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

Jan 9, 2019 – 11:25 AM EST

PDB ID	:	6IRA
EMDB ID:	:	EMD-9714
Title	:	Structure of the human GluN1/GluN2A NMDA receptor in the glutamate/glycine-bound state at pH 7.8
Authors	:	Zhang, J.; Chang, S.; Zhang, X.; Zhu, S.
Deposited on	:	2018-11-12
Resolution	:	4.50 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.

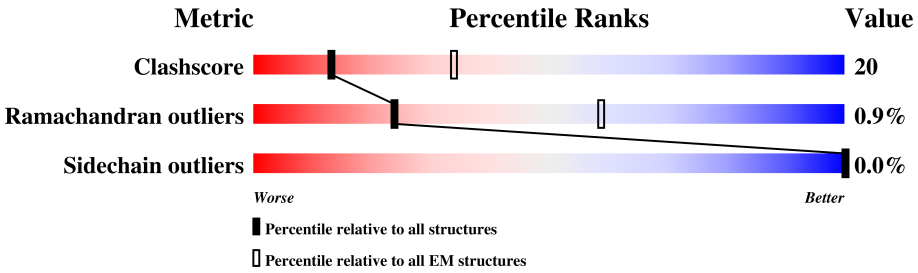
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

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 4.50 Å.

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



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	B	853	63% 25% 12%
1	D	853	63% 25% 12%
2	A	847	66% 26% • 7%
2	C	847	66% 26% • 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23932 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 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	751	Total 5791	C 3744	N 949	O 1062	S 36	1	0
1	B	751	Total 5791	C 3744	N 949	O 1062	S 36	1	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	656	ARG	GLU	engineered mutation	UNP Q12879
D	657	ARG	GLU	engineered mutation	UNP Q12879
D	843	LYS	-	expression tag	UNP Q12879
D	844	SER	-	expression tag	UNP Q12879
D	845	ARG	-	expression tag	UNP Q12879
D	846	ALA	-	expression tag	UNP Q12879
D	847	GLU	-	expression tag	UNP Q12879
D	848	ALA	-	expression tag	UNP Q12879
D	849	LYS	-	expression tag	UNP Q12879
D	850	ARG	-	expression tag	UNP Q12879
D	851	MET	-	expression tag	UNP Q12879
D	852	LYS	-	expression tag	UNP Q12879
D	853	GLY	-	expression tag	UNP Q12879
B	656	ARG	GLU	engineered mutation	UNP Q12879
B	657	ARG	GLU	engineered mutation	UNP Q12879
B	843	LYS	-	expression tag	UNP Q12879
B	844	SER	-	expression tag	UNP Q12879
B	845	ARG	-	expression tag	UNP Q12879
B	846	ALA	-	expression tag	UNP Q12879
B	847	GLU	-	expression tag	UNP Q12879
B	848	ALA	-	expression tag	UNP Q12879
B	849	LYS	-	expression tag	UNP Q12879
B	850	ARG	-	expression tag	UNP Q12879
B	851	MET	-	expression tag	UNP Q12879
B	852	LYS	-	expression tag	UNP Q12879
B	853	GLY	-	expression tag	UNP Q12879

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	789	Total 6175	C 3935	N 1071	O 1134	S 35	1	0
2	C	789	Total 6175	C 3935	N 1071	O 1134	S 35	1	0

There are 2 discrepancies between the modelled and reference sequences:

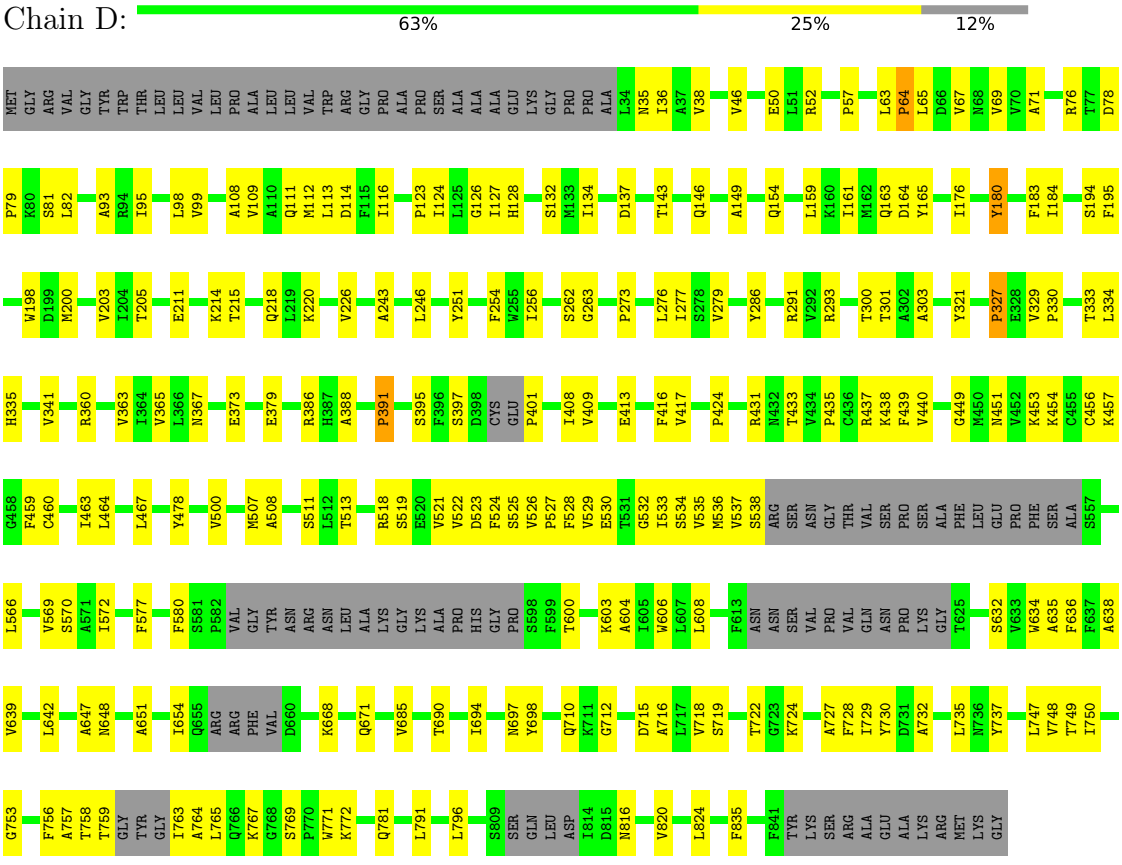
Chain	Residue	Modelled	Actual	Comment	Reference
A	612	ARG	GLY	engineered mutation	UNP Q05586
C	612	ARG	GLY	engineered mutation	UNP Q05586

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.

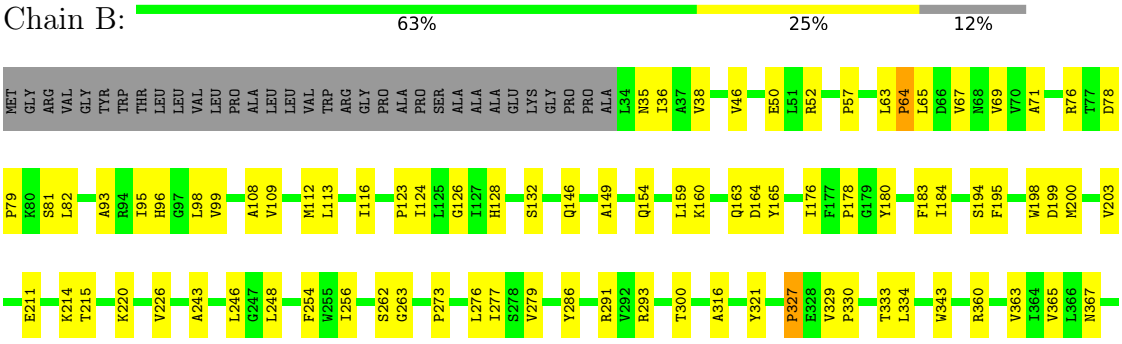
- Molecule 1: Glutamate receptor ionotropic, NMDA 2A

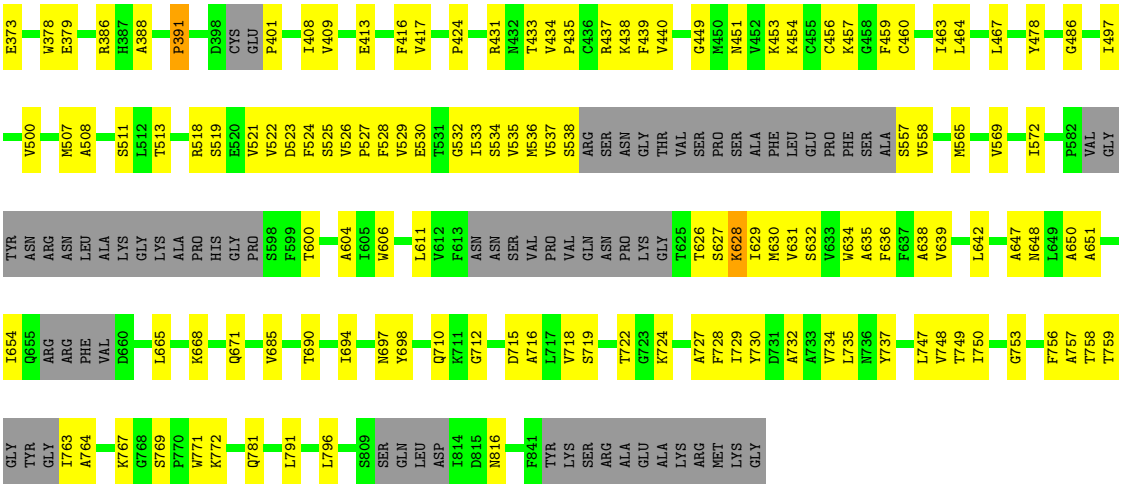
Chain D:



- Molecule 1: Glutamate receptor ionotropic, NMDA 2A

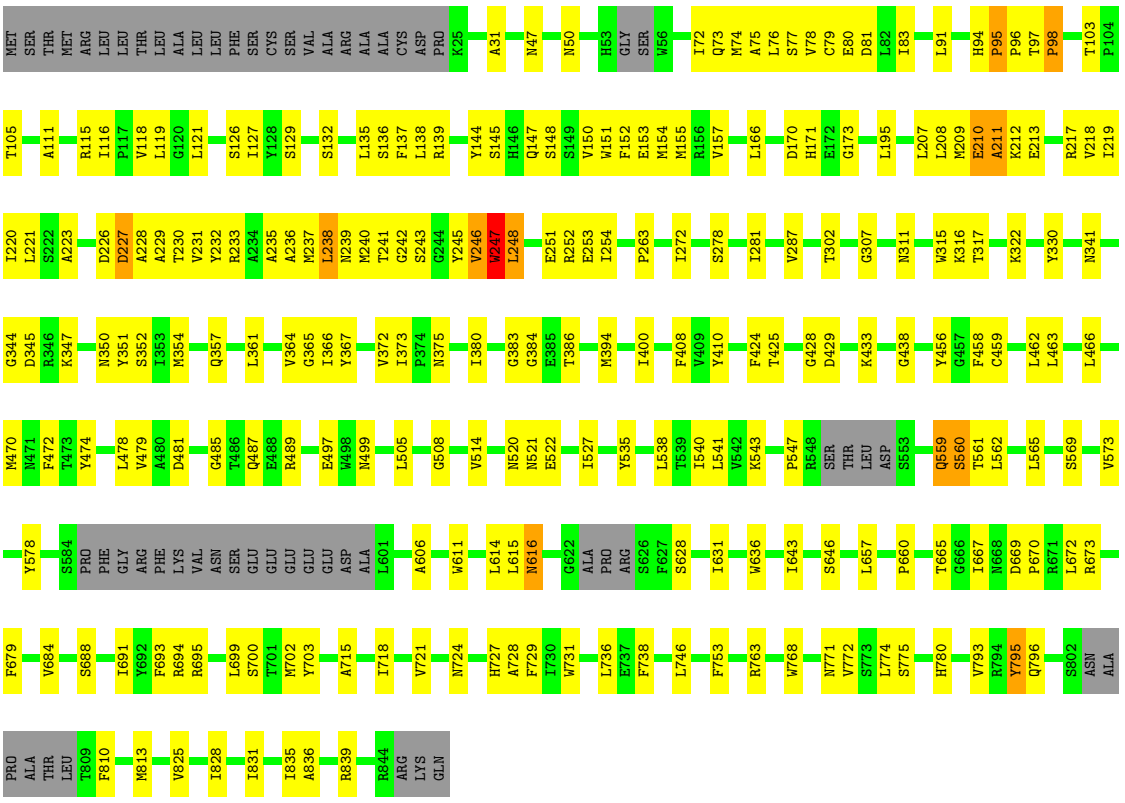
Chain B:





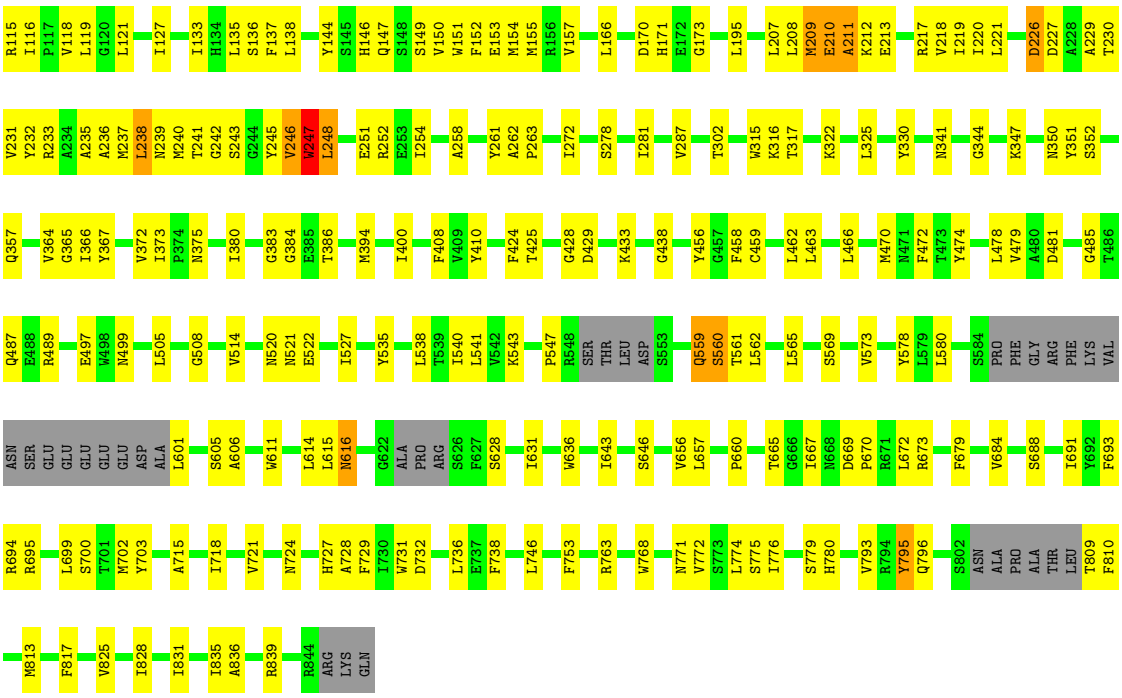
• Molecule 2: Glutamate receptor ionotropic, NMDA 1

Chain A:



• Molecule 2: Glutamate receptor ionotropic, NMDA 1

Chain C:


R115 I116 P117 V118 L119 G120 L121
I127
I133 H134 L135 S136 F137 L138
Y144 S145 H146 Q147 S148 S149 V150 W151 F152 E153 M154 M155 R156 V157
L166
D170 H171 E172 G173
L195
L207 L208 M209 E210 A211 K212 E213
R217 Y218 I219 I220 L221
D226 D227 A228 A229 T230
V231 Y232 R233 A234 A235 A236 M237 L238 N239 M240 T241 G242 S243 G244 Y245 V246 W247 L248
E251 R252 E253 I254
A258
Y261 A262 P263
I272
S278
I281
V287
T302
W315 K316 T317
K322
L325
Y330
M341
G344
K347
N350 Y351 S352
Q357
V364 G365 I366 Y367
V372 I373 P374 N375
I380
G383 G384 E385 T386
M394
I400
F408 V409 Y410
F424 T425
G428 D429
K433
G438
Y456 G457 F458 C459
L462 L463
L466
M470 N471 F472 T473 Y474
L478 V479 A480 D481
G485 T486
Q487 E488 R489
E497 W498 N499
L505
G508
V514
N520 N521 E522
I527
Y535
L538 T539 I540 L541 V542 K543
P547 R548 SER THR LEU ASP S553
Q559 S560 T561 L562
L565
S569
V573
Y578 L579 L580
S584 PRO PHE GLY ARG PHE LYS VAL
ASN SER GLU GLU GLU GLU GLU ASP ALA L601
S605 A606
W611
L614 L615 N616
G622 ALA PRO ARG S626 F627 S628
I631
W636
I643
S646
V656 L657
P660
T665 G666 I667 N668 D669 P670 R671 L672 R673
F679
V684
S688
I691 Y692 F693
R694 R695
L699 S700 T701 M702 Y703
A715
I718
V721
N724
H727 A728 F729 I730 W731 D732
L736 E737 F738
L746
F753
R763
W768
N771 V772 S773 L774 S775 I776
S779 H780
V793 R794 Y795 Q796
S802 ASN ALA PRO ALA THR LEU T809 F810
M813
F817
V825
I828
I831
I835 A836
R839
R844 ARG LYS GLN

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	131990	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 ($e^-/Å^2$)	63	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	B	0.48	0/5921	0.70	11/8037 (0.1%)
1	D	0.48	0/5921	0.70	10/8037 (0.1%)
2	A	0.44	0/6304	0.73	11/8531 (0.1%)
2	C	0.44	0/6304	0.72	11/8531 (0.1%)
All	All	0.46	0/24450	0.71	43/33136 (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	B	0	7
1	D	0	4
2	A	0	3
2	C	0	3
All	All	0	17

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	246	VAL	O-C-N	-15.63	97.69	122.70
2	A	246	VAL	O-C-N	-15.62	97.70	122.70
2	C	246	VAL	CA-C-N	10.81	140.99	117.20
2	A	246	VAL	CA-C-N	10.80	140.97	117.20
2	A	95	PRO	N-CA-CB	7.60	112.42	103.30
2	C	95	PRO	N-CA-CB	7.59	112.40	103.30
1	D	753	GLY	O-C-N	-7.58	110.57	122.70
1	B	753	GLY	O-C-N	-7.55	110.61	122.70
1	B	64	PRO	N-CA-C	-6.59	94.97	112.10
1	D	64	PRO	N-CA-C	-6.58	94.98	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	401	PRO	N-CA-CB	6.45	111.04	103.30
1	D	401	PRO	N-CA-CB	6.42	111.00	103.30
2	C	96	PRO	N-CA-CB	6.24	110.79	103.30
2	A	96	PRO	N-CA-CB	6.23	110.78	103.30
1	B	628	LYS	CA-C-N	-6.21	103.54	117.20
1	D	327	PRO	N-CA-CB	6.20	110.73	103.30
2	C	547	PRO	N-CA-CB	6.17	110.70	103.30
2	A	547	PRO	N-CA-CB	6.14	110.67	103.30
1	B	327	PRO	N-CA-CB	6.13	110.66	103.30
1	B	391	PRO	N-CA-CB	6.09	110.61	103.30
1	D	391	PRO	N-CA-CB	6.06	110.57	103.30
2	A	660	PRO	N-CA-CB	6.03	110.53	103.30
2	C	660	PRO	N-CA-CB	6.02	110.53	103.30
1	D	636	PHE	CB-CA-C	5.83	122.06	110.40
1	B	636	PHE	CB-CA-C	5.81	122.02	110.40
1	B	424	PRO	N-CA-CB	5.80	110.26	103.30
1	D	424	PRO	N-CA-CB	5.80	110.26	103.30
1	D	176	ILE	CG1-CB-CG2	-5.77	98.71	111.40
1	D	57	PRO	N-CA-CB	5.64	110.07	103.30
1	D	330	PRO	N-CA-CB	5.64	110.07	103.30
1	B	57	PRO	N-CA-CB	5.64	110.06	103.30
1	B	176	ILE	CG1-CB-CG2	-5.62	99.03	111.40
1	B	330	PRO	N-CA-CB	5.60	110.02	103.30
2	C	247	TRP	O-C-N	-5.60	113.74	122.70
2	A	247	TRP	O-C-N	-5.57	113.78	122.70
2	A	98	PRO	N-CA-CB	5.56	109.97	103.30
2	A	210	GLU	N-CA-C	-5.56	96.00	111.00
2	C	210	GLU	N-CA-C	-5.55	96.01	111.00
2	C	98	PRO	N-CA-CB	5.53	109.94	103.30
2	A	227	ASP	N-CA-CB	-5.21	101.22	110.60
2	A	559	GLN	N-CA-C	5.08	124.70	111.00
2	C	209	MET	O-C-N	5.03	130.75	122.70
2	C	559	GLN	N-CA-C	5.03	124.58	111.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	247	TRP	Mainchain
2	A	248	LEU	Peptide
2	A	795	TYR	Peptide
1	B	165	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	B	199	ASP	Peptide
1	B	200	MET	Peptide
1	B	333	THR	Peptide
1	B	343	TRP	Peptide
1	B	611	LEU	Peptide
1	B	628	LYS	Mainchain
2	C	247	TRP	Mainchain
2	C	248	LEU	Peptide
2	C	795	TYR	Peptide
1	D	165	TYR	Peptide
1	D	180	TYR	Peptide
1	D	200	MET	Peptide
1	D	333	THR	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	B	5791	0	5617	256	0
1	D	5791	0	5617	253	0
2	A	6175	0	6111	227	0
2	C	6175	0	6110	241	0
All	All	23932	0	23455	932	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 20.

All (932) 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:D:522:VAL:CG1	1:D:765:LEU:O	1.70	1.37
1:B:533:ILE:CG1	1:B:757:ALA:HB3	1.58	1.33
2:A:208:LEU:O	2:A:211:ALA:HB3	1.19	1.33
1:B:63:LEU:HD21	1:B:300:THR:CB	1.58	1.33
2:A:227:ASP:O	2:A:230:THR:HB	1.25	1.32
1:D:63:LEU:HD21	1:D:300:THR:CB	1.57	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:HD11	1:B:300:THR:CG2	1.60	1.31
1:D:533:ILE:CG1	1:D:757:ALA:HB3	1.58	1.30
1:D:63:LEU:HD11	1:D:300:THR:CG2	1.63	1.26
2:A:218:VAL:CA	2:A:246:VAL:HG21	1.64	1.26
2:C:218:VAL:CA	2:C:246:VAL:HG21	1.64	1.25
2:C:208:LEU:O	2:C:211:ALA:HB3	1.19	1.25
2:C:243:SER:HB3	2:C:384:GLY:N	1.51	1.24
2:C:218:VAL:HA	2:C:246:VAL:CG2	1.69	1.22
2:A:243:SER:HB3	2:A:384:GLY:N	1.51	1.22
1:B:63:LEU:CD2	1:B:300:THR:HB	1.68	1.22
1:D:63:LEU:CD2	1:D:300:THR:HB	1.69	1.22
2:A:218:VAL:HA	2:A:246:VAL:CG2	1.69	1.21
1:B:536:MET:O	1:B:727:ALA:HB1	1.08	1.21
2:C:227:ASP:O	2:C:230:THR:HB	1.32	1.21
1:D:536:MET:O	1:D:727:ALA:HB1	1.04	1.19
1:D:63:LEU:CD1	1:D:67:VAL:HG21	1.74	1.18
2:A:217:ARG:O	2:A:246:VAL:HG23	1.44	1.17
1:B:526:VAL:CG1	1:B:527:PRO:HD2	1.74	1.17
1:B:63:LEU:CD1	1:B:67:VAL:HG21	1.74	1.17
1:D:63:LEU:CD1	1:D:300:THR:HG22	1.75	1.17
2:A:207:LEU:O	2:A:210:GLU:HB3	1.45	1.16
1:D:816:ASN:ND2	2:C:559:GLN:HE22	1.45	1.15
1:D:526:VAL:CG1	1:D:527:PRO:HD2	1.75	1.15
2:C:217:ARG:O	2:C:246:VAL:HG23	1.44	1.15
2:A:559:GLN:HE22	1:B:816:ASN:ND2	1.46	1.14
1:D:535:VAL:HG22	1:D:729:ILE:CG1	1.75	1.14
1:D:63:LEU:HD12	1:D:67:VAL:HG21	1.15	1.13
2:A:243:SER:CB	2:A:384:GLY:H	1.61	1.13
2:C:207:LEU:O	2:C:210:GLU:HB3	1.45	1.13
2:C:243:SER:CB	2:C:384:GLY:H	1.62	1.13
1:B:63:LEU:CD1	1:B:300:THR:HG22	1.79	1.12
1:B:535:VAL:HG22	1:B:729:ILE:HG12	1.15	1.12
1:B:536:MET:HA	1:B:749:THR:HA	1.14	1.12
1:B:63:LEU:HD12	1:B:67:VAL:CG2	1.82	1.10
1:D:536:MET:O	1:D:727:ALA:CB	2.00	1.10
1:D:536:MET:HA	1:D:749:THR:HA	1.13	1.10
2:A:246:VAL:O	2:A:247:TRP:CD1	2.05	1.09
2:C:246:VAL:O	2:C:247:TRP:CD1	2.05	1.09
1:D:522:VAL:HG13	1:D:765:LEU:O	1.33	1.09
2:A:223:ALA:HB1	2:A:227:ASP:OD2	1.52	1.09
1:D:63:LEU:HD12	1:D:67:VAL:CG2	1.82	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:ILE:CG2	1:D:729:ILE:CG2	2.30	1.09
1:B:63:LEU:HD12	1:B:67:VAL:HG21	1.15	1.08
1:B:533:ILE:HG12	1:B:757:ALA:HB3	1.10	1.08
1:D:535:VAL:HG22	1:D:729:ILE:HG12	1.08	1.07
2:C:243:SER:CA	2:C:383:GLY:HA3	1.84	1.07
1:B:463:ILE:HD13	1:B:528:PHE:CE2	1.90	1.06
2:A:243:SER:CA	2:A:383:GLY:HA3	1.84	1.06
1:B:536:MET:O	1:B:727:ALA:CB	2.03	1.06
2:A:228:ALA:HB1	2:A:232:TYR:CE2	1.91	1.06
2:A:217:ARG:O	2:A:246:VAL:CG2	2.03	1.06
2:C:217:ARG:O	2:C:246:VAL:CG2	2.03	1.05
2:A:243:SER:HA	2:A:383:GLY:HA3	1.37	1.05
1:D:533:ILE:HG12	1:D:757:ALA:HB3	1.10	1.05
2:C:243:SER:HA	2:C:383:GLY:HA3	1.37	1.04
1:D:526:VAL:HG13	1:D:527:PRO:HD2	1.39	1.04
2:C:229:ALA:O	2:C:233:ARG:N	1.91	1.03
1:D:533:ILE:HG12	1:D:757:ALA:CB	1.90	1.02
1:B:529:VAL:CG1	1:B:530:GLU:H	1.71	1.02
1:D:463:ILE:HD13	1:D:528:PHE:CE2	1.94	1.02
2:C:232:TYR:CE2	2:C:262:ALA:N	2.29	1.01
1:D:529:VAL:CG1	1:D:530:GLU:H	1.71	1.01
1:B:521:VAL:O	1:B:767:LYS:HE3	1.60	1.00
2:C:219:ILE:H	2:C:246:VAL:CG1	1.73	1.00
1:D:536:MET:HA	1:D:749:THR:CA	1.91	1.00
1:D:521:VAL:O	1:D:767:LYS:HE3	1.59	1.00
1:B:533:ILE:HG12	1:B:757:ALA:CB	1.90	1.00
1:B:526:VAL:HG13	1:B:527:PRO:HD2	1.38	0.99
1:B:536:MET:HA	1:B:749:THR:CA	1.92	0.99
2:A:226:ASP:O	2:A:230:THR:OG1	1.79	0.99
2:A:219:ILE:H	2:A:246:VAL:CG1	1.74	0.98
1:B:533:ILE:CG2	1:B:729:ILE:CG2	2.40	0.98
2:A:615:LEU:O	2:A:616:ASN:HB2	1.63	0.98
1:B:529:VAL:CG1	1:B:530:GLU:N	2.26	0.98
2:A:218:VAL:HA	2:A:246:VAL:HG21	1.00	0.98
2:A:208:LEU:O	2:A:211:ALA:CB	2.12	0.97
2:C:218:VAL:HA	2:C:246:VAL:HG21	1.00	0.97
2:C:208:LEU:O	2:C:211:ALA:CB	2.12	0.97
2:C:615:LEU:O	2:C:616:ASN:HB2	1.64	0.97
1:B:533:ILE:N	1:B:756:PHE:O	1.97	0.96
1:B:535:VAL:HG22	1:B:729:ILE:CG1	1.95	0.96
1:D:533:ILE:HD11	1:D:690:THR:HG22	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:ILE:N	1:D:756:PHE:O	1.97	0.96
1:D:522:VAL:HG11	1:D:765:LEU:O	1.64	0.96
2:A:246:VAL:O	2:A:247:TRP:CG	2.20	0.95
1:D:537:VAL:O	1:D:748:VAL:O	1.85	0.94
1:D:535:VAL:CG2	1:D:729:ILE:HG12	1.97	0.94
1:D:529:VAL:HG12	1:D:530:GLU:N	1.80	0.94
1:B:533:ILE:CG1	1:B:757:ALA:CB	2.45	0.94
2:C:227:ASP:O	2:C:231:VAL:HG23	1.66	0.94
1:B:529:VAL:HG12	1:B:530:GLU:N	1.80	0.94
1:B:537:VAL:O	1:B:748:VAL:O	1.85	0.93
2:C:243:SER:HB3	2:C:384:GLY:H	1.09	0.93
2:C:232:TYR:CZ	2:C:262:ALA:N	2.27	0.93
2:C:246:VAL:O	2:C:247:TRP:CG	2.20	0.93
1:D:529:VAL:CG1	1:D:530:GLU:N	2.26	0.93
1:B:463:ILE:HD11	1:B:528:PHE:CZ	2.03	0.93
1:D:816:ASN:HD21	2:C:559:GLN:HE22	1.11	0.92
2:A:228:ALA:O	2:A:232:TYR:N	2.03	0.92
2:A:559:GLN:HE22	1:B:816:ASN:HD21	1.04	0.92
2:C:219:ILE:H	2:C:246:VAL:HG11	1.30	0.91
1:D:533:ILE:CG1	1:D:757:ALA:CB	2.45	0.91
2:A:219:ILE:H	2:A:246:VAL:HG11	1.31	0.91
1:D:529:VAL:HG13	1:D:530:GLU:H	1.35	0.91
1:D:533:ILE:HG22	1:D:729:ILE:CG2	2.00	0.91
2:C:615:LEU:O	2:C:616:ASN:CB	2.17	0.91
1:B:536:MET:CB	1:B:749:THR:HG22	2.01	0.91
1:D:536:MET:CB	1:D:749:THR:HG22	2.01	0.90
2:A:227:ASP:O	2:A:230:THR:CB	2.18	0.90
2:A:228:ALA:HB1	2:A:232:TYR:HE2	1.34	0.90
1:B:529:VAL:HG13	1:B:530:GLU:H	1.34	0.90
2:A:615:LEU:O	2:A:616:ASN:CB	2.16	0.89
1:D:63:LEU:CD1	1:D:67:VAL:CG2	2.47	0.89
2:A:218:VAL:HA	2:A:246:VAL:CB	2.03	0.89
2:C:229:ALA:CA	2:C:232:TYR:HB3	2.03	0.89
1:B:533:ILE:HD11	1:B:690:THR:HG22	1.53	0.89
2:C:219:ILE:N	2:C:246:VAL:HG11	1.87	0.89
2:A:227:ASP:O	2:A:231:VAL:HG23	1.74	0.88
1:B:533:ILE:HB	1:B:756:PHE:O	1.74	0.88
1:B:463:ILE:CD1	1:B:528:PHE:CZ	2.57	0.88
2:A:559:GLN:NE2	1:B:816:ASN:HD21	1.71	0.88
1:D:526:VAL:HG12	1:D:527:PRO:HD2	1.55	0.87
1:D:533:ILE:HB	1:D:756:PHE:O	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:243:SER:HB3	2:A:384:GLY:H	1.09	0.87
1:D:463:ILE:HD11	1:D:528:PHE:CZ	2.09	0.87
1:B:500:VAL:HG11	1:B:522:VAL:HG21	1.54	0.87
2:C:218:VAL:HA	2:C:246:VAL:CB	2.03	0.87
1:D:533:ILE:HG23	1:D:729:ILE:HG22	1.56	0.87
2:A:219:ILE:N	2:A:246:VAL:HG11	1.88	0.87
1:B:526:VAL:HG12	1:B:527:PRO:HD2	1.54	0.86
1:B:63:LEU:CD1	1:B:67:VAL:CG2	2.47	0.86
1:B:64:PRO:CD	1:B:65:LEU:H	1.89	0.86
1:B:534:SER:HB2	1:B:732:ALA:CB	2.05	0.86
1:D:816:ASN:HD21	2:C:559:GLN:NE2	1.71	0.86
2:A:77:SER:O	2:A:81:ASP:HB2	1.77	0.85
2:A:211:ALA:HB1	2:A:240:MET:HE1	1.58	0.85
1:B:535:VAL:HB	1:B:750:ILE:HB	1.57	0.85
1:D:536:MET:CA	1:D:749:THR:HA	2.05	0.85
1:D:536:MET:HB2	1:D:749:THR:HG22	1.57	0.85
1:D:535:VAL:HB	1:D:750:ILE:HD13	1.58	0.85
2:A:466:LEU:O	2:A:470:MET:HB2	1.77	0.85
1:D:535:VAL:HB	1:D:750:ILE:HB	1.57	0.85
1:B:536:MET:HB2	1:B:749:THR:HG22	1.58	0.84
1:B:535:VAL:HB	1:B:750:ILE:HD13	1.59	0.84
2:C:77:SER:O	2:C:81:ASP:HB2	1.77	0.84
1:D:533:ILE:CG2	1:D:729:ILE:HG21	2.07	0.84
2:C:466:LEU:O	2:C:470:MET:HB2	1.77	0.84
1:D:463:ILE:CD1	1:D:528:PHE:CZ	2.61	0.84
1:B:536:MET:CA	1:B:749:THR:HA	2.06	0.84
1:D:534:SER:O	1:D:729:ILE:HA	1.76	0.84
1:D:535:VAL:H	1:D:750:ILE:CG2	1.90	0.83
1:D:533:ILE:CD1	1:D:690:THR:HG22	2.08	0.83
1:B:63:LEU:HD11	1:B:300:THR:HG22	0.85	0.83
1:B:463:ILE:HD13	1:B:528:PHE:HE2	1.41	0.82
1:D:533:ILE:HG23	1:D:729:ILE:CG2	2.05	0.82
1:B:463:ILE:HD11	1:B:528:PHE:HZ	1.39	0.82
1:D:816:ASN:ND2	2:C:559:GLN:NE2	2.25	0.82
2:C:211:ALA:HB1	2:C:240:MET:HE1	1.60	0.81
1:B:535:VAL:H	1:B:750:ILE:CG2	1.92	0.81
1:D:64:PRO:CD	1:D:65:LEU:H	1.89	0.81
1:B:519:SER:HA	1:B:524:PHE:HE2	1.45	0.80
1:B:534:SER:O	1:B:729:ILE:HA	1.82	0.80
1:B:565:MET:HG3	2:C:817:PHE:CE1	2.16	0.80
1:D:109:VAL:O	1:D:112:MET:HB2	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:243:SER:N	2:A:383:GLY:HA3	1.97	0.80
2:A:559:GLN:O	2:A:562:LEU:N	2.15	0.80
1:B:533:ILE:CA	1:B:756:PHE:O	2.30	0.80
1:D:533:ILE:CB	1:D:756:PHE:O	2.31	0.79
1:B:533:ILE:HG13	1:B:757:ALA:HB3	1.63	0.79
1:D:533:ILE:CA	1:D:756:PHE:O	2.30	0.79
1:D:816:ASN:CG	2:C:559:GLN:HE22	1.84	0.79
2:A:235:ALA:O	2:A:238:LEU:N	2.16	0.78
1:B:109:VAL:O	1:B:112:MET:HB2	1.82	0.78
2:C:243:SER:N	2:C:383:GLY:HA3	1.97	0.78
1:D:535:VAL:CA	1:D:750:ILE:HB	2.13	0.78
2:A:218:VAL:HA	2:A:246:VAL:HG11	1.66	0.78
1:B:534:SER:HB2	1:B:732:ALA:HB2	1.64	0.78
2:C:235:ALA:O	2:C:238:LEU:N	2.16	0.78
1:B:463:ILE:CD1	1:B:528:PHE:CE2	2.65	0.78
1:B:533:ILE:CB	1:B:756:PHE:O	2.32	0.78
2:C:559:GLN:O	2:C:562:LEU:N	2.15	0.78
1:D:463:ILE:HD11	1:D:528:PHE:HZ	1.47	0.78
1:D:533:ILE:HG13	1:D:757:ALA:HB3	1.63	0.78
1:B:533:ILE:HG23	1:B:729:ILE:HG22	1.66	0.78
1:B:533:ILE:CD1	1:B:690:THR:HG22	2.14	0.78
1:B:535:VAL:CA	1:B:750:ILE:HB	2.14	0.78
1:D:654:ILE:HG12	2:C:657:LEU:HD11	1.66	0.78
2:A:559:GLN:NE2	1:B:816:ASN:ND2	2.27	0.77
2:C:232:TYR:CE2	2:C:261:TYR:C	2.56	0.77
1:B:532:GLY:HA2	1:B:757:ALA:O	1.84	0.77
1:B:533:ILE:HG22	1:B:729:ILE:CG2	2.14	0.77
1:B:533:ILE:HG23	1:B:729:ILE:CG2	2.15	0.77
1:D:532:GLY:HA2	1:D:757:ALA:O	1.84	0.77
1:B:522:VAL:CG1	1:B:523:ASP:N	2.48	0.77
2:A:195:LEU:HD21	2:A:210:GLU:OE2	1.85	0.77
1:B:64:PRO:CG	1:B:65:LEU:H	1.98	0.77
1:D:536:MET:CG	1:D:749:THR:HG22	2.15	0.77
1:D:535:VAL:HG22	1:D:729:ILE:CD1	2.14	0.76
2:C:195:LEU:HD21	2:C:210:GLU:OE2	1.85	0.76
2:A:559:GLN:HE22	1:B:816:ASN:CG	1.89	0.76
2:C:226:ASP:O	2:C:230:THR:OG1	2.04	0.76
2:C:76:LEU:O	2:C:80:GLU:HB2	1.86	0.76
2:C:218:VAL:HA	2:C:246:VAL:HG11	1.66	0.76
1:D:522:VAL:CG1	1:D:523:ASP:N	2.48	0.76
2:C:410:TYR:HB2	2:C:456:TYR:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:LEU:HD21	1:D:300:THR:HB	0.79	0.76
1:D:522:VAL:HG12	1:D:523:ASP:N	2.01	0.75
1:D:64:PRO:CG	1:D:65:LEU:H	1.98	0.75
1:B:536:MET:CG	1:B:749:THR:HG22	2.15	0.75
2:A:410:TYR:HB2	2:A:456:TYR:HB2	1.68	0.75
2:A:223:ALA:CB	2:A:227:ASP:OD2	2.32	0.75
1:B:63:LEU:CD1	1:B:300:THR:CG2	2.53	0.75
1:B:537:VAL:HG12	1:B:727:ALA:CB	2.16	0.75
1:B:537:VAL:HG12	1:B:727:ALA:HB2	1.69	0.75
1:D:535:VAL:HA	1:D:728:PHE:O	1.86	0.75
2:A:352:SER:HA	2:A:365:GLY:O	1.87	0.75
1:B:521:VAL:C	1:B:767:LYS:HE3	2.07	0.75
1:D:433:THR:HA	1:D:456:CYS:O	1.87	0.74
1:D:500:VAL:HG11	1:D:522:VAL:HG21	1.69	0.74
2:A:76:LEU:O	2:A:80:GLU:HB2	1.86	0.74
1:D:463:ILE:CD1	1:D:528:PHE:CE2	2.70	0.74
2:C:352:SER:HA	2:C:365:GLY:O	1.87	0.74
1:D:63:LEU:HD11	1:D:300:THR:HG22	0.80	0.74
2:A:218:VAL:HA	2:A:246:VAL:CG1	2.17	0.74
2:A:540:ILE:HA	2:A:729:PHE:O	1.88	0.73
1:B:522:VAL:O	1:B:524:PHE:CE2	2.41	0.73
1:B:532:GLY:CA	1:B:757:ALA:O	2.36	0.73
2:C:218:VAL:HA	2:C:246:VAL:CG1	2.17	0.73
1:B:533:ILE:HG22	1:B:729:ILE:HG23	1.70	0.73
1:B:522:VAL:HG12	1:B:523:ASP:N	2.01	0.73
1:D:533:ILE:HG22	1:D:729:ILE:HG23	1.69	0.73
2:A:207:LEU:O	2:A:210:GLU:CB	2.31	0.73
2:C:229:ALA:HA	2:C:232:TYR:HB3	1.69	0.73
1:D:522:VAL:O	1:D:524:PHE:CE2	2.41	0.73
1:D:532:GLY:CA	1:D:757:ALA:O	2.37	0.73
1:D:463:ILE:HD13	1:D:528:PHE:HE2	1.49	0.73
1:B:36:ILE:O	1:B:69:VAL:HA	1.87	0.73
1:B:535:VAL:CB	1:B:750:ILE:HB	2.18	0.73
2:C:227:ASP:C	2:C:230:THR:HB	2.09	0.73
1:D:519:SER:HA	1:D:524:PHE:HE2	1.52	0.73
1:D:535:VAL:CB	1:D:750:ILE:HB	2.17	0.72
1:B:535:VAL:HA	1:B:728:PHE:O	1.88	0.72
1:B:535:VAL:CG2	1:B:729:ILE:HG12	2.09	0.72
2:C:540:ILE:HA	2:C:729:PHE:O	1.88	0.72
2:C:195:LEU:CD2	2:C:210:GLU:OE2	2.39	0.71
2:A:235:ALA:O	2:A:236:ALA:C	2.27	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:534:SER:O	1:D:729:ILE:HG23	1.90	0.71
2:C:235:ALA:O	2:C:236:ALA:C	2.27	0.71
1:D:408:ILE:HG12	1:D:507:MET:HB2	1.71	0.71
1:D:534:SER:HB2	1:D:732:ALA:CB	2.21	0.70
1:D:36:ILE:O	1:D:69:VAL:HA	1.90	0.70
1:D:600:THR:O	1:D:604:ALA:HB3	1.91	0.70
1:D:211:GLU:HB2	1:D:215:THR:HG23	1.71	0.70
2:A:657:LEU:HD11	1:B:654:ILE:HG12	1.74	0.70
2:C:218:VAL:CG2	2:C:246:VAL:HG21	2.21	0.70
2:A:218:VAL:CB	2:A:246:VAL:HG21	2.21	0.70
1:B:433:THR:HA	1:B:456:CYS:O	1.92	0.70
2:C:170:ASP:HB2	2:C:173:GLY:H	1.56	0.70
2:A:195:LEU:CD2	2:A:210:GLU:OE2	2.39	0.70
1:B:435:PRO:HA	1:B:454:LYS:O	1.92	0.70
2:C:218:VAL:CA	2:C:246:VAL:HG11	2.21	0.70
2:C:479:VAL:HG12	2:C:481:ASP:H	1.57	0.70
1:D:220:LYS:HE2	1:B:220:LYS:HE2	1.73	0.70
1:B:408:ILE:HG12	1:B:507:MET:HB2	1.73	0.70
1:D:537:VAL:HG12	1:D:727:ALA:CB	2.21	0.70
2:C:229:ALA:O	2:C:233:ARG:CB	2.39	0.69
1:B:536:MET:HE3	1:B:749:THR:CG2	2.22	0.69
2:A:218:VAL:CA	2:A:246:VAL:HG11	2.21	0.69
2:C:218:VAL:CB	2:C:246:VAL:HG21	2.21	0.69
2:A:211:ALA:CB	2:A:240:MET:HE1	2.21	0.69
2:C:207:LEU:O	2:C:210:GLU:CB	2.31	0.69
2:A:170:ASP:HB2	2:A:173:GLY:H	1.56	0.69
1:B:113:LEU:O	1:B:116:ILE:HB	1.92	0.69
1:D:211:GLU:HB3	1:D:214:LYS:HB2	1.73	0.69
1:B:211:GLU:HB2	1:B:215:THR:HG23	1.73	0.68
1:B:521:VAL:O	1:B:767:LYS:CE	2.39	0.68
2:A:218:VAL:CG2	2:A:246:VAL:HG21	2.21	0.68
2:C:220:ILE:HG12	2:C:248:LEU:HB2	1.75	0.68
1:D:321:TYR:HE1	2:C:73:GLN:HE21	1.42	0.68
2:A:479:VAL:HG12	2:A:481:ASP:H	1.57	0.68
1:B:211:GLU:HB3	1:B:214:LYS:HB2	1.75	0.68
2:A:541:LEU:HD22	2:A:746:LEU:HD22	1.75	0.67
1:D:526:VAL:CG1	1:D:527:PRO:CD	2.66	0.67
1:B:526:VAL:CG1	1:B:527:PRO:CD	2.66	0.67
1:D:64:PRO:CG	1:D:65:LEU:N	2.57	0.67
2:C:541:LEU:HD22	2:C:746:LEU:HD22	1.75	0.67
2:A:220:ILE:HG12	2:A:248:LEU:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:SER:CB	1:B:732:ALA:CB	2.72	0.67
2:A:218:VAL:HG22	2:A:246:VAL:CG2	2.25	0.67
2:C:218:VAL:HG22	2:C:246:VAL:CG2	2.25	0.67
1:D:535:VAL:HB	1:D:750:ILE:CD1	2.25	0.67
1:D:409:VAL:HG22	1:D:478:TYR:HB2	1.77	0.66
1:B:569:VAL:HG11	1:B:631:VAL:HG13	1.78	0.66
2:A:615:LEU:O	2:A:616:ASN:ND2	2.28	0.66
2:A:119:LEU:HA	2:A:138:LEU:O	1.96	0.65
2:A:242:GLY:O	2:A:245:TYR:HD2	1.79	0.65
1:D:438:LYS:O	1:D:451:ASN:HA	1.95	0.65
2:A:219:ILE:H	2:A:246:VAL:HG12	1.61	0.65
1:B:535:VAL:HB	1:B:750:ILE:CD1	2.26	0.65
2:A:232:TYR:OH	2:A:253:GLU:HB3	1.96	0.65
2:C:242:GLY:O	2:C:245:TYR:HD2	1.80	0.65
1:B:409:VAL:HG22	1:B:478:TYR:HB2	1.78	0.65
2:A:208:LEU:CD1	2:A:238:LEU:HD12	2.27	0.65
1:B:534:SER:HB2	1:B:732:ALA:HB1	1.78	0.65
2:C:119:LEU:HA	2:C:138:LEU:O	1.96	0.65
2:C:144:TYR:O	2:C:147:GLN:HB2	1.96	0.65
1:D:113:LEU:O	1:D:116:ILE:HB	1.97	0.65
2:C:229:ALA:C	2:C:232:TYR:HB3	2.16	0.65
2:C:208:LEU:HB2	2:C:238:LEU:HD13	1.79	0.65
2:C:218:VAL:HG22	2:C:246:VAL:HG21	1.80	0.64
1:D:435:PRO:HA	1:D:454:LYS:O	1.98	0.64
2:A:144:TYR:O	2:A:147:GLN:HB2	1.96	0.64
2:C:211:ALA:CB	2:C:240:MET:HE1	2.26	0.64
1:B:63:LEU:HD21	1:B:300:THR:HB	0.75	0.64
1:B:648:ASN:O	1:B:651:ALA:HB3	1.97	0.64
1:D:648:ASN:O	1:D:651:ALA:HB3	1.97	0.64
1:B:64:PRO:CG	1:B:65:LEU:N	2.57	0.64
2:A:218:VAL:HG22	2:A:246:VAL:HG21	1.79	0.64
2:C:208:LEU:CD1	2:C:238:LEU:HD12	2.27	0.64
2:C:611:TRP:HE3	2:C:615:LEU:HD11	1.64	0.64
2:C:615:LEU:O	2:C:616:ASN:ND2	2.30	0.63
2:C:219:ILE:H	2:C:246:VAL:HG12	1.61	0.63
1:D:63:LEU:HD21	1:D:300:THR:CA	2.28	0.63
2:A:208:LEU:HB2	2:A:238:LEU:HD13	1.79	0.63
2:C:229:ALA:HA	2:C:232:TYR:CD2	2.33	0.63
1:B:533:ILE:CB	1:B:757:ALA:HB3	2.28	0.63
1:D:64:PRO:HG2	1:D:65:LEU:H	1.63	0.63
1:B:536:MET:HG3	1:B:749:THR:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:211:ALA:O	2:A:213:GLU:N	2.32	0.62
1:B:533:ILE:HG13	1:B:757:ALA:CB	2.25	0.62
2:A:243:SER:HB2	2:A:384:GLY:H	1.62	0.62
1:B:533:ILE:CG2	1:B:729:ILE:HG21	2.27	0.62
1:B:98:LEU:HB2	1:B:124:ILE:HG12	1.80	0.62
1:D:367:ASN:ND2	1:D:373:GLU:OE1	2.32	0.62
1:B:367:ASN:ND2	1:B:373:GLU:OE1	2.31	0.62
2:A:228:ALA:CB	2:A:232:TYR:HE2	2.12	0.62
1:B:64:PRO:HG2	1:B:65:LEU:H	1.63	0.62
2:C:836:ALA:HA	2:C:839:ARG:HD2	1.80	0.62
1:B:535:VAL:HB	1:B:750:ILE:CB	2.29	0.62
1:B:639:VAL:O	1:B:642:LEU:HB2	1.98	0.62
1:D:536:MET:HE3	1:D:749:THR:CG2	2.30	0.62
2:A:836:ALA:HA	2:A:839:ARG:HD2	1.80	0.62
2:C:810:PHE:H	2:C:813:MET:HB2	1.65	0.62
1:D:533:ILE:CD1	1:D:690:THR:CG2	2.76	0.62
1:D:38:VAL:HA	1:D:99:VAL:HB	1.81	0.62
1:B:534:SER:CB	1:B:732:ALA:HB1	2.30	0.61
1:B:164:ASP:O	1:B:453:LYS:NZ	2.33	0.61
1:D:536:MET:HG3	1:D:749:THR:HG22	1.81	0.61
1:D:533:ILE:CB	1:D:757:ALA:HB3	2.28	0.61
2:A:611:TRP:HE3	2:A:615:LEU:HD11	1.65	0.61
2:C:211:ALA:O	2:C:213:GLU:N	2.32	0.61
1:D:440:VAL:O	1:D:449:GLY:HA2	2.00	0.61
1:B:440:VAL:O	1:B:449:GLY:HA2	2.01	0.61
1:D:164:ASP:O	1:D:453:LYS:NZ	2.33	0.61
2:A:380:ILE:HA	2:A:386:THR:HG22	1.83	0.60
2:A:810:PHE:H	2:A:813:MET:HB2	1.65	0.60
1:D:431:ARG:NH2	2:C:694:ARG:O	2.34	0.60
2:C:380:ILE:HA	2:C:386:THR:HG22	1.84	0.60
1:D:537:VAL:HG12	1:D:727:ALA:HB2	1.82	0.60
1:D:523:ASP:HB3	1:D:772:LYS:HE2	1.83	0.60
1:B:535:VAL:N	1:B:750:ILE:HB	2.17	0.60
1:D:36:ILE:HB	1:D:69:VAL:HG22	1.84	0.60
2:A:240:MET:HA	2:A:245:TYR:CE1	2.37	0.60
2:C:350:ASN:HA	2:C:367:TYR:O	2.02	0.60
2:C:543:LYS:NZ	2:C:724:ASN:OD1	2.34	0.60
1:D:273:PRO:HG2	1:D:276:LEU:HD21	1.83	0.60
1:D:533:ILE:HG13	1:D:757:ALA:CB	2.25	0.60
2:A:543:LYS:NZ	2:A:724:ASN:OD1	2.34	0.60
1:B:534:SER:CB	1:B:732:ALA:HB2	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:350:ASN:HA	2:A:367:TYR:O	2.02	0.60
2:C:243:SER:HB2	2:C:384:GLY:H	1.62	0.60
1:D:534:SER:HB2	1:D:732:ALA:HB2	1.84	0.60
1:B:256:ILE:HG12	1:B:277:ILE:HB	1.84	0.59
2:A:438:GLY:HA3	2:A:478:LEU:HD12	1.84	0.59
1:D:535:VAL:H	1:D:750:ILE:HG21	1.68	0.59
1:D:535:VAL:N	1:D:750:ILE:HB	2.16	0.59
1:D:63:LEU:HB2	1:D:65:LEU:O	2.03	0.59
2:C:240:MET:HA	2:C:245:TYR:CE1	2.36	0.59
2:A:208:LEU:HB2	2:A:238:LEU:CD1	2.33	0.59
1:D:535:VAL:HB	1:D:750:ILE:CB	2.29	0.59
1:D:63:LEU:HD21	1:D:300:THR:CG2	2.30	0.59
2:A:208:LEU:C	2:A:211:ALA:HB3	2.16	0.59
1:D:570:SER:HB3	1:D:608:LEU:HD11	1.83	0.59
1:D:63:LEU:CD1	1:D:300:THR:CG2	2.55	0.58
1:D:536:MET:CE	1:D:749:THR:CG2	2.81	0.58
2:A:615:LEU:O	2:A:616:ASN:CG	2.40	0.58
1:B:647:ALA:O	1:B:651:ALA:N	2.37	0.58
2:C:438:GLY:HA3	2:C:478:LEU:HD12	1.84	0.58
1:B:64:PRO:HG2	1:B:65:LEU:N	2.18	0.58
1:B:36:ILE:HB	1:B:69:VAL:HG22	1.85	0.58
1:D:639:VAL:O	1:D:642:LEU:HB2	2.03	0.58
1:B:63:LEU:HB2	1:B:65:LEU:O	2.03	0.58
2:C:208:LEU:HB2	2:C:238:LEU:CD1	2.33	0.58
2:C:615:LEU:O	2:C:616:ASN:CG	2.42	0.58
1:D:536:MET:HA	1:D:749:THR:CB	2.33	0.58
2:A:207:LEU:HA	2:A:210:GLU:OE1	2.03	0.58
2:C:487:GLN:HA	2:C:497:GLU:O	2.04	0.58
1:D:46:VAL:O	1:D:50:GLU:N	2.34	0.58
2:A:508:GLY:HA2	2:A:763:ARG:HH22	1.68	0.58
1:B:35:ASN:ND2	1:B:93:ALA:O	2.36	0.58
2:A:694:ARG:O	1:B:431:ARG:NH2	2.36	0.58
1:B:38:VAL:HA	1:B:99:VAL:HB	1.85	0.58
2:A:233:ARG:HB3	2:A:233:ARG:CZ	2.33	0.58
2:A:157:VAL:HG21	2:A:372:VAL:HG11	1.85	0.58
1:B:536:MET:CE	1:B:749:THR:CG2	2.81	0.58
2:C:521:ASN:H	2:C:695:ARG:HH12	1.52	0.57
1:B:46:VAL:O	1:B:50:GLU:N	2.35	0.57
1:B:523:ASP:HB3	1:B:772:LYS:HE2	1.86	0.57
2:C:152:PHE:O	2:C:155:MET:HB2	2.04	0.57
2:C:207:LEU:HA	2:C:210:GLU:OE1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:769:SER:HB2	1:D:771:TRP:HD1	1.69	0.57
2:A:211:ALA:C	2:A:213:GLU:H	2.08	0.57
2:A:521:ASN:H	2:A:695:ARG:HH12	1.52	0.57
2:A:831:ILE:HG23	2:A:835:ILE:HD12	1.86	0.57
1:B:464:LEU:HD23	1:B:467:LEU:HD12	1.86	0.57
2:C:211:ALA:C	2:C:213:GLU:H	2.08	0.57
2:A:487:GLN:HA	2:A:497:GLU:O	2.04	0.57
1:D:35:ASN:ND2	1:D:93:ALA:O	2.37	0.57
2:A:520:ASN:HB3	2:A:695:ARG:HH22	1.69	0.57
1:B:273:PRO:HG2	1:B:276:LEU:HD21	1.86	0.57
1:B:638:ALA:O	1:B:642:LEU:N	2.37	0.57
1:D:98:LEU:HB2	1:D:124:ILE:HG12	1.86	0.57
1:D:64:PRO:HG2	1:D:65:LEU:N	2.18	0.57
2:A:229:ALA:O	2:A:230:THR:C	2.43	0.57
1:D:535:VAL:H	1:D:750:ILE:HB	1.70	0.57
2:C:227:ASP:O	2:C:230:THR:CB	2.28	0.57
1:D:149:ALA:HB1	1:D:154:GLN:HE21	1.70	0.57
1:B:533:ILE:CD1	1:B:690:THR:CG2	2.83	0.56
2:C:157:VAL:HG21	2:C:372:VAL:HG11	1.86	0.56
2:C:508:GLY:HA2	2:C:763:ARG:HH22	1.68	0.56
2:C:520:ASN:HB3	2:C:695:ARG:HH22	1.69	0.56
1:D:535:VAL:CB	1:D:750:ILE:HD13	2.33	0.56
2:C:424:PHE:HB3	2:C:428:GLY:HA2	1.87	0.56
1:B:535:VAL:H	1:B:750:ILE:HG21	1.69	0.56
1:B:533:ILE:O	1:B:756:PHE:O	2.23	0.56
2:A:233:ARG:NH1	2:A:233:ARG:HB2	2.21	0.56
1:B:149:ALA:HB1	1:B:154:GLN:HE21	1.71	0.56
1:B:536:MET:HA	1:B:749:THR:CB	2.34	0.56
1:B:63:LEU:HD13	1:B:67:VAL:CG2	2.35	0.56
2:A:227:ASP:O	2:A:231:VAL:N	2.38	0.56
2:C:831:ILE:HG23	2:C:835:ILE:HD12	1.86	0.56
1:D:647:ALA:O	1:D:651:ALA:N	2.38	0.56
1:D:63:LEU:HD13	1:D:67:VAL:CG2	2.35	0.56
2:C:243:SER:CB	2:C:384:GLY:N	2.32	0.56
1:B:439:PHE:HB3	1:B:449:GLY:HA3	1.88	0.56
1:B:632:SER:O	1:B:635:ALA:HB3	2.06	0.56
2:A:152:PHE:O	2:A:155:MET:HB2	2.04	0.56
1:B:63:LEU:HD21	1:B:300:THR:CG2	2.31	0.56
1:B:694:ILE:HA	1:B:697:ASN:HB2	1.88	0.56
2:A:115:ARG:HG2	2:A:135:LEU:HD13	1.88	0.55
2:A:91:LEU:HB3	2:A:121:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:115:ARG:HG2	2:C:135:LEU:HD13	1.88	0.55
1:B:530:GLU:CD	2:C:535:TYR:HB3	2.27	0.55
2:C:628:SER:HA	2:C:631:ILE:HD12	1.89	0.55
1:D:632:SER:O	1:D:635:ALA:HB3	2.06	0.55
1:B:535:VAL:H	1:B:750:ILE:HB	1.71	0.55
1:D:52:ARG:HA	1:D:293:ARG:HH21	1.70	0.55
2:A:243:SER:N	2:A:383:GLY:CA	2.68	0.55
1:B:438:LYS:O	1:B:451:ASN:HA	2.05	0.55
1:B:668:LYS:HA	1:B:671:GLN:HB2	1.89	0.55
1:D:256:ILE:HG12	1:D:277:ILE:HB	1.88	0.55
1:D:35:ASN:HB3	1:D:95:ILE:HG12	1.88	0.55
1:D:533:ILE:O	1:D:756:PHE:O	2.24	0.55
1:B:750:ILE:HG23	1:B:750:ILE:O	2.07	0.55
2:A:237:MET:C	2:A:239:ASN:H	2.09	0.55
2:A:424:PHE:HB3	2:A:428:GLY:HA2	1.87	0.55
1:D:464:LEU:HD23	1:D:467:LEU:HD12	1.88	0.55
2:A:208:LEU:HD13	2:A:238:LEU:HD12	1.89	0.55
1:B:600:THR:O	1:B:604:ALA:HB3	2.06	0.55
2:C:91:LEU:HB3	2:C:121:LEU:HD11	1.88	0.55
2:A:628:SER:HA	2:A:631:ILE:HD12	1.88	0.55
2:A:715:ALA:HA	2:A:718:ILE:HD12	1.89	0.55
1:B:35:ASN:HB3	1:B:95:ILE:HG12	1.88	0.55
2:C:237:MET:C	2:C:239:ASN:H	2.09	0.55
1:D:321:TYR:HA	2:C:72:ILE:HD13	1.89	0.55
1:D:38:VAL:O	1:D:71:ALA:HA	2.06	0.55
1:D:535:VAL:H	1:D:750:ILE:CB	2.19	0.55
2:C:243:SER:N	2:C:383:GLY:CA	2.68	0.55
1:B:63:LEU:HD12	1:B:67:VAL:HG23	1.85	0.54
1:B:665:LEU:O	1:B:671:GLN:NE2	2.41	0.54
2:A:233:ARG:CB	2:A:233:ARG:CZ	2.85	0.54
1:B:277:ILE:HG12	1:B:365:VAL:HG22	1.88	0.54
2:A:665:THR:N	2:A:669:ASP:OD2	2.36	0.54
2:C:302:THR:HG21	2:C:316:LYS:HB2	1.90	0.54
1:D:694:ILE:HA	1:D:697:ASN:HB2	1.89	0.54
2:C:208:LEU:HD13	2:C:238:LEU:HD12	1.89	0.54
2:A:302:THR:HG21	2:A:316:LYS:HB2	1.89	0.54
1:D:522:VAL:HG12	1:D:523:ASP:O	2.08	0.54
1:B:513:THR:OG1	1:B:518:ARG:NH1	2.40	0.54
1:B:522:VAL:CG1	1:B:523:ASP:H	2.21	0.54
1:B:569:VAL:HG13	1:B:631:VAL:HG22	1.90	0.54
1:B:535:VAL:CB	1:B:750:ILE:HD13	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:SER:HB2	1:B:771:TRP:HD1	1.72	0.54
2:C:208:LEU:C	2:C:211:ALA:HB3	2.15	0.54
1:B:522:VAL:HG12	1:B:523:ASP:O	2.08	0.54
1:B:38:VAL:O	1:B:71:ALA:HA	2.08	0.54
2:C:505:LEU:O	2:C:763:ARG:NH2	2.41	0.54
1:D:750:ILE:HG23	1:D:750:ILE:O	2.07	0.54
1:B:532:GLY:HA3	1:B:758:THR:HA	1.90	0.54
2:C:715:ALA:HA	2:C:718:ILE:HD12	1.89	0.54
1:B:535:VAL:H	1:B:750:ILE:CB	2.20	0.53
1:B:533:ILE:CG2	1:B:729:ILE:HG23	2.27	0.53
1:B:534:SER:O	1:B:729:ILE:HG23	2.09	0.53
1:D:534:SER:CB	1:D:732:ALA:CB	2.86	0.53
1:D:522:VAL:CG1	1:D:523:ASP:H	2.21	0.53
1:D:439:PHE:HB3	1:D:449:GLY:HA3	1.90	0.53
2:A:79:CYS:HA	2:A:83:ILE:HB	1.90	0.53
1:B:184:ILE:HG23	1:B:203:VAL:HG21	1.90	0.53
2:C:665:THR:N	2:C:669:ASP:OD2	2.35	0.53
1:D:538:SER:HA	1:D:747:LEU:HD23	1.91	0.53
1:B:626:THR:O	1:B:629:ILE:HB	2.09	0.53
2:C:208:LEU:HD12	2:C:238:LEU:CD1	2.39	0.53
2:A:233:ARG:NH1	2:A:233:ARG:CB	2.72	0.52
2:A:218:VAL:C	2:A:246:VAL:HG11	2.29	0.52
2:C:218:VAL:C	2:C:246:VAL:HG11	2.29	0.52
1:D:534:SER:HB2	1:D:732:ALA:HB1	1.89	0.52
2:C:364:VAL:O	2:C:375:ASN:N	2.42	0.52
2:C:562:LEU:HD23	2:C:565:LEU:HD12	1.92	0.52
1:D:638:ALA:O	1:D:642:LEU:N	2.41	0.52
1:D:532:GLY:HA3	1:D:758:THR:HA	1.90	0.52
2:A:208:LEU:HD12	2:A:238:LEU:CD1	2.39	0.52
2:A:472:PHE:HB2	2:A:474:TYR:CZ	2.44	0.52
2:A:505:LEU:O	2:A:763:ARG:NH2	2.41	0.52
1:B:52:ARG:HA	1:B:293:ARG:HH21	1.74	0.52
2:C:278:SER:HA	2:C:281:ILE:HD12	1.92	0.52
2:C:79:CYS:HA	2:C:83:ILE:HB	1.90	0.52
1:D:668:LYS:HA	1:D:671:GLN:HB2	1.91	0.52
2:A:278:SER:HA	2:A:281:ILE:HD12	1.92	0.52
2:C:366:ILE:HB	2:C:373:ILE:HB	1.92	0.52
1:D:534:SER:CB	1:D:732:ALA:HB1	2.40	0.52
2:A:364:VAL:O	2:A:375:ASN:N	2.42	0.52
2:C:232:TYR:HE2	2:C:261:TYR:C	2.10	0.52
2:C:522:GLU:H	2:C:695:ARG:NH2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:THR:OG1	1:D:518:ARG:NH1	2.42	0.52
2:A:118:VAL:O	2:A:137:PHE:HA	2.10	0.52
2:A:147:GLN:O	2:A:150:VAL:HB	2.10	0.52
1:B:538:SER:HA	1:B:747:LEU:HD23	1.90	0.52
2:C:208:LEU:O	2:C:240:MET:HE3	2.09	0.52
2:A:351:TYR:HB2	2:A:367:TYR:HB2	1.92	0.51
2:A:559:GLN:O	2:A:561:THR:N	2.43	0.51
1:B:279:VAL:HG22	1:B:363:VAL:HG22	1.92	0.51
1:B:46:VAL:HG13	1:B:71:ALA:HB3	1.92	0.51
2:C:433:LYS:HE2	2:C:456:TYR:HE1	1.76	0.51
2:A:522:GLU:H	2:A:695:ARG:NH2	2.08	0.51
1:B:108:ALA:O	1:B:112:MET:N	2.39	0.51
2:C:472:PHE:HB2	2:C:474:TYR:CZ	2.44	0.51
2:C:559:GLN:O	2:C:561:THR:N	2.44	0.51
1:D:279:VAL:HG22	1:D:363:VAL:HG22	1.92	0.51
1:B:413:GLU:OE1	1:B:511:SER:OG	2.25	0.51
2:A:366:ILE:HB	2:A:373:ILE:HB	1.92	0.51
2:A:721:VAL:HG11	2:A:746:LEU:HD21	1.93	0.51
2:A:208:LEU:CB	2:A:238:LEU:HD13	2.40	0.51
2:C:147:GLN:O	2:C:150:VAL:HB	2.10	0.51
2:C:251:GLU:HA	2:C:254:ILE:HD12	1.92	0.51
2:C:721:VAL:HG11	2:C:746:LEU:HD21	1.93	0.51
1:D:526:VAL:HG13	1:D:527:PRO:CD	2.27	0.51
2:A:144:TYR:OH	2:A:252:ARG:NE	2.44	0.51
2:A:228:ALA:O	2:A:232:TYR:CD2	2.63	0.51
2:A:562:LEU:HD23	2:A:565:LEU:HD12	1.92	0.51
2:C:229:ALA:O	2:C:233:ARG:HB2	2.09	0.51
1:D:226:VAL:HG22	1:D:254:PHE:HB2	1.92	0.51
1:B:63:LEU:HD11	1:B:300:THR:HG21	1.78	0.51
2:A:237:MET:O	2:A:239:ASN:N	2.44	0.51
2:C:232:TYR:OH	2:C:258:ALA:O	2.28	0.51
2:C:351:TYR:HB2	2:C:367:TYR:HB2	1.92	0.51
2:A:251:GLU:HA	2:A:254:ILE:HD12	1.92	0.50
2:C:118:VAL:O	2:C:137:PHE:HA	2.10	0.50
1:D:536:MET:N	1:D:728:PHE:O	2.37	0.50
2:C:226:ASP:O	2:C:227:ASP:C	2.50	0.50
1:D:108:ALA:O	1:D:112:MET:N	2.40	0.50
2:C:237:MET:O	2:C:239:ASN:N	2.44	0.50
2:C:217:ARG:C	2:C:246:VAL:CG2	2.79	0.50
1:D:277:ILE:HG12	1:D:365:VAL:HG22	1.92	0.50
1:D:730:TYR:HB2	1:D:735:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:243:SER:CB	2:A:384:GLY:N	2.32	0.50
1:B:759:THR:HG21	2:C:780:HIS:CE1	2.47	0.50
2:C:795:TYR:HB2	2:C:796:GLN:HG3	1.93	0.50
2:A:433:LYS:HE2	2:A:456:TYR:HE1	1.76	0.50
2:A:485:GLY:HA2	2:A:499:ASN:HB2	1.93	0.50
2:C:208:LEU:CB	2:C:238:LEU:HD13	2.40	0.50
2:C:485:GLY:HA2	2:C:499:ASN:HB2	1.93	0.50
2:C:144:TYR:OH	2:C:252:ARG:NE	2.44	0.50
1:B:558:VAL:HG22	2:C:809:THR:HG23	1.93	0.50
1:B:63:LEU:HB3	1:B:65:LEU:HB2	1.94	0.50
2:C:693:PHE:O	2:C:703:TYR:OH	2.26	0.50
1:D:535:VAL:HB	1:D:750:ILE:CG1	2.42	0.50
2:A:208:LEU:HD12	2:A:238:LEU:HD12	1.94	0.50
1:B:460:CYS:HA	1:B:463:ILE:HD12	1.93	0.50
1:B:526:VAL:HG13	1:B:527:PRO:CD	2.27	0.50
1:B:730:TYR:HB2	1:B:735:LEU:HD11	1.94	0.50
1:D:460:CYS:HA	1:D:463:ILE:HD12	1.94	0.50
2:A:795:TYR:HB2	2:A:796:GLN:HG3	1.93	0.49
2:C:211:ALA:C	2:C:213:GLU:N	2.66	0.49
1:D:63:LEU:HB3	1:D:65:LEU:HB2	1.94	0.49
2:A:394:MET:HG3	2:A:768:TRP:HZ2	1.77	0.49
2:A:489:ARG:HH21	1:B:195:PHE:H	1.59	0.49
1:B:527:PRO:HG2	1:B:527:PRO:O	2.12	0.49
1:D:538:SER:HA	1:D:747:LEU:HA	1.95	0.49
1:B:486:GLY:HA3	1:B:497:ILE:HD12	1.94	0.49
1:D:527:PRO:O	1:D:527:PRO:HG2	2.12	0.49
2:A:211:ALA:C	2:A:213:GLU:N	2.66	0.49
1:D:459:PHE:HE1	1:D:791:LEU:HB3	1.76	0.49
2:A:543:LYS:HZ1	2:A:724:ASN:HA	1.77	0.49
1:B:500:VAL:CG1	1:B:522:VAL:HG21	2.35	0.49
1:B:535:VAL:HB	1:B:750:ILE:CG1	2.43	0.49
1:B:459:PHE:HE1	1:B:791:LEU:HB3	1.78	0.49
2:C:505:LEU:HD12	2:C:527:ILE:HD13	1.95	0.49
1:D:528:PHE:C	1:D:528:PHE:CD1	2.86	0.49
1:B:536:MET:N	1:B:728:PHE:O	2.42	0.49
2:C:243:SER:HB3	2:C:383:GLY:C	2.28	0.49
2:A:111:ALA:HA	2:A:116:ILE:HD12	1.95	0.49
2:A:73:GLN:O	2:A:75:ALA:N	2.46	0.49
1:B:537:VAL:O	1:B:748:VAL:N	2.46	0.49
2:C:232:TYR:CZ	2:C:258:ALA:O	2.66	0.49
1:B:759:THR:HG21	2:C:780:HIS:ND1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:759:THR:HG22	2:A:535:TYR:HE2	1.78	0.48
2:A:738:PHE:CZ	2:A:793:VAL:HA	2.48	0.48
1:B:528:PHE:C	1:B:528:PHE:CD1	2.86	0.48
2:C:218:VAL:N	2:C:246:VAL:HG21	2.22	0.48
2:C:394:MET:HG3	2:C:768:TRP:HZ2	1.77	0.48
2:A:693:PHE:O	2:A:703:TYR:OH	2.26	0.48
1:D:220:LYS:HZ2	1:B:246:LEU:HA	1.78	0.48
2:C:111:ALA:HA	2:C:116:ILE:HD12	1.95	0.48
2:C:217:ARG:O	2:C:246:VAL:CB	2.61	0.48
2:A:463:LEU:HD21	2:A:514:VAL:HG21	1.96	0.48
2:A:541:LEU:O	2:A:728:ALA:HA	2.13	0.48
2:C:463:LEU:HD21	2:C:514:VAL:HG21	1.96	0.48
1:D:521:VAL:C	1:D:767:LYS:HE3	2.32	0.48
2:A:217:ARG:O	2:A:246:VAL:CB	2.61	0.48
2:A:459:CYS:HA	2:A:462:LEU:HD12	1.96	0.48
2:C:541:LEU:O	2:C:728:ALA:HA	2.13	0.48
2:C:559:GLN:HB2	2:C:562:LEU:HD12	1.95	0.48
1:D:134:ILE:HD11	1:D:146:GLN:HB2	1.95	0.48
1:D:536:MET:HE2	1:D:749:THR:HG23	1.95	0.48
1:D:537:VAL:O	1:D:748:VAL:N	2.46	0.48
1:B:538:SER:HA	1:B:747:LEU:HA	1.94	0.48
1:B:508:ALA:HB3	1:B:764:ALA:HB3	1.95	0.48
2:C:272:ILE:HD12	2:C:350:ASN:HB3	1.96	0.48
2:C:738:PHE:CZ	2:C:793:VAL:HA	2.48	0.48
1:D:533:ILE:HD12	1:D:690:THR:CG2	2.43	0.48
1:D:78:ASP:O	1:D:81:SER:OG	2.25	0.48
1:B:712:GLY:N	1:B:715:ASP:OD2	2.47	0.48
2:C:111:ALA:HB1	2:C:116:ILE:HB	1.96	0.48
2:C:209:MET:O	2:C:210:GLU:C	2.51	0.48
2:C:538:LEU:HB2	2:C:753:PHE:HB2	1.96	0.48
2:C:73:GLN:O	2:C:75:ALA:N	2.46	0.48
1:D:111:GLN:O	1:D:114:ASP:HB2	2.14	0.48
1:D:530:GLU:CD	2:A:535:TYR:HB3	2.34	0.48
1:D:710:GLN:HE22	1:D:716:ALA:HA	1.79	0.48
1:B:627:SER:HA	1:B:630:MET:HG2	1.96	0.47
1:D:46:VAL:HG13	1:D:71:ALA:HB3	1.96	0.47
2:A:538:LEU:HB2	2:A:753:PHE:HB2	1.96	0.47
2:A:208:LEU:O	2:A:240:MET:HE3	2.14	0.47
2:C:229:ALA:HA	2:C:232:TYR:CB	2.40	0.47
2:C:341:ASN:HA	2:C:347:LYS:HE3	1.97	0.47
2:A:505:LEU:HD12	2:A:527:ILE:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:559:GLN:HB2	2:A:562:LEU:HD12	1.95	0.47
2:C:459:CYS:HA	2:C:462:LEU:HD12	1.96	0.47
1:B:719:SER:O	1:B:724:LYS:N	2.46	0.47
1:D:128:HIS:HA	1:D:132:SER:HB3	1.95	0.47
2:A:72:ILE:HD13	1:B:321:TYR:HA	1.96	0.47
1:B:565:MET:HG3	2:C:817:PHE:HE1	1.77	0.47
2:A:209:MET:O	2:A:210:GLU:C	2.51	0.47
2:A:341:ASN:HA	2:A:347:LYS:HE3	1.97	0.47
1:B:291:ARG:HE	1:B:360:ARG:HH11	1.62	0.47
1:B:537:VAL:CG1	1:B:727:ALA:CB	2.91	0.47
2:A:272:ILE:HD12	2:A:350:ASN:HB3	1.96	0.47
1:D:719:SER:O	1:D:724:LYS:N	2.45	0.47
1:B:286:TYR:OH	1:B:379:GLU:OE2	2.29	0.47
1:B:565:MET:HG3	2:C:817:PHE:CD1	2.48	0.47
1:B:388:ALA:O	1:B:437:ARG:NH1	2.48	0.47
1:B:535:VAL:HG22	1:B:729:ILE:CD1	2.44	0.47
2:C:208:LEU:CD1	2:C:238:LEU:CD1	2.93	0.47
2:A:111:ALA:HB1	2:A:116:ILE:HB	1.96	0.46
2:A:75:ALA:HA	2:A:78:VAL:HB	1.98	0.46
1:D:634:TRP:O	1:D:638:ALA:N	2.46	0.46
1:D:537:VAL:HA	1:D:727:ALA:HB2	1.97	0.46
2:A:150:VAL:O	2:A:153:GLU:HB2	2.15	0.46
2:A:195:LEU:HD22	2:A:210:GLU:OE2	2.16	0.46
2:A:218:VAL:N	2:A:246:VAL:HG21	2.22	0.46
2:C:235:ALA:O	2:C:237:MET:N	2.48	0.46
2:C:219:ILE:N	2:C:246:VAL:CG1	2.53	0.46
1:D:413:GLU:OE1	1:D:511:SER:OG	2.27	0.46
1:D:820:VAL:O	1:D:824:LEU:N	2.35	0.46
2:A:243:SER:HB3	2:A:383:GLY:C	2.28	0.46
1:B:128:HIS:HA	1:B:132:SER:HB3	1.97	0.46
2:C:150:VAL:O	2:C:153:GLU:HB2	2.16	0.46
2:C:825:VAL:HA	2:C:828:ILE:HD12	1.97	0.46
1:B:262:SER:OG	1:B:263:GLY:N	2.48	0.46
1:B:434:VAL:O	1:B:456:CYS:HB2	2.16	0.46
1:D:123:PRO:HG3	1:D:334:LEU:HD12	1.96	0.46
2:A:217:ARG:C	2:A:246:VAL:CG2	2.79	0.46
2:A:315:TRP:HB3	2:A:317:THR:H	1.81	0.46
1:B:522:VAL:HG13	1:B:523:ASP:H	1.81	0.46
1:B:710:GLN:HE22	1:B:716:ALA:HA	1.81	0.46
2:C:151:TRP:O	2:C:154:MET:HB2	2.16	0.46
1:D:577:PHE:HA	1:D:580:PHE:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:825:VAL:HA	2:A:828:ILE:HD12	1.97	0.46
1:B:694:ILE:O	1:B:698:TYR:N	2.35	0.46
2:C:208:LEU:HD12	2:C:238:LEU:HD12	1.94	0.46
1:D:533:ILE:HG22	1:D:729:ILE:HG21	1.79	0.46
1:B:226:VAL:HG22	1:B:254:PHE:HB2	1.97	0.46
1:D:262:SER:OG	1:D:263:GLY:N	2.49	0.46
2:A:235:ALA:O	2:A:237:MET:N	2.48	0.46
2:C:315:TRP:HB3	2:C:317:THR:H	1.81	0.46
2:A:151:TRP:O	2:A:154:MET:HB2	2.15	0.45
1:B:78:ASP:O	1:B:81:SER:OG	2.25	0.45
2:A:208:LEU:CD1	2:A:238:LEU:CD1	2.93	0.45
2:A:578:TYR:OH	2:A:606:ALA:N	2.49	0.45
1:B:163:GLN:HA	1:B:198:TRP:HH2	1.81	0.45
2:C:521:ASN:H	2:C:695:ARG:NH1	2.14	0.45
2:C:75:ALA:HA	2:C:78:VAL:HB	1.98	0.45
1:D:137:ASP:H	2:C:133:ILE:HD11	1.82	0.45
1:D:569:VAL:HA	1:D:572:ILE:HD12	1.99	0.45
1:D:694:ILE:O	1:D:698:TYR:N	2.35	0.45
2:A:357:GLN:HE22	2:A:380:ILE:H	1.64	0.45
2:A:643:ILE:O	2:A:646:SER:OG	2.29	0.45
2:C:226:ASP:C	2:C:230:THR:HG1	2.15	0.45
1:D:63:LEU:HD12	1:D:67:VAL:HG23	1.85	0.45
1:B:533:ILE:CG2	1:B:729:ILE:HG22	2.27	0.45
2:C:208:LEU:CB	2:C:238:LEU:CD1	2.94	0.45
2:C:731:TRP:HB3	2:C:732:ASP:H	1.62	0.45
1:D:533:ILE:CG2	1:D:729:ILE:HG23	2.29	0.45
2:A:138:LEU:HD22	2:A:344:GLY:HA3	1.99	0.45
1:D:522:VAL:HG13	1:D:523:ASP:H	1.81	0.45
1:B:126:GLY:HA3	1:B:146:GLN:HG2	1.98	0.45
1:B:534:SER:OG	1:B:732:ALA:CB	2.65	0.45
2:C:578:TYR:OH	2:C:606:ALA:N	2.49	0.45
2:A:521:ASN:H	2:A:695:ARG:NH1	2.14	0.45
2:C:543:LYS:HZ1	2:C:724:ASN:HA	1.81	0.45
1:D:535:VAL:HG22	1:D:729:ILE:HD11	1.96	0.45
2:A:208:LEU:CB	2:A:238:LEU:CD1	2.94	0.45
1:B:417:VAL:HA	1:B:457:LYS:O	2.16	0.45
2:C:611:TRP:CE3	2:C:615:LEU:HD11	2.49	0.45
1:D:416:PHE:HA	1:D:459:PHE:HB2	1.99	0.45
2:A:611:TRP:CE3	2:A:615:LEU:HD11	2.49	0.45
2:A:136:SER:HB3	2:A:322:LYS:HE2	1.99	0.45
2:A:228:ALA:O	2:A:231:VAL:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:PRO:HG3	1:B:334:LEU:HD12	1.99	0.45
2:C:601:LEU:O	2:C:605:SER:OG	2.30	0.45
2:C:738:PHE:HZ	2:C:793:VAL:HA	1.81	0.45
1:D:127:ILE:HG22	1:D:128:HIS:CD2	2.52	0.45
2:A:738:PHE:HZ	2:A:793:VAL:HA	1.81	0.44
2:A:73:GLN:HE21	1:B:321:TYR:HE1	1.65	0.44
2:C:210:GLU:HB3	2:C:211:ALA:H	1.55	0.44
2:A:688:SER:HA	2:A:691:ILE:HD12	1.99	0.44
1:B:416:PHE:HA	1:B:459:PHE:HB2	2.00	0.44
1:B:513:THR:O	1:B:518:ARG:NH1	2.47	0.44
1:B:536:MET:HG3	1:B:749:THR:CG2	2.47	0.44
1:B:654:ILE:HD12	2:C:656:VAL:HG21	1.99	0.44
2:A:237:MET:C	2:A:239:ASN:N	2.70	0.44
2:C:195:LEU:HD22	2:C:210:GLU:OE2	2.15	0.44
2:A:228:ALA:CB	2:A:232:TYR:CE2	2.81	0.44
2:C:357:GLN:HE22	2:C:380:ILE:H	1.64	0.44
2:C:463:LEU:HD23	2:C:466:LEU:HD12	2.00	0.44
1:D:194:SER:HA	2:C:489:ARG:HH21	1.83	0.44
2:A:218:VAL:HG22	2:A:246:VAL:HG22	1.99	0.44
2:C:241:THR:HB	2:C:263:PRO:HG3	2.00	0.44
2:A:367:TYR:HE1	2:A:372:VAL:HG22	1.82	0.44
1:B:246:LEU:HD13	1:B:248:LEU:HD12	2.00	0.44
2:C:118:VAL:HB	2:C:137:PHE:HD1	1.83	0.44
2:C:138:LEU:HD22	2:C:344:GLY:HA3	1.99	0.44
2:C:688:SER:HA	2:C:691:ILE:HD12	1.99	0.44
1:D:163:GLN:HA	1:D:198:TRP:HH2	1.82	0.44
1:D:835:PHE:CE2	2:C:580:LEU:HD13	2.52	0.44
2:A:241:THR:HB	2:A:263:PRO:HG3	2.00	0.44
2:C:367:TYR:HE1	2:C:372:VAL:HG22	1.82	0.44
1:B:557:SER:OG	2:C:809:THR:HG21	2.17	0.44
1:D:533:ILE:HG21	1:D:729:ILE:HG21	1.96	0.44
1:D:737:TYR:CE1	1:D:796:LEU:HA	2.53	0.44
2:A:31:ALA:HA	2:A:91:LEU:H	1.83	0.44
1:B:291:ARG:HE	1:B:360:ARG:NH1	2.16	0.44
1:B:63:LEU:C	1:B:65:LEU:N	2.63	0.44
2:C:208:LEU:HA	2:C:211:ALA:HB2	2.00	0.44
2:C:237:MET:C	2:C:239:ASN:N	2.70	0.44
1:D:126:GLY:HA3	1:D:146:GLN:HG2	1.99	0.44
2:A:670:PRO:HA	2:A:673:ARG:HB2	2.00	0.43
1:D:603:LYS:HA	1:D:606:TRP:HD1	1.83	0.43
1:D:534:SER:CB	1:D:732:ALA:HB2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:463:LEU:HD23	2:A:466:LEU:HD12	2.00	0.43
2:A:210:GLU:HB3	2:A:211:ALA:H	1.55	0.43
2:C:227:ASP:O	2:C:231:VAL:N	2.37	0.43
1:D:184:ILE:HG23	1:D:203:VAL:HG21	2.00	0.43
1:D:536:MET:HG3	1:D:749:THR:CG2	2.47	0.43
1:D:781:GLN:HA	2:A:521:ASN:HD21	1.83	0.43
1:B:534:SER:OG	1:B:732:ALA:HB1	2.18	0.43
2:C:425:THR:OG1	2:C:429:ASP:N	2.37	0.43
1:B:113:LEU:HA	1:B:116:ILE:HD12	2.00	0.43
1:D:246:LEU:HA	1:B:220:LYS:HZ2	1.84	0.43
1:B:737:TYR:CE1	1:B:796:LEU:HA	2.54	0.43
2:C:643:ILE:O	2:C:646:SER:OG	2.29	0.43
2:C:31:ALA:HA	2:C:91:LEU:H	1.83	0.43
1:D:291:ARG:HE	1:D:360:ARG:NH1	2.16	0.43
1:D:737:TYR:HE1	1:D:796:LEU:HA	1.84	0.43
1:B:63:LEU:HD13	1:B:67:VAL:HG21	1.83	0.43
2:C:136:SER:HB3	2:C:322:LYS:HE2	1.99	0.43
2:C:670:PRO:HA	2:C:673:ARG:HB2	2.00	0.43
2:C:667:ILE:HA	2:C:672:LEU:HD12	2.01	0.43
1:D:523:ASP:HB3	1:D:772:LYS:CE	2.47	0.43
2:A:118:VAL:HB	2:A:137:PHE:HD1	1.83	0.43
2:A:208:LEU:HA	2:A:211:ALA:HB2	2.01	0.43
2:C:166:LEU:HB2	2:C:221:LEU:HD23	2.00	0.43
1:D:534:SER:OG	1:D:732:ALA:HB1	2.18	0.43
2:A:559:GLN:O	2:A:560:SER:C	2.57	0.43
1:B:718:VAL:O	1:B:722:THR:N	2.47	0.43
1:B:781:GLN:HA	2:C:521:ASN:HD21	1.84	0.43
1:D:388:ALA:O	1:D:437:ARG:NH1	2.52	0.43
2:A:227:ASP:C	2:A:231:VAL:HG23	2.37	0.43
2:A:287:VAL:HA	2:A:330:TYR:CZ	2.54	0.43
1:D:63:LEU:CB	1:D:65:LEU:O	2.67	0.43
1:D:536:MET:CE	1:D:749:THR:HG23	2.48	0.43
1:B:79:PRO:HA	1:B:82:LEU:HD12	2.01	0.43
2:C:47:ASN:HA	2:C:50:ASN:HD22	1.84	0.43
1:D:718:VAL:O	1:D:722:THR:N	2.48	0.43
1:D:508:ALA:HB3	1:D:764:ALA:HB3	2.00	0.43
2:A:233:ARG:HH11	2:A:233:ARG:HB2	1.83	0.42
2:A:679:PHE:HA	2:A:727:HIS:CD2	2.54	0.42
1:B:536:MET:HE3	1:B:735:LEU:HB3	2.01	0.42
1:B:76:ARG:HD3	1:B:78:ASP:HB2	2.00	0.42
2:C:700:SER:HA	2:C:703:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:712:GLY:N	1:D:715:ASP:OD2	2.52	0.42
1:D:759:THR:HG21	2:A:780:HIS:CE1	2.54	0.42
2:A:126:SER:O	2:A:129:SER:OG	2.29	0.42
2:A:700:SER:HA	2:A:703:TYR:CE2	2.54	0.42
1:D:525:SER:HG	1:D:763:ILE:N	2.17	0.42
1:B:569:VAL:HA	1:B:572:ILE:HD12	2.01	0.42
2:A:425:THR:OG1	2:A:429:ASP:N	2.37	0.42
2:A:520:ASN:HB3	2:A:695:ARG:NH2	2.34	0.42
2:C:146:HIS:O	2:C:149:SER:OG	2.30	0.42
2:C:229:ALA:O	2:C:232:TYR:HB3	2.18	0.42
1:D:246:LEU:HD23	1:B:220:LYS:HZ3	1.85	0.42
2:C:229:ALA:O	2:C:233:ARG:HB3	2.18	0.42
2:C:559:GLN:O	2:C:560:SER:C	2.58	0.42
2:C:679:PHE:HA	2:C:727:HIS:CD2	2.54	0.42
1:B:63:LEU:CD2	1:B:300:THR:CB	2.55	0.42
1:B:627:SER:C	1:B:629:ILE:N	2.72	0.42
2:C:127:ILE:HG12	2:C:171:HIS:HB2	2.02	0.42
2:C:287:VAL:HA	2:C:330:TYR:CZ	2.54	0.42
1:D:143:THR:HA	1:D:335:HIS:HE1	1.84	0.42
1:D:164:ASP:HB2	1:D:386:ARG:NH1	2.34	0.42
2:A:771:ASN:HA	2:A:774:LEU:HD12	2.02	0.42
2:C:771:ASN:HA	2:C:774:LEU:HD12	2.02	0.42
1:D:159:LEU:HD23	1:D:159:LEU:HA	1.89	0.42
1:D:65:LEU:HD12	1:D:303:ALA:HB1	2.01	0.42
2:A:166:LEU:HB2	2:A:221:LEU:HD23	2.00	0.42
2:A:47:ASN:HA	2:A:50:ASN:HD22	1.84	0.42
2:A:132:SER:HB3	1:B:178:PRO:HG2	2.01	0.42
1:B:734:VAL:HA	1:B:737:TYR:HD2	1.83	0.42
1:D:205:THR:O	1:D:218:GLN:NE2	2.36	0.42
1:D:534:SER:O	1:D:729:ILE:CA	2.59	0.42
2:A:614:LEU:HD21	2:A:636:TRP:HB3	2.02	0.42
1:B:159:LEU:HD23	1:B:159:LEU:HA	1.89	0.42
1:B:536:MET:CE	1:B:749:THR:HG23	2.49	0.42
1:B:63:LEU:CB	1:B:65:LEU:O	2.67	0.42
2:A:127:ILE:HG12	2:A:171:HIS:HB2	2.02	0.42
2:A:667:ILE:HA	2:A:672:LEU:HD12	2.01	0.42
2:A:684:VAL:H	2:A:731:TRP:HZ2	1.68	0.42
1:B:164:ASP:HB2	1:B:386:ARG:NH1	2.35	0.42
1:D:500:VAL:CG1	1:D:522:VAL:HG21	2.47	0.42
2:A:103:THR:O	2:A:105:THR:N	2.51	0.41
2:A:522:GLU:H	2:A:695:ARG:HH22	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:541:LEU:HD21	2:A:736:LEU:HD22	2.02	0.41
1:B:634:TRP:O	1:B:638:ALA:N	2.51	0.41
2:C:211:ALA:CB	2:C:240:MET:CE	2.96	0.41
1:D:417:VAL:HA	1:D:457:LYS:O	2.20	0.41
2:A:772:VAL:O	2:A:775:SER:OG	2.31	0.41
2:C:684:VAL:H	2:C:731:TRP:HZ2	1.68	0.41
1:D:180:TYR:HA	1:D:183:PHE:CD2	2.55	0.41
1:D:286:TYR:OH	1:D:379:GLU:OE2	2.30	0.41
2:A:699:LEU:O	2:A:702:MET:HB2	2.20	0.41
2:C:520:ASN:HB3	2:C:695:ARG:NH2	2.34	0.41
2:A:307:GLY:O	2:A:311:ASN:ND2	2.41	0.41
2:C:217:ARG:C	2:C:246:VAL:HG21	2.40	0.41
2:C:541:LEU:HD21	2:C:736:LEU:HD22	2.02	0.41
2:C:614:LEU:HD21	2:C:636:TRP:HB3	2.02	0.41
2:A:400:ILE:HD13	2:A:463:LEU:HD13	2.02	0.41
2:A:489:ARG:HH21	1:B:194:SER:HA	1.86	0.41
1:D:301:THR:HG21	1:D:341:VAL:HG13	2.03	0.41
1:D:63:LEU:C	1:D:65:LEU:N	2.63	0.41
2:A:139:ARG:N	2:A:345:ASP:OD1	2.47	0.41
1:B:180:TYR:HA	1:B:183:PHE:CD2	2.56	0.41
1:D:79:PRO:HA	1:D:82:LEU:HD12	2.02	0.41
2:A:228:ALA:C	2:A:232:TYR:HD2	2.24	0.41
2:A:631:ILE:HG13	1:B:606:TRP:HH2	1.85	0.41
1:B:759:THR:HG22	2:C:535:TYR:HE2	1.86	0.41
2:C:569:SER:O	2:C:573:VAL:HG23	2.21	0.41
1:D:161:ILE:HA	1:D:386:ARG:HH12	1.85	0.41
2:A:145:SER:O	2:A:148:SER:OG	2.23	0.41
2:A:354:MET:HB3	2:A:361:LEU:HD22	2.03	0.41
2:A:408:PHE:HA	2:A:458:PHE:HD2	1.86	0.41
1:B:525:SER:OG	1:B:763:ILE:HB	2.20	0.41
1:B:96:HIS:HE1	1:B:316:ALA:N	2.19	0.41
2:C:408:PHE:HA	2:C:458:PHE:HD2	1.86	0.41
2:C:210:GLU:O	2:C:213:GLU:HG3	2.21	0.41
2:C:699:LEU:O	2:C:702:MET:HB2	2.20	0.41
1:B:243:ALA:HA	1:B:246:LEU:HD12	2.03	0.41
1:B:533:ILE:HD12	1:B:690:THR:CG2	2.50	0.41
2:C:522:GLU:H	2:C:695:ARG:HH22	1.68	0.41
1:D:251:TYR:OH	1:D:397:SER:N	2.51	0.41
1:D:735:LEU:HB3	1:D:749:THR:HG21	2.02	0.41
1:B:63:LEU:HD21	1:B:300:THR:CA	2.38	0.41
1:B:65:LEU:HD23	1:B:65:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:229:ALA:O	2:C:233:ARG:CA	2.64	0.41
2:C:400:ILE:HD13	2:C:463:LEU:HD13	2.02	0.41
1:D:195:PHE:H	2:C:489:ARG:HH21	1.69	0.41
1:D:251:TYR:CE2	1:D:395:SER:HA	2.56	0.41
1:D:750:ILE:CG2	1:D:750:ILE:O	2.69	0.40
2:A:569:SER:O	2:A:573:VAL:HG23	2.21	0.40
1:D:286:TYR:CZ	1:D:360:ARG:HD3	2.57	0.40
1:D:76:ARG:HD3	1:D:78:ASP:HB2	2.04	0.40
2:C:207:LEU:CA	2:C:210:GLU:OE1	2.69	0.40
1:D:243:ALA:HA	1:D:246:LEU:HB2	2.03	0.40
1:D:566:LEU:HD22	1:D:608:LEU:HD22	2.04	0.40
1:D:685:VAL:H	1:D:730:TYR:HE1	1.69	0.40
2:A:228:ALA:O	2:A:232:TYR:HD2	2.03	0.40
1:B:685:VAL:H	1:B:730:TYR:HE1	1.69	0.40
2:C:325:LEU:HD23	2:C:325:LEU:HA	1.90	0.40
2:C:615:LEU:HD23	2:C:615:LEU:HA	1.86	0.40
2:C:772:VAL:O	2:C:775:SER:OG	2.31	0.40
1:D:64:PRO:HG2	1:D:65:LEU:HG	2.02	0.40
1:B:160:LYS:HD2	1:B:378:TRP:HH2	1.86	0.40
1:B:64:PRO:HG2	1:B:65:LEU:HG	2.02	0.40
1:B:647:ALA:HA	1:B:650:ALA:HB3	2.03	0.40
2:C:210:GLU:O	2:C:213:GLU:CG	2.70	0.40
2:C:776[B]:ILE:HD13	2:C:776[B]:ILE:HA	1.86	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	B	736/853 (86%)	656 (89%)	77 (10%)	3 (0%)	36	76
1	D	736/853 (86%)	658 (89%)	75 (10%)	3 (0%)	36	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	778/847 (92%)	693 (89%)	75 (10%)	10 (1%)	13 53
2	C	778/847 (92%)	692 (89%)	76 (10%)	10 (1%)	13 53
All	All	3028/3400 (89%)	2699 (89%)	303 (10%)	26 (1%)	24 60

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	327	PRO
1	D	329	VAL
2	A	95	PRO
2	A	98	PRO
2	A	212	LYS
2	A	616	ASN
1	B	327	PRO
1	B	329	VAL
2	C	95	PRO
2	C	98	PRO
2	C	212	LYS
2	C	616	ASN
2	A	97	THR
2	A	211	ALA
2	A	560	SER
2	C	97	THR
2	C	211	ALA
2	C	560	SER
2	A	74	MET
2	C	74	MET
2	A	238	LEU
2	C	238	LEU
1	D	391	PRO
2	A	94	HIS
1	B	391	PRO
2	C	94	HIS

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	B	612/738 (83%)	612 (100%)	0	100 100
1	D	612/738 (83%)	612 (100%)	0	100 100
2	A	660/731 (90%)	660 (100%)	0	100 100
2	C	660/731 (90%)	659 (100%)	1 (0%)	94 96
All	All	2544/2938 (87%)	2543 (100%)	1 (0%)	100 100

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

Mol	Chain	Res	Type
2	C	226	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	35	ASN
1	D	42	HIS
1	D	96	HIS
1	D	128	HIS
1	D	380	ASN
1	D	387	HIS
1	D	687	ASN
1	D	736	ASN
2	A	38	HIS
2	A	61	ASN
2	A	134	HIS
2	A	161	ASN
2	A	357	GLN
2	A	520	ASN
2	A	559	GLN
1	B	35	ASN
1	B	42	HIS
1	B	96	HIS
1	B	128	HIS
1	B	358	HIS
1	B	380	ASN
1	B	387	HIS
1	B	736	ASN
2	C	38	HIS
2	C	61	ASN
2	C	134	HIS

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Mol	Chain	Res	Type
2	C	161	ASN
2	C	357	GLN
2	C	520	ASN
2	C	559	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.