:LEU:CD1	2:B:81:LEU:CG	2.77	0.61
1:C:226:ASP:O	1:C:229:THR:OG1	2.17	0.61
3:D:543:PHE:CD1	3:D:639:TYR:CE1	2.89	0.61
3:D:605:LEU:HD12	3:D:629:ALA:HB1	1.73	0.61
3:D:37:VAL:CG1	3:D:68:MET:O	2.48	0.61
1:A:150:VAL:HG21	1:A:351:TYR:CD2	2.35	0.61
1:A:532:LYS:O	1:A:755:GLY:HA2	2.00	0.61
2:B:182:THR:HG21	2:B:190:TRP:CH2	2.35	0.61
2:B:559:MET:CG	2:B:563:ILE:CD1	2.78	0.61
1:C:568:VAL:CG1	1:C:608:SER:CB	2.78	0.61
1:A:496:TRP:CH2	1:A:524:TYR:CG	2.88	0.61
1:A:86:GLN:HE21	1:A:306:ARG:CA	2.08	0.61
2:B:753:LEU:CD2	2:B:760:LYS:CB	2.79	0.61
1:C:415:THR:HG22	1:C:416:SER:N	2.16	0.61
1:C:78:VAL:CA	1:C:82:LEU:HB2	2.25	0.61
2:B:559:MET:HG2	2:B:563:ILE:CD1	2.30	0.61
2:B:179:ILE:HG21	2:B:195:TYR:HH	0.64	0.60
2:B:640:PHE:O	2:B:643:GLN:N	2.34	0.60
2:B:775:GLU:O	2:B:778:GLU:N	2.33	0.60
1:C:692:ARG:HD3	1:C:701:TYR:OH	2.01	0.60
1:A:496:TRP:CZ2	1:A:524:TYR:HB3	2.36	0.60
1:A:709:TYR:OH	1:A:724:LEU:HD12	1.97	0.60
2:B:277:ASP:OD2	2:B:354:VAL:CG1	2.47	0.60
2:B:541:PHE:HB3	2:B:545:VAL:HG11	1.82	0.60
1:C:58:ILE:HG21	1:C:296:PHE:CE2	2.37	0.60
1:A:709:TYR:CZ	1:A:724:LEU:CD1	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:TYR:CE2	1:A:752:PHE:CD2	2.89	0.60
1:A:736:PHE:CD1	1:A:794:GLN:OE1	2.54	0.60
2:B:270:SER:O	2:B:356:LEU:O	2.19	0.60
1:C:606:TRP:HZ3	1:C:609:TRP:HE3	1.47	0.60
1:A:117:PRO:HD3	1:A:315:TRP:HZ3	1.66	0.60
2:B:154:MET:HE3	2:B:248:ILE:HG13	1.83	0.60
1:C:194:VAL:O	1:C:195:LEU:CD2	2.47	0.60
1:C:142:PRO:HG3	1:C:349:ALA:HB3	1.83	0.60
1:A:496:TRP:HE1	1:A:504:LEU:HD23	1.66	0.60
2:B:163:SER:CB	2:B:194:ASN:HD22	2.15	0.60
2:B:516:PHE:CE2	2:B:749:TYR:HB2	2.37	0.60
1:A:664:GLY:HA3	1:A:670:LEU:HD13	1.83	0.60
1:A:94:HIS:HB3	1:A:95:PRO:HD2	1.84	0.60
2:B:164:VAL:HG21	2:B:179:ILE:HD12	1.83	0.60
3:D:225:LEU:HD12	3:D:251:TRP:HZ3	1.66	0.60
3:D:77:ILE:HD11	3:D:106:ILE:HD11	1.83	0.60
2:B:135:THR:OG1	2:B:137:PHE:CD2	2.49	0.60
2:B:502:ILE:HG12	2:B:512:PHE:CE2	2.36	0.60
2:B:541:PHE:HB3	2:B:545:VAL:CG1	2.31	0.60
2:B:164:VAL:HG21	2:B:179:ILE:HD11	1.83	0.60
1:A:292:ILE:HG13	1:A:321:PHE:CZ	2.37	0.59
2:B:151:LEU:CD2	2:B:182:THR:CG2	2.75	0.59
2:B:193:GLN:HG3	2:B:214:ILE:HG23	1.83	0.59
2:B:164:VAL:HG22	2:B:220:LEU:CD1	2.25	0.59
2:B:584:GLY:O	2:B:587:PHE:CD1	2.46	0.59
2:B:678:THR:O	2:B:679:GLU:C	2.38	0.59
1:C:73:GLN:O	1:C:77:SER:HB2	2.02	0.59
1:A:247:TRP:HB3	1:A:266:ILE:CG1	2.31	0.59
2:B:125:MET:CE	2:B:251:SER:O	2.49	0.59
1:A:283:ASP:OD2	1:A:334:VAL:N	2.35	0.59
2:B:178:PHE:O	2:B:181:THR:N	2.34	0.59
1:C:34:SER:HA	1:C:96:PRO:HD3	1.85	0.59
1:A:449:VAL:HG12	1:A:451:GLN:HG2	1.84	0.59
1:A:570:VAL:O	1:A:573:VAL:HG23	2.02	0.59
2:B:194:ASN:CG	2:B:214:ILE:CG1	2.56	0.59
2:B:25:PHE:CB	2:B:26:PRO:HD3	2.33	0.59
3:D:430:ARG:O	3:D:472:TYR:CB	2.49	0.59
1:A:205:THR:HG23	1:A:238:LEU:HD13	1.72	0.59
1:A:810:ASN:HB3	3:D:631:PHE:CE1	2.36	0.59
3:D:170:TYR:HE1	3:D:199:HIS:HB3	1.68	0.59
1:A:208:LEU:HD22	1:A:235:ALA:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:PHE:CE1	1:A:774:ILE:CG1	2.86	0.59
2:B:505:GLU:CD	2:B:680:ARG:NH1	2.56	0.59
1:C:627:ALA:O	1:C:630:LEU:CB	2.49	0.59
3:D:543:PHE:CE1	3:D:639:TYR:CE1	2.91	0.59
1:A:500:MET:HE3	1:A:521:ARG:CG	2.32	0.59
1:A:511:ILE:C	1:A:758:ILE:HD11	2.23	0.59
1:C:109:TYR:HD1	3:D:105:GLN:CD	2.04	0.59
1:C:295:LEU:HD22	1:C:321:PHE:CE1	2.29	0.59
1:A:818:VAL:CG1	3:D:558:MET:HE3	2.32	0.59
3:D:663:LYS:O	3:D:666:ARG:O	2.20	0.59
2:B:49:TRP:O	2:B:53:MET:CB	2.42	0.59
2:B:548:MET:HA	2:B:551:VAL:HB	1.84	0.59
3:D:301:THR:HB	3:D:333:TYR:CE2	2.38	0.59
3:D:603:TRP:HA	3:D:603:TRP:HE3	1.68	0.59
1:A:122:THR:CG2	1:A:277:GLU:CD	2.71	0.59
1:A:575:LEU:HD13	1:A:622:PRO:CB	2.22	0.59
2:B:166:THR:O	2:B:197:THR:OG1	2.16	0.59
2:B:178:PHE:O	2:B:179:ILE:C	2.37	0.59
2:B:247:TRP:CB	2:B:268:LEU:HD23	2.33	0.59
1:A:574:MET:CE	2:B:819:SER:HG	2.15	0.59
1:A:577:LEU:O	2:B:823:PHE:CE1	2.56	0.59
1:C:264:ASP:OD1	1:C:265:GLY:N	2.35	0.59
3:D:411:ILE:HD12	3:D:789:TRP:HZ3	1.64	0.59
1:A:122:THR:HG23	1:A:277:GLU:CD	2.23	0.59
1:A:205:THR:HA	1:A:208:LEU:HD13	1.85	0.59
1:A:419:THR:O	1:A:452:CYS:SG	2.60	0.59
2:B:777:GLU:N	2:B:777:GLU:OE1	2.34	0.59
1:C:149:LEU:O	1:C:153:GLU:N	2.35	0.59
1:A:124:ARG:HH12	1:A:271:LEU:HB2	1.62	0.58
2:B:182:THR:HG22	2:B:190:TRP:HZ3	1.48	0.58
2:B:541:PHE:HB3	2:B:545:VAL:HG21	1.85	0.58
1:A:621:ALA:H	2:B:594:TRP:HH2	1.48	0.58
2:B:669:ARG:NE	2:B:696:PHE:CD2	2.71	0.58
2:B:521:ILE:HG12	2:B:745:ALA:CB	2.33	0.58
3:D:322:SER:O	3:D:325:TYR:HB3	2.03	0.58
1:A:549:LEU:O	1:A:553:MET:HB2	2.04	0.58
7:B:1102:BMK:C14	1:C:649:LEU:CD1	2.81	0.58
2:B:197:THR:O	2:B:207:THR:HG22	2.02	0.58
2:B:521:ILE:H	2:B:745:ALA:HB3	1.68	0.58
2:B:618:ILE:HG12	1:C:822:ILE:HG22	1.84	0.58
3:D:170:TYR:CE1	3:D:199:HIS:HB3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:HB3	1:A:244:GLY:O	2.02	0.58
3:D:741:LEU:CD1	3:D:741:LEU:H	2.17	0.58
3:D:522:PHE:CE1	3:D:755:TYR:CB	2.86	0.58
1:A:526:GLU:O	1:A:527:PHE:HD1	1.86	0.58
2:B:686:TYR:HB2	2:B:689:MET:HB3	1.86	0.58
2:B:799:GLN:O	2:B:799:GLN:HG2	2.04	0.58
1:A:500:MET:CE	1:A:521:ARG:CB	2.74	0.58
1:A:516:THR:HG23	1:A:754:SER:CB	2.33	0.58
2:B:154:MET:HE1	2:B:218:VAL:HG11	1.85	0.58
2:B:559:MET:O	2:B:563:ILE:CD1	2.51	0.58
2:B:702:GLN:OE1	2:B:702:GLN:N	2.27	0.58
1:C:354:MET:HA	1:C:362:VAL:O	2.03	0.58
1:C:542:LYS:N	1:C:743:ASP:O	2.34	0.58
3:D:565:VAL:O	3:D:569:VAL:CG2	2.51	0.58
1:A:541:LYS:CB	1:A:745:VAL:CG2	2.81	0.58
2:B:541:PHE:HB3	2:B:545:VAL:CG2	2.34	0.58
2:B:621:ILE:CG2	1:C:818:VAL:CG1	2.76	0.58
1:C:654:VAL:C	1:C:656:ARG:H	2.06	0.58
1:A:500:MET:O	1:A:503:LEU:HB3	2.04	0.58
1:A:525:ILE:CD1	1:A:527:PHE:HE1	2.17	0.58
2:B:163:SER:HB2	2:B:194:ASN:HB3	1.85	0.58
2:B:197:THR:O	2:B:198:LEU:CB	2.51	0.58
2:B:264:PHE:CE1	2:B:268:LEU:HD11	2.38	0.58
2:B:49:TRP:CE3	2:B:49:TRP:HA	2.39	0.58
1:C:195:LEU:HB3	1:C:207:LEU:HD21	1.85	0.58
2:B:768:LEU:CB	1:C:519:ASN:CB	2.60	0.58
1:A:709:TYR:CZ	1:A:724:LEU:HD11	2.30	0.58
1:A:516:THR:HG23	1:A:754:SER:OG	2.03	0.58
2:B:120:HIS:ND1	2:B:280:ILE:CD1	2.67	0.58
2:B:49:TRP:HE3	2:B:49:TRP:HA	1.69	0.58
2:B:634:THR:HA	2:B:637:LEU:HB2	1.85	0.58
2:B:775:GLU:HA	2:B:778:GLU:HG2	1.85	0.58
1:C:637:PHE:HE1	1:C:641:ILE:CD1	2.16	0.58
1:A:208:LEU:HB3	1:A:240:MET:CE	2.33	0.58
1:A:122:THR:HG21	1:A:277:GLU:CG	2.33	0.58
1:A:525:ILE:C	1:A:762:LYS:CE	2.71	0.58
2:B:33:ILE:HG23	2:B:64:LEU:O	2.03	0.58
2:B:486:GLY:C	2:B:490:TYR:HD2	2.06	0.58
2:B:458:THR:CG2	2:B:766:ALA:HB1	2.32	0.58
1:A:648:ASN:CG	2:B:800:LEU:HD11	2.24	0.58
1:C:265:GLY:HA3	1:C:381:TRP:C	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:SER:HB2	1:C:96:PRO:CG	2.34	0.58
3:D:77:ILE:HG12	3:D:110:ILE:HD11	1.84	0.58
3:D:526:GLY:O	3:D:726:ALA:N	2.36	0.58
1:A:86:GLN:HE22	1:A:306:ARG:CB	2.05	0.58
1:C:142:PRO:HD2	1:C:349:ALA:CB	2.33	0.58
3:D:502:ALA:H	3:D:758:ALA:HB3	1.69	0.58
1:C:637:PHE:CG	3:D:818:LEU:CD2	2.85	0.58
1:A:157:LEU:HD22	1:A:372:ILE:CD1	2.32	0.57
1:A:124:ARG:HH11	1:A:271:LEU:HB3	1.69	0.57
2:B:196:ILE:HD11	2:B:211:LEU:HG	1.84	0.57
1:C:109:TYR:CD1	3:D:105:GLN:NE2	2.71	0.57
1:A:113:PHE:CE1	2:B:100:ALA:HB2	2.35	0.57
1:C:653:LEU:C	1:C:653:LEU:HD12	2.24	0.57
2:B:504:GLU:OE2	1:C:775:LEU:HB3	2.04	0.57
1:C:809:GLU:O	1:C:812:ALA:HB3	2.04	0.57
1:A:150:VAL:CG2	1:A:351:TYR:HD2	2.17	0.57
1:A:664:GLY:CA	1:A:670:LEU:HD13	2.35	0.57
1:A:671:ARG:O	1:A:673:PRO:HD3	2.03	0.57
2:B:42:GLU:CB	2:B:63:THR:HG22	2.31	0.57
3:D:305:GLU:O	3:D:306:HIS:CD2	2.57	0.57
3:D:512:ARG:HA	3:D:515:VAL:HG22	1.85	0.57
3:D:408:PRO:CG	3:D:790:LEU:HD23	2.34	0.57
1:A:142:PRO:HG3	1:A:349:ALA:HB3	1.85	0.57
1:C:787:ASP:O	1:C:791:VAL:HB	2.03	0.57
1:C:412:ARG:NH1	1:C:454:TYR:OH	2.37	0.57
1:C:609:TRP:O	1:C:610:ARG:C	2.43	0.57
1:C:716:ILE:HD13	1:C:737:GLU:HG3	1.85	0.57
1:A:530:PRO:HB3	1:A:755:GLY:CA	2.32	0.57
2:B:501:THR:OG1	6:B:1101:GLU:N	2.37	0.57
2:B:180:LYS:NZ	2:B:195:TYR:CZ	2.72	0.57
1:C:606:TRP:HA	1:C:606:TRP:CE3	2.39	0.57
3:D:554:MET:HA	3:D:554:MET:HE2	1.87	0.57
2:B:112:THR:O	2:B:113:PHE:HB2	2.04	0.57
1:C:142:PRO:HD3	1:C:346:ARG:O	2.05	0.57
1:A:497:ASN:HA	1:A:501:GLY:HA3	1.85	0.57
2:B:540:PRO:HB2	1:C:804:ALA:HB3	1.85	0.57
5:C:1002:NAG:C8	5:C:1002:NAG:H3	2.12	0.57
3:D:301:THR:HB	3:D:333:TYR:CD1	2.39	0.57
3:D:409:PHE:CE1	3:D:755:TYR:OH	2.50	0.57
1:C:630:LEU:HD23	3:D:825:SER:OG	2.04	0.57
1:A:124:ARG:HG2	1:A:141:VAL:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:548:MET:O	2:B:552:MET:N	2.38	0.57
1:C:449:VAL:CG1	1:C:450:PRO:N	2.68	0.57
1:C:34:SER:HB2	1:C:96:PRO:HD3	1.86	0.57
3:D:253:VAL:HG12	3:D:254:PRO:O	2.05	0.57
2:B:152:ASN:HB3	2:B:375:LEU:CB	2.35	0.57
2:B:523:VAL:CA	2:B:738:ILE:HD11	2.34	0.57
2:B:64:LEU:HD12	2:B:81:LEU:CD2	2.15	0.57
2:B:669:ARG:HD2	2:B:696:PHE:CE2	2.36	0.57
3:D:606:VAL:HA	3:D:628:TRP:CH2	2.40	0.57
5:A:1002:NAG:C8	5:A:1002:NAG:H3	2.15	0.56
5:A:1006:NAG:H3	5:A:1006:NAG:C8	2.15	0.56
1:A:115:ARG:CB	1:A:315:TRP:HB3	2.31	0.56
1:A:541:LYS:O	1:A:743:ASP:O	2.23	0.56
2:B:247:TRP:HB2	2:B:268:LEU:HD23	1.86	0.56
2:B:504:GLU:O	2:B:507:SER:HB2	2.04	0.56
2:B:520:GLY:CA	2:B:743:ILE:HG13	2.27	0.56
1:C:634:TRP:HA	1:C:637:PHE:CD2	2.40	0.56
3:D:409:PHE:CD2	3:D:755:TYR:CE2	2.83	0.56
3:D:500:TYR:HE2	3:D:765:TRP:NE1	2.02	0.56
1:A:811:MET:H	3:D:631:PHE:HE2	1.53	0.56
2:B:354:VAL:HA	2:B:369:LYS:HA	1.86	0.56
2:B:424:CYS:CB	2:B:442:LYS:O	2.52	0.56
2:B:495:MET:HE2	2:B:753:LEU:HD11	1.88	0.56
2:B:552:MET:HE3	2:B:622:TRP:CZ3	2.35	0.56
2:B:736:VAL:CG1	2:B:737:THR:N	2.68	0.56
1:C:631:GLY:O	1:C:635:ALA:HB3	2.06	0.56
1:C:634:TRP:CA	1:C:637:PHE:HD2	2.16	0.56
3:D:606:VAL:HA	3:D:628:TRP:CZ3	2.40	0.56
2:B:130:LYS:CB	2:B:137:PHE:CE2	2.88	0.56
2:B:529:ALA:HB3	2:B:645:ARG:O	2.05	0.56
2:B:541:PHE:CE1	1:C:803:PRO:HB2	2.40	0.56
1:A:540:VAL:N	1:A:745:VAL:O	2.38	0.56
1:A:560:LEU:HB2	2:B:805:MET:CE	2.35	0.56
2:B:485:ILE:HD11	2:B:506:ARG:NE	2.20	0.56
2:B:659:GLN:OE1	2:B:686:TYR:CE2	2.58	0.56
3:D:569:VAL:O	3:D:572:TYR:CB	2.53	0.56
1:A:243:ALA:HB2	1:A:383:GLY:HA3	1.85	0.56
1:A:46:VAL:O	1:A:49:ALA:HB3	2.05	0.56
1:A:531:PHE:CE1	1:A:774:ILE:CB	2.89	0.56
2:B:244:GLY:O	2:B:245:PHE:HD1	1.88	0.56
2:B:765:LEU:HD13	1:C:519:ASN:CG	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:60:UNK:CB	4:G:65:UNK:HA	2.35	0.56
2:B:514:VAL:N	2:B:515:PRO:CD	2.64	0.56
1:C:132:SER:CB	3:D:172:PRO:HB2	2.30	0.56
1:A:815:PHE:HE2	3:D:554:MET:HG2	1.64	0.56
3:D:804:SER:O	3:D:805:GLN:C	2.44	0.56
1:A:621:ALA:HB2	2:B:594:TRP:CZ2	2.41	0.56
1:A:710:GLU:N	1:A:710:GLU:OE1	2.38	0.56
2:B:659:GLN:CD	2:B:686:TYR:OH	2.43	0.56
3:D:525:THR:OG1	3:D:725:ASP:OD1	2.23	0.56
2:B:249:VAL:CG2	2:B:268:LEU:CD2	2.84	0.56
2:B:268:LEU:CD1	2:B:268:LEU:H	2.18	0.56
2:B:640:PHE:CD1	2:B:643:GLN:CB	2.88	0.56
2:B:765:LEU:CD2	1:C:523:GLN:CG	2.75	0.56
3:D:545:GLU:N	3:D:546:PRO:CD	2.67	0.56
3:D:600:TRP:O	3:D:603:TRP:HB2	2.06	0.56
2:B:207:THR:O	2:B:211:LEU:HG	2.06	0.56
1:C:274:GLY:N	1:C:280:HIS:NE2	2.32	0.56
1:C:291:ALA:HB3	1:C:325:LEU:HD13	1.86	0.56
1:C:628:ARG:CZ	1:C:628:ARG:HB2	2.36	0.56
3:D:627:VAL:O	3:D:630:PHE:HD2	1.89	0.56
1:A:32:VAL:HG22	1:A:65:VAL:HG12	1.87	0.56
1:A:690:TYR:CE2	1:A:752:PHE:CZ	2.94	0.56
2:B:163:SER:O	2:B:220:LEU:N	2.36	0.56
2:B:271:VAL:HG21	2:B:355:VAL:HA	1.86	0.56
2:B:640:PHE:HD1	2:B:643:GLN:CB	2.18	0.56
1:A:331:PRO:O	1:A:337:ARG:HA	2.06	0.56
1:C:477:VAL:HG11	1:C:499:MET:HB2	1.88	0.56
3:D:387:LEU:C	3:D:389:PRO:HD2	2.24	0.56
1:A:34:SER:HA	1:A:96:PRO:CD	2.36	0.55
2:B:163:SER:CB	2:B:194:ASN:HB3	2.35	0.55
2:B:355:VAL:N	2:B:368:GLY:O	2.30	0.55
1:C:291:ALA:HB2	1:C:325:LEU:CD1	2.36	0.55
1:A:365:GLY:HA2	1:A:375:ASN:HB2	1.87	0.55
1:A:611:VAL:CG1	1:A:635:ALA:HA	2.36	0.55
1:C:575:LEU:HA	1:C:630:LEU:CD1	2.35	0.55
3:D:409:PHE:HZ	3:D:727:ALA:HB1	1.71	0.55
1:C:560:LEU:HD23	1:C:560:LEU:N	2.21	0.55
3:D:563:SER:OG	3:D:594:THR:OG1	2.23	0.55
1:A:651:ALA:HA	1:A:654:VAL:HG23	1.88	0.55
1:C:782:PHE:CZ	1:C:786:LEU:HD11	2.42	0.55
3:D:507:THR:HG23	3:D:753:THR:HG21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:522:PHE:CZ	3:D:755:TYR:CB	2.89	0.55
1:A:249:VAL:HG22	1:A:267:ILE:O	2.06	0.55
2:B:197:THR:HG23	2:B:198:LEU:HG	1.88	0.55
2:B:541:PHE:CD1	2:B:541:PHE:N	2.75	0.55
2:B:496:ALA:H	2:B:752:ALA:HB3	1.71	0.55
2:B:761:ARG:CB	2:B:762:PRO:HD3	2.37	0.55
1:C:329:LYS:HD2	1:C:329:LYS:O	2.07	0.55
2:B:765:LEU:HD12	1:C:523:GLN:NE2	2.19	0.55
3:D:525:THR:HG22	3:D:754:GLY:HA2	1.89	0.55
3:D:540:PRO:HD2	3:D:810:ASN:CB	2.36	0.55
1:A:292:ILE:HG13	1:A:321:PHE:CE1	2.42	0.55
2:B:473:HIS:CD2	6:B:1101:GLU:OXT	2.60	0.55
2:B:120:HIS:NE2	2:B:280:ILE:HD11	2.18	0.55
2:B:559:MET:HG2	2:B:563:ILE:HD12	1.89	0.55
2:B:659:GLN:OE1	2:B:686:TYR:HE2	1.90	0.55
1:C:425:THR:HG23	1:C:431:ILE:CG1	2.35	0.55
1:A:606:TRP:CZ2	3:D:623:ILE:HD11	2.41	0.55
2:B:538:LEU:CB	2:B:541:PHE:CD1	2.90	0.55
2:B:659:GLN:NE2	2:B:686:TYR:HH	2.02	0.55
2:B:664:TYR:C	2:B:666:PRO:HD2	2.27	0.55
3:D:325:TYR:HD1	3:D:326:GLU:N	2.03	0.55
2:B:125:MET:HE1	2:B:251:SER:HB2	1.88	0.55
2:B:520:GLY:CA	2:B:743:ILE:HG21	2.36	0.55
1:A:205:THR:HG21	1:A:238:LEU:HD11	1.70	0.55
1:A:653:LEU:O	1:A:654:VAL:C	2.44	0.55
2:B:197:THR:O	2:B:198:LEU:CD1	2.54	0.55
2:B:205:ALA:HA	2:B:208:LEU:HB2	1.89	0.55
2:B:164:VAL:HA	2:B:220:LEU:HB2	1.89	0.55
1:C:164:ILE:HG12	1:C:193:LYS:CB	2.37	0.55
3:D:408:PRO:HG3	3:D:790:LEU:HD23	1.88	0.55
1:A:133:ILE:CG2	2:B:128:ALA:HB1	2.36	0.55
2:B:673:VAL:HG21	2:B:718:TYR:CZ	2.41	0.55
1:A:560:LEU:HB2	2:B:805:MET:HE2	1.89	0.54
1:A:530:PRO:HB2	1:A:755:GLY:HA3	1.77	0.54
2:B:120:HIS:ND1	2:B:280:ILE:CG1	2.70	0.54
1:C:34:SER:HB2	1:C:96:PRO:CD	2.38	0.54
3:D:543:PHE:CE1	3:D:639:TYR:HE1	2.25	0.54
3:D:507:THR:CG2	3:D:753:THR:HG21	2.37	0.54
1:A:682:VAL:HG23	1:A:729:TRP:CE3	2.42	0.54
1:C:73:GLN:O	1:C:77:SER:N	2.37	0.54
3:D:744:ILE:O	3:D:747:GLY:N	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HG	1:A:249:VAL:HG12	1.88	0.54
2:B:162:PHE:HD1	2:B:216:SER:N	2.04	0.54
2:B:410:ILE:HG23	2:B:441:LYS:C	2.27	0.54
2:B:526:SER:CB	2:B:734:LYS:O	2.55	0.54
1:A:794:GLN:O	1:A:795:GLU:HG2	2.07	0.54
2:B:247:TRP:HB2	2:B:268:LEU:CD2	2.37	0.54
2:B:520:GLY:HA3	2:B:743:ILE:HB	1.89	0.54
1:C:53:HIS:CG	1:C:293:HIS:CE1	2.90	0.54
2:B:765:LEU:CD1	1:C:519:ASN:OD1	2.55	0.54
3:D:522:PHE:CZ	3:D:755:TYR:HB2	2.43	0.54
1:A:500:MET:HE3	1:A:521:ARG:HD3	1.90	0.54
1:A:113:PHE:CZ	2:B:100:ALA:HB3	2.39	0.54
1:A:534:GLN:CB	1:A:732:ALA:HB2	2.35	0.54
2:B:192:VAL:HG11	2:B:195:TYR:CE2	2.42	0.54
2:B:351:PRO:HG3	2:B:370:TRP:HZ3	1.67	0.54
2:B:46:ARG:HH21	2:B:63:THR:HB	1.73	0.54
1:C:630:LEU:HD22	1:C:634:TRP:CZ2	2.42	0.54
1:A:535:GLY:O	1:A:731:SER:HB2	2.07	0.54
2:B:531:THR:CB	2:B:640:PHE:CZ	2.91	0.54
2:B:517:VAL:O	2:B:748:GLY:HA2	2.07	0.54
1:A:574:MET:CE	2:B:819:SER:OG	2.55	0.54
2:B:78:VAL:O	2:B:82:MET:HG2	2.07	0.54
1:C:168:SER:HA	1:C:197:PHE:CE1	2.42	0.54
1:A:496:TRP:NE1	1:A:504:LEU:HD23	2.23	0.54
2:B:278:TYR:HB2	2:B:283:ARG:NH1	2.22	0.54
1:C:575:LEU:N	1:C:634:TRP:CH2	2.74	0.54
3:D:559:LEU:O	3:D:563:SER:N	2.40	0.54
1:A:365:GLY:HA2	1:A:375:ASN:H	1.72	0.54
2:B:136:PHE:O	2:B:137:PHE:CD1	2.61	0.54
5:C:1002:NAG:C3	5:C:1002:NAG:H83	2.20	0.54
1:C:637:PHE:CE1	1:C:641:ILE:HD11	2.42	0.54
3:D:331:LYS:O	3:D:334:LEU:HB3	2.08	0.54
5:A:1004:NAG:O7	5:A:1004:NAG:O3	2.25	0.53
1:A:782:PHE:CE2	1:A:786:LEU:CD1	2.91	0.53
2:B:770:PHE:N	2:B:770:PHE:CD1	2.72	0.53
1:C:32:VAL:HG22	1:C:65:VAL:HG12	1.89	0.53
1:A:511:ILE:O	1:A:758:ILE:CG1	2.55	0.53
2:B:758:ARG:O	2:B:759:TRP:C	2.42	0.53
5:C:1006:NAG:C3	5:C:1006:NAG:H83	2.18	0.53
1:C:534:GLN:NE2	1:C:730:ASP:OD1	2.31	0.53
2:B:636:ASN:ND2	1:C:803:PRO:HB3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:HB2	1:A:315:TRP:CB	2.33	0.53
1:A:287:VAL:HG22	1:A:330:TYR:HB3	1.90	0.53
2:B:759:TRP:C	2:B:762:PRO:HD2	2.29	0.53
1:C:295:LEU:O	1:C:298:MET:HB2	2.09	0.53
1:C:669:ARG:O	1:C:672:ASN:O	2.26	0.53
1:C:770:VAL:O	1:C:774:ILE:HG12	2.08	0.53
2:B:244:GLY:O	2:B:245:PHE:CD1	2.61	0.53
2:B:29:ASN:CB	2:B:87:ILE:HA	2.38	0.53
2:B:541:PHE:HZ	2:B:636:ASN:HB2	1.73	0.53
2:B:758:ARG:O	2:B:762:PRO:CD	2.55	0.53
1:C:342:GLU:CD	3:D:170:TYR:HE2	2.07	0.53
1:C:697:LEU:O	1:C:698:SER:C	2.46	0.53
3:D:565:VAL:O	3:D:569:VAL:CB	2.56	0.53
2:B:162:PHE:HD2	2:B:219:ILE:HG12	1.67	0.53
2:B:120:HIS:NE2	2:B:280:ILE:HD13	2.24	0.53
2:B:765:LEU:HD21	1:C:523:GLN:HA	1.89	0.53
1:C:283:ASP:CG	1:C:335:THR:HG22	2.29	0.53
1:C:576:TYR:CE1	1:C:600:THR:HB	2.44	0.53
3:D:301:THR:HB	3:D:333:TYR:CZ	2.44	0.53
1:A:259:LEU:C	1:A:262:ALA:HB3	2.29	0.53
1:A:440:ASP:CB	1:A:449:VAL:CG2	2.87	0.53
2:B:249:VAL:HG21	2:B:268:LEU:CD2	2.37	0.53
1:C:630:LEU:CD2	3:D:825:SER:OG	2.57	0.53
3:D:200:LEU:HD12	3:D:211:ILE:CB	2.39	0.53
3:D:332:ARG:C	3:D:335:ILE:CG1	2.76	0.53
3:D:543:PHE:N	3:D:543:PHE:CD1	2.73	0.53
1:A:124:ARG:CG	1:A:141:VAL:HB	2.38	0.53
1:A:54:PHE:N	1:A:54:PHE:CD1	2.73	0.53
2:B:521:ILE:CD1	2:B:653:LEU:HD11	2.37	0.53
3:D:554:MET:HA	3:D:554:MET:CE	2.39	0.53
1:A:150:VAL:CG2	1:A:351:TYR:CD2	2.92	0.53
1:A:479:ASP:CB	1:A:498:GLY:HA2	2.39	0.53
1:A:525:ILE:C	1:A:762:LYS:HZ3	2.09	0.53
1:A:76:LEU:HD23	1:A:76:LEU:C	2.29	0.53
1:C:292:ILE:HG12	1:C:321:PHE:CZ	2.43	0.53
1:A:775:LEU:CD2	3:D:510:GLU:HA	2.38	0.53
1:A:803:PRO:HG2	3:D:542:ALA:O	2.09	0.53
1:C:673:PRO:HG2	1:C:703:HIS:CB	2.19	0.53
1:C:745:VAL:HG12	1:C:746:THR:N	2.24	0.53
1:A:401:VAL:CG2	1:A:477:VAL:HB	2.38	0.53
2:B:759:TRP:N	2:B:759:TRP:CD1	2.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:VAL:HG11	1:C:110:THR:HG22	1.90	0.53
3:D:77:ILE:CD1	3:D:106:ILE:HD11	2.38	0.53
3:D:284:LEU:N	3:D:285:PRO:HD3	2.22	0.53
3:D:500:TYR:OH	3:D:764:GLY:HA2	2.09	0.53
1:A:510:MET:HG3	1:A:760:MET:SD	2.49	0.52
2:B:541:PHE:HZ	1:C:803:PRO:HB3	1.66	0.52
1:A:220:ILE:HG12	1:A:248:LEU:HD12	1.91	0.52
1:A:678:ILE:CG2	1:A:724:LEU:CD2	2.84	0.52
2:B:219:ILE:N	2:B:246:VAL:O	2.39	0.52
2:B:522:SER:HB3	2:B:743:ILE:CG2	2.35	0.52
3:D:734:GLY:O	3:D:793:ILE:CA	2.57	0.52
1:A:32:VAL:HA	1:A:65:VAL:HG12	1.91	0.52
2:B:634:THR:CG2	7:B:1102:BMK:C15	2.87	0.52
2:B:410:ILE:HG22	2:B:443:CYS:SG	2.49	0.52
1:C:365:GLY:HA2	1:C:375:ASN:H	1.75	0.52
3:D:562:VAL:CA	3:D:565:VAL:CG2	2.87	0.52
1:A:111:ALA:O	1:A:114:TYR:N	2.41	0.52
2:B:120:HIS:CG	2:B:280:ILE:HD13	2.44	0.52
2:B:284:VAL:O	2:B:288:LEU:HG	2.09	0.52
2:B:396:ILE:O	2:B:465:LEU:HD23	2.10	0.52
2:B:636:ASN:ND2	1:C:803:PRO:CG	2.72	0.52
2:B:720:ALA:CB	2:B:743:ILE:HG21	2.33	0.52
1:C:113:PHE:HD1	3:D:102:ALA:CB	2.22	0.52
1:C:478:ALA:CB	1:C:502:GLU:OE2	2.57	0.52
3:D:567:VAL:O	3:D:571:GLU:CB	2.57	0.52
3:D:543:PHE:CD1	3:D:639:TYR:CD1	2.97	0.52
1:A:530:PRO:HA	1:A:756:PHE:C	2.29	0.52
1:A:775:LEU:HD21	3:D:510:GLU:N	2.25	0.52
1:C:109:TYR:CE1	3:D:105:GLN:CD	2.82	0.52
3:D:563:SER:OG	3:D:594:THR:CB	2.57	0.52
3:D:37:VAL:HG23	3:D:95:GLY:O	2.10	0.52
1:A:142:PRO:HG3	1:A:349:ALA:CB	2.40	0.52
1:A:796:CYS:SG	1:A:797:ASP:N	2.82	0.52
2:B:296:SER:O	2:B:300:GLU:HB2	2.10	0.52
2:B:592:ALA:O	2:B:596:LEU:CB	2.58	0.52
2:B:638:ALA:O	2:B:641:MET:CG	2.57	0.52
2:B:516:PHE:CZ	2:B:749:TYR:HB2	2.43	0.52
3:D:301:THR:HB	3:D:333:TYR:CE1	2.45	0.52
1:A:248:LEU:HD23	1:A:267:ILE:HB	1.92	0.52
1:A:63:THR:HG1	5:A:1001:NAG:C6	2.21	0.52
1:A:682:VAL:HG22	1:A:729:TRP:CZ3	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:ASN:ND2	1:C:523:GLN:HE21	2.08	0.52
1:C:295:LEU:HB2	1:C:324:VAL:HG11	1.91	0.52
2:B:768:LEU:CD2	1:C:519:ASN:CA	2.41	0.52
1:C:575:LEU:CA	1:C:634:TRP:CH2	2.78	0.52
2:B:568:SER:C	2:B:570:VAL:N	2.60	0.52
3:D:765:TRP:HB2	3:D:769:VAL:HG21	1.91	0.52
1:A:560:LEU:HB3	2:B:809:PHE:HE2	1.74	0.52
1:A:678:ILE:HG21	1:A:724:LEU:CD2	2.40	0.52
2:B:197:THR:C	2:B:198:LEU:HD12	2.30	0.52
2:B:491:LYS:O	2:B:491:LYS:HD2	2.10	0.52
2:B:495:MET:HE3	2:B:753:LEU:HD11	1.92	0.52
1:C:25:LYS:O	1:C:59:GLN:HB2	2.10	0.52
1:C:326:MET:HA	1:C:340:PHE:HD2	1.75	0.52
1:C:621:ALA:HB1	1:C:622:PRO:HD2	1.91	0.52
3:D:168:THR:HG21	3:D:174:TYR:HB2	1.92	0.52
3:D:224:LEU:HD23	3:D:252:ILE:HB	1.91	0.52
1:A:26:ILE:HG13	1:A:59:GLN:HG2	1.88	0.51
2:B:720:ALA:HB3	2:B:743:ILE:CG2	2.37	0.51
1:C:778:HIS:ND1	1:C:783:MET:HG2	2.24	0.51
3:D:301:THR:CB	3:D:333:TYR:CG	2.93	0.51
1:A:457:CYS:HB3	1:A:512:VAL:HG12	1.92	0.51
2:B:787:ILE:C	2:B:788:CYS:SG	2.88	0.51
1:C:53:HIS:NE2	1:C:293:HIS:CD2	2.57	0.51
1:C:637:PHE:HE1	1:C:641:ILE:HD11	1.74	0.51
2:B:147:ALA:O	2:B:151:LEU:HD13	2.10	0.51
2:B:516:PHE:HD2	2:B:517:VAL:HG23	1.75	0.51
2:B:673:VAL:HG12	2:B:698:GLN:NE2	2.26	0.51
1:C:150:VAL:O	1:C:154:MET:N	2.35	0.51
1:A:124:ARG:NH1	1:A:271:LEU:HB3	2.24	0.51
1:A:283:ASP:CG	1:A:334:VAL:H	2.13	0.51
1:A:500:MET:HE3	1:A:521:ARG:CD	2.40	0.51
2:B:169:PHE:CB	2:B:170:PRO:HD2	2.29	0.51
2:B:485:ILE:CD1	2:B:506:ARG:HE	2.21	0.51
2:B:672:THR:H	2:B:693:MET:HG2	1.75	0.51
3:D:405:GLU:HB3	3:D:412:VAL:HG23	1.91	0.51
1:A:468:MET:HG2	1:A:470:PHE:HD1	1.76	0.51
1:A:496:TRP:NE1	1:A:500:MET:SD	2.83	0.51
2:B:399:LEU:HB2	2:B:484:MET:CE	2.40	0.51
1:C:330:TYR:N	1:C:331:PRO:HD3	2.24	0.51
1:C:478:ALA:N	1:C:502:GLU:OE2	2.34	0.51
1:C:694:GLN:HB2	1:C:697:LEU:CD1	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:VAL:HG13	1:C:88:TYR:CD1	2.45	0.51
1:A:326:MET:HA	1:A:340:PHE:HD2	1.76	0.51
1:A:30:GLY:HA2	1:A:63:THR:O	2.11	0.51
1:A:528:SER:HB2	1:A:758:ILE:HG22	1.92	0.51
2:B:268:LEU:CD1	2:B:268:LEU:N	2.73	0.51
2:B:274:ASP:CB	2:B:276:TRP:CE2	2.94	0.51
2:B:69:THR:CB	2:B:98:GLN:OE1	2.59	0.51
1:C:477:VAL:CB	1:C:499:MET:HG3	2.40	0.51
3:D:565:VAL:O	3:D:569:VAL:N	2.32	0.51
1:C:30:GLY:HA2	1:C:63:THR:O	2.11	0.51
1:C:477:VAL:CG2	1:C:499:MET:CG	2.88	0.51
1:C:531:PHE:C	1:C:531:PHE:CD1	2.84	0.51
1:A:551:SER:CB	1:A:649:LEU:CD1	2.88	0.51
2:B:192:VAL:CB	2:B:195:TYR:HE2	2.24	0.51
2:B:512:PHE:HB3	2:B:751:ILE:H	1.75	0.51
2:B:517:VAL:HG12	2:B:518:GLU:N	2.25	0.51
1:C:481:LYS:HG3	1:C:684:GLN:OE1	2.11	0.51
1:C:75:ALA:O	1:C:78:VAL:N	2.35	0.51
3:D:360:ILE:HG22	3:D:368:TRP:HE3	1.75	0.51
1:A:788:LYS:O	1:A:792:ARG:CB	2.59	0.51
2:B:154:MET:HE3	2:B:248:ILE:CG1	2.40	0.51
1:A:204:LEU:HD12	1:A:231:VAL:HA	1.92	0.51
1:A:477:VAL:HG23	1:A:502:GLU:HG3	1.93	0.51
1:A:32:VAL:HG22	1:A:65:VAL:CG1	2.41	0.51
1:A:535:GLY:O	1:A:731:SER:CB	2.59	0.51
2:B:151:LEU:O	2:B:155:GLU:HG2	2.11	0.51
2:B:643:GLN:C	2:B:645:ARG:H	2.14	0.51
1:C:288:VAL:O	1:C:292:ILE:HG13	2.11	0.51
1:C:634:TRP:C	1:C:637:PHE:HD2	2.14	0.51
1:A:818:VAL:CG1	3:D:558:MET:HE1	2.41	0.51
1:A:811:MET:HB2	3:D:631:PHE:HD2	1.75	0.51
1:A:367:PHE:HD1	1:A:372:ILE:HA	1.76	0.50
2:B:31:ALA:O	2:B:90:VAL:CB	2.59	0.50
2:B:787:ILE:O	2:B:788:CYS:SG	2.69	0.50
1:C:78:VAL:HB	1:C:110:THR:HG21	1.93	0.50
1:A:53:HIS:CD2	1:A:293:HIS:CB	2.94	0.50
1:A:578:LEU:CG	1:A:627:ALA:HB2	2.38	0.50
1:A:775:LEU:HD23	3:D:510:GLU:HA	1.91	0.50
2:B:172:TYR:CD1	2:B:173:ARG:N	2.79	0.50
2:B:753:LEU:CD2	2:B:760:LYS:HG2	2.26	0.50
1:C:67:HIS:CE1	1:C:95:PRO:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLU:O	1:A:280:HIS:N	2.45	0.50
1:A:140:THR:O	1:A:346:ARG:CD	2.59	0.50
1:A:399:LYS:HA	1:A:473:GLU:O	2.11	0.50
2:B:759:TRP:O	2:B:763:ILE:N	2.35	0.50
5:D:1002:NAG:C8	5:D:1002:NAG:H3	2.19	0.50
3:D:73:PRO:O	3:D:77:ILE:HD12	2.12	0.50
1:A:105:THR:CA	1:A:128:TYR:HE2	2.20	0.50
1:A:536:LEU:N	1:A:536:LEU:HD12	2.26	0.50
1:A:606:TRP:NE1	3:D:623:ILE:CG1	2.74	0.50
2:B:124:SER:C	2:B:139:PHE:CB	2.79	0.50
2:B:522:SER:O	2:B:717:ILE:HG23	2.12	0.50
1:C:78:VAL:HG11	1:C:110:THR:HG21	1.93	0.50
1:C:80:GLU:O	1:C:84:SER:HB3	2.12	0.50
3:D:321:GLU:O	3:D:324:VAL:CG1	2.55	0.50
3:D:559:LEU:HD21	3:D:598:ALA:CB	2.35	0.50
2:B:249:VAL:HG23	2:B:268:LEU:HD23	1.94	0.50
2:B:485:ILE:O	2:B:489:VAL:HG23	2.12	0.50
2:B:559:MET:HB2	2:B:618:ILE:HD13	1.93	0.50
1:C:132:SER:CA	3:D:172:PRO:HB3	2.38	0.50
1:A:140:THR:O	1:A:346:ARG:HD3	2.12	0.50
1:A:436:CYS:HA	1:A:474:VAL:O	2.11	0.50
2:B:121:GLY:O	2:B:125:MET:HG2	2.12	0.50
2:B:197:THR:HG23	2:B:198:LEU:CD1	2.42	0.50
2:B:534:PRO:CD	2:B:804:ASN:OD1	2.60	0.50
2:B:660:ARG:N	2:B:661:PRO:HD3	2.25	0.50
1:C:481:LYS:O	1:C:499:MET:HB2	2.12	0.50
1:A:357:GLN:HG3	1:A:380:ILE:HG21	1.94	0.50
3:D:494:VAL:HA	3:D:499:ALA:O	2.12	0.50
3:D:562:VAL:O	3:D:565:VAL:HG23	2.11	0.50
1:A:211:ALA:HB3	1:A:240:MET:HE1	1.93	0.50
1:A:67:HIS:ND1	1:A:67:HIS:O	2.45	0.50
2:B:397:VAL:HG23	2:B:467:LEU:HA	1.94	0.50
1:C:77:SER:O	1:C:81:ASP:HB3	2.12	0.50
3:D:111:SER:HG	3:D:137:MET:H	1.60	0.50
1:A:133:ILE:HG22	2:B:128:ALA:HB1	1.94	0.50
2:B:204:ASP:O	2:B:207:THR:OG1	2.28	0.50
2:B:768:LEU:N	2:B:768:LEU:CD1	2.75	0.50
1:C:634:TRP:N	1:C:634:TRP:CD1	2.79	0.50
1:A:575:LEU:CD1	1:A:622:PRO:CB	2.85	0.49
1:A:526:GLU:N	1:A:762:LYS:HD3	2.27	0.49
2:B:267:GLY:HA2	2:B:358:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:ASN:CB	2:B:363:GLU:O	2.60	0.49
2:B:57:PHE:CG	2:B:292:THR:CG2	2.78	0.49
1:A:292:ILE:CG1	1:A:321:PHE:HE1	2.23	0.49
1:A:496:TRP:CZ2	1:A:524:TYR:CB	2.96	0.49
1:A:510:MET:CG	1:A:760:MET:SD	3.00	0.49
3:D:408:PRO:CG	3:D:790:LEU:CD2	2.90	0.49
1:A:283:ASP:OD2	1:A:335:THR:HG22	2.12	0.49
1:A:609:TRP:CZ3	1:A:612:LEU:CD1	2.93	0.49
1:A:690:TYR:CE2	1:A:752:PHE:CE2	2.99	0.49
2:B:249:VAL:HG21	2:B:268:LEU:HD21	1.94	0.49
1:C:73:GLN:O	1:C:77:SER:CB	2.60	0.49
1:A:267:ILE:N	1:A:267:ILE:HD13	2.27	0.49
1:A:302:THR:O	1:A:315:TRP:NE1	2.39	0.49
1:A:786:LEU:O	1:A:790:TRP:HD1	1.95	0.49
2:B:247:TRP:CB	2:B:268:LEU:CB	2.70	0.49
2:B:512:PHE:O	1:C:529:LYS:CE	2.60	0.49
2:B:724:ASN:OD1	2:B:737:THR:HG21	2.13	0.49
1:A:330:TYR:H	1:A:331:PRO:HD3	1.78	0.49
1:A:58:ILE:HD11	1:A:293:HIS:CD2	2.47	0.49
1:A:530:PRO:CA	1:A:756:PHE:O	2.57	0.49
2:B:31:ALA:O	2:B:90:VAL:HA	2.13	0.49
2:B:659:GLN:CD	2:B:686:TYR:HH	2.16	0.49
1:C:394:MET:SD	1:C:766:TRP:NE1	2.86	0.49
1:C:551:SER:O	1:C:555:PRO:HD2	2.12	0.49
3:D:630:PHE:CD1	3:D:630:PHE:C	2.86	0.49
2:B:204:ASP:OD1	2:B:204:ASP:N	2.44	0.49
2:B:30:ILE:HA	2:B:89:GLY:O	2.13	0.49
3:D:741:LEU:CD1	3:D:741:LEU:N	2.75	0.49
4:F:18:UNK:HA	4:F:77:UNK:C	2.42	0.49
1:A:34:SER:HB2	1:A:96:PRO:HG2	1.70	0.49
1:A:540:VAL:CG2	1:A:541:LYS:N	2.74	0.49
1:A:609:TRP:HA	1:A:609:TRP:CE3	2.48	0.49
2:B:593:VAL:O	2:B:597:TRP:HB2	2.13	0.49
2:B:74:ILE:HG21	2:B:105:LEU:CD2	2.31	0.49
1:C:53:HIS:CE1	1:C:293:HIS:CD2	3.00	0.49
1:C:701:TYR:HA	1:C:704:MET:HE2	1.95	0.49
3:D:505:SER:O	3:D:755:TYR:CE1	2.66	0.49
1:A:103:THR:O	1:A:105:THR:N	2.44	0.49
2:B:235:ALA:HA	2:B:238:LEU:HB2	1.95	0.49
2:B:523:VAL:CG2	2:B:717:ILE:CD1	2.87	0.49
1:C:354:MET:SD	1:C:361:LEU:CB	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:VAL:CG1	1:C:110:THR:HG21	2.42	0.49
1:C:823:VAL:O	1:C:826:ILE:HG13	2.13	0.49
3:D:540:PRO:HD2	3:D:810:ASN:HB2	1.95	0.49
3:D:606:VAL:CB	3:D:628:TRP:CH2	2.92	0.49
2:B:405:VAL:CG1	2:B:406:ILE:N	2.76	0.49
2:B:643:GLN:O	2:B:645:ARG:N	2.37	0.49
2:B:664:TYR:HB3	2:B:666:PRO:HD2	1.95	0.49
3:D:165:SER:OG	3:D:195:GLU:HB3	2.13	0.49
3:D:283:ASP:CA	3:D:285:PRO:HD2	2.42	0.49
1:A:496:TRP:O	1:A:497:ASN:CB	2.60	0.49
1:A:516:THR:HG23	1:A:754:SER:HB3	1.94	0.49
1:A:533:TYR:HA	1:A:754:SER:O	2.13	0.49
2:B:397:VAL:CG2	2:B:467:LEU:HA	2.43	0.49
2:B:402:ALA:N	2:B:403:PRO:CD	2.75	0.49
2:B:634:THR:HG21	7:B:1102:BMK:C15	2.43	0.49
1:C:276:ASN:HB3	1:C:279:ALA:CB	2.41	0.49
1:C:292:ILE:HG12	1:C:321:PHE:HZ	1.78	0.49
1:C:464:LEU:HD22	1:C:468:MET:HE2	1.95	0.49
1:A:147:GLN:NE2	1:A:250:GLY:HA2	2.28	0.48
1:A:531:PHE:CE1	1:A:774:ILE:HG12	2.36	0.48
1:C:50:ASN:O	1:C:55:THR:OG1	2.31	0.48
3:D:540:PRO:CD	3:D:810:ASN:HB2	2.42	0.48
1:A:103:THR:N	1:A:104:PRO:CD	2.76	0.48
1:A:221:LEU:CD1	1:A:253:GLU:HG2	2.44	0.48
1:A:540:VAL:O	1:A:745:VAL:O	2.31	0.48
1:C:290:GLN:OE1	1:C:330:TYR:HB2	2.13	0.48
1:C:575:LEU:HB3	1:C:634:TRP:HZ3	1.77	0.48
1:C:75:ALA:O	1:C:78:VAL:HB	2.12	0.48
3:D:636:LEU:HD12	3:D:639:TYR:HD2	1.78	0.48
2:B:29:ASN:O	2:B:88:HIS:N	2.31	0.48
1:C:128:TYR:HB2	1:C:139:ARG:NH2	2.29	0.48
1:C:673:PRO:HG3	1:C:679:TYR:OH	2.12	0.48
1:C:792:ARG:O	1:C:793:TYR:C	2.48	0.48
3:D:325:TYR:CD1	3:D:325:TYR:C	2.85	0.48
1:A:123:THR:O	1:A:139:ARG:CD	2.60	0.48
2:B:179:ILE:HG22	2:B:195:TYR:OH	1.98	0.48
2:B:425:ARG:O	2:B:466:TYR:HA	2.13	0.48
2:B:534:PRO:CG	2:B:804:ASN:OD1	2.61	0.48
5:A:1006:NAG:C3	5:A:1006:NAG:H83	2.18	0.48
1:A:794:GLN:O	1:A:795:GLU:CG	2.61	0.48
1:A:80:GLU:HG2	1:A:81:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:PHE:CE2	2:B:224:SER:OG	2.44	0.48
2:B:192:VAL:CG2	2:B:195:TYR:HE2	2.11	0.48
2:B:541:PHE:HE1	1:C:803:PRO:CB	2.24	0.48
2:B:639:ALA:O	2:B:642:ILE:HB	2.14	0.48
1:C:168:SER:CA	1:C:197:PHE:CE1	2.96	0.48
1:C:481:LYS:HB2	1:C:498:GLY:CA	2.37	0.48
3:D:361:LEU:HD23	3:D:362:LEU:N	2.28	0.48
1:A:221:LEU:HD11	1:A:253:GLU:HG2	1.95	0.48
1:A:552:PHE:CD1	1:A:552:PHE:C	2.86	0.48
2:B:194:ASN:ND2	2:B:211:LEU:CD2	2.69	0.48
3:D:34:VAL:HG13	3:D:93:VAL:HB	1.95	0.48
1:A:500:MET:CE	1:A:521:ARG:CG	2.92	0.48
1:A:496:TRP:HE1	1:A:504:LEU:CD2	2.27	0.48
2:B:256:ASN:OD1	2:B:256:ASN:N	2.40	0.48
2:B:401:GLU:O	2:B:406:ILE:HD11	2.13	0.48
2:B:539:GLU:N	2:B:540:PRO:HD2	2.29	0.48
2:B:683:ARG:HD3	2:B:690:HIS:CE1	2.49	0.48
1:C:455:GLY:HA2	1:C:790:TRP:CH2	2.48	0.48
1:C:696:GLU:H	1:C:696:GLU:CD	2.16	0.48
1:A:602:SER:O	1:A:606:TRP:CE3	2.67	0.48
2:B:621:ILE:HD13	2:B:621:ILE:HA	1.65	0.48
1:C:229:THR:HG22	1:C:258:ALA:HA	1.95	0.48
3:D:410:VAL:HG22	3:D:454:CYS:HB2	1.95	0.48
3:D:606:VAL:CA	3:D:628:TRP:CH2	2.96	0.48
1:A:539:LEU:HG	1:A:539:LEU:O	2.13	0.48
2:B:801:ASP:HB3	2:B:804:ASN:HB3	1.95	0.48
1:C:301:ILE:HG23	1:C:317:THR:OG1	2.12	0.48
1:C:26:ILE:CG1	1:C:61:ASN:HB2	2.44	0.48
3:D:606:VAL:N	3:D:628:TRP:HZ3	2.12	0.48
3:D:834:LEU:O	3:D:835:PHE:C	2.52	0.48
1:A:146:HIS:CE1	1:A:345:ASP:HB2	2.48	0.48
1:A:277:GLU:O	1:A:278:SER:C	2.50	0.48
1:A:34:SER:HB2	1:A:96:PRO:HG3	0.49	0.48
2:B:119:ILE:CB	2:B:283:ARG:HB3	2.44	0.48
2:B:484:MET:O	2:B:488:VAL:HG23	2.14	0.48
2:B:458:THR:HG21	2:B:770:PHE:CZ	2.49	0.48
2:B:775:GLU:HA	2:B:778:GLU:CG	2.44	0.48
3:D:202:MET:HG2	3:D:202:MET:O	2.13	0.48
3:D:408:PRO:HG2	3:D:790:LEU:CD2	2.44	0.48
1:A:150:VAL:HG22	1:A:367:PHE:CD2	2.49	0.47
2:B:243:TYR:HD1	2:B:243:TYR:H	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:542:SER:HA	2:B:546:TRP:HB2	1.96	0.47
1:A:648:ASN:ND2	2:B:800:LEU:HD11	2.29	0.47
1:C:535:GLY:O	1:C:731:SER:OG	2.31	0.47
3:D:807:ASP:O	3:D:808:ILE:C	2.52	0.47
1:A:500:MET:HE3	1:A:521:ARG:HG2	1.96	0.47
1:A:519:ASN:HA	1:A:522:ALA:HB3	1.96	0.47
2:B:719:ASP:OD2	6:B:1101:GLU:N	2.47	0.47
2:B:125:MET:HE1	2:B:251:SER:C	2.34	0.47
2:B:636:ASN:ND2	1:C:803:PRO:HG2	2.29	0.47
3:D:559:LEU:C	3:D:559:LEU:HD23	2.33	0.47
3:D:562:VAL:CA	3:D:565:VAL:HG23	2.42	0.47
3:D:600:TRP:HA	3:D:603:TRP:HB2	1.96	0.47
4:F:164:UNK:HA	4:F:176:UNK:HA	1.96	0.47
1:A:394:MET:HE1	1:A:765:PRO:CG	2.45	0.47
2:B:163:SER:O	2:B:220:LEU:HB2	2.13	0.47
2:B:775:GLU:O	2:B:776:MET:C	2.50	0.47
1:C:731:SER:O	1:C:735:GLU:HG2	2.14	0.47
3:D:565:VAL:O	3:D:569:VAL:HB	2.14	0.47
1:A:202:LYS:O	1:A:204:LEU:CD2	2.62	0.47
2:B:680:ARG:HG3	2:B:683:ARG:HH21	1.79	0.47
2:B:758:ARG:C	2:B:760:LYS:N	2.66	0.47
1:C:291:ALA:CB	1:C:325:LEU:HD12	2.36	0.47
1:C:79:CYS:SG	3:D:74:LYS:CB	3.03	0.47
3:D:570:PHE:O	3:D:574:SER:N	2.32	0.47
1:A:538:ILE:HG22	1:A:540:VAL:HG12	1.95	0.47
1:A:70:ASN:HA	2:B:314:GLY:O	2.15	0.47
2:B:541:PHE:HE1	1:C:803:PRO:HB2	1.77	0.47
1:A:286:ALA:CB	1:A:330:TYR:CZ	2.86	0.47
1:A:426:ILE:HD12	1:A:426:ILE:C	2.35	0.47
1:A:681:THR:HG22	1:A:704:MET:SD	2.55	0.47
2:B:151:LEU:HA	2:B:154:MET:HB2	1.95	0.47
2:B:172:TYR:CG	2:B:173:ARG:N	2.82	0.47
2:B:197:THR:O	2:B:207:THR:HG21	2.15	0.47
2:B:621:ILE:HG21	1:C:818:VAL:CG1	2.27	0.47
2:B:640:PHE:O	2:B:641:MET:C	2.53	0.47
1:C:667:ASP:CG	1:C:668:PRO:HD2	2.34	0.47
1:C:83:ILE:HD13	1:C:114:TYR:CE2	2.49	0.47
3:D:507:THR:HG22	3:D:508:ILE:H	1.79	0.47
3:D:53:ASP:O	3:D:54:PHE:C	2.52	0.47
1:C:628:ARG:HD2	3:D:596:GLY:HA3	1.96	0.47
3:D:543:PHE:HE1	3:D:643:LEU:HD11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1006:NAG:C1	5:C:1006:NAG:C8	2.92	0.47
1:C:483:GLY:HA2	1:C:497:ASN:O	2.15	0.47
1:A:220:ILE:HG12	1:A:248:LEU:HB2	1.97	0.47
1:A:150:VAL:HG22	1:A:367:PHE:CE2	2.50	0.47
2:B:194:ASN:ND2	2:B:211:LEU:HD23	2.18	0.47
2:B:520:GLY:CA	2:B:743:ILE:CB	2.93	0.47
2:B:532:VAL:O	2:B:533:SER:HB2	2.15	0.47
1:C:103:THR:CB	1:C:104:PRO:HD3	2.44	0.47
1:C:117:PRO:HG2	1:C:321:PHE:HD2	1.79	0.47
3:D:177:PHE:O	3:D:181:VAL:HG23	2.14	0.47
3:D:399:LEU:O	3:D:401:ILE:HG13	2.13	0.47
3:D:409:PHE:CZ	3:D:727:ALA:HB1	2.49	0.47
3:D:58:PRO:HG2	3:D:303:LEU:HD12	1.86	0.47
3:D:670:PHE:CG	3:D:672:PRO:HD2	2.50	0.47
1:A:379:ILE:HG21	1:A:381:TRP:CE2	2.50	0.47
2:B:31:ALA:CB	2:B:90:VAL:HG12	2.40	0.47
2:B:370:TRP:CD1	2:B:375:LEU:HA	2.50	0.47
1:A:292:ILE:O	1:A:295:LEU:HB3	2.14	0.47
1:A:113:PHE:CE2	1:A:312:THR:HA	2.50	0.47
2:B:677:SER:OG	6:B:1101:GLU:OE2	2.30	0.47
2:B:50:THR:O	2:B:54:SER:HB2	2.14	0.47
1:C:503:LEU:CD1	1:C:508:ALA:O	2.59	0.47
1:A:291:ALA:HA	1:A:324:VAL:HG22	1.96	0.47
1:A:517:ILE:CD1	1:A:530:PRO:HB3	2.45	0.47
2:B:249:VAL:HB	2:B:270:SER:HA	1.97	0.47
1:C:77:SER:O	1:C:81:ASP:CB	2.63	0.47
3:D:505:SER:HA	3:D:755:TYR:CE1	2.50	0.47
1:A:736:PHE:CE1	1:A:794:GLN:CG	2.98	0.46
1:A:811:MET:HB2	3:D:631:PHE:CE2	2.49	0.46
1:A:93:SER:HB2	1:A:277:GLU:OE1	2.14	0.46
2:B:634:THR:HG23	7:B:1102:BMK:C15	2.45	0.46
2:B:657:LYS:O	2:B:668:PHE:HE1	1.98	0.46
2:B:680:ARG:O	2:B:684:ASN:ND2	2.44	0.46
2:B:775:GLU:HG2	2:B:776:MET:HE3	1.98	0.46
1:C:576:TYR:O	1:C:577:LEU:C	2.53	0.46
1:A:287:VAL:CG2	1:A:330:TYR:CD2	2.92	0.46
1:A:621:ALA:CB	1:A:622:PRO:HD3	2.38	0.46
2:B:448:CYS:SG	2:B:497:VAL:CG1	3.03	0.46
1:C:94:HIS:N	1:C:122:THR:OG1	2.33	0.46
1:C:201:THR:CB	1:C:204:LEU:HD21	2.45	0.46
3:D:627:VAL:HG13	3:D:630:PHE:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASP:OD1	1:A:130:ASP:C	2.48	0.46
1:A:146:HIS:HE1	1:A:345:ASP:HB2	1.81	0.46
1:A:408:PHE:CD2	1:A:514:PRO:HB3	2.50	0.46
1:A:496:TRP:HZ2	1:A:524:TYR:HB3	1.79	0.46
2:B:588:THR:O	2:B:592:ALA:CB	2.63	0.46
2:B:693:MET:C	2:B:693:MET:SD	2.94	0.46
2:B:31:ALA:H	2:B:90:VAL:HG12	1.79	0.46
1:C:184:LEU:CB	1:C:189:SER:HA	2.46	0.46
3:D:432:GLN:HA	3:D:445:TYR:HA	1.97	0.46
4:G:21:UNK:HA	4:G:79:UNK:O	2.16	0.46
1:A:53:HIS:CD2	1:A:293:HIS:CD2	3.03	0.46
1:A:551:SER:O	1:A:645:TYR:HE1	1.98	0.46
1:A:793:TYR:HB3	1:A:794:GLN:NE2	2.31	0.46
1:A:830:PHE:O	1:A:834:ALA:N	2.38	0.46
2:B:32:VAL:HG13	2:B:91:VAL:CG2	2.43	0.46
2:B:682:ILE:HG22	2:B:690:HIS:HB2	1.97	0.46
2:B:519:THR:CG2	2:B:721:ALA:HB3	2.41	0.46
2:B:31:ALA:O	2:B:90:VAL:HB	2.13	0.46
1:C:123:THR:O	1:C:123:THR:OG1	2.33	0.46
1:C:92:VAL:HG11	1:C:104:PRO:HB3	1.97	0.46
1:A:485:GLN:HA	1:A:496:TRP:HA	1.97	0.46
2:B:768:LEU:CB	1:C:519:ASN:CA	2.93	0.46
3:D:148:GLN:O	3:D:152:MET:HG3	2.15	0.46
1:A:105:THR:HG23	2:B:107:PHE:HE1	1.81	0.46
1:A:46:VAL:HG21	1:A:62:ALA:HB2	1.98	0.46
1:A:80:GLU:O	1:A:84:SER:OG	2.31	0.46
2:B:164:VAL:HG23	2:B:220:LEU:HD12	0.60	0.46
2:B:405:VAL:HA	2:B:445:LYS:O	2.16	0.46
2:B:491:LYS:HD3	2:B:491:LYS:HA	1.58	0.46
2:B:512:PHE:CD2	2:B:750:GLY:HA3	2.50	0.46
1:C:30:GLY:O	1:C:90:ILE:HA	2.15	0.46
1:A:204:LEU:HD11	1:A:231:VAL:HA	1.98	0.46
1:A:736:PHE:CE1	1:A:794:GLN:HG2	2.50	0.46
2:B:473:HIS:CG	6:B:1101:GLU:OXT	2.68	0.46
2:B:182:THR:HG23	2:B:190:TRP:HZ3	1.75	0.46
2:B:201:SER:OG	2:B:202:TYR:CD1	2.64	0.46
2:B:411:ASP:C	2:B:411:ASP:OD1	2.50	0.46
2:B:495:MET:HE2	2:B:753:LEU:CD1	2.46	0.46
1:C:574:MET:HG3	3:D:822:MET:SD	2.56	0.46
3:D:639:TYR:CD1	3:D:639:TYR:C	2.88	0.46
3:D:657:SER:O	3:D:744:ILE:HD11	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:VAL:HG22	1:A:541:LYS:N	2.30	0.46
1:A:30:GLY:O	1:A:90:ILE:HA	2.15	0.46
2:B:163:SER:O	2:B:220:LEU:CB	2.64	0.46
3:D:561:ILE:O	3:D:565:VAL:CG2	2.38	0.46
3:D:630:PHE:CG	3:D:631:PHE:N	2.83	0.46
5:A:1002:NAG:H83	5:A:1002:NAG:C3	2.20	0.46
1:A:517:ILE:HD11	1:A:530:PRO:HB3	1.98	0.46
2:B:264:PHE:HE1	2:B:268:LEU:HD21	1.81	0.46
2:B:522:SER:HB3	2:B:720:ALA:HB2	1.97	0.46
2:B:659:GLN:C	2:B:661:PRO:HD3	2.37	0.46
2:B:759:TRP:HD1	2:B:759:TRP:N	2.14	0.46
1:C:113:PHE:CE1	3:D:102:ALA:HB3	2.51	0.46
1:A:170:ASP:O	1:A:174:ARG:HG3	2.16	0.46
1:A:550:ASP:OD1	1:A:652:PHE:CD1	2.69	0.46
1:A:259:LEU:O	1:A:359:ARG:NH2	2.49	0.45
1:A:379:ILE:CG2	1:A:381:TRP:NE1	2.80	0.45
1:A:54:PHE:O	1:A:54:PHE:HD1	1.99	0.45
2:B:523:VAL:O	2:B:738:ILE:CD1	2.64	0.45
1:C:117:PRO:HG2	1:C:321:PHE:CD2	2.51	0.45
1:C:283:ASP:CB	1:C:335:THR:HG22	2.46	0.45
1:C:795:GLU:HG3	1:C:796:CYS:N	2.31	0.45
3:D:531:VAL:O	3:D:741:LEU:HA	2.16	0.45
1:A:291:ALA:CB	1:A:325:LEU:HD13	2.46	0.45
1:A:525:ILE:O	1:A:762:LYS:NZ	2.43	0.45
1:A:626:SER:HA	1:A:629:ILE:HD11	1.98	0.45
2:B:448:CYS:SG	2:B:497:VAL:HG11	2.56	0.45
2:B:31:ALA:CA	2:B:90:VAL:HG12	2.45	0.45
1:C:204:LEU:O	1:C:208:LEU:HD12	2.17	0.45
1:C:273:ASN:CB	1:C:335:THR:HA	2.46	0.45
1:C:57:LYS:C	1:C:58:ILE:HG13	2.35	0.45
1:C:606:TRP:HA	1:C:606:TRP:HE3	1.80	0.45
1:C:80:GLU:O	1:C:84:SER:CB	2.64	0.45
2:B:249:VAL:HG23	2:B:268:LEU:CD2	2.45	0.45
5:C:1004:NAG:H3	5:C:1004:NAG:C8	2.22	0.45
1:C:298:MET:SD	1:C:320:LEU:CD2	3.02	0.45
1:C:630:LEU:O	1:C:634:TRP:CG	2.69	0.45
3:D:55:HIS:HB3	3:D:56:HIS:H	1.51	0.45
1:A:803:PRO:HG3	3:D:642:ASN:ND2	2.31	0.45
5:A:1006:NAG:C1	5:A:1006:NAG:C8	2.94	0.45
1:A:503:LEU:HD11	1:A:761:ARG:CA	2.46	0.45
1:A:53:HIS:HD2	1:A:293:HIS:CB	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ALA:N	2:B:90:VAL:HG12	2.32	0.45
1:C:23:ASP:N	1:C:24:PRO:CD	2.79	0.45
1:C:439:PRO:CD	1:C:476:LEU:HB2	2.45	0.45
1:C:438:GLY:HA2	1:C:476:LEU:HD12	1.98	0.45
1:C:519:ASN:HD21	1:C:523:GLN:HE21	1.65	0.45
1:C:667:ASP:HA	1:C:668:PRO:HD3	1.84	0.45
3:D:147:GLN:O	3:D:151:VAL:HG23	2.16	0.45
3:D:345:SER:O	3:D:353:MET:CB	2.65	0.45
3:D:594:THR:CG2	3:D:598:ALA:HB2	2.35	0.45
1:A:249:VAL:HG13	1:A:266:ILE:HD11	1.98	0.45
2:B:247:TRP:HB3	2:B:268:LEU:HD23	1.98	0.45
2:B:643:GLN:C	2:B:645:ARG:N	2.69	0.45
1:C:58:ILE:HG21	1:C:296:PHE:HE2	1.81	0.45
1:A:34:SER:CA	1:A:96:PRO:CD	2.92	0.45
2:B:160:HIS:CG	2:B:160:HIS:O	2.70	0.45
2:B:559:MET:SD	2:B:618:ILE:HG21	2.57	0.45
2:B:592:ALA:HA	2:B:595:LEU:CB	2.47	0.45
2:B:669:ARG:HD3	2:B:696:PHE:CE2	2.52	0.45
2:B:768:LEU:HD23	1:C:519:ASN:CB	2.38	0.45
1:C:782:PHE:CE2	1:C:786:LEU:CD1	2.96	0.45
3:D:360:ILE:HG22	3:D:368:TRP:CE3	2.51	0.45
1:A:330:TYR:N	1:A:331:PRO:CD	2.78	0.45
1:A:524:TYR:O	1:A:762:LYS:HE2	2.15	0.45
2:B:53:MET:HA	2:B:53:MET:HE1	1.92	0.45
2:B:618:ILE:HG12	1:C:822:ILE:CG2	2.45	0.45
2:B:91:VAL:HG21	2:B:284:VAL:HG13	1.99	0.45
1:C:679:TYR:H	1:C:703:HIS:CE1	2.33	0.45
1:A:381:TRP:HB3	1:A:382:PRO:CD	2.42	0.45
1:A:512:VAL:HG22	1:A:758:ILE:HD11	1.99	0.45
2:B:490:TYR:O	2:B:491:LYS:HB3	2.16	0.45
1:C:323:ARG:HA	1:C:323:ARG:HD3	1.67	0.45
1:C:438:GLY:HA2	1:C:439:PRO:HD2	1.80	0.45
1:C:674:SER:HB3	1:C:677:PHE:CB	2.42	0.45
1:A:225:GLU:OE2	1:A:255:SER:OG	2.21	0.45
1:A:286:ALA:CB	1:A:330:TYR:OH	2.62	0.45
1:A:357:GLN:HE21	1:A:380:ILE:HB	1.82	0.45
1:A:510:MET:HA	1:A:760:MET:HG2	1.99	0.45
2:B:166:THR:CB	2:B:172:TYR:HB2	2.47	0.45
2:B:169:PHE:CB	2:B:170:PRO:HD3	2.39	0.45
2:B:262:TYR:C	2:B:262:TYR:CD2	2.87	0.45
2:B:42:GLU:O	2:B:46:ARG:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:VAL:HG12	1:C:67:HIS:NE2	2.31	0.45
3:D:543:PHE:O	3:D:546:PRO:CG	2.59	0.45
3:D:566:ALA:O	3:D:570:PHE:N	2.41	0.45
1:A:124:ARG:O	1:A:143:PRO:HA	2.17	0.45
1:A:254:ILE:HD11	1:A:270:GLN:HG3	1.99	0.45
2:B:192:VAL:HG22	2:B:193:GLN:N	2.30	0.45
2:B:194:ASN:HB2	2:B:214:ILE:CG1	2.45	0.45
1:C:575:LEU:C	1:C:575:LEU:HD23	2.37	0.45
4:G:41:UNK:C	4:G:43:UNK:N	2.79	0.45
1:A:251:GLU:O	1:A:254:ILE:HG12	2.17	0.44
1:A:119:ILE:HD13	1:A:288:VAL:HG21	1.63	0.44
2:B:120:HIS:CG	2:B:280:ILE:CD1	3.00	0.44
2:B:221:LEU:N	2:B:221:LEU:HD12	2.33	0.44
2:B:405:VAL:O	2:B:406:ILE:CD1	2.63	0.44
2:B:517:VAL:CG1	2:B:518:GLU:N	2.80	0.44
2:B:525:VAL:HG21	2:B:650:VAL:HG22	1.94	0.44
1:A:291:ALA:HB2	1:A:325:LEU:HA	1.98	0.44
1:A:767:LYS:HD3	1:A:768:GLN:N	2.32	0.44
2:B:163:SER:HB2	2:B:194:ASN:HD22	1.79	0.44
2:B:176:ILE:O	2:B:180:LYS:HG2	2.17	0.44
2:B:533:SER:HA	2:B:534:PRO:HD2	1.47	0.44
2:B:522:SER:OG	2:B:720:ALA:HA	2.17	0.44
2:B:512:PHE:CG	2:B:750:GLY:HA3	2.51	0.44
1:C:425:THR:CG2	1:C:431:ILE:HG13	2.38	0.44
1:C:53:HIS:HA	1:C:53:HIS:HD1	1.72	0.44
1:C:565:GLY:O	1:C:569:HIS:HE1	1.87	0.44
3:D:162:TYR:O	3:D:192:TRP:HB2	2.17	0.44
3:D:526:GLY:HA2	3:D:753:THR:HG22	1.99	0.44
1:A:554:GLN:HB2	1:A:555:PRO:CD	2.48	0.44
1:A:788:LYS:CD	1:A:788:LYS:C	2.85	0.44
1:A:807:THR:O	1:A:807:THR:HG22	2.17	0.44
2:B:157:TYR:OH	2:B:246:VAL:CG1	2.59	0.44
2:B:247:TRP:CD2	2:B:268:LEU:HB3	2.47	0.44
1:A:511:ILE:O	1:A:758:ILE:HG13	2.16	0.44
1:A:811:MET:HE2	3:D:631:PHE:CD2	2.48	0.44
2:B:243:TYR:N	2:B:243:TYR:CD1	2.86	0.44
2:B:490:TYR:O	2:B:491:LYS:CB	2.64	0.44
1:C:78:VAL:CB	1:C:110:THR:HG21	2.48	0.44
1:C:315:TRP:CZ3	1:C:317:THR:O	2.66	0.44
1:A:115:ARG:HB2	1:A:315:TRP:H	1.81	0.44
2:B:157:TYR:OH	2:B:246:VAL:CG2	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:459:VAL:O	2:B:459:VAL:CG1	2.64	0.44
2:B:50:THR:HA	2:B:53:MET:HB2	1.99	0.44
1:C:142:PRO:CG	1:C:349:ALA:CB	2.92	0.44
1:C:367:PHE:HD1	1:C:372:ILE:HA	1.82	0.44
1:A:93:SER:HB3	1:A:121:LEU:HD12	1.98	0.44
1:A:607:PHE:C	1:A:607:PHE:CD1	2.91	0.44
1:C:678:ILE:N	1:C:725:HIS:HD2	2.02	0.44
1:A:27:VAL:HG13	1:A:88:TYR:CG	2.50	0.44
1:A:94:HIS:CB	1:A:95:PRO:HD2	2.47	0.44
2:B:651:THR:CB	2:B:655:ASP:OD2	2.63	0.44
1:C:569:HIS:H	1:C:569:HIS:HD1	1.64	0.44
1:C:636:LEU:C	1:C:636:LEU:HD22	2.36	0.44
3:D:198:ILE:HD12	3:D:215:LEU:HD23	2.00	0.44
3:D:759:ILE:HG22	3:D:760:GLN:N	2.33	0.44
2:B:198:LEU:HB2	2:B:207:THR:HG23	1.92	0.44
2:B:65:LEU:HD23	2:B:66:VAL:N	2.32	0.44
2:B:659:GLN:CD	2:B:686:TYR:CE2	2.91	0.44
1:C:134:HIS:N	1:C:134:HIS:CD2	2.85	0.44
2:B:512:PHE:HD1	1:C:529:LYS:CE	2.30	0.44
1:C:697:LEU:C	1:C:699:THR:N	2.65	0.44
5:D:1003:NAG:H61	5:D:1004:NAG:C7	2.48	0.44
3:D:408:PRO:HG3	3:D:790:LEU:CD2	2.48	0.44
3:D:58:PRO:CG	3:D:303:LEU:HD12	2.44	0.44
3:D:667:PRO:HG2	3:D:668:ASN:ND2	2.31	0.44
1:A:126:SER:OG	1:A:143:PRO:HB2	2.18	0.44
1:A:124:ARG:CZ	1:A:271:LEU:HD22	2.47	0.44
1:A:440:ASP:CB	1:A:447:PRO:HD2	2.48	0.44
1:A:834:ALA:C	1:A:836:LYS:H	2.21	0.44
2:B:114:ILE:HG23	2:B:115:PRO:HD2	2.00	0.44
2:B:682:ILE:CG2	2:B:690:HIS:HB2	2.47	0.44
1:C:46:VAL:HG21	1:C:62:ALA:HB2	1.98	0.44
1:C:76:LEU:C	1:C:78:VAL:N	2.70	0.44
4:G:67:UNK:O	4:G:84:UNK:N	2.51	0.44
1:A:53:HIS:CG	1:A:293:HIS:CD2	3.05	0.43
1:A:34:SER:C	1:A:96:PRO:HG2	2.38	0.43
2:B:154:MET:CA	2:B:158:ASP:CB	2.85	0.43
2:B:58:ASP:O	2:B:59:VAL:HG23	2.18	0.43
1:C:731:SER:O	1:C:735:GLU:CG	2.66	0.43
3:D:168:THR:HG22	3:D:169:THR:N	2.33	0.43
3:D:666:ARG:HA	3:D:667:PRO:HD2	1.80	0.43
1:A:124:ARG:HG2	1:A:141:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:CYS:SG	2:B:72:LYS:HB2	2.58	0.43
2:B:151:LEU:HD23	2:B:190:TRP:CZ2	2.43	0.43
2:B:58:ASP:O	2:B:59:VAL:CG2	2.66	0.43
2:B:685:ASN:HB3	2:B:686:TYR:CD1	2.53	0.43
1:C:575:LEU:HB3	1:C:634:TRP:CZ3	2.46	0.43
1:A:60:LEU:HD11	1:A:293:HIS:HE1	1.83	0.43
1:A:811:MET:N	3:D:631:PHE:HE2	2.03	0.43
1:A:78:VAL:O	1:A:82:LEU:HB2	2.17	0.43
2:B:236:ARG:NH1	2:B:263:GLU:OE1	2.51	0.43
2:B:264:PHE:CE1	2:B:268:LEU:HD21	2.53	0.43
2:B:659:GLN:NE2	2:B:686:TYR:CE2	2.80	0.43
2:B:768:LEU:O	2:B:771:VAL:HB	2.18	0.43
1:C:141:VAL:HB	1:C:142:PRO:HD2	2.00	0.43
1:C:273:ASN:HA	1:C:273:ASN:HD22	1.70	0.43
4:F:13:UNK:O	4:F:108:UNK:N	2.52	0.43
1:A:709:TYR:CE1	1:A:724:LEU:CD1	3.01	0.43
1:A:736:PHE:HE1	1:A:794:GLN:NE2	2.14	0.43
2:B:401:GLU:O	2:B:405:VAL:O	2.36	0.43
2:B:425:ARG:NH1	2:B:466:TYR:HB3	2.34	0.43
2:B:559:MET:CB	2:B:618:ILE:HD13	2.49	0.43
2:B:761:ARG:N	2:B:762:PRO:CD	2.81	0.43
1:A:668:PRO:HG3	2:B:785:THR:CB	2.49	0.43
1:C:408:PHE:HA	1:C:456:PHE:HB3	2.00	0.43
2:B:768:LEU:CG	1:C:519:ASN:CA	2.96	0.43
1:C:649:LEU:C	1:C:649:LEU:HD23	2.39	0.43
3:D:627:VAL:HG13	3:D:630:PHE:CE2	2.53	0.43
1:A:106:PRO:HB3	2:B:107:PHE:CE2	2.40	0.43
1:A:425:THR:OG1	1:A:427:ASN:O	2.26	0.43
2:B:108:VAL:O	2:B:112:THR:HG23	2.18	0.43
2:B:173:ARG:HA	2:B:173:ARG:HD3	1.32	0.43
2:B:196:ILE:HD11	2:B:211:LEU:CD2	2.49	0.43
2:B:249:VAL:CG2	2:B:268:LEU:HD23	2.49	0.43
1:C:678:ILE:H	1:C:725:HIS:CD2	2.16	0.43
1:C:697:LEU:O	1:C:700:MET:N	2.50	0.43
4:F:111:UNK:HA	4:F:141:UNK:O	2.19	0.43
1:A:202:LYS:C	1:A:204:LEU:HD23	2.38	0.43
1:A:204:LEU:HD11	1:A:230:ALA:O	2.17	0.43
1:A:408:PHE:HD2	1:A:514:PRO:HB3	1.84	0.43
1:A:496:TRP:CZ3	1:A:524:TYR:CD2	3.06	0.43
1:A:810:ASN:HB2	3:D:631:PHE:CE2	2.40	0.43
1:A:815:PHE:HE1	3:D:558:MET:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:TYR:CE2	2:B:389:HIS:CD2	3.06	0.43
2:B:355:VAL:HG12	2:B:367:VAL:CB	2.47	0.43
2:B:401:GLU:O	2:B:406:ILE:CD1	2.67	0.43
3:D:595:ILE:HB	3:D:596:GLY:H	1.64	0.43
4:F:141:UNK:CA	4:F:142:UNK:C	2.96	0.43
1:A:249:VAL:CG1	1:A:266:ILE:HD11	2.48	0.43
1:A:379:ILE:CG2	1:A:381:TRP:CE2	3.02	0.43
2:B:109:SER:O	2:B:110:SER:C	2.56	0.43
2:B:405:VAL:HG12	2:B:406:ILE:N	2.33	0.43
2:B:468:VAL:CG2	2:B:484:MET:CG	2.59	0.43
1:C:227:ASP:O	1:C:231:VAL:HG23	2.18	0.43
1:C:611:VAL:O	1:C:642:VAL:HG21	2.19	0.43
1:A:128:TYR:HB3	1:A:137:PHE:CD2	2.54	0.43
1:A:65:VAL:HG13	1:A:67:HIS:H	1.83	0.43
2:B:523:VAL:CG2	2:B:717:ILE:HD11	2.48	0.43
2:B:559:MET:SD	2:B:618:ILE:CG2	3.07	0.43
1:C:274:GLY:CA	1:C:280:HIS:CE1	2.88	0.43
3:D:236:PHE:HD2	3:D:268:PHE:CD1	2.37	0.43
3:D:332:ARG:CB	3:D:335:ILE:HD11	2.49	0.43
3:D:409:PHE:CD1	3:D:755:TYR:OH	2.67	0.43
3:D:559:LEU:C	3:D:559:LEU:CD2	2.87	0.43
3:D:627:VAL:HA	3:D:630:PHE:HD2	1.83	0.43
4:F:39:UNK:HA	4:F:45:UNK:HA	2.01	0.43
1:A:794:GLN:C	1:A:795:GLU:CG	2.86	0.43
2:B:759:TRP:O	2:B:762:PRO:HD2	2.19	0.43
1:C:667:ASP:OD2	1:C:668:PRO:HD2	2.19	0.43
3:D:505:SER:CA	3:D:755:TYR:CE1	3.02	0.43
3:D:559:LEU:CD2	3:D:598:ALA:HB1	2.39	0.43
3:D:726:ALA:O	3:D:730:ASN:ND2	2.34	0.43
4:F:86:UNK:HA	4:F:104:UNK:HA	2.01	0.43
1:A:303:ASP:HB3	1:A:304:PRO:HD2	2.01	0.43
2:B:50:THR:O	2:B:54:SER:N	2.52	0.43
2:B:540:PRO:CB	1:C:803:PRO:O	2.67	0.43
3:D:195:GLU:CD	3:D:220:SER:HB3	2.39	0.43
3:D:761:LYS:HD2	3:D:761:LYS:HA	1.48	0.43
1:A:105:THR:CA	1:A:128:TYR:CE2	2.98	0.42
1:A:809:GLU:O	1:A:812:ALA:HB3	2.18	0.42
1:A:79:CYS:O	1:A:83:ILE:HB	2.19	0.42
2:B:154:MET:HE3	2:B:248:ILE:CD1	2.48	0.42
2:B:501:THR:HG23	2:B:747:THR:HG21	2.01	0.42
2:B:458:THR:HG21	2:B:770:PHE:HZ	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:HIS:N	1:A:122:THR:HG1	2.07	0.42
1:A:164:ILE:HG23	1:A:193:LYS:O	2.18	0.42
1:A:554:GLN:HB2	1:A:555:PRO:HD3	2.01	0.42
1:A:520:GLU:CB	1:A:693:ARG:NH2	2.81	0.42
1:C:401:VAL:HG21	1:C:477:VAL:HG23	2.01	0.42
1:C:538:ILE:O	1:C:746:THR:HA	2.19	0.42
3:D:155:ILE:HD11	3:D:359:ILE:HG12	2.01	0.42
3:D:514:GLU:O	3:D:761:LYS:NZ	2.49	0.42
1:A:121:LEU:HD11	1:A:281:ILE:HG12	1.97	0.42
1:A:400:ILE:HD12	1:A:512:VAL:HG23	1.99	0.42
1:A:525:ILE:HA	1:A:762:LYS:CD	2.48	0.42
2:B:194:ASN:OD1	2:B:214:ILE:CD1	2.67	0.42
2:B:520:GLY:O	2:B:743:ILE:HG22	2.15	0.42
3:D:229:LYS:O	3:D:232:ALA:HB3	2.19	0.42
3:D:402:VAL:HB	3:D:472:TYR:CZ	2.54	0.42
3:D:667:PRO:HG3	3:D:698:TYR:CZ	2.55	0.42
3:D:522:PHE:CE1	3:D:755:TYR:HB3	2.54	0.42
1:A:410:TYR:O	1:A:453:CYS:HA	2.20	0.42
1:A:501:GLY:O	1:A:502:GLU:C	2.54	0.42
1:A:815:PHE:CE2	3:D:554:MET:CB	2.89	0.42
2:B:673:VAL:HG21	2:B:718:TYR:OH	2.19	0.42
3:D:225:LEU:HD21	3:D:227:CYS:SG	2.59	0.42
3:D:560:LEU:C	3:D:560:LEU:HD22	2.36	0.42
3:D:688:ILE:HG22	3:D:696:HIS:HB2	2.00	0.42
4:F:38:UNK:HA	4:F:87:UNK:HA	2.01	0.42
1:A:221:LEU:HD23	1:A:247:TRP:CZ3	2.54	0.42
1:A:621:ALA:HB1	1:A:628:ARG:CB	2.50	0.42
2:B:203:THR:HG23	2:B:203:THR:O	2.19	0.42
1:C:108:SER:HG	1:C:134:HIS:CE1	2.38	0.42
3:D:202:MET:HA	3:D:207:ILE:CB	2.49	0.42
3:D:403:THR:HG22	3:D:471:LEU:HD11	2.01	0.42
1:A:124:ARG:CG	1:A:141:VAL:CB	2.96	0.42
1:A:437:ASN:HB2	1:A:475:HIS:HB2	2.00	0.42
1:A:574:MET:HE1	2:B:819:SER:HB2	2.00	0.42
1:A:575:LEU:O	1:A:575:LEU:HD12	2.20	0.42
2:B:141:ALA:O	2:B:142:SER:C	2.55	0.42
2:B:137:PHE:O	2:B:346:GLY:HA3	2.20	0.42
3:D:452:GLY:HA2	3:D:789:TRP:CE2	2.55	0.42
3:D:606:VAL:CA	3:D:628:TRP:CZ3	3.02	0.42
1:A:540:VAL:HG23	1:A:719:VAL:CG1	2.50	0.42
1:A:54:PHE:O	1:A:54:PHE:CD1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:LEU:O	1:A:569:HIS:HB2	2.20	0.42
2:B:251:SER:HA	2:B:254:THR:HB	2.02	0.42
5:C:1006:NAG:H3	5:C:1006:NAG:C8	2.15	0.42
1:C:483:GLY:HA3	1:C:500:MET:HB2	2.00	0.42
1:A:329:LYS:O	1:A:330:TYR:CB	2.63	0.42
1:A:50:ASN:OD1	1:A:60:LEU:HB2	2.20	0.42
1:A:525:ILE:HD11	1:A:527:PHE:HE1	1.78	0.42
2:B:52:ASP:HB3	2:B:285:ARG:HD2	2.02	0.42
2:B:516:PHE:CD2	2:B:517:VAL:HG23	2.53	0.42
2:B:615:SER:O	2:B:619:VAL:CG2	2.63	0.42
1:C:126:SER:HB2	1:C:172:GLU:CD	2.40	0.42
1:C:348:PHE:CD1	1:C:348:PHE:N	2.87	0.42
1:C:785:GLU:O	1:C:789:THR:OG1	2.10	0.42
1:C:133:ILE:HG23	3:D:130:ALA:CB	2.50	0.42
3:D:556:PHE:HA	3:D:556:PHE:HD1	1.69	0.42
1:C:622:PRO:HD3	3:D:600:TRP:HH2	1.84	0.42
3:D:606:VAL:CA	3:D:628:TRP:HH2	2.33	0.42
1:A:557:GLN:O	1:A:558:SER:C	2.57	0.42
2:B:196:ILE:HD11	2:B:211:LEU:CG	2.49	0.42
2:B:197:THR:HG23	2:B:198:LEU:CG	2.49	0.42
1:C:496:TRP:HA	1:C:501:GLY:HA3	2.01	0.42
3:D:301:THR:CB	3:D:333:TYR:CD2	3.03	0.42
3:D:594:THR:HG22	3:D:598:ALA:CB	2.50	0.42
3:D:643:LEU:HA	3:D:643:LEU:HD23	1.88	0.42
4:F:63:UNK:HA	4:F:76:UNK:HA	2.02	0.42
4:G:122:UNK:HA	4:G:148:UNK:CB	2.49	0.42
1:A:266:ILE:HG23	1:A:266:ILE:O	2.20	0.42
1:A:606:TRP:CD1	3:D:623:ILE:HG12	2.54	0.42
2:B:125:MET:HE3	2:B:251:SER:HB2	1.96	0.42
2:B:240:LEU:O	2:B:245:PHE:CB	2.63	0.42
2:B:157:TYR:HH	2:B:246:VAL:HG11	1.84	0.42
2:B:353:LEU:HB2	2:B:370:TRP:HB3	2.02	0.42
2:B:680:ARG:CG	2:B:683:ARG:HH21	2.33	0.42
3:D:108:ASP:O	3:D:112:VAL:HG23	2.20	0.42
3:D:200:LEU:CD2	3:D:201:ASP:N	2.68	0.42
3:D:562:VAL:O	3:D:566:ALA:N	2.37	0.42
1:A:696:GLU:CD	1:A:696:GLU:H	2.17	0.41
2:B:295:ALA:O	2:B:299:LEU:N	2.53	0.41
2:B:468:VAL:HG23	2:B:484:MET:HG2	1.89	0.41
2:B:501:THR:HG22	2:B:502:ILE:N	2.35	0.41
2:B:505:GLU:HG2	2:B:680:ARG:HH12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:553:LEU:O	2:B:556:VAL:HB	2.19	0.41
1:C:78:VAL:CG1	1:C:110:THR:CG2	2.95	0.41
1:C:477:VAL:CG2	1:C:499:MET:CB	2.82	0.41
1:C:673:PRO:CG	1:C:703:HIS:HB3	2.44	0.41
3:D:151:VAL:O	3:D:155:ILE:HG13	2.20	0.41
3:D:538:VAL:HA	3:D:646:PHE:HZ	1.79	0.41
3:D:639:TYR:O	3:D:639:TYR:CD1	2.73	0.41
1:A:194:VAL:O	1:A:195:LEU:HD23	2.21	0.41
1:A:54:PHE:CD1	1:A:293:HIS:HD2	2.38	0.41
1:A:651:ALA:O	1:A:654:VAL:HB	2.20	0.41
1:C:481:LYS:HD2	1:C:684:GLN:HB2	2.01	0.41
1:C:576:TYR:HA	1:C:579:ASP:HB3	2.02	0.41
3:D:325:TYR:CD1	3:D:326:GLU:CA	3.03	0.41
3:D:431:LYS:O	3:D:446:ILE:N	2.52	0.41
1:A:122:THR:HG21	1:A:277:GLU:CD	2.35	0.41
1:A:736:PHE:HD1	1:A:794:GLN:OE1	2.01	0.41
2:B:199:ASP:HB3	2:B:200:THR:H	1.67	0.41
2:B:736:VAL:CG1	2:B:737:THR:H	2.31	0.41
1:C:771:SER:O	1:C:772:LEU:C	2.58	0.41
1:A:121:LEU:HD13	1:A:281:ILE:HG13	1.99	0.41
1:A:133:ILE:CG2	2:B:128:ALA:CB	2.91	0.41
1:A:464:LEU:O	1:A:468:MET:CB	2.69	0.41
1:A:496:TRP:N	1:A:496:TRP:CE3	2.86	0.41
1:A:790:TRP:N	1:A:790:TRP:CD1	2.87	0.41
2:B:520:GLY:O	2:B:720:ALA:N	2.48	0.41
2:B:523:VAL:HG13	2:B:717:ILE:HG13	2.01	0.41
2:B:754:GLN:HB3	2:B:757:SER:CB	2.50	0.41
3:D:218:LEU:HD12	3:D:218:LEU:C	2.41	0.41
1:A:216:ALA:O	1:A:217:ARG:HD3	2.20	0.41
1:A:561:TRP:CG	1:A:562:LEU:N	2.87	0.41
2:B:144:LYS:HA	2:B:178:PHE:CD2	2.56	0.41
2:B:163:SER:OG	2:B:194:ASN:ND2	2.52	0.41
2:B:271:VAL:CG2	2:B:354:VAL:O	2.68	0.41
2:B:31:ALA:HB3	2:B:90:VAL:HG11	2.01	0.41
1:C:29:ILE:HD11	1:C:60:LEU:HD23	2.02	0.41
3:D:396:ASP:CB	3:D:467:PHE:CA	2.92	0.41
3:D:545:GLU:H	3:D:545:GLU:HG2	1.67	0.41
1:A:198:GLU:CG	1:A:199:PRO:HD2	2.49	0.41
1:A:208:LEU:HB3	1:A:240:MET:HE1	2.02	0.41
1:A:217:ARG:HA	1:A:217:ARG:HD3	1.76	0.41
1:A:559:THR:HG22	1:A:559:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:LEU:HD11	2:B:45:ILE:CD1	2.50	0.41
2:B:502:ILE:HG12	2:B:512:PHE:CE1	2.53	0.41
2:B:559:MET:CB	2:B:618:ILE:HG21	2.49	0.41
2:B:672:THR:H	2:B:693:MET:CG	2.32	0.41
2:B:728:GLY:HA2	2:B:786:GLY:HA3	2.03	0.41
2:B:74:ILE:CG2	2:B:105:LEU:CD2	2.95	0.41
1:C:446:ARG:N	1:C:447:PRO:CD	2.83	0.41
1:C:629:ILE:O	1:C:633:VAL:N	2.46	0.41
3:D:168:THR:CG2	3:D:174:TYR:HB2	2.51	0.41
3:D:200:LEU:CD1	3:D:211:ILE:CB	2.98	0.41
3:D:225:LEU:HD12	3:D:251:TRP:CZ3	2.52	0.41
3:D:252:ILE:HA	3:D:273:ILE:O	2.20	0.41
1:A:550:ASP:O	1:A:553:MET:HB3	2.21	0.41
2:B:156:GLU:OE2	2:B:157:TYR:HB3	2.20	0.41
2:B:214:ILE:N	2:B:214:ILE:CD1	2.79	0.41
2:B:55:LEU:HD23	2:B:55:LEU:HA	1.93	0.41
1:C:265:GLY:HA3	1:C:381:TRP:O	2.21	0.41
1:C:627:ALA:O	1:C:630:LEU:CA	2.69	0.41
3:D:725:ASP:OD1	3:D:726:ALA:N	2.54	0.41
4:G:73:UNK:N	4:G:78:UNK:O	2.54	0.41
1:A:718:ALA:HB1	1:A:724:LEU:HG	2.02	0.41
2:B:271:VAL:HG23	2:B:354:VAL:O	2.20	0.41
2:B:538:LEU:CB	2:B:541:PHE:CE1	3.04	0.41
2:B:58:ASP:C	2:B:59:VAL:HG23	2.41	0.41
1:C:342:GLU:OE1	3:D:170:TYR:CE2	2.73	0.41
3:D:815:PHE:CD1	3:D:815:PHE:N	2.88	0.41
1:A:357:GLN:HG2	1:A:380:ILE:HD13	2.03	0.41
2:B:34:LEU:HA	2:B:34:LEU:HD23	1.89	0.41
2:B:424:CYS:N	2:B:442:LYS:O	2.54	0.41
1:C:415:THR:CG2	1:C:416:SER:N	2.83	0.41
1:C:27:VAL:HB	1:C:59:GLN:O	2.21	0.41
3:D:58:PRO:HG3	3:D:303:LEU:CD1	2.45	0.41
1:A:718:ALA:O	1:A:723:LYS:N	2.54	0.41
2:B:197:THR:OG1	2:B:198:LEU:N	2.54	0.41
2:B:31:ALA:O	2:B:90:VAL:CA	2.69	0.41
2:B:780:GLU:O	2:B:784:LEU:N	2.54	0.41
1:C:622:PRO:HG3	3:D:600:TRP:HH2	1.81	0.41
2:B:520:GLY:C	2:B:743:ILE:HB	2.41	0.41
2:B:520:GLY:CA	2:B:743:ILE:HB	2.51	0.41
1:C:531:PHE:CE1	1:C:756:PHE:CB	3.04	0.41
1:C:572:ALA:HB1	1:C:604:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:LEU:O	1:C:87:VAL:HG22	2.21	0.41
3:D:667:PRO:HG3	3:D:698:TYR:CE2	2.56	0.41
2:B:151:LEU:CD2	2:B:190:TRP:CZ2	3.04	0.40
2:B:197:THR:HG23	2:B:198:LEU:HD12	2.03	0.40
2:B:350:ASN:O	2:B:351:PRO:C	2.59	0.40
2:B:494:VAL:HG12	2:B:495:MET:HG3	2.01	0.40
2:B:502:ILE:HG21	2:B:512:PHE:CE1	2.52	0.40
2:B:64:LEU:HD12	2:B:81:LEU:HD13	1.75	0.40
2:B:830:TYR:O	2:B:831:LYS:C	2.59	0.40
1:C:633:VAL:HG12	1:C:634:TRP:HD1	1.86	0.40
1:C:663:THR:N	1:C:667:ASP:HB2	2.36	0.40
1:A:199:PRO:HA	1:A:227:ASP:OD2	2.21	0.40
1:A:570:VAL:O	1:A:572:ALA:N	2.54	0.40
1:A:26:ILE:HA	1:A:59:GLN:C	2.42	0.40
2:B:765:LEU:HG	1:C:523:GLN:HG2	2.02	0.40
4:G:61:UNK:O	4:G:62:UNK:C	2.69	0.40
1:A:105:THR:HB	1:A:128:TYR:OH	2.21	0.40
1:A:165:LEU:HD22	1:A:180:LEU:HD13	2.02	0.40
1:A:204:LEU:HD11	1:A:231:VAL:N	2.36	0.40
1:A:512:VAL:HG22	1:A:758:ILE:CD1	2.51	0.40
1:C:367:PHE:CZ	1:C:369:GLY:O	2.75	0.40
3:D:462:ALA:O	3:D:466:LYS:N	2.48	0.40
3:D:541:SER:HA	3:D:544:LEU:CG	2.48	0.40
3:D:554:MET:CA	3:D:554:MET:CE	2.99	0.40
4:G:198:UNK:HA	4:G:209:UNK:HA	2.03	0.40
1:A:208:LEU:CD2	1:A:235:ALA:HA	2.50	0.40
1:A:257:SER:O	1:A:258:ALA:C	2.60	0.40
1:A:287:VAL:HG21	1:A:338:ILE:CD1	2.52	0.40
1:A:626:SER:CA	1:A:629:ILE:HD12	2.47	0.40
1:A:540:VAL:HG23	1:A:719:VAL:HG13	2.02	0.40
2:B:634:THR:HG21	7:B:1102:BMK:C11	2.52	0.40
2:B:456:SER:OG	2:B:457:LYS:N	2.54	0.40
2:B:502:ILE:C	2:B:503:ASN:HD22	2.24	0.40
2:B:540:PRO:C	1:C:804:ALA:HB3	2.42	0.40
1:C:408:PHE:HB3	1:C:457:CYS:SG	2.62	0.40
1:C:415:THR:CG2	1:C:416:SER:H	2.32	0.40
1:C:771:SER:O	1:C:774:ILE:N	2.55	0.40
3:D:185:ILE:CB	3:D:192:TRP:HE1	2.34	0.40
3:D:328:HIS:CD2	3:D:328:HIS:C	2.93	0.40
1:A:266:ILE:HG22	1:A:356:LEU:HG	2.04	0.40
1:A:504:LEU:HA	1:A:504:LEU:HD13	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LEU:HD12	1:A:627:ALA:CA	2.05	0.40
1:A:753:ARG:H	1:A:753:ARG:HG3	1.72	0.40
2:B:260:ILE:HA	2:B:261:PRO:HD3	1.96	0.40
2:B:332:ASN:HA	2:B:341:SER:HA	2.04	0.40
2:B:621:ILE:HG23	1:C:818:VAL:CG1	2.46	0.40
3:D:194:LEU:HD11	3:D:197:VAL:CG2	2.52	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	793/814 (97%)	754 (95%)	33 (4%)	6 (1%)	22	66
1	C	794/814 (98%)	758 (96%)	28 (4%)	8 (1%)	18	61
2	B	791/832 (95%)	729 (92%)	49 (6%)	13 (2%)	11	53
3	D	791/837 (94%)	754 (95%)	32 (4%)	5 (1%)	28	71
All	All	3169/3297 (96%)	2995 (94%)	142 (4%)	32 (1%)	23	61

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447	PRO
1	A	658	PRO
2	B	169	PHE
2	B	515	PRO
2	B	534	PRO
1	C	392	TYR
1	C	655	LEU
1	C	698	SER
1	C	800	SER

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Mol	Chain	Res	Type
3	D	28	PRO
1	A	24	PRO
2	B	569	PRO
1	C	802	ALA
3	D	808	ILE
2	B	199	ASP
2	B	254	THR
2	B	265	PRO
3	D	58	PRO
1	A	263	PRO
2	B	198	LEU
2	B	533	SER
2	B	607	VAL
1	C	98	PRO
1	A	541	LYS
1	A	555	PRO
2	B	188	VAL
2	B	264	PHE
1	C	439	PRO
1	C	450	PRO
3	D	43	VAL
2	B	320	ASP
3	D	388	TYR

### 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	537/698 (77%)	493 (92%)	44 (8%)	13	46
1	C	471/698 (68%)	425 (90%)	46 (10%)	9	37
2	B	494/725 (68%)	441 (89%)	53 (11%)	8	33
3	D	373/735 (51%)	336 (90%)	37 (10%)	9	36
All	All	1875/2856 (66%)	1695 (90%)	180 (10%)	14	38

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	PHE
1	A	60	LEU
1	A	79	CYS
1	A	99	THR
1	A	101	HIS
1	A	113	PHE
1	A	138	LEU
1	A	139	ARG
1	A	160	TRP
1	A	202	LYS
1	A	204	LEU
1	A	210	GLU
1	A	266	ILE
1	A	330	TYR
1	A	356	LEU
1	A	392	TYR
1	A	393	GLN
1	A	397	ARG
1	A	398	LEU
1	A	417	ASP
1	A	426	ILE
1	A	452	CYS
1	A	468	MET
1	A	469	ASP
1	A	482	PHE
1	A	496	TRP
1	A	500	MET
1	A	528	SER
1	A	532	LYS
1	A	549	LEU
1	A	571	VAL
1	A	574	MET
1	A	601	LEU
1	A	607	PHE
1	A	625	PHE
1	A	665	ILE
1	A	744	LEU
1	A	767	LYS
1	A	768	GLN
1	A	785	GLU
1	A	788	LYS
1	A	796	CYS
1	A	809	GLU

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Mol	Chain	Res	Type
1	A	833	ILE
2	B	40	ILE
2	B	53	MET
2	B	57	PHE
2	B	72	LYS
2	B	86	LYS
2	B	98	GLN
2	B	156	GLU
2	B	157	TYR
2	B	159	TRP
2	B	173	ARG
2	B	176	ILE
2	B	186	SER
2	B	190	TRP
2	B	195	TYR
2	B	223	CYS
2	B	243	TYR
2	B	264	PHE
2	B	268	LEU
2	B	283	ARG
2	B	303	SER
2	B	332	ASN
2	B	352	LYS
2	B	354	VAL
2	B	356	LEU
2	B	399	LEU
2	B	491	LYS
2	B	492	ARG
2	B	500	LEU
2	B	504	GLU
2	B	512	PHE
2	B	524	MET
2	B	525	VAL
2	B	539	GLU
2	B	541	PHE
2	B	564	PHE
2	B	597	TRP
2	B	621	ILE
2	B	640	PHE
2	B	641	MET
2	B	662	HIS
2	B	686	TYR

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Mol	Chain	Res	Type
2	B	692	TYR
2	B	718	TYR
2	B	738	ILE
2	B	743	ILE
2	B	760	LYS
2	B	765	LEU
2	B	768	LEU
2	B	788	CYS
2	B	789	HIS
2	B	801	ASP
2	B	804	ASN
2	B	811	MET
1	C	26	ILE
1	C	53	HIS
1	C	58	ILE
1	C	59	GLN
1	C	79	CYS
1	C	81	ASP
1	C	139	ARG
1	C	203	ASN
1	C	212	LYS
1	C	260	ARG
1	C	272	ILE
1	C	273	ASN
1	C	277	GLU
1	C	301	ILE
1	C	308	CYS
1	C	323	ARG
1	C	329	LYS
1	C	335	THR
1	C	426	ILE
1	C	477	VAL
1	C	500	MET
1	C	534	GLN
1	C	560	LEU
1	C	574	MET
1	C	577	LEU
1	C	601	LEU
1	C	606	TRP
1	C	628	ARG
1	C	636	LEU
1	C	637	PHE

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Mol	Chain	Res	Type
1	C	639	MET
1	C	667	ASP
1	C	670	LEU
1	C	695	VAL
1	C	724	LEU
1	C	742	CYS
1	C	753	ARG
1	C	767	LYS
1	C	771	SER
1	C	775	LEU
1	C	783	MET
1	C	788	LYS
1	C	796	CYS
1	C	829	ILE
1	C	830	PHE
1	C	831	ILE
3	D	37	VAL
3	D	55	HIS
3	D	72	ASP
3	D	137	MET
3	D	182	ARG
3	D	200	LEU
3	D	218	LEU
3	D	316	CYS
3	D	325	TYR
3	D	328	HIS
3	D	333	TYR
3	D	365	GLU
3	D	370	ARG
3	D	543	PHE
3	D	544	LEU
3	D	545	GLU
3	D	547	PHE
3	D	548	SER
3	D	550	ASP
3	D	552	TRP
3	D	555	MET
3	D	556	PHE
3	D	560	LEU
3	D	565	VAL
3	D	568	PHE
3	D	573	PHE

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Mol	Chain	Res	Type
3	D	595	ILE
3	D	600	TRP
3	D	601	LEU
3	D	602	LEU
3	D	603	TRP
3	D	605	LEU
3	D	614	GLN
3	D	630	PHE
3	D	639	TYR
3	D	794	CYS
3	D	795	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	86	GLN
1	A	146	HIS
1	A	196	GLN
1	A	293	HIS
1	A	648	ASN
1	A	810	ASN
2	B	120	HIS
2	B	194	ASN
2	B	389	HIS
2	B	473	HIS
2	B	503	ASN
2	B	636	ASN
2	B	659	GLN
2	B	675	GLN
1	C	53	HIS
1	C	59	GLN
1	C	451	GLN
1	C	523	GLN
1	C	703	HIS
1	C	725	HIS
3	D	154	ASN
3	D	199	HIS
3	D	306	HIS
3	D	328	HIS
3	D	668	ASN
3	D	691	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	1001	1,5	14,14,15	0.28	0	15,19,21	0.57	0
5	NAG	A	1002	5	14,14,15	0.29	0	15,19,21	0.56	0
5	NAG	A	1003	1,5	14,14,15	0.29	0	15,19,21	0.57	0
5	NAG	A	1004	5	14,14,15	0.29	0	15,19,21	0.58	0
5	NAG	A	1005	1,5	14,14,15	0.30	0	15,19,21	0.58	0
5	NAG	A	1006	5	14,14,15	0.29	0	15,19,21	0.57	0
6	GLU	B	1101	-	1,9,9	0.11	0	1,11,11	0.10	0
7	BMK	B	1102	-	16,20,20	2.23	3 (18%)	18,31,31	1.23	1 (5%)
5	NAG	C	1001	1,5	14,14,15	0.28	0	15,19,21	0.57	0
5	NAG	C	1002	5	14,14,15	0.27	0	15,19,21	0.57	0
5	NAG	C	1003	1,5	14,14,15	0.29	0	15,19,21	0.57	0
5	NAG	C	1004	5	14,14,15	0.28	0	15,19,21	0.57	0
5	NAG	C	1005	1,5	14,14,15	0.29	0	15,19,21	0.57	0
5	NAG	C	1006	5	14,14,15	0.29	0	15,19,21	0.56	0
5	NAG	D	1001	3,5	14,14,15	0.28	0	15,19,21	0.57	0
5	NAG	D	1002	5	14,14,15	0.29	0	15,19,21	0.57	0
5	NAG	D	1003	3,5	14,14,15	0.29	0	15,19,21	0.57	0
5	NAG	D	1004	5	14,14,15	0.29	0	15,19,21	0.57	0



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1001	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1002	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1003	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1004	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1005	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1006	5	-	0/6/23/26	0/1/1/1
6	GLU	B	1101	-	-	0/3/9/9	0/0/0/0
7	BMK	B	1102	-	-	0/0/25/25	0/2/4/4
5	NAG	C	1001	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1002	5	-	0/6/23/26	0/1/1/1
5	NAG	C	1003	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1004	5	-	0/6/23/26	0/1/1/1
5	NAG	C	1005	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1006	5	-	0/6/23/26	0/1/1/1
5	NAG	D	1001	3,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1002	5	-	0/6/23/26	0/1/1/1
5	NAG	D	1003	3,5	-	2/6/23/26	0/1/1/1
5	NAG	D	1004	5	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1102	BMK	C-C5	-2.19	1.49	1.53
7	B	1102	BMK	C3-C2	5.07	1.46	1.39
7	B	1102	BMK	C6-C5	6.66	1.49	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1102	BMK	C13-C9-C3	-3.49	116.54	121.01

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1003	NAG	C8-C7-N2-C2
5	D	1003	NAG	O7-C7-N2-C2

There are no ring outliers.

12 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1001	NAG	3	0
5	A	1002	NAG	3	0
5	A	1004	NAG	1	0
5	A	1006	NAG	4	0
6	B	1101	GLU	7	0
7	B	1102	BMK	8	0
5	C	1002	NAG	3	0
5	C	1004	NAG	2	0
5	C	1006	NAG	4	0
5	D	1002	NAG	2	0
5	D	1003	NAG	1	0
5	D	1004	NAG	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	134:UNK	C	135:UNK	N	14.40