Full wwPDB EM Validation Report

Nov 1, 2022 – 07:22 PM EDT

PDB ID	:	5KBU
EMDB ID	:	EMD-8231
Title	:	Cryo-EM structure of GluA2-2xSTZ complex at 7.8 Angstrom resolution
Authors	:	Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.
Deposited on	:	2016-06-03
Resolution	:	7.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

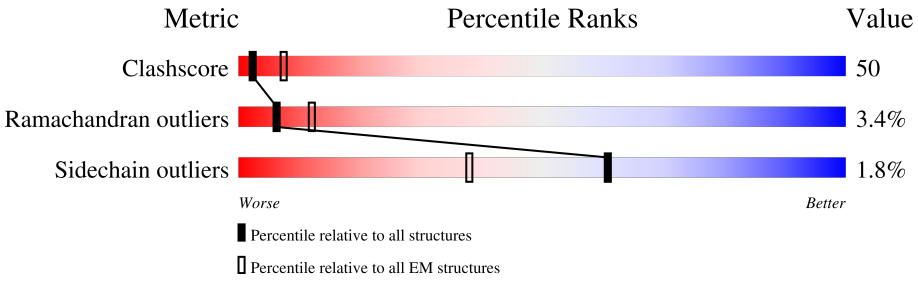
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1034	22% 60% 29% • • 6%
1	B	1034	11% 56% 18% • 25%
1	C	1034	24% 60% 29% • • 6%
1	D	1034	13% 56% 18% • 25%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25678 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 Glutamate receptor 2,Voltage-dependent calcium channel gamma-2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	973	Total	C	N	O	S	0	0
			7110	4589	1138	1346	37		
1	B	779	Total	C	N	O	S	0	0
			5647	3635	902	1083	27		
1	C	973	Total	C	N	O	S	0	0
			7110	4589	1138	1346	37		
1	D	779	Total	C	N	O	S	0	0
			5647	3635	902	1083	27		

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	382	LEU	VAL	engineered mutation	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	engineered mutation	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	758	LEU	VAL	engineered mutation	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	1047	ASP	ASN	conflict	UNP O88602
A	1208	THR	-	expression tag	UNP O88602
A	1209	GLY	-	expression tag	UNP O88602
A	1210	GLY	-	expression tag	UNP O88602
A	1211	LEU	-	expression tag	UNP O88602
A	1212	VAL	-	expression tag	UNP O88602
A	1213	PRO	-	expression tag	UNP O88602

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1214	ARG	-	expression tag	UNP O88602
A	1215	GLY	-	expression tag	UNP O88602
B	241	GLU	ASN	engineered mutation	UNP P19491
B	382	LEU	VAL	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	engineered mutation	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	758	LEU	VAL	engineered mutation	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	1047	ASP	ASN	conflict	UNP O88602
B	1208	THR	-	expression tag	UNP O88602
B	1209	GLY	-	expression tag	UNP O88602
B	1210	GLY	-	expression tag	UNP O88602
B	1211	LEU	-	expression tag	UNP O88602
B	1212	VAL	-	expression tag	UNP O88602
B	1213	PRO	-	expression tag	UNP O88602
B	1214	ARG	-	expression tag	UNP O88602
B	1215	GLY	-	expression tag	UNP O88602
C	241	GLU	ASN	engineered mutation	UNP P19491
C	382	LEU	VAL	engineered mutation	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	engineered mutation	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	758	LEU	VAL	engineered mutation	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	1047	ASP	ASN	conflict	UNP O88602
C	1208	THR	-	expression tag	UNP O88602
C	1209	GLY	-	expression tag	UNP O88602

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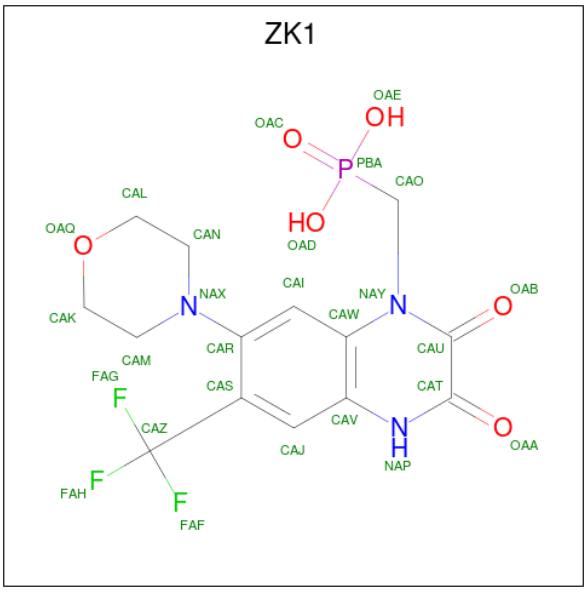
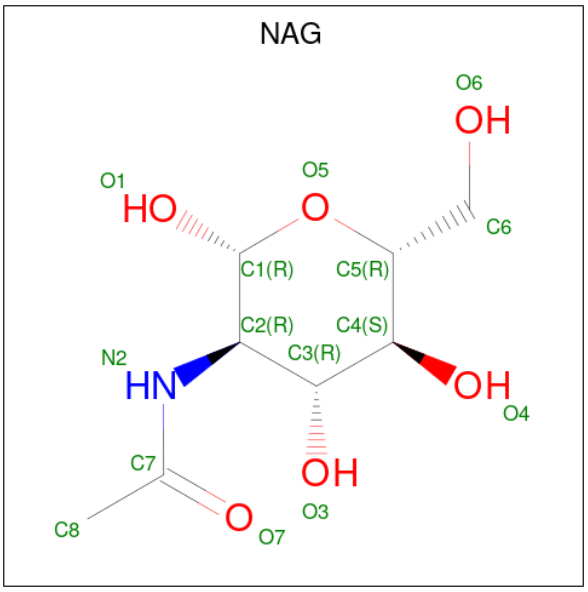
Chain	Residue	Modelled	Actual	Comment	Reference
C	1210	GLY	-	expression tag	UNP O88602
C	1211	LEU	-	expression tag	UNP O88602
C	1212	VAL	-	expression tag	UNP O88602
C	1213	PRO	-	expression tag	UNP O88602
C	1214	ARG	-	expression tag	UNP O88602
C	1215	GLY	-	expression tag	UNP O88602
D	241	GLU	ASN	engineered mutation	UNP P19491
D	382	LEU	VAL	engineered mutation	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	engineered mutation	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	758	LEU	VAL	engineered mutation	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	1047	ASP	ASN	conflict	UNP O88602
D	1208	THR	-	expression tag	UNP O88602
D	1209	GLY	-	expression tag	UNP O88602
D	1210	GLY	-	expression tag	UNP O88602
D	1211	LEU	-	expression tag	UNP O88602
D	1212	VAL	-	expression tag	UNP O88602
D	1213	PRO	-	expression tag	UNP O88602
D	1214	ARG	-	expression tag	UNP O88602
D	1215	GLY	-	expression tag	UNP O88602

- Molecule 2 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: $C_{14}H_{15}F_3N_3O_6P$).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



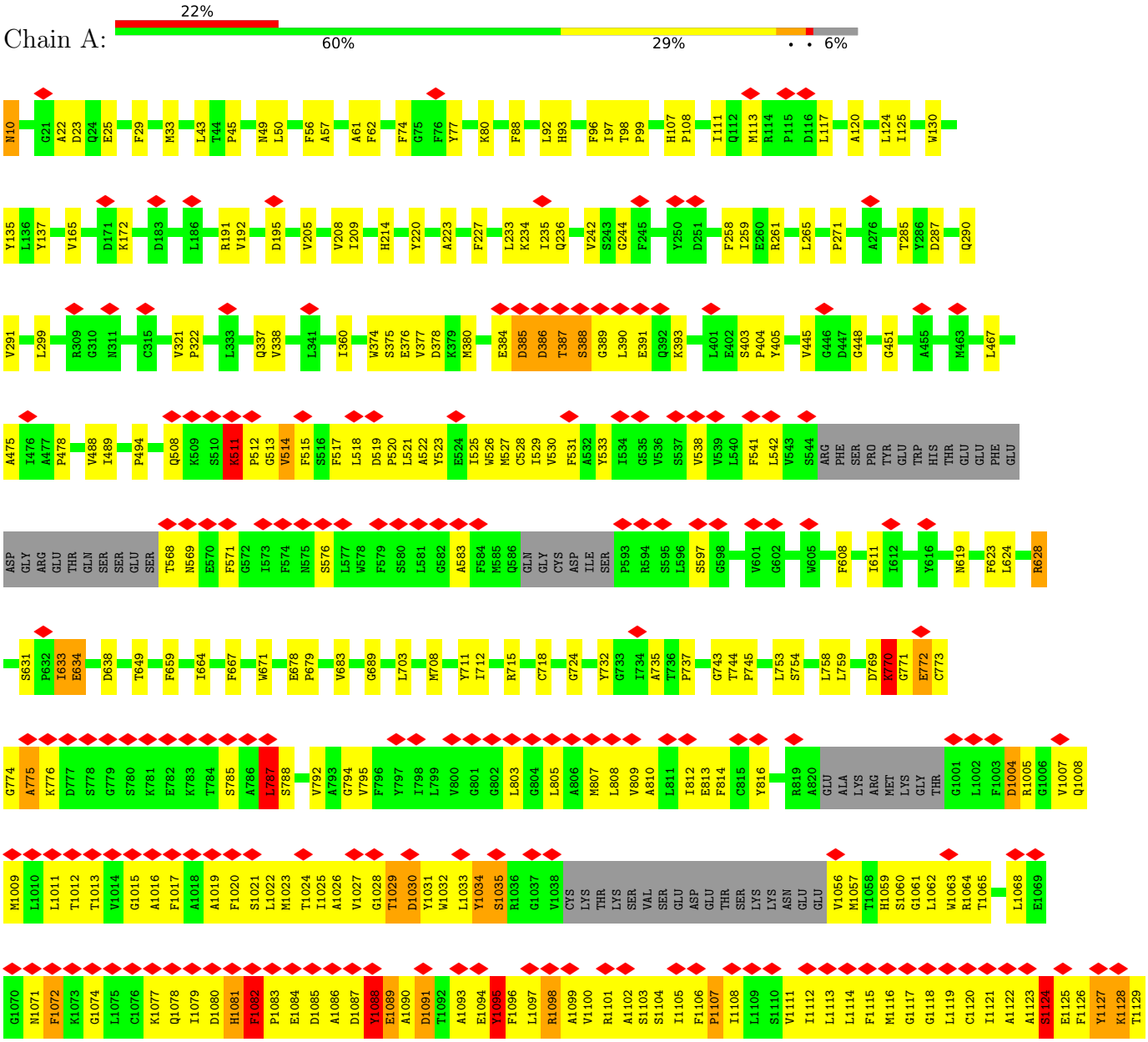
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

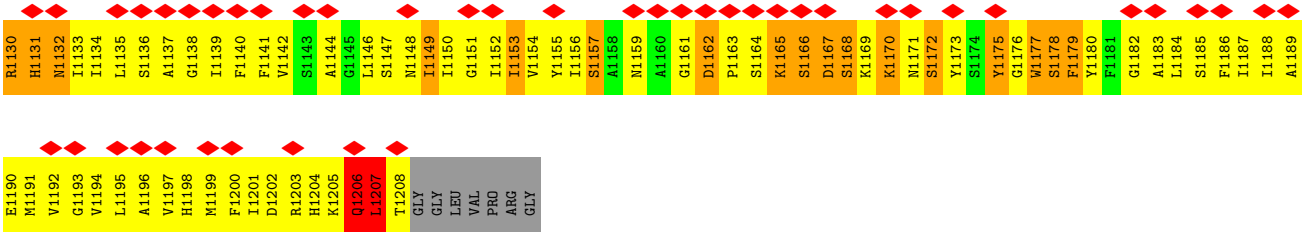
3 Residue-property plots (i)

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

- Molecule 1: Glutamate receptor 2,Voltage-dependent calcium channel gamma-2 subunit

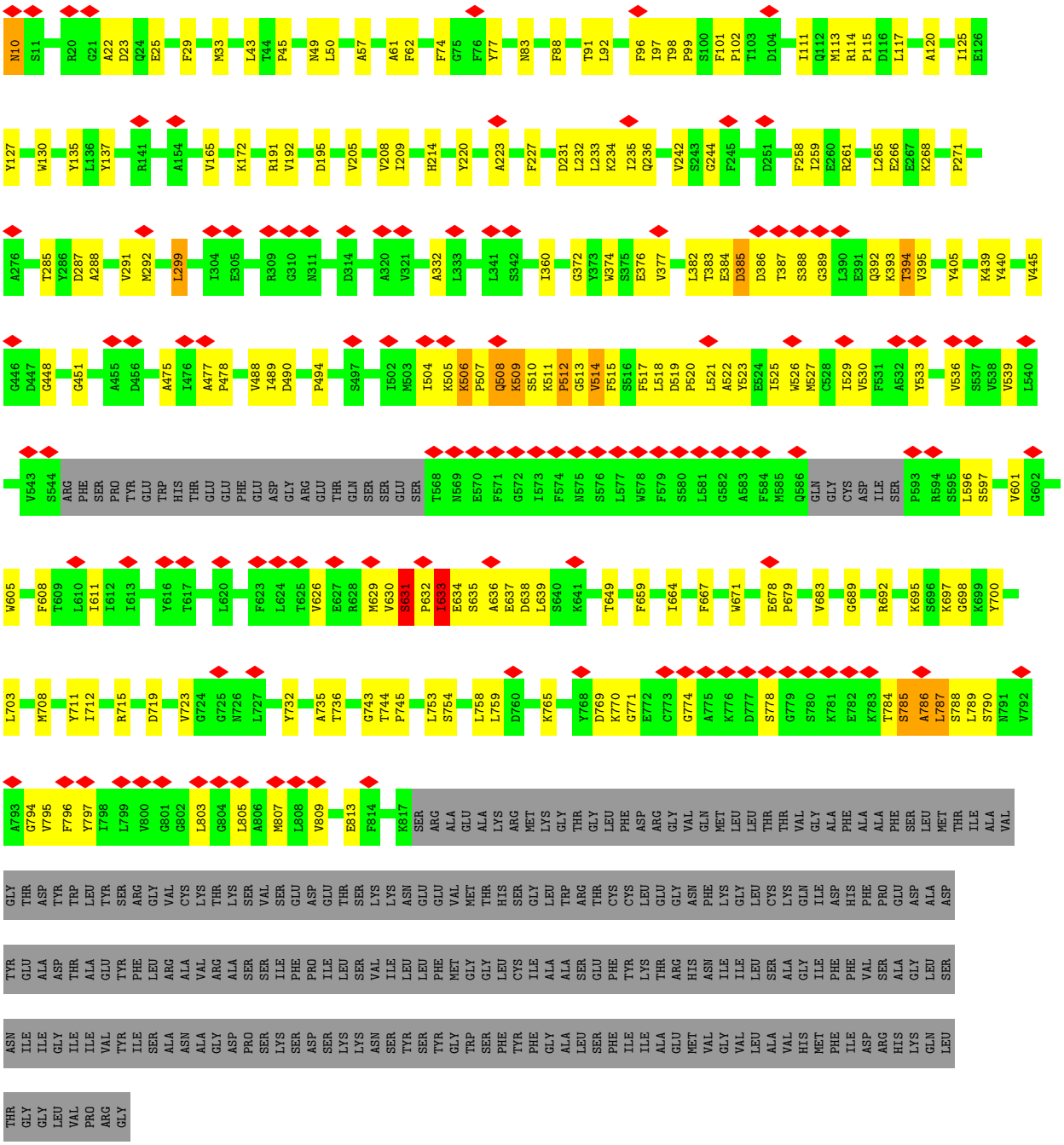
Chain A:





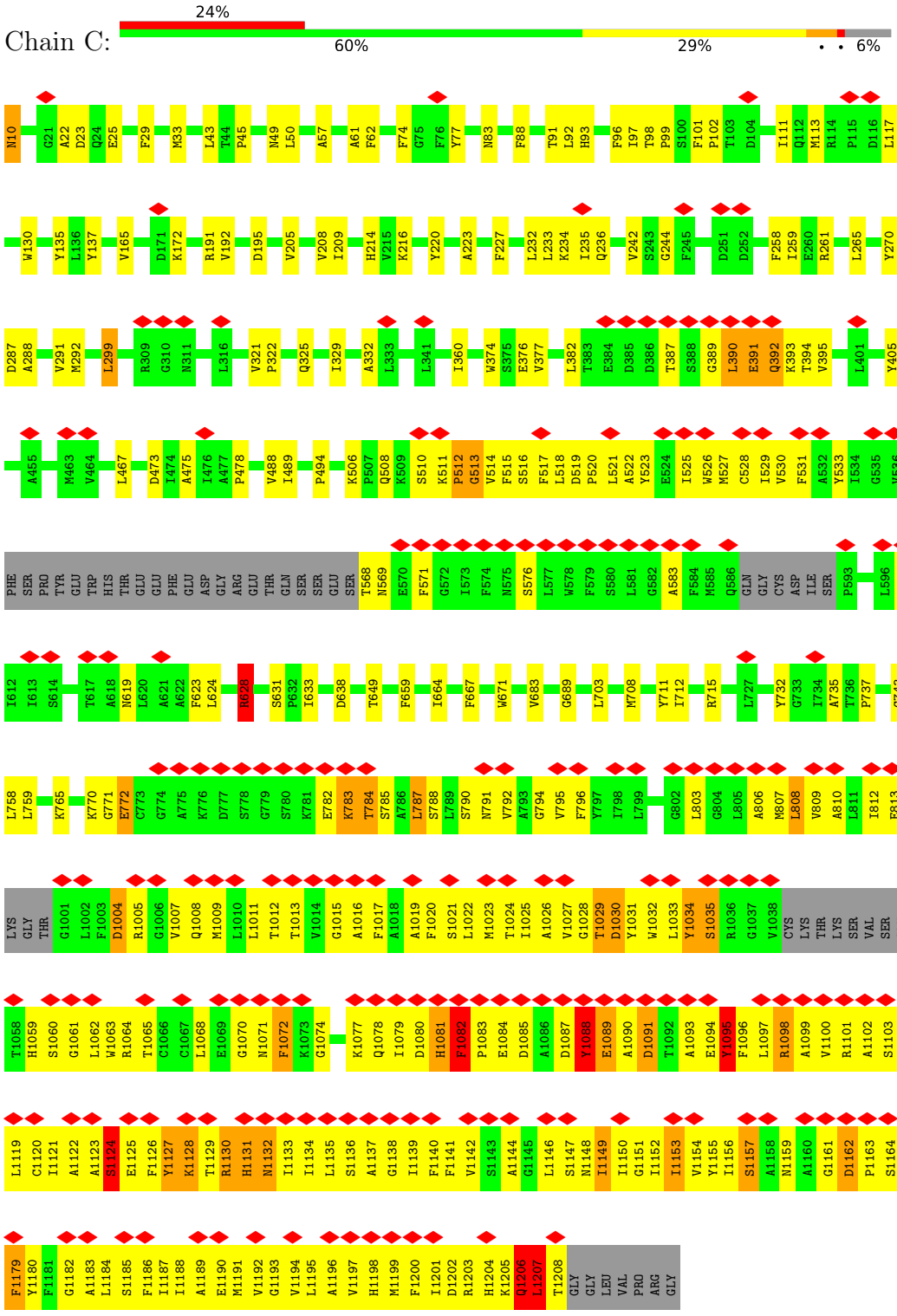
• Molecule 1: Glutamate receptor 2,Voltage-dependent calcium channel gamma-2 subunit

Chain B:



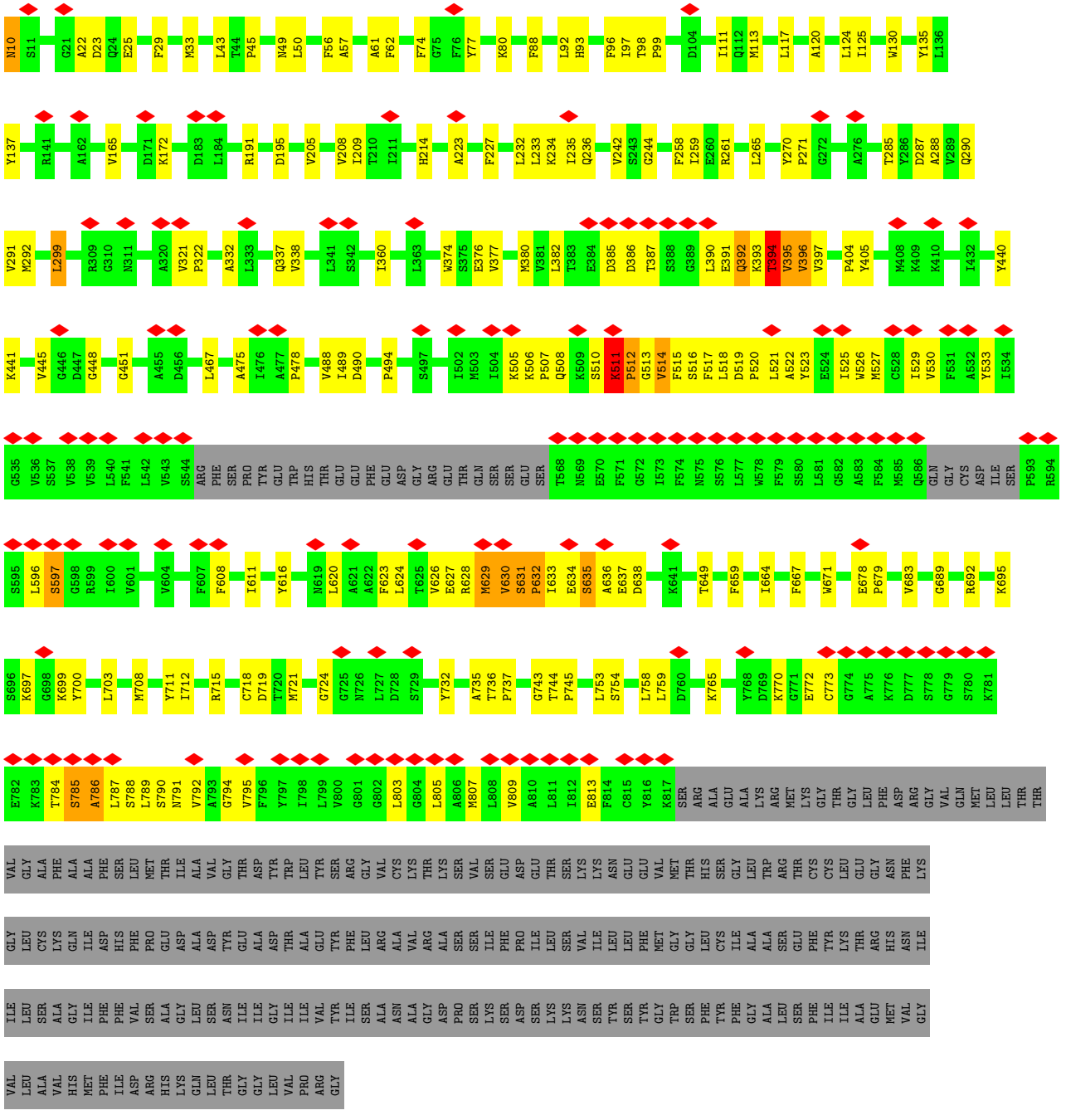
• Molecule 1: Glutamate receptor 2,Voltage-dependent calcium channel gamma-2 subunit

Chain C:



• Molecule 1: Glutamate receptor 2,Voltage-dependent calcium channel gamma-2 subunit

Chain D:


N10 S11 G21 A22 D23 Q24 E25 F29 M33 L43 T44 P45 M49 L50 F56 A57 A61 F62 F74 G75 F76 Y77 K80 F88 L92 H93 F96 I97 T98 P99 D104 I111 Q112 M113 L117 A120 L124 I125 W130 Y135 L136
Y137 R141 A162 V165 D171 K172 D183 L184 R191 D195 V205 V208 I209 T210 I211 H214 A223 F227 L232 L233 K234 I235 Q236 V242 S243 G244 F258 I259 E260 R261 L265 Y270 P271 G272 A276 T285 Y286 D287 A288 V289 Q290
V291 M292 L299 R309 G310 N311 A320 V321 P322 A332 L333 Q337 V338 L341 S342 I360 L363 W374 S375 E376 V377 M380 V381 L382 T383 E384 D385 D386 T387 S388 G389 L390 E391 Q392 K393 T394 V395 V396 V397 P404 Y405 M408 K409 K410 I432 Y440
K441 V445 G446 D447 G448 G451 A455 D456 L467 A475 I476 A477 P478 V488 I489 D490 P494 S497 I502 M503 I504 K505 K506 P507 Q508 K509 S510 K511 P512 G513 V514 F515 S516 F517 L518 D519 P520 L521 A522 Y523 E524 I525 W526 M527 C528 I529 V530 F531 A532 Y533 I534
G535 V536 S537 V538 V539 L540 F541 L542 V543 S544 ARG PHE SER PRO TYR GLU TRP HIS THR GLU GLU PHE GLU ASP GLY ARG GLU THR GLN SER SER GLU SER T568 N569 E570 F571 G572 I573 F574 N575 S576 L577 W578 F579 S580 L581 G582 A583 F584 M585 Q586 GLN GLY CYS ASP ILE SER P593 R594
S595 L596 S597 G598 R599 I600 V601 V604 F607 F608 I611 Y616 N619 L620 A621 A622 F623 L624 T625 V626 E627 R628 M629 V630 S631 P632 I633 E634 S635 A636 E637 D638 K641 T649 F659 I664 F667 W671 E678 P679 V683 G689 R692 K695
S696 K697 G698 K699 Y700 L703 M708 Y711 I712 R715 C718 D719 T720 M721 G724 G725 N726 L727 D728 S729 Y732 A735 T736 P737 G743 T744 P745 L753 S754 L758 L759 D760 K765 Y768 D769 K770 G771 E772 C773 G774 A775 K776 D777 S778 G779 S780 K781
E782 K783 T784 S785 A786 L787 S788 L789 S790 N791 V792 A793 G794 V795 F796 Y797 I798 L799 V800 G801 G802 L803 G804 L805 A806 M807 L808 V809 A810 L811 I812 E813 F814 C815 Y816 K817 SER ARG ALA GLU ALA LYS ARG MET LYS GLY THR GLY LEU PHE ASP ARG GLY VAL GLN MET LEU LEU THR THR
VAL GLY ALA PHE ALA ALA PHE SER LEU MET THR ILE ALA VAL GLY THR ASP TYR TRP LEU TYR SER ARG GLY VAL CYS LYS THR LYS SER VAL SER GLU ASP GLU THR SER LYS LYS ASN GLU GLU VAL MET THR HIS SER GLY LEU TRP ARG THR CYS CYS LEU GLU GLY ASN PHE LYS
GLY LEU CYS LYS GLN ILE ASP HIS PHE PRO GLU ASP ALA ASP TYR GLU ALA ASP THR ALA GLU TYR PHE LEU ARG ALA VAL ARG ALA SER SER ILE PHE PRO ILE LEU SER VAL ILE LEU LEU PHE MET GLY GLY LEU CYS ILE ALA ALA SER GLU PHE TYR LYS THR ARG HIS ASN ILE
ILE LEU SER ALA GLY PHE PHE VAL SER ALA GLY LEU SER ASN ILE ILE GLY ILE ILE VAL TYR ILE SER ALA ASN ALA GLY ASP PRO SER LYS SER ASP SER LYS LYS ASN SER TYR SER TYR GLY TRP SER PHE TYR PHE GLY ALA LEU SER PHE ILE ILE ALA GLU MET VAL GLY
VAL LEU ALA VAL HIS MET PHE ILE ASP ARG HIS LYS GLN LEU THR GLY GLY LEU VAL PRO ARG GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	10293	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 ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	367.19998, 367.19998, 367.19998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZK1, 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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.33	2/7267 (0.0%)	0.60	15/9925 (0.2%)
1	B	0.24	0/5768	0.37	2/7888 (0.0%)
1	C	0.34	2/7267 (0.0%)	0.54	16/9925 (0.2%)
1	D	0.23	0/5768	0.36	1/7888 (0.0%)
All	All	0.30	4/26070 (0.0%)	0.49	34/35626 (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	3
1	C	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1157	SER	C-N	-10.31	1.10	1.34
1	A	1157	SER	C-N	-10.30	1.10	1.34
1	C	808	LEU	C-N	8.81	1.54	1.34
1	A	787	LEU	C-N	-5.18	1.22	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	787	LEU	O-C-N	-28.18	77.62	122.70
1	C	628	ARG	NE-CZ-NH1	-13.77	113.42	120.30
1	A	628	ARG	NE-CZ-NH2	-12.47	114.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	628	ARG	NE-CZ-NH2	11.86	126.23	120.30
1	A	628	ARG	NE-CZ-NH1	11.01	125.80	120.30
1	A	1107	PRO	CA-N-CD	-8.70	99.33	111.50
1	C	1107	PRO	CA-N-CD	-8.69	99.34	111.50
1	C	1206	GLN	O-C-N	-8.14	109.67	122.70
1	A	1206	GLN	O-C-N	-8.12	109.70	122.70
1	A	1207	LEU	O-C-N	-8.09	109.75	122.70
1	C	1207	LEU	O-C-N	-8.09	109.76	122.70
1	C	1157	SER	C-N-CA	7.72	141.00	121.70
1	A	1157	SER	C-N-CA	7.71	140.97	121.70
1	C	1157	SER	O-C-N	-6.95	111.59	122.70
1	A	1082	PHE	N-CA-C	6.94	129.74	111.00
1	C	1082	PHE	N-CA-C	6.93	129.71	111.00
1	A	1157	SER	O-C-N	-6.92	111.62	122.70
1	A	1179	PHE	O-C-N	6.18	132.59	122.70
1	C	1179	PHE	O-C-N	6.18	132.59	122.70
1	A	628	ARG	CD-NE-CZ	5.76	131.67	123.60
1	C	628	ARG	CD-NE-CZ	5.32	131.05	123.60
1	A	1004	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	1004	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	1179	PHE	C-N-CA	-5.26	108.55	121.70
1	C	1179	PHE	C-N-CA	-5.26	108.55	121.70
1	D	511	LYS	C-N-CD	5.10	139.10	128.40
1	C	511	LYS	C-N-CD	5.07	139.05	128.40
1	B	511	LYS	C-N-CD	5.07	139.04	128.40
1	C	631	SER	C-N-CD	5.07	139.04	128.40
1	B	631	SER	C-N-CD	5.06	139.02	128.40
1	A	511	LYS	C-N-CD	5.05	139.01	128.40
1	C	506	LYS	C-N-CD	5.05	139.01	128.40
1	C	1034	TYR	CB-CA-C	-5.04	100.33	110.40
1	A	1034	TYR	CB-CA-C	-5.02	100.36	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1206	GLN	Mainchain
1	A	1207	LEU	Mainchain
1	A	787	LEU	Mainchain
1	C	1206	GLN	Mainchain
1	C	1207	LEU	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7110	0	6571	1036	0
1	B	5647	0	5177	227	0
1	C	7110	0	6573	1039	0
1	D	5647	0	5177	238	0
2	A	27	0	13	0	0
2	B	27	0	13	1	0
2	C	27	0	13	0	0
2	D	27	0	13	0	0
3	A	14	0	13	2	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	2	0
All	All	25678	0	23602	2456	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 50.

All (2456) 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:C:1114:LEU:CD1	1:C:1141:PHE:CZ	1.75	1.69
1:A:1114:LEU:CD1	1:A:1141:PHE:CZ	1.75	1.68
1:C:1134:ILE:CG2	1:C:1200:PHE:HB3	1.21	1.66
1:A:1083:PRO:HG2	1:A:1098:ARG:CG	1.16	1.62
1:A:1114:LEU:HD13	1:A:1141:PHE:CZ	1.31	1.60
1:C:1164:SER:HA	1:C:1165:LYS:CG	1.27	1.60
1:C:512:PRO:CB	1:C:790:SER:HB2	1.23	1.59
1:A:1134:ILE:CG2	1:A:1200:PHE:HB3	1.21	1.58
1:C:512:PRO:HB3	1:C:790:SER:CB	1.19	1.58
1:C:1083:PRO:HG2	1:C:1098:ARG:CG	1.16	1.57
1:C:611:ILE:HD12	1:D:517:PHE:CE1	1.36	1.57
1:A:1114:LEU:HD13	1:A:1141:PHE:CE1	1.38	1.55
1:C:568:THR:CB	1:C:1202:ASP:HB2	1.31	1.55
1:D:514:VAL:HG22	1:D:794:GLY:CA	1.30	1.55
1:A:542:LEU:CD2	1:A:1197:VAL:HG11	1.22	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:SER:HA	1:A:1165:LYS:CG	1.27	1.55
1:A:1083:PRO:CG	1:A:1098:ARG:HG3	1.06	1.53
1:C:1114:LEU:HD13	1:C:1141:PHE:CE1	1.38	1.52
1:C:541:PHE:CZ	1:C:1198:HIS:CG	1.98	1.51
1:C:1114:LEU:HD13	1:C:1141:PHE:CZ	1.31	1.50
1:C:1083:PRO:CG	1:C:1098:ARG:HG3	1.06	1.50
1:A:1102:ALA:O	1:A:1106:PHE:CD2	1.65	1.48
1:C:1102:ALA:O	1:C:1106:PHE:CD2	1.65	1.48
1:A:1182:GLY:O	1:A:1186:PHE:CD2	1.67	1.48
1:A:1083:PRO:CA	1:A:1097:LEU:HB2	1.45	1.47
1:A:1022:LEU:CD2	1:A:1185:SER:HB3	1.44	1.46
1:C:1182:GLY:O	1:C:1186:PHE:CD2	1.67	1.46
1:A:1031:TYR:CE1	1:A:1059:HIS:CD2	2.05	1.45
1:C:1164:SER:CA	1:C:1165:LYS:HG3	1.45	1.45
1:C:1022:LEU:CD2	1:C:1185:SER:HB3	1.44	1.45
1:D:512:PRO:HB3	1:D:790:SER:CB	1.43	1.45
1:D:512:PRO:CB	1:D:790:SER:HB2	1.45	1.45
1:C:1114:LEU:CD1	1:C:1141:PHE:CE2	2.00	1.44
1:A:1114:LEU:CD1	1:A:1141:PHE:CE2	2.00	1.44
1:C:1031:TYR:CE1	1:C:1059:HIS:CD2	2.05	1.44
1:A:771:GLY:HA2	1:A:772:GLU:CB	1.45	1.43
1:C:1121:ILE:HD12	1:C:1134:ILE:CG1	1.46	1.43
1:A:568:THR:CB	1:A:1202:ASP:HB2	1.46	1.43
1:A:1164:SER:CA	1:A:1165:LYS:HG3	1.45	1.43
1:A:1121:ILE:HD12	1:A:1134:ILE:CG1	1.46	1.42
1:C:1083:PRO:CA	1:C:1097:LEU:HB2	1.45	1.42
1:D:718:CYS:HB3	1:D:773:CYS:SG	1.60	1.42
1:A:542:LEU:CD2	1:A:1197:VAL:CG1	1.98	1.41
1:C:1197:VAL:CG1	1:C:1200:PHE:HE2	1.33	1.40
1:C:1083:PRO:HG3	1:C:1097:LEU:C	1.04	1.40
1:C:1197:VAL:HG13	1:C:1200:PHE:CE2	1.54	1.40
1:C:1129:THR:HB	1:C:1133:ILE:CD1	1.50	1.40
1:A:623:PHE:HE1	1:B:785:SER:CB	1.33	1.39
1:A:1083:PRO:HG3	1:A:1097:LEU:C	1.04	1.39
1:A:1197:VAL:HG13	1:A:1200:PHE:CE2	1.54	1.39
1:A:1129:THR:HB	1:A:1133:ILE:CD1	1.50	1.38
1:A:1197:VAL:CG1	1:A:1200:PHE:HE2	1.33	1.38
1:C:541:PHE:CE2	1:C:1198:HIS:CD2	2.11	1.38
1:C:541:PHE:CZ	1:C:1198:HIS:ND1	1.90	1.37
1:A:1111:VAL:O	1:A:1115:PHE:CD2	1.80	1.34
1:C:512:PRO:HB3	1:C:790:SER:CA	1.54	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:PRO:CA	1:C:790:SER:HB2	1.54	1.33
1:C:1104:SER:O	1:C:1107:PRO:CD	1.76	1.33
1:C:1111:VAL:O	1:C:1115:PHE:CD2	1.80	1.33
1:A:1083:PRO:CG	1:A:1097:LEU:C	1.96	1.33
1:D:508:GLN:HB3	1:D:629:MET:SD	1.68	1.33
1:A:771:GLY:CA	1:A:772:GLU:HB2	1.47	1.32
1:C:1121:ILE:CD1	1:C:1134:ILE:HG12	1.60	1.32
1:C:1127:TYR:CZ	1:C:1130:ARG:HA	1.64	1.32
1:C:1083:PRO:CG	1:C:1097:LEU:C	1.96	1.31
1:C:1131:HIS:O	1:C:1133:ILE:N	1.62	1.31
1:C:1134:ILE:HG22	1:C:1200:PHE:CB	1.57	1.31
1:A:1134:ILE:HG22	1:A:1200:PHE:CB	1.57	1.31
1:C:809:VAL:HA	1:C:812:ILE:CD1	1.60	1.31
1:A:1104:SER:O	1:A:1107:PRO:CD	1.76	1.30
1:A:1131:HIS:O	1:A:1133:ILE:N	1.62	1.30
1:A:1127:TYR:CZ	1:A:1130:ARG:HA	1.64	1.30
1:A:1083:PRO:CD	1:A:1098:ARG:HG3	1.62	1.30
1:A:1121:ILE:CD1	1:A:1134:ILE:HG12	1.60	1.30
1:C:611:ILE:CD1	1:D:517:PHE:CE1	2.13	1.30
1:C:531:PHE:HE2	1:C:1187:ILE:CG1	1.45	1.29
1:C:782:GLU:HA	1:C:783:LYS:CB	1.51	1.29
1:A:809:VAL:HA	1:A:812:ILE:CD1	1.60	1.29
1:C:568:THR:CB	1:C:1202:ASP:CB	2.11	1.29
1:C:1114:LEU:HD13	1:C:1141:PHE:CE2	1.65	1.28
1:A:1020:PHE:CE1	1:A:1108:ILE:HA	1.68	1.28
1:C:1020:PHE:CZ	1:C:1108:ILE:HG23	1.67	1.28
1:A:1134:ILE:CG2	1:A:1200:PHE:CB	2.08	1.28
1:A:1020:PHE:CZ	1:A:1108:ILE:HG23	1.67	1.27
1:C:1020:PHE:CE1	1:C:1108:ILE:HA	1.68	1.27
1:B:507:PRO:O	1:B:508:GLN:HG3	1.10	1.26
1:C:1083:PRO:CD	1:C:1098:ARG:HG3	1.62	1.26
1:A:1102:ALA:O	1:A:1106:PHE:HD2	0.93	1.26
1:A:541:PHE:CZ	1:A:1198:HIS:CG	2.22	1.26
1:C:1197:VAL:O	1:C:1200:PHE:CD2	1.89	1.26
1:D:508:GLN:CB	1:D:629:MET:SD	2.23	1.25
1:A:1019:ALA:HB2	1:A:1188:ILE:CG2	1.65	1.25
1:C:1134:ILE:CG2	1:C:1200:PHE:CB	2.08	1.25
1:A:1019:ALA:CB	1:A:1188:ILE:HG22	1.67	1.25
1:A:1197:VAL:O	1:A:1200:PHE:CD2	1.89	1.25
1:C:1019:ALA:HB2	1:C:1188:ILE:CG2	1.65	1.25
1:A:1114:LEU:HD13	1:A:1141:PHE:CE2	1.65	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1197:VAL:CG1	1:A:1200:PHE:CE2	2.14	1.23
1:A:1177:TRP:O	1:A:1179:PHE:N	1.70	1.23
1:C:1102:ALA:O	1:C:1106:PHE:HD2	0.93	1.23
1:A:519:ASP:O	1:B:787:LEU:HD21	1.35	1.22
1:C:1120:CYS:HA	1:C:1126:PHE:CD1	1.74	1.22
1:C:1177:TRP:O	1:C:1179:PHE:N	1.70	1.22
1:C:568:THR:O	1:C:1202:ASP:HB3	1.37	1.22
1:A:1120:CYS:HA	1:A:1126:PHE:CD1	1.74	1.22
1:C:1019:ALA:CB	1:C:1188:ILE:HG22	1.67	1.22
1:C:1197:VAL:HA	1:C:1200:PHE:CD2	1.75	1.21
1:A:1016:ALA:HA	1:A:1192:VAL:CG1	1.69	1.21
1:C:1016:ALA:HA	1:C:1192:VAL:CG1	1.70	1.21
1:A:1197:VAL:HA	1:A:1200:PHE:CD2	1.75	1.21
1:A:623:PHE:CE1	1:B:785:SER:CB	2.24	1.20
1:A:1114:LEU:HD11	1:A:1141:PHE:CE2	1.71	1.20
1:C:1031:TYR:HE1	1:C:1059:HIS:CD2	1.49	1.20
1:C:1114:LEU:HD13	1:C:1141:PHE:CD1	1.76	1.20
1:A:1114:LEU:HD13	1:A:1141:PHE:CD1	1.76	1.20
1:C:1129:THR:CB	1:C:1133:ILE:HD11	1.72	1.20
1:A:1063:TRP:NE1	1:A:1081:HIS:CE1	2.10	1.19
1:C:1017:PHE:CE1	1:C:1115:PHE:HB3	1.77	1.19
1:A:1189:ALA:O	1:A:1192:VAL:HG22	1.43	1.19
1:A:1034:TYR:O	1:A:1173:TYR:HB3	1.38	1.19
1:C:1197:VAL:CG1	1:C:1200:PHE:CE2	2.14	1.19
1:A:1121:ILE:CG2	1:A:1133:ILE:CG2	2.19	1.18
1:A:1017:PHE:CE1	1:A:1115:PHE:HB3	1.77	1.18
1:A:1194:VAL:O	1:A:1198:HIS:HD2	1.24	1.18
1:C:1063:TRP:NE1	1:C:1081:HIS:CE1	2.10	1.18
1:C:1121:ILE:CG2	1:C:1133:ILE:CG2	2.19	1.18
1:A:531:PHE:HE2	1:A:1187:ILE:HG12	1.09	1.17
1:D:514:VAL:CG2	1:D:794:GLY:HA2	1.73	1.17
1:C:1034:TYR:O	1:C:1173:TYR:HB3	1.38	1.17
1:A:1129:THR:CB	1:A:1133:ILE:HD11	1.72	1.17
1:C:1189:ALA:O	1:C:1192:VAL:HG22	1.43	1.17
1:C:1107:PRO:HD2	1:C:1108:ILE:H	1.08	1.17
1:C:1194:VAL:O	1:C:1198:HIS:HD2	1.24	1.17
1:A:1016:ALA:HB2	1:A:1192:VAL:HB	1.16	1.16
1:C:1129:THR:HB	1:C:1133:ILE:CG1	1.75	1.15
1:A:1129:THR:HB	1:A:1133:ILE:CG1	1.75	1.15
1:A:568:THR:CB	1:A:1202:ASP:CB	2.25	1.15
1:B:611:ILE:HD12	1:C:517:PHE:CE1	1.81	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:787:LEU:HD13	1:C:788:SER:H	1.11	1.15
1:A:1104:SER:O	1:A:1107:PRO:CG	1.94	1.15
1:D:718:CYS:CB	1:D:773:CYS:SG	2.33	1.15
1:A:1031:TYR:HE1	1:A:1059:HIS:CD2	1.49	1.15
1:A:1121:ILE:HG22	1:A:1133:ILE:HB	1.27	1.15
1:C:1121:ILE:HG22	1:C:1133:ILE:HB	1.27	1.15
1:C:538:VAL:CG2	1:C:1194:VAL:HG22	1.76	1.14
1:A:541:PHE:CZ	1:A:1198:HIS:ND1	2.15	1.14
1:C:1104:SER:O	1:C:1107:PRO:CG	1.94	1.14
1:A:1126:PHE:HB3	1:A:1127:TYR:HA	1.26	1.14
1:A:1169:LYS:H	1:A:1172:SER:HB3	1.01	1.14
1:C:531:PHE:CZ	1:C:1187:ILE:HD11	1.81	1.14
1:A:1013:THR:O	1:A:1017:PHE:CD2	2.01	1.14
1:C:1020:PHE:O	1:C:1023:MET:HG2	1.46	1.14
1:A:1020:PHE:O	1:A:1023:MET:HG2	1.46	1.14
1:A:1182:GLY:O	1:A:1186:PHE:HD2	0.79	1.14
1:A:1107:PRO:HD2	1:A:1108:ILE:H	1.08	1.13
1:C:1013:THR:O	1:C:1017:PHE:CD2	2.01	1.13
1:D:514:VAL:CG2	1:D:794:GLY:CA	2.24	1.13
1:B:632:PRO:O	1:B:633:ILE:HG23	1.48	1.12
1:B:611:ILE:HD12	1:C:517:PHE:HE1	0.96	1.12
1:C:394:THR:CG2	1:C:395:VAL:H	1.63	1.12
1:C:394:THR:HG22	1:C:395:VAL:N	1.61	1.12
1:C:531:PHE:HE2	1:C:1187:ILE:HG12	0.98	1.12
1:A:1016:ALA:CB	1:A:1192:VAL:HB	1.79	1.12
1:A:1082:PHE:O	1:A:1097:LEU:HD13	1.50	1.12
1:A:1121:ILE:HB	1:A:1134:ILE:HG13	1.29	1.12
1:A:541:PHE:CE2	1:A:1198:HIS:CD2	2.38	1.11
1:B:611:ILE:CD1	1:C:517:PHE:HE1	1.63	1.11
1:C:1016:ALA:CB	1:C:1192:VAL:HB	1.79	1.11
1:C:541:PHE:CZ	1:C:1198:HIS:CE1	2.38	1.11
1:C:1114:LEU:HD12	1:C:1141:PHE:CZ	1.73	1.11
1:A:1111:VAL:HA	1:A:1114:LEU:CD2	1.80	1.11
1:C:1127:TYR:H	1:C:1128:LYS:HA	1.02	1.11
1:A:1176:GLY:HA2	1:A:1177:TRP:CB	1.75	1.11
1:A:810:ALA:O	1:A:814:PHE:CD2	2.04	1.11
1:C:1111:VAL:HA	1:C:1114:LEU:CD2	1.80	1.11
1:A:1152:ILE:CG1	1:A:1186:PHE:CE2	2.34	1.10
1:C:1016:ALA:CA	1:C:1192:VAL:HG11	1.80	1.10
1:C:1129:THR:HG22	1:C:1133:ILE:HG13	1.34	1.10
1:C:1182:GLY:O	1:C:1186:PHE:HD2	0.79	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:ILE:HG21	1:B:723:VAL:HG11	1.30	1.10
1:C:531:PHE:CE2	1:C:1187:ILE:HG12	1.84	1.10
1:C:1062:LEU:O	1:C:1081:HIS:HA	1.50	1.10
1:A:809:VAL:HA	1:A:812:ILE:HD11	1.32	1.10
1:A:1016:ALA:CA	1:A:1192:VAL:HG11	1.80	1.10
1:A:1081:HIS:CD2	1:A:1101:ARG:CD	2.35	1.10
1:C:1114:LEU:HD11	1:C:1141:PHE:CE2	1.71	1.10
1:C:1121:ILE:HB	1:C:1134:ILE:HG13	1.30	1.10
1:C:1152:ILE:CG1	1:C:1186:PHE:CE2	2.34	1.10
1:C:1169:LYS:H	1:C:1172:SER:HB3	1.01	1.10
1:B:394:THR:HG22	1:B:395:VAL:H	1.06	1.10
1:C:538:VAL:HG21	1:C:1194:VAL:HG22	1.28	1.10
1:C:1126:PHE:HB3	1:C:1127:TYR:HA	1.26	1.10
1:C:809:VAL:HA	1:C:812:ILE:CG1	1.82	1.10
1:C:810:ALA:O	1:C:814:PHE:CD2	2.04	1.10
1:C:1029:THR:HB	1:C:1178:SER:CB	1.82	1.10
1:C:1121:ILE:CG2	1:C:1133:ILE:HB	1.82	1.09
1:C:1152:ILE:HG13	1:C:1186:PHE:CE2	1.87	1.09
1:A:1127:TYR:H	1:A:1128:LYS:HA	1.02	1.09
1:A:1152:ILE:HG13	1:A:1186:PHE:CE2	1.87	1.09
1:C:1082:PHE:O	1:C:1097:LEU:HD13	1.50	1.09
1:C:1129:THR:CG2	1:C:1133:ILE:HG13	1.82	1.09
1:A:1111:VAL:O	1:A:1115:PHE:HD2	1.20	1.09
1:B:507:PRO:O	1:B:508:GLN:CG	1.99	1.09
1:B:507:PRO:HG2	1:B:631:SER:HB3	1.33	1.09
1:A:809:VAL:HA	1:A:812:ILE:CG1	1.81	1.09
1:C:520:PRO:O	1:D:787:LEU:CD2	2.01	1.09
1:C:1081:HIS:CD2	1:C:1101:ARG:CD	2.35	1.09
1:C:1083:PRO:HG3	1:C:1098:ARG:N	1.67	1.09
1:A:531:PHE:HE2	1:A:1187:ILE:CG1	1.64	1.08
1:A:1062:LEU:O	1:A:1081:HIS:HA	1.50	1.08
1:A:1020:PHE:HE1	1:A:1108:ILE:HA	0.96	1.08
1:A:1114:LEU:HD22	1:A:1141:PHE:HA	1.36	1.08
1:C:812:ILE:O	1:C:816:TYR:CD2	2.06	1.08
1:A:1083:PRO:HG2	1:A:1098:ARG:CB	1.83	1.08
1:A:542:LEU:HD23	1:A:1197:VAL:HG11	1.11	1.08
1:A:1029:THR:HB	1:A:1178:SER:CB	1.82	1.08
1:A:1121:ILE:CG2	1:A:1133:ILE:HB	1.82	1.08
1:A:1129:THR:CG2	1:A:1133:ILE:HG13	1.82	1.08
1:A:1176:GLY:CA	1:A:1177:TRP:HB2	1.83	1.08
1:C:1029:THR:HB	1:C:1178:SER:HB3	1.33	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:TYR:N	1:A:1128:LYS:HA	1.62	1.07
1:A:1114:LEU:HD12	1:A:1141:PHE:CZ	1.73	1.07
1:C:1016:ALA:HB2	1:C:1192:VAL:HB	1.16	1.07
1:C:1083:PRO:HG2	1:C:1098:ARG:CB	1.83	1.07
1:A:1083:PRO:HG3	1:A:1098:ARG:N	1.67	1.07
1:A:1127:TYR:HB2	1:A:1129:THR:H	0.92	1.07
1:B:509:LYS:HG2	1:B:510:SER:H	1.12	1.07
1:C:531:PHE:CE2	1:C:1187:ILE:CG1	2.37	1.07
1:C:1176:GLY:HA2	1:C:1177:TRP:CB	1.75	1.07
1:A:812:ILE:O	1:A:816:TYR:CD2	2.06	1.07
1:B:508:GLN:HG2	1:B:629:MET:HG3	1.34	1.07
1:C:1020:PHE:HE1	1:C:1108:ILE:HA	0.97	1.07
1:C:1176:GLY:CA	1:C:1177:TRP:HB2	1.83	1.07
1:C:1199:MET:HA	1:C:1202:ASP:OD2	1.56	1.06
1:A:1156:ILE:HB	1:A:1175:TYR:OH	1.54	1.06
1:A:1020:PHE:CD1	1:A:1111:VAL:HG11	1.90	1.06
1:C:541:PHE:CE1	1:C:1198:HIS:CE1	2.42	1.06
1:C:1083:PRO:HA	1:C:1097:LEU:CB	1.85	1.06
1:B:507:PRO:HG2	1:B:631:SER:CB	1.84	1.06
1:C:1009:MET:SD	1:C:1199:MET:SD	2.54	1.06
1:C:1164:SER:CA	1:C:1165:LYS:CG	2.15	1.06
1:A:568:THR:O	1:A:1202:ASP:HB3	1.54	1.06
1:A:1083:PRO:HA	1:A:1097:LEU:CB	1.85	1.06
1:C:568:THR:C	1:C:1202:ASP:CB	2.23	1.06
1:C:1020:PHE:CD1	1:C:1111:VAL:HG11	1.90	1.06
1:C:1081:HIS:CD2	1:C:1101:ARG:HD3	1.91	1.06
1:D:508:GLN:CA	1:D:629:MET:SD	2.44	1.06
1:C:1127:TYR:HB2	1:C:1129:THR:H	0.92	1.05
1:A:1009:MET:SD	1:A:1199:MET:SD	2.54	1.05
1:A:1029:THR:HB	1:A:1178:SER:HB3	1.33	1.05
1:C:1127:TYR:N	1:C:1128:LYS:HA	1.62	1.05
1:C:1156:ILE:HB	1:C:1175:TYR:OH	1.54	1.05
1:A:1020:PHE:CE1	1:A:1111:VAL:HB	1.91	1.05
1:A:809:VAL:O	1:A:813:GLU:HG3	1.56	1.05
1:B:506:LYS:HG2	1:B:719:ASP:HA	1.35	1.05
1:C:1020:PHE:CE1	1:C:1111:VAL:HB	1.91	1.05
1:A:1020:PHE:HZ	1:A:1108:ILE:CG2	1.70	1.05
1:C:809:VAL:HA	1:C:812:ILE:HD11	1.32	1.05
1:C:1127:TYR:CE2	1:C:1130:ARG:HG3	1.92	1.05
1:A:1197:VAL:CA	1:A:1200:PHE:CD2	2.40	1.04
1:A:1063:TRP:CE2	1:A:1081:HIS:CE1	2.46	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1199:MET:HA	1:A:1202:ASP:OD2	1.56	1.04
1:C:568:THR:C	1:C:1202:ASP:HB3	1.75	1.04
1:C:1176:GLY:HA2	1:C:1177:TRP:HB2	1.05	1.04
1:A:542:LEU:HD21	1:A:1197:VAL:HG11	1.05	1.04
1:A:1023:MET:CE	1:A:1148:ASN:HD21	1.71	1.04
1:A:1084:GLU:HG2	1:A:1085:ASP:H	1.22	1.04
1:C:1197:VAL:CA	1:C:1200:PHE:CE2	2.41	1.04
1:A:1021:SER:O	1:A:1024:THR:HG22	1.58	1.04
1:A:1127:TYR:CE2	1:A:1130:ARG:HG3	1.92	1.04
1:B:630:VAL:HG22	1:B:631:SER:H	1.22	1.04
1:A:1197:VAL:O	1:A:1200:PHE:CE2	2.10	1.03
1:C:517:PHE:CZ	1:C:526:TRP:CH2	2.45	1.03
1:A:1013:THR:O	1:A:1017:PHE:HD2	1.37	1.03
1:C:1004:ASP:O	1:C:1008:GLN:CB	2.06	1.03
1:A:1022:LEU:CD2	1:A:1185:SER:CB	2.35	1.03
1:A:1114:LEU:CD1	1:A:1141:PHE:CE1	2.15	1.03
1:A:1129:THR:HG22	1:A:1133:ILE:HG13	1.34	1.03
1:C:1022:LEU:HD22	1:C:1185:SER:HB3	1.41	1.03
1:C:1063:TRP:CE2	1:C:1081:HIS:CE1	2.46	1.03
1:C:1114:LEU:HD22	1:C:1141:PHE:HA	1.36	1.03
1:C:1197:VAL:O	1:C:1200:PHE:CE2	2.10	1.03
1:C:1197:VAL:CA	1:C:1200:PHE:CD2	2.40	1.03
1:A:1004:ASP:O	1:A:1008:GLN:CB	2.06	1.03
1:C:1021:SER:O	1:C:1024:THR:HG22	1.58	1.03
1:A:1081:HIS:CD2	1:A:1101:ARG:HD3	1.91	1.03
1:A:1197:VAL:CA	1:A:1200:PHE:CE2	2.41	1.03
1:C:809:VAL:O	1:C:813:GLU:HG3	1.56	1.03
1:C:1022:LEU:HD23	1:C:1185:SER:CB	1.88	1.03
1:C:1020:PHE:HZ	1:C:1108:ILE:CG2	1.70	1.02
1:A:1196:ALA:HA	1:A:1199:MET:HE3	1.40	1.02
1:C:611:ILE:CD1	1:D:517:PHE:HE1	1.60	1.02
1:C:1022:LEU:CD2	1:C:1185:SER:CB	2.35	1.02
1:C:1023:MET:CE	1:C:1148:ASN:HD21	1.71	1.02
1:A:1022:LEU:HD23	1:A:1185:SER:CB	1.88	1.02
1:B:506:LYS:HG2	1:B:719:ASP:CA	1.89	1.02
1:A:1114:LEU:HD22	1:A:1141:PHE:CA	1.89	1.02
1:B:626:VAL:HB	1:C:628:ARG:HH11	1.24	1.02
1:C:1009:MET:O	1:C:1013:THR:HG23	1.59	1.02
1:C:1031:TYR:CD1	1:C:1059:HIS:CD2	2.48	1.02
1:C:541:PHE:CE1	1:C:1198:HIS:ND1	2.27	1.02
1:C:1127:TYR:HE2	1:C:1130:ARG:HG3	1.20	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1131:HIS:HD2	1:C:1207:LEU:HD12	1.25	1.02
1:A:1121:ILE:CD1	1:A:1134:ILE:HA	1.90	1.01
1:A:1121:ILE:HG21	1:A:1133:ILE:CG2	1.90	1.01
1:B:611:ILE:CD1	1:C:517:PHE:CE1	2.40	1.01
1:C:541:PHE:CE2	1:C:1198:HIS:CG	2.38	1.01
1:C:1121:ILE:CD1	1:C:1134:ILE:HA	1.90	1.01
1:C:1121:ILE:HG21	1:C:1133:ILE:CG2	1.90	1.01
1:A:1121:ILE:HG21	1:A:1133:ILE:HG22	1.43	1.01
1:C:1083:PRO:HG3	1:C:1097:LEU:O	1.58	1.01
1:C:1189:ALA:O	1:C:1192:VAL:CG2	2.08	1.01
1:A:1023:MET:HE3	1:A:1148:ASN:ND2	1.76	1.01
1:C:1083:PRO:HG3	1:C:1097:LEU:CA	1.90	1.01
1:A:1009:MET:O	1:A:1013:THR:HG23	1.59	1.01
1:A:1164:SER:CA	1:A:1165:LYS:CG	2.15	1.01
1:C:1104:SER:C	1:C:1107:PRO:HD3	1.81	1.01
1:C:1104:SER:C	1:C:1107:PRO:CD	2.29	1.01
1:C:1159:ASN:ND2	1:C:1175:TYR:CE1	2.29	1.01
1:A:1104:SER:C	1:A:1107:PRO:CD	2.29	1.01
1:A:1121:ILE:CG2	1:A:1133:ILE:CB	2.39	1.01
1:C:1016:ALA:HA	1:C:1192:VAL:HG11	1.03	1.01
1:A:1114:LEU:HD13	1:A:1141:PHE:CD2	1.96	1.00
1:C:1083:PRO:CG	1:C:1098:ARG:CG	1.97	1.00
1:C:1196:ALA:HA	1:C:1199:MET:HE3	1.40	1.00
1:A:531:PHE:CE2	1:A:1187:ILE:HG12	1.96	1.00
1:A:1020:PHE:CG	1:A:1111:VAL:HG11	1.96	1.00
1:A:1104:SER:C	1:A:1107:PRO:HD3	1.81	1.00
1:C:1114:LEU:HD13	1:C:1141:PHE:CD2	1.96	1.00
1:C:1114:LEU:HD22	1:C:1141:PHE:CA	1.89	1.00
1:A:1159:ASN:ND2	1:A:1175:TYR:CE1	2.29	1.00
1:A:1189:ALA:O	1:A:1192:VAL:CG2	2.08	1.00
1:C:1034:TYR:CE2	1:C:1059:HIS:HB3	1.96	1.00
1:C:1104:SER:O	1:C:1107:PRO:HG2	1.60	1.00
1:A:1022:LEU:HD22	1:A:1185:SER:HB3	1.41	1.00
1:A:1031:TYR:CD1	1:A:1059:HIS:CD2	2.48	1.00
1:C:1121:ILE:CG2	1:C:1133:ILE:CB	2.39	1.00
1:A:1083:PRO:CG	1:A:1097:LEU:O	2.06	1.00
1:A:1176:GLY:HA2	1:A:1177:TRP:HB2	1.05	1.00
1:A:1127:TYR:HB2	1:A:1129:THR:N	1.76	1.00
1:A:1016:ALA:HA	1:A:1192:VAL:HG11	1.03	0.99
1:B:507:PRO:CB	1:B:630:VAL:O	2.10	0.99
1:C:1083:PRO:CG	1:C:1097:LEU:O	2.06	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1121:ILE:HG21	1:C:1133:ILE:HG22	1.43	0.99
1:C:1114:LEU:CD1	1:C:1141:PHE:CE1	2.15	0.99
1:A:1197:VAL:HA	1:A:1200:PHE:HD2	1.23	0.99
1:C:1127:TYR:HB2	1:C:1129:THR:N	1.76	0.99
1:A:1083:PRO:HG3	1:A:1097:LEU:CA	1.90	0.99
1:A:1083:PRO:HG3	1:A:1097:LEU:O	1.58	0.99
1:C:568:THR:CA	1:C:1202:ASP:HB2	1.91	0.99
1:C:1020:PHE:CG	1:C:1111:VAL:HG11	1.96	0.99
1:A:611:ILE:HD12	1:B:517:PHE:CE1	1.97	0.99
1:A:771:GLY:CA	1:A:772:GLU:CB	2.18	0.98
1:A:1029:THR:O	1:A:1031:TYR:N	1.96	0.98
1:A:1034:TYR:CE2	1:A:1059:HIS:HB3	1.96	0.98
1:A:1063:TRP:CZ2	1:A:1081:HIS:HE1	1.81	0.98
1:A:1104:SER:O	1:A:1107:PRO:HD2	1.60	0.98
1:A:611:ILE:HD12	1:B:517:PHE:HE1	1.25	0.98
1:C:611:ILE:HD11	1:D:517:PHE:CZ	1.99	0.98
1:C:1127:TYR:CB	1:C:1129:THR:H	1.77	0.98
1:A:1083:PRO:CA	1:A:1097:LEU:CB	2.41	0.98
1:A:1104:SER:O	1:A:1107:PRO:HG2	1.60	0.98
1:C:1194:VAL:O	1:C:1198:HIS:CD2	2.16	0.98
1:D:508:GLN:HG2	1:D:629:MET:HG3	1.45	0.98
1:A:812:ILE:O	1:A:816:TYR:HD2	1.44	0.98
1:A:1182:GLY:C	1:A:1186:PHE:HD2	1.67	0.98
1:C:1111:VAL:O	1:C:1115:PHE:HD2	1.21	0.98
1:A:1127:TYR:HE2	1:A:1130:ARG:HG3	1.20	0.98
1:B:507:PRO:HG2	1:B:631:SER:CA	1.94	0.98
1:C:1063:TRP:CZ2	1:C:1081:HIS:HE1	1.81	0.98
1:C:1104:SER:O	1:C:1107:PRO:HD2	1.60	0.98
1:D:514:VAL:HG22	1:D:794:GLY:HA3	1.39	0.98
1:B:507:PRO:HB2	1:B:630:VAL:O	1.64	0.97
1:C:611:ILE:CD1	1:D:517:PHE:CZ	2.47	0.97
1:C:782:GLU:CA	1:C:783:LYS:CB	2.41	0.97
1:C:812:ILE:O	1:C:816:TYR:HD2	1.44	0.97
1:A:519:ASP:O	1:B:787:LEU:CD2	2.11	0.97
1:A:1131:HIS:HD2	1:A:1207:LEU:HD12	1.25	0.97
1:A:1020:PHE:HZ	1:A:1108:ILE:HG23	0.98	0.97
1:A:1153:ILE:HG12	1:A:1156:ILE:HD11	1.45	0.97
1:C:512:PRO:CB	1:C:790:SER:CB	2.01	0.97
1:A:1194:VAL:O	1:A:1198:HIS:CD2	2.16	0.97
1:A:1197:VAL:HA	1:A:1200:PHE:CE2	2.00	0.97
1:D:517:PHE:CE2	1:D:526:TRP:CH2	2.53	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1083:PRO:CA	1:C:1097:LEU:CB	2.41	0.97
1:C:1084:GLU:HG2	1:C:1085:ASP:H	1.22	0.97
1:A:718:CYS:HB3	1:A:776:LYS:CB	1.95	0.97
1:A:1111:VAL:HA	1:A:1114:LEU:HD21	1.47	0.96
1:B:394:THR:HG22	1:B:395:VAL:N	1.80	0.96
1:C:1083:PRO:HA	1:C:1097:LEU:HB2	0.98	0.96
1:B:394:THR:HG23	1:B:439:LYS:C	1.85	0.96
1:C:1056:VAL:HG12	1:C:1057:MET:N	1.80	0.96
1:C:1129:THR:HB	1:C:1133:ILE:HD11	0.96	0.96
1:C:1197:VAL:HA	1:C:1200:PHE:CE2	2.00	0.96
1:A:1056:VAL:HG12	1:A:1057:MET:N	1.80	0.96
1:C:1029:THR:O	1:C:1031:TYR:N	1.96	0.96
1:C:1022:LEU:HD23	1:C:1185:SER:HB3	0.98	0.96
1:A:1017:PHE:HE1	1:A:1115:PHE:HB3	1.25	0.96
1:A:1083:PRO:HA	1:A:1097:LEU:HB2	0.98	0.96
1:A:1034:TYR:CD2	1:A:1059:HIS:HB3	2.00	0.96
1:A:1016:ALA:CA	1:A:1192:VAL:CG1	2.42	0.96
1:A:1063:TRP:HE1	1:A:1081:HIS:CE1	1.75	0.96
1:A:1127:TYR:CB	1:A:1129:THR:H	1.77	0.96
1:C:1063:TRP:HE1	1:C:1081:HIS:CE1	1.75	0.96
1:C:1153:ILE:HG12	1:C:1156:ILE:HD11	1.45	0.96
1:C:1020:PHE:HZ	1:C:1108:ILE:HG23	0.98	0.96
1:C:1034:TYR:CD2	1:C:1059:HIS:HB3	2.00	0.95
1:A:1121:ILE:HD12	1:A:1134:ILE:CB	1.96	0.95
1:C:1182:GLY:C	1:C:1186:PHE:HD2	1.67	0.95
1:D:631:SER:HB3	1:D:632:PRO:HD2	1.48	0.95
1:D:718:CYS:CB	1:D:773:CYS:HG	1.74	0.95
1:A:1029:THR:CB	1:A:1178:SER:HB3	1.97	0.95
1:A:1129:THR:HB	1:A:1133:ILE:HD11	0.96	0.95
1:C:1129:THR:CB	1:C:1133:ILE:CG1	2.45	0.95
1:A:531:PHE:CZ	1:A:1187:ILE:HD11	2.02	0.95
1:C:1111:VAL:HA	1:C:1114:LEU:HD21	1.47	0.95
1:D:508:GLN:HB3	1:D:629:MET:CE	1.95	0.95
1:A:511:LYS:H	1:A:512:PRO:HD3	1.30	0.95
1:A:809:VAL:HA	1:A:812:ILE:HG12	1.49	0.95
1:C:512:PRO:CB	1:C:790:SER:CA	2.39	0.95
1:C:568:THR:CB	1:C:1202:ASP:CA	2.44	0.95
1:C:1029:THR:CB	1:C:1178:SER:HB3	1.97	0.95
1:A:787:LEU:HG	1:A:788:SER:H	1.30	0.95
1:A:1022:LEU:HD23	1:A:1185:SER:HB3	0.98	0.95
1:A:1056:VAL:HG12	1:A:1057:MET:H	1.32	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1129:THR:CB	1:A:1133:ILE:CG1	2.45	0.95
1:A:1004:ASP:O	1:A:1008:GLN:N	2.00	0.94
1:C:1062:LEU:O	1:C:1081:HIS:CA	2.15	0.94
1:A:520:PRO:O	1:B:787:LEU:HG	1.66	0.94
1:A:1062:LEU:O	1:A:1081:HIS:CA	2.15	0.94
1:C:1121:ILE:HD12	1:C:1134:ILE:CB	1.96	0.94
1:A:1035:SER:HA	1:A:1173:TYR:CD2	2.02	0.94
1:C:1013:THR:O	1:C:1017:PHE:HD2	1.37	0.94
1:C:1056:VAL:HG12	1:C:1057:MET:H	1.32	0.94
1:C:1023:MET:HE3	1:C:1148:ASN:ND2	1.82	0.94
1:C:1004:ASP:O	1:C:1008:GLN:N	2.00	0.94
1:C:809:VAL:HA	1:C:812:ILE:HG12	1.49	0.94
1:A:1114:LEU:HD13	1:A:1141:PHE:CG	2.03	0.94
1:A:1197:VAL:HG13	1:A:1200:PHE:CZ	2.03	0.94
1:A:1197:VAL:C	1:A:1200:PHE:CD2	2.41	0.94
1:C:1007:VAL:O	1:C:1011:LEU:HG	1.67	0.94
1:A:541:PHE:CZ	1:A:1198:HIS:CE1	2.55	0.94
1:A:1199:MET:O	1:A:1202:ASP:OD1	1.86	0.93
1:C:1035:SER:HA	1:C:1173:TYR:CD2	2.02	0.93
1:C:1121:ILE:HD13	1:C:1134:ILE:HA	1.48	0.93
1:A:1007:VAL:O	1:A:1011:LEU:HG	1.67	0.93
1:C:394:THR:HG22	1:C:395:VAL:H	0.78	0.93
1:C:1197:VAL:HA	1:C:1200:PHE:HD2	1.23	0.93
1:A:1020:PHE:CD1	1:A:1111:VAL:CG1	2.51	0.93
1:C:1124:SER:HB3	1:C:1125:GLU:C	1.88	0.93
1:D:718:CYS:HB3	1:D:773:CYS:HG	1.19	0.93
1:A:1121:ILE:CD1	1:A:1134:ILE:CG1	2.31	0.93
1:C:1020:PHE:CD1	1:C:1111:VAL:CG1	2.51	0.93
1:C:1114:LEU:HD13	1:C:1141:PHE:CG	2.03	0.93
1:C:541:PHE:HZ	1:C:1198:HIS:CG	1.64	0.92
1:C:1199:MET:O	1:C:1202:ASP:OD1	1.86	0.92
1:D:518:LEU:O	1:D:521:LEU:O	1.86	0.92
1:C:1197:VAL:C	1:C:1200:PHE:CD2	2.41	0.92
1:A:541:PHE:HZ	1:A:1198:HIS:CG	1.85	0.92
1:A:1081:HIS:CD2	1:A:1101:ARG:HD2	2.03	0.92
1:A:1124:SER:HB3	1:A:1125:GLU:C	1.88	0.92
1:B:394:THR:HG23	1:B:439:LYS:O	1.67	0.92
1:C:1102:ALA:HB1	1:C:1106:PHE:HE2	1.34	0.92
1:A:1121:ILE:HD13	1:A:1134:ILE:HA	1.48	0.92
1:B:508:GLN:HG2	1:B:629:MET:CG	1.99	0.92
1:A:1124:SER:HB3	1:A:1126:PHE:N	1.85	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:VAL:CA	1:A:812:ILE:HG12	1.99	0.92
1:C:1197:VAL:HG13	1:C:1200:PHE:CZ	2.03	0.92
1:B:633:ILE:HB	1:B:634:GLU:CB	1.99	0.92
1:C:1197:VAL:CB	1:C:1200:PHE:HE2	1.83	0.92
1:A:1121:ILE:HG23	1:A:1133:ILE:HG21	1.52	0.91
1:C:1009:MET:HG3	1:C:1203:ARG:HH21	1.35	0.91
1:C:1023:MET:CE	1:C:1148:ASN:ND2	2.32	0.91
1:C:1177:TRP:O	1:C:1180:TYR:N	2.02	0.91
1:C:1017:PHE:HE1	1:C:1115:PHE:HB3	1.25	0.91
1:A:1129:THR:CB	1:A:1133:ILE:CD1	2.39	0.91
1:C:1124:SER:HB3	1:C:1126:PHE:N	1.85	0.91
1:A:1177:TRP:O	1:A:1180:TYR:N	2.02	0.91
1:C:809:VAL:CA	1:C:812:ILE:HG12	1.99	0.91
1:A:1023:MET:CE	1:A:1148:ASN:ND2	2.32	0.91
1:A:1131:HIS:ND1	1:A:1132:ASN:N	2.17	0.91
1:A:810:ALA:O	1:A:814:PHE:HD2	1.51	0.91
1:A:1102:ALA:HB1	1:A:1106:PHE:HE2	1.34	0.91
1:C:1020:PHE:CD1	1:C:1111:VAL:CB	2.53	0.91
1:C:1131:HIS:ND1	1:C:1132:ASN:N	2.17	0.91
1:C:1156:ILE:CB	1:C:1175:TYR:OH	2.19	0.91
1:A:1169:LYS:N	1:A:1172:SER:HB3	1.86	0.91
1:A:1020:PHE:CD1	1:A:1111:VAL:CB	2.53	0.91
1:C:1081:HIS:CD2	1:C:1101:ARG:HD2	2.04	0.91
1:C:1120:CYS:HA	1:C:1126:PHE:CE1	2.05	0.91
1:A:1107:PRO:HD2	1:A:1108:ILE:N	1.86	0.91
1:A:1103:SER:O	1:A:1107:PRO:HG3	1.71	0.90
1:A:514:VAL:HG13	1:A:794:GLY:HA3	1.53	0.90
1:A:1156:ILE:CB	1:A:1175:TYR:OH	2.19	0.90
1:C:1121:ILE:CD1	1:C:1134:ILE:CG1	2.31	0.90
1:A:568:THR:C	1:A:1202:ASP:CB	2.39	0.90
1:A:1096:PHE:CD1	1:A:1097:LEU:HA	2.07	0.90
1:A:1120:CYS:HA	1:A:1126:PHE:CE1	2.05	0.90
1:A:1121:ILE:HG23	1:A:1133:ILE:CG2	2.00	0.90
1:C:517:PHE:CE2	1:C:526:TRP:CH2	2.60	0.90
1:A:1114:LEU:CD2	1:A:1141:PHE:HA	2.01	0.90
1:C:1016:ALA:CA	1:C:1192:VAL:CG1	2.42	0.90
1:C:1031:TYR:CE1	1:C:1059:HIS:HD2	1.88	0.90
1:A:541:PHE:CE1	1:A:1198:HIS:CE1	2.60	0.90
1:A:542:LEU:HD23	1:A:1197:VAL:CG1	1.82	0.90
1:A:568:THR:C	1:A:1202:ASP:HB3	1.91	0.90
1:A:1114:LEU:CD1	1:A:1141:PHE:CD2	2.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1114:LEU:CD2	1:C:1141:PHE:HA	2.01	0.90
1:A:1153:ILE:O	1:A:1156:ILE:HG12	1.72	0.89
1:C:531:PHE:HZ	1:C:1187:ILE:HD11	1.30	0.89
1:C:1016:ALA:HA	1:C:1192:VAL:CB	2.02	0.89
1:C:1111:VAL:CG2	1:C:1144:ALA:HB1	2.02	0.89
1:A:1197:VAL:CB	1:A:1200:PHE:HE2	1.83	0.89
1:C:1096:PHE:CD1	1:C:1097:LEU:HA	2.07	0.89
1:A:808:LEU:O	1:A:812:ILE:HG23	1.71	0.89
1:A:1111:VAL:CG2	1:A:1144:ALA:HB1	2.02	0.89
1:C:1127:TYR:CZ	1:C:1130:ARG:CA	2.54	0.89
1:A:1004:ASP:O	1:A:1008:GLN:HB2	1.71	0.89
1:A:1031:TYR:CE1	1:A:1059:HIS:HD2	1.88	0.89
1:C:541:PHE:CE2	1:C:1198:HIS:NE2	2.39	0.89
1:C:1103:SER:O	1:C:1107:PRO:HG3	1.71	0.89
1:C:1121:ILE:HG22	1:C:1133:ILE:CB	2.02	0.89
1:A:1009:MET:HG3	1:A:1203:ARG:HH21	1.35	0.89
1:A:1016:ALA:HA	1:A:1192:VAL:CB	2.02	0.89
1:B:394:THR:CG2	1:B:395:VAL:H	1.86	0.89
1:C:1121:ILE:HG23	1:C:1133:ILE:HG21	1.52	0.89
1:C:1169:LYS:N	1:C:1172:SER:HB3	1.86	0.89
1:A:1129:THR:CG2	1:A:1133:ILE:CG1	2.51	0.89
1:C:521:LEU:HA	1:D:787:LEU:HD23	1.51	0.89
1:A:1127:TYR:CZ	1:A:1130:ARG:CA	2.54	0.88
1:C:531:PHE:CE2	1:C:1187:ILE:HD11	2.07	0.88
1:C:1004:ASP:O	1:C:1008:GLN:HB2	1.71	0.88
1:C:1129:THR:CG2	1:C:1133:ILE:CG1	2.51	0.88
1:C:1153:ILE:O	1:C:1156:ILE:HG12	1.72	0.88
1:C:1170:LYS:HB3	1:C:1171:ASN:HB2	1.55	0.88
1:C:1107:PRO:HD2	1:C:1108:ILE:N	1.86	0.88
1:C:1164:SER:HA	1:C:1165:LYS:HG2	1.56	0.88
1:A:1083:PRO:N	1:A:1097:LEU:HB2	1.89	0.88
1:C:1197:VAL:HG13	1:C:1200:PHE:HE2	0.93	0.88
1:C:1114:LEU:CD1	1:C:1141:PHE:CD2	2.54	0.88
1:C:1083:PRO:CD	1:C:1098:ARG:CG	2.41	0.87
1:A:1154:VAL:HG12	1:B:797:TYR:OH	1.72	0.87
1:C:520:PRO:O	1:D:787:LEU:HD22	1.71	0.87
1:D:508:GLN:HA	1:D:629:MET:SD	2.14	0.87
1:B:507:PRO:CG	1:B:631:SER:HA	2.05	0.87
1:C:1104:SER:C	1:C:1107:PRO:CG	2.43	0.87
1:C:1121:ILE:HB	1:C:1134:ILE:CG1	2.04	0.87
1:C:1121:ILE:HG23	1:C:1133:ILE:CG2	2.00	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:THR:C	1:C:1202:ASP:HB2	1.90	0.87
1:A:1111:VAL:CG2	1:A:1144:ALA:CB	2.53	0.87
1:C:1062:LEU:CD2	1:C:1155:TYR:CE2	2.57	0.87
1:C:1153:ILE:HA	1:C:1156:ILE:HG12	1.57	0.87
1:A:1104:SER:C	1:A:1107:PRO:CG	2.43	0.87
1:A:1196:ALA:HA	1:A:1199:MET:CE	2.04	0.87
1:A:531:PHE:CE2	1:A:1187:ILE:CG1	2.54	0.87
1:D:517:PHE:CZ	1:D:526:TRP:CH2	2.63	0.87
1:C:1106:PHE:N	1:C:1107:PRO:HD3	1.90	0.87
1:C:1111:VAL:CG2	1:C:1144:ALA:CB	2.53	0.87
1:A:1083:PRO:HG2	1:A:1098:ARG:CD	2.06	0.86
1:A:1114:LEU:HD12	1:A:1115:PHE:N	1.91	0.86
1:C:1083:PRO:N	1:C:1097:LEU:HB2	1.89	0.86
1:C:1104:SER:HA	1:C:1107:PRO:HG3	1.56	0.86
1:A:538:VAL:HG21	1:A:1194:VAL:HG22	1.57	0.86
1:A:718:CYS:CB	1:A:776:LYS:CB	2.52	0.86
1:A:1062:LEU:CD2	1:A:1155:TYR:CE2	2.57	0.86
1:A:1106:PHE:N	1:A:1107:PRO:HD3	1.90	0.86
1:C:1056:VAL:CG1	1:C:1057:MET:H	1.89	0.86
1:C:531:PHE:CE2	1:C:1187:ILE:CD1	2.57	0.86
1:C:1196:ALA:HA	1:C:1199:MET:CE	2.04	0.86
1:A:1104:SER:HA	1:A:1107:PRO:HG3	1.57	0.86
1:A:1170:LYS:HB3	1:A:1171:ASN:HB2	1.55	0.86
1:A:1121:ILE:CG2	1:A:1133:ILE:HG21	2.05	0.86
1:A:1121:ILE:HB	1:A:1134:ILE:CG1	2.04	0.86
1:A:1197:VAL:C	1:A:1200:PHE:CE2	2.49	0.86
1:B:632:PRO:O	1:B:633:ILE:CG2	2.23	0.86
1:C:787:LEU:CD1	1:C:788:SER:H	1.88	0.86
1:A:1121:ILE:HD12	1:A:1134:ILE:HG12	0.86	0.86
1:B:509:LYS:HG2	1:B:510:SER:N	1.91	0.85
1:C:1063:TRP:CZ2	1:C:1081:HIS:CE1	2.64	0.85
1:C:1088:TYR:O	1:C:1090:ALA:HA	1.76	0.85
1:B:633:ILE:HB	1:B:634:GLU:CA	2.06	0.85
1:A:538:VAL:CG2	1:A:1194:VAL:HG22	2.06	0.85
1:A:568:THR:CB	1:A:1202:ASP:CA	2.54	0.85
1:A:1096:PHE:CZ	1:A:1097:LEU:HD23	2.11	0.85
1:C:520:PRO:O	1:D:787:LEU:HD23	1.74	0.85
1:C:1029:THR:C	1:C:1031:TYR:H	1.78	0.85
1:A:1056:VAL:CG1	1:A:1057:MET:H	1.89	0.85
1:A:1134:ILE:CB	1:A:1200:PHE:HB3	2.06	0.85
1:A:1088:TYR:O	1:A:1090:ALA:HA	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:PHE:CD1	1:A:1111:VAL:HB	2.12	0.85
1:C:1096:PHE:CZ	1:C:1097:LEU:HD23	2.11	0.85
1:C:1121:ILE:HD12	1:C:1134:ILE:HG12	0.86	0.85
1:C:1134:ILE:CB	1:C:1200:PHE:HB3	2.06	0.85
1:A:1029:THR:C	1:A:1031:TYR:H	1.78	0.85
1:D:510:SER:O	1:D:511:LYS:HG3	1.76	0.85
1:A:542:LEU:HD22	1:A:1197:VAL:CG1	2.04	0.85
1:C:810:ALA:O	1:C:814:PHE:HD2	1.51	0.85
1:C:1121:ILE:CG2	1:C:1133:ILE:HG22	2.00	0.84
1:D:517:PHE:CZ	1:D:526:TRP:HH2	1.94	0.84
1:D:632:PRO:C	1:D:633:ILE:HD12	1.96	0.84
1:C:1022:LEU:HD22	1:C:1185:SER:CB	2.05	0.84
1:C:1083:PRO:HG2	1:C:1098:ARG:CD	2.05	0.84
1:C:1114:LEU:HD12	1:C:1115:PHE:N	1.91	0.84
1:A:1182:GLY:C	1:A:1186:PHE:CD2	2.47	0.84
1:D:630:VAL:HG23	1:D:631:SER:N	1.91	0.84
1:A:1063:TRP:CZ2	1:A:1081:HIS:CE1	2.64	0.84
1:A:1096:PHE:CG	1:A:1097:LEU:HA	2.12	0.84
1:C:517:PHE:CZ	1:C:526:TRP:HH2	1.93	0.84
1:C:1096:PHE:CG	1:C:1097:LEU:HA	2.12	0.84
1:A:809:VAL:CA	1:A:812:ILE:HD11	2.07	0.84
1:A:1153:ILE:HA	1:A:1156:ILE:HG12	1.57	0.84
1:C:1121:ILE:CG2	1:C:1133:ILE:HG21	2.05	0.84
1:C:1121:ILE:CG1	1:C:1134:ILE:HG12	2.07	0.84
1:C:1153:ILE:O	1:C:1156:ILE:CG1	2.25	0.84
1:C:568:THR:O	1:C:1202:ASP:CB	2.22	0.84
1:C:1197:VAL:C	1:C:1200:PHE:CE2	2.49	0.84
1:A:1117:GLY:O	1:A:1121:ILE:HG23	1.77	0.84
1:C:1134:ILE:HG21	1:C:1200:PHE:HB3	1.54	0.84
1:A:1022:LEU:HD22	1:A:1185:SER:CB	2.05	0.84
1:A:1152:ILE:O	1:A:1156:ILE:HG23	1.77	0.84
1:C:518:LEU:O	1:C:521:LEU:O	1.95	0.84
1:C:1152:ILE:O	1:C:1156:ILE:HG23	1.77	0.84
1:C:1117:GLY:O	1:C:1121:ILE:HG23	1.77	0.84
1:B:507:PRO:HG2	1:B:630:VAL:O	1.77	0.83
1:C:1153:ILE:CA	1:C:1156:ILE:HG12	2.09	0.83
1:A:541:PHE:CZ	1:A:1198:HIS:CD2	2.65	0.83
1:A:1121:ILE:HG22	1:A:1133:ILE:CB	2.02	0.83
1:A:1121:ILE:CG1	1:A:1134:ILE:HG12	2.07	0.83
1:B:509:LYS:CG	1:B:510:SER:H	1.91	0.83
1:C:1134:ILE:HG21	1:C:1200:PHE:CA	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:LEU:CD2	1:A:1197:VAL:HG13	2.07	0.83
1:A:1107:PRO:CD	1:A:1108:ILE:H	1.91	0.83
1:A:1121:ILE:CG2	1:A:1133:ILE:HG22	2.00	0.83
1:B:507:PRO:CG	1:B:630:VAL:O	2.26	0.83
1:A:1153:ILE:O	1:A:1156:ILE:CG1	2.25	0.83
1:C:1111:VAL:HG23	1:C:1144:ALA:HB1	1.60	0.83
1:C:541:PHE:CZ	1:C:1198:HIS:CD2	2.48	0.83
1:C:809:VAL:CA	1:C:812:ILE:HD11	2.07	0.83
1:C:1121:ILE:CB	1:C:1134:ILE:HG13	2.09	0.83
1:C:512:PRO:CA	1:C:790:SER:CB	2.47	0.82
1:C:1009:MET:SD	1:C:1199:MET:HB3	2.20	0.82
1:C:1029:THR:CG2	1:C:1178:SER:HB3	2.09	0.82
1:A:1134:ILE:HG21	1:A:1200:PHE:HB3	1.54	0.82
1:A:1097:LEU:O	1:A:1098:ARG:HB2	1.79	0.82
1:A:1121:ILE:CB	1:A:1134:ILE:HG13	2.09	0.82
1:C:1107:PRO:CD	1:C:1108:ILE:H	1.91	0.82
1:A:517:PHE:HE1	1:D:611:ILE:HD12	1.41	0.82
1:A:633:ILE:HG22	1:A:634:GLU:H	1.45	0.82
1:A:1029:THR:HB	1:A:1178:SER:HB2	1.62	0.82
1:A:1152:ILE:HD11	1:A:1186:PHE:CE2	2.15	0.82
1:C:1029:THR:HB	1:C:1178:SER:HB2	1.62	0.82
1:C:1170:LYS:N	1:C:1171:ASN:O	2.12	0.82
1:D:631:SER:HB3	1:D:632:PRO:CD	2.09	0.82
1:C:1134:ILE:CB	1:C:1200:PHE:CB	2.57	0.82
1:A:1134:ILE:CB	1:A:1200:PHE:CB	2.57	0.82
1:A:1134:ILE:HG21	1:A:1200:PHE:CA	2.09	0.82
1:A:1153:ILE:CA	1:A:1156:ILE:HG12	2.09	0.82
1:A:1163:PRO:C	1:A:1165:LYS:HG2	2.01	0.82
1:A:386:ASP:O	1:A:388:SER:N	2.13	0.81
1:B:372:GLY:HA2	1:B:383:THR:HG23	1.61	0.81
1:B:518:LEU:O	1:B:521:LEU:O	1.98	0.81
1:C:1027:VAL:HA	1:C:1032:TRP:HZ2	1.45	0.81
1:C:1065:THR:HG23	1:C:1082:PHE:CZ	2.16	0.81
1:A:1083:PRO:CG	1:A:1098:ARG:CG	1.97	0.81
1:A:1083:PRO:CD	1:A:1098:ARG:CG	2.41	0.81
1:C:1020:PHE:O	1:C:1023:MET:CG	2.28	0.81
1:C:1115:PHE:CE1	1:C:1141:PHE:HE2	1.98	0.81
1:C:1152:ILE:HD11	1:C:1186:PHE:CE2	2.15	0.81
1:C:1163:PRO:C	1:C:1165:LYS:HG2	2.01	0.81
1:C:1182:GLY:C	1:C:1186:PHE:CD2	2.47	0.81
1:D:514:VAL:HG22	1:D:794:GLY:HA2	0.83	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:THR:CG2	1:A:1178:SER:HB3	2.10	0.81
1:C:1008:GLN:O	1:C:1012:THR:HG23	1.80	0.81
1:C:1020:PHE:CD1	1:C:1111:VAL:HB	2.12	0.81
1:D:518:LEU:HA	1:D:526:TRP:HE1	1.46	0.81
1:A:541:PHE:CE1	1:A:1198:HIS:ND1	2.48	0.81
1:A:1164:SER:HA	1:A:1165:LYS:HG2	1.55	0.81
1:B:394:THR:CG2	1:B:439:LYS:O	2.29	0.81
1:A:542:LEU:HD21	1:A:1197:VAL:CG1	1.82	0.81
1:A:1008:GLN:O	1:A:1012:THR:HG23	1.80	0.81
1:C:568:THR:CB	1:C:1202:ASP:C	2.48	0.81
1:A:1065:THR:HG23	1:A:1082:PHE:CZ	2.16	0.81
1:C:1020:PHE:HB2	1:C:1111:VAL:HG11	1.63	0.81
1:C:1097:LEU:O	1:C:1098:ARG:HB2	1.79	0.81
1:A:1020:PHE:HB2	1:A:1111:VAL:HG11	1.63	0.80
1:A:1062:LEU:HD21	1:A:1155:TYR:CD2	2.15	0.80
1:C:517:PHE:CE2	1:C:526:TRP:CZ2	2.68	0.80
1:C:1081:HIS:CG	1:C:1101:ARG:HD3	2.16	0.80
1:C:1170:LYS:HB3	1:C:1171:ASN:CB	2.10	0.80
1:A:1009:MET:SD	1:A:1199:MET:HB3	2.20	0.80
1:A:1170:LYS:HB3	1:A:1171:ASN:CB	2.10	0.80
1:A:1168:SER:HA	1:A:1171:ASN:OD1	1.82	0.80
1:B:507:PRO:CG	1:B:631:SER:HB3	2.10	0.80
1:C:1152:ILE:CD1	1:C:1186:PHE:CE2	2.64	0.80
1:A:1111:VAL:HG23	1:A:1144:ALA:HB1	1.61	0.80
1:A:1115:PHE:CE1	1:A:1141:PHE:HE2	1.98	0.80
1:A:1131:HIS:CD2	1:A:1207:LEU:HD12	2.15	0.80
1:A:1020:PHE:CZ	1:A:1108:ILE:CG2	2.53	0.80
1:A:1153:ILE:HA	1:A:1156:ILE:CD1	2.12	0.80
1:C:1107:PRO:O	1:C:1111:VAL:HG23	1.81	0.80
1:A:388:SER:O	1:A:390:LEU:N	2.14	0.80
1:A:1020:PHE:CE1	1:A:1108:ILE:CA	2.59	0.80
1:A:1081:HIS:CG	1:A:1101:ARG:HD3	2.16	0.80
1:C:514:VAL:HG22	1:C:794:GLY:CA	2.12	0.80
1:D:512:PRO:CG	1:D:790:SER:HB2	2.11	0.80
1:A:1153:ILE:C	1:A:1156:ILE:HG12	2.03	0.80
1:C:1200:PHE:CZ	1:C:1201:ILE:HG13	2.17	0.80
1:A:1027:VAL:HA	1:A:1032:TRP:HZ2	1.45	0.80
1:C:1071:ASN:O	1:C:1072:PHE:HB2	1.81	0.80
1:C:1135:LEU:HD23	1:C:1200:PHE:CE1	2.17	0.80
1:C:1153:ILE:HA	1:C:1156:ILE:CD1	2.12	0.80
1:B:504:ILE:HD13	1:B:633:ILE:CG2	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:PHE:CD1	1:A:1115:PHE:CD1	2.70	0.79
1:B:508:GLN:CG	1:B:629:MET:HG3	2.11	0.79
1:A:531:PHE:HZ	1:A:1187:ILE:HD11	1.44	0.79
1:A:1020:PHE:O	1:A:1023:MET:CG	2.28	0.79
1:C:809:VAL:CA	1:C:812:ILE:CG1	2.59	0.79
1:C:1062:LEU:HD21	1:C:1155:TYR:CD2	2.16	0.79
1:A:1126:PHE:HB3	1:A:1127:TYR:CA	2.10	0.79
1:A:633:ILE:HG23	1:A:638:ASP:CB	2.12	0.79
1:A:1152:ILE:CD1	1:A:1186:PHE:CE2	2.64	0.79
1:C:1083:PRO:CG	1:C:1098:ARG:N	2.36	0.79
1:A:1071:ASN:O	1:A:1072:PHE:HB2	1.81	0.79
1:A:1107:PRO:O	1:A:1111:VAL:HG23	1.81	0.79
1:A:1135:LEU:HD23	1:A:1200:PHE:CE1	2.17	0.79
1:C:1017:PHE:CD1	1:C:1115:PHE:CD1	2.70	0.79
1:C:1129:THR:CB	1:C:1133:ILE:CD1	2.39	0.79
1:C:1130:ARG:O	1:C:1131:HIS:ND1	2.16	0.79
1:C:1168:SER:HA	1:C:1171:ASN:OD1	1.82	0.79
1:A:1111:VAL:O	1:A:1114:LEU:HG	1.83	0.79
1:A:1130:ARG:O	1:A:1131:HIS:ND1	2.16	0.79
1:C:1153:ILE:C	1:C:1156:ILE:HG12	2.03	0.79
1:C:1200:PHE:CE1	1:C:1201:ILE:HG13	2.18	0.79
1:D:510:SER:O	1:D:511:LYS:CG	2.31	0.79
1:C:1020:PHE:CE1	1:C:1108:ILE:CA	2.59	0.79
1:C:1197:VAL:CA	1:C:1200:PHE:HD2	1.90	0.79
1:A:568:THR:CA	1:A:1202:ASP:HB2	2.13	0.79
1:A:1020:PHE:CB	1:A:1111:VAL:HG11	2.13	0.79
1:A:1200:PHE:CE1	1:A:1201:ILE:HG13	2.18	0.79
1:C:1020:PHE:CZ	1:C:1108:ILE:CG2	2.53	0.79
1:A:1083:PRO:CG	1:A:1098:ARG:N	2.36	0.78
1:A:1165:LYS:O	1:A:1166:SER:OG	2.01	0.78
1:A:511:LYS:H	1:A:512:PRO:CD	1.95	0.78
1:A:1032:TRP:O	1:A:1179:PHE:HE2	1.66	0.78
1:A:1134:ILE:HG21	1:A:1200:PHE:N	1.98	0.78
1:C:541:PHE:HE2	1:C:1198:HIS:CD2	1.94	0.78
1:C:1111:VAL:O	1:C:1114:LEU:HG	1.83	0.78
1:C:1165:LYS:O	1:C:1166:SER:OG	2.01	0.78
1:A:787:LEU:HG	1:A:788:SER:N	1.96	0.78
1:C:1120:CYS:CA	1:C:1126:PHE:CD1	2.64	0.78
1:A:1200:PHE:CZ	1:A:1201:ILE:HG13	2.17	0.78
1:C:1087:ASP:HB2	1:D:699:LYS:HZ2	1.49	0.78
1:A:1131:HIS:HD2	1:A:1207:LEU:CD1	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:ILE:HD11	1:D:788:SER:O	1.83	0.78
1:C:1118:GLY:HA2	1:C:1121:ILE:HG12	1.66	0.78
1:D:508:GLN:HG2	1:D:629:MET:CG	2.13	0.78
1:A:1056:VAL:CG1	1:A:1057:MET:N	2.46	0.78
1:A:1127:TYR:CE2	1:A:1130:ARG:HA	2.18	0.78
1:A:1170:LYS:HE2	1:A:1170:LYS:HA	1.64	0.78
1:A:1170:LYS:N	1:A:1171:ASN:O	2.12	0.78
1:C:1032:TRP:O	1:C:1179:PHE:HE2	1.66	0.78
1:C:1032:TRP:O	1:C:1179:PHE:CE2	2.37	0.78
1:C:1134:ILE:HG21	1:C:1200:PHE:N	1.98	0.78
1:C:1027:VAL:HA	1:C:1032:TRP:CZ2	2.19	0.78
1:D:394:THR:HG22	1:D:440:TYR:HA	1.64	0.78
1:C:538:VAL:HG23	1:C:1194:VAL:HG22	1.62	0.78
1:C:1170:LYS:HE2	1:C:1170:LYS:HA	1.64	0.78
1:A:542:LEU:HD22	1:A:1197:VAL:HG13	1.66	0.77
1:C:1126:PHE:HB3	1:C:1127:TYR:CA	2.10	0.77
1:C:1189:ALA:C	1:C:1192:VAL:HG22	2.05	0.77
1:A:1121:ILE:HG21	1:A:1133:ILE:CB	2.09	0.77
1:C:1023:MET:HE1	1:C:1148:ASN:HD21	1.47	0.77
1:C:1159:ASN:CG	1:C:1175:TYR:HE1	1.88	0.77
1:C:1149:ILE:O	1:C:1149:ILE:HD13	1.85	0.77
1:A:1016:ALA:CA	1:A:1192:VAL:CB	2.62	0.77
1:A:1189:ALA:C	1:A:1192:VAL:HG22	2.05	0.77
1:D:510:SER:O	1:D:511:LYS:CB	2.31	0.77
1:B:692:ARG:HG3	1:B:700:TYR:CD2	2.19	0.77
1:C:1111:VAL:HG23	1:C:1144:ALA:CB	2.14	0.77
1:A:1118:GLY:HA2	1:A:1121:ILE:HG12	1.65	0.77
1:C:1020:PHE:CB	1:C:1111:VAL:HG11	2.13	0.77
1:B:506:LYS:HG2	1:B:719:ASP:CB	2.15	0.77
1:D:692:ARG:HG3	1:D:700:TYR:CD2	2.19	0.77
1:C:1083:PRO:HD2	1:C:1098:ARG:HG3	1.66	0.77
1:C:1104:SER:HA	1:C:1107:PRO:CG	2.15	0.77
1:C:1131:HIS:HD2	1:C:1207:LEU:CD1	1.97	0.77
1:A:1032:TRP:O	1:A:1179:PHE:CE2	2.37	0.77
1:A:1153:ILE:HA	1:A:1156:ILE:CG1	2.15	0.77
1:A:1197:VAL:HG12	1:A:1200:PHE:CE2	2.19	0.77
1:C:1016:ALA:CB	1:C:1192:VAL:CB	2.62	0.77
1:C:1168:SER:HA	1:C:1171:ASN:CG	2.06	0.77
1:D:390:LEU:O	1:D:392:GLN:N	2.18	0.77
1:C:1104:SER:CA	1:C:1107:PRO:HG3	2.15	0.76
1:A:1118:GLY:HA2	1:A:1121:ILE:CD1	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1017:PHE:CE1	1:C:1115:PHE:CB	2.65	0.76
1:D:635:SER:OG	1:D:638:ASP:CG	2.24	0.76
1:A:1027:VAL:HA	1:A:1032:TRP:CZ2	2.19	0.76
1:A:1104:SER:HA	1:A:1107:PRO:CG	2.15	0.76
1:A:1156:ILE:HB	1:A:1175:TYR:HH	1.49	0.76
1:A:1068:LEU:HD23	1:A:1074:GLY:CA	2.15	0.76
1:A:1083:PRO:HD2	1:A:1098:ARG:HG3	1.66	0.76
1:B:507:PRO:HG2	1:B:631:SER:HA	1.66	0.76
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.68	0.76
1:A:1129:THR:O	1:A:1133:ILE:CD1	2.34	0.76
1:A:1149:ILE:O	1:A:1149:ILE:HD13	1.85	0.76
1:C:1127:TYR:N	1:C:1128:LYS:CA	2.47	0.76
1:C:1129:THR:CA	1:C:1133:ILE:HD11	2.16	0.76
1:D:508:GLN:HB3	1:D:629:MET:HE3	1.67	0.76
1:A:1031:TYR:HE1	1:A:1059:HIS:NE2	1.83	0.76
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.67	0.76
1:C:611:ILE:HD11	1:D:517:PHE:HZ	1.49	0.76
1:C:1068:LEU:HD23	1:C:1074:GLY:CA	2.15	0.76
1:A:1159:ASN:CG	1:A:1175:TYR:HE1	1.88	0.76
1:C:1027:VAL:O	1:C:1063:TRP:HZ3	1.69	0.76
1:C:1127:TYR:CE2	1:C:1130:ARG:HA	2.18	0.76
1:C:1129:THR:O	1:C:1133:ILE:HD12	1.86	0.76
1:C:1131:HIS:CD2	1:C:1207:LEU:HD12	2.15	0.76
1:A:1027:VAL:O	1:A:1063:TRP:HZ3	1.69	0.76
1:A:1129:THR:CA	1:A:1133:ILE:HD11	2.16	0.76
1:C:521:LEU:HA	1:D:787:LEU:CD2	2.16	0.76
1:C:1029:THR:CB	1:C:1178:SER:CB	2.57	0.76
1:C:1031:TYR:HE1	1:C:1059:HIS:NE2	1.83	0.76
1:C:1121:ILE:HG21	1:C:1133:ILE:CB	2.09	0.76
1:D:394:THR:HG22	1:D:440:TYR:CA	2.15	0.76
1:A:541:PHE:CE2	1:A:1198:HIS:CG	2.65	0.76
1:A:809:VAL:C	1:A:812:ILE:HG12	2.06	0.76
1:C:541:PHE:HZ	1:C:1198:HIS:CB	1.99	0.76
1:C:771:GLY:C	1:C:772:GLU:HG3	2.05	0.76
1:C:1152:ILE:HG13	1:C:1186:PHE:CD2	2.21	0.76
1:A:1126:PHE:CB	1:A:1127:TYR:HA	2.04	0.75
1:B:513:GLY:C	1:B:515:PHE:H	1.90	0.75
1:C:1105:ILE:C	1:C:1107:PRO:HD3	2.07	0.75
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.68	0.75
1:D:394:THR:O	1:D:396:VAL:N	2.20	0.75
1:A:1035:SER:HA	1:A:1173:TYR:HD2	1.46	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1083:PRO:CB	1:A:1098:ARG:HG3	2.12	0.75
1:A:1104:SER:CA	1:A:1107:PRO:HG3	2.15	0.75
1:A:1129:THR:O	1:A:1133:ILE:HD12	1.86	0.75
1:B:786:ALA:C	1:B:787:LEU:HD13	2.07	0.75
1:C:1129:THR:O	1:C:1133:ILE:CD1	2.34	0.75
1:A:809:VAL:O	1:A:813:GLU:CG	2.35	0.75
1:A:1017:PHE:CE1	1:A:1115:PHE:CB	2.65	0.75
1:A:1029:THR:CB	1:A:1178:SER:CB	2.57	0.75
1:C:1084:GLU:HG2	1:C:1085:ASP:OD2	1.87	0.75
1:C:1118:GLY:HA2	1:C:1121:ILE:CD1	2.16	0.75
1:A:1009:MET:HA	1:A:1199:MET:SD	2.27	0.75
1:A:1167:ASP:O	1:A:1171:ASN:ND2	2.18	0.75
1:A:1111:VAL:HG23	1:A:1144:ALA:CB	2.14	0.75
1:A:1114:LEU:HB3	1:A:1140:PHE:HB2	1.68	0.75
1:C:512:PRO:HA	1:C:790:SER:HB2	1.64	0.75
1:C:1035:SER:HA	1:C:1173:TYR:HD2	1.46	0.75
1:D:512:PRO:HB3	1:D:790:SER:CA	2.17	0.75
1:A:1134:ILE:HG21	1:A:1200:PHE:CB	2.12	0.75
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.68	0.75
1:A:1168:SER:HA	1:A:1171:ASN:CG	2.06	0.75
1:C:1153:ILE:O	1:C:1153:ILE:HD13	1.87	0.75
1:C:1153:ILE:HA	1:C:1156:ILE:CG1	2.15	0.75
1:A:1176:GLY:HA3	1:A:1179:PHE:HB2	1.69	0.75
1:C:512:PRO:HB3	1:C:790:SER:HA	1.61	0.75
1:C:1016:ALA:CA	1:C:1192:VAL:CB	2.62	0.75
1:C:1176:GLY:HA3	1:C:1179:PHE:HB2	1.69	0.75
1:A:1020:PHE:HD1	1:A:1111:VAL:HG21	1.51	0.74
1:A:1146:LEU:O	1:A:1149:ILE:HG22	1.86	0.74
1:A:1152:ILE:HG13	1:A:1186:PHE:CD2	2.21	0.74
1:C:1020:PHE:HD1	1:C:1111:VAL:HG21	1.51	0.74
1:A:809:VAL:CA	1:A:812:ILE:CG1	2.59	0.74
1:A:1084:GLU:HG2	1:A:1085:ASP:OD2	1.87	0.74
1:A:1122:ALA:O	1:A:1123:ALA:HB3	1.87	0.74
1:A:1153:ILE:O	1:A:1153:ILE:HD13	1.87	0.74
1:A:525:ILE:HG12	1:B:789:LEU:HD13	1.68	0.74
1:C:1009:MET:SD	1:C:1199:MET:CG	2.75	0.74
1:C:1197:VAL:HG12	1:C:1200:PHE:CE2	2.19	0.74
1:D:630:VAL:O	1:D:631:SER:OG	2.06	0.74
1:A:1105:ILE:C	1:A:1107:PRO:HD3	2.07	0.74
1:B:633:ILE:HB	1:B:634:GLU:HA	1.70	0.74
1:C:809:VAL:C	1:C:812:ILE:HG12	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1146:LEU:O	1:C:1149:ILE:HG22	1.86	0.74
1:A:568:THR:C	1:A:1202:ASP:HB2	2.04	0.74
1:A:1016:ALA:CB	1:A:1192:VAL:CB	2.62	0.74
1:A:1156:ILE:CG2	1:A:1179:PHE:CE1	2.70	0.74
1:A:1172:SER:OG	1:A:1173:TYR:N	2.20	0.74
1:B:392:GLN:O	1:B:394:THR:N	2.21	0.74
1:B:508:GLN:HG2	1:B:629:MET:SD	2.26	0.74
1:C:1019:ALA:HB1	1:C:1189:ALA:N	2.03	0.74
1:C:1170:LYS:N	1:C:1171:ASN:HB3	2.03	0.74
1:D:517:PHE:CE2	1:D:526:TRP:CZ2	2.75	0.74
1:C:1114:LEU:HB3	1:C:1140:PHE:HB2	1.68	0.74
1:C:1156:ILE:CG2	1:C:1179:PHE:CE1	2.70	0.74
1:C:1172:SER:OG	1:C:1173:TYR:N	2.20	0.74
1:A:1009:MET:SD	1:A:1199:MET:CG	2.75	0.74
1:B:630:VAL:HG22	1:B:631:SER:N	2.02	0.74
1:D:630:VAL:HG23	1:D:631:SER:H	1.53	0.74
1:C:1009:MET:HA	1:C:1199:MET:SD	2.27	0.74
1:C:1156:ILE:HB	1:C:1175:TYR:HH	1.50	0.74
1:A:1131:HIS:O	1:A:1132:ASN:C	2.25	0.74
1:A:1131:HIS:CD2	1:A:1207:LEU:CD1	2.71	0.74
1:A:1170:LYS:N	1:A:1171:ASN:HB3	2.03	0.74
1:C:1122:ALA:O	1:C:1123:ALA:HB3	1.87	0.74
1:B:394:THR:CG2	1:B:439:LYS:C	2.56	0.73
1:C:514:VAL:HG22	1:C:794:GLY:HA3	1.70	0.73
1:C:1170:LYS:O	1:C:1170:LYS:HD3	1.88	0.73
1:A:1114:LEU:HB3	1:A:1140:PHE:CB	2.19	0.73
1:C:1126:PHE:CB	1:C:1127:TYR:HA	2.04	0.73
1:A:1019:ALA:HB1	1:A:1189:ALA:N	2.03	0.73
1:A:1170:LYS:O	1:A:1170:LYS:HD3	1.88	0.73
1:C:518:LEU:HA	1:C:526:TRP:HE1	1.54	0.73
1:C:611:ILE:HG21	1:D:795:VAL:HG21	1.70	0.73
1:A:1177:TRP:O	1:A:1178:SER:C	2.27	0.73
1:C:1167:ASP:O	1:C:1171:ASN:ND2	2.18	0.73
1:A:1031:TYR:CD1	1:A:1059:HIS:HD2	2.02	0.73
1:A:1020:PHE:CZ	1:A:1108:ILE:HA	2.24	0.73
1:C:809:VAL:O	1:C:813:GLU:CG	2.35	0.73
1:A:1121:ILE:CD1	1:A:1134:ILE:CA	2.66	0.73
1:C:1159:ASN:OD1	1:C:1175:TYR:HE1	1.71	0.73
1:C:787:LEU:HD13	1:C:788:SER:N	1.95	0.72
1:C:1004:ASP:C	1:C:1008:GLN:HB2	2.10	0.72
1:A:1111:VAL:HG22	1:A:1144:ALA:CB	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1020:PHE:CZ	1:C:1108:ILE:HA	2.24	0.72
1:C:1111:VAL:HA	1:C:1114:LEU:CG	2.19	0.72
1:C:1134:ILE:HB	1:C:1200:PHE:HB2	1.71	0.72
1:A:1134:ILE:HB	1:A:1200:PHE:HB2	1.71	0.72
1:C:1121:ILE:CD1	1:C:1134:ILE:CA	2.66	0.72
1:A:633:ILE:HG23	1:A:638:ASP:HB3	1.70	0.72
1:C:1177:TRP:C	1:C:1179:PHE:N	2.42	0.72
1:A:1009:MET:HG3	1:A:1203:ARG:NH2	2.04	0.72
1:A:1159:ASN:OD1	1:A:1175:TYR:HE1	1.71	0.72
1:C:1114:LEU:HB3	1:C:1140:PHE:CB	2.19	0.72
1:A:1121:ILE:HD12	1:A:1134:ILE:CA	2.19	0.72
1:A:1169:LYS:H	1:A:1172:SER:CB	1.93	0.72
1:A:1016:ALA:CA	1:A:1192:VAL:HB	2.20	0.72
1:A:1032:TRP:N	1:A:1060:SER:O	2.21	0.72
1:A:1111:VAL:HA	1:A:1114:LEU:CG	2.19	0.72
1:A:1197:VAL:HG13	1:A:1200:PHE:HE2	0.93	0.72
1:C:1084:GLU:HG2	1:C:1085:ASP:N	2.03	0.72
1:A:633:ILE:CG2	1:A:638:ASP:HB2	2.19	0.72
1:A:1032:TRP:HB2	1:A:1061:GLY:HA2	1.72	0.72
1:C:1016:ALA:CA	1:C:1192:VAL:HB	2.20	0.72
1:C:1096:PHE:HA	1:C:1097:LEU:C	2.09	0.72
1:C:1163:PRO:O	1:C:1165:LYS:HG2	1.90	0.72
1:A:1127:TYR:CE2	1:A:1130:ARG:CA	2.73	0.72
1:A:1131:HIS:C	1:A:1133:ILE:N	2.43	0.72
1:B:507:PRO:HG3	1:B:631:SER:HA	1.70	0.72
1:C:1152:ILE:HG12	1:C:1186:PHE:CZ	2.24	0.72
1:D:508:GLN:CG	1:D:629:MET:SD	2.78	0.72
1:A:1127:TYR:CE1	1:A:1130:ARG:HA	2.24	0.71
1:A:1163:PRO:O	1:A:1165:LYS:HG2	1.90	0.71
1:C:1121:ILE:HD12	1:C:1134:ILE:CA	2.19	0.71
1:C:1124:SER:CA	1:C:1125:GLU:HB3	2.21	0.71
1:B:513:GLY:O	1:B:515:PHE:N	2.24	0.71
1:C:1009:MET:HG3	1:C:1203:ARG:NH2	2.04	0.71
1:C:1032:TRP:N	1:C:1060:SER:O	2.21	0.71
1:C:1177:TRP:O	1:C:1178:SER:C	2.27	0.71
1:A:1068:LEU:HD23	1:A:1074:GLY:HA3	1.71	0.71
1:A:1114:LEU:HD22	1:A:1141:PHE:N	2.04	0.71
1:A:1134:ILE:CG2	1:A:1200:PHE:CA	2.67	0.71
1:A:1150:ILE:O	1:A:1154:VAL:HG13	1.91	0.71
1:B:633:ILE:HD13	1:B:633:ILE:N	2.04	0.71
1:C:1032:TRP:HB2	1:C:1061:GLY:HA2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1199:MET:O	1:C:1202:ASP:CG	2.28	0.71
1:A:1104:SER:CA	1:A:1107:PRO:CG	2.68	0.71
1:A:1134:ILE:HB	1:A:1200:PHE:CB	2.20	0.71
1:A:1023:MET:HE1	1:A:1148:ASN:HD21	1.51	0.71
1:C:1062:LEU:HD21	1:C:1155:TYR:CE2	2.23	0.71
1:C:1083:PRO:HD2	1:C:1098:ARG:CG	2.19	0.71
1:A:1127:TYR:CB	1:A:1133:ILE:CD1	2.69	0.71
1:A:1152:ILE:HG12	1:A:1186:PHE:CZ	2.24	0.71
1:C:1150:ILE:O	1:C:1154:VAL:HG13	1.91	0.71
1:A:1004:ASP:C	1:A:1008:GLN:HB2	2.10	0.71
1:A:1199:MET:O	1:A:1202:ASP:CG	2.28	0.71
1:C:512:PRO:CB	1:C:790:SER:C	2.59	0.71
1:C:1111:VAL:HG22	1:C:1144:ALA:CB	2.19	0.71
1:D:718:CYS:SG	1:D:773:CYS:HA	2.31	0.71
1:A:809:VAL:HG12	1:A:813:GLU:OE2	1.91	0.71
1:A:1124:SER:CA	1:A:1125:GLU:HB3	2.20	0.71
1:C:571:PHE:CB	1:C:1205:LYS:NZ	2.54	0.71
1:A:812:ILE:HB	1:A:816:TYR:HE2	1.55	0.71
1:A:1062:LEU:HD21	1:A:1155:TYR:CE2	2.22	0.71
1:A:1118:GLY:CA	1:A:1121:ILE:HG12	2.21	0.71
1:C:812:ILE:HB	1:C:816:TYR:HE2	1.55	0.71
1:C:1152:ILE:CG1	1:C:1186:PHE:CZ	2.74	0.71
1:C:1156:ILE:CG2	1:C:1179:PHE:CD1	2.74	0.71
1:A:1083:PRO:N	1:A:1097:LEU:CB	2.54	0.70
1:C:809:VAL:HG12	1:C:813:GLU:OE2	1.91	0.70
1:C:1114:LEU:HD22	1:C:1141:PHE:N	2.04	0.70
1:C:1127:TYR:CB	1:C:1133:ILE:CD1	2.69	0.70
1:C:1134:ILE:CG2	1:C:1200:PHE:CA	2.66	0.70
1:C:1156:ILE:HG23	1:C:1179:PHE:CE1	2.26	0.70
1:A:813:GLU:OE2	1:D:596:LEU:HB3	1.91	0.70
1:A:1096:PHE:HA	1:A:1097:LEU:C	2.09	0.70
1:A:1156:ILE:HG23	1:A:1179:PHE:CE1	2.26	0.70
1:C:1083:PRO:CB	1:C:1098:ARG:HG3	2.12	0.70
1:C:1131:HIS:CD2	1:C:1207:LEU:CD1	2.71	0.70
1:C:1134:ILE:HB	1:C:1200:PHE:CB	2.21	0.70
1:A:1197:VAL:CA	1:A:1200:PHE:HD2	1.90	0.70
1:C:541:PHE:CE2	1:C:1198:HIS:CE1	2.76	0.70
1:C:1104:SER:CA	1:C:1107:PRO:CG	2.68	0.70
1:A:1083:PRO:HD2	1:A:1098:ARG:CG	2.19	0.70
1:A:1127:TYR:HD2	1:A:1128:LYS:C	1.95	0.70
1:C:611:ILE:HD12	1:D:517:PHE:HE1	0.69	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1126:PHE:O	1:C:1128:LYS:HE3	1.92	0.70
1:C:1127:TYR:CE2	1:C:1130:ARG:CA	2.73	0.70
1:C:1127:TYR:CE1	1:C:1130:ARG:HA	2.24	0.70
1:C:1164:SER:CA	1:C:1165:LYS:HG2	2.17	0.70
1:D:518:LEU:HA	1:D:526:TRP:NE1	2.05	0.70
1:C:1131:HIS:CG	1:C:1132:ASN:H	2.09	0.70
1:A:1083:PRO:CB	1:A:1097:LEU:HB2	2.22	0.70
1:C:531:PHE:HE2	1:C:1187:ILE:CD1	1.99	0.70
1:C:1118:GLY:HA2	1:C:1121:ILE:CG1	2.22	0.70
1:A:774:GLY:O	1:A:775:ALA:HB2	1.92	0.70
1:A:1084:GLU:HG2	1:A:1085:ASP:N	2.03	0.70
1:A:1126:PHE:O	1:A:1128:LYS:HE3	1.92	0.70
1:C:1115:PHE:O	1:C:1119:LEU:HG	1.92	0.70
1:C:1068:LEU:HD23	1:C:1074:GLY:HA3	1.72	0.69
1:C:1105:ILE:C	1:C:1107:PRO:CD	2.60	0.69
1:C:1118:GLY:CA	1:C:1121:ILE:HG12	2.21	0.69
1:C:1127:TYR:HD2	1:C:1128:LYS:C	1.95	0.69
1:A:1105:ILE:C	1:A:1107:PRO:CD	2.60	0.69
1:A:1156:ILE:CG2	1:A:1179:PHE:CD1	2.74	0.69
1:D:394:THR:HG22	1:D:440:TYR:C	2.12	0.69
1:A:1197:VAL:CA	1:A:1200:PHE:HE2	1.93	0.69
1:B:611:ILE:HD11	1:C:517:PHE:CE1	2.26	0.69
1:C:538:VAL:HG21	1:C:1194:VAL:CG2	2.17	0.69
1:C:1129:THR:CB	1:C:1133:ILE:HG13	2.17	0.69
1:A:628:ARG:NH1	1:D:627:GLU:H	1.91	0.69
1:A:1032:TRP:HA	1:A:1178:SER:OG	1.92	0.69
1:A:1120:CYS:CA	1:A:1126:PHE:CD1	2.64	0.69
1:C:1131:HIS:O	1:C:1132:ASN:C	2.25	0.69
1:A:541:PHE:CE2	1:A:1198:HIS:NE2	2.60	0.69
1:C:1004:ASP:O	1:C:1008:GLN:HB3	1.93	0.69
1:A:568:THR:CB	1:A:1202:ASP:C	2.61	0.69
1:A:1023:MET:HE1	1:A:1107:PRO:HB2	1.74	0.69
1:A:1129:THR:CB	1:A:1133:ILE:HG13	2.17	0.69
1:A:1152:ILE:CG1	1:A:1186:PHE:CZ	2.74	0.69
1:A:1156:ILE:HG13	1:A:1157:SER:N	2.08	0.69
1:C:1032:TRP:HA	1:C:1178:SER:OG	1.93	0.69
1:C:1083:PRO:HA	1:C:1097:LEU:CD1	2.23	0.69
1:C:1095:TYR:O	1:C:1099:ALA:HB2	1.93	0.69
1:A:1016:ALA:N	1:A:1192:VAL:CG1	2.56	0.69
1:A:1115:PHE:O	1:A:1119:LEU:HG	1.92	0.69
1:A:1102:ALA:O	1:A:1106:PHE:CE2	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:TYR:N	1:A:1128:LYS:CA	2.47	0.68
1:A:1095:TYR:O	1:A:1099:ALA:HB2	1.93	0.68
1:C:1021:SER:O	1:C:1025:ILE:HG12	1.93	0.68
1:A:1021:SER:O	1:A:1025:ILE:HG12	1.93	0.68
1:A:1118:GLY:HA2	1:A:1121:ILE:CG1	2.22	0.68
1:C:1156:ILE:HG13	1:C:1157:SER:N	2.08	0.68
1:D:718:CYS:SG	1:D:773:CYS:CB	2.82	0.68
1:A:1106:PHE:N	1:A:1107:PRO:CD	2.56	0.68
1:A:1127:TYR:CD2	1:A:1129:THR:N	2.62	0.68
1:A:1151:GLY:O	1:A:1154:VAL:HG22	1.93	0.68
1:C:1083:PRO:HG2	1:C:1097:LEU:O	1.92	0.68
1:C:1127:TYR:CD2	1:C:1129:THR:N	2.62	0.68
1:C:1151:GLY:O	1:C:1154:VAL:HG22	1.93	0.68
1:A:1063:TRP:HA	1:A:1081:HIS:H	1.59	0.68
1:A:1083:PRO:HG2	1:A:1097:LEU:O	1.92	0.68
1:C:1152:ILE:HD11	1:C:1186:PHE:HE2	1.59	0.68
1:C:1071:ASN:O	1:C:1072:PHE:CB	2.42	0.68
1:C:1087:ASP:HB2	1:D:699:LYS:NZ	2.07	0.68
1:C:1088:TYR:O	1:C:1089:GLU:HB2	1.93	0.68
1:C:1063:TRP:HA	1:C:1081:HIS:H	1.59	0.68
1:C:1083:PRO:N	1:C:1097:LEU:CB	2.54	0.68
1:A:1088:TYR:O	1:A:1089:GLU:HB2	1.93	0.68
1:C:1023:MET:HE1	1:C:1148:ASN:ND2	2.07	0.68
1:A:1083:PRO:HA	1:A:1097:LEU:CD1	2.23	0.68
1:C:1016:ALA:N	1:C:1192:VAL:CG1	2.56	0.68
1:D:510:SER:O	1:D:511:LYS:HB2	1.93	0.68
1:C:1169:LYS:H	1:C:1172:SER:CB	1.93	0.67
1:D:517:PHE:HD1	1:D:616:TYR:HH	1.42	0.67
1:A:1004:ASP:O	1:A:1008:GLN:HB3	1.93	0.67
1:A:1062:LEU:HD23	1:A:1155:TYR:CE2	2.30	0.67
1:A:1031:TYR:CE1	1:A:1059:HIS:NE2	2.61	0.67
1:A:1097:LEU:O	1:A:1098:ARG:CB	2.42	0.67
1:C:1097:LEU:O	1:C:1098:ARG:CB	2.42	0.67
1:A:1017:PHE:CE1	1:A:1115:PHE:CD1	2.83	0.67
1:A:1102:ALA:C	1:A:1106:PHE:HD2	1.91	0.67
1:C:1017:PHE:CE1	1:C:1115:PHE:CD1	2.83	0.67
1:C:1106:PHE:N	1:C:1107:PRO:CD	2.56	0.67
1:C:1023:MET:HE1	1:C:1107:PRO:HB2	1.77	0.67
1:C:1103:SER:O	1:C:1147:SER:OG	2.12	0.67
1:C:1114:LEU:HD22	1:C:1141:PHE:CG	2.29	0.67
1:A:571:PHE:CB	1:A:1205:LYS:NZ	2.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:PHE:CG	1:A:1111:VAL:CG1	2.75	0.67
1:A:1100:VAL:HG22	1:A:1154:VAL:CG2	2.25	0.67
1:A:1164:SER:CA	1:A:1165:LYS:HG2	2.17	0.67
1:D:514:VAL:HG13	1:D:794:GLY:C	2.14	0.67
1:C:568:THR:CA	1:C:1202:ASP:CB	2.61	0.67
1:D:505:LYS:HG2	1:D:506:LYS:H	1.59	0.67
1:A:1197:VAL:CG1	1:A:1200:PHE:CZ	2.73	0.67
1:C:1083:PRO:HG3	1:C:1097:LEU:CB	2.25	0.67
1:D:514:VAL:HA	1:D:794:GLY:HA3	1.77	0.67
1:C:1107:PRO:CD	1:C:1108:ILE:N	2.55	0.67
1:A:633:ILE:HD13	1:A:633:ILE:N	2.09	0.66
1:A:1114:LEU:HD22	1:A:1141:PHE:CG	2.29	0.66
1:C:1083:PRO:CB	1:C:1097:LEU:HB2	2.22	0.66
1:A:1071:ASN:O	1:A:1072:PHE:CB	2.42	0.66
1:A:1102:ALA:C	1:A:1106:PHE:CD2	2.65	0.66
1:A:1127:TYR:HB2	1:A:1133:ILE:HD11	1.76	0.66
1:C:1141:PHE:HB2	1:C:1193:GLY:HA2	1.77	0.66
1:C:1141:PHE:CB	1:C:1193:GLY:CA	2.73	0.66
1:C:1199:MET:CA	1:C:1202:ASP:OD2	2.39	0.66
1:D:635:SER:OG	1:D:638:ASP:OD2	2.11	0.66
1:A:1141:PHE:HB2	1:A:1193:GLY:HA2	1.77	0.66
1:C:541:PHE:CD1	1:C:1198:HIS:CE1	2.83	0.66
1:A:1170:LYS:H	1:A:1171:ASN:C	1.97	0.66
1:C:1102:ALA:C	1:C:1106:PHE:HD2	1.91	0.66
1:C:1127:TYR:HB2	1:C:1133:ILE:HD11	1.76	0.66
1:D:506:LYS:HB3	1:D:719:ASP:HA	1.76	0.66
1:A:1107:PRO:HB3	1:A:1147:SER:HB3	1.78	0.66
1:C:1100:VAL:HG22	1:C:1154:VAL:CG2	2.25	0.66
1:A:1124:SER:CB	1:A:1125:GLU:HB3	2.26	0.66
1:A:1152:ILE:HD11	1:A:1186:PHE:HE2	1.59	0.66
1:C:1062:LEU:HD23	1:C:1155:TYR:CE2	2.30	0.66
1:C:1107:PRO:HB3	1:C:1147:SER:HB3	1.78	0.66
1:C:1156:ILE:HG22	1:C:1179:PHE:CD1	2.31	0.66
1:C:1102:ALA:C	1:C:1106:PHE:CD2	2.65	0.66
1:A:1130:ARG:HG2	1:A:1130:ARG:HH11	1.61	0.66
1:C:571:PHE:CB	1:C:1205:LYS:HZ2	2.09	0.66
1:A:1020:PHE:CD1	1:A:1111:VAL:HG21	2.31	0.65
1:A:1083:PRO:HG3	1:A:1097:LEU:CB	2.25	0.65
1:A:1152:ILE:HG12	1:A:1186:PHE:CE2	2.31	0.65
1:C:1020:PHE:CG	1:C:1111:VAL:CG1	2.75	0.65
1:C:1020:PHE:C	1:C:1023:MET:HG2	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1156:ILE:HG22	1:A:1179:PHE:CD1	2.31	0.65
1:A:1167:ASP:N	1:A:1167:ASP:OD1	2.28	0.65
1:C:1102:ALA:O	1:C:1106:PHE:CE2	2.41	0.65
1:A:1124:SER:HA	1:A:1125:GLU:HB3	1.78	0.65
1:A:1129:THR:O	1:A:1133:ILE:HG13	1.96	0.65
1:A:1141:PHE:CB	1:A:1193:GLY:CA	2.73	0.65
1:C:1111:VAL:C	1:C:1114:LEU:HG	2.17	0.65
1:A:1094:GLU:O	1:A:1095:TYR:HB3	1.97	0.65
1:A:1107:PRO:CD	1:A:1108:ILE:N	2.55	0.65
1:A:1164:SER:N	1:A:1165:LYS:HG2	2.11	0.65
1:B:505:LYS:HG2	1:B:506:LYS:H	1.61	0.65
1:C:1100:VAL:HG22	1:C:1154:VAL:HG21	1.78	0.65
1:C:1124:SER:HA	1:C:1125:GLU:HB3	1.78	0.65
1:C:1129:THR:O	1:C:1133:ILE:HG13	1.96	0.65
1:C:1164:SER:N	1:C:1165:LYS:HG2	2.11	0.65
1:C:1167:ASP:N	1:C:1167:ASP:OD1	2.28	0.65
1:C:1170:LYS:H	1:C:1171:ASN:C	1.97	0.65
1:A:1020:PHE:C	1:A:1023:MET:HG2	2.17	0.65
1:A:1071:ASN:O	1:A:1072:PHE:CD2	2.50	0.65
1:C:1124:SER:CB	1:C:1125:GLU:HB3	2.26	0.65
1:D:505:LYS:HG2	1:D:506:LYS:N	2.10	0.65
1:D:634:GLU:O	1:D:635:SER:HB3	1.96	0.65
1:A:1079:ILE:O	1:A:1080:ASP:HB2	1.97	0.65
1:B:508:GLN:HA	1:B:629:MET:SD	2.37	0.65
1:C:1071:ASN:O	1:C:1072:PHE:CD2	2.50	0.65
1:A:1071:ASN:O	1:A:1072:PHE:HD2	1.80	0.65
1:C:1175:TYR:O	1:C:1177:TRP:HB2	1.97	0.65
1:A:1028:GLY:HA2	1:A:1063:TRP:CZ3	2.32	0.65
1:A:1124:SER:HB3	1:A:1125:GLU:CA	2.27	0.65
1:C:512:PRO:HB2	1:C:790:SER:C	2.16	0.65
1:C:520:PRO:O	1:D:787:LEU:CB	2.45	0.65
1:C:1031:TYR:CE1	1:C:1059:HIS:CG	2.81	0.65
1:C:1156:ILE:HG22	1:C:1179:PHE:CE1	2.32	0.65
1:D:508:GLN:HG2	1:D:629:MET:SD	2.37	0.65
1:A:1156:ILE:HG22	1:A:1179:PHE:CE1	2.32	0.64
1:A:1175:TYR:O	1:A:1177:TRP:HB2	1.97	0.64
1:A:1103:SER:O	1:A:1147:SER:OG	2.12	0.64
1:A:1128:LYS:NZ	1:A:1128:LYS:HB2	2.12	0.64
1:A:1141:PHE:HB2	1:A:1193:GLY:CA	2.27	0.64
1:B:632:PRO:C	1:B:633:ILE:HD13	2.18	0.64
1:C:1128:LYS:HB2	1:C:1128:LYS:NZ	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1141:PHE:HB2	1:C:1193:GLY:CA	2.27	0.64
1:D:514:VAL:CA	1:D:794:GLY:HA3	2.27	0.64
1:A:531:PHE:CE2	1:A:1187:ILE:HD11	2.33	0.64
1:A:1127:TYR:CE2	1:A:1130:ARG:N	2.65	0.64
1:C:1127:TYR:CB	1:C:1129:THR:N	2.50	0.64
1:C:1141:PHE:CB	1:C:1193:GLY:HA2	2.27	0.64
1:C:521:LEU:HD22	1:C:526:TRP:CD2	2.32	0.64
1:A:1096:PHE:HA	1:A:1097:LEU:O	1.98	0.64
1:A:1111:VAL:C	1:A:1114:LEU:HG	2.17	0.64
1:A:1154:VAL:HG23	1:A:1155:TYR:N	2.11	0.64
1:C:809:VAL:CA	1:C:812:ILE:CD1	2.55	0.64
1:C:1182:GLY:CA	1:C:1186:PHE:CE2	2.81	0.64
1:A:1141:PHE:CB	1:A:1193:GLY:HA2	2.27	0.64
1:C:1130:ARG:HG2	1:C:1130:ARG:HH11	1.61	0.64
1:C:1154:VAL:HG23	1:C:1155:TYR:N	2.11	0.64
1:C:1020:PHE:CD1	1:C:1111:VAL:HG21	2.31	0.64
1:C:1071:ASN:O	1:C:1072:PHE:HD2	1.80	0.64
1:C:1094:GLU:O	1:C:1095:TYR:HB3	1.97	0.64
1:A:1127:TYR:HB2	1:A:1133:ILE:CD1	2.28	0.64
1:C:1027:VAL:O	1:C:1032:TRP:NE1	2.30	0.64
1:C:1197:VAL:CG1	1:C:1200:PHE:CZ	2.73	0.64
1:C:519:ASP:HB2	1:C:520:PRO:HD3	1.79	0.64
1:C:568:THR:CB	1:C:1202:ASP:O	2.46	0.64
1:C:1031:TYR:CD1	1:C:1059:HIS:HD2	2.02	0.64
1:C:1079:ILE:O	1:C:1080:ASP:HB2	1.97	0.64
1:A:1083:PRO:CG	1:A:1098:ARG:CB	2.60	0.63
1:A:1100:VAL:HG22	1:A:1154:VAL:HG21	1.78	0.63
1:A:1121:ILE:HD12	1:A:1134:ILE:HA	1.71	0.63
1:A:1199:MET:CA	1:A:1202:ASP:OD2	2.39	0.63
1:B:632:PRO:C	1:B:633:ILE:HG23	2.17	0.63
1:A:1177:TRP:C	1:A:1179:PHE:N	2.41	0.63
1:C:525:ILE:HG12	1:D:789:LEU:HD13	1.81	0.63
1:C:633:ILE:HG23	1:C:638:ASP:HB2	1.80	0.63
1:C:1127:TYR:CE2	1:C:1130:ARG:N	2.65	0.63
1:A:1017:PHE:HA	1:A:1115:PHE:CE1	2.33	0.63
1:A:1019:ALA:CB	1:A:1188:ILE:CG2	2.48	0.63
1:A:1027:VAL:O	1:A:1032:TRP:NE1	2.30	0.63
1:A:1127:TYR:CD2	1:A:1128:LYS:C	2.72	0.63
1:C:812:ILE:HG13	1:C:813:GLU:N	2.13	0.63
1:A:568:THR:O	1:A:1202:ASP:CB	2.36	0.63
1:A:1009:MET:SD	1:A:1199:MET:CB	2.87	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:ALA:HB2	1:A:1188:ILE:HG22	0.77	0.63
1:A:1129:THR:O	1:A:1133:ILE:CG1	2.46	0.63
1:C:1017:PHE:HA	1:C:1115:PHE:CE1	2.33	0.63
1:C:1096:PHE:HA	1:C:1097:LEU:O	1.98	0.63
1:D:521:LEU:HD23	1:D:525:ILE:HB	1.80	0.63
1:A:521:LEU:HD23	1:A:525:ILE:HB	1.80	0.63
1:A:1138:GLY:HA3	1:A:1197:VAL:HG22	1.81	0.63
1:B:521:LEU:HD23	1:B:525:ILE:HB	1.80	0.63
1:C:1016:ALA:N	1:C:1192:VAL:HG11	2.13	0.63
1:C:1028:GLY:HA2	1:C:1063:TRP:CZ3	2.32	0.63
1:C:1088:TYR:C	1:C:1090:ALA:HA	2.19	0.63
1:C:1124:SER:HB3	1:C:1125:GLU:CA	2.27	0.63
1:A:1159:ASN:CG	1:A:1175:TYR:CE1	2.68	0.63
1:C:1083:PRO:CG	1:C:1098:ARG:CB	2.60	0.63
1:A:1200:PHE:CE1	1:A:1201:ILE:CG1	2.82	0.63
1:A:1121:ILE:HG21	1:A:1133:ILE:HB	1.73	0.63
1:A:1182:GLY:CA	1:A:1186:PHE:CE2	2.81	0.63
1:B:507:PRO:C	1:B:508:GLN:HG3	2.11	0.63
1:A:633:ILE:HG23	1:A:638:ASP:HB2	1.77	0.63
1:A:1088:TYR:C	1:A:1090:ALA:HA	2.19	0.63
1:C:1004:ASP:O	1:C:1008:GLN:CA	2.47	0.63
1:C:1200:PHE:CE1	1:C:1201:ILE:CG1	2.82	0.63
1:A:1016:ALA:HB1	1:A:1141:PHE:CE2	2.34	0.62
1:A:1182:GLY:HA3	1:A:1186:PHE:HE2	1.64	0.62
1:C:1131:HIS:O	1:C:1134:ILE:N	2.32	0.62
1:A:1153:ILE:O	1:A:1156:ILE:HG13	1.99	0.62
1:C:1150:ILE:O	1:C:1153:ILE:HG22	1.99	0.62
1:A:521:LEU:HD22	1:A:526:TRP:CD2	2.35	0.62
1:C:1063:TRP:NE1	1:C:1081:HIS:ND1	2.47	0.62
1:C:1146:LEU:HD11	1:C:1150:ILE:HD11	1.81	0.62
1:D:519:ASP:HB2	1:D:520:PRO:HD3	1.80	0.62
1:D:521:LEU:HD22	1:D:526:TRP:CD2	2.34	0.62
1:A:1016:ALA:N	1:A:1192:VAL:HG11	2.13	0.62
1:A:1031:TYR:HD1	1:A:1059:HIS:HB2	1.64	0.62
1:A:1146:LEU:HD11	1:A:1150:ILE:HD11	1.81	0.62
1:C:1127:TYR:HB2	1:C:1133:ILE:CD1	2.28	0.62
1:C:1127:TYR:CD2	1:C:1128:LYS:C	2.72	0.62
1:D:514:VAL:CG2	1:D:794:GLY:HA3	2.10	0.62
1:C:1031:TYR:HD1	1:C:1059:HIS:HB2	1.64	0.62
1:C:1121:ILE:CG1	1:C:1134:ILE:CG1	2.75	0.62
1:C:1138:GLY:HA3	1:C:1197:VAL:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1105:ILE:N	1:A:1107:PRO:HD3	2.15	0.62
1:A:1111:VAL:C	1:A:1115:PHE:CD2	2.69	0.62
1:B:521:LEU:HD22	1:B:526:TRP:CD2	2.35	0.62
1:C:1016:ALA:C	1:C:1115:PHE:HE1	2.03	0.62
1:A:1022:LEU:HD22	1:A:1185:SER:CA	2.30	0.62
1:C:541:PHE:CZ	1:C:1198:HIS:CB	2.77	0.62
1:C:1182:GLY:HA3	1:C:1186:PHE:HE2	1.64	0.62
1:A:569:ASN:CB	1:A:1005:ARG:HG2	2.30	0.62
1:A:1016:ALA:C	1:A:1115:PHE:HE1	2.03	0.62
1:A:1150:ILE:O	1:A:1153:ILE:HG22	1.99	0.62
1:C:518:LEU:HA	1:C:526:TRP:NE1	2.14	0.62
1:C:1016:ALA:HB1	1:C:1141:PHE:CE2	2.34	0.62
1:C:1034:TYR:CE2	1:C:1059:HIS:CB	2.80	0.62
1:C:1111:VAL:C	1:C:1115:PHE:HD2	2.02	0.62
1:D:50:LEU:HD23	1:D:57:ALA:HB1	1.82	0.62
1:D:507:PRO:O	1:D:508:GLN:HB2	1.99	0.62
1:A:522:ALA:HB3	1:A:525:ILE:HG13	1.82	0.62
1:A:1146:LEU:O	1:A:1146:LEU:HD13	2.00	0.62
1:C:394:THR:CG2	1:C:395:VAL:N	2.35	0.62
1:A:1111:VAL:HA	1:A:1114:LEU:HG	1.81	0.62
1:A:1131:HIS:O	1:A:1134:ILE:N	2.32	0.62
1:C:1020:PHE:HE1	1:C:1108:ILE:CA	1.91	0.62
1:C:1111:VAL:C	1:C:1115:PHE:CD2	2.70	0.62
1:B:507:PRO:CG	1:B:631:SER:CA	2.66	0.61
1:C:1111:VAL:HA	1:C:1114:LEU:HG	1.81	0.61
1:C:1129:THR:O	1:C:1133:ILE:CG1	2.46	0.61
1:A:1004:ASP:O	1:A:1008:GLN:CA	2.47	0.61
1:C:1019:ALA:CB	1:C:1188:ILE:CG2	2.48	0.61
1:C:1105:ILE:N	1:C:1107:PRO:HD3	2.15	0.61
1:C:1153:ILE:O	1:C:1156:ILE:HG13	1.98	0.61
1:A:1127:TYR:CE2	1:A:1130:ARG:CG	2.76	0.61
1:A:1127:TYR:CB	1:A:1129:THR:N	2.50	0.61
1:A:1134:ILE:HG22	1:A:1200:PHE:HB3	0.62	0.61
1:C:541:PHE:CD2	1:C:1198:HIS:NE2	2.67	0.61
1:C:1009:MET:SD	1:C:1199:MET:CB	2.87	0.61
1:A:531:PHE:CE2	1:A:1187:ILE:CD1	2.82	0.61
1:A:619:ASN:OD1	1:B:787:LEU:HD12	1.99	0.61
1:B:786:ALA:O	1:B:787:LEU:HD13	2.00	0.61
1:C:1118:GLY:O	1:C:1121:ILE:HG12	2.00	0.61
1:C:1146:LEU:O	1:C:1146:LEU:HD13	2.00	0.61
1:D:489:ILE:HD12	1:D:735:ALA:HB1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:ILE:HG13	1:A:813:GLU:N	2.13	0.61
1:A:1118:GLY:O	1:A:1121:ILE:HG12	2.00	0.61
1:A:1202:ASP:OD1	1:A:1203:ARG:N	2.34	0.61
1:C:1029:THR:C	1:C:1031:TYR:N	2.48	0.61
1:C:1127:TYR:OH	1:C:1130:ARG:HA	2.00	0.61
1:A:1083:PRO:HA	1:A:1097:LEU:HD12	1.83	0.61
1:A:1121:ILE:CG1	1:A:1134:ILE:CG1	2.75	0.61
1:C:50:LEU:HD23	1:C:57:ALA:HB1	1.82	0.61
1:C:516:SER:OG	1:C:791:ASN:CG	2.39	0.61
1:A:628:ARG:NH2	1:D:623:PHE:HD1	1.98	0.61
1:A:1118:GLY:C	1:A:1121:ILE:HG12	2.21	0.61
1:C:1202:ASP:OD1	1:C:1203:ARG:N	2.34	0.61
1:A:1103:SER:O	1:A:1107:PRO:CG	2.48	0.61
1:B:50:LEU:HD23	1:B:57:ALA:HB1	1.83	0.61
1:A:1114:LEU:HB2	1:A:1141:PHE:CD1	2.36	0.61
1:B:394:THR:HG22	1:B:440:TYR:HA	1.82	0.61
1:C:1031:TYR:CE1	1:C:1059:HIS:NE2	2.61	0.61
1:C:1115:PHE:CE1	1:C:1141:PHE:CE2	2.86	0.61
1:C:1134:ILE:HG22	1:C:1200:PHE:HB3	0.62	0.61
1:C:1022:LEU:HD22	1:C:1185:SER:CA	2.30	0.61
1:C:1121:ILE:CB	1:C:1134:ILE:CG1	2.75	0.61
1:C:1127:TYR:CE2	1:C:1130:ARG:CG	2.76	0.61
1:C:809:VAL:HG12	1:C:813:GLU:CD	2.22	0.60
1:C:1020:PHE:CD1	1:C:1111:VAL:CG2	2.84	0.60
1:C:390:LEU:O	1:C:392:GLN:N	2.34	0.60
1:D:522:ALA:HB3	1:D:525:ILE:HG13	1.83	0.60
1:A:1020:PHE:CZ	1:A:1108:ILE:CA	2.83	0.60
1:A:1063:TRP:NE1	1:A:1081:HIS:ND1	2.47	0.60
1:B:505:LYS:HD3	1:B:698:GLY:N	2.16	0.60
1:C:521:LEU:HD23	1:C:525:ILE:HB	1.83	0.60
1:D:514:VAL:HG22	1:D:794:GLY:C	2.16	0.60
1:A:50:LEU:HD23	1:A:57:ALA:HB1	1.82	0.60
1:A:809:VAL:HG12	1:A:813:GLU:CD	2.22	0.60
1:C:1020:PHE:CZ	1:C:1108:ILE:CA	2.83	0.60
1:A:519:ASP:HB2	1:A:520:PRO:HD3	1.82	0.60
1:B:522:ALA:HB3	1:B:525:ILE:HG13	1.82	0.60
1:C:765:LYS:O	1:C:770:LYS:HB2	2.01	0.60
1:C:1131:HIS:C	1:C:1133:ILE:N	2.43	0.60
1:A:1031:TYR:CE1	1:A:1059:HIS:CG	2.81	0.60
1:D:514:VAL:CB	1:D:794:GLY:HA3	2.30	0.60
1:A:475:ALA:HB3	1:A:735:ALA:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:GLN:O	1:B:509:LYS:HB2	2.01	0.60
1:C:1118:GLY:HA2	1:C:1121:ILE:HD11	1.84	0.60
1:C:1118:GLY:C	1:C:1121:ILE:HG12	2.21	0.60
1:A:571:PHE:CB	1:A:1205:LYS:HZ2	2.14	0.60
1:A:1020:PHE:CD1	1:A:1111:VAL:CG2	2.84	0.60
1:C:1177:TRP:C	1:C:1179:PHE:H	2.04	0.60
1:A:1077:LYS:O	1:A:1079:ILE:HG13	2.02	0.60
1:A:1083:PRO:CG	1:A:1097:LEU:CB	2.79	0.60
1:A:1088:TYR:HD2	1:A:1089:GLU:H	1.50	0.60
1:C:522:ALA:HB3	1:C:525:ILE:HG13	1.83	0.60
1:C:1136:SER:O	1:C:1139:ILE:HG12	2.01	0.60
1:C:1083:PRO:CG	1:C:1097:LEU:CB	2.79	0.60
1:C:1155:TYR:CD1	1:C:1179:PHE:HZ	2.20	0.60
1:C:1159:ASN:CG	1:C:1175:TYR:CE1	2.68	0.60
1:A:628:ARG:HH12	1:D:627:GLU:H	1.50	0.59
1:A:1136:SER:O	1:A:1139:ILE:HG12	2.01	0.59
1:C:514:VAL:HG22	1:C:794:GLY:HA2	1.84	0.59
1:C:1077:LYS:O	1:C:1079:ILE:HG13	2.02	0.59
1:A:611:ILE:CD1	1:B:517:PHE:CE1	2.78	0.59
1:A:1017:PHE:N	1:A:1115:PHE:HE1	2.01	0.59
1:C:1114:LEU:HB2	1:C:1141:PHE:CD1	2.36	0.59
1:C:1152:ILE:HD11	1:C:1186:PHE:CZ	2.37	0.59
1:C:1168:SER:HB3	1:C:1172:SER:HB3	1.84	0.59
1:C:1183:ALA:O	1:C:1187:ILE:HD12	2.02	0.59
1:A:568:THR:CB	1:A:1202:ASP:O	2.50	0.59
1:C:475:ALA:HB3	1:C:735:ALA:HB3	1.84	0.59
1:A:810:ALA:C	1:A:814:PHE:CD2	2.76	0.59
1:B:626:VAL:CB	1:C:628:ARG:HH11	2.08	0.59
1:C:520:PRO:HA	1:C:623:PHE:HE2	1.67	0.59
1:A:1020:PHE:HB2	1:A:1115:PHE:HZ	1.68	0.59
1:A:1034:TYR:CE2	1:A:1059:HIS:CB	2.80	0.59
1:A:1179:PHE:O	1:A:1183:ALA:N	2.35	0.59
1:B:505:LYS:HE3	1:B:506:LYS:HE3	1.83	0.59
1:A:1118:GLY:HA2	1:A:1121:ILE:HD11	1.84	0.59
1:A:1136:SER:O	1:A:1140:PHE:HD1	1.86	0.59
1:C:1164:SER:N	1:C:1165:LYS:CG	2.65	0.59
1:A:1063:TRP:HA	1:A:1081:HIS:N	2.17	0.59
1:A:1079:ILE:HD12	1:A:1082:PHE:HE1	1.67	0.59
1:C:394:THR:HG23	1:C:439:LYS:C	2.23	0.59
1:C:1063:TRP:HA	1:C:1081:HIS:N	2.17	0.59
1:C:1197:VAL:CA	1:C:1200:PHE:HE2	1.93	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:PHE:CE1	1:D:611:ILE:HD12	2.32	0.59
1:A:1183:ALA:O	1:A:1187:ILE:HD12	2.02	0.59
1:C:1079:ILE:HD12	1:C:1082:PHE:HE1	1.67	0.59
1:C:1083:PRO:HA	1:C:1097:LEU:HD12	1.83	0.59
1:A:795:VAL:HG21	1:D:611:ILE:HG21	1.84	0.59
1:C:1063:TRP:HZ2	1:C:1081:HIS:HE1	1.46	0.59
1:C:1194:VAL:CG1	1:C:1198:HIS:NE2	2.66	0.59
1:A:808:LEU:O	1:A:812:ILE:HG12	2.03	0.58
1:A:1152:ILE:HD11	1:A:1186:PHE:CZ	2.37	0.58
1:C:1131:HIS:C	1:C:1133:ILE:H	2.04	0.58
1:A:538:VAL:HG23	1:A:1194:VAL:HG22	1.85	0.58
1:A:1152:ILE:CD1	1:A:1186:PHE:HE2	2.12	0.58
1:A:1194:VAL:HG12	1:A:1198:HIS:NE2	2.18	0.58
1:C:1122:ALA:O	1:C:1123:ALA:CB	2.51	0.58
1:A:1013:THR:HB	1:A:1017:PHE:HE2	1.69	0.58
1:A:1111:VAL:C	1:A:1115:PHE:HD2	2.02	0.58
1:A:1115:PHE:CE1	1:A:1141:PHE:CE2	2.86	0.58
1:A:1127:TYR:OH	1:A:1130:ARG:HA	2.00	0.58
1:A:1168:SER:HB3	1:A:1172:SER:HB3	1.84	0.58
1:C:1019:ALA:HB2	1:C:1188:ILE:HG22	0.77	0.58
1:C:1020:PHE:HB2	1:C:1115:PHE:HZ	1.68	0.58
1:C:1081:HIS:HD2	1:C:1101:ARG:HD2	1.67	0.58
1:A:1068:LEU:HD23	1:A:1074:GLY:HA2	1.85	0.58
1:A:10:ASN:N	1:A:10:ASN:HD22	2.01	0.58
1:A:1135:LEU:HD23	1:A:1200:PHE:CZ	2.38	0.58
1:C:1129:THR:HB	1:C:1133:ILE:HG12	1.78	0.58
1:D:631:SER:CB	1:D:632:PRO:HD2	2.30	0.58
1:A:1194:VAL:CG1	1:A:1198:HIS:NE2	2.66	0.58
1:C:1098:ARG:O	1:C:1101:ARG:N	2.37	0.58
1:D:695:LYS:HG2	1:D:695:LYS:O	2.04	0.58
1:A:1183:ALA:O	1:A:1187:ILE:CD1	2.52	0.58
1:A:611:ILE:CD1	1:B:517:PHE:CZ	2.87	0.58
1:C:810:ALA:C	1:C:814:PHE:CD2	2.76	0.58
1:A:1089:GLU:HB3	1:A:1091:ASP:N	2.19	0.58
1:A:1131:HIS:O	1:A:1133:ILE:CA	2.50	0.58
1:B:513:GLY:C	1:B:515:PHE:N	2.55	0.58
1:C:569:ASN:CB	1:C:1005:ARG:HG2	2.34	0.58
1:A:1155:TYR:CD1	1:A:1179:PHE:HZ	2.20	0.58
1:B:235:ILE:HD13	1:B:242:VAL:HG21	1.85	0.58
1:B:514:VAL:HG22	1:B:794:GLY:CA	2.33	0.58
1:C:1089:GLU:HB3	1:C:1091:ASP:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1135:LEU:HD23	1:C:1200:PHE:CZ	2.38	0.57
1:C:1183:ALA:O	1:C:1187:ILE:CD1	2.52	0.57
1:A:1121:ILE:CB	1:A:1134:ILE:CG1	2.75	0.57
1:A:1122:ALA:O	1:A:1123:ALA:CB	2.51	0.57
1:C:394:THR:HG23	1:C:439:LYS:O	2.03	0.57
1:C:512:PRO:N	1:C:790:SER:HB2	2.16	0.57
1:C:1023:MET:CE	1:C:1148:ASN:CG	2.73	0.57
1:C:1194:VAL:HG12	1:C:1198:HIS:NE2	2.18	0.57
1:A:1023:MET:CE	1:A:1148:ASN:CG	2.73	0.57
1:A:1089:GLU:HB2	1:A:1090:ALA:HA	1.86	0.57
1:A:1131:HIS:CG	1:A:1132:ASN:H	2.09	0.57
1:C:1013:THR:HB	1:C:1017:PHE:HE2	1.69	0.57
1:C:1096:PHE:CZ	1:C:1097:LEU:CD2	2.86	0.57
1:C:1114:LEU:CD1	1:C:1141:PHE:CD1	2.67	0.57
1:C:1169:LYS:O	1:C:1170:LYS:HB2	2.04	0.57
1:A:812:ILE:C	1:A:816:TYR:CD2	2.78	0.57
1:A:1098:ARG:O	1:A:1101:ARG:N	2.37	0.57
1:B:10:ASN:HD22	1:B:10:ASN:N	2.01	0.57
1:C:1136:SER:O	1:C:1140:PHE:HD1	1.86	0.57
1:D:235:ILE:HD13	1:D:242:VAL:HG21	1.86	0.57
1:D:507:PRO:HD3	1:D:721:MET:SD	2.44	0.57
1:A:235:ILE:HD13	1:A:242:VAL:HG21	1.85	0.57
1:A:1023:MET:HE3	1:A:1148:ASN:CG	2.24	0.57
1:A:1029:THR:C	1:A:1031:TYR:N	2.48	0.57
1:A:1129:THR:HB	1:A:1133:ILE:HG12	1.78	0.57
1:A:1177:TRP:C	1:A:1179:PHE:H	2.04	0.57
1:C:809:VAL:O	1:C:812:ILE:CG1	2.53	0.57
1:C:809:VAL:CB	1:C:812:ILE:HD11	2.35	0.57
1:C:1152:ILE:HG23	1:C:1179:PHE:HD1	1.69	0.57
1:C:235:ILE:HD13	1:C:242:VAL:HG21	1.85	0.57
1:C:1103:SER:O	1:C:1107:PRO:CG	2.48	0.57
1:A:809:VAL:CB	1:A:812:ILE:HD11	2.35	0.57
1:A:1023:MET:HE1	1:A:1148:ASN:ND2	2.14	0.57
1:A:1094:GLU:HG3	1:A:1098:ARG:NH2	2.20	0.57
1:C:10:ASN:HD22	1:C:10:ASN:N	2.02	0.57
1:C:389:GLY:C	1:C:391:GLU:H	2.08	0.57
1:C:1017:PHE:N	1:C:1115:PHE:HE1	2.01	0.57
1:C:1032:TRP:HA	1:C:1178:SER:HG	1.69	0.57
1:C:1111:VAL:O	1:C:1115:PHE:CE2	2.53	0.57
1:C:1200:PHE:CZ	1:C:1201:ILE:CG1	2.88	0.57
1:A:93:HIS:ND1	1:A:322:PRO:HB3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:GLY:O	1:A:515:PHE:N	2.37	0.57
1:A:809:VAL:O	1:A:812:ILE:CG1	2.53	0.57
1:A:1023:MET:N	1:A:1185:SER:HB2	2.20	0.57
1:C:517:PHE:CZ	1:C:526:TRP:CZ2	2.92	0.57
1:C:1068:LEU:HD23	1:C:1074:GLY:HA2	1.85	0.57
1:D:10:ASN:HD22	1:D:10:ASN:N	2.02	0.57
1:D:99:PRO:HA	1:D:113:MET:HB2	1.87	0.57
1:D:512:PRO:CB	1:D:790:SER:C	2.74	0.57
1:A:513:GLY:C	1:A:515:PHE:H	2.07	0.57
1:A:1012:THR:OG1	1:A:1199:MET:SD	2.62	0.57
1:A:1131:HIS:C	1:A:1133:ILE:H	2.04	0.57
1:C:1007:VAL:O	1:C:1007:VAL:HG12	2.04	0.57
1:C:1020:PHE:HB2	1:C:1115:PHE:CZ	2.40	0.57
1:B:489:ILE:HD12	1:B:735:ALA:HB1	1.87	0.57
1:C:1012:THR:OG1	1:C:1199:MET:SD	2.62	0.57
1:C:1031:TYR:CD1	1:C:1059:HIS:CG	2.93	0.57
1:D:633:ILE:HD12	1:D:633:ILE:N	2.20	0.57
1:C:77:TYR:CE2	1:C:98:THR:HG21	2.40	0.56
1:C:99:PRO:HA	1:C:113:MET:HB2	1.87	0.56
1:C:1179:PHE:O	1:C:1183:ALA:N	2.35	0.56
1:D:77:TYR:CE2	1:D:98:THR:HG21	2.40	0.56
1:D:508:GLN:C	1:D:629:MET:SD	2.83	0.56
1:B:394:THR:CG2	1:B:440:TYR:HA	2.34	0.56
1:C:1023:MET:HA	1:C:1185:SER:OG	2.05	0.56
1:C:1089:GLU:HB2	1:C:1090:ALA:HA	1.86	0.56
1:A:99:PRO:HA	1:A:113:MET:HB2	1.87	0.56
1:A:1169:LYS:O	1:A:1170:LYS:HB2	2.05	0.56
1:A:1201:ILE:HG22	1:A:1205:LYS:HE3	1.86	0.56
1:B:504:ILE:CD1	1:B:633:ILE:CG2	2.81	0.56
1:C:576:SER:CB	1:C:1198:HIS:HE1	2.18	0.56
1:C:812:ILE:C	1:C:816:TYR:HD2	2.08	0.56
1:D:512:PRO:HB2	1:D:790:SER:C	2.26	0.56
1:D:785:SER:O	1:D:786:ALA:HB2	2.05	0.56
1:A:1032:TRP:HA	1:A:1178:SER:HG	1.69	0.56
1:A:1095:TYR:CD2	1:A:1096:PHE:N	2.73	0.56
1:A:1096:PHE:CZ	1:A:1097:LEU:CD2	2.86	0.56
1:A:1111:VAL:CA	1:A:1114:LEU:HG	2.36	0.56
1:A:1152:ILE:HG23	1:A:1179:PHE:HD1	1.69	0.56
1:B:514:VAL:HG22	1:B:794:GLY:HA3	1.85	0.56
1:B:633:ILE:HG21	1:B:723:VAL:CG1	2.21	0.56
1:C:1034:TYR:O	1:C:1173:TYR:CB	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:521:LEU:HD22	1:D:526:TRP:CG	2.41	0.56
1:A:77:TYR:CE2	1:A:98:THR:HG21	2.40	0.56
1:A:1020:PHE:HB2	1:A:1115:PHE:CZ	2.40	0.56
1:A:1111:VAL:HA	1:A:1114:LEU:HD23	1.83	0.56
1:A:1114:LEU:HB2	1:A:1141:PHE:CE1	2.41	0.56
1:A:1127:TYR:CG	1:A:1129:THR:N	2.74	0.56
1:C:1023:MET:N	1:C:1185:SER:HB2	2.20	0.56
1:A:1164:SER:N	1:A:1165:LYS:CG	2.65	0.56
1:B:99:PRO:HA	1:B:113:MET:HB2	1.87	0.56
1:C:808:LEU:O	1:C:812:ILE:HG23	2.05	0.56
1:C:1084:GLU:H	1:C:1097:LEU:HD12	1.70	0.56
1:A:209:ILE:HA	1:A:214:HIS:CD2	2.41	0.56
1:A:1084:GLU:H	1:A:1097:LEU:HD12	1.70	0.56
1:C:521:LEU:HD22	1:C:526:TRP:CG	2.40	0.56
1:C:1095:TYR:CD2	1:C:1096:PHE:N	2.73	0.56
1:C:1197:VAL:O	1:C:1200:PHE:CG	2.57	0.56
1:D:512:PRO:HB3	1:D:790:SER:HB2	0.65	0.56
1:C:376:GLU:HG3	1:C:377:VAL:HG13	1.88	0.56
1:C:1064:ARG:HG2	1:C:1078:GLN:HA	1.88	0.56
1:C:1127:TYR:N	1:C:1127:TYR:CD2	2.73	0.56
1:C:1127:TYR:CG	1:C:1129:THR:N	2.74	0.56
1:A:769:ASP:C	1:A:771:GLY:H	2.09	0.56
1:A:1023:MET:HA	1:A:1185:SER:OG	2.05	0.56
1:A:1082:PHE:C	1:A:1097:LEU:HD13	2.25	0.56
1:A:1127:TYR:N	1:A:1127:TYR:CD2	2.73	0.56
1:B:521:LEU:HD22	1:B:526:TRP:CG	2.41	0.56
1:C:227:PHE:CD1	1:C:244:GLY:HA3	2.41	0.56
1:A:1088:TYR:N	1:A:1088:TYR:CD2	2.73	0.56
1:B:695:LYS:O	1:B:695:LYS:HG2	2.04	0.56
1:C:812:ILE:C	1:C:816:TYR:CD2	2.78	0.56
1:A:376:GLU:HG3	1:A:377:VAL:HG13	1.88	0.55
1:A:1088:TYR:CD2	1:A:1089:GLU:N	2.73	0.55
1:A:1200:PHE:CZ	1:A:1201:ILE:CG1	2.88	0.55
1:C:1023:MET:HE1	1:C:1148:ASN:OD1	2.06	0.55
1:C:1111:VAL:CA	1:C:1114:LEU:HG	2.36	0.55
1:C:1114:LEU:HB2	1:C:1141:PHE:CE1	2.41	0.55
1:D:227:PHE:CD1	1:D:244:GLY:HA3	2.41	0.55
1:D:376:GLU:HG3	1:D:377:VAL:HG13	1.88	0.55
1:A:227:PHE:CD1	1:A:244:GLY:HA3	2.41	0.55
1:A:521:LEU:HD22	1:A:526:TRP:CG	2.41	0.55
1:A:769:ASP:O	1:A:771:GLY:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:LEU:CD2	1:A:1155:TYR:HE2	2.17	0.55
1:C:209:ILE:HA	1:C:214:HIS:CD2	2.41	0.55
1:C:1094:GLU:HG3	1:C:1098:ARG:NH2	2.20	0.55
1:C:1115:PHE:CZ	1:C:1141:PHE:HE2	2.25	0.55
1:C:1170:LYS:HB3	1:C:1171:ASN:HB3	1.88	0.55
1:D:209:ILE:HA	1:D:214:HIS:CD2	2.41	0.55
1:A:1023:MET:CE	1:A:1148:ASN:OD1	2.54	0.55
1:C:1031:TYR:O	1:C:1177:TRP:HB3	2.06	0.55
1:C:1152:ILE:CD1	1:C:1186:PHE:HE2	2.12	0.55
1:A:1031:TYR:O	1:A:1177:TRP:HB3	2.06	0.55
1:A:1118:GLY:O	1:A:1121:ILE:CG1	2.54	0.55
1:A:1124:SER:CB	1:A:1125:GLU:CB	2.84	0.55
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.41	0.55
1:C:512:PRO:HB2	1:C:790:SER:O	2.06	0.55
1:C:1096:PHE:CE1	1:C:1097:LEU:HD23	2.41	0.55
1:D:516:SER:OG	1:D:791:ASN:CG	2.45	0.55
1:A:1007:VAL:O	1:A:1007:VAL:HG12	2.04	0.55
1:A:1096:PHE:CE1	1:A:1097:LEU:HD23	2.41	0.55
1:B:209:ILE:HA	1:B:214:HIS:CD2	2.41	0.55
1:B:506:LYS:HG2	1:B:719:ASP:HB2	1.88	0.55
1:C:1023:MET:CE	1:C:1148:ASN:OD1	2.54	0.55
1:C:1121:ILE:HD12	1:C:1134:ILE:HA	1.72	0.55
1:C:1201:ILE:HG22	1:C:1205:LYS:HE3	1.87	0.55
1:A:808:LEU:O	1:A:812:ILE:CG2	2.51	0.55
1:A:1115:PHE:CZ	1:A:1141:PHE:HE2	2.25	0.55
1:A:1124:SER:CB	1:A:1126:PHE:CD1	2.90	0.55
1:B:376:GLU:HG3	1:B:377:VAL:HG13	1.88	0.55
1:C:1062:LEU:CD2	1:C:1155:TYR:HE2	2.17	0.55
1:C:1118:GLY:O	1:C:1121:ILE:CG1	2.54	0.55
1:D:718:CYS:SG	1:D:773:CYS:CA	2.95	0.55
1:A:1027:VAL:O	1:A:1063:TRP:CZ3	2.56	0.55
1:A:1176:GLY:CA	1:A:1177:TRP:CB	2.59	0.55
1:B:77:TYR:CE2	1:B:98:THR:HG21	2.41	0.55
1:D:753:LEU:HD22	1:D:758:LEU:HD13	1.89	0.55
1:A:1102:ALA:HB1	1:A:1106:PHE:CE2	2.27	0.55
1:A:1141:PHE:CB	1:A:1193:GLY:HA3	2.37	0.55
1:C:753:LEU:HD22	1:C:758:LEU:HD13	1.89	0.55
1:C:1035:SER:CA	1:C:1173:TYR:CD2	2.85	0.55
1:A:391:GLU:C	1:A:393:LYS:H	2.10	0.55
1:B:788:SER:OG	1:B:790:SER:OG	2.12	0.55
1:C:1124:SER:CB	1:C:1125:GLU:CB	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1141:PHE:CB	1:C:1193:GLY:HA3	2.37	0.55
1:C:1153:ILE:CG1	1:C:1156:ILE:HD11	2.29	0.55
1:A:1030:ASP:O	1:A:1031:TYR:CD1	2.60	0.55
1:A:1089:GLU:CB	1:A:1090:ALA:CA	2.85	0.55
1:A:1200:PHE:CD1	1:A:1201:ILE:N	2.76	0.55
1:C:1102:ALA:HB1	1:C:1106:PHE:CE2	2.27	0.55
1:C:1114:LEU:CD1	1:C:1141:PHE:CG	2.84	0.55
1:A:1007:VAL:O	1:A:1011:LEU:CG	2.48	0.54
1:A:1083:PRO:CG	1:A:1097:LEU:HB2	2.38	0.54
1:A:1189:ALA:O	1:A:1192:VAL:HG23	2.05	0.54
1:C:771:GLY:O	1:C:772:GLU:HG3	2.06	0.54
1:C:1068:LEU:CD2	1:C:1074:GLY:HA3	2.37	0.54
1:C:1089:GLU:CB	1:C:1090:ALA:CA	2.85	0.54
1:C:1204:HIS:O	1:C:1208:THR:HG23	2.08	0.54
1:A:1204:HIS:O	1:A:1208:THR:HG23	2.08	0.54
1:B:62:PHE:HE2	1:B:92:LEU:HD12	1.72	0.54
1:C:91:THR:HG21	1:D:56:PHE:CE2	2.42	0.54
1:C:1182:GLY:HA3	1:C:1186:PHE:CE2	2.42	0.54
1:A:62:PHE:HE2	1:A:92:LEU:HD12	1.73	0.54
1:A:1114:LEU:HD11	1:A:1141:PHE:CD2	2.34	0.54
1:B:299:LEU:HD11	1:B:332:ALA:HB2	1.88	0.54
1:B:635:SER:O	1:B:636:ALA:C	2.44	0.54
1:C:1135:LEU:C	1:C:1135:LEU:HD13	2.28	0.54
1:B:519:ASP:HB2	1:B:520:PRO:HD3	1.90	0.54
1:C:1030:ASP:O	1:C:1031:TYR:CD1	2.60	0.54
1:D:505:LYS:CG	1:D:506:LYS:H	2.21	0.54
1:B:506:LYS:CG	1:B:719:ASP:HA	2.25	0.54
1:C:62:PHE:HE2	1:C:92:LEU:HD12	1.73	0.54
1:C:489:ILE:HD12	1:C:735:ALA:HB1	1.88	0.54
1:C:1127:TYR:HD2	1:C:1128:LYS:CA	2.21	0.54
1:B:692:ARG:CG	1:B:700:TYR:CD2	2.89	0.54
1:C:1200:PHE:CD1	1:C:1201:ILE:N	2.76	0.54
1:D:394:THR:CG2	1:D:440:TYR:C	2.76	0.54
1:A:753:LEU:HD22	1:A:758:LEU:HD13	1.89	0.54
1:A:754:SER:HB3	1:A:759:LEU:HD12	1.90	0.54
1:A:1135:LEU:HD13	1:A:1135:LEU:C	2.27	0.54
1:A:1064:ARG:HG2	1:A:1078:GLN:HA	1.88	0.54
1:A:1192:VAL:HG23	1:A:1193:GLY:N	2.23	0.54
1:C:1124:SER:CB	1:C:1126:PHE:CD1	2.90	0.54
1:A:1135:LEU:HD13	1:A:1135:LEU:O	2.08	0.54
1:C:1027:VAL:O	1:C:1063:TRP:CZ3	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:635:SER:O	1:D:638:ASP:N	2.25	0.54
1:A:541:PHE:HZ	1:A:1198:HIS:CB	2.19	0.54
1:A:1068:LEU:CD2	1:A:1074:GLY:HA3	2.37	0.54
1:C:1088:TYR:HD2	1:C:1089:GLU:H	1.50	0.54
1:D:765:LYS:O	1:D:770:LYS:HB2	2.08	0.54
1:A:1197:VAL:O	1:A:1200:PHE:CG	2.57	0.53
1:B:753:LEU:HD22	1:B:758:LEU:HD13	1.89	0.53
1:C:754:SER:HB3	1:C:759:LEU:HD12	1.90	0.53
1:C:1127:TYR:HD2	1:C:1128:LYS:HA	1.73	0.53
1:A:812:ILE:C	1:A:816:TYR:HD2	2.08	0.53
1:A:1031:TYR:CD1	1:A:1059:HIS:CG	2.93	0.53
1:C:809:VAL:O	1:C:812:ILE:HG13	2.07	0.53
1:C:1177:TRP:HA	1:C:1177:TRP:CE3	2.42	0.53
1:D:475:ALA:HB3	1:D:735:ALA:HB3	1.90	0.53
1:A:1190:GLU:O	1:A:1194:VAL:HG23	2.08	0.53
1:C:1083:PRO:CG	1:C:1097:LEU:HB2	2.38	0.53
1:C:1190:GLU:O	1:C:1194:VAL:HG23	2.08	0.53
1:A:1193:GLY:O	1:A:1197:VAL:HG23	2.09	0.53
1:B:636:ALA:O	1:B:639:LEU:N	2.37	0.53
1:C:1082:PHE:C	1:C:1097:LEU:HD13	2.25	0.53
1:C:1192:VAL:HG23	1:C:1193:GLY:N	2.23	0.53
1:D:692:ARG:CG	1:D:700:TYR:CD2	2.90	0.53
1:A:774:GLY:O	1:A:775:ALA:CB	2.57	0.53
1:C:809:VAL:C	1:C:812:ILE:CG1	2.77	0.53
1:A:1035:SER:CA	1:A:1173:TYR:CD2	2.85	0.53
1:D:62:PHE:HE2	1:D:92:LEU:HD12	1.73	0.53
1:A:1161:GLY:O	1:A:1163:PRO:N	2.42	0.53
1:D:337:GLN:HE22	3:D:1302:NAG:H2	1.74	0.53
1:D:754:SER:HB3	1:D:759:LEU:HD12	1.91	0.53
1:A:809:VAL:HG13	1:A:812:ILE:HD11	1.90	0.53
1:B:506:LYS:CG	1:B:719:ASP:HB2	2.39	0.53
1:C:521:LEU:CA	1:D:787:LEU:HD23	2.31	0.53
1:C:1135:LEU:HD13	1:C:1135:LEU:O	2.08	0.53
1:A:1034:TYR:O	1:A:1173:TYR:CB	2.32	0.53
1:B:626:VAL:HB	1:C:628:ARG:NH1	2.08	0.53
1:C:1029:THR:HG21	1:C:1178:SER:CA	2.39	0.53
1:C:1088:TYR:CD2	1:C:1088:TYR:N	2.73	0.53
1:A:542:LEU:HD21	1:A:1197:VAL:HG21	1.91	0.53
1:C:541:PHE:CZ	1:C:1198:HIS:HA	2.43	0.53
1:C:1056:VAL:CG1	1:C:1057:MET:N	2.46	0.53
1:A:809:VAL:O	1:A:812:ILE:HG13	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:LEU:HD23	1:A:1140:PHE:CE2	2.44	0.52
1:A:1127:TYR:HD2	1:A:1128:LYS:CA	2.21	0.52
1:C:1139:ILE:HG13	1:C:1140:PHE:CD1	2.44	0.52
1:C:1170:LYS:N	1:C:1171:ASN:CB	2.73	0.52
1:D:405:TYR:CG	1:D:478:PRO:HG3	2.44	0.52
1:A:523:TYR:O	1:A:527:MET:HG2	2.09	0.52
1:A:1029:THR:HG21	1:A:1178:SER:CA	2.39	0.52
1:A:1127:TYR:CD1	1:A:1133:ILE:HD12	2.44	0.52
1:A:1146:LEU:HD13	1:A:1146:LEU:C	2.30	0.52
1:C:1153:ILE:HD11	1:D:789:LEU:HD21	1.90	0.52
1:C:1170:LYS:CB	1:C:1171:ASN:CB	2.85	0.52
1:D:205:VAL:O	1:D:209:ILE:HG13	2.09	0.52
1:A:628:ARG:HH11	1:D:626:VAL:HB	1.74	0.52
1:A:1127:TYR:HD2	1:A:1128:LYS:HA	1.73	0.52
1:A:1141:PHE:HB3	1:A:1193:GLY:CA	2.39	0.52
1:C:512:PRO:HA	1:C:790:SER:CB	2.30	0.52
1:C:1113:LEU:HD23	1:C:1140:PHE:CE2	2.44	0.52
1:A:1177:TRP:HA	1:A:1177:TRP:CE3	2.42	0.52
1:C:205:VAL:O	1:C:209:ILE:HG13	2.09	0.52
1:C:1189:ALA:O	1:C:1192:VAL:HG23	2.05	0.52
1:A:513:GLY:C	1:A:515:PHE:N	2.63	0.52
1:A:809:VAL:CG1	1:A:813:GLU:OE2	2.58	0.52
1:A:1170:LYS:HB3	1:A:1171:ASN:HB3	1.88	0.52
1:C:216:LYS:NZ	1:C:473:ASP:OD2	2.43	0.52
1:C:809:VAL:HG13	1:C:812:ILE:HD11	1.90	0.52
1:D:630:VAL:CG2	1:D:631:SER:H	2.17	0.52
1:C:523:TYR:O	1:C:527:MET:HG2	2.10	0.52
1:C:1127:TYR:CD1	1:C:1133:ILE:HD12	2.44	0.52
1:A:1020:PHE:HE1	1:A:1108:ILE:CA	1.91	0.52
1:A:1032:TRP:CH2	1:A:1062:LEU:HD11	2.45	0.52
1:C:405:TYR:CG	1:C:478:PRO:HG3	2.44	0.52
1:C:1032:TRP:CH2	1:C:1062:LEU:HD11	2.45	0.52
1:C:1153:ILE:HG23	1:C:1154:VAL:N	2.25	0.52
1:C:1161:GLY:O	1:C:1162:ASP:C	2.49	0.52
1:C:1161:GLY:O	1:C:1163:PRO:N	2.42	0.52
1:A:405:TYR:CG	1:A:478:PRO:HG3	2.45	0.52
1:A:541:PHE:HZ	1:A:1198:HIS:HA	1.75	0.52
1:A:571:PHE:CB	1:A:1205:LYS:HZ3	2.23	0.52
1:A:1079:ILE:HD12	1:A:1082:PHE:CE1	2.45	0.52
1:A:1161:GLY:O	1:A:1162:ASP:C	2.49	0.52
1:B:754:SER:HB3	1:B:759:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:512:PRO:CB	1:D:790:SER:CB	2.34	0.52
1:A:337:GLN:NE2	3:A:1302:NAG:H2	2.25	0.52
1:A:405:TYR:CD1	1:A:478:PRO:HG3	2.45	0.52
1:A:769:ASP:C	1:A:771:GLY:N	2.64	0.52
1:A:1016:ALA:HA	1:A:1192:VAL:CG2	2.40	0.52
1:A:1027:VAL:C	1:A:1063:TRP:HZ3	2.13	0.52
1:A:1071:ASN:C	1:A:1072:PHE:CD2	2.83	0.52
1:B:405:TYR:CG	1:B:478:PRO:HG3	2.45	0.52
1:C:809:VAL:CG1	1:C:813:GLU:OE2	2.58	0.52
1:A:568:THR:CA	1:A:1202:ASP:CB	2.80	0.51
1:A:1063:TRP:HZ2	1:A:1081:HIS:HE1	1.46	0.51
1:A:1114:LEU:HB3	1:A:1140:PHE:HB3	1.91	0.51
1:C:83:ASN:ND2	1:D:80:LYS:HA	2.26	0.51
1:C:1083:PRO:CG	1:C:1098:ARG:CA	2.88	0.51
1:C:1146:LEU:HD13	1:C:1146:LEU:C	2.30	0.51
1:C:1193:GLY:O	1:C:1197:VAL:HG23	2.09	0.51
1:D:631:SER:CB	1:D:632:PRO:CD	2.85	0.51
1:A:809:VAL:C	1:A:812:ILE:CG1	2.77	0.51
1:A:1083:PRO:CG	1:A:1098:ARG:CA	2.89	0.51
1:C:1079:ILE:HD12	1:C:1082:PHE:CE1	2.45	0.51
1:C:1088:TYR:HD2	1:C:1089:GLU:N	2.07	0.51
1:A:1027:VAL:C	1:A:1032:TRP:HE1	2.13	0.51
1:C:1027:VAL:C	1:C:1063:TRP:HZ3	2.13	0.51
1:D:512:PRO:CB	1:D:790:SER:CA	2.82	0.51
1:A:517:PHE:HE1	1:D:611:ILE:CD1	2.17	0.51
1:A:1026:ALA:HB1	1:A:1182:GLY:N	2.26	0.51
1:A:1127:TYR:HB3	1:A:1133:ILE:CD1	2.40	0.51
1:B:523:TYR:O	1:B:527:MET:HG2	2.10	0.51
1:B:630:VAL:CG2	1:B:631:SER:H	2.05	0.51
1:C:517:PHE:HZ	1:C:526:TRP:CH2	2.21	0.51
1:C:520:PRO:O	1:D:787:LEU:HB3	2.10	0.51
1:C:1023:MET:HE3	1:C:1148:ASN:HD21	1.47	0.51
1:C:1071:ASN:C	1:C:1072:PHE:CD2	2.83	0.51
1:A:810:ALA:C	1:A:814:PHE:HD2	2.12	0.51
1:A:1153:ILE:HG23	1:A:1154:VAL:N	2.25	0.51
1:B:205:VAL:O	1:B:209:ILE:HG13	2.10	0.51
1:C:1007:VAL:O	1:C:1011:LEU:CG	2.48	0.51
1:C:1027:VAL:C	1:C:1032:TRP:HE1	2.13	0.51
1:C:1141:PHE:HB3	1:C:1193:GLY:CA	2.39	0.51
1:D:523:TYR:O	1:D:527:MET:HG2	2.10	0.51
1:A:337:GLN:HE22	3:A:1302:NAG:H2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:GLY:CA	1:A:772:GLU:HB3	2.28	0.51
1:A:1081:HIS:HD2	1:A:1101:ARG:HD2	1.67	0.51
1:A:1130:ARG:HH11	1:A:1130:ARG:CG	2.24	0.51
1:A:1170:LYS:N	1:A:1171:ASN:CB	2.73	0.51
1:B:405:TYR:CD1	1:B:478:PRO:HG3	2.46	0.51
1:D:405:TYR:CD1	1:D:478:PRO:HG3	2.45	0.51
1:A:541:PHE:CZ	1:A:1198:HIS:HA	2.46	0.51
1:A:1138:GLY:HA3	1:A:1197:VAL:CG2	2.40	0.51
1:B:475:ALA:HB3	1:B:735:ALA:HB3	1.93	0.51
1:B:494:PRO:HA	1:B:732:TYR:O	2.10	0.51
1:B:515:PHE:HD1	1:B:518:LEU:HD12	1.76	0.51
1:C:74:PHE:CZ	1:C:285:THR:HG23	2.46	0.51
1:C:1020:PHE:CE1	1:C:1111:VAL:CB	2.73	0.51
1:A:1170:LYS:CA	1:A:1171:ASN:CB	2.89	0.51
1:A:1199:MET:O	1:A:1203:ARG:HG2	2.11	0.51
1:B:596:LEU:HB3	1:C:813:GLU:OE2	2.11	0.51
1:C:1114:LEU:HB3	1:C:1140:PHE:HB3	1.91	0.51
1:C:1131:HIS:O	1:C:1133:ILE:CA	2.50	0.51
1:D:290:GLN:HG2	1:D:338:VAL:HG21	1.93	0.51
1:A:1139:ILE:HG13	1:A:1140:PHE:CD1	2.45	0.51
1:C:515:PHE:HD1	1:C:518:LEU:HD12	1.76	0.51
1:A:205:VAL:O	1:A:209:ILE:HG13	2.10	0.51
1:A:515:PHE:HD1	1:A:518:LEU:HD12	1.76	0.51
1:B:611:ILE:HG21	1:C:795:VAL:HG21	1.93	0.51
1:C:1026:ALA:HB1	1:C:1182:GLY:N	2.26	0.51
1:C:1089:GLU:CB	1:C:1090:ALA:HA	2.41	0.51
1:D:74:PHE:CZ	1:D:285:THR:HG23	2.46	0.51
1:A:611:ILE:HG21	1:B:795:VAL:HG21	1.92	0.50
1:B:43:LEU:O	1:B:45:PRO:HD3	2.11	0.50
1:B:74:PHE:CZ	1:B:285:THR:HG23	2.46	0.50
1:B:611:ILE:HD11	1:C:517:PHE:CZ	2.45	0.50
1:C:571:PHE:CB	1:C:1205:LYS:HZ3	2.22	0.50
1:C:1199:MET:O	1:C:1203:ARG:HG2	2.11	0.50
1:D:633:ILE:HB	1:D:638:ASP:OD1	2.11	0.50
1:D:634:GLU:CB	1:D:724:GLY:N	2.74	0.50
1:A:1114:LEU:HD11	1:A:1115:PHE:CE2	2.47	0.50
1:B:765:LYS:O	1:B:770:LYS:HB2	2.10	0.50
1:C:405:TYR:CD1	1:C:478:PRO:HG3	2.45	0.50
1:C:1063:TRP:CE2	1:C:1081:HIS:ND1	2.80	0.50
1:C:1182:GLY:CA	1:C:1186:PHE:CD2	2.95	0.50
1:A:1088:TYR:HD2	1:A:1089:GLU:N	2.07	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:ASP:C	1:B:771:GLY:H	2.15	0.50
1:C:810:ALA:C	1:C:814:PHE:HD2	2.12	0.50
1:C:1127:TYR:HB3	1:C:1133:ILE:CD1	2.40	0.50
1:D:515:PHE:HD1	1:D:518:LEU:HD12	1.76	0.50
1:A:1114:LEU:CD1	1:A:1141:PHE:CD1	2.67	0.50
1:C:1016:ALA:HA	1:C:1192:VAL:CG2	2.40	0.50
1:A:1020:PHE:CE1	1:A:1111:VAL:CB	2.73	0.50
1:A:1024:THR:O	1:A:1027:VAL:HG22	2.11	0.50
1:A:1127:TYR:CG	1:A:1133:ILE:HD12	2.47	0.50
1:A:1148:ASN:HD22	1:A:1186:PHE:HE1	1.60	0.50
1:C:1114:LEU:HD11	1:C:1115:PHE:CE2	2.47	0.50
1:D:517:PHE:HD1	1:D:616:TYR:OH	1.93	0.50
1:A:1021:SER:O	1:A:1024:THR:CG2	2.47	0.50
1:A:1033:LEU:HD12	1:A:1033:LEU:O	2.12	0.50
1:B:507:PRO:CB	1:B:630:VAL:C	2.80	0.50
1:B:536:VAL:HG22	1:C:803:LEU:HD21	1.94	0.50
1:C:1138:GLY:HA3	1:C:1197:VAL:CG2	2.40	0.50
1:A:56:PHE:CE2	1:B:91:THR:HG21	2.47	0.50
1:A:80:LYS:HA	1:B:83:ASN:ND2	2.27	0.50
1:A:1134:ILE:CB	1:A:1200:PHE:HB2	2.34	0.50
1:A:1152:ILE:CD1	1:A:1186:PHE:CZ	2.95	0.50
1:C:1130:ARG:HH11	1:C:1130:ARG:CG	2.24	0.50
1:A:489:ILE:HD12	1:A:735:ALA:HB1	1.94	0.49
1:A:542:LEU:HD21	1:A:1197:VAL:CG2	2.42	0.49
1:A:1026:ALA:HB1	1:A:1182:GLY:CA	2.42	0.49
1:C:1026:ALA:HB1	1:C:1182:GLY:CA	2.42	0.49
1:C:1170:LYS:CA	1:C:1171:ASN:CB	2.89	0.49
1:D:337:GLN:NE2	3:D:1302:NAG:H2	2.26	0.49
1:A:525:ILE:HG12	1:B:789:LEU:CD1	2.40	0.49
1:A:787:LEU:CG	1:A:788:SER:H	2.05	0.49
1:A:1083:PRO:HD2	1:A:1098:ARG:HG2	1.94	0.49
1:A:1089:GLU:O	1:A:1095:TYR:HE2	1.95	0.49
1:A:1154:VAL:CG2	1:A:1155:TYR:N	2.75	0.49
1:C:494:PRO:HA	1:C:732:TYR:O	2.11	0.49
1:C:659:PHE:HB3	1:C:671:TRP:HB2	1.95	0.49
1:C:445:VAL:HG13	1:C:448:GLY:HA2	1.95	0.49
1:C:1024:THR:O	1:C:1027:VAL:HG22	2.11	0.49
1:C:1127:TYR:CG	1:C:1133:ILE:HD12	2.47	0.49
1:D:526:TRP:O	1:D:529:ILE:HG22	2.13	0.49
1:B:629:MET:HA	1:B:629:MET:CE	2.42	0.49
1:C:1137:ALA:O	1:C:1141:PHE:HD1	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1154:VAL:CG2	1:C:1155:TYR:N	2.75	0.49
1:A:633:ILE:HG22	1:A:634:GLU:N	2.22	0.49
1:A:1139:ILE:HG13	1:A:1140:PHE:N	2.28	0.49
1:A:1170:LYS:CB	1:A:1171:ASN:CB	2.85	0.49
1:C:1033:LEU:HD12	1:C:1033:LEU:O	2.12	0.49
1:D:506:LYS:HB3	1:D:719:ASP:CA	2.41	0.49
1:A:74:PHE:CZ	1:A:285:THR:HG23	2.47	0.49
1:A:526:TRP:O	1:A:529:ILE:HG22	2.13	0.49
1:A:1012:THR:OG1	1:A:1199:MET:CE	2.61	0.49
1:A:1090:ALA:O	1:A:1091:ASP:HB2	2.13	0.49
1:A:1137:ALA:O	1:A:1141:PHE:HD1	1.96	0.49
1:A:1149:ILE:HD13	1:A:1149:ILE:C	2.32	0.49
1:B:386:ASP:C	1:B:388:SER:H	2.16	0.49
1:A:1029:THR:CG2	1:A:1178:SER:CB	2.88	0.49
1:A:1183:ALA:O	1:A:1187:ILE:HG13	2.13	0.49
1:C:1023:MET:HE3	1:C:1148:ASN:CG	2.33	0.49
1:C:1148:ASN:HD22	1:C:1186:PHE:HE1	1.60	0.49
1:A:494:PRO:HA	1:A:732:TYR:O	2.12	0.49
1:A:1035:SER:CA	1:A:1173:TYR:HD2	2.22	0.49
1:A:1146:LEU:CD1	1:A:1150:ILE:HD11	2.42	0.49
1:B:526:TRP:O	1:B:529:ILE:HG22	2.12	0.49
1:C:1183:ALA:O	1:C:1187:ILE:HG13	2.13	0.49
1:D:195:ASP:HA	1:D:223:ALA:HB3	1.95	0.49
1:A:541:PHE:CE2	1:A:1198:HIS:CE1	2.96	0.49
1:A:608:PHE:HZ	1:B:796:PHE:CZ	2.30	0.49
1:B:659:PHE:HB3	1:B:671:TRP:HB2	1.95	0.49
1:C:43:LEU:O	1:C:45:PRO:HD3	2.12	0.49
1:D:50:LEU:HD22	1:D:61:ALA:HB2	1.95	0.49
1:D:93:HIS:ND1	1:D:322:PRO:HB3	2.28	0.49
1:A:810:ALA:HB2	1:D:597:SER:OG	2.12	0.49
1:B:50:LEU:HD22	1:B:61:ALA:HB2	1.95	0.49
1:D:395:VAL:O	1:D:397:VAL:HG23	2.13	0.49
1:A:1153:ILE:HA	1:A:1156:ILE:HD11	1.94	0.48
1:B:384:GLU:O	1:B:385:ASP:CB	2.60	0.48
1:C:127:TYR:CE2	1:C:382:LEU:HD21	2.47	0.48
1:C:1206:GLN:O	1:C:1207:LEU:C	2.52	0.48
1:C:1207:LEU:O	1:C:1208:THR:C	2.51	0.48
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.94	0.48
1:A:664:ILE:HB	1:A:667:PHE:HD2	1.78	0.48
1:A:1016:ALA:N	1:A:1192:VAL:HG12	2.28	0.48
1:A:1159:ASN:ND2	1:A:1175:TYR:CD1	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1207:LEU:O	1:A:1208:THR:C	2.51	0.48
1:C:619:ASN:HA	1:D:624:LEU:HD13	1.95	0.48
1:C:1083:PRO:HD2	1:C:1098:ARG:HG2	1.94	0.48
1:D:43:LEU:O	1:D:45:PRO:HD3	2.12	0.48
1:D:393:LYS:O	1:D:395:VAL:N	2.45	0.48
1:A:445:VAL:HG13	1:A:448:GLY:HA2	1.95	0.48
1:A:517:PHE:CZ	1:A:526:TRP:CH2	3.01	0.48
1:A:1033:LEU:HD12	1:A:1033:LEU:C	2.34	0.48
1:A:1111:VAL:O	1:A:1115:PHE:CE2	2.53	0.48
1:A:1170:LYS:CB	1:A:1171:ASN:HB2	2.37	0.48
1:A:1182:GLY:CA	1:A:1186:PHE:CD2	2.95	0.48
1:B:445:VAL:HG13	1:B:448:GLY:HA2	1.95	0.48
1:C:1188:ILE:O	1:C:1192:VAL:HG13	2.13	0.48
1:D:445:VAL:HG13	1:D:448:GLY:HA2	1.95	0.48
1:D:628:ARG:HG3	1:D:628:ARG:O	2.14	0.48
1:D:659:PHE:HB3	1:D:671:TRP:HB2	1.95	0.48
1:A:43:LEU:O	1:A:45:PRO:HD3	2.12	0.48
1:A:1152:ILE:HG23	1:A:1179:PHE:CD1	2.48	0.48
1:A:1153:ILE:C	1:A:1153:ILE:HD13	2.33	0.48
1:A:1182:GLY:HA3	1:A:1186:PHE:CE2	2.42	0.48
1:A:1188:ILE:O	1:A:1192:VAL:HG13	2.13	0.48
1:C:664:ILE:HB	1:C:667:PHE:HD2	1.79	0.48
1:C:810:ALA:HB1	1:C:814:PHE:HE2	1.79	0.48
1:C:1177:TRP:O	1:C:1179:PHE:CA	2.55	0.48
1:A:1206:GLN:O	1:A:1207:LEU:C	2.52	0.48
1:C:783:LYS:N	1:C:784:THR:HA	2.28	0.48
1:C:1089:GLU:O	1:C:1095:TYR:HE2	1.95	0.48
1:C:1129:THR:N	1:C:1133:ILE:HD11	2.28	0.48
1:A:576:SER:CB	1:A:1198:HIS:HE1	2.27	0.48
1:B:539:VAL:HG13	1:C:807:MET:SD	2.53	0.48
1:C:50:LEU:HD22	1:C:61:ALA:HB2	1.94	0.48
1:C:1088:TYR:CD2	1:C:1089:GLU:N	2.73	0.48
1:C:1141:PHE:HB3	1:C:1193:GLY:HA3	1.95	0.48
1:D:664:ILE:HB	1:D:667:PHE:HD2	1.79	0.48
1:A:50:LEU:HD22	1:A:61:ALA:HB2	1.95	0.48
1:A:258:PHE:HD2	1:A:259:ILE:HD12	1.79	0.48
1:A:1127:TYR:CD2	1:A:1130:ARG:N	2.82	0.48
1:A:1153:ILE:CG1	1:A:1156:ILE:HD11	2.29	0.48
1:C:1007:VAL:HG12	1:C:1011:LEU:HG	1.96	0.48
1:C:1070:GLY:HA2	1:C:1071:ASN:HA	1.48	0.48
1:C:1127:TYR:CD2	1:C:1130:ARG:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1153:ILE:C	1:C:1153:ILE:HD13	2.33	0.48
1:C:1200:PHE:CG	1:C:1201:ILE:N	2.81	0.48
1:C:1090:ALA:O	1:C:1091:ASP:HB2	2.13	0.48
1:C:1111:VAL:HA	1:C:1114:LEU:HD23	1.83	0.48
1:C:1114:LEU:HD11	1:C:1141:PHE:CD2	2.34	0.48
1:C:1139:ILE:HG13	1:C:1140:PHE:N	2.28	0.48
1:C:1149:ILE:HD13	1:C:1149:ILE:C	2.32	0.48
1:C:1153:ILE:HA	1:C:1156:ILE:HD11	1.94	0.48
1:A:628:ARG:CZ	1:D:623:PHE:HD1	2.27	0.48
1:A:1089:GLU:CB	1:A:1090:ALA:HA	2.41	0.48
1:A:1141:PHE:HB3	1:A:1193:GLY:HA3	1.95	0.48
1:B:514:VAL:HG13	1:B:794:GLY:HA3	1.96	0.48
1:C:541:PHE:HZ	1:C:1198:HIS:CA	2.26	0.48
1:C:1033:LEU:HD12	1:C:1033:LEU:C	2.34	0.48
1:A:1156:ILE:CG2	1:A:1175:TYR:OH	2.62	0.48
1:A:1177:TRP:O	1:A:1179:PHE:CA	2.55	0.48
1:B:195:ASP:HA	1:B:223:ALA:HB3	1.96	0.48
1:B:509:LYS:CG	1:B:510:SER:N	2.60	0.48
1:C:521:LEU:HD22	1:C:526:TRP:CE2	2.49	0.48
1:C:526:TRP:O	1:C:529:ILE:HG22	2.13	0.48
1:C:810:ALA:O	1:C:814:PHE:CE2	2.65	0.48
1:C:1127:TYR:CD2	1:C:1128:LYS:HA	2.49	0.48
1:A:1015:GLY:C	1:A:1192:VAL:HG11	2.34	0.47
1:B:97:ILE:HG13	1:B:111:ILE:HB	1.96	0.47
1:C:541:PHE:CZ	1:C:1198:HIS:CA	2.96	0.47
1:C:1138:GLY:O	1:C:1142:VAL:HG23	2.14	0.47
1:C:1164:SER:HA	1:C:1165:LYS:HG3	0.51	0.47
1:D:494:PRO:HA	1:D:732:TYR:O	2.14	0.47
1:A:1151:GLY:O	1:A:1154:VAL:CG2	2.61	0.47
1:B:664:ILE:HB	1:B:667:PHE:HD2	1.79	0.47
1:D:510:SER:C	1:D:511:LYS:HG3	2.33	0.47
1:A:711:TYR:O	1:A:715:ARG:HG2	2.14	0.47
1:A:1089:GLU:HB2	1:A:1090:ALA:CA	2.45	0.47
1:A:1138:GLY:O	1:A:1142:VAL:HG23	2.14	0.47
1:B:258:PHE:HD2	1:B:259:ILE:HD12	1.79	0.47
1:C:1012:THR:OG1	1:C:1199:MET:CE	2.61	0.47
1:A:530:VAL:O	1:A:533:TYR:HB3	2.15	0.47
1:A:634:GLU:O	1:A:724:GLY:HA3	2.15	0.47
1:A:810:ALA:HB1	1:A:814:PHE:HE2	1.79	0.47
1:A:1194:VAL:HG12	1:A:1198:HIS:CD2	2.50	0.47
1:A:1200:PHE:CG	1:A:1201:ILE:N	2.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1004:ASP:HB3	1:C:1008:GLN:HB2	1.97	0.47
1:C:1124:SER:HB2	1:C:1126:PHE:HB2	1.96	0.47
1:D:258:PHE:HD2	1:D:259:ILE:HD12	1.79	0.47
1:A:1124:SER:HB2	1:A:1126:PHE:HB2	1.96	0.47
1:B:29:PHE:O	1:B:33:MET:HG2	2.14	0.47
1:C:1017:PHE:CE1	1:C:1115:PHE:HD1	2.31	0.47
1:C:1156:ILE:CG2	1:C:1175:TYR:OH	2.62	0.47
1:D:711:TYR:O	1:D:715:ARG:HG2	2.14	0.47
1:A:1017:PHE:CE1	1:A:1115:PHE:CG	3.02	0.47
1:A:1114:LEU:HD12	1:A:1114:LEU:C	2.34	0.47
1:C:1017:PHE:CE1	1:C:1115:PHE:CG	3.02	0.47
1:A:1007:VAL:HG12	1:A:1011:LEU:HG	1.96	0.47
1:A:1015:GLY:C	1:A:1192:VAL:CG1	2.83	0.47
1:A:1083:PRO:HA	1:A:1097:LEU:CG	2.44	0.47
1:A:1129:THR:N	1:A:1133:ILE:HD11	2.28	0.47
1:A:1171:ASN:O	1:A:1172:SER:CB	2.63	0.47
1:B:504:ILE:HD13	1:B:633:ILE:HG22	1.93	0.47
1:B:506:LYS:CG	1:B:719:ASP:CA	2.78	0.47
1:C:29:PHE:O	1:C:33:MET:HG2	2.15	0.47
1:C:530:VAL:O	1:C:533:TYR:HB3	2.15	0.47
1:C:711:TYR:O	1:C:715:ARG:HG2	2.14	0.47
1:C:1023:MET:HE1	1:C:1148:ASN:CG	2.35	0.47
1:C:1114:LEU:HD12	1:C:1114:LEU:C	2.34	0.47
1:C:1124:SER:HB2	1:C:1126:PHE:CD1	2.50	0.47
1:C:1152:ILE:CD1	1:C:1186:PHE:CZ	2.95	0.47
1:C:1169:LYS:O	1:C:1169:LYS:HG3	2.15	0.47
1:D:29:PHE:O	1:D:33:MET:HG2	2.15	0.47
1:D:124:LEU:HD13	1:D:380:MET:HE1	1.96	0.47
1:D:512:PRO:HB3	1:D:790:SER:C	2.34	0.47
1:A:195:ASP:HA	1:A:223:ALA:HB3	1.96	0.47
1:C:135:TYR:CE1	1:C:137:TYR:HB3	2.50	0.47
1:C:809:VAL:HG22	1:C:812:ILE:HD11	1.97	0.47
1:C:1146:LEU:CD1	1:C:1150:ILE:HD11	2.42	0.47
1:B:519:ASP:N	1:B:520:PRO:CD	2.78	0.47
1:B:530:VAL:O	1:B:533:TYR:HB3	2.15	0.47
1:C:195:ASP:HA	1:C:223:ALA:HB3	1.96	0.47
1:C:299:LEU:HD11	1:C:332:ALA:HB2	1.97	0.47
1:C:1098:ARG:O	1:C:1101:ARG:HB3	2.15	0.47
1:C:1194:VAL:HG12	1:C:1198:HIS:CD2	2.50	0.47
1:A:1004:ASP:HB3	1:A:1008:GLN:HB2	1.96	0.47
1:A:1164:SER:HA	1:A:1165:LYS:HG3	0.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:LYS:O	1:A:1169:LYS:HG3	2.15	0.47
1:B:711:TYR:O	1:B:715:ARG:HG2	2.14	0.47
1:C:208:VAL:HG12	1:C:214:HIS:HB3	1.97	0.47
1:C:1021:SER:O	1:C:1024:THR:CG2	2.47	0.47
1:C:1151:GLY:C	1:C:1154:VAL:HG22	2.35	0.47
1:A:124:LEU:HD13	1:A:380:MET:HE1	1.96	0.46
1:A:521:LEU:CD2	1:A:525:ILE:HB	2.45	0.46
1:A:1023:MET:HE1	1:A:1148:ASN:OD1	2.14	0.46
1:A:1134:ILE:CD1	1:A:1203:ARG:HG3	2.45	0.46
1:A:1149:ILE:HG23	1:A:1150:ILE:N	2.31	0.46
1:B:636:ALA:O	1:B:638:ASP:N	2.48	0.46
1:C:97:ILE:HG13	1:C:111:ILE:HB	1.97	0.46
1:C:258:PHE:HD2	1:C:259:ILE:HD12	1.79	0.46
1:C:1013:THR:C	1:C:1017:PHE:HD2	2.13	0.46
1:C:1015:GLY:C	1:C:1192:VAL:HG11	2.34	0.46
1:C:1017:PHE:CA	1:C:1115:PHE:CE1	2.98	0.46
1:C:1134:ILE:CD1	1:C:1203:ARG:HG3	2.45	0.46
1:C:1135:LEU:CD2	1:C:1200:PHE:CZ	2.99	0.46
1:C:1167:ASP:C	1:C:1171:ASN:HD21	2.14	0.46
1:A:1124:SER:HB2	1:A:1126:PHE:CD1	2.50	0.46
1:A:1201:ILE:CG2	1:A:1205:LYS:HE3	2.45	0.46
1:C:22:ALA:HB1	1:C:25:GLU:HB2	1.97	0.46
1:C:1026:ALA:O	1:C:1178:SER:HB2	2.16	0.46
1:C:1089:GLU:HB2	1:C:1090:ALA:CA	2.45	0.46
1:C:1164:SER:N	1:C:1165:LYS:HA	2.30	0.46
1:A:135:TYR:CE1	1:A:137:TYR:HB3	2.50	0.46
1:A:1127:TYR:CB	1:A:1133:ILE:HD12	2.45	0.46
1:A:1156:ILE:CA	1:A:1175:TYR:OH	2.64	0.46
1:A:1164:SER:N	1:A:1165:LYS:HA	2.30	0.46
1:C:1029:THR:CG2	1:C:1178:SER:CB	2.88	0.46
1:D:208:VAL:HG12	1:D:214:HIS:HB3	1.97	0.46
1:A:1026:ALA:O	1:A:1178:SER:HB2	2.16	0.46
1:A:1062:LEU:O	1:A:1081:HIS:N	2.48	0.46
1:A:1063:TRP:CE2	1:A:1081:HIS:ND1	2.79	0.46
1:C:783:LYS:H	1:C:784:THR:HA	1.81	0.46
1:C:1087:ASP:OD2	1:D:697:LYS:HD2	2.16	0.46
1:D:514:VAL:CG1	1:D:794:GLY:C	2.84	0.46
1:D:530:VAL:O	1:D:533:TYR:HB3	2.15	0.46
1:A:97:ILE:HG13	1:A:111:ILE:HB	1.97	0.46
1:A:1098:ARG:O	1:A:1101:ARG:HB3	2.15	0.46
1:A:1151:GLY:C	1:A:1154:VAL:HG22	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1135:LEU:CD2	1:A:1200:PHE:CZ	2.99	0.46
1:B:536:VAL:HG21	1:B:605:TRP:CE3	2.51	0.46
1:C:23:ASP:HB3	1:C:271:PRO:HB2	1.98	0.46
1:C:520:PRO:HA	1:C:623:PHE:CE2	2.50	0.46
1:C:1015:GLY:C	1:C:1192:VAL:CG1	2.83	0.46
1:C:1134:ILE:HG22	1:C:1200:PHE:CG	2.39	0.46
1:D:394:THR:O	1:D:395:VAL:C	2.54	0.46
1:D:394:THR:CG2	1:D:440:TYR:CA	2.92	0.46
1:D:490:ASP:HB2	1:D:736:THR:HG23	1.97	0.46
1:D:517:PHE:CD1	1:D:616:TYR:OH	2.68	0.46
1:A:541:PHE:HE2	1:A:1198:HIS:CD2	2.23	0.46
1:A:1121:ILE:HD13	1:A:1134:ILE:CA	2.31	0.46
1:A:1129:THR:CA	1:A:1133:ILE:CD1	2.89	0.46
1:C:467:LEU:HD22	1:C:737:PRO:HD3	1.96	0.46
1:C:1141:PHE:HB2	1:C:1193:GLY:HA3	1.96	0.46
1:C:1170:LYS:HA	1:C:1170:LYS:CE	2.39	0.46
1:C:1201:ILE:CG2	1:C:1205:LYS:HE3	2.45	0.46
1:A:1084:GLU:CG	1:A:1085:ASP:H	2.05	0.46
1:D:22:ALA:HB1	1:D:25:GLU:HB2	1.98	0.46
1:D:23:ASP:HB3	1:D:271:PRO:HB2	1.98	0.46
1:A:22:ALA:HB1	1:A:25:GLU:HB2	1.98	0.46
1:A:812:ILE:HG13	1:A:813:GLU:H	1.81	0.46
1:A:1017:PHE:CE1	1:A:1115:PHE:HD1	2.31	0.46
1:A:1017:PHE:CA	1:A:1115:PHE:CE1	2.98	0.46
1:A:1134:ILE:HG22	1:A:1200:PHE:CG	2.39	0.46
1:B:117:LEU:HD12	1:B:120:ALA:HB3	1.98	0.46
1:C:62:PHE:CE2	1:C:92:LEU:HD12	2.51	0.46
1:C:619:ASN:CA	1:D:624:LEU:HD13	2.46	0.46
1:C:809:VAL:O	1:C:812:ILE:HG12	2.15	0.46
1:D:117:LEU:HD12	1:D:120:ALA:HB3	1.98	0.46
1:A:62:PHE:CE2	1:A:92:LEU:HD12	2.51	0.46
1:A:209:ILE:CD1	1:A:234:LYS:HB2	2.46	0.46
1:A:619:ASN:OD1	1:B:787:LEU:CD1	2.63	0.46
1:A:1031:TYR:HB3	1:A:1177:TRP:CD1	2.51	0.46
1:B:208:VAL:HG12	1:B:214:HIS:HB3	1.97	0.46
1:B:388:SER:HA	1:B:389:GLY:HA2	1.61	0.46
1:C:1096:PHE:CG	1:C:1097:LEU:CA	2.94	0.46
1:C:1152:ILE:HG23	1:C:1179:PHE:CD1	2.48	0.46
1:C:1156:ILE:CA	1:C:1175:TYR:OH	2.64	0.46
1:D:62:PHE:CE2	1:D:92:LEU:HD12	2.51	0.46
1:D:135:TYR:CE1	1:D:137:TYR:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ASP:HB3	1:B:271:PRO:HB2	1.98	0.45
1:B:601:VAL:HG23	1:C:806:ALA:CB	2.47	0.45
1:C:209:ILE:CD1	1:C:234:LYS:HB2	2.46	0.45
1:C:1031:TYR:HB3	1:C:1177:TRP:CD1	2.51	0.45
1:C:1171:ASN:O	1:C:1172:SER:CB	2.63	0.45
1:D:97:ILE:HG13	1:D:111:ILE:HB	1.97	0.45
1:D:512:PRO:HB2	1:D:790:SER:O	2.16	0.45
1:D:521:LEU:HD22	1:D:526:TRP:CE2	2.52	0.45
1:A:683:VAL:HG11	1:A:689:GLY:HA2	1.99	0.45
1:A:1127:TYR:CD2	1:A:1128:LYS:HA	2.49	0.45
1:C:512:PRO:HG2	1:C:513:GLY:H	1.79	0.45
1:C:517:PHE:HZ	1:C:526:TRP:HH2	1.54	0.45
1:A:208:VAL:HG12	1:A:214:HIS:HB3	1.97	0.45
1:A:628:ARG:HB2	1:D:626:VAL:HG21	1.98	0.45
1:A:809:VAL:HG22	1:A:812:ILE:HD11	1.97	0.45
1:A:1124:SER:OG	1:A:1125:GLU:HB3	2.16	0.45
1:B:774:GLY:O	1:B:778:SER:N	2.47	0.45
1:C:117:LEU:HD12	1:C:120:ALA:HB3	1.97	0.45
1:C:394:THR:O	1:C:395:VAL:HG23	2.16	0.45
1:C:528:CYS:SG	1:C:1153:ILE:HG13	2.56	0.45
1:C:683:VAL:HG11	1:C:689:GLY:HA2	1.98	0.45
1:C:1170:LYS:CB	1:C:1171:ASN:HB2	2.37	0.45
1:A:1032:TRP:O	1:A:1179:PHE:CD2	2.69	0.45
1:B:135:TYR:CE1	1:B:137:TYR:HB3	2.50	0.45
1:B:507:PRO:HG2	1:B:630:VAL:C	2.37	0.45
1:C:1115:PHE:CZ	1:C:1141:PHE:CE2	3.04	0.45
1:D:683:VAL:HG11	1:D:689:GLY:HA2	1.98	0.45
1:A:628:ARG:HH12	1:D:627:GLU:N	2.14	0.45
1:B:683:VAL:HG11	1:B:689:GLY:HA2	1.99	0.45
1:C:387:THR:C	1:C:389:GLY:H	2.19	0.45
1:C:1032:TRP:O	1:C:1179:PHE:CD2	2.69	0.45
1:C:1124:SER:OG	1:C:1125:GLU:HB3	2.16	0.45
1:C:1148:ASN:ND2	1:C:1186:PHE:HE1	2.14	0.45
1:A:29:PHE:O	1:A:33:MET:HG2	2.15	0.45
1:A:384:GLU:O	1:A:385:ASP:CB	2.64	0.45
1:A:1115:PHE:CZ	1:A:1141:PHE:CE2	3.04	0.45
1:A:1202:ASP:OD1	1:A:1203:ARG:HG2	2.17	0.45
1:B:22:ALA:HB1	1:B:25:GLU:HB2	1.98	0.45
1:B:165:VAL:O	1:B:165:VAL:HG22	2.17	0.45
1:B:505:LYS:HG2	1:B:506:LYS:N	2.28	0.45
1:B:521:LEU:HD22	1:B:526:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1128:LYS:HB2	1:C:1128:LYS:HZ1	1.79	0.45
1:C:1149:ILE:HG23	1:C:1150:ILE:N	2.31	0.45
1:C:1017:PHE:N	1:C:1115:PHE:CE1	2.84	0.45
1:C:1151:GLY:O	1:C:1154:VAL:CG2	2.61	0.45
1:C:1062:LEU:O	1:C:1081:HIS:N	2.48	0.45
1:C:1129:THR:CA	1:C:1133:ILE:CD1	2.89	0.45
1:C:1146:LEU:CD1	1:C:1150:ILE:CD1	2.95	0.45
1:D:514:VAL:CG1	1:D:794:GLY:O	2.64	0.45
1:A:611:ILE:HD12	1:B:517:PHE:CZ	2.42	0.45
1:A:1096:PHE:CG	1:A:1097:LEU:CA	2.94	0.45
1:A:1100:VAL:HG22	1:A:1154:VAL:HG23	1.98	0.45
1:A:1102:ALA:CB	1:A:1106:PHE:HE2	2.18	0.45
1:C:261:ARG:O	1:C:265:LEU:HG	2.17	0.45
1:D:62:PHE:CE2	1:D:88:PHE:HB3	2.52	0.45
1:D:209:ILE:CD1	1:D:234:LYS:HB2	2.47	0.45
1:B:515:PHE:CD1	1:B:518:LEU:HD12	2.52	0.45
1:C:1016:ALA:N	1:C:1192:VAL:HG12	2.28	0.45
1:C:1029:THR:HG21	1:C:1178:SER:HB3	1.97	0.45
1:C:1112:ILE:O	1:C:1116:MET:HG2	2.17	0.45
1:D:125:ILE:HG23	1:D:130:TRP:HB2	1.99	0.45
1:D:620:LEU:HA	1:D:623:PHE:HD2	1.82	0.45
1:A:1079:ILE:CD1	1:A:1082:PHE:HE1	2.30	0.44
1:A:1089:GLU:O	1:A:1095:TYR:CE2	2.70	0.44
1:A:1189:ALA:CA	1:A:1192:VAL:HG22	2.47	0.44
1:B:505:LYS:HD3	1:B:697:LYS:C	2.37	0.44
1:C:809:VAL:HG12	1:C:813:GLU:CG	2.48	0.44
1:C:1020:PHE:CZ	1:C:1108:ILE:CB	3.00	0.44
1:C:1083:PRO:HG2	1:C:1098:ARG:NE	2.32	0.44
1:C:1189:ALA:CA	1:C:1192:VAL:HG22	2.47	0.44
1:A:1125:GLU:O	1:A:1126:PHE:CD2	2.70	0.44
1:A:1148:ASN:ND2	1:A:1186:PHE:HE1	2.14	0.44
1:B:636:ALA:C	1:B:638:ASP:N	2.70	0.44
1:C:1017:PHE:CZ	1:C:1119:LEU:HD21	2.53	0.44
1:C:1159:ASN:ND2	1:C:1175:TYR:CD1	2.81	0.44
1:A:521:LEU:HD22	1:A:526:TRP:CE2	2.52	0.44
1:A:809:VAL:O	1:A:812:ILE:HG12	2.15	0.44
1:A:1112:ILE:O	1:A:1116:MET:HG2	2.17	0.44
1:A:1146:LEU:CD1	1:A:1150:ILE:CD1	2.95	0.44
1:B:787:LEU:HD13	1:B:787:LEU:N	2.31	0.44
1:C:321:VAL:HA	1:C:322:PRO:HD3	1.86	0.44
1:C:1184:LEU:O	1:C:1188:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:ARG:O	1:D:265:LEU:HG	2.17	0.44
1:D:488:VAL:HG23	1:D:489:ILE:HG23	2.00	0.44
1:D:635:SER:O	1:D:636:ALA:C	2.55	0.44
1:A:130:TRP:CE2	1:A:191:ARG:HD3	2.53	0.44
1:A:1114:LEU:HD11	1:A:1115:PHE:CD2	2.53	0.44
1:A:1141:PHE:HB2	1:A:1193:GLY:HA3	1.96	0.44
1:B:62:PHE:CE2	1:B:88:PHE:HB3	2.52	0.44
1:B:130:TRP:CH2	1:B:191:ARG:HB3	2.53	0.44
1:B:209:ILE:CD1	1:B:234:LYS:HB2	2.47	0.44
1:C:125:ILE:HG23	1:C:130:TRP:HB2	1.99	0.44
1:C:1084:GLU:CG	1:C:1085:ASP:H	2.05	0.44
1:A:117:LEU:HD12	1:A:120:ALA:HB3	1.98	0.44
1:A:1020:PHE:CZ	1:A:1108:ILE:CB	3.00	0.44
1:A:1083:PRO:HG2	1:A:1098:ARG:NE	2.32	0.44
1:A:1150:ILE:HA	1:A:1153:ILE:HG22	2.00	0.44
1:A:1177:TRP:CE3	1:A:1177:TRP:CA	3.01	0.44
1:B:62:PHE:CE2	1:B:92:LEU:HD12	2.51	0.44
1:B:261:ARG:O	1:B:265:LEU:HG	2.17	0.44
1:B:490:ASP:HB2	1:B:736:THR:HG23	1.98	0.44
1:C:96:PHE:CE2	1:C:98:THR:HB	2.53	0.44
1:C:521:LEU:CD2	1:C:525:ILE:HB	2.47	0.44
1:C:1016:ALA:HA	1:C:1192:VAL:HG21	1.99	0.44
1:C:1121:ILE:HD13	1:C:1134:ILE:CA	2.31	0.44
1:C:1152:ILE:HG12	1:C:1186:PHE:CE2	2.31	0.44
1:D:635:SER:O	1:D:637:GLU:N	2.51	0.44
1:B:125:ILE:HG23	1:B:130:TRP:HB2	1.99	0.44
1:B:525:ILE:HD13	1:C:792:VAL:HG21	1.99	0.44
1:D:521:LEU:CD2	1:D:525:ILE:HB	2.46	0.44
1:A:23:ASP:HB3	1:A:271:PRO:HB2	1.98	0.44
1:A:49:ASN:C	1:A:50:LEU:HD12	2.38	0.44
1:A:809:VAL:HG12	1:A:813:GLU:CG	2.48	0.44
1:C:93:HIS:ND1	1:C:322:PRO:HB3	2.33	0.44
1:C:1125:GLU:O	1:C:1126:PHE:CD2	2.70	0.44
1:D:287:ASP:O	1:D:291:VAL:HG23	2.18	0.44
1:A:519:ASP:N	1:A:520:PRO:CD	2.81	0.44
1:A:541:PHE:HZ	1:A:1198:HIS:CA	2.30	0.44
1:A:633:ILE:CG2	1:A:638:ASP:CB	2.82	0.44
1:A:809:VAL:CG1	1:A:812:ILE:HD11	2.48	0.44
1:A:1016:ALA:HA	1:A:1192:VAL:HG21	1.98	0.44
1:A:1083:PRO:CG	1:A:1097:LEU:CA	2.77	0.44
1:B:96:PHE:CE2	1:B:98:THR:HB	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:PHE:CE2	1:C:88:PHE:HB3	2.52	0.44
1:C:389:GLY:O	1:C:391:GLU:N	2.50	0.44
1:C:521:LEU:HB3	1:C:526:TRP:CE2	2.53	0.44
1:C:1079:ILE:CD1	1:C:1082:PHE:HE1	2.29	0.44
1:C:1114:LEU:HD11	1:C:1115:PHE:CD2	2.53	0.44
1:C:1202:ASP:OD1	1:C:1203:ARG:HG2	2.17	0.44
1:D:130:TRP:CE2	1:D:191:ARG:HD3	2.53	0.44
1:A:125:ILE:HG23	1:A:130:TRP:HB2	1.99	0.44
1:A:261:ARG:O	1:A:265:LEU:HG	2.18	0.44
1:A:1129:THR:H	1:A:1133:ILE:HD11	1.83	0.44
1:B:394:THR:CG2	1:B:440:TYR:CA	2.96	0.44
1:C:49:ASN:C	1:C:50:LEU:HD12	2.38	0.44
1:C:512:PRO:CB	1:C:790:SER:HA	2.34	0.44
1:C:1177:TRP:CE3	1:C:1177:TRP:CA	3.01	0.44
1:D:49:ASN:C	1:D:50:LEU:HD12	2.38	0.44
1:A:62:PHE:CE2	1:A:88:PHE:HB3	2.52	0.43
1:A:809:VAL:HA	1:A:812:ILE:HD13	1.82	0.43
1:A:1130:ARG:CG	1:A:1130:ARG:NH1	2.81	0.43
1:A:1184:LEU:O	1:A:1188:ILE:HG13	2.18	0.43
1:B:488:VAL:HG23	1:B:489:ILE:HG23	2.00	0.43
1:B:514:VAL:HG22	1:B:794:GLY:HA2	1.99	0.43
1:C:809:VAL:CG1	1:C:812:ILE:HD11	2.48	0.43
1:A:96:PHE:CE2	1:A:98:THR:HB	2.53	0.43
1:A:528:CYS:SG	1:A:1153:ILE:HG13	2.58	0.43
1:B:519:ASP:N	1:B:520:PRO:HD2	2.33	0.43
1:B:632:PRO:C	1:B:633:ILE:CD1	2.86	0.43
1:C:270:TYR:HA	1:C:271:PRO:HD2	1.87	0.43
1:C:512:PRO:CG	1:C:513:GLY:H	2.31	0.43
1:C:515:PHE:CD1	1:C:518:LEU:HD12	2.52	0.43
1:C:525:ILE:HD13	1:D:792:VAL:HG21	2.00	0.43
1:C:1127:TYR:CB	1:C:1133:ILE:HD12	2.45	0.43
1:A:130:TRP:CH2	1:A:191:ARG:HB3	2.53	0.43
1:A:488:VAL:HG23	1:A:489:ILE:HG23	2.00	0.43
1:A:515:PHE:CD1	1:A:518:LEU:HD12	2.52	0.43
1:A:541:PHE:CD1	1:A:1198:HIS:CE1	3.04	0.43
1:A:1167:ASP:C	1:A:1171:ASN:HD21	2.14	0.43
1:C:130:TRP:CE2	1:C:191:ARG:HD3	2.53	0.43
1:A:290:GLN:HG2	1:A:338:VAL:HG21	2.00	0.43
1:A:1121:ILE:O	1:A:1134:ILE:HD11	2.18	0.43
1:B:508:GLN:HE21	1:B:629:MET:HG3	1.84	0.43
1:C:1121:ILE:O	1:C:1134:ILE:HD11	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1129:THR:H	1:C:1133:ILE:HD11	1.83	0.43
1:C:1170:LYS:N	1:C:1171:ASN:CA	2.82	0.43
1:A:810:ALA:O	1:A:814:PHE:CE2	2.65	0.43
1:A:1017:PHE:CZ	1:A:1119:LEU:HD21	2.53	0.43
1:A:1129:THR:CG2	1:A:1133:ILE:HG12	2.44	0.43
1:B:130:TRP:CE2	1:B:191:ARG:HD3	2.54	0.43
1:B:633:ILE:CB	1:B:634:GLU:CB	2.85	0.43
1:C:488:VAL:HG23	1:C:489:ILE:HG23	2.00	0.43
1:A:1032:TRP:CB	1:A:1061:GLY:HA2	2.46	0.43
1:C:1089:GLU:O	1:C:1095:TYR:CE2	2.70	0.43
1:C:1156:ILE:HA	1:C:1159:ASN:OD1	2.19	0.43
1:D:96:PHE:CE2	1:D:98:THR:HB	2.53	0.43
1:A:1156:ILE:HA	1:A:1159:ASN:OD1	2.19	0.43
1:A:1164:SER:C	1:A:1165:LYS:HG3	2.29	0.43
1:B:518:LEU:HA	1:B:526:TRP:HE1	1.83	0.43
1:C:165:VAL:O	1:C:165:VAL:HG22	2.18	0.43
1:C:1009:MET:CE	1:C:1199:MET:HB3	2.49	0.43
1:C:1031:TYR:HD1	1:C:1059:HIS:CB	2.31	0.43
1:C:1124:SER:CB	1:C:1125:GLU:CA	2.96	0.43
1:C:1150:ILE:HA	1:C:1153:ILE:HG22	2.00	0.43
1:C:1183:ALA:O	1:C:1187:ILE:CG1	2.67	0.43
1:A:97:ILE:N	1:A:97:ILE:HD12	2.34	0.43
1:A:165:VAL:HG22	1:A:165:VAL:O	2.18	0.43
1:A:321:VAL:HA	1:A:322:PRO:HD3	1.86	0.43
1:D:97:ILE:N	1:D:97:ILE:HD12	2.34	0.43
1:B:394:THR:CG2	1:B:395:VAL:N	2.53	0.43
1:C:97:ILE:HD12	1:C:97:ILE:N	2.34	0.43
1:D:165:VAL:HG22	1:D:165:VAL:O	2.18	0.43
1:A:771:GLY:HA2	1:A:772:GLU:HB2	0.57	0.43
1:A:1023:MET:HA	1:A:1185:SER:HG	1.83	0.43
1:B:97:ILE:HD12	1:B:97:ILE:N	2.34	0.43
1:B:521:LEU:CD2	1:B:525:ILE:HB	2.45	0.43
1:C:130:TRP:CH2	1:C:191:ARG:HB3	2.53	0.43
1:C:1100:VAL:HG22	1:C:1154:VAL:HG23	1.98	0.43
1:A:209:ILE:HD11	1:A:235:ILE:HG23	2.01	0.42
1:A:287:ASP:O	1:A:291:VAL:HG23	2.18	0.42
1:A:795:VAL:HG12	1:D:608:PHE:CD1	2.54	0.42
1:A:1019:ALA:CB	1:A:1189:ALA:N	2.78	0.42
1:A:1151:GLY:HA2	1:A:1154:VAL:HG22	2.01	0.42
1:B:209:ILE:HD11	1:B:235:ILE:HG23	2.01	0.42
1:B:360:ILE:HD11	1:B:374:TRP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:ASP:O	1:C:291:VAL:HG23	2.18	0.42
1:C:1151:GLY:HA2	1:C:1154:VAL:HG22	2.01	0.42
1:D:382:LEU:HD12	1:D:382:LEU:N	2.34	0.42
1:A:521:LEU:HB3	1:A:526:TRP:CE2	2.54	0.42
1:A:1020:PHE:CD1	1:A:1023:MET:SD	3.13	0.42
1:A:1031:TYR:HE1	1:A:1059:HIS:CG	2.18	0.42
1:A:1159:ASN:OD1	1:A:1175:TYR:CE1	2.61	0.42
1:C:1111:VAL:CA	1:C:1114:LEU:HD21	2.35	0.42
1:A:533:TYR:CZ	1:A:583:ALA:HB1	2.55	0.42
1:A:628:ARG:NH1	1:D:623:PHE:HA	2.33	0.42
1:A:1170:LYS:N	1:A:1171:ASN:CA	2.82	0.42
1:B:506:LYS:H	1:B:506:LYS:HG3	1.74	0.42
1:C:541:PHE:HZ	1:C:1198:HIS:HA	1.81	0.42
1:C:1020:PHE:CB	1:C:1115:PHE:CZ	3.02	0.42
1:A:360:ILE:HD11	1:A:374:TRP:HB2	2.01	0.42
1:A:541:PHE:CZ	1:A:1201:ILE:HD12	2.54	0.42
1:A:809:VAL:HG12	1:A:813:GLU:HG3	2.02	0.42
1:A:1009:MET:HE1	1:A:1199:MET:HB3	2.02	0.42
1:A:1183:ALA:O	1:A:1187:ILE:CG1	2.67	0.42
1:B:49:ASN:C	1:B:50:LEU:HD12	2.38	0.42
1:C:1153:ILE:CG2	1:C:1154:VAL:N	2.82	0.42
1:D:270:TYR:HA	1:D:271:PRO:HD2	1.87	0.42
1:D:299:LEU:HD11	1:D:332:ALA:HB2	2.01	0.42
1:D:809:VAL:O	1:D:813:GLU:HG3	2.19	0.42
1:A:385:ASP:C	1:A:387:THR:N	2.73	0.42
1:A:514:VAL:HG13	1:A:794:GLY:CA	2.38	0.42
1:A:568:THR:CB	1:A:1202:ASP:HA	2.47	0.42
1:A:1009:MET:CE	1:A:1199:MET:HB3	2.49	0.42
1:B:287:ASP:O	1:B:291:VAL:HG23	2.18	0.42
1:C:1111:VAL:HG23	1:C:1144:ALA:HB2	1.98	0.42
1:C:1159:ASN:OD1	1:C:1175:TYR:CE1	2.61	0.42
1:C:1170:LYS:CB	1:C:1171:ASN:HB3	2.50	0.42
1:A:233:LEU:HD23	1:A:236:GLN:OE1	2.19	0.42
1:A:517:PHE:CE1	1:D:611:ILE:CD1	2.99	0.42
1:A:812:ILE:O	1:A:816:TYR:CE2	2.69	0.42
1:A:1187:ILE:O	1:A:1191:MET:HG2	2.20	0.42
1:D:519:ASP:N	1:D:520:PRO:CD	2.82	0.42
1:A:628:ARG:NH2	1:D:623:PHE:CD1	2.84	0.42
1:A:795:VAL:HG12	1:D:608:PHE:HD1	1.85	0.42
1:A:1131:HIS:CG	1:A:1132:ASN:N	2.77	0.42
1:A:1182:GLY:HA2	1:A:1185:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:ASP:N	1:C:520:PRO:CD	2.82	0.42
1:C:708:MET:O	1:C:712:ILE:HG12	2.20	0.42
1:C:1019:ALA:CB	1:C:1189:ALA:N	2.78	0.42
1:C:1065:THR:HG23	1:C:1082:PHE:HZ	1.80	0.42
1:C:1182:GLY:HA2	1:C:1185:SER:OG	2.19	0.42
1:C:1187:ILE:O	1:C:1191:MET:HG2	2.20	0.42
1:D:130:TRP:CH2	1:D:191:ARG:HB3	2.54	0.42
1:A:1017:PHE:N	1:A:1115:PHE:CE1	2.84	0.42
1:A:1030:ASP:O	1:A:1059:HIS:HD2	2.03	0.42
1:A:1170:LYS:CA	1:A:1171:ASN:HB3	2.50	0.42
1:B:233:LEU:HD23	1:B:236:GLN:OE1	2.19	0.42
1:B:512:PRO:HB2	1:B:513:GLY:H	1.72	0.42
1:C:812:ILE:HG13	1:C:813:GLU:H	1.81	0.42
1:C:1020:PHE:CD1	1:C:1023:MET:SD	3.12	0.42
1:A:718:CYS:HB2	1:A:776:LYS:CB	2.45	0.42
1:A:770:LYS:HG3	1:A:770:LYS:O	2.20	0.42
1:A:1026:ALA:CB	1:A:1182:GLY:CA	2.98	0.42
1:B:708:MET:O	1:B:712:ILE:HG12	2.19	0.42
1:C:232:LEU:O	1:C:236:GLN:HB2	2.20	0.42
1:C:233:LEU:HD23	1:C:236:GLN:OE1	2.20	0.42
1:C:360:ILE:HD11	1:C:374:TRP:HB2	2.01	0.42
1:C:1020:PHE:CE2	1:C:1108:ILE:HG23	2.40	0.42
1:A:1013:THR:C	1:A:1017:PHE:HD2	2.13	0.42
1:A:1083:PRO:CD	1:A:1098:ARG:N	2.83	0.42
1:A:1111:VAL:CG2	1:A:1144:ALA:HB2	2.47	0.42
1:A:1128:LYS:HB2	1:A:1128:LYS:HZ1	1.83	0.42
1:A:1148:ASN:ND2	1:A:1186:PHE:CE1	2.88	0.42
1:C:533:TYR:CZ	1:C:583:ALA:HB1	2.54	0.42
1:C:1026:ALA:CB	1:C:1182:GLY:CA	2.98	0.42
1:D:321:VAL:HA	1:D:322:PRO:HD3	1.86	0.42
1:D:360:ILE:HD11	1:D:374:TRP:HB2	2.01	0.42
1:D:515:PHE:CD1	1:D:518:LEU:HD12	2.52	0.42
1:B:521:LEU:HB3	1:B:526:TRP:CE2	2.55	0.41
1:B:608:PHE:HD1	1:C:795:VAL:HG12	1.85	0.41
1:A:744:THR:HB	1:A:745:PRO:HD3	2.02	0.41
1:A:1171:ASN:O	1:A:1172:SER:OG	2.30	0.41
1:B:608:PHE:HZ	1:C:796:PHE:CZ	2.38	0.41
1:B:633:ILE:CB	1:B:634:GLU:HA	2.41	0.41
1:C:1023:MET:HA	1:C:1185:SER:HG	1.85	0.41
1:D:233:LEU:HD23	1:D:236:GLN:OE1	2.20	0.41
1:A:1104:SER:HA	1:A:1107:PRO:HG2	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:GLU:O	1:A:1125:GLU:HG3	2.20	0.41
1:B:394:THR:HG22	1:B:439:LYS:O	2.16	0.41
1:B:809:VAL:O	1:B:813:GLU:HG3	2.19	0.41
1:D:394:THR:HG22	1:D:441:LYS:N	2.36	0.41
1:D:630:VAL:CG2	1:D:631:SER:N	2.61	0.41
1:D:805:LEU:O	1:D:809:VAL:HG23	2.20	0.41
1:A:391:GLU:C	1:A:393:LYS:N	2.74	0.41
1:A:1020:PHE:CB	1:A:1115:PHE:CZ	3.02	0.41
1:A:1121:ILE:HG21	1:A:1133:ILE:C	2.41	0.41
1:A:1153:ILE:CG2	1:A:1154:VAL:N	2.82	0.41
1:B:232:LEU:O	1:B:236:GLN:HB2	2.20	0.41
1:B:805:LEU:O	1:B:809:VAL:HG23	2.20	0.41
1:C:288:ALA:O	1:C:292:MET:HG3	2.21	0.41
1:C:568:THR:CB	1:C:1202:ASP:HA	2.46	0.41
1:C:803:LEU:O	1:C:807:MET:HG2	2.21	0.41
1:C:1020:PHE:HA	1:C:1023:MET:HG2	2.03	0.41
1:C:1027:VAL:CA	1:C:1032:TRP:HZ2	2.25	0.41
1:D:521:LEU:HB3	1:D:526:TRP:CE2	2.55	0.41
1:D:708:MET:O	1:D:712:ILE:HG12	2.20	0.41
1:A:375:SER:HB3	1:A:378:ASP:HB2	2.03	0.41
1:A:708:MET:O	1:A:712:ILE:HG12	2.20	0.41
1:A:1013:THR:C	1:A:1017:PHE:CD2	2.86	0.41
1:A:1114:LEU:CD2	1:A:1141:PHE:N	2.80	0.41
1:B:288:ALA:O	1:B:292:MET:HG3	2.21	0.41
1:B:633:ILE:CB	1:B:634:GLU:CA	2.83	0.41
2:B:1301:ZK1:HAI	2:B:1301:ZK1:HAOA	1.81	0.41
1:C:809:VAL:HG12	1:C:813:GLU:HG3	2.02	0.41
1:D:232:LEU:O	1:D:236:GLN:HB2	2.21	0.41
1:D:744:THR:HB	1:D:745:PRO:HD3	2.03	0.41
1:A:1016:ALA:C	1:A:1115:PHE:CE1	2.89	0.41
1:A:1031:TYR:HD1	1:A:1059:HIS:CB	2.31	0.41
1:A:1086:ALA:C	1:A:1088:TYR:N	2.74	0.41
1:C:209:ILE:HD11	1:C:235:ILE:HG23	2.01	0.41
1:C:1083:PRO:CD	1:C:1098:ARG:N	2.83	0.41
1:C:1121:ILE:HG21	1:C:1133:ILE:HB	1.73	0.41
1:C:1125:GLU:O	1:C:1125:GLU:HG3	2.19	0.41
1:D:508:GLN:CB	1:D:629:MET:CE	2.80	0.41
1:A:107:HIS:HA	1:A:108:PRO:HD3	1.92	0.41
1:A:385:ASP:O	1:A:387:THR:N	2.53	0.41
1:A:403:SER:HA	1:A:404:PRO:HA	1.87	0.41
1:A:678:GLU:HA	1:A:679:PRO:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:THR:O	1:A:1017:PHE:CE2	2.66	0.41
1:B:127:TYR:CE2	1:B:382:LEU:HD21	2.56	0.41
1:C:744:THR:HB	1:C:745:PRO:HD3	2.02	0.41
1:C:1121:ILE:HG21	1:C:1133:ILE:C	2.41	0.41
1:C:1170:LYS:CA	1:C:1171:ASN:HB3	2.50	0.41
1:D:209:ILE:HD11	1:D:235:ILE:HG23	2.01	0.41
1:A:1111:VAL:HG23	1:A:1144:ALA:HB2	1.98	0.41
1:A:1191:MET:O	1:A:1195:LEU:HG	2.21	0.41
1:B:803:LEU:O	1:B:807:MET:HG2	2.20	0.41
1:C:101:PHE:HA	1:C:102:PRO:HD3	1.94	0.41
1:C:1111:VAL:O	1:C:1114:LEU:CG	2.62	0.41
1:D:467:LEU:HD22	1:D:737:PRO:HD3	2.02	0.41
1:D:678:GLU:HA	1:D:679:PRO:C	2.41	0.41
1:A:611:ILE:HD11	1:B:517:PHE:HZ	1.86	0.41
1:A:758:LEU:HD23	1:A:758:LEU:O	2.21	0.41
1:B:101:PHE:HA	1:B:102:PRO:HD3	1.94	0.41
1:B:758:LEU:O	1:B:758:LEU:HD23	2.21	0.41
1:C:1030:ASP:O	1:C:1059:HIS:HD2	2.03	0.41
1:C:1130:ARG:CG	1:C:1130:ARG:NH1	2.81	0.41
1:C:1148:ASN:ND2	1:C:1186:PHE:CE1	2.88	0.41
1:C:1164:SER:C	1:C:1165:LYS:HG3	2.29	0.41
1:D:404:PRO:HB3	1:D:711:TYR:CE1	2.56	0.41
1:D:505:LYS:NZ	1:D:697:LYS:HA	2.35	0.41
1:A:1020:PHE:CE2	1:A:1108:ILE:HG23	2.40	0.41
1:B:744:THR:HB	1:B:745:PRO:HD3	2.02	0.41
1:C:192:VAL:HB	1:C:220:TYR:CD1	2.56	0.41
1:C:1013:THR:C	1:C:1017:PHE:CD2	2.86	0.41
1:C:1017:PHE:CD1	1:C:1115:PHE:HD1	2.34	0.41
1:C:1124:SER:OG	1:C:1126:PHE:CD1	2.70	0.41
1:A:805:LEU:O	1:A:809:VAL:HG23	2.21	0.40
1:B:114:ARG:HA	1:B:115:PRO:HD3	1.92	0.40
1:B:192:VAL:HB	1:B:220:TYR:CD1	2.56	0.40
1:B:505:LYS:HE3	1:B:506:LYS:CE	2.51	0.40
1:C:1081:HIS:HD2	1:C:1101:ARG:CD	2.16	0.40
1:C:1172:SER:HG	1:C:1173:TYR:H	1.63	0.40
1:C:1195:LEU:O	1:C:1199:MET:HG3	2.21	0.40
1:A:192:VAL:HB	1:A:220:TYR:CD1	2.56	0.40
1:A:467:LEU:HD22	1:A:737:PRO:HD3	2.02	0.40
1:A:624:LEU:O	1:A:628:ARG:HG3	2.20	0.40
1:A:628:ARG:CZ	1:D:623:PHE:HA	2.52	0.40
1:A:792:VAL:HG21	1:D:525:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1195:LEU:O	1:A:1199:MET:HG3	2.21	0.40
1:B:231:ASP:HB3	1:B:234:LYS:HE2	2.04	0.40
1:B:477:ALA:HB1	1:B:478:PRO:CD	2.52	0.40
1:B:608:PHE:CD1	1:C:795:VAL:HG12	2.57	0.40
1:C:1020:PHE:CA	1:C:1023:MET:HG2	2.52	0.40
1:D:508:GLN:CG	1:D:629:MET:HG3	2.34	0.40
1:A:1029:THR:HG21	1:A:1178:SER:HB3	1.97	0.40
1:A:1124:SER:CB	1:A:1126:PHE:N	2.72	0.40
1:C:624:LEU:O	1:C:628:ARG:HG3	2.21	0.40
1:D:10:ASN:N	1:D:10:ASN:ND2	2.70	0.40
1:A:511:LYS:N	1:A:512:PRO:CD	2.73	0.40
1:A:803:LEU:O	1:A:807:MET:HG2	2.21	0.40
1:A:1089:GLU:CB	1:A:1090:ALA:C	2.90	0.40
1:B:678:GLU:HA	1:B:679:PRO:C	2.41	0.40
1:C:325:GLN:O	1:C:329:ILE:HG13	2.22	0.40
1:C:531:PHE:CE2	1:C:1187:ILE:HG13	2.45	0.40
1:C:758:LEU:O	1:C:758:LEU:HD23	2.21	0.40
1:C:1083:PRO:HA	1:C:1097:LEU:CG	2.44	0.40
1:A:1124:SER:CB	1:A:1125:GLU:CA	2.96	0.40
1:B:266:GLU:HG2	1:B:268:LYS:H	1.86	0.40
1:D:288:ALA:O	1:D:292:MET:HG3	2.21	0.40
1:D:803:LEU:O	1:D:807:MET:HG2	2.21	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	963/1034 (93%)	844 (88%)	78 (8%)	41 (4%)	2 22
1	B	773/1034 (75%)	699 (90%)	56 (7%)	18 (2%)	6 34
1	C	963/1034 (93%)	845 (88%)	82 (8%)	36 (4%)	3 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	773/1034 (75%)	693 (90%)	57 (7%)	23 (3%)	4 28
All	All	3472/4136 (84%)	3081 (89%)	273 (8%)	118 (3%)	6 26

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	LYS
1	A	385	ASP
1	A	387	THR
1	A	389	GLY
1	A	511	LYS
1	A	633	ILE
1	A	634	GLU
1	A	772	GLU
1	A	775	ALA
1	A	785	SER
1	A	1030	ASP
1	A	1089	GLU
1	A	1091	ASP
1	A	1095	TYR
1	A	1132	ASN
1	A	1165	LYS
1	A	1166	SER
1	A	1170	LYS
1	A	1178	SER
1	B	172	LYS
1	B	385	ASP
1	B	393	LYS
1	B	508	GLN
1	B	514	VAL
1	B	633	ILE
1	B	785	SER
1	C	172	LYS
1	C	391	GLU
1	C	512	PRO
1	C	1030	ASP
1	C	1089	GLU
1	C	1091	ASP
1	C	1095	TYR
1	C	1132	ASN
1	C	1165	LYS
1	C	1166	SER

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Mol	Chain	Res	Type
1	C	1170	LYS
1	C	1178	SER
1	D	172	LYS
1	D	385	ASP
1	D	391	GLU
1	D	394	THR
1	D	395	VAL
1	D	511	LYS
1	D	514	VAL
1	D	630	VAL
1	D	631	SER
1	D	635	SER
1	A	514	VAL
1	A	770	LYS
1	A	1072	PHE
1	A	1098	ARG
1	A	1124	SER
1	A	1172	SER
1	B	394	THR
1	B	509	LYS
1	B	784	THR
1	C	393	LYS
1	C	783	LYS
1	C	1072	PHE
1	C	1098	ARG
1	C	1124	SER
1	C	1172	SER
1	D	387	THR
1	D	392	GLN
1	D	512	PRO
1	D	513	GLY
1	D	632	PRO
1	D	784	THR
1	A	388	SER
1	A	787	LEU
1	A	1029	THR
1	A	1081	HIS
1	A	1088	TYR
1	A	1093	ALA
1	A	1131	HIS
1	B	512	PRO
1	C	390	LEU

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Mol	Chain	Res	Type
1	C	508	GLN
1	C	785	SER
1	C	1029	THR
1	C	1081	HIS
1	C	1088	TYR
1	C	1093	ALA
1	C	1131	HIS
1	D	785	SER
1	D	786	ALA
1	A	597	SER
1	A	1175	TYR
1	B	597	SER
1	B	637	GLU
1	C	392	GLN
1	C	597	SER
1	C	1175	TYR
1	D	386	ASP
1	D	396	VAL
1	D	597	SER
1	A	386	ASP
1	A	508	GLN
1	A	1082	PHE
1	A	1162	ASP
1	B	387	THR
1	B	786	ALA
1	C	510	SER
1	C	513	GLY
1	C	784	THR
1	C	1082	PHE
1	C	1162	ASP
1	A	1087	ASP
1	A	743	GLY
1	B	631	SER
1	B	743	GLY
1	C	743	GLY
1	D	743	GLY
1	A	451	GLY
1	B	451	GLY
1	C	451	GLY
1	D	451	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	693/876 (79%)	676 (98%)	17 (2%)	47	68
1	B	546/876 (62%)	540 (99%)	6 (1%)	73	84
1	C	693/876 (79%)	676 (98%)	17 (2%)	47	68
1	D	546/876 (62%)	541 (99%)	5 (1%)	78	87
All	All	2478/3504 (71%)	2433 (98%)	45 (2%)	61	77

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	299	LEU
1	A	631	SER
1	A	770	LYS
1	A	773	CYS
1	A	1035	SER
1	A	1088	TYR
1	A	1095	TYR
1	A	1124	SER
1	A	1127	TYR
1	A	1128	LYS
1	A	1130	ARG
1	A	1149	ILE
1	A	1153	ILE
1	A	1167	ASP
1	A	1168	SER
1	A	1177	TRP
1	B	10	ASN
1	B	299	LEU
1	B	506	LYS
1	B	631	SER
1	B	633	ILE
1	B	787	LEU
1	C	10	ASN

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Mol	Chain	Res	Type
1	C	299	LEU
1	C	628	ARG
1	C	772	GLU
1	C	787	LEU
1	C	1035	SER
1	C	1088	TYR
1	C	1095	TYR
1	C	1124	SER
1	C	1127	TYR
1	C	1128	LYS
1	C	1130	ARG
1	C	1149	ILE
1	C	1153	ILE
1	C	1167	ASP
1	C	1168	SER
1	C	1177	TRP
1	D	10	ASN
1	D	299	LEU
1	D	394	THR
1	D	629	MET
1	D	772	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	GLN
1	A	1059	HIS
1	A	1081	HIS
1	A	1148	ASN
1	A	1198	HIS
1	B	83	ASN
1	B	619	ASN
1	C	83	ASN
1	C	1059	HIS
1	C	1081	HIS
1	C	1148	ASN
1	C	1198	HIS
1	D	337	GLN
1	D	344	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
2	ZK1	C	1301	-	28,29,29	3.49	12 (42%)	42,45,45	1.62	7 (16%)
3	NAG	C	1302	1	14,14,15	0.48	0	17,19,21	0.96	1 (5%)
3	NAG	D	1302	1	14,14,15	0.51	0	17,19,21	0.72	0
2	ZK1	A	1301	-	28,29,29	3.50	12 (42%)	42,45,45	1.63	7 (16%)
2	ZK1	B	1301	-	28,29,29	3.48	11 (39%)	42,45,45	1.61	7 (16%)
3	NAG	A	1302	1	14,14,15	0.48	0	17,19,21	0.75	0
2	ZK1	D	1301	-	28,29,29	3.50	12 (42%)	42,45,45	1.62	7 (16%)
3	NAG	B	1302	1	14,14,15	0.50	0	17,19,21	0.74	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
2	ZK1	C	1301	-	-	5/13/23/23	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	D	1302	1	-	2/6/23/26	0/1/1/1
2	ZK1	A	1301	-	-	5/13/23/23	0/3/3/3
2	ZK1	B	1301	-	-	5/13/23/23	0/3/3/3
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
2	ZK1	D	1301	-	-	5/13/23/23	0/3/3/3
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	ZK1	OAA-CAT	9.35	1.41	1.23
2	D	1301	ZK1	OAA-CAT	9.32	1.41	1.23
2	B	1301	ZK1	OAA-CAT	9.27	1.41	1.23
2	C	1301	ZK1	OAA-CAT	9.25	1.41	1.23
2	C	1301	ZK1	OAB-CAU	8.46	1.41	1.23
2	B	1301	ZK1	OAB-CAU	8.43	1.40	1.23
2	D	1301	ZK1	OAB-CAU	8.42	1.40	1.23
2	A	1301	ZK1	OAB-CAU	8.39	1.40	1.23
2	C	1301	ZK1	PBA-OAC	7.25	1.65	1.50
2	A	1301	ZK1	PBA-OAC	7.24	1.65	1.50
2	D	1301	ZK1	PBA-OAC	7.17	1.65	1.50
2	B	1301	ZK1	PBA-OAC	7.15	1.65	1.50
2	A	1301	ZK1	CAT-NAP	6.08	1.44	1.35
2	D	1301	ZK1	CAT-NAP	6.05	1.44	1.35
2	C	1301	ZK1	CAT-NAP	5.97	1.44	1.35
2	B	1301	ZK1	CAT-NAP	5.91	1.44	1.35
2	D	1301	ZK1	PBA-OAE	4.71	1.65	1.54
2	B	1301	ZK1	PBA-OAE	4.68	1.65	1.54
2	A	1301	ZK1	PBA-OAE	4.65	1.65	1.54
2	C	1301	ZK1	PBA-OAE	4.60	1.65	1.54
2	C	1301	ZK1	PBA-OAD	-3.66	1.46	1.54
2	D	1301	ZK1	PBA-OAD	-3.62	1.46	1.54
2	A	1301	ZK1	PBA-OAD	-3.61	1.46	1.54
2	B	1301	ZK1	PBA-OAD	-3.59	1.46	1.54
2	B	1301	ZK1	CAJ-CAS	3.39	1.44	1.39
2	A	1301	ZK1	CAJ-CAS	3.39	1.44	1.39
2	C	1301	ZK1	CAJ-CAS	3.33	1.44	1.39
2	D	1301	ZK1	CAJ-CAS	3.32	1.44	1.39
2	A	1301	ZK1	CAW-NAY	3.31	1.47	1.41
2	B	1301	ZK1	CAW-NAY	3.31	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1301	ZK1	CAW-NAY	3.22	1.46	1.41
2	C	1301	ZK1	CAW-NAY	3.20	1.46	1.41
2	D	1301	ZK1	CAM-NAX	2.18	1.50	1.46
2	D	1301	ZK1	PBA-CAO	2.18	1.86	1.81
2	A	1301	ZK1	CAM-NAX	2.16	1.50	1.46
2	A	1301	ZK1	CAR-NAX	2.16	1.46	1.41
2	B	1301	ZK1	PBA-CAO	2.16	1.86	1.81
2	C	1301	ZK1	CAR-NAX	2.16	1.46	1.41
2	A	1301	ZK1	PBA-CAO	2.15	1.86	1.81
2	C	1301	ZK1	PBA-CAO	2.15	1.86	1.81
2	D	1301	ZK1	CAR-NAX	2.14	1.46	1.41
2	C	1301	ZK1	CAM-NAX	2.13	1.50	1.46
2	B	1301	ZK1	CAM-NAX	2.13	1.50	1.46
2	B	1301	ZK1	CAR-NAX	2.12	1.46	1.41
2	D	1301	ZK1	CAN-NAX	2.04	1.49	1.46
2	A	1301	ZK1	CAI-CAW	2.03	1.42	1.39
2	C	1301	ZK1	CAI-CAW	2.01	1.42	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1301	ZK1	CAN-NAX-CAM	4.57	121.61	111.52
2	A	1301	ZK1	CAN-NAX-CAM	4.53	121.51	111.52
2	D	1301	ZK1	CAN-NAX-CAM	4.50	121.45	111.52
2	B	1301	ZK1	CAN-NAX-CAM	4.50	121.44	111.52
2	A	1301	ZK1	CAO-NAY-CAU	3.95	120.35	116.51
2	B	1301	ZK1	CAO-NAY-CAU	3.93	120.34	116.51
2	C	1301	ZK1	CAO-NAY-CAU	3.92	120.33	116.51
2	D	1301	ZK1	CAO-NAY-CAU	3.92	120.33	116.51
2	A	1301	ZK1	CAV-NAP-CAT	-3.80	119.96	124.80
2	D	1301	ZK1	CAV-NAP-CAT	-3.75	120.02	124.80
2	C	1301	ZK1	CAV-NAP-CAT	-3.73	120.05	124.80
2	B	1301	ZK1	CAV-NAP-CAT	-3.65	120.15	124.80
2	A	1301	ZK1	CAU-CAT-NAP	2.53	120.10	117.49
2	D	1301	ZK1	CAU-CAT-NAP	2.49	120.06	117.49
2	C	1301	ZK1	CAU-CAT-NAP	2.47	120.03	117.49
2	B	1301	ZK1	CAU-CAT-NAP	2.46	120.03	117.49
2	A	1301	ZK1	CAI-CAR-NAX	-2.39	118.99	122.52
2	B	1301	ZK1	CAI-CAR-NAX	-2.37	119.01	122.52
2	C	1301	ZK1	CAI-CAR-NAX	-2.35	119.04	122.52
2	D	1301	ZK1	CAI-CAR-NAX	-2.33	119.08	122.52
2	D	1301	ZK1	CAW-NAY-CAU	-2.30	119.94	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1301	ZK1	CAT-CAU-NAY	2.26	119.91	117.32
2	C	1301	ZK1	CAT-CAU-NAY	2.24	119.89	117.32
2	A	1301	ZK1	CAT-CAU-NAY	2.24	119.89	117.32
2	A	1301	ZK1	CAW-NAY-CAU	-2.24	120.02	122.79
2	C	1301	ZK1	CAW-NAY-CAU	-2.22	120.04	122.79
2	B	1301	ZK1	CAT-CAU-NAY	2.16	119.80	117.32
3	C	1302	NAG	C1-O5-C5	2.16	115.12	112.19
2	B	1301	ZK1	CAW-NAY-CAU	-2.15	120.12	122.79

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	ZK1	NAY-CAO-PBA-OAC
2	A	1301	ZK1	NAY-CAO-PBA-OAE
2	B	1301	ZK1	NAY-CAO-PBA-OAC
2	B	1301	ZK1	NAY-CAO-PBA-OAE
2	C	1301	ZK1	NAY-CAO-PBA-OAC
2	C	1301	ZK1	NAY-CAO-PBA-OAE
2	D	1301	ZK1	NAY-CAO-PBA-OAC
2	D	1301	ZK1	NAY-CAO-PBA-OAE
3	A	1302	NAG	C8-C7-N2-C2
3	A	1302	NAG	O7-C7-N2-C2
3	D	1302	NAG	C8-C7-N2-C2
3	D	1302	NAG	O7-C7-N2-C2
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2
2	B	1301	ZK1	CAI-CAR-NAX-CAN
2	C	1301	ZK1	CAI-CAR-NAX-CAN
2	A	1301	ZK1	CAI-CAR-NAX-CAN
2	D	1301	ZK1	CAI-CAR-NAX-CAN
2	A	1301	ZK1	CAS-CAR-NAX-CAN
2	B	1301	ZK1	CAS-CAR-NAX-CAN
2	C	1301	ZK1	CAS-CAR-NAX-CAN
2	D	1301	ZK1	CAS-CAR-NAX-CAN
2	A	1301	ZK1	NAY-CAO-PBA-OAD
2	B	1301	ZK1	NAY-CAO-PBA-OAD
2	C	1301	ZK1	NAY-CAO-PBA-OAD
2	D	1301	ZK1	NAY-CAO-PBA-OAD

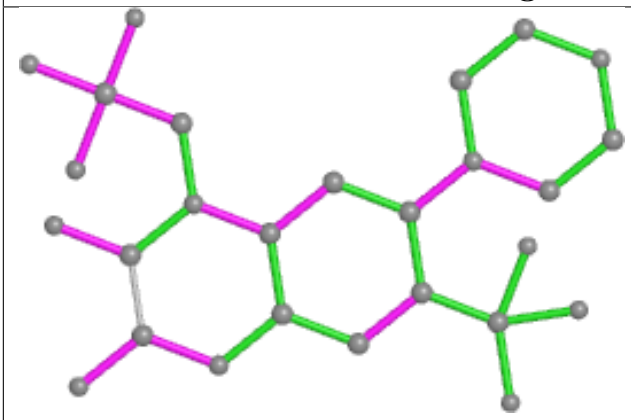
There are no ring outliers.

3 monomers are involved in 5 short contacts:

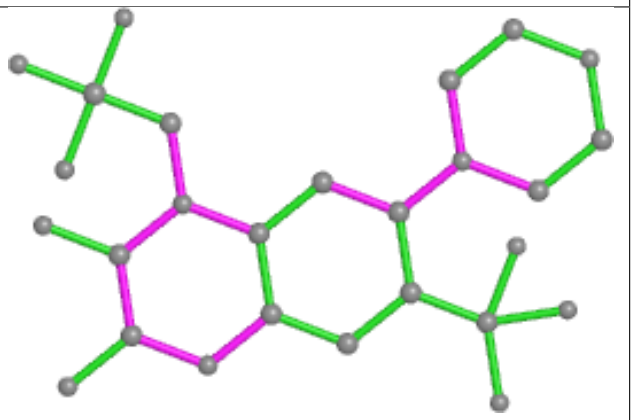
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1302	NAG	2	0
2	B	1301	ZK1	1	0
3	A	1302	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

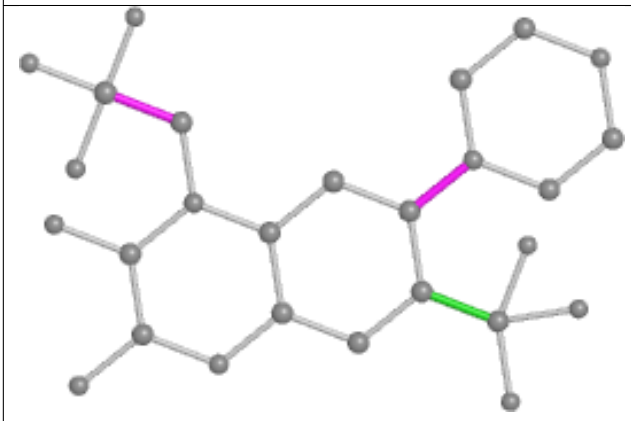
Ligand ZK1 C 1301



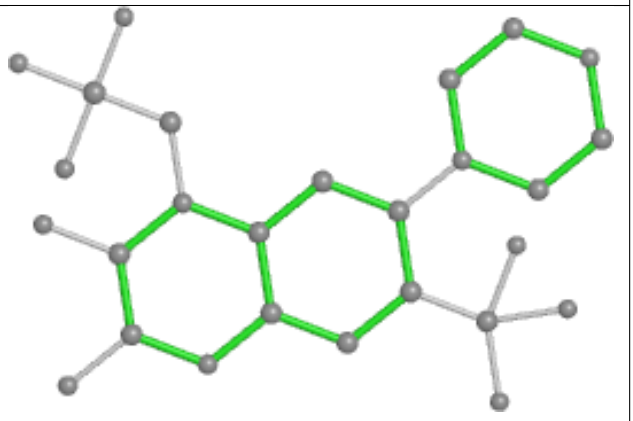
Bond lengths



Bond angles

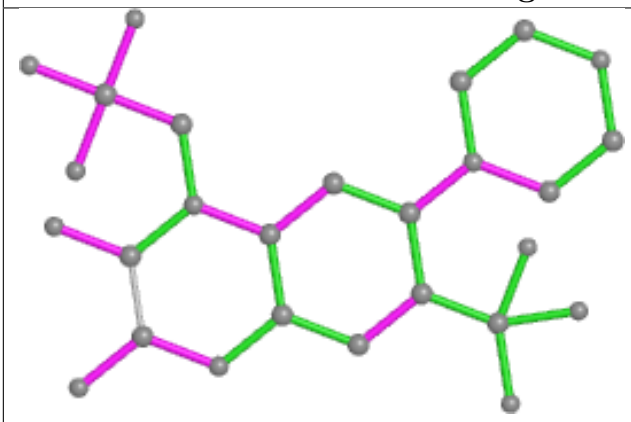


Torsions

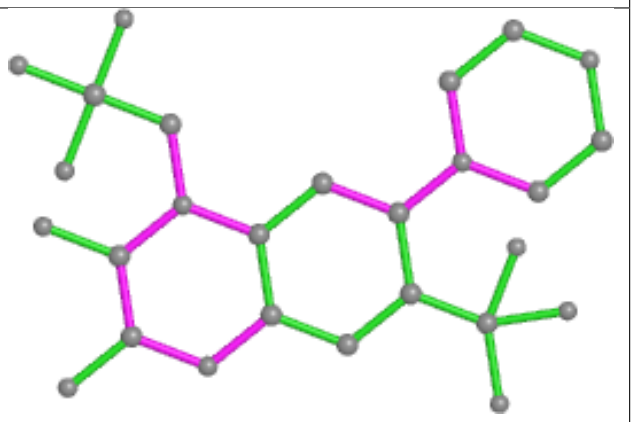


Rings

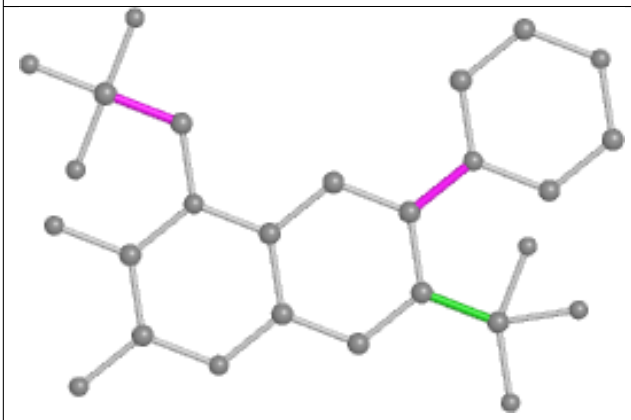
Ligand ZK1 A 1301



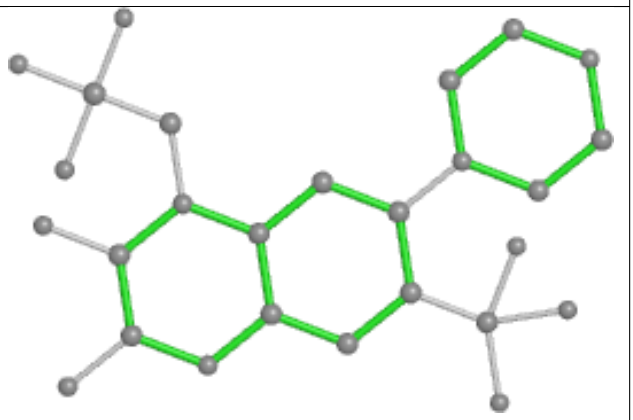
Bond lengths



Bond angles

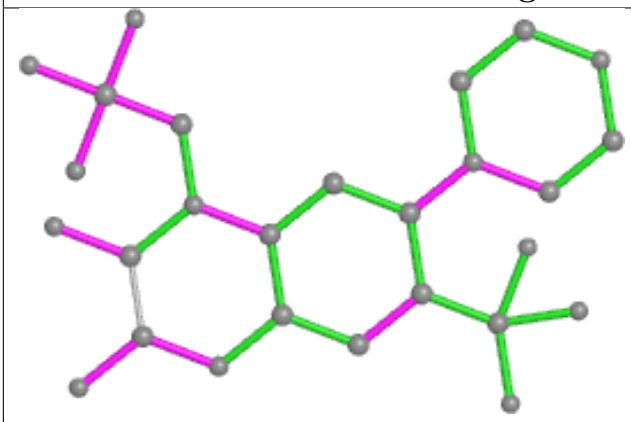


Torsions

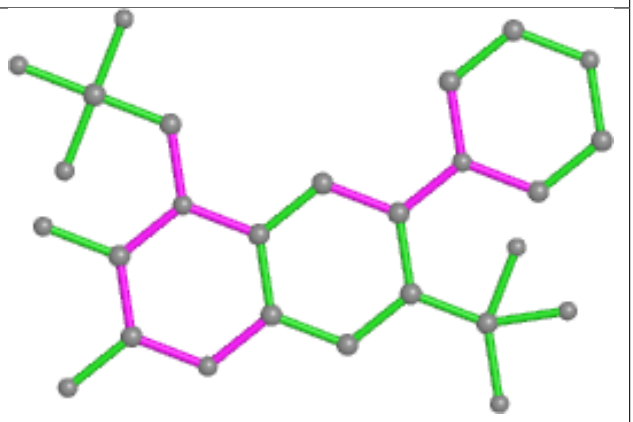


Rings

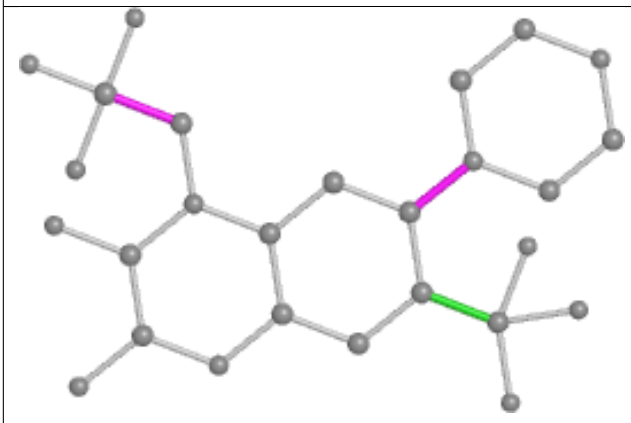
Ligand ZK1 B 1301



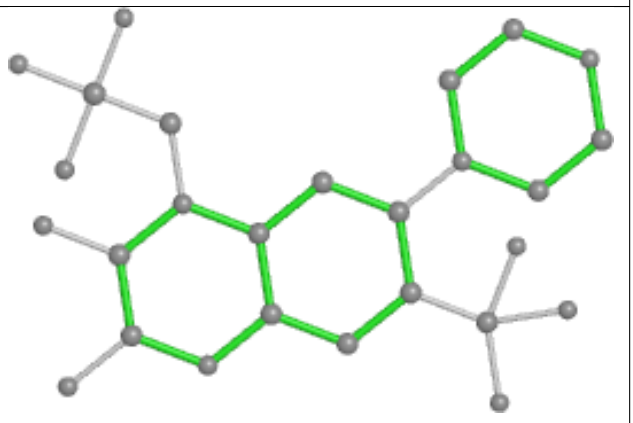
Bond lengths



Bond angles

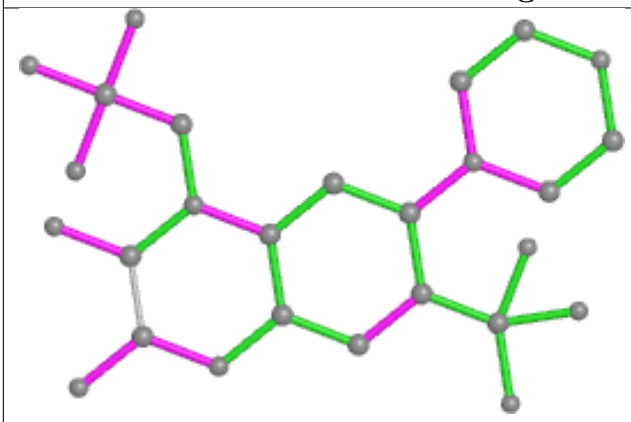


Torsions

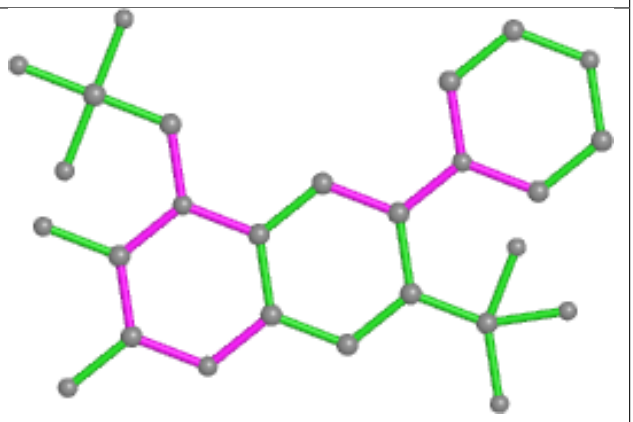


Rings

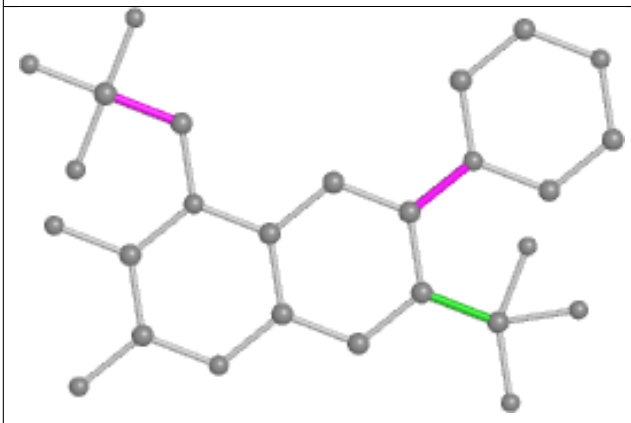
Ligand ZK1 D 1301



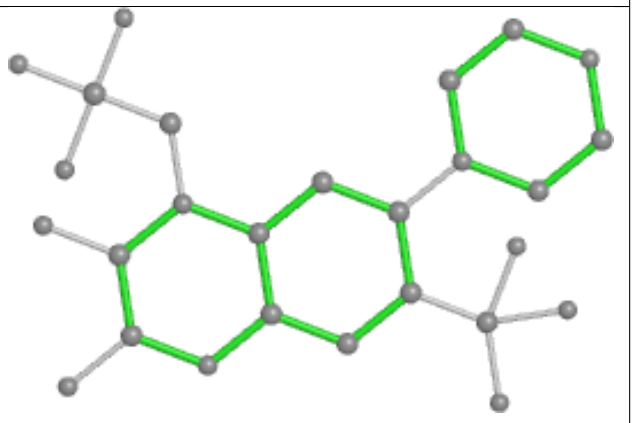
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1157:SER	C	1158:ALA	N	1.10
1	C	1157:SER	C	1158:ALA	N	1.10

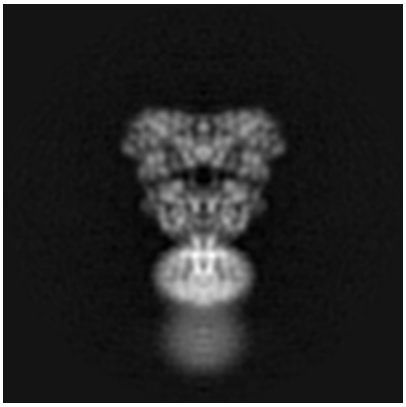
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8231. These allow visual inspection of the internal detail of the map and identification of artifacts.

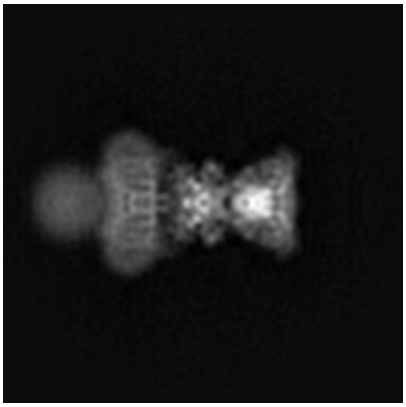
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

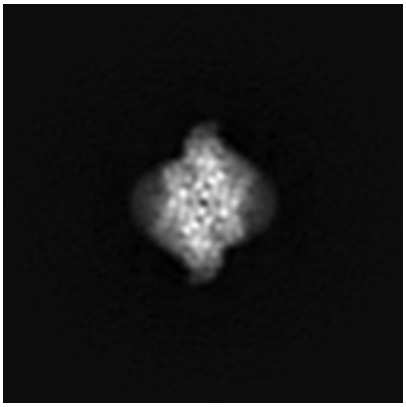
6.1.1 Primary map



X



Y



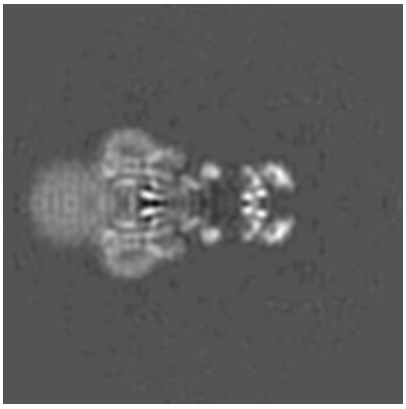
Z

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

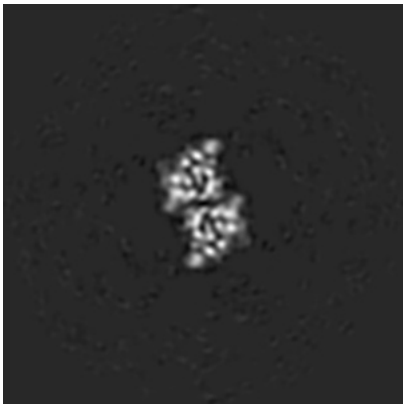
6.2 Central slices

6.2.1 Primary map

X Index: 180



Y Index: 180

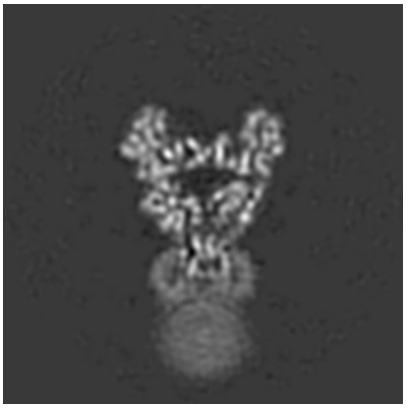


Z Index: 180

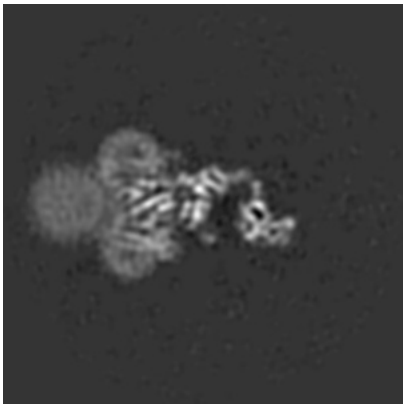
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

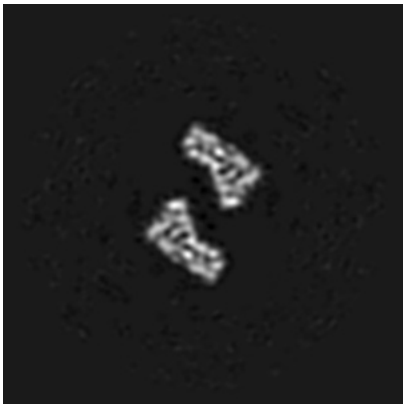
6.3.1 Primary map



X Index: 176



Y Index: 173

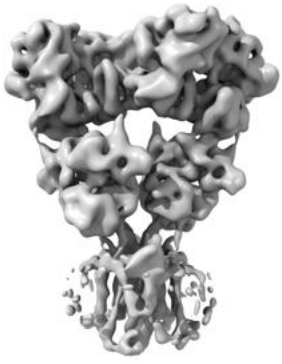


Z Index: 250

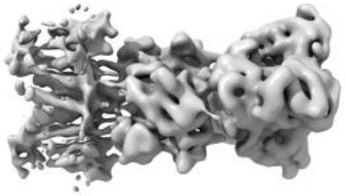
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

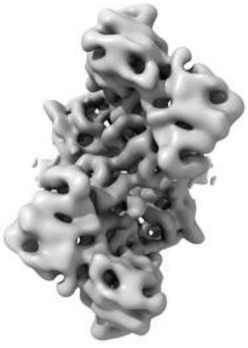
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

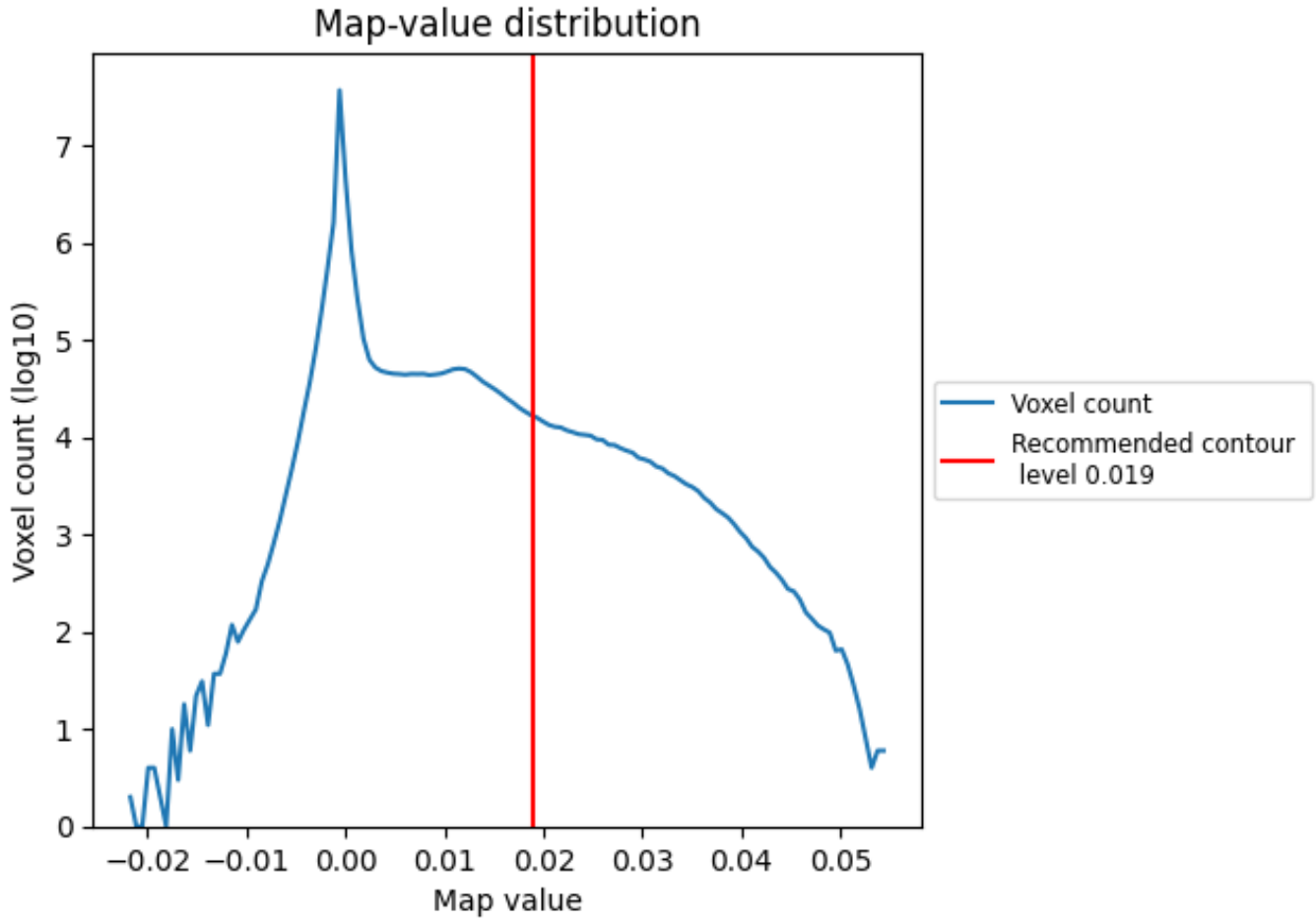
6.5 Mask visualisation (i)

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

7 Map analysis

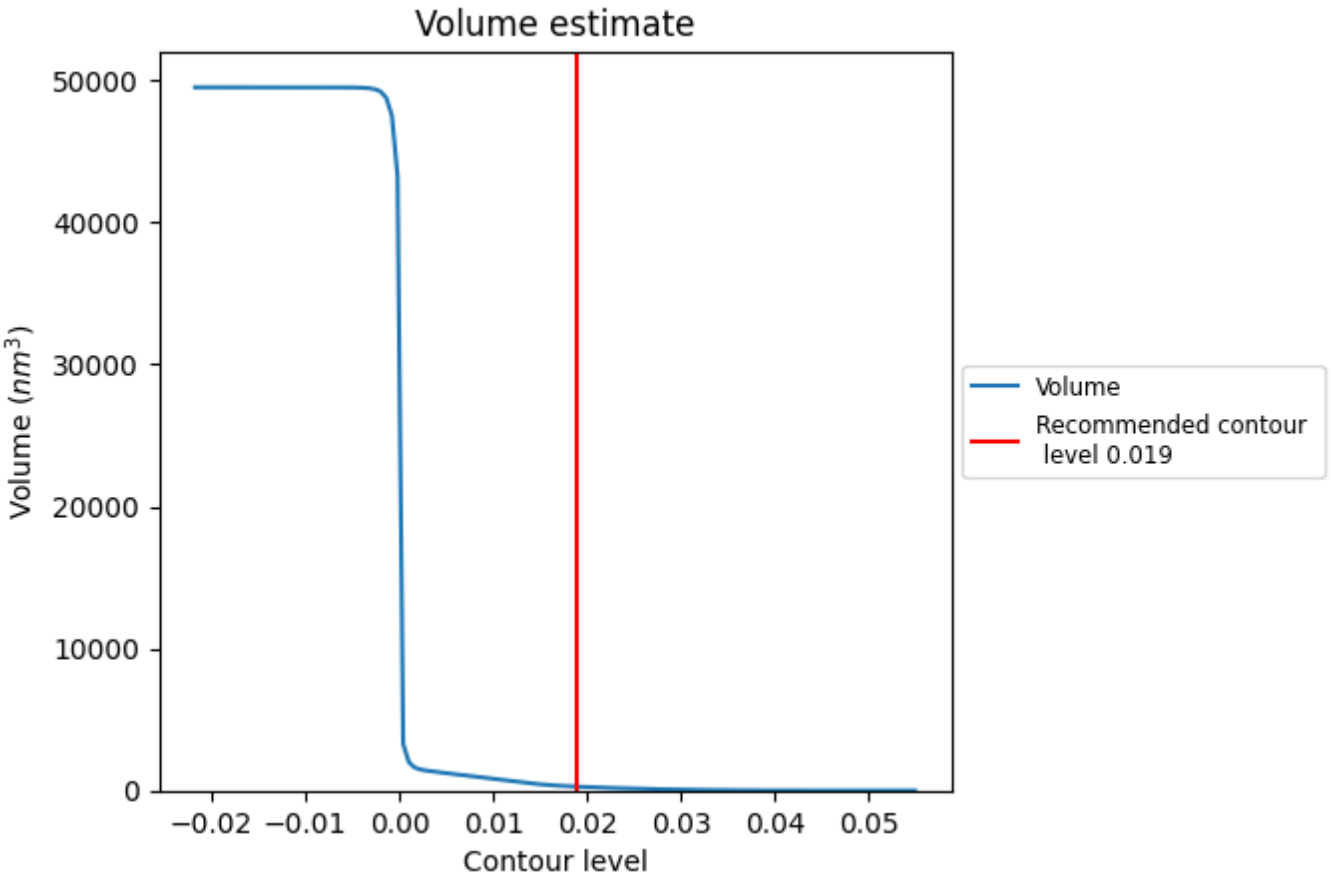
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

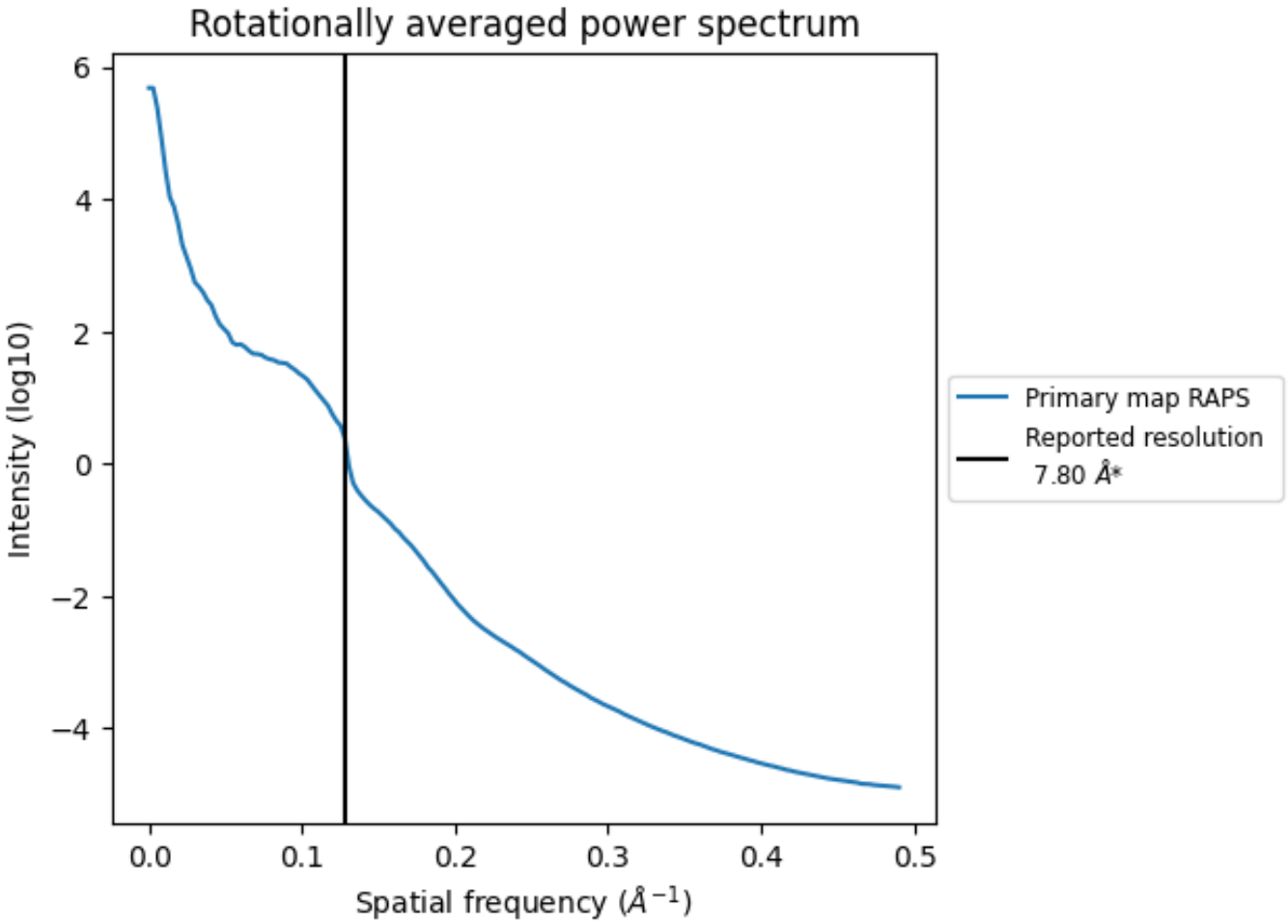
7.2 Volume estimate



The volume at the recommended contour level is 273 nm^3; this corresponds to an approximate mass of 246 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.128 $Å^{-1}$

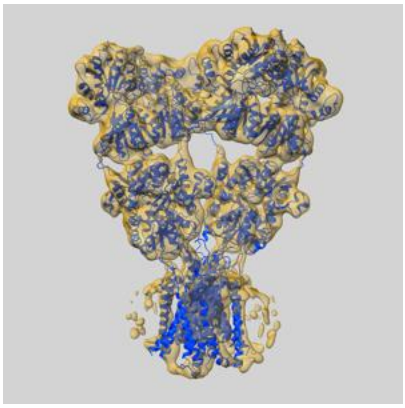
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

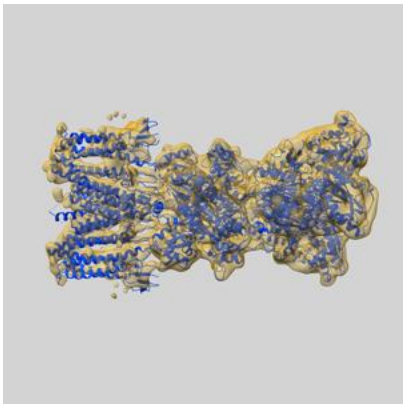
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8231 and PDB model 5KBU. Per-residue inclusion information can be found in section 3 on page 8.

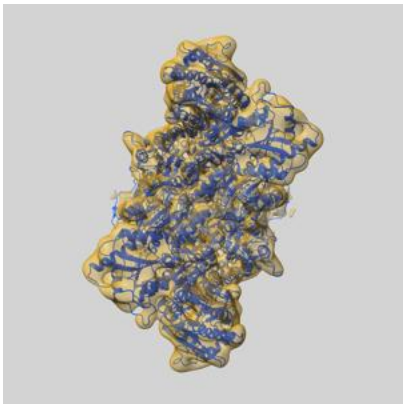
9.1 Map-model overlay



X



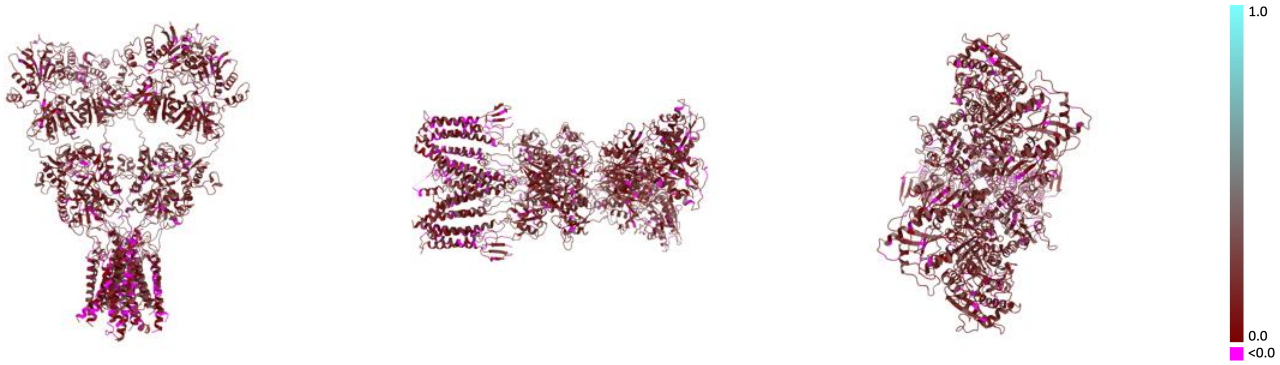
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

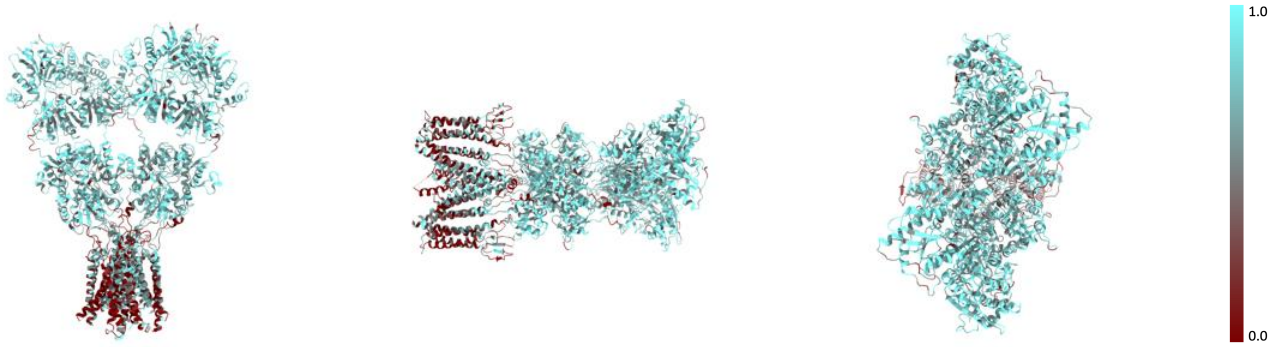
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

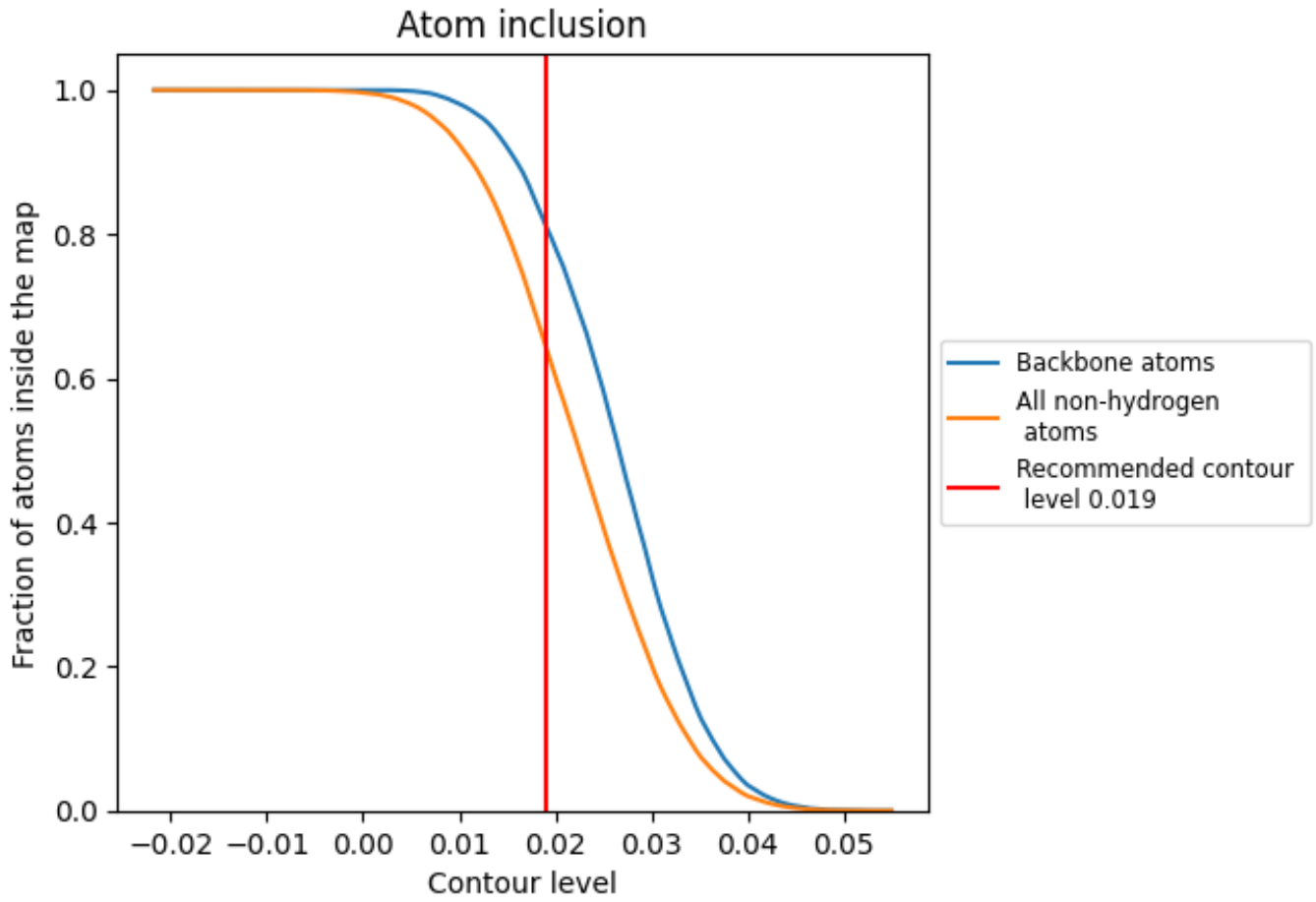
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.019).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6430	0.1530
A	0.6181	0.1570
B	0.6918	0.1610
C	0.6039	0.1420
D	0.6746	0.1530