Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Jan 9, 2019 – 11:23 AM EST

PDB ID	:	6IRG
EMDB ID:	:	EMD-9716
Title	:	Structure of the human GluN1/GluN2A NMDA receptor in the glutamate/glycine-bound state at pH 6.3, Class II
Authors	:	Zhang, J.; Chang, S.; Zhang, X.; Zhu, S.
Deposited on	:	2018-11-12
Resolution	:	5.50 Å(reported)
Based on PDB ID	:	4PE5, 5TQ0, 5H8F

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

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

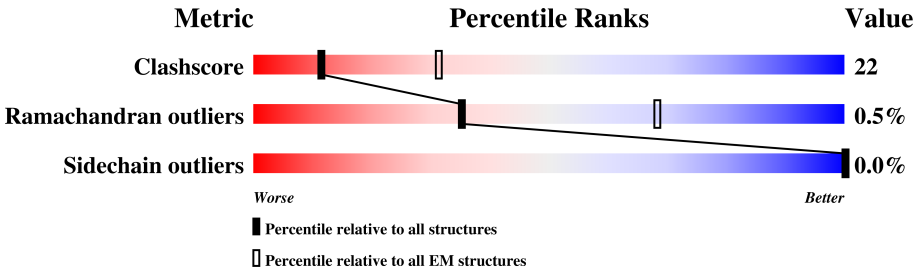
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

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 5.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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

Mol	Chain	Length	Quality of chain
1	A	847	63% 29% • 7%
1	C	847	62% 30% • 7%
2	B	841	63% 26% 11%
2	D	841	63% 26% 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23912 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 ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	787	Total	C	N	O	S	1	0
			6168	3931	1070	1132	35		
1	A	787	Total	C	N	O	S	1	0
			6168	3931	1070	1132	35		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	612	ARG	GLY	engineered mutation	UNP Q05586
A	612	ARG	GLY	engineered mutation	UNP Q05586

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	752	Total	C	N	O	S	1	0
			5788	3740	950	1062	36		
2	D	752	Total	C	N	O	S	1	0
			5788	3740	950	1062	36		

There are 4 discrepancies between the modelled and reference sequences:

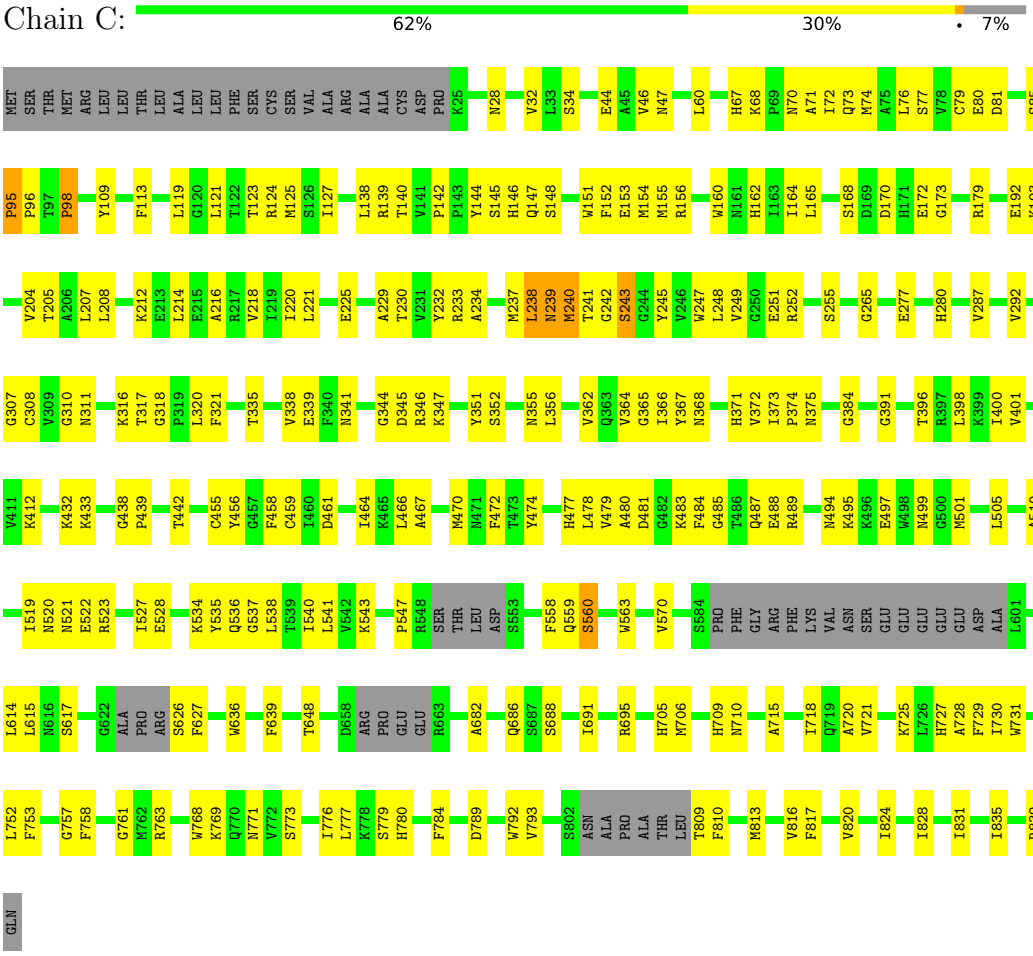
Chain	Residue	Modelled	Actual	Comment	Reference
B	656	ARG	GLU	engineered mutation	UNP Q12879
B	657	ARG	GLU	engineered mutation	UNP Q12879
D	656	ARG	GLU	engineered mutation	UNP Q12879
D	657	ARG	GLU	engineered mutation	UNP Q12879

3 Residue-property plots (i)

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

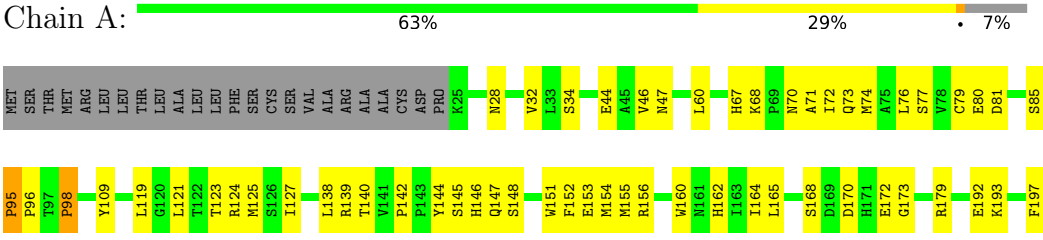
• Molecule 1: Glutamate receptor ionotropic, NMDA 1

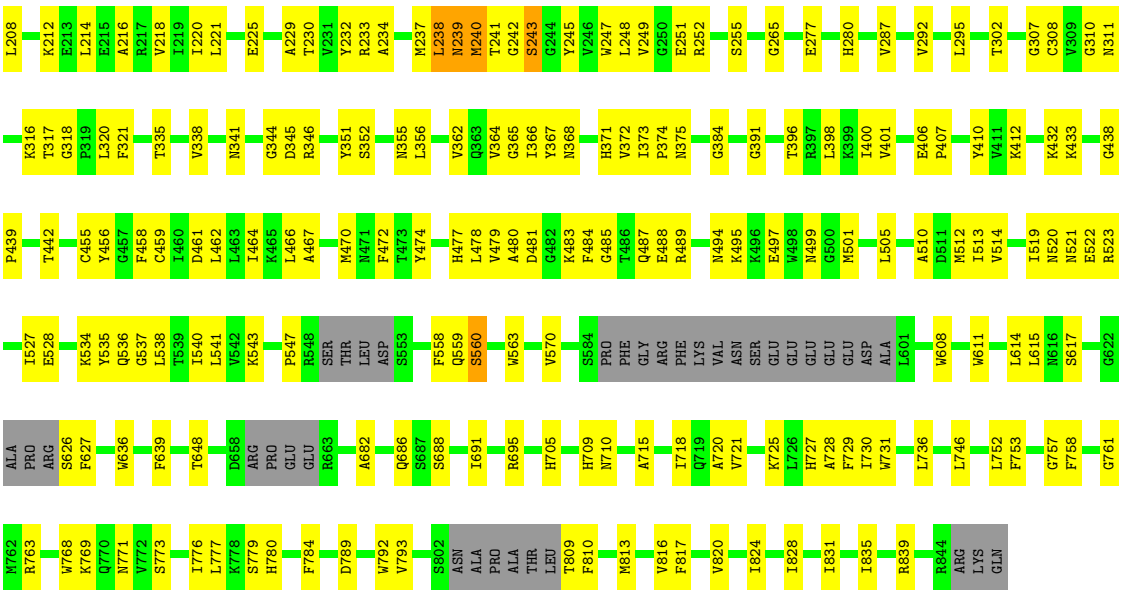
Chain C:



• Molecule 1: Glutamate receptor ionotropic, NMDA 1

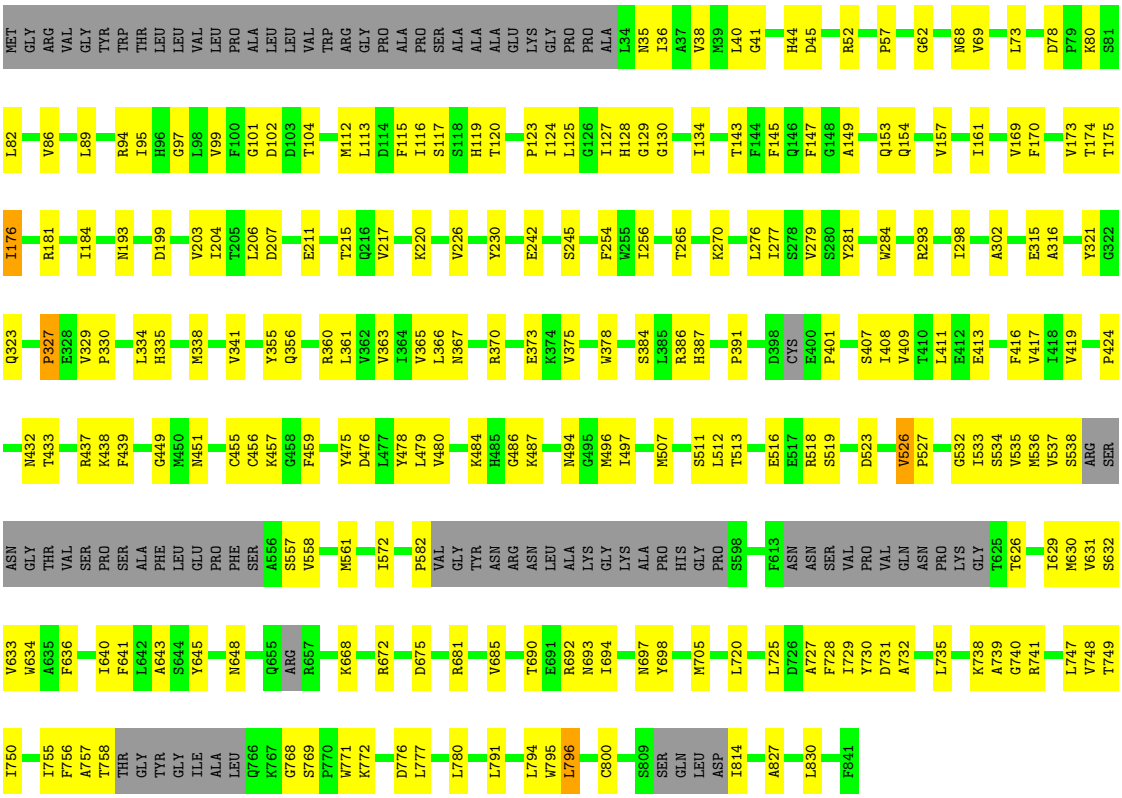
Chain A:





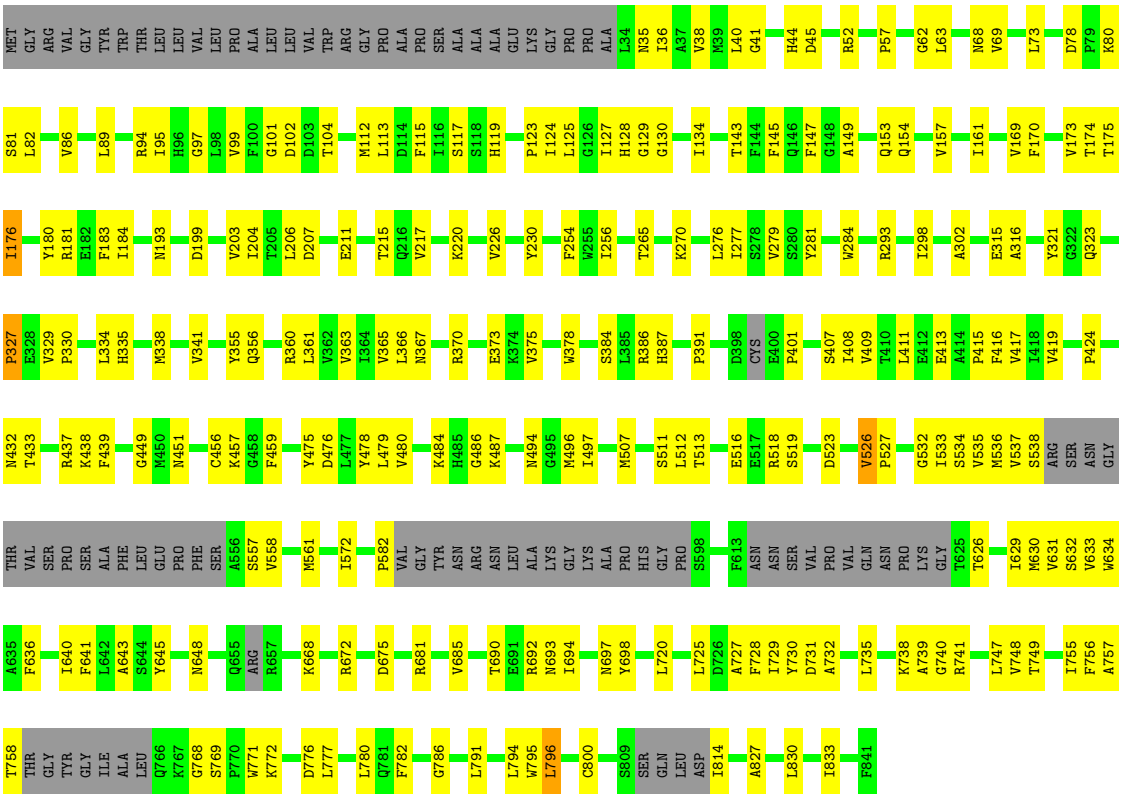
• Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain B:



• Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain D:


MET GLY ARG VAL GLY TYR TRP THR LEU LEU VAL VAL LEU PRO ALA LEU LEU VAL TRP ARG GLY PRO ALA PRO SER ALA ALA ALA GLU LYS GLY PRO PRO ALA L34 N35 I36 A37 V38 M39 L40 G41 H44 D45 R52 P57 G62 L63 N68 V69 L73 D78 P79 K80
S81 L82 V86 L89 R94 I95 H96 G97 L98 V99 F100 G101 D102 D103 T104 M112 L113 D114 F115 I116 S117 S118 H119 P123 I124 L125 G126 I127 H128 G129 G130 I134 T143 F144 F145 Q146 F147 G148 A149 Q153 Q154 V157 I161 V169 F170 V173 T174 T175
I176 Y180 R181 E182 F183 I184 N193 D199 V203 I204 T205 L206 D207 E211 T215 Q216 V217 K220 V226 Y230 F254 W255 I256 T265 K270 L276 I277 S278 V279 S280 Y281 W284 R293 I298 A302 E315 A316 Y321 G322 Q323
P327 E328 V329 P330 L334 H335 M338 V341 Y355 Q356 R360 L361 W362 V363 I364 V365 L366 N367 R370 E373 K374 V375 W378 S384 L385 R386 H387 P391 D398 CYS E400 P401 S407 I408 V409 T410 L411 E412 E413 A414 P415 F416 V417 I418 V419 P424
N432 T433 R437 K438 F439 G449 M450 N451 C456 K457 G458 F459 Y475 D476 L477 Y478 L479 V480 K484 H485 G486 K487 N494 G495 M496 I497 M507 S511 L512 T513 E516 E517 R518 S519 D523 V526 P527 G532 I533 S534 V535 M536 V537 S538 ARG SER ASN GLY
THR VAL SER PRO SER ALA PHE LEU GLU PRO PHE SER A556 S557 V558 M561 I572 P582 VAL GLY TYR ASN ARG ASN LEU ALA LYS GLY LYS ALA PRO HIS GLY PRO S598 F613 ASN ASN SER VAL PRO VAL GLN ASN PRO LYS GLY T625 T626 I629 M630 V631 S632 V633 W634
A635 F636 I640 F641 L642 A643 S644 Y645 N648 Q655 ARG R657 K668 R672 D675 R681 V685 T690 E691 R692 N693 I694 N697 Y698 L720 L725 D726 A727 F728 I729 Y730 D731 A732 L735 K738 A739 G740 R741 L747 V748 T749 I755 F756 A757
T758 THR GLY TYR GLY ILE ALA LEU Q766 K767 G768 S769 P770 W771 K772 D776 L777 L780 Q781 F782 G786 L791 L794 W795 L796 C800 S809 SER GLN LEU ASP I814 A827 L830 I833 F841

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	148840	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 ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
1	A	0.33	0/6297	0.60	6/8519 (0.1%)
1	C	0.33	0/6297	0.59	5/8519 (0.1%)
2	B	0.32	0/5918	0.59	9/8033 (0.1%)
2	D	0.32	0/5918	0.59	9/8033 (0.1%)
All	All	0.32	0/24430	0.59	29/33104 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	B	0	4
2	D	0	4
All	All	0	10

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	95	PRO	N-CA-CB	8.25	113.19	103.30
1	A	95	PRO	N-CA-CB	8.20	113.14	103.30
2	D	526	VAL	C-N-CD	7.86	144.91	128.40
2	B	526	VAL	C-N-CD	7.75	144.68	128.40
2	D	327	PRO	N-CA-CB	6.55	111.16	103.30
2	B	327	PRO	N-CA-CB	6.55	111.16	103.30
2	B	424	PRO	N-CA-CB	6.28	110.83	103.30
2	D	391	PRO	N-CA-CB	6.26	110.82	103.30
2	D	424	PRO	N-CA-CB	6.26	110.82	103.30
2	B	391	PRO	N-CA-CB	6.24	110.79	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	547	PRO	N-CA-CB	6.09	110.61	103.30
1	C	98	PRO	N-CA-CB	6.08	110.59	103.30
1	A	547	PRO	N-CA-CB	6.07	110.58	103.30
1	A	98	PRO	N-CA-CB	6.05	110.56	103.30
2	D	401	PRO	N-CA-CB	5.97	110.47	103.30
2	B	401	PRO	N-CA-CB	5.96	110.45	103.30
1	C	96	PRO	N-CA-CB	5.79	110.25	103.30
1	A	96	PRO	N-CA-CB	5.79	110.24	103.30
2	B	330	PRO	N-CA-CB	5.61	110.03	103.30
2	D	330	PRO	N-CA-CB	5.58	110.00	103.30
2	B	57	PRO	N-CA-CB	5.57	109.98	103.30
2	D	57	PRO	N-CA-CB	5.55	109.96	103.30
2	D	796	LEU	CA-CB-CG	5.42	127.76	115.30
2	B	796	LEU	CA-CB-CG	5.40	127.73	115.30
1	A	243	SER	C-N-CA	5.19	133.20	122.30
2	B	176	ILE	CG1-CB-CG2	-5.09	100.20	111.40
2	D	176	ILE	CG1-CB-CG2	-5.08	100.22	111.40
1	A	238	LEU	C-N-CA	5.07	134.37	121.70
1	C	238	LEU	C-N-CA	5.05	134.33	121.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	TYR	Mainchain
2	B	170	PHE	Peptide
2	B	44	HIS	Peptide
2	B	62	GLY	Peptide
2	B	796	LEU	Peptide
1	C	232	TYR	Mainchain
2	D	170	PHE	Peptide
2	D	44	HIS	Peptide
2	D	62	GLY	Peptide
2	D	796	LEU	Peptide

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	6168	0	6120	290	0
1	C	6168	0	6119	298	0
2	B	5788	0	5594	351	0
2	D	5788	0	5594	350	0
All	All	23912	0	23427	1019	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 22.

All (1019) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:PHE:CZ	2:D:561:MET:HE2	1.40	1.54
1:C:817:PHE:CZ	2:B:561:MET:HE3	1.41	1.53
1:C:611:TRP:CB	2:B:629:ILE:HG23	1.39	1.52
2:D:537:VAL:CG1	2:D:727:ALA:HB2	1.35	1.52
2:B:537:VAL:CG1	2:B:727:ALA:HB2	1.35	1.51
2:B:537:VAL:HG12	2:B:727:ALA:CB	1.39	1.51
2:D:537:VAL:HG12	2:D:727:ALA:CB	1.39	1.49
1:A:611:TRP:CB	2:D:629:ILE:HG23	1.42	1.47
1:C:817:PHE:CE1	2:B:561:MET:HE3	1.50	1.46
1:C:608:TRP:CZ2	2:B:626:THR:O	1.69	1.45
2:B:534:SER:CB	2:B:732:ALA:CB	1.95	1.44
1:A:608:TRP:CZ2	2:D:626:THR:O	1.70	1.44
1:C:817:PHE:CZ	2:B:561:MET:HB3	1.53	1.44
2:D:534:SER:CB	2:D:732:ALA:CB	1.95	1.43
2:D:534:SER:HB2	2:D:732:ALA:CB	1.51	1.41
1:A:817:PHE:CZ	2:D:561:MET:HB3	1.57	1.40
1:C:608:TRP:CH2	2:B:626:THR:O	1.76	1.38
2:D:537:VAL:CG1	2:D:727:ALA:CB	1.98	1.37
2:B:534:SER:HB2	2:B:732:ALA:CB	1.51	1.37
2:B:630:MET:O	2:B:634:TRP:CE3	1.80	1.35
1:A:608:TRP:CH2	2:D:626:THR:O	1.79	1.34
2:D:630:MET:O	2:D:634:TRP:CE3	1.80	1.34
2:B:534:SER:CB	2:B:732:ALA:HB2	1.56	1.32
2:B:537:VAL:CG1	2:B:727:ALA:CB	1.98	1.31
2:B:534:SER:OG	2:B:732:ALA:CB	1.81	1.28
2:D:534:SER:OG	2:D:732:ALA:CB	1.81	1.26
2:D:534:SER:CB	2:D:732:ALA:HB2	1.56	1.26
1:C:611:TRP:CB	2:B:629:ILE:CG2	2.14	1.25
2:B:535:VAL:HA	2:B:728:PHE:O	1.33	1.25
1:C:233:ARG:O	1:C:237:MET:HG2	1.11	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:839:ARG:CZ	2:B:582:PRO:HG3	1.67	1.25
1:C:243:SER:OG	1:C:384:GLY:N	1.69	1.24
1:A:817:PHE:CE1	2:D:561:MET:HE2	1.71	1.24
1:A:817:PHE:CE2	2:D:561:MET:HE2	1.71	1.24
1:A:233:ARG:O	1:A:237:MET:HG2	1.11	1.24
1:C:608:TRP:CG	2:B:629:ILE:HD11	1.38	1.22
2:D:535:VAL:HA	2:D:728:PHE:O	1.33	1.21
1:A:611:TRP:CB	2:D:629:ILE:CG2	2.17	1.21
1:C:608:TRP:CG	2:B:629:ILE:CD1	2.06	1.21
2:B:534:SER:CB	2:B:732:ALA:HB1	1.65	1.20
1:C:521:ASN:CA	2:B:780:LEU:HD13	1.69	1.20
2:B:537:VAL:CG2	2:B:748:VAL:O	1.90	1.19
2:D:537:VAL:CG2	2:D:748:VAL:O	1.90	1.19
1:A:839:ARG:CZ	2:D:582:PRO:HG3	1.73	1.19
2:B:537:VAL:O	2:B:748:VAL:N	1.74	1.19
2:D:537:VAL:O	2:D:748:VAL:N	1.74	1.19
1:A:521:ASN:CA	2:D:780:LEU:HD13	1.72	1.18
1:C:608:TRP:CB	2:B:629:ILE:HD11	1.72	1.18
2:D:534:SER:CB	2:D:732:ALA:HB1	1.65	1.17
1:C:809:THR:CG2	2:B:558:VAL:N	2.08	1.16
1:C:615:LEU:HD12	2:B:632:SER:OG	1.44	1.16
1:C:521:ASN:HA	2:B:780:LEU:CD1	1.76	1.16
1:A:615:LEU:HD12	2:D:632:SER:OG	1.50	1.12
1:C:608:TRP:CA	2:B:629:ILE:HD11	1.79	1.12
1:A:777:LEU:HD13	2:D:516:GLU:HA	1.21	1.11
2:D:538:SER:HA	2:D:747:LEU:HA	1.29	1.11
1:A:521:ASN:HA	2:D:780:LEU:CD1	1.79	1.11
1:A:817:PHE:CE1	2:D:561:MET:CE	2.33	1.10
1:A:817:PHE:CZ	2:D:561:MET:CE	2.34	1.10
1:C:817:PHE:CZ	2:B:561:MET:CE	2.34	1.10
2:B:630:MET:O	2:B:634:TRP:CZ3	2.04	1.10
2:D:630:MET:O	2:D:634:TRP:CZ3	2.04	1.09
1:C:208:LEU:HB3	1:C:238:LEU:HD11	1.11	1.09
2:D:536:MET:HA	2:D:749:THR:HA	1.12	1.09
1:A:809:THR:CG2	2:D:558:VAL:N	2.14	1.08
2:B:536:MET:HA	2:B:749:THR:HA	1.12	1.08
2:B:538:SER:HA	2:B:747:LEU:HA	1.29	1.08
2:B:536:MET:HA	2:B:749:THR:CA	1.83	1.08
1:C:817:PHE:HZ	2:B:561:MET:CB	1.64	1.08
1:C:817:PHE:CE1	2:B:561:MET:CE	2.36	1.08
1:C:777:LEU:HD13	2:B:516:GLU:HA	1.17	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:PHE:HZ	2:D:561:MET:CB	1.67	1.07
1:C:611:TRP:CG	2:B:629:ILE:CG2	2.37	1.07
1:A:243:SER:HB3	1:A:384:GLY:N	1.69	1.07
1:C:615:LEU:HD13	2:B:633:VAL:N	1.69	1.07
2:D:533:ILE:HG12	2:D:690:THR:HG22	1.35	1.07
2:B:535:VAL:HG22	2:B:729:ILE:HG12	1.32	1.07
2:B:534:SER:OG	2:B:732:ALA:HB1	1.48	1.07
1:C:813:MET:SD	2:B:641:PHE:HE1	1.77	1.07
2:D:536:MET:HA	2:D:749:THR:CA	1.83	1.07
1:A:615:LEU:HD13	2:D:633:VAL:N	1.70	1.06
2:B:536:MET:HG3	2:B:749:THR:HG22	1.37	1.06
1:A:243:SER:HB3	1:A:384:GLY:H	0.89	1.06
2:D:535:VAL:HG22	2:D:729:ILE:HG12	1.32	1.05
1:A:208:LEU:HB3	1:A:238:LEU:HD11	1.10	1.05
2:D:526:VAL:HG23	2:D:776:ASP:OD1	1.54	1.05
2:D:536:MET:HG3	2:D:749:THR:HG22	1.37	1.05
1:C:608:TRP:HA	2:B:629:ILE:CD1	1.87	1.04
1:A:233:ARG:O	1:A:237:MET:CG	2.06	1.04
2:B:533:ILE:HG12	2:B:690:THR:HG22	1.35	1.04
2:D:537:VAL:N	2:D:748:VAL:O	1.91	1.04
1:C:839:ARG:NH2	2:B:582:PRO:CG	2.22	1.03
1:A:608:TRP:HA	2:D:629:ILE:CD1	1.88	1.03
2:B:537:VAL:N	2:B:748:VAL:O	1.91	1.02
2:B:536:MET:O	2:B:727:ALA:CA	2.08	1.02
1:A:611:TRP:CG	2:D:629:ILE:CG2	2.42	1.02
1:A:611:TRP:HB3	2:D:629:ILE:CG2	1.87	1.02
1:C:817:PHE:CE2	2:B:561:MET:HE3	1.93	1.02
2:D:537:VAL:HG13	2:D:727:ALA:CB	1.88	1.02
1:A:813:MET:SD	2:D:641:PHE:HE1	1.82	1.02
2:B:526:VAL:HG23	2:B:776:ASP:OD1	1.59	1.02
2:B:537:VAL:HG13	2:B:727:ALA:CB	1.88	1.02
2:D:536:MET:O	2:D:727:ALA:CA	2.07	1.02
1:C:233:ARG:O	1:C:237:MET:CG	2.06	1.02
1:C:615:LEU:HD13	2:B:632:SER:C	1.80	1.01
1:C:817:PHE:CZ	2:B:561:MET:CB	2.40	1.01
1:C:813:MET:SD	2:B:641:PHE:CE1	2.54	1.00
2:B:536:MET:O	2:B:727:ALA:HB1	1.62	1.00
2:D:537:VAL:HG22	2:D:748:VAL:O	1.60	1.00
1:C:611:TRP:CG	2:B:629:ILE:HG21	1.97	1.00
2:B:537:VAL:HG22	2:B:748:VAL:O	1.60	0.99
2:D:534:SER:OG	2:D:732:ALA:HB1	1.48	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:LEU:HD13	2:D:632:SER:C	1.81	0.99
1:A:817:PHE:CZ	2:D:561:MET:CB	2.42	0.99
1:A:521:ASN:HA	2:D:780:LEU:HD13	0.99	0.99
2:B:536:MET:CA	2:B:749:THR:HA	1.92	0.98
2:D:536:MET:O	2:D:727:ALA:HB1	1.62	0.98
2:D:536:MET:CA	2:D:749:THR:HA	1.92	0.98
2:B:536:MET:O	2:B:727:ALA:CB	2.13	0.97
1:C:608:TRP:HZ2	2:B:626:THR:O	1.36	0.97
1:A:608:TRP:HA	2:D:629:ILE:HD11	1.46	0.97
1:C:608:TRP:HA	2:B:629:ILE:HD11	1.41	0.97
1:C:611:TRP:HB3	2:B:629:ILE:CG2	1.83	0.96
1:A:611:TRP:HB2	2:D:629:ILE:HG23	1.46	0.96
1:A:839:ARG:NH2	2:D:582:PRO:CG	2.28	0.96
2:D:537:VAL:CA	2:D:748:VAL:O	2.14	0.96
1:A:608:TRP:HZ2	2:D:626:THR:O	1.36	0.96
2:B:537:VAL:CA	2:B:748:VAL:O	2.14	0.96
1:A:611:TRP:HB3	2:D:629:ILE:HG23	0.96	0.96
1:A:817:PHE:HZ	2:D:561:MET:HB3	0.88	0.95
2:D:536:MET:O	2:D:727:ALA:CB	2.13	0.95
2:B:536:MET:CG	2:B:749:THR:HG22	1.96	0.95
2:D:536:MET:O	2:D:727:ALA:HA	1.67	0.94
1:A:611:TRP:CG	2:D:629:ILE:HG21	2.03	0.94
2:B:533:ILE:CG2	2:B:729:ILE:HG23	1.97	0.94
1:C:839:ARG:CZ	2:B:582:PRO:CG	2.45	0.94
1:C:608:TRP:HH2	2:B:626:THR:O	1.46	0.94
2:D:533:ILE:CG2	2:D:729:ILE:HG23	1.97	0.94
1:A:608:TRP:CA	2:D:629:ILE:HD11	1.80	0.94
2:D:536:MET:CG	2:D:749:THR:HG22	1.96	0.94
1:A:813:MET:SD	2:D:641:PHE:CE1	2.59	0.94
1:C:521:ASN:HA	2:B:780:LEU:HD13	0.95	0.93
1:A:521:ASN:OD1	2:D:777:LEU:HD22	1.66	0.93
1:C:615:LEU:CD1	2:B:632:SER:OG	2.16	0.93
1:A:234:ALA:O	1:A:237:MET:HB2	1.67	0.93
1:C:234:ALA:O	1:C:237:MET:HB2	1.67	0.93
2:B:631:VAL:HA	2:B:634:TRP:HE3	1.34	0.93
2:B:536:MET:O	2:B:727:ALA:HA	1.67	0.93
1:C:521:ASN:OD1	2:B:777:LEU:HD22	1.69	0.92
2:D:631:VAL:HA	2:D:634:TRP:HE3	1.34	0.92
1:A:608:TRP:HH2	2:D:626:THR:O	1.51	0.92
1:C:817:PHE:HZ	2:B:561:MET:HB3	0.83	0.91
1:A:535:TYR:CE1	2:D:527:PRO:HG3	2.04	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:608:TRP:CZ2	2:B:626:THR:C	2.44	0.91
2:B:630:MET:C	2:B:634:TRP:CZ3	2.44	0.91
2:D:630:MET:C	2:D:634:TRP:CZ3	2.44	0.91
1:C:611:TRP:HB2	2:B:629:ILE:HG23	1.47	0.91
2:B:533:ILE:HG12	2:B:690:THR:CG2	2.02	0.90
1:C:466:LEU:O	1:C:470:MET:HB2	1.71	0.90
1:C:611:TRP:HB3	2:B:629:ILE:HG23	0.91	0.90
1:A:817:PHE:CD1	2:D:561:MET:CE	2.55	0.90
1:A:839:ARG:CZ	2:D:582:PRO:CG	2.50	0.90
1:C:521:ASN:HB2	2:B:780:LEU:HB3	1.51	0.90
1:A:466:LEU:O	1:A:470:MET:HB2	1.71	0.89
2:B:220:LYS:NZ	2:D:217:VAL:HG22	1.87	0.89
1:C:817:PHE:CE2	2:B:561:MET:CE	2.53	0.89
1:C:817:PHE:CD1	2:B:561:MET:HE3	2.06	0.89
1:C:809:THR:HG21	2:B:558:VAL:H	1.37	0.89
2:D:533:ILE:HG12	2:D:690:THR:CG2	2.02	0.89
2:D:537:VAL:HG13	2:D:727:ALA:HB1	1.55	0.89
1:A:521:ASN:HB2	2:D:780:LEU:HB3	1.55	0.89
1:C:817:PHE:CD1	2:B:561:MET:CE	2.56	0.88
1:C:839:ARG:NH2	2:B:582:PRO:HG3	1.85	0.88
1:C:777:LEU:HB3	2:B:516:GLU:HB2	1.55	0.88
2:B:433:THR:HA	2:B:456:CYS:O	1.74	0.88
1:A:615:LEU:CD1	2:D:632:SER:OG	2.22	0.87
1:A:817:PHE:CE2	2:D:561:MET:CE	2.57	0.87
1:A:608:TRP:CZ2	2:D:626:THR:C	2.48	0.87
2:B:217:VAL:HG22	2:D:220:LYS:NZ	1.89	0.87
1:C:535:TYR:CE1	2:B:527:PRO:HG3	2.10	0.87
2:D:433:THR:HA	2:D:456:CYS:O	1.74	0.87
1:A:243:SER:CB	1:A:384:GLY:H	1.83	0.87
2:D:537:VAL:HG23	2:D:748:VAL:O	1.75	0.86
2:B:537:VAL:HG13	2:B:727:ALA:HB1	1.55	0.86
1:A:611:TRP:HB2	2:D:629:ILE:CG2	2.04	0.86
1:A:777:LEU:HB3	2:D:516:GLU:HB2	1.58	0.85
2:B:526:VAL:CG2	2:B:776:ASP:OD1	2.23	0.85
2:D:534:SER:HB2	2:D:732:ALA:HB1	1.37	0.85
2:D:630:MET:O	2:D:634:TRP:HE3	1.59	0.85
2:D:535:VAL:CA	2:D:728:PHE:O	2.23	0.85
2:B:533:ILE:HD12	2:B:757:ALA:HB2	1.59	0.84
2:B:534:SER:N	2:B:732:ALA:HB2	1.92	0.84
2:B:537:VAL:C	2:B:748:VAL:O	2.17	0.84
1:A:164:ILE:HB	1:A:218:VAL:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:534:SER:CA	2:B:732:ALA:HB2	2.08	0.83
2:B:535:VAL:CA	2:B:728:PHE:O	2.23	0.83
2:D:534:SER:CA	2:D:732:ALA:HB2	2.08	0.83
2:D:534:SER:N	2:D:732:ALA:HB2	1.92	0.83
1:C:164:ILE:HB	1:C:218:VAL:O	1.78	0.83
2:D:537:VAL:C	2:D:748:VAL:O	2.17	0.83
1:C:230:THR:HA	1:C:233:ARG:HD2	1.61	0.83
2:B:537:VAL:HG23	2:B:748:VAL:O	1.75	0.82
2:D:537:VAL:O	2:D:748:VAL:O	1.97	0.82
2:B:533:ILE:CG2	2:B:729:ILE:CG2	2.58	0.82
2:B:533:ILE:HD12	2:B:757:ALA:CB	2.08	0.82
2:B:630:MET:O	2:B:634:TRP:HE3	1.59	0.82
2:B:537:VAL:O	2:B:748:VAL:O	1.97	0.82
1:A:230:THR:HA	1:A:233:ARG:HD2	1.60	0.82
1:C:777:LEU:HD13	2:B:516:GLU:CA	2.08	0.82
2:D:526:VAL:CG2	2:D:776:ASP:OD1	2.27	0.82
2:D:533:ILE:HD12	2:D:757:ALA:CB	2.08	0.82
2:D:533:ILE:CG2	2:D:729:ILE:CG2	2.58	0.82
2:D:533:ILE:HD12	2:D:757:ALA:HB2	1.59	0.82
1:C:809:THR:HG21	2:B:558:VAL:N	1.85	0.82
1:C:816:VAL:HG11	2:B:641:PHE:CZ	2.15	0.81
1:C:611:TRP:HB2	2:B:629:ILE:CG2	2.04	0.81
1:A:535:TYR:HE1	2:D:527:PRO:HG3	1.46	0.81
1:A:809:THR:HG21	2:D:558:VAL:H	1.43	0.81
1:A:816:VAL:HG11	2:D:641:PHE:CZ	2.15	0.81
2:B:536:MET:CB	2:B:749:THR:HG22	2.11	0.81
2:D:536:MET:CB	2:D:749:THR:HG22	2.11	0.81
1:A:839:ARG:NH2	2:D:582:PRO:HG3	1.92	0.81
2:D:631:VAL:HA	2:D:634:TRP:CE3	2.16	0.81
1:C:611:TRP:CD1	2:B:629:ILE:HG21	2.16	0.80
2:D:534:SER:O	2:D:729:ILE:HA	1.81	0.80
2:B:536:MET:HG3	2:B:749:THR:CG2	2.12	0.80
2:B:220:LYS:HZ3	2:D:217:VAL:HG22	1.43	0.79
2:D:536:MET:HG3	2:D:749:THR:CG2	2.12	0.79
2:B:631:VAL:HA	2:B:634:TRP:CE3	2.16	0.79
2:B:534:SER:O	2:B:729:ILE:HA	1.81	0.79
1:C:239:ASN:O	1:C:241:THR:N	2.15	0.79
1:A:242:GLY:N	1:A:245:TYR:CD2	2.52	0.78
1:A:817:PHE:CE1	2:D:561:MET:HE3	2.19	0.78
2:D:533:ILE:CG1	2:D:690:THR:HG22	2.12	0.77
1:A:777:LEU:CD1	2:D:519:SER:OG	2.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:TRP:CD1	2:D:629:ILE:HG21	2.20	0.77
1:C:608:TRP:CH2	2:B:626:THR:C	2.57	0.77
1:C:233:ARG:C	1:C:237:MET:HG2	2.02	0.77
2:D:438:LYS:O	2:D:451:ASN:HA	1.86	0.76
2:D:537:VAL:O	2:D:748:VAL:C	2.24	0.76
2:D:536:MET:HA	2:D:749:THR:CB	2.14	0.76
1:A:233:ARG:C	1:A:237:MET:HG2	2.02	0.76
1:A:242:GLY:N	1:A:245:TYR:HD2	1.83	0.76
1:C:240:MET:CE	1:C:245:TYR:CE1	2.69	0.76
2:B:533:ILE:CG1	2:B:690:THR:HG22	2.13	0.76
2:B:537:VAL:O	2:B:748:VAL:C	2.24	0.76
2:D:535:VAL:HG22	2:D:729:ILE:CG1	2.15	0.76
1:C:243:SER:CB	1:C:384:GLY:H	1.98	0.76
2:B:535:VAL:HG22	2:B:729:ILE:CG1	2.15	0.75
2:B:536:MET:HA	2:B:749:THR:CB	2.14	0.75
2:B:630:MET:C	2:B:634:TRP:CE3	2.59	0.75
1:A:240:MET:CE	1:A:245:TYR:CE1	2.70	0.75
2:B:533:ILE:HA	2:B:730:TYR:O	1.86	0.75
1:C:208:LEU:HB3	1:C:238:LEU:CD1	2.06	0.75
2:B:438:LYS:O	2:B:451:ASN:HA	1.85	0.74
1:C:208:LEU:CB	1:C:238:LEU:HD11	2.06	0.74
2:D:630:MET:C	2:D:634:TRP:CE3	2.59	0.74
1:A:817:PHE:CD1	2:D:561:MET:HE2	2.20	0.74
2:B:534:SER:HB2	2:B:732:ALA:CA	2.18	0.74
1:C:535:TYR:HE1	2:B:527:PRO:HG3	1.49	0.74
2:D:533:ILE:HA	2:D:730:TYR:O	1.87	0.74
1:A:817:PHE:CD2	2:D:561:MET:HE2	2.20	0.74
1:A:817:PHE:CD1	2:D:561:MET:HE3	2.22	0.74
1:A:608:TRP:CH2	2:D:626:THR:C	2.62	0.73
1:A:208:LEU:HB3	1:A:238:LEU:CD1	2.05	0.73
1:C:72:ILE:HG13	2:D:323:GLN:HE21	1.54	0.73
1:A:208:LEU:CB	1:A:238:LEU:HD11	2.05	0.73
2:B:536:MET:HB2	2:B:735:LEU:HD22	1.70	0.73
1:A:240:MET:HE3	1:A:245:TYR:CE1	2.23	0.73
1:C:780:HIS:HB3	2:B:758:THR:O	1.89	0.73
2:D:534:SER:HB2	2:D:732:ALA:CA	2.17	0.73
2:D:536:MET:HB2	2:D:735:LEU:HD22	1.70	0.73
1:A:240:MET:CE	1:A:245:TYR:HE1	2.02	0.73
2:B:630:MET:HB3	2:B:634:TRP:CZ3	2.23	0.73
2:D:630:MET:HB3	2:D:634:TRP:CZ3	2.23	0.72
1:C:608:TRP:CE2	2:B:629:ILE:HD12	1.83	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:630:MET:C	2:D:634:TRP:HZ3	1.91	0.72
1:C:839:ARG:NH2	2:B:582:PRO:CD	2.53	0.72
1:C:240:MET:CE	1:C:245:TYR:HE1	2.01	0.72
1:C:817:PHE:CD2	2:B:561:MET:CE	2.72	0.72
1:A:72:ILE:HG13	2:B:323:GLN:HE21	1.54	0.72
2:B:217:VAL:HG22	2:D:220:LYS:HZ3	1.54	0.72
1:C:777:LEU:CD1	2:B:519:SER:OG	2.37	0.71
2:B:534:SER:HB2	2:B:732:ALA:HB1	1.38	0.71
1:C:144:TYR:O	1:C:147:GLN:HB2	1.90	0.71
2:B:537:VAL:O	2:B:747:LEU:C	2.29	0.71
2:D:537:VAL:O	2:D:747:LEU:C	2.29	0.71
1:A:144:TYR:O	1:A:147:GLN:HB2	1.90	0.71
2:B:533:ILE:HG22	2:B:729:ILE:HG23	1.73	0.71
1:A:608:TRP:CH2	2:D:629:ILE:HB	2.21	0.71
2:D:533:ILE:HG22	2:D:729:ILE:HG23	1.73	0.70
1:C:817:PHE:CD2	2:B:561:MET:HE2	2.26	0.70
1:A:410:TYR:HB2	1:A:456:TYR:HB2	1.73	0.70
1:A:230:THR:HG22	1:A:233:ARG:NH1	2.06	0.70
2:B:533:ILE:O	2:B:756:PHE:N	2.25	0.70
2:B:630:MET:C	2:B:634:TRP:HZ3	1.91	0.70
1:C:410:TYR:HB2	1:C:456:TYR:HB2	1.73	0.70
1:C:240:MET:HE3	1:C:245:TYR:CE1	2.25	0.70
1:C:240:MET:HE1	1:C:245:TYR:HE1	1.56	0.70
1:A:809:THR:HG22	2:D:557:SER:OG	1.92	0.69
2:B:534:SER:HB2	2:B:732:ALA:HB2	1.32	0.69
1:C:615:LEU:HD11	2:B:633:VAL:HG23	1.74	0.69
1:A:777:LEU:HD13	2:D:516:GLU:CA	2.12	0.69
1:C:809:THR:HG22	2:B:558:VAL:N	2.06	0.69
1:A:406:GLU:HG2	1:A:410:TYR:HA	1.74	0.69
1:C:608:TRP:CZ2	2:B:626:THR:HA	2.27	0.69
1:C:230:THR:HG22	1:C:233:ARG:NH1	2.08	0.69
1:A:777:LEU:HD11	2:D:519:SER:OG	1.92	0.69
1:C:809:THR:HG22	2:B:557:SER:OG	1.93	0.69
1:C:242:GLY:O	1:C:245:TYR:HD2	1.76	0.68
1:C:243:SER:OG	1:C:384:GLY:CA	2.42	0.68
1:A:780:HIS:HB3	2:D:758:THR:O	1.93	0.68
2:B:536:MET:C	2:B:727:ALA:HB1	2.14	0.68
2:D:538:SER:C	2:D:748:VAL:H	1.97	0.68
1:A:615:LEU:HD11	2:D:633:VAL:HG23	1.75	0.67
2:B:538:SER:C	2:B:748:VAL:H	1.97	0.67
1:A:817:PHE:CD2	2:D:561:MET:CE	2.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:GLU:HG2	1:C:410:TYR:HA	1.75	0.67
2:D:536:MET:C	2:D:727:ALA:HB1	2.14	0.67
1:A:240:MET:HE1	1:A:245:TYR:HE1	1.60	0.67
1:C:777:LEU:HD11	2:B:519:SER:OG	1.94	0.67
2:D:533:ILE:O	2:D:756:PHE:N	2.25	0.67
1:C:615:LEU:CD1	2:B:633:VAL:N	2.55	0.67
2:D:537:VAL:CB	2:D:727:ALA:HB2	2.23	0.67
2:D:534:SER:HB2	2:D:732:ALA:HB2	1.32	0.67
2:D:537:VAL:CB	2:D:748:VAL:O	2.43	0.67
1:C:817:PHE:CE1	2:B:561:MET:HB3	2.26	0.67
1:C:540:ILE:HA	1:C:729:PHE:O	1.95	0.67
1:A:535:TYR:HE1	2:D:527:PRO:CG	2.08	0.67
1:A:535:TYR:CE1	2:D:527:PRO:CG	2.77	0.66
1:C:242:GLY:N	1:C:245:TYR:CD2	2.63	0.66
2:B:52:ARG:HA	2:B:293:ARG:HH21	1.61	0.66
2:B:630:MET:HB3	2:B:634:TRP:HZ3	1.60	0.66
2:D:537:VAL:O	2:D:748:VAL:CA	2.43	0.66
1:A:839:ARG:NH2	2:D:582:PRO:CD	2.58	0.66
2:B:537:VAL:CB	2:B:748:VAL:O	2.43	0.66
1:A:817:PHE:CE1	2:D:561:MET:HB3	2.25	0.66
1:A:221:LEU:HD12	1:A:249:VAL:HG22	1.78	0.66
2:B:537:VAL:O	2:B:748:VAL:CA	2.43	0.66
1:A:608:TRP:HA	2:D:629:ILE:HD13	1.76	0.66
1:A:560:SER:HA	1:A:563:TRP:HD1	1.61	0.65
2:B:217:VAL:HG22	2:D:220:LYS:HZ1	1.59	0.65
2:D:630:MET:HB3	2:D:634:TRP:HZ3	1.60	0.65
1:C:521:ASN:CB	2:B:780:LEU:HD13	2.27	0.65
1:C:824:ILE:CG2	2:B:572:ILE:CD1	2.74	0.65
1:C:221:LEU:HD12	1:C:249:VAL:HG22	1.78	0.65
1:C:816:VAL:HG11	2:B:641:PHE:HZ	1.60	0.65
1:A:828:ILE:HD11	2:D:572:ILE:CD1	2.26	0.65
1:C:560:SER:HA	1:C:563:TRP:HD1	1.61	0.65
2:B:125:LEU:HA	2:B:145:PHE:O	1.97	0.65
1:C:608:TRP:CZ2	2:B:626:THR:CA	2.80	0.65
2:D:52:ARG:HA	2:D:293:ARG:HH21	1.61	0.65
2:D:537:VAL:H	2:D:748:VAL:C	1.99	0.65
2:B:35:ASN:HA	2:B:68:ASN:O	1.97	0.65
1:C:817:PHE:CG	2:B:561:MET:CE	2.79	0.65
2:B:537:VAL:H	2:B:748:VAL:C	1.99	0.65
1:A:540:ILE:HA	1:A:729:PHE:O	1.95	0.64
2:B:537:VAL:CB	2:B:727:ALA:HB2	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:PHE:O	2:D:119:HIS:HB2	1.98	0.64
1:C:608:TRP:HA	2:B:629:ILE:HD13	1.78	0.64
2:D:35:ASN:HA	2:D:68:ASN:O	1.97	0.64
1:A:816:VAL:HG11	2:D:641:PHE:HZ	1.60	0.64
1:C:828:ILE:HD11	2:B:572:ILE:HG12	1.78	0.64
1:A:817:PHE:CG	2:D:561:MET:CE	2.81	0.64
2:B:735:LEU:O	2:B:739:ALA:HB2	1.98	0.64
2:D:533:ILE:N	2:D:756:PHE:O	2.27	0.64
2:D:735:LEU:O	2:D:739:ALA:HB2	1.98	0.64
2:B:631:VAL:CA	2:B:634:TRP:HE3	2.10	0.64
1:C:77:SER:O	1:C:81:ASP:HB2	1.98	0.64
2:D:125:LEU:HA	2:D:145:PHE:O	1.96	0.64
1:A:615:LEU:HD11	2:D:633:VAL:CG2	2.28	0.63
1:A:608:TRP:CZ2	2:D:626:THR:HA	2.33	0.63
1:A:77:SER:O	1:A:81:ASP:HB2	1.98	0.63
1:A:828:ILE:HD11	2:D:572:ILE:HD13	1.81	0.63
1:C:828:ILE:HD11	2:B:572:ILE:CD1	2.29	0.63
1:C:813:MET:CE	2:B:641:PHE:CE1	2.82	0.62
1:C:439:PRO:HG2	1:C:442:THR:HG22	1.82	0.62
1:A:521:ASN:OD1	2:D:777:LEU:CD2	2.43	0.62
1:A:813:MET:CE	2:D:641:PHE:CE1	2.82	0.62
1:A:125:MET:SD	1:A:252:ARG:NH2	2.72	0.62
1:C:615:LEU:HD11	2:B:633:VAL:CG2	2.30	0.62
1:A:519:ILE:HG22	2:D:780:LEU:HD21	1.81	0.62
1:A:510:ALA:O	1:A:763:ARG:NH2	2.32	0.62
2:B:115:PHE:O	2:B:119:HIS:HB2	1.98	0.62
1:A:617:SER:HB3	2:D:632:SER:HB2	1.82	0.62
1:C:510:ALA:O	1:C:763:ARG:NH2	2.32	0.62
1:A:439:PRO:HG2	1:A:442:THR:HG22	1.81	0.62
2:B:537:VAL:HG12	2:B:727:ALA:HB3	1.71	0.62
1:A:152:PHE:O	1:A:155:MET:HB2	2.00	0.62
2:B:536:MET:O	2:B:728:PHE:N	2.33	0.62
1:A:234:ALA:C	1:A:237:MET:HB2	2.20	0.62
1:C:125:MET:SD	1:C:252:ARG:NH2	2.72	0.62
1:C:239:ASN:O	1:C:241:THR:OG1	2.13	0.61
1:A:809:THR:N	2:D:558:VAL:HG22	2.12	0.61
1:C:152:PHE:O	1:C:155:MET:HB2	2.00	0.61
1:C:824:ILE:HG21	2:B:572:ILE:CD1	2.30	0.61
2:D:38:VAL:HG22	2:D:99:VAL:HB	1.82	0.61
1:C:521:ASN:OD1	2:B:777:LEU:CD2	2.44	0.61
2:B:220:LYS:HZ1	2:D:217:VAL:HG22	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:ILE:HD11	2:D:572:ILE:HG12	1.81	0.61
1:C:535:TYR:HE1	2:B:527:PRO:CG	2.12	0.61
1:C:828:ILE:HD11	2:B:572:ILE:CG1	2.29	0.61
1:C:809:THR:N	2:B:558:VAL:HG22	2.10	0.61
1:C:234:ALA:C	1:C:237:MET:HB2	2.20	0.61
1:C:535:TYR:CE1	2:B:527:PRO:CG	2.83	0.61
1:C:617:SER:HB3	2:B:632:SER:HB2	1.83	0.61
1:A:521:ASN:CB	2:D:780:LEU:HD13	2.31	0.61
1:A:810:PHE:HE2	2:D:645:TYR:HH	1.49	0.60
2:D:536:MET:O	2:D:728:PHE:N	2.33	0.60
1:A:242:GLY:O	1:A:245:TYR:HD2	1.83	0.60
2:B:38:VAL:HG22	2:B:99:VAL:HB	1.82	0.60
2:B:630:MET:CB	2:B:634:TRP:HZ3	2.14	0.60
1:A:615:LEU:CD1	2:D:633:VAL:N	2.56	0.60
2:D:630:MET:CB	2:D:634:TRP:HZ3	2.14	0.60
2:D:631:VAL:CA	2:D:634:TRP:HE3	2.10	0.60
1:C:648:THR:HG22	2:B:643:ALA:CB	2.31	0.60
1:A:828:ILE:HD11	2:D:572:ILE:CG1	2.31	0.60
1:C:839:ARG:NH2	2:B:582:PRO:HG2	2.15	0.60
1:C:351:TYR:HB2	1:C:367:TYR:HB2	1.84	0.60
2:D:537:VAL:N	2:D:749:THR:HA	2.17	0.60
1:A:824:ILE:CG2	2:D:572:ILE:CD1	2.79	0.60
2:D:175:THR:HG22	2:D:206:LEU:HB2	1.84	0.60
2:B:36:ILE:HB	2:B:69:VAL:HG22	1.84	0.59
2:B:496:MET:HG3	2:B:512:LEU:HD21	1.84	0.59
2:D:36:ILE:HB	2:D:69:VAL:HG22	1.84	0.59
1:A:538:LEU:HB2	1:A:753:PHE:HB2	1.84	0.59
1:C:828:ILE:HD11	2:B:572:ILE:HD13	1.84	0.59
1:C:824:ILE:CG2	2:B:572:ILE:HD13	2.31	0.59
1:A:372:VAL:HG12	1:A:374:PRO:HD3	1.84	0.59
2:B:533:ILE:N	2:B:756:PHE:O	2.27	0.59
1:A:824:ILE:HG12	2:D:634:TRP:CZ2	2.37	0.59
1:A:817:PHE:CZ	2:D:561:MET:CG	2.85	0.59
1:C:366:ILE:HB	1:C:373:ILE:HB	1.85	0.59
1:C:824:ILE:HG23	2:B:572:ILE:HD13	1.84	0.59
1:C:372:VAL:HG12	1:C:374:PRO:HD3	1.84	0.59
2:D:537:VAL:HG12	2:D:727:ALA:HB3	1.71	0.59
2:B:537:VAL:N	2:B:749:THR:HA	2.17	0.59
1:A:648:THR:HG22	2:D:643:ALA:CB	2.33	0.59
1:A:366:ILE:HB	1:A:373:ILE:HB	1.85	0.59
2:D:532:GLY:O	2:D:731:ASP:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:TYR:HB2	1:A:367:TYR:HB2	1.84	0.59
2:B:407:SER:HA	2:B:476:ASP:HB2	1.84	0.59
1:C:817:PHE:CZ	2:B:561:MET:CG	2.85	0.58
1:A:824:ILE:HG12	2:D:634:TRP:HZ2	1.68	0.58
2:D:537:VAL:H	2:D:749:THR:HA	1.68	0.58
1:A:125:MET:O	1:A:139:ARG:NH2	2.36	0.58
1:A:608:TRP:CZ2	2:D:626:THR:CA	2.86	0.58
2:B:157:VAL:HG21	2:B:361:LEU:HD13	1.85	0.58
1:C:828:ILE:CD1	2:B:572:ILE:HG12	2.34	0.58
2:B:175:THR:HG22	2:B:206:LEU:HB2	1.84	0.58
2:B:532:GLY:O	2:B:731:ASP:HA	2.03	0.58
1:C:824:ILE:HG12	2:B:634:TRP:CZ2	2.38	0.58
1:C:212:LYS:HG2	1:C:212:LYS:O	2.04	0.58
2:D:407:SER:HA	2:D:476:ASP:HB2	1.84	0.58
2:D:496:MET:HG3	2:D:512:LEU:HD21	1.84	0.58
2:D:416:PHE:HA	2:D:459:PHE:HB2	1.85	0.58
1:C:538:LEU:HB2	1:C:753:PHE:HB2	1.84	0.58
1:C:119:LEU:HA	1:C:138:LEU:O	2.04	0.58
1:C:813:MET:SD	2:B:641:PHE:CD1	2.97	0.58
2:B:537:VAL:H	2:B:749:THR:HA	1.68	0.58
2:B:534:SER:OG	2:B:732:ALA:HB2	1.76	0.57
1:C:817:PHE:CD2	2:B:561:MET:HE3	2.38	0.57
2:D:486:GLY:HA3	2:D:497:ILE:HD12	1.87	0.57
2:B:211:GLU:HB2	2:B:215:THR:HG23	1.87	0.57
1:C:608:TRP:CH2	2:B:629:ILE:HB	2.27	0.57
2:B:533:ILE:HD12	2:B:757:ALA:HB3	1.85	0.57
2:B:486:GLY:HA3	2:B:497:ILE:HD12	1.87	0.57
1:A:144:TYR:HE1	1:A:251:GLU:HB2	1.70	0.57
2:B:416:PHE:HA	2:B:459:PHE:HB2	1.85	0.57
1:C:824:ILE:HG12	2:B:634:TRP:HZ2	1.70	0.57
2:D:533:ILE:HD12	2:D:757:ALA:HB3	1.85	0.57
1:A:212:LYS:HG2	1:A:212:LYS:O	2.04	0.57
1:C:125:MET:O	1:C:139:ARG:NH2	2.36	0.57
1:A:28:ASN:ND2	1:A:85:SER:O	2.31	0.56
1:C:608:TRP:CA	2:B:629:ILE:CD1	2.56	0.56
2:D:270:LYS:O	2:D:370:ARG:NH1	2.38	0.56
2:D:211:GLU:HB2	2:D:215:THR:HG23	1.87	0.56
1:C:70:ASN:ND2	2:D:321:TYR:O	2.38	0.56
2:D:409:VAL:HG22	2:D:478:TYR:HB2	1.87	0.56
2:D:157:VAL:HG21	2:D:361:LEU:HD13	1.85	0.56
2:B:45:ASP:HA	2:B:73:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:ASP:OD2	2:B:772:LYS:NZ	2.39	0.56
1:C:810:PHE:H	1:C:813:MET:HB2	1.71	0.56
2:D:102:ASP:HB2	2:D:129:GLY:HA3	1.87	0.56
2:D:45:ASP:HA	2:D:73:LEU:HD11	1.87	0.56
1:A:119:LEU:HA	1:A:138:LEU:O	2.04	0.56
2:B:532:GLY:HA3	2:B:755:ILE:CG2	2.36	0.56
2:D:532:GLY:HA3	2:D:755:ILE:CG2	2.36	0.56
1:A:521:ASN:HB2	2:D:780:LEU:CB	2.34	0.56
2:B:270:LYS:O	2:B:370:ARG:NH1	2.38	0.56
1:C:519:ILE:HG22	2:B:780:LEU:HD21	1.86	0.56
2:B:413:GLU:H	2:B:417:VAL:HB	1.70	0.56
2:B:486:GLY:O	2:B:692:ARG:NH2	2.39	0.56
2:D:413:GLU:H	2:D:417:VAL:HB	1.70	0.56
1:A:809:THR:HG22	2:D:558:VAL:N	2.12	0.56
2:B:533:ILE:HG23	2:B:729:ILE:CG2	2.36	0.56
2:B:533:ILE:HG21	2:B:729:ILE:CG2	2.35	0.56
2:B:89:LEU:HB3	2:B:95:ILE:HD12	1.87	0.56
1:A:810:PHE:H	1:A:813:MET:HB2	1.71	0.56
2:B:409:VAL:HG22	2:B:478:TYR:HB2	1.87	0.56
1:C:242:GLY:N	1:C:245:TYR:HD2	2.03	0.56
2:B:265:THR:HG21	2:B:284:TRP:HE1	1.71	0.56
1:A:70:ASN:ND2	2:B:321:TYR:O	2.39	0.56
1:C:521:ASN:HB2	2:B:780:LEU:CB	2.31	0.56
1:C:144:TYR:HE1	1:C:251:GLU:HB2	1.70	0.55
1:C:817:PHE:CE2	2:B:561:MET:HE2	2.36	0.55
1:C:820:VAL:HG13	2:B:634:TRP:HE1	1.70	0.55
2:D:265:THR:HG21	2:D:284:TRP:HE1	1.71	0.55
1:A:142:PRO:HB3	1:A:345:ASP:HB3	1.89	0.55
2:B:102:ASP:HB2	2:B:129:GLY:HA3	1.87	0.55
2:D:279:VAL:HG22	2:D:363:VAL:HG22	1.88	0.55
2:D:486:GLY:O	2:D:692:ARG:NH2	2.39	0.55
1:C:142:PRO:HB3	1:C:345:ASP:HB3	1.89	0.55
2:D:169:VAL:HA	2:D:199:ASP:HB2	1.88	0.55
2:D:533:ILE:HG23	2:D:729:ILE:CG2	2.36	0.55
2:D:523:ASP:OD2	2:D:772:LYS:NZ	2.39	0.55
1:C:138:LEU:HD22	1:C:344:GLY:HA3	1.88	0.55
1:C:467:ALA:HB2	1:C:474:TYR:HE2	1.72	0.55
1:A:138:LEU:HD22	1:A:344:GLY:HA3	1.88	0.55
1:A:467:ALA:HB2	1:A:474:TYR:HE2	1.72	0.55
1:C:28:ASN:ND2	1:C:85:SER:O	2.31	0.55
2:B:279:VAL:HG22	2:B:363:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ARG:NH1	1:C:251:GLU:OE1	2.40	0.55
1:A:824:ILE:HG21	2:D:572:ILE:CD1	2.37	0.54
1:A:828:ILE:CD1	2:D:572:ILE:HG12	2.36	0.54
2:B:123:PRO:HG3	2:B:334:LEU:HD12	1.89	0.54
1:C:234:ALA:HA	1:C:237:MET:HB2	1.90	0.54
1:A:824:ILE:HG23	2:D:572:ILE:HD13	1.90	0.54
1:C:145:SER:OG	1:C:179:ARG:NH1	2.40	0.54
2:D:533:ILE:HG21	2:D:729:ILE:CG2	2.35	0.54
1:A:124:ARG:NH1	1:A:251:GLU:OE1	2.40	0.54
1:A:520:ASN:HD22	1:A:523:ARG:HD2	1.73	0.54
2:B:169:VAL:HA	2:B:199:ASP:HB2	1.88	0.54
1:C:505:LEU:HD12	1:C:527:ILE:HD13	1.90	0.54
1:C:615:LEU:HD22	2:B:633:VAL:HA	1.89	0.54
2:D:94:ARG:NH1	2:D:315:GLU:OE1	2.40	0.54
2:D:89:LEU:HB3	2:D:95:ILE:HD12	1.87	0.54
1:A:145:SER:OG	1:A:179:ARG:NH1	2.40	0.54
2:B:94:ARG:NH1	2:B:315:GLU:OE1	2.40	0.54
1:A:839:ARG:NH2	2:D:582:PRO:HG2	2.19	0.54
2:D:184:ILE:HG12	2:D:203:VAL:HG11	1.90	0.54
1:A:813:MET:SD	2:D:641:PHE:CD1	3.01	0.54
1:A:234:ALA:HA	1:A:237:MET:HB2	1.90	0.54
1:C:79:CYS:HB3	2:D:80:LYS:HE3	1.89	0.54
1:A:242:GLY:O	1:A:245:TYR:CD2	2.61	0.54
1:A:239:ASN:O	1:A:241:THR:N	2.41	0.54
1:C:145:SER:O	1:C:148:SER:OG	2.21	0.54
1:C:71:ALA:HB3	2:D:323:GLN:HE22	1.73	0.54
1:C:242:GLY:O	1:C:245:TYR:CD2	2.58	0.53
1:C:520:ASN:HD22	1:C:523:ARG:HD2	1.73	0.53
1:C:831:ILE:HG23	1:C:835:ILE:HD12	1.89	0.53
2:D:123:PRO:HG3	2:D:334:LEU:HD12	1.89	0.53
1:A:127:ILE:HG13	1:A:172:GLU:HG3	1.91	0.53
1:A:505:LEU:HD12	1:A:527:ILE:HD13	1.90	0.53
1:A:79:CYS:HB3	2:B:80:LYS:HE3	1.89	0.53
2:D:361:LEU:HB2	2:D:378:TRP:HB2	1.91	0.53
1:A:489:ARG:HA	1:A:495:LYS:O	2.09	0.53
1:A:731:TRP:HB2	1:A:736:LEU:HD11	1.90	0.53
2:B:361:LEU:HB2	2:B:378:TRP:HB2	1.91	0.53
1:C:810:PHE:HE2	2:B:645:TYR:HH	1.55	0.53
2:B:537:VAL:HG12	2:B:727:ALA:HB2	0.59	0.53
2:D:537:VAL:HG12	2:D:727:ALA:HB2	0.59	0.53
2:B:184:ILE:HG12	2:B:203:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:117:SER:HB2	2:D:143:THR:H	1.73	0.53
1:A:824:ILE:CG2	2:D:572:ILE:HD13	2.38	0.53
1:A:831:ILE:HG23	1:A:835:ILE:HD12	1.89	0.53
1:C:127:ILE:HG13	1:C:172:GLU:HG3	1.91	0.53
2:B:533:ILE:CD1	2:B:757:ALA:CB	2.84	0.53
1:C:731:TRP:HB2	1:C:736:LEU:HD11	1.90	0.53
1:A:682:ALA:HB1	1:A:710:ASN:HA	1.91	0.53
1:A:71:ALA:HB3	2:B:323:GLN:HE22	1.74	0.52
2:B:432:ASN:HB2	2:B:457:LYS:HE2	1.91	0.52
1:A:488:GLU:HB2	1:A:499:ASN:HD21	1.75	0.52
2:B:768:GLY:H	2:B:772:LYS:HZ2	1.58	0.52
1:C:682:ALA:HB1	1:C:710:ASN:HA	1.91	0.52
1:C:817:PHE:CD1	2:B:561:MET:HE1	2.40	0.52
2:D:533:ILE:CD1	2:D:757:ALA:CB	2.84	0.52
1:A:432:LYS:HD3	1:A:464:ILE:HD12	1.91	0.52
1:A:335:THR:OG1	1:A:346:ARG:NH1	2.42	0.52
1:A:148:SER:HA	1:A:151:TRP:HD1	1.75	0.52
2:B:173:VAL:HG22	2:B:204:ILE:HB	1.92	0.52
1:C:489:ARG:HA	1:C:495:LYS:O	2.09	0.52
1:A:520:ASN:HD21	1:A:688:SER:HB2	1.75	0.52
2:B:117:SER:HB2	2:B:143:THR:H	1.73	0.52
1:C:520:ASN:HD21	1:C:688:SER:HB2	1.75	0.52
2:D:173:VAL:HG22	2:D:204:ILE:HB	1.92	0.52
1:A:121:LEU:O	1:A:140:THR:OG1	2.28	0.52
1:A:410:TYR:O	1:A:455:CYS:HA	2.10	0.52
2:B:277:ILE:HG12	2:B:365:VAL:HG22	1.91	0.52
1:C:148:SER:HA	1:C:151:TRP:HD1	1.75	0.52
1:C:335:THR:OG1	1:C:346:ARG:NH1	2.42	0.52
1:C:302:THR:HG21	1:C:316:LYS:HB2	1.91	0.51
2:D:432:ASN:HB2	2:D:457:LYS:HE2	1.91	0.51
1:A:302:THR:HG21	1:A:316:LYS:HB2	1.91	0.51
1:C:488:GLU:HB2	1:C:499:ASN:HD21	1.75	0.51
1:A:308:CYS:HB2	2:B:80:LYS:HG3	1.93	0.51
1:C:308:CYS:HB2	2:D:80:LYS:HG3	1.92	0.51
1:C:410:TYR:O	1:C:455:CYS:HA	2.10	0.51
2:D:277:ILE:HG12	2:D:365:VAL:HG22	1.91	0.51
1:C:559:GLN:NE2	2:D:814:ILE:O	2.43	0.51
1:A:817:PHE:CG	2:D:561:MET:HE2	2.45	0.51
2:B:256:ILE:HG12	2:B:277:ILE:HD12	1.93	0.51
2:B:302:ALA:HB1	2:B:334:LEU:HD22	1.93	0.51
2:D:768:GLY:H	2:D:772:LYS:HZ2	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:GLY:HA2	2:B:128:HIS:H	1.76	0.51
2:B:694:ILE:O	2:B:698:TYR:N	2.37	0.51
2:D:298:ILE:HG12	2:D:341:VAL:HG11	1.93	0.51
1:C:277:GLU:HA	1:C:280:HIS:HD2	1.76	0.51
1:C:432:LYS:HD3	1:C:464:ILE:HD12	1.91	0.51
1:C:398:LEU:HB3	1:C:512:MET:HG3	1.93	0.51
1:C:484:PHE:O	1:C:501:MET:N	2.41	0.51
1:C:536:GLN:HB2	1:C:758:PHE:HE2	1.75	0.51
2:B:791:LEU:HD23	2:B:794:LEU:HD12	1.93	0.51
1:A:536:GLN:HB2	1:A:758:PHE:HE2	1.75	0.51
1:C:541:LEU:O	1:C:728:ALA:HA	2.10	0.51
1:C:483:LYS:HD3	1:C:686:GLN:HB2	1.92	0.51
2:D:82:LEU:O	2:D:86:VAL:HB	2.11	0.51
1:A:487:GLN:HA	1:A:497:GLU:O	2.11	0.50
1:A:541:LEU:O	1:A:728:ALA:HA	2.10	0.50
1:A:615:LEU:HD22	2:D:633:VAL:HA	1.92	0.50
2:D:101:GLY:HA2	2:D:128:HIS:H	1.76	0.50
2:D:256:ILE:HG12	2:D:277:ILE:HD12	1.93	0.50
1:A:559:GLN:NE2	2:B:814:ILE:O	2.44	0.50
1:A:777:LEU:HB3	2:D:516:GLU:CB	2.37	0.50
2:B:533:ILE:CD1	2:B:757:ALA:HB3	2.41	0.50
1:C:121:LEU:O	1:C:140:THR:OG1	2.28	0.50
1:C:777:LEU:HB3	2:B:516:GLU:CB	2.36	0.50
1:C:310:GLY:N	2:D:78:ASP:OD2	2.44	0.50
2:D:153:GLN:NE2	2:D:356:GLN:O	2.36	0.50
2:D:720:LEU:HB3	2:D:747:LEU:HD22	1.93	0.50
1:A:540:ILE:HG12	1:A:730:ILE:HG12	1.92	0.50
1:C:540:ILE:HG12	1:C:730:ILE:HG12	1.92	0.50
2:D:668:LYS:HD3	2:D:672:ARG:HD2	1.94	0.50
1:A:91:LEU:HB3	1:A:121:LEU:HD21	1.94	0.50
1:A:151:TRP:O	1:A:154:MET:HB2	2.11	0.50
1:C:91:LEU:HB3	1:C:121:LEU:HD21	1.94	0.50
1:C:151:TRP:O	1:C:154:MET:HB2	2.11	0.50
2:B:413:GLU:OE1	2:B:511:SER:N	2.43	0.50
2:D:533:ILE:CD1	2:D:757:ALA:HB3	2.41	0.50
1:A:277:GLU:HA	1:A:280:HIS:HD2	1.76	0.50
2:B:82:LEU:O	2:B:86:VAL:HB	2.11	0.50
1:C:487:GLN:HA	1:C:497:GLU:O	2.11	0.50
1:A:820:VAL:HG13	2:D:634:TRP:HE1	1.77	0.50
1:A:483:LYS:HD3	1:A:686:GLN:HB2	1.92	0.50
2:B:334:LEU:HB3	2:B:338:MET:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:720:LEU:HB3	2:B:747:LEU:HD22	1.93	0.50
2:D:302:ALA:HB1	2:D:334:LEU:HD22	1.93	0.50
2:D:769:SER:HB2	2:D:771:TRP:HD1	1.77	0.50
2:D:827:ALA:O	2:D:830:LEU:HB2	2.11	0.50
1:C:570:VAL:HG22	1:C:614:LEU:HD13	1.94	0.49
1:A:310:GLY:N	2:B:78:ASP:OD2	2.44	0.49
2:B:668:LYS:HD3	2:B:672:ARG:HD2	1.94	0.49
2:B:769:SER:HB2	2:B:771:TRP:HD1	1.77	0.49
1:C:438:GLY:HA3	1:C:478:LEU:HB2	1.95	0.49
2:B:298:ILE:HG12	2:B:341:VAL:HG11	1.93	0.49
1:C:543:LYS:HG2	1:C:721:VAL:HG13	1.95	0.49
1:C:46:VAL:HG13	1:C:60:LEU:HD13	1.94	0.49
1:A:398:LEU:HB3	1:A:512:MET:HG3	1.93	0.49
2:D:791:LEU:HD23	2:D:794:LEU:HD12	1.93	0.49
1:A:570:VAL:HG22	1:A:614:LEU:HD13	1.94	0.49
2:B:281:TYR:HE1	2:B:360:ARG:H	1.60	0.49
2:B:827:ALA:O	2:B:830:LEU:HB2	2.12	0.49
1:C:170:ASP:HB2	1:C:173:GLY:H	1.78	0.49
1:C:307:GLY:O	1:C:311:ASN:ND2	2.37	0.49
1:A:519:ILE:CG2	2:D:780:LEU:HD21	2.41	0.49
1:A:193:LYS:HE3	1:A:214:LEU:HD21	1.95	0.49
1:A:234:ALA:HA	1:A:237:MET:CG	2.43	0.49
1:A:715:ALA:HA	1:A:718:ILE:HD12	1.95	0.49
1:C:162:HIS:ND1	1:C:192:GLU:OE2	2.46	0.49
1:A:364:VAL:HA	1:A:375:ASN:HB2	1.94	0.49
2:B:408:ILE:HD12	2:B:475:TYR:HB3	1.95	0.49
2:D:513:THR:OG1	2:D:518:ARG:NH1	2.46	0.49
1:A:648:THR:HG22	2:D:643:ALA:HB1	1.94	0.49
1:A:162:HIS:ND1	1:A:192:GLU:OE2	2.46	0.48
1:A:341:ASN:HD22	1:A:345:ASP:HB2	1.78	0.48
1:C:839:ARG:NH2	2:B:582:PRO:HD2	2.28	0.48
2:D:35:ASN:O	2:D:97:GLY:N	2.46	0.48
1:A:461:ASP:OD2	1:A:792:TRP:NE1	2.40	0.48
1:A:46:VAL:HG13	1:A:60:LEU:HD13	1.94	0.48
2:B:127:ILE:HA	2:B:147:PHE:HB2	1.95	0.48
1:C:193:LYS:HE3	1:C:214:LEU:HD21	1.94	0.48
2:B:35:ASN:O	2:B:97:GLY:N	2.46	0.48
1:C:146:HIS:NE2	1:C:345:ASP:OD2	2.43	0.48
2:D:276:LEU:HB2	2:D:366:LEU:HD12	1.94	0.48
2:D:334:LEU:HB3	2:D:338:MET:HG2	1.94	0.48
2:D:41:GLY:H	2:D:102:ASP:HA	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:367:ASN:ND2	2:B:373:GLU:OE1	2.46	0.48
2:B:411:LEU:HD21	2:B:484:LYS:HA	1.95	0.48
2:B:741:ARG:NH2	2:B:795:TRP:O	2.41	0.48
1:C:521:ASN:H	1:C:695:ARG:HH12	1.62	0.48
2:D:281:TYR:HE1	2:D:360:ARG:H	1.60	0.48
2:D:408:ILE:HD12	2:D:475:TYR:HB3	1.95	0.48
2:D:741:ARG:NH2	2:D:795:TRP:O	2.41	0.48
1:A:229:ALA:O	1:A:233:ARG:HG3	2.12	0.48
1:A:543:LYS:HG2	1:A:721:VAL:HG13	1.95	0.48
2:B:276:LEU:HB2	2:B:366:LEU:HD12	1.94	0.48
1:C:229:ALA:O	1:C:233:ARG:HG3	2.13	0.48
1:C:292:VAL:HA	1:C:295:LEU:HD12	1.96	0.48
1:C:317:THR:HG22	1:C:320:LEU:HD12	1.95	0.48
1:C:461:ASP:OD2	1:C:792:TRP:NE1	2.40	0.48
1:C:720:ALA:O	1:C:725:LYS:N	2.46	0.48
2:D:367:ASN:ND2	2:D:373:GLU:OE1	2.46	0.48
2:D:413:GLU:OE1	2:D:511:SER:N	2.43	0.48
1:A:438:GLY:HA3	1:A:478:LEU:HB2	1.95	0.48
1:A:32:VAL:HB	1:A:92:VAL:HA	1.96	0.48
1:C:396:THR:HB	1:C:472:PHE:HA	1.96	0.48
1:C:715:ALA:HA	1:C:718:ILE:HD12	1.95	0.48
2:D:534:SER:OG	2:D:732:ALA:HB2	1.76	0.48
1:A:292:VAL:HA	1:A:295:LEU:HD12	1.96	0.48
1:A:317:THR:HG22	1:A:320:LEU:HD12	1.95	0.48
2:B:174:THR:HG22	2:B:230:TYR:HB2	1.95	0.48
2:B:513:THR:OG1	2:B:518:ARG:NH1	2.46	0.48
1:C:234:ALA:HA	1:C:237:MET:CG	2.43	0.48
1:C:352:SER:HA	1:C:365:GLY:O	2.13	0.48
2:B:41:GLY:H	2:B:102:ASP:HA	1.79	0.48
1:C:364:VAL:HA	1:C:375:ASN:HB2	1.94	0.48
2:D:681:ARG:HB3	2:D:725:LEU:HD23	1.95	0.48
2:D:536:MET:HA	2:D:749:THR:HG22	1.96	0.48
1:A:145:SER:O	1:A:148:SER:OG	2.22	0.48
1:A:146:HIS:NE2	1:A:345:ASP:OD2	2.43	0.48
2:D:127:ILE:HA	2:D:147:PHE:HB2	1.95	0.48
1:A:396:THR:HB	1:A:472:PHE:HA	1.96	0.47
1:A:720:ALA:O	1:A:725:LYS:N	2.46	0.47
2:B:777:LEU:HD23	2:B:780:LEU:HD12	1.96	0.47
2:D:174:THR:HG22	2:D:230:TYR:HB2	1.96	0.47
2:D:78:ASP:O	2:D:81:SER:OG	2.28	0.47
2:B:536:MET:HA	2:B:749:THR:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:VAL:HB	1:C:92:VAL:HA	1.96	0.47
1:A:352:SER:HA	1:A:365:GLY:O	2.13	0.47
2:D:694:ILE:HA	2:D:697:ASN:HB2	1.96	0.47
1:A:617:SER:HB3	2:D:632:SER:CB	2.45	0.47
2:B:636:PHE:CE2	2:B:640:ILE:HD11	2.49	0.47
2:B:536:MET:N	2:B:728:PHE:O	2.47	0.47
2:B:536:MET:HA	2:B:749:THR:HG22	1.96	0.47
2:D:534:SER:OG	2:D:732:ALA:HB3	2.02	0.47
2:D:636:PHE:CE2	2:D:640:ILE:HD11	2.50	0.47
1:A:521:ASN:H	1:A:695:ARG:HH12	1.62	0.47
1:C:558:PHE:HA	2:D:814:ILE:HG13	1.96	0.47
1:A:611:TRP:CB	2:D:629:ILE:HG21	2.22	0.47
1:C:234:ALA:CA	1:C:237:MET:HB2	2.45	0.47
1:C:809:THR:HG22	2:B:557:SER:C	2.34	0.47
2:D:411:LEU:HD21	2:D:484:LYS:HA	1.95	0.47
1:A:234:ALA:CA	1:A:237:MET:HB2	2.45	0.47
2:D:777:LEU:HD23	2:D:780:LEU:HD12	1.96	0.47
1:A:170:ASP:HB2	1:A:173:GLY:H	1.78	0.47
1:A:626:SER:OG	1:A:627:PHE:N	2.48	0.47
1:A:705:HIS:HA	1:A:709:HIS:HD2	1.79	0.47
2:B:36:ILE:HG12	2:B:97:GLY:HA3	1.96	0.47
1:C:341:ASN:HD22	1:C:345:ASP:HB2	1.78	0.47
1:C:626:SER:OG	1:C:627:PHE:N	2.48	0.47
2:D:536:MET:CA	2:D:749:THR:HG22	2.45	0.47
2:B:437:ARG:HD3	2:B:451:ASN:HB3	1.97	0.47
1:C:317:THR:O	1:C:321:PHE:N	2.41	0.47
2:D:35:ASN:HB3	2:D:95:ILE:HG23	1.97	0.47
1:A:513:ILE:HB	1:A:761:GLY:HA3	1.96	0.47
2:B:116:ILE:O	2:B:120:THR:OG1	2.24	0.47
2:B:161:ILE:HA	2:B:386:ARG:HH22	1.79	0.47
2:B:740:GLY:HA2	2:B:800:CYS:H	1.80	0.47
1:C:648:THR:HG22	2:B:643:ALA:HB1	1.96	0.47
1:A:485:GLY:HA2	1:A:686:GLN:HB3	1.96	0.47
2:B:681:ARG:HB3	2:B:725:LEU:HD23	1.95	0.47
2:D:536:MET:HA	2:D:749:THR:CG2	2.44	0.47
2:D:685:VAL:H	2:D:730:TYR:HE1	1.63	0.47
1:C:617:SER:HB3	2:B:632:SER:CB	2.44	0.46
1:C:513:ILE:HB	1:C:761:GLY:HA3	1.96	0.46
2:D:36:ILE:HG12	2:D:97:GLY:HA3	1.96	0.46
2:D:532:GLY:HA3	2:D:755:ILE:HG21	1.97	0.46
2:D:536:MET:N	2:D:728:PHE:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:536:MET:C	2:D:749:THR:HA	2.36	0.46
2:D:740:GLY:HA2	2:D:800:CYS:H	1.80	0.46
1:A:162:HIS:HB3	1:A:216:ALA:HB2	1.97	0.46
1:A:317:THR:O	1:A:321:PHE:N	2.41	0.46
2:B:104:THR:OG1	2:B:130:GLY:N	2.44	0.46
1:C:485:GLY:HA2	1:C:686:GLN:HB3	1.96	0.46
2:D:298:ILE:HG23	2:D:341:VAL:HG21	1.97	0.46
2:D:437:ARG:HD3	2:D:451:ASN:HB3	1.97	0.46
2:B:298:ILE:HG23	2:B:341:VAL:HG21	1.97	0.46
2:B:685:VAL:H	2:B:730:TYR:HE1	1.63	0.46
1:C:705:HIS:HA	1:C:709:HIS:HD2	1.79	0.46
2:B:536:MET:CA	2:B:749:THR:HG22	2.45	0.46
2:B:645:TYR:HA	2:B:648:ASN:HB2	1.97	0.46
2:D:672:ARG:HB3	2:D:675:ASP:HB2	1.97	0.46
2:B:694:ILE:HA	2:B:697:ASN:HB2	1.96	0.46
1:A:615:LEU:HD13	2:D:633:VAL:CA	2.45	0.46
1:A:773:SER:HA	1:A:776[A]:ILE:HD12	1.98	0.46
2:B:35:ASN:HB3	2:B:95:ILE:HG23	1.97	0.46
1:C:648:THR:HG22	2:B:643:ALA:HB2	1.97	0.46
1:C:34:SER:HB3	1:C:67:HIS:HD2	1.81	0.46
1:C:773:SER:HA	1:C:776[A]:ILE:HD12	1.98	0.46
1:A:558:PHE:HA	2:B:814:ILE:HG13	1.96	0.46
1:A:76:LEU:O	1:A:80:GLU:HB2	2.16	0.46
1:C:401:VAL:HG22	1:C:477:HIS:HB2	1.98	0.46
1:C:76:LEU:O	1:C:80:GLU:HB2	2.16	0.46
2:D:533:ILE:HG23	2:D:729:ILE:HG23	1.92	0.46
1:A:172:GLU:OE1	1:A:252:ARG:NH1	2.43	0.46
1:A:439:PRO:HG3	1:A:480:ALA:HA	1.98	0.46
1:C:534:LYS:O	1:C:757:GLY:HA2	2.16	0.46
1:C:636:TRP:HA	1:C:639:PHE:HD2	1.81	0.45
1:A:534:LYS:O	1:A:757:GLY:HA2	2.16	0.45
1:A:34:SER:HB3	1:A:67:HIS:HD2	1.81	0.45
2:B:94:ARG:HB3	2:B:316:ALA:HB3	1.99	0.45
2:B:532:GLY:HA3	2:B:755:ILE:HG21	1.97	0.45
1:C:162:HIS:HB3	1:C:216:ALA:HB2	1.97	0.45
2:D:161:ILE:HA	2:D:386:ARG:HH22	1.80	0.45
2:D:536:MET:O	2:D:727:ALA:C	2.53	0.45
2:B:537:VAL:HG23	2:B:748:VAL:HB	1.99	0.45
2:D:537:VAL:HG23	2:D:748:VAL:HB	1.98	0.45
1:A:839:ARG:NH2	2:D:582:PRO:HD2	2.32	0.45
2:D:645:TYR:HA	2:D:648:ASN:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:VAL:HG12	1:A:481:ASP:H	1.82	0.45
1:A:494:ASN:HB3	2:B:193:ASN:HB3	1.99	0.45
1:A:68:LYS:HD2	1:A:74:MET:HA	1.99	0.45
2:B:672:ARG:HB3	2:B:675:ASP:HB2	1.97	0.45
2:B:536:MET:C	2:B:749:THR:HA	2.36	0.45
1:A:636:TRP:HA	1:A:639:PHE:HD2	1.81	0.45
2:B:536:MET:O	2:B:727:ALA:C	2.53	0.45
2:D:411:LEU:HD23	2:D:480:VAL:HB	1.99	0.45
2:D:538:SER:CA	2:D:748:VAL:H	2.30	0.45
2:B:176:ILE:HD12	2:B:207:ASP:HA	1.99	0.45
1:C:789:ASP:HA	1:C:793:VAL:HB	1.98	0.45
1:A:220:ILE:HA	1:A:248:LEU:HB2	1.99	0.45
2:D:738:LYS:HA	2:D:741:ARG:HB2	1.98	0.45
1:A:341:ASN:N	1:A:345:ASP:O	2.42	0.44
2:B:437:ARG:HB3	2:B:451:ASN:HB3	2.00	0.44
1:C:234:ALA:O	1:C:238:LEU:N	2.50	0.44
2:D:113:LEU:HD13	2:D:124:ILE:HG21	2.00	0.44
1:A:519:ILE:HG22	2:D:780:LEU:CD2	2.48	0.44
2:B:536:MET:CB	2:B:735:LEU:HD22	2.44	0.44
2:D:94:ARG:HB3	2:D:316:ALA:HB3	1.99	0.44
1:A:401:VAL:HG22	1:A:477:HIS:HB2	1.98	0.44
2:D:226:VAL:HG22	2:D:254:PHE:HB2	2.00	0.44
1:A:234:ALA:O	1:A:238:LEU:N	2.50	0.44
1:A:484:PHE:O	1:A:501:MET:N	2.41	0.44
1:A:789:ASP:HA	1:A:793:VAL:HB	1.98	0.44
2:D:40:LEU:HB2	2:D:73:LEU:HD23	2.00	0.44
2:B:411:LEU:HD23	2:B:480:VAL:HB	1.99	0.44
1:C:220:ILE:HA	1:C:248:LEU:HB2	1.99	0.44
1:A:287:VAL:HG21	1:A:338:VAL:HG11	2.00	0.44
1:C:839:ARG:NH1	2:B:582:PRO:HG3	2.24	0.44
2:B:735:LEU:O	2:B:739:ALA:CB	2.65	0.44
2:B:40:LEU:HB2	2:B:73:LEU:HD23	2.00	0.44
1:C:287:VAL:HG21	1:C:338:VAL:HG11	2.00	0.44
1:C:439:PRO:HG3	1:C:480:ALA:HA	1.99	0.44
1:C:68:LYS:HD2	1:C:74:MET:HA	1.99	0.44
2:D:694:ILE:O	2:D:698:TYR:N	2.37	0.44
2:B:533:ILE:HD11	2:B:693:ASN:HD22	1.83	0.44
1:C:519:ILE:CG2	2:B:780:LEU:HD21	2.47	0.44
2:D:437:ARG:HB3	2:D:451:ASN:HB3	2.00	0.44
1:A:307:GLY:O	1:A:311:ASN:ND2	2.37	0.44
1:A:160:TRP:HZ3	1:A:391:GLY:H	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:535:VAL:H	2:B:750:ILE:HB	1.22	0.44
1:C:479:VAL:HG12	1:C:481:ASP:H	1.82	0.44
1:A:608:TRP:CA	2:D:629:ILE:CD1	2.55	0.43
2:B:226:VAL:HG22	2:B:254:PHE:HB2	2.00	0.43
2:B:153:GLN:NE2	2:B:356:GLN:O	2.36	0.43
2:B:439:PHE:HB3	2:B:449:GLY:HA3	2.00	0.43
2:D:176:ILE:HD12	2:D:207:ASP:HA	1.99	0.43
1:A:168:SER:HA	1:A:197:PHE:HB2	2.00	0.43
1:A:396:THR:HA	1:A:472:PHE:HD1	1.83	0.43
2:B:738:LYS:HA	2:B:741:ARG:HB2	1.98	0.43
1:C:494:ASN:HB3	2:D:193:ASN:HB3	2.00	0.43
1:C:528:GLU:OE1	1:C:769:LYS:NZ	2.51	0.43
2:B:533:ILE:CG1	2:B:757:ALA:HB3	2.49	0.43
1:C:225:GLU:OE2	1:C:255:SER:OG	2.36	0.43
1:C:240:MET:HE1	1:C:245:TYR:CE1	2.41	0.43
1:A:522:GLU:H	1:A:695:ARG:NH2	2.16	0.43
2:B:408:ILE:HG12	2:B:507:MET:HB2	2.01	0.43
2:B:538:SER:CA	2:B:748:VAL:H	2.30	0.43
1:C:168:SER:HA	1:C:197:PHE:HB2	2.00	0.43
2:D:384:SER:HB2	2:D:386:ARG:HE	1.84	0.43
2:D:533:ILE:HD11	2:D:693:ASN:HD22	1.83	0.43
1:A:648:THR:HG22	2:D:643:ALA:HB2	2.01	0.43
1:C:824:ILE:CG2	2:B:572:ILE:HD11	2.47	0.43
2:D:143:THR:HA	2:D:335:HIS:CE1	2.53	0.43
2:B:113:LEU:HD13	2:B:124:ILE:HG21	2.00	0.43
1:C:265:GLY:N	1:C:356:LEU:O	2.36	0.43
1:A:768:TRP:HZ3	1:A:771:ASN:HD22	1.66	0.43
2:B:181:ARG:HA	2:B:184:ILE:HD12	2.01	0.43
1:A:153:GLU:HA	1:A:156:ARG:HE	1.84	0.43
1:A:528:GLU:OE1	1:A:769:LYS:NZ	2.51	0.43
1:C:221:LEU:HD11	1:C:247:TRP:HE3	1.84	0.43
1:C:779:SER:HA	1:C:784:PHE:HD2	1.84	0.43
2:D:408:ILE:HG12	2:D:507:MET:HB2	2.01	0.43
1:A:225:GLU:OE2	1:A:255:SER:OG	2.36	0.43
2:B:487:LYS:HD2	2:B:494:ASN:HD22	1.84	0.43
1:C:153:GLU:HA	1:C:156:ARG:HE	1.84	0.43
1:C:339:GLU:O	1:C:347:LYS:N	2.40	0.43
1:C:368:ASN:HD22	1:C:371:HIS:CD2	2.37	0.43
1:C:505:LEU:O	1:C:763:ARG:NH2	2.52	0.43
1:C:541:LEU:HD22	1:C:746:LEU:HD22	2.01	0.43
1:C:522:GLU:H	1:C:695:ARG:NH2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:181:ARG:HA	2:D:184:ILE:HD12	2.01	0.43
1:A:205:THR:HA	1:A:208:LEU:HD12	2.01	0.42
1:A:241:THR:C	1:A:245:TYR:CD2	2.92	0.42
2:B:134:ILE:HG21	2:B:355:TYR:HE1	1.83	0.42
1:C:172:GLU:OE1	1:C:252:ARG:NH1	2.43	0.42
1:A:204:VAL:HG12	1:A:208:LEU:HG	2.01	0.42
1:C:153:GLU:O	1:C:156:ARG:HG2	2.19	0.42
1:C:396:THR:HA	1:C:472:PHE:HD1	1.83	0.42
2:D:134:ILE:HG21	2:D:355:TYR:HE1	1.83	0.42
2:D:63:LEU:HD23	2:D:63:LEU:HA	1.87	0.42
2:D:533:ILE:HG13	2:D:757:ALA:HB3	2.02	0.42
1:A:541:LEU:HD22	1:A:746:LEU:HD22	2.01	0.42
2:B:384:SER:HB2	2:B:386:ARG:HE	1.84	0.42
1:A:308:CYS:O	2:B:78:ASP:HB3	2.19	0.42
1:C:160:TRP:HZ3	1:C:391:GLY:H	1.66	0.42
2:D:439:PHE:HB3	2:D:449:GLY:HA3	2.00	0.42
1:A:265:GLY:N	1:A:356:LEU:O	2.36	0.42
1:A:153:GLU:O	1:A:156:ARG:HG2	2.19	0.42
2:D:533:ILE:CG1	2:D:757:ALA:HB3	2.49	0.42
2:D:537:VAL:CG1	2:D:727:ALA:HB1	2.09	0.42
1:A:543:LYS:HE3	1:A:727:HIS:HA	2.02	0.42
2:B:143:THR:HA	2:B:335:HIS:CE1	2.54	0.42
1:C:407:PRO:HG2	1:C:458:PHE:HE2	1.84	0.42
1:C:768:TRP:HZ3	1:C:771:ASN:HD22	1.66	0.42
1:A:824:ILE:CG1	2:D:634:TRP:HZ2	2.32	0.42
1:A:433:LYS:HE2	1:A:456:TYR:HE1	1.85	0.42
1:A:505:LEU:O	1:A:763:ARG:NH2	2.52	0.42
2:D:433:THR:HB	2:D:456:CYS:H	1.84	0.42
1:A:355:ASN:H	1:A:362:VAL:H	1.68	0.42
2:B:433:THR:HB	2:B:456:CYS:H	1.84	0.42
1:C:318:GLY:HA2	1:C:321:PHE:HD2	1.85	0.42
1:C:543:LYS:HE3	1:C:727:HIS:HA	2.02	0.42
1:A:400:ILE:HG12	1:A:512:MET:HB2	2.02	0.42
2:B:242:GLU:O	2:B:245:SER:OG	2.30	0.42
2:B:533:ILE:HG13	2:B:757:ALA:HB3	2.01	0.42
1:C:123:THR:OG1	1:C:139:ARG:NE	2.53	0.42
1:C:153:GLU:HA	1:C:156:ARG:NE	2.35	0.42
1:C:308:CYS:O	2:D:78:ASP:HB3	2.20	0.42
1:C:44:GLU:HA	1:C:47:ASN:HD22	1.85	0.42
1:C:615:LEU:HD13	2:B:633:VAL:CA	2.48	0.42
1:A:123:THR:OG1	1:A:139:ARG:NE	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLY:HA2	1:A:321:PHE:HD2	1.85	0.41
1:A:368:ASN:HD22	1:A:371:HIS:CD2	2.37	0.41
1:A:400:ILE:HD12	1:A:474:TYR:HB3	2.01	0.41
2:B:433:THR:HG22	2:B:457:LYS:HG3	2.03	0.41
2:B:630:MET:CB	2:B:634:TRP:CZ3	2.95	0.41
1:C:234:ALA:HA	1:C:237:MET:HG3	2.02	0.41
1:C:355:ASN:H	1:C:362:VAL:H	1.68	0.41
2:D:149:ALA:HB1	2:D:154:GLN:HE21	1.85	0.41
2:D:536:MET:HB2	2:D:749:THR:HG22	1.97	0.41
1:A:212:LYS:CG	1:A:212:LYS:O	2.69	0.41
1:A:234:ALA:HA	1:A:237:MET:HG3	2.02	0.41
1:A:407:PRO:HG2	1:A:458:PHE:HE2	1.84	0.41
1:A:615:LEU:CD1	2:D:632:SER:HG	2.31	0.41
1:C:400:ILE:HD12	1:C:474:TYR:HB3	2.02	0.41
1:C:438:GLY:HA3	1:C:478:LEU:HD12	2.02	0.41
2:D:735:LEU:O	2:D:739:ALA:CB	2.65	0.41
1:A:221:LEU:HD11	1:A:247:TRP:HE3	1.84	0.41
1:A:809:THR:HG22	2:D:557:SER:C	2.40	0.41
2:B:149:ALA:HB1	2:B:154:GLN:HE21	1.85	0.41
1:C:459:CYS:HB3	1:C:514:VAL:HG12	2.02	0.41
1:A:817:PHE:CD2	2:D:561:MET:HE1	2.53	0.41
1:A:153:GLU:HA	1:A:156:ARG:NE	2.35	0.41
1:A:438:GLY:HA3	1:A:478:LEU:HD12	2.02	0.41
1:C:205:THR:HA	1:C:208:LEU:HD12	2.01	0.41
1:C:810:PHE:HE2	2:B:645:TYR:OH	2.03	0.41
2:D:533:ILE:HB	2:D:756:PHE:O	2.20	0.41
1:C:204:VAL:HG12	1:C:208:LEU:HG	2.01	0.41
1:C:433:LYS:HE2	1:C:456:TYR:HE1	1.85	0.41
1:A:816:VAL:CG1	2:D:641:PHE:HZ	2.32	0.41
1:C:688:SER:HA	1:C:691:ILE:HD12	2.02	0.41
2:D:487:LYS:HD2	2:D:494:ASN:HD22	1.84	0.41
1:A:68:LYS:HZ3	1:A:76:LEU:HB2	1.86	0.41
1:C:341:ASN:N	1:C:345:ASP:O	2.42	0.41
1:C:400:ILE:HG12	1:C:512:MET:HB2	2.02	0.41
2:D:256:ILE:HA	2:D:277:ILE:HB	2.02	0.41
2:D:535:VAL:CG2	2:D:729:ILE:HG12	2.24	0.41
1:A:44:GLU:HA	1:A:47:ASN:HD22	1.85	0.41
1:A:459:CYS:HB3	1:A:514:VAL:HG12	2.02	0.41
1:A:688:SER:HA	1:A:691:ILE:HD12	2.02	0.41
1:A:109:TYR:HB3	2:B:112:MET:SD	2.60	0.41
2:B:533:ILE:HB	2:B:756:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:GLY:C	1:C:245:TYR:HD2	2.23	0.41
1:C:537:GLY:H	1:C:752:LEU:HD22	1.86	0.41
2:D:375:VAL:HA	2:D:387:HIS:CD2	2.56	0.41
1:A:839:ARG:NH1	2:D:582:PRO:HG3	2.27	0.41
2:D:536:MET:CB	2:D:735:LEU:HD22	2.44	0.41
1:A:459:CYS:HA	1:A:462:LEU:HD12	2.03	0.41
2:B:536:MET:HB2	2:B:749:THR:HG22	1.97	0.41
1:C:195:LEU:HD13	1:C:207:LEU:HB3	2.03	0.41
2:D:690:THR:HA	2:D:693:ASN:HD22	1.86	0.41
1:A:367:TYR:HE1	1:A:372:VAL:HG22	1.86	0.41
1:A:412:LYS:HB2	1:A:456:TYR:HE2	1.86	0.41
1:A:537:GLY:H	1:A:752:LEU:HD22	1.86	0.41
1:A:779:SER:HA	1:A:784:PHE:HD2	1.84	0.41
2:D:104:THR:OG1	2:D:130:GLY:N	2.44	0.41
2:D:433:THR:HG22	2:D:457:LYS:HG3	2.03	0.41
2:B:281:TYR:CD1	2:B:360:ARG:HB2	2.56	0.41
2:B:375:VAL:HA	2:B:387:HIS:CD2	2.56	0.41
1:C:824:ILE:CG1	2:B:634:TRP:HZ2	2.31	0.41
1:C:109:TYR:HB3	2:D:112:MET:SD	2.61	0.41
2:D:419:VAL:HG21	2:D:479:LEU:HD11	2.03	0.41
1:A:777:LEU:HD13	2:D:519:SER:OG	2.17	0.41
1:C:813:MET:HE3	2:B:641:PHE:CE1	2.57	0.40
1:C:706:MET:O	1:C:710:ASN:ND2	2.47	0.40
1:C:113:PHE:CE2	2:D:112:MET:HE2	2.57	0.40
2:D:180:TYR:HA	2:D:183:PHE:HD2	1.86	0.40
2:D:534:SER:HB2	2:D:732:ALA:HA	1.99	0.40
1:A:72:ILE:HG23	2:B:119:HIS:HB3	2.03	0.40
2:B:690:THR:HA	2:B:693:ASN:HD22	1.86	0.40
1:C:165:LEU:HD23	1:C:220:ILE:HB	2.03	0.40
1:C:234:ALA:HA	1:C:237:MET:CB	2.52	0.40
1:C:824:ILE:HG21	2:B:572:ILE:HD11	2.01	0.40
2:D:830:LEU:HD23	2:D:833:ILE:HD12	2.04	0.40
2:B:256:ILE:HA	2:B:277:ILE:HB	2.02	0.40
2:B:419:VAL:HG21	2:B:479:LEU:HD11	2.03	0.40
1:C:816:VAL:HG11	2:B:641:PHE:CE2	2.56	0.40
2:D:415:PRO:HG3	2:D:741:ARG:HH22	1.86	0.40
2:D:782:PHE:O	2:D:786:GLY:N	2.55	0.40
2:B:534:SER:HB2	2:B:732:ALA:HA	1.99	0.40
1:C:341:ASN:HA	1:C:347:LYS:HE3	2.04	0.40
1:C:412:LYS:HB2	1:C:456:TYR:HE2	1.86	0.40
1:A:165:LEU:HD23	1:A:220:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:433:THR:HG21	2:B:455:CYS:HB3	2.04	0.40
2:B:533:ILE:HG23	2:B:729:ILE:HG23	1.92	0.40
1:C:277:GLU:HA	1:C:280:HIS:CD2	2.56	0.40
2:D:630:MET:HB3	2:D:634:TRP:CH2	2.57	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	776/847 (92%)	702 (90%)	68 (9%)	6 (1%)	21	65
1	C	776/847 (92%)	703 (91%)	67 (9%)	6 (1%)	21	65
2	B	737/841 (88%)	659 (89%)	76 (10%)	2 (0%)	43	81
2	D	737/841 (88%)	659 (89%)	76 (10%)	2 (0%)	43	81
All	All	3026/3376 (90%)	2723 (90%)	287 (10%)	16 (0%)	35	74

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	95	PRO
1	C	98	PRO
1	C	240	MET
1	A	95	PRO
1	A	98	PRO
1	A	240	MET
2	B	329	VAL
2	D	329	VAL
1	C	239	ASN
1	A	239	ASN
2	B	327	PRO

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Mol	Chain	Res	Type
2	D	327	PRO
1	C	73	GLN
1	C	560	SER
1	A	73	GLN
1	A	560	SER

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	661/731 (90%)	661 (100%)	0	100 100
1	C	661/731 (90%)	660 (100%)	1 (0%)	94 96
2	B	609/729 (84%)	609 (100%)	0	100 100
2	D	609/729 (84%)	609 (100%)	0	100 100
All	All	2540/2920 (87%)	2539 (100%)	1 (0%)	100 100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	243	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	47	ASN
1	C	70	ASN
1	C	73	GLN
1	C	280	HIS
1	C	341	ASN
1	C	371	HIS
1	C	499	ASN
1	C	520	ASN
1	C	705	HIS
1	C	709	HIS

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Mol	Chain	Res	Type
1	A	47	ASN
1	A	70	ASN
1	A	73	GLN
1	A	280	HIS
1	A	341	ASN
1	A	371	HIS
1	A	499	ASN
1	A	520	ASN
1	A	705	HIS
1	A	709	HIS
2	B	42	HIS
2	B	96	HIS
2	B	323	GLN
2	B	358	HIS
2	B	367	ASN
2	B	494	ASN
2	B	693	ASN
2	B	766	GLN
2	D	42	HIS
2	D	96	HIS
2	D	323	GLN
2	D	358	HIS
2	D	367	ASN
2	D	494	ASN
2	D	693	ASN
2	D	766	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.