wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:56 PM BST

PDB ID	:	4BOM
EMDB ID:	:	EMD-2380
Title	:	Structure of herpesvirus fusion glycoprotein B-bilayer complex revealing the protein-membrane and lateral protein-protein interaction
Authors	:	Maurer, U.E.; Zeev-Ben-Mordehai, Z.; Pandurangan, A.P.; Cairns, T.M.; Hannah, B.P.; Whitbeck, J.C.; Eisenberg, R.J.; Cohen, G.H.; Topf, M.; Huiskonen, J.T.; Grunewald, K.
Deposited on	:	2013-05-21
Resolution	:	27.00 Å(reported)
Based on PDB ID	:	3NWF

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

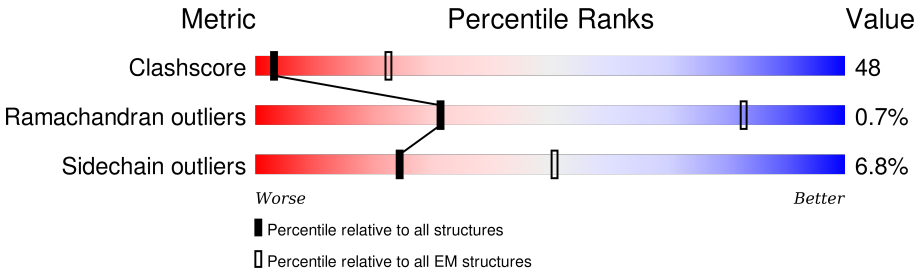
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 27.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	622	40% 52%
1	B	622	42% 51% 5%
1	C	622	41% 52%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14745 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 ENVELOPE GLYCOPROTEIN B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	608	Total	C	N	O	S	0	1
			4915	3097	869	927	22		
1	B	608	Total	C	N	O	S	0	1
			4915	3097	869	927	22		
1	C	608	Total	C	N	O	S	0	1
			4915	3097	869	927	22		

There are 6 discrepancies between the modelled and reference sequences:

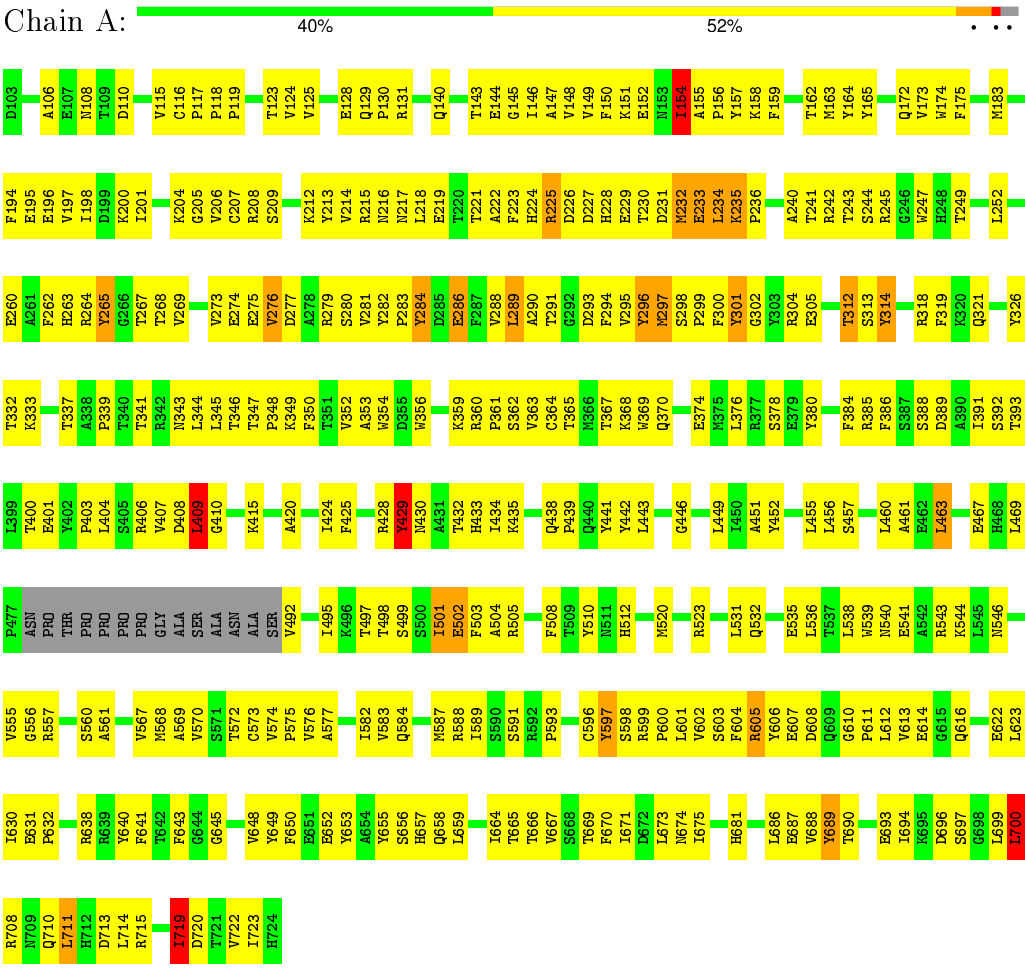
Chain	Residue	Modelled	Actual	Comment	Reference
A	313	SER	THR	CONFLICT	UNP P06437
A	443	LEU	GLN	CONFLICT	UNP P06437
B	313	SER	THR	CONFLICT	UNP P06437
B	443	LEU	GLN	CONFLICT	UNP P06437
C	313	SER	THR	CONFLICT	UNP P06437
C	443	LEU	GLN	CONFLICT	UNP P06437

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

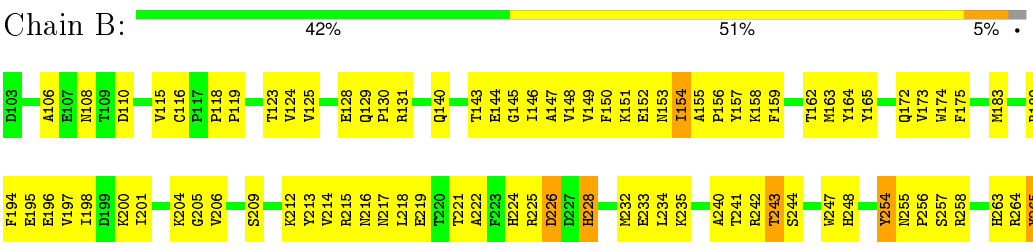
- Molecule 1: ENVELOPE GLYCOPROTEIN B

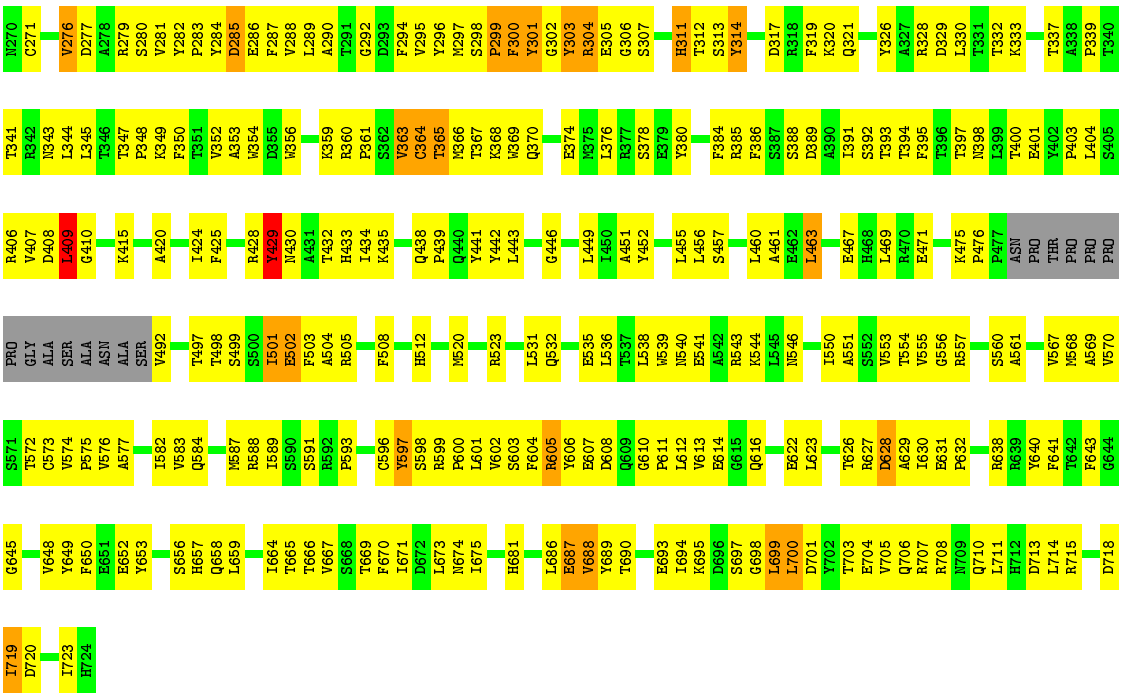
Chain A:



- Molecule 1: ENVELOPE GLYCOPROTEIN B

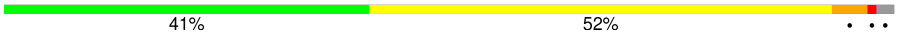
Chain B:

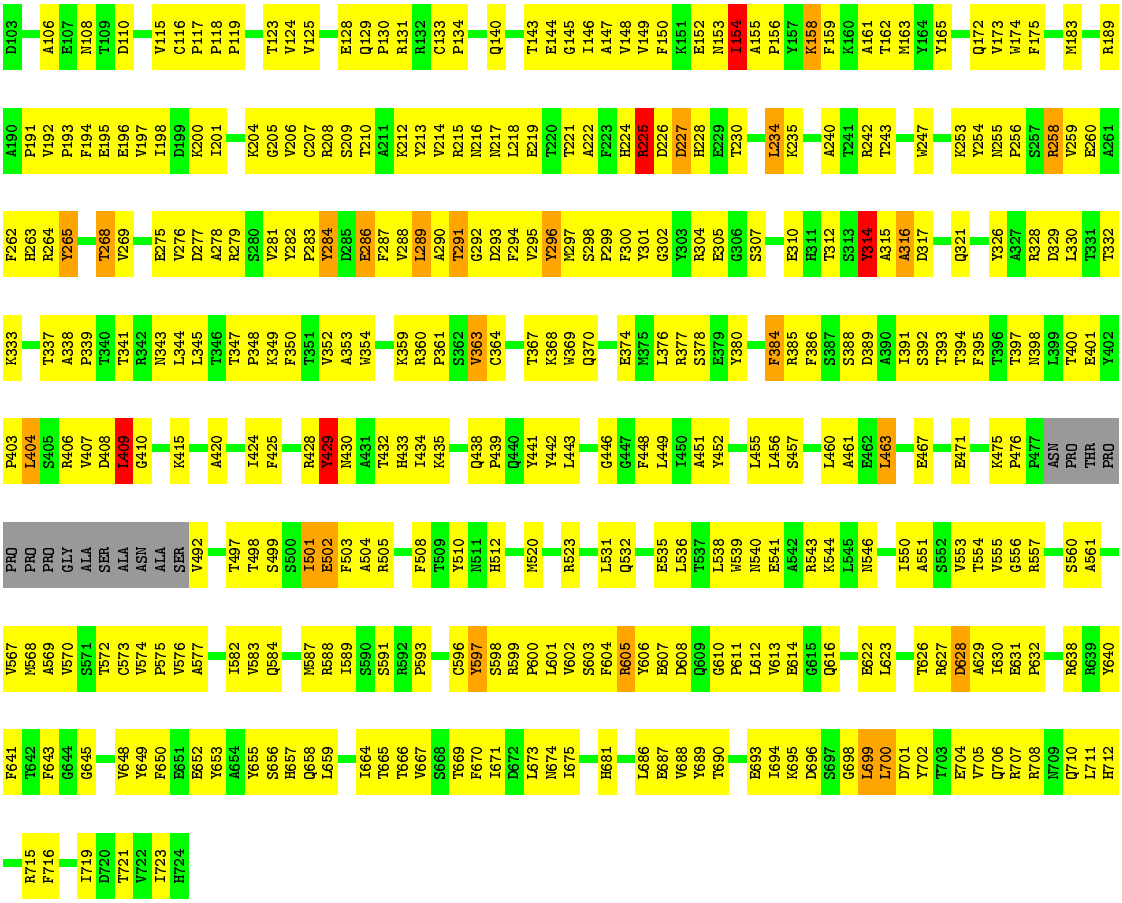




• Molecule 1: ENVELOPE GLYCOPROTEIN B

Chain C:





4 Experimental information (i)

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	LOW PASS FILTER TO THE FIRST ZERO CROSSING OF THE CTF	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	Depositor
Image detector	ULTRASCAN 4000	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	1.04	0/5036	1.12	3/6840 (0.0%)
1	B	1.04	0/5036	1.10	1/6840 (0.0%)
1	C	1.04	0/5036	1.11	1/6840 (0.0%)
All	All	1.04	0/15108	1.11	5/20520 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16
1	B	0	13
1	C	0	12
All	All	0	41

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	702	TYR	CA-CB-CG	-6.86	100.36	113.40
1	B	429	TYR	CA-CB-CG	-6.57	100.92	113.40
1	C	429	TYR	CA-CB-CG	-6.56	100.94	113.40
1	A	429	TYR	CA-CB-CG	-6.54	100.97	113.40
1	A	702	TYR	CB-CG-CD1	-5.92	117.45	121.00

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	ILE	Peptide
1	A	225	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	228	HIS	Peptide
1	A	284	TYR	Peptide
1	A	362	SER	Peptide
1	A	363	VAL	Peptide
1	A	365	THR	Peptide
1	A	409	LEU	Peptide
1	A	429	TYR	Peptide
1	A	460	LEU	Peptide
1	A	501	ILE	Peptide
1	A	628	ASP	Peptide
1	A	700	LEU	Peptide
1	A	701	ASP	Peptide
1	A	702	TYR	Peptide
1	A	719	ILE	Peptide
1	B	154	ILE	Peptide
1	B	284	TYR	Peptide
1	B	299	PRO	Peptide
1	B	311	HIS	Peptide
1	B	363	VAL	Peptide
1	B	364	CYS	Peptide
1	B	365	THR	Peptide
1	B	409	LEU	Peptide
1	B	429	TYR	Peptide
1	B	460	LEU	Peptide
1	B	501	ILE	Peptide
1	B	628	ASP	Peptide
1	B	719	ILE	Peptide
1	C	154	ILE	Peptide
1	C	225	ARG	Peptide
1	C	314	TYR	Peptide
1	C	316	ALA	Peptide
1	C	363	VAL	Peptide
1	C	409	LEU	Peptide
1	C	429	TYR	Peptide
1	C	460	LEU	Peptide
1	C	501	ILE	Peptide
1	C	628	ASP	Peptide
1	C	699	LEU	Peptide
1	C	719	ILE	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	4915	0	4740	548	0
1	B	4915	0	4740	554	0
1	C	4915	0	4740	551	0
All	All	14745	0	14220	1396	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 48.

All (1396) 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:B:699:LEU:HD13	1:C:281:VAL:HG13	1.26	1.14
1:C:408:ASP:HB2	1:C:492:VAL:HG13	1.14	1.14
1:B:706:GLN:HG3	1:C:699:LEU:HD21	1.26	1.13
1:B:700:LEU:HB2	1:C:279:ARG:HG2	1.32	1.11
1:A:397:THR:HG21	1:A:442:TYR:HB3	1.33	1.11
1:B:397:THR:HG21	1:B:442:TYR:HB3	1.33	1.10
1:A:408:ASP:HB2	1:A:492:VAL:HG13	1.19	1.10
1:C:154:ILE:HG13	1:C:155:ALA:HA	1.22	1.10
1:A:700:LEU:HG	1:B:158:LYS:HE3	1.28	1.09
1:C:363:VAL:HG11	1:C:409:LEU:HD13	1.08	1.08
1:B:700:LEU:HG	1:C:158:LYS:HE3	1.36	1.08
1:C:363:VAL:HG13	1:C:364:CYS:HA	1.34	1.07
1:B:408:ASP:HB2	1:B:492:VAL:HG13	1.16	1.07
1:A:699:LEU:HA	1:A:700:LEU:HD13	1.12	1.06
1:B:711:LEU:HD21	1:C:242:ARG:HB2	1.35	1.06
1:C:397:THR:HG21	1:C:442:TYR:HB3	1.33	1.06
1:A:701:ASP:H	1:B:158:LYS:HE2	1.14	1.05
1:A:240:ALA:HB3	1:A:243:THR:HG21	1.37	1.05
1:A:700:LEU:HD21	1:B:156:PRO:HB3	1.40	1.04
1:C:240:ALA:HB3	1:C:243:THR:HG21	1.37	1.04
1:A:154:ILE:HG13	1:A:155:ALA:HA	1.39	1.03
1:A:711:LEU:HD11	1:B:240:ALA:HB3	1.40	1.03
1:C:291:THR:HG23	1:C:293:ASP:H	1.22	1.03
1:A:391:ILE:HG22	1:A:393:THR:HG23	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:LEU:HD21	1:B:240:ALA:HB1	1.42	1.02
1:A:313:SER:HB2	1:A:314:TYR:HA	1.40	1.00
1:B:391:ILE:HG22	1:B:393:THR:HG23	1.41	1.00
1:C:391:ILE:HG22	1:C:393:THR:HG23	1.41	1.00
1:A:723:ILE:HB	1:C:217:ASN:HB3	1.42	1.00
1:C:312:THR:HG23	1:C:314:TYR:HB2	1.44	0.99
1:C:299:PRO:HA	1:C:354:TRP:HE1	1.27	0.99
1:C:286:GLU:HG2	1:C:294:PHE:HD2	1.27	0.99
1:A:707:ARG:HG2	1:B:242:ARG:HG2	1.46	0.98
1:A:209:SER:HB3	1:A:224:HIS:HB3	1.46	0.97
1:C:605:ARG:HD3	1:C:607:GLU:H	1.26	0.96
1:B:688:VAL:HG13	1:C:369:TRP:CH2	2.02	0.95
1:A:298:SER:HB2	1:A:301:TYR:CD1	2.01	0.95
1:A:719:ILE:HG23	1:A:720:ASP:HA	1.48	0.95
1:B:605:ARG:HD3	1:B:607:GLU:H	1.31	0.95
1:C:204:LYS:HB3	1:C:206:VAL:HG22	1.49	0.95
1:C:601:LEU:HD23	1:C:627:ARG:HD3	1.50	0.94
1:A:601:LEU:HD23	1:A:627:ARG:HD3	1.49	0.94
1:A:605:ARG:HD3	1:A:607:GLU:H	1.31	0.94
1:B:601:LEU:HD23	1:B:627:ARG:HD3	1.50	0.93
1:B:700:LEU:CG	1:C:158:LYS:HE3	1.99	0.93
1:A:711:LEU:HD13	1:B:243:THR:HG23	1.51	0.92
1:A:172:GLN:HB2	1:A:183:MET:HB2	1.50	0.92
1:A:699:LEU:HB3	1:A:700:LEU:HD22	1.52	0.91
1:B:708:ARG:HE	1:C:290:ALA:HA	1.34	0.91
1:C:297:MET:HB2	1:C:345:LEU:HD22	1.51	0.91
1:C:299:PRO:HA	1:C:354:TRP:NE1	1.86	0.91
1:A:224:HIS:HB2	1:A:269:VAL:HB	1.53	0.91
1:C:456:LEU:CD2	1:C:461:ALA:HA	2.01	0.91
1:B:688:VAL:HG11	1:C:448:PHE:HE2	1.36	0.90
1:A:298:SER:HB2	1:A:301:TYR:CE1	2.07	0.90
1:A:456:LEU:CD2	1:A:461:ALA:HA	2.01	0.90
1:B:242:ARG:HH12	1:C:284:TYR:HD2	1.20	0.90
1:C:388:SER:HB3	1:C:391:ILE:HB	1.53	0.90
1:B:456:LEU:CD2	1:B:461:ALA:HA	2.01	0.90
1:C:408:ASP:CB	1:C:492:VAL:HG13	2.02	0.90
1:C:374:GLU:HB2	1:C:428:ARG:HH12	1.37	0.90
1:A:408:ASP:CB	1:A:492:VAL:HG13	2.03	0.89
1:C:154:ILE:HG13	1:C:156:PRO:HD3	1.52	0.89
1:B:311:HIS:CE1	1:B:313:SER:HB3	2.08	0.89
1:B:408:ASP:CB	1:B:492:VAL:HG13	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:LEU:HD22	1:C:290:ALA:H	1.38	0.88
1:B:388:SER:HB3	1:B:391:ILE:HB	1.53	0.88
1:A:374:GLU:HB2	1:A:428:ARG:HH12	1.37	0.88
1:A:175:PHE:CD2	1:A:258:ARG:HG3	2.08	0.88
1:A:707:ARG:HG2	1:B:242:ARG:HA	1.54	0.88
1:B:374:GLU:HB2	1:B:428:ARG:HH12	1.37	0.88
1:A:456:LEU:HD21	1:A:461:ALA:HA	1.55	0.88
1:A:388:SER:HB3	1:A:391:ILE:HB	1.53	0.87
1:C:286:GLU:HG2	1:C:294:PHE:CD2	2.09	0.87
1:B:700:LEU:HB3	1:C:279:ARG:NH1	1.90	0.87
1:B:706:GLN:HG3	1:C:699:LEU:CD2	2.03	0.87
1:B:363:VAL:HG21	1:B:409:LEU:HD13	1.57	0.87
1:A:708:ARG:HH11	1:B:244:SER:HB2	1.37	0.87
1:C:456:LEU:HD21	1:C:461:ALA:HA	1.55	0.86
1:B:456:LEU:HD21	1:B:461:ALA:HA	1.55	0.86
1:C:363:VAL:HG13	1:C:364:CYS:CA	2.04	0.86
1:B:116:CYS:HB3	1:B:560:SER:HB2	1.58	0.85
1:B:363:VAL:CG2	1:B:409:LEU:HD13	2.06	0.85
1:A:116:CYS:HB3	1:A:560:SER:HB2	1.58	0.85
1:B:699:LEU:HA	1:C:156:PRO:HB3	1.55	0.85
1:A:602:VAL:HG21	1:A:623:LEU:HD22	1.59	0.85
1:C:116:CYS:HB3	1:C:560:SER:HB2	1.58	0.85
1:A:158:LYS:HE3	1:C:700:LEU:HD13	1.58	0.85
1:C:602:VAL:HG21	1:C:623:LEU:HD22	1.58	0.85
1:A:175:PHE:CZ	1:A:258:ARG:HA	2.11	0.85
1:B:297:MET:HG2	1:B:354:TRP:HH2	1.39	0.84
1:A:699:LEU:CA	1:A:700:LEU:HD13	2.03	0.84
1:B:711:LEU:CD2	1:C:242:ARG:HB2	2.08	0.84
1:B:281:VAL:HG13	1:B:282:TYR:HD1	1.41	0.84
1:C:603:SER:HB3	1:C:612:LEU:HD21	1.58	0.83
1:A:708:ARG:NH1	1:B:244:SER:HB2	1.91	0.83
1:A:603:SER:HB3	1:A:612:LEU:HD21	1.58	0.83
1:C:225:ARG:HA	1:C:254:TYR:CD2	2.14	0.83
1:A:328:ARG:NH2	1:A:333:LYS:HD3	1.93	0.83
1:A:397:THR:HG23	1:A:443:LEU:O	1.79	0.83
1:B:603:SER:HB3	1:B:612:LEU:HD21	1.58	0.82
1:B:706:GLN:CG	1:C:699:LEU:HD21	2.06	0.82
1:C:288:VAL:CG1	1:C:292:GLY:HA2	2.09	0.82
1:C:154:ILE:CG1	1:C:155:ALA:HA	2.05	0.82
1:B:689:TYR:HD2	1:B:694:ILE:HD11	1.44	0.82
1:C:328:ARG:NH2	1:C:333:LYS:HD3	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:VAL:HG21	1:B:623:LEU:HD22	1.58	0.82
1:A:699:LEU:HD23	1:A:700:LEU:HD22	1.61	0.82
1:B:700:LEU:CD1	1:C:158:LYS:HE3	2.10	0.82
1:A:299:PRO:HA	1:A:354:TRP:HE1	1.44	0.81
1:C:286:GLU:HG3	1:C:295:VAL:O	1.80	0.81
1:C:298:SER:HB3	1:C:300:PHE:CD2	2.15	0.81
1:B:397:THR:HG23	1:B:443:LEU:O	1.79	0.81
1:A:290:ALA:HB3	1:C:716:PHE:CE2	2.15	0.81
1:B:688:VAL:HG11	1:C:448:PHE:CE2	2.14	0.81
1:A:714:LEU:HD21	1:C:296:TYR:HB3	1.61	0.81
1:B:699:LEU:HD13	1:C:281:VAL:CG1	2.10	0.81
1:A:687:GLU:OE2	1:C:499:SER:HB2	1.80	0.81
1:A:293:ASP:HA	1:B:713:ASP:OD2	1.81	0.80
1:B:697:SER:HA	1:C:154:ILE:HG21	1.63	0.80
1:C:397:THR:HG23	1:C:443:LEU:O	1.80	0.80
1:C:159:PHE:CZ	1:C:299:PRO:HG3	2.16	0.80
1:A:700:LEU:HB2	1:B:279:ARG:NH2	1.97	0.80
1:C:616:GLN:OE1	1:C:627:ARG:HA	1.82	0.80
1:A:711:LEU:HD11	1:B:240:ALA:CB	2.11	0.80
1:B:616:GLN:OE1	1:B:627:ARG:HA	1.82	0.80
1:B:700:LEU:HD12	1:C:158:LYS:HG2	1.64	0.80
1:A:616:GLN:OE1	1:A:627:ARG:HA	1.82	0.80
1:A:707:ARG:CG	1:B:242:ARG:HA	2.12	0.79
1:C:204:LYS:CB	1:C:206:VAL:HG22	2.12	0.79
1:B:305:GLU:HG3	1:B:306:GLY:H	1.45	0.79
1:B:700:LEU:CB	1:C:279:ARG:HG2	2.12	0.79
1:A:279:ARG:NH2	1:C:700:LEU:HD12	1.97	0.79
1:B:700:LEU:HD21	1:B:704:GLU:CD	2.03	0.79
1:B:601:LEU:HD23	1:B:627:ARG:CD	2.13	0.79
1:A:707:ARG:O	1:B:242:ARG:HB3	1.82	0.78
1:C:601:LEU:HD23	1:C:627:ARG:CD	2.13	0.78
1:B:328:ARG:NH2	1:B:333:LYS:HD3	1.99	0.78
1:A:700:LEU:HG	1:B:158:LYS:CE	2.13	0.78
1:B:687:GLU:OE1	1:B:690:THR:HG22	1.83	0.78
1:A:699:LEU:CB	1:A:700:LEU:HD22	2.13	0.78
1:B:297:MET:HG2	1:B:354:TRP:CH2	2.19	0.78
1:A:699:LEU:HA	1:A:700:LEU:CD1	2.06	0.77
1:A:707:ARG:HG2	1:B:242:ARG:CG	2.14	0.77
1:A:276:VAL:HG11	1:C:715:ARG:NH1	2.00	0.77
1:B:708:ARG:HH21	1:C:290:ALA:HB2	1.49	0.77
1:A:616:GLN:CD	1:A:627:ARG:HA	2.05	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:ILE:HG23	1:A:720:ASP:CA	2.14	0.77
1:A:601:LEU:HD23	1:A:627:ARG:CD	2.13	0.77
1:B:700:LEU:HD23	1:B:704:GLU:HB3	1.67	0.77
1:C:240:ALA:HB3	1:C:243:THR:CG2	2.15	0.76
1:A:711:LEU:HG	1:B:241:THR:O	1.84	0.76
1:C:616:GLN:CD	1:C:627:ARG:HA	2.05	0.76
1:A:605:ARG:CD	1:A:607:GLU:H	1.99	0.76
1:A:543:ARG:HA	1:A:550:ILE:HG12	1.66	0.76
1:B:364:CYS:HB2	1:B:409:LEU:HB3	1.66	0.76
1:B:605:ARG:CD	1:B:607:GLU:H	1.99	0.76
1:A:312:THR:HG23	1:A:314:TYR:HB2	1.68	0.76
1:B:688:VAL:HG13	1:C:369:TRP:CZ2	2.21	0.76
1:C:253:LYS:HA	1:C:268:THR:HG21	1.65	0.76
1:B:209:SER:HB2	1:B:224:HIS:HB3	1.67	0.76
1:B:543:ARG:HA	1:B:550:ILE:HG12	1.66	0.76
1:A:499:SER:HB2	1:B:687:GLU:OE2	1.85	0.76
1:A:699:LEU:CG	1:A:700:LEU:HD22	2.16	0.76
1:B:708:ARG:NH1	1:C:277:ASP:HB2	2.01	0.76
1:B:616:GLN:CD	1:B:627:ARG:HA	2.05	0.76
1:A:713:ASP:HB2	1:C:294:PHE:CD1	2.21	0.75
1:C:690:THR:OG1	1:C:693:GLU:HG3	1.85	0.75
1:A:425:PHE:CE2	1:A:430:ASN:HA	2.22	0.75
1:A:240:ALA:HB3	1:A:243:THR:CG2	2.16	0.75
1:B:299:PRO:CA	1:B:354:TRP:HE1	2.00	0.75
1:C:296:TYR:H	1:C:296:TYR:HD1	1.34	0.75
1:B:551:ALA:O	1:B:555:VAL:HG22	1.87	0.75
1:C:425:PHE:CE2	1:C:430:ASN:HA	2.22	0.75
1:A:233:GLU:O	1:A:249:THR:HG22	1.87	0.75
1:C:286:GLU:CD	1:C:294:PHE:HB3	2.06	0.75
1:C:551:ALA:O	1:C:555:VAL:HG22	1.87	0.75
1:A:158:LYS:NZ	1:C:700:LEU:HD22	2.03	0.74
1:A:707:ARG:NE	1:B:242:ARG:HA	2.02	0.74
1:A:175:PHE:CE2	1:A:258:ARG:HA	2.21	0.74
1:A:551:ALA:O	1:A:555:VAL:HG22	1.87	0.74
1:A:614:GLU:HG3	1:A:627:ARG:NH2	2.03	0.74
1:C:614:GLU:HG3	1:C:627:ARG:NH2	2.03	0.74
1:C:314:TYR:HB3	1:C:315:ALA:O	1.88	0.74
1:C:543:ARG:HA	1:C:550:ILE:HG12	1.66	0.74
1:B:700:LEU:HB2	1:C:279:ARG:CG	2.16	0.73
1:C:695:LYS:NZ	1:C:702:TYR:HB3	2.01	0.73
1:C:163:MET:HG3	1:C:276:VAL:HG21	1.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:LEU:HD11	1:B:156:PRO:HG3	1.70	0.73
1:A:242:ARG:O	1:C:711:LEU:HD21	1.87	0.73
1:A:700:LEU:CD2	1:B:156:PRO:HB3	2.18	0.73
1:B:707:ARG:HH21	1:C:242:ARG:HG2	1.53	0.73
1:B:614:GLU:HG3	1:B:627:ARG:NH2	2.03	0.73
1:B:425:PHE:CE2	1:B:430:ASN:HA	2.22	0.73
1:A:154:ILE:CG1	1:A:155:ALA:HA	2.18	0.73
1:A:312:THR:HG23	1:A:314:TYR:CB	2.18	0.73
1:A:313:SER:HB2	1:A:314:TYR:HD1	1.53	0.73
1:C:289:LEU:HD22	1:C:290:ALA:N	2.03	0.73
1:C:286:GLU:CG	1:C:294:PHE:HB3	2.19	0.73
1:A:531:LEU:O	1:A:535:GLU:HG2	1.89	0.73
1:B:719:ILE:HB	1:B:720:ASP:O	1.87	0.73
1:B:531:LEU:O	1:B:535:GLU:HG2	1.89	0.73
1:B:157:TYR:CE2	1:B:300:PHE:HE1	2.07	0.72
1:A:597:TYR:HD1	1:A:599:ARG:H	1.36	0.72
1:C:531:LEU:O	1:C:535:GLU:HG2	1.89	0.72
1:B:605:ARG:NH1	1:B:610:GLY:H	1.88	0.72
1:A:289:LEU:HD22	1:A:290:ALA:H	1.54	0.72
1:A:690:THR:OG1	1:A:693:GLU:HG3	1.89	0.72
1:C:605:ARG:CD	1:C:607:GLU:H	1.99	0.72
1:A:312:THR:CG2	1:A:314:TYR:HB2	2.20	0.72
1:A:605:ARG:NH1	1:A:610:GLY:H	1.87	0.72
1:A:206:VAL:HG12	1:A:233:GLU:OE2	1.90	0.72
1:C:297:MET:CE	1:C:298:SER:H	2.03	0.71
1:B:689:TYR:CD2	1:B:694:ILE:HD11	2.24	0.71
1:B:256:PRO:HG3	1:B:265:TYR:C	2.10	0.71
1:C:605:ARG:NH1	1:C:610:GLY:H	1.88	0.71
1:A:290:ALA:HB3	1:C:716:PHE:HE2	1.53	0.71
1:A:699:LEU:CD2	1:A:700:LEU:HD22	2.20	0.71
1:B:601:LEU:CD2	1:B:627:ARG:HD3	2.20	0.71
1:A:297:MET:HG2	1:A:345:LEU:HD22	1.71	0.71
1:B:294:PHE:CZ	1:C:710:GLN:HB3	2.25	0.71
1:B:597:TYR:HD1	1:B:599:ARG:H	1.36	0.71
1:B:698:GLY:O	1:C:156:PRO:HG3	1.91	0.71
1:C:597:TYR:HD1	1:C:599:ARG:H	1.36	0.71
1:B:193:PRO:O	1:B:197:VAL:HG23	1.91	0.71
1:B:172:GLN:HB2	1:B:183:MET:HB2	1.71	0.71
1:C:360:ARG:HB2	1:C:361:PRO:HD3	1.73	0.71
1:B:175:PHE:CZ	1:B:258:ARG:HA	2.26	0.70
1:A:193:PRO:O	1:A:197:VAL:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:VAL:CG1	1:C:364:CYS:HA	2.19	0.70
1:A:638:ARG:HG3	1:A:649:TYR:HE1	1.56	0.70
1:A:689:TYR:CD2	1:A:694:ILE:HD11	2.25	0.70
1:A:256:PRO:HG3	1:A:265:TYR:C	2.12	0.70
1:B:674:ASN:O	1:C:523:ARG:HD2	1.90	0.70
1:A:290:ALA:HB2	1:C:715:ARG:NH2	2.06	0.70
1:A:546:ASN:O	1:A:550:ILE:HD13	1.92	0.70
1:A:674:ASN:O	1:B:523:ARG:HD2	1.90	0.70
1:B:638:ARG:HG3	1:B:649:TYR:HE1	1.56	0.70
1:A:217:ASN:ND2	1:B:723:ILE:H	1.89	0.70
1:B:360:ARG:HB2	1:B:361:PRO:HD3	1.74	0.70
1:B:217:ASN:CG	1:C:723:ILE:HG22	2.12	0.70
1:B:700:LEU:HB3	1:C:279:ARG:CZ	2.21	0.70
1:A:707:ARG:HG2	1:B:242:ARG:CA	2.22	0.70
1:B:708:ARG:NH2	1:C:290:ALA:HB2	2.05	0.70
1:A:523:ARG:HD2	1:C:674:ASN:O	1.90	0.70
1:B:285:ASP:HA	1:B:298:SER:HB2	1.74	0.70
1:C:546:ASN:O	1:C:550:ILE:HD13	1.92	0.70
1:B:546:ASN:O	1:B:550:ILE:HD13	1.92	0.69
1:A:601:LEU:CD2	1:A:627:ARG:HD3	2.20	0.69
1:B:613:VAL:HG12	1:B:614:GLU:O	1.93	0.69
1:C:193:PRO:O	1:C:197:VAL:HG23	1.91	0.69
1:C:156:PRO:HG2	1:C:158:LYS:NZ	2.07	0.69
1:C:601:LEU:CD2	1:C:627:ARG:HD3	2.20	0.69
1:C:638:ARG:HG3	1:C:649:TYR:HE1	1.56	0.69
1:C:329:ASP:HB3	1:C:332:THR:OG1	1.93	0.69
1:A:550:ILE:O	1:A:553:VAL:HG12	1.93	0.69
1:C:613:VAL:HG12	1:C:614:GLU:O	1.93	0.69
1:A:329:ASP:HB3	1:A:332:THR:OG1	1.93	0.69
1:A:715:ARG:HD2	1:B:243:THR:CG2	2.22	0.69
1:C:161:ALA:HB3	1:C:276:VAL:HB	1.75	0.69
1:A:711:LEU:CD1	1:B:243:THR:HG23	2.20	0.69
1:A:613:VAL:HG12	1:A:614:GLU:O	1.92	0.69
1:C:228:HIS:O	1:C:230:THR:HG23	1.93	0.69
1:B:550:ILE:O	1:B:553:VAL:HG12	1.93	0.69
1:C:163:MET:HG3	1:C:276:VAL:CG2	2.22	0.69
1:A:207:CYS:O	1:A:231:ASP:HB2	1.92	0.68
1:A:723:ILE:CB	1:C:217:ASN:HB3	2.20	0.68
1:A:301:TYR:HD1	1:A:301:TYR:H	1.41	0.68
1:B:388:SER:OG	1:B:391:ILE:HG13	1.93	0.68
1:C:550:ILE:O	1:C:553:VAL:HG12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:CYS:CB	1:B:409:LEU:HB3	2.22	0.68
1:A:699:LEU:HD23	1:A:700:LEU:CD2	2.23	0.68
1:A:289:LEU:HD22	1:A:290:ALA:N	2.09	0.68
1:B:329:ASP:HB3	1:B:332:THR:OG1	1.93	0.68
1:A:406:ARG:O	1:A:492:VAL:HA	1.93	0.68
1:B:711:LEU:HD21	1:C:242:ARG:CB	2.19	0.68
1:A:605:ARG:NH2	1:A:611:PRO:HD2	2.09	0.68
1:A:276:VAL:HG11	1:C:715:ARG:CZ	2.24	0.68
1:B:605:ARG:NH2	1:B:611:PRO:HD2	2.09	0.68
1:B:281:VAL:HG13	1:B:282:TYR:CD1	2.26	0.68
1:C:603:SER:CB	1:C:612:LEU:HD21	2.24	0.68
1:C:388:SER:OG	1:C:391:ILE:HG13	1.93	0.67
1:C:145:GLY:HA3	1:C:452:TYR:CZ	2.30	0.67
1:A:555:VAL:HG23	1:A:557:ARG:H	1.59	0.67
1:B:145:GLY:HA3	1:B:452:TYR:CZ	2.29	0.67
1:A:299:PRO:CA	1:A:354:TRP:HE1	2.07	0.67
1:A:194:PHE:O	1:A:198:ILE:HD13	1.95	0.67
1:B:699:LEU:CA	1:C:156:PRO:HB3	2.25	0.67
1:A:360:ARG:HB2	1:A:361:PRO:HD3	1.75	0.67
1:A:388:SER:OG	1:A:391:ILE:HG13	1.93	0.67
1:C:605:ARG:HD2	1:C:607:GLU:O	1.95	0.67
1:A:603:SER:CB	1:A:612:LEU:HD21	2.25	0.67
1:A:289:LEU:HD13	1:A:290:ALA:N	2.08	0.67
1:B:538:LEU:HD21	1:C:539:TRP:CD2	2.30	0.67
1:A:172:GLN:CB	1:A:183:MET:HB2	2.24	0.67
1:A:145:GLY:HA3	1:A:452:TYR:CZ	2.29	0.67
1:C:695:LYS:HZ1	1:C:702:TYR:HB3	1.58	0.67
1:B:603:SER:CB	1:B:612:LEU:HD21	2.24	0.67
1:B:700:LEU:H	1:C:279:ARG:CZ	2.06	0.67
1:A:699:LEU:HD12	1:A:699:LEU:H	1.59	0.67
1:B:555:VAL:HG23	1:B:557:ARG:H	1.60	0.67
1:A:538:LEU:HD21	1:B:539:TRP:CD2	2.30	0.67
1:A:289:LEU:HD13	1:A:290:ALA:H	1.59	0.67
1:C:143:THR:HG22	1:C:144:GLU:O	1.95	0.67
1:C:194:PHE:O	1:C:198:ILE:HD13	1.94	0.67
1:B:700:LEU:CD2	1:B:704:GLU:HB3	2.25	0.66
1:A:701:ASP:H	1:B:158:LYS:CE	2.02	0.66
1:B:143:THR:HG22	1:B:144:GLU:O	1.95	0.66
1:C:406:ARG:O	1:C:492:VAL:HA	1.94	0.66
1:A:707:ARG:CD	1:B:242:ARG:HA	2.24	0.66
1:A:539:TRP:CD2	1:C:538:LEU:HD21	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:VAL:HG23	1:C:557:ARG:H	1.60	0.66
1:A:156:PRO:HG2	1:C:700:LEU:HG	1.76	0.66
1:B:719:ILE:HB	1:B:720:ASP:C	2.16	0.66
1:B:499:SER:HB2	1:C:687:GLU:OE2	1.95	0.66
1:B:194:PHE:O	1:B:198:ILE:HD13	1.95	0.66
1:B:204:LYS:CB	1:B:206:VAL:HG22	2.26	0.66
1:B:224:HIS:HB2	1:B:269:VAL:HB	1.78	0.66
1:C:425:PHE:CE1	1:C:429:TYR:HB3	2.31	0.66
1:B:700:LEU:HD12	1:C:158:LYS:CG	2.25	0.66
1:B:425:PHE:CE1	1:B:429:TYR:HB3	2.31	0.66
1:B:699:LEU:HB3	1:C:156:PRO:HB3	1.78	0.66
1:B:707:ARG:NH2	1:C:242:ARG:HG2	2.11	0.66
1:B:297:MET:HB2	1:B:345:LEU:HD22	1.78	0.66
1:C:172:GLN:HB2	1:C:183:MET:HB2	1.78	0.66
1:B:520:MET:HE2	1:B:520:MET:HA	1.79	0.66
1:B:106:ALA:HA	1:B:643:PHE:CE2	2.31	0.66
1:A:313:SER:CB	1:A:314:TYR:HA	2.14	0.65
1:A:711:LEU:HB2	1:B:242:ARG:O	1.96	0.65
1:B:294:PHE:HZ	1:C:710:GLN:HB3	1.59	0.65
1:A:700:LEU:HB2	1:B:279:ARG:CZ	2.26	0.65
1:A:700:LEU:CG	1:B:158:LYS:HE3	2.16	0.65
1:A:425:PHE:CE1	1:A:429:TYR:HB3	2.31	0.65
1:A:290:ALA:HB2	1:C:715:ARG:CZ	2.26	0.65
1:B:406:ARG:O	1:B:492:VAL:HA	1.95	0.65
1:C:520:MET:HE2	1:C:520:MET:HA	1.78	0.65
1:B:700:LEU:HG	1:C:158:LYS:CE	2.22	0.65
1:A:714:LEU:HG	1:C:286:GLU:OE1	1.97	0.65
1:C:605:ARG:NH2	1:C:611:PRO:HD2	2.12	0.65
1:C:291:THR:HG23	1:C:293:ASP:N	2.03	0.65
1:A:707:ARG:NH1	1:B:243:THR:H	1.95	0.65
1:C:254:TYR:HB2	1:C:268:THR:HG23	1.79	0.65
1:B:700:LEU:CD1	1:C:158:LYS:HB3	2.27	0.64
1:A:106:ALA:HA	1:A:643:PHE:CE2	2.33	0.64
1:A:143:THR:HG22	1:A:144:GLU:O	1.95	0.64
1:A:151:LYS:HD2	1:C:688:VAL:CG1	2.27	0.64
1:B:321:GLN:HE21	1:B:341:THR:HG21	1.62	0.64
1:A:321:GLN:HE21	1:A:341:THR:HG21	1.62	0.64
1:A:713:ASP:OD2	1:C:293:ASP:HA	1.96	0.64
1:A:707:ARG:CG	1:B:242:ARG:HG2	2.24	0.64
1:C:106:ALA:HA	1:C:643:PHE:CE2	2.31	0.64
1:C:189:ARG:HH11	1:C:349:LYS:HD3	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:LEU:HB3	1:C:156:PRO:HA	1.79	0.64
1:A:605:ARG:HD2	1:A:607:GLU:O	1.98	0.64
1:A:659:LEU:N	1:A:659:LEU:HD12	2.13	0.64
1:C:701:ASP:O	1:C:705:VAL:HG23	1.98	0.64
1:A:699:LEU:HB2	1:C:702:TYR:HE2	1.62	0.64
1:C:297:MET:HE2	1:C:298:SER:H	1.62	0.64
1:B:605:ARG:HD2	1:B:607:GLU:O	1.98	0.64
1:B:289:LEU:HB2	1:B:292:GLY:H	1.63	0.64
1:A:281:VAL:HB	1:A:282:TYR:CD2	2.33	0.64
1:C:321:GLN:HE21	1:C:341:THR:HG21	1.62	0.64
1:A:715:ARG:HD2	1:B:243:THR:HG23	1.79	0.63
1:B:540:ASN:O	1:B:543:ARG:HG2	1.98	0.63
1:B:321:GLN:NE2	1:B:341:THR:HG21	2.13	0.63
1:B:189:ARG:HH11	1:B:349:LYS:HD3	1.63	0.63
1:A:106:ALA:HA	1:A:643:PHE:HE2	1.62	0.63
1:A:364:CYS:HB2	1:A:409:LEU:HB3	1.79	0.63
1:A:189:ARG:HH11	1:A:349:LYS:HD3	1.63	0.63
1:A:707:ARG:HG2	1:B:242:ARG:CB	2.29	0.63
1:B:156:PRO:HG2	1:B:158:LYS:HZ2	1.63	0.63
1:B:157:TYR:CZ	1:B:300:PHE:HE1	2.17	0.63
1:C:321:GLN:NE2	1:C:341:THR:HG21	2.13	0.63
1:A:540:ASN:O	1:A:543:ARG:HG2	1.98	0.63
1:B:706:GLN:O	1:B:710:GLN:HG3	1.97	0.63
1:C:540:ASN:O	1:C:543:ARG:HG2	1.98	0.63
1:B:659:LEU:N	1:B:659:LEU:HD12	2.13	0.63
1:A:673:LEU:HG	1:A:675:ILE:HG12	1.81	0.63
1:B:699:LEU:H	1:B:699:LEU:HD12	1.63	0.63
1:A:408:ASP:HB2	1:A:492:VAL:CG1	2.13	0.63
1:A:290:ALA:N	1:C:708:ARG:HH21	1.97	0.63
1:A:321:GLN:NE2	1:A:341:THR:HG21	2.13	0.63
1:A:520:MET:HA	1:A:520:MET:HE2	1.80	0.62
1:B:311:HIS:HE1	1:B:313:SER:HB3	1.58	0.62
1:B:225:ARG:HG3	1:B:254:TYR:CE2	2.34	0.62
1:C:154:ILE:CG1	1:C:156:PRO:HD3	2.26	0.62
1:B:699:LEU:HD22	1:C:281:VAL:O	2.00	0.62
1:C:442:TYR:O	1:C:449:LEU:HD12	1.99	0.62
1:A:706:GLN:HA	1:A:706:GLN:OE1	1.99	0.62
1:B:589:ILE:HD11	1:B:630:ILE:HD13	1.82	0.62
1:B:401:GLU:HB2	1:B:476:PRO:HD3	1.81	0.62
1:B:442:TYR:O	1:B:449:LEU:HD12	1.99	0.62
1:C:401:GLU:HB2	1:C:476:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:SER:O	1:A:593:PRO:HD3	1.99	0.62
1:A:401:GLU:HB2	1:A:476:PRO:HD3	1.81	0.62
1:C:572:THR:HG22	1:C:573:CYS:N	2.14	0.62
1:C:659:LEU:HD12	1:C:659:LEU:N	2.13	0.62
1:A:699:LEU:HD12	1:A:699:LEU:N	2.14	0.62
1:A:589:ILE:HD11	1:A:630:ILE:HD13	1.82	0.62
1:A:224:HIS:CE1	1:A:225:ARG:HB2	2.35	0.62
1:A:208:ARG:HA	1:A:231:ASP:HB3	1.82	0.62
1:C:288:VAL:HG11	1:C:292:GLY:HA2	1.80	0.62
1:C:591:SER:O	1:C:593:PRO:HD3	1.99	0.62
1:A:572:THR:HG22	1:A:573:CYS:N	2.14	0.61
1:B:438:GLN:HB3	1:B:439:PRO:HD2	1.82	0.61
1:A:124:VAL:HG13	1:A:568:MET:O	2.01	0.61
1:B:363:VAL:HG21	1:B:409:LEU:CD1	2.28	0.61
1:B:605:ARG:HG3	1:B:611:PRO:O	2.00	0.61
1:B:456:LEU:HD23	1:B:457:SER:O	2.01	0.61
1:C:673:LEU:HG	1:C:675:ILE:HG12	1.81	0.61
1:A:204:LYS:CB	1:A:206:VAL:HG22	2.31	0.61
1:A:297:MET:CE	1:A:319:PHE:HB2	2.30	0.61
1:B:572:THR:HG22	1:B:573:CYS:N	2.14	0.61
1:B:673:LEU:HG	1:B:675:ILE:HG12	1.81	0.61
1:B:591:SER:O	1:B:593:PRO:HD3	1.99	0.61
1:C:614:GLU:HG3	1:C:627:ARG:CZ	2.31	0.61
1:A:674:ASN:HB3	1:B:523:ARG:HH11	1.65	0.61
1:B:189:ARG:NH1	1:B:349:LYS:HD3	2.16	0.61
1:A:442:TYR:O	1:A:449:LEU:HD12	1.99	0.61
1:A:713:ASP:OD2	1:C:294:PHE:HD1	1.83	0.61
1:A:722:VAL:HA	1:C:217:ASN:ND2	2.16	0.61
1:A:605:ARG:HG3	1:A:611:PRO:O	2.00	0.61
1:C:589:ILE:HD11	1:C:630:ILE:HD13	1.82	0.61
1:C:124:VAL:HG13	1:C:568:MET:O	2.01	0.61
1:A:282:TYR:HB2	1:A:283:PRO:HD2	1.83	0.61
1:A:523:ARG:HH11	1:C:674:ASN:HB3	1.65	0.61
1:C:289:LEU:CD2	1:C:290:ALA:H	2.12	0.61
1:B:305:GLU:HG3	1:B:306:GLY:N	2.16	0.61
1:B:705:VAL:HG23	1:C:279:ARG:HH12	1.64	0.61
1:A:305:GLU:OE1	1:A:359:LYS:HE3	2.01	0.61
1:C:438:GLN:HB3	1:C:439:PRO:HD2	1.83	0.61
1:B:163:MET:SD	1:B:289:LEU:HD13	2.40	0.61
1:A:158:LYS:HZ2	1:C:700:LEU:HD22	1.65	0.61
1:A:260:GLU:O	1:A:262:PHE:HD1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ARG:NH1	1:C:349:LYS:HD3	2.16	0.60
1:B:344:LEU:N	1:B:344:LEU:HD12	2.16	0.60
1:B:124:VAL:HG13	1:B:568:MET:O	2.01	0.60
1:C:664:ILE:HG22	1:C:665:THR:O	2.02	0.60
1:A:397:THR:HG22	1:A:398:ASN:N	2.16	0.60
1:A:438:GLN:HB3	1:A:439:PRO:HD2	1.83	0.60
1:C:344:LEU:N	1:C:344:LEU:HD12	2.16	0.60
1:B:106:ALA:HA	1:B:643:PHE:HE2	1.66	0.60
1:C:106:ALA:HA	1:C:643:PHE:HE2	1.66	0.60
1:C:291:THR:HG21	1:C:293:ASP:HB2	1.82	0.60
1:C:605:ARG:HG3	1:C:611:PRO:O	2.01	0.60
1:A:288:VAL:HG12	1:A:289:LEU:O	2.01	0.60
1:B:674:ASN:HB3	1:C:523:ARG:HH11	1.65	0.60
1:A:456:LEU:HD23	1:A:457:SER:O	2.01	0.60
1:B:204:LYS:HB2	1:B:206:VAL:HG22	1.83	0.60
1:C:368:LYS:HG2	1:C:368:LYS:O	2.01	0.60
1:B:397:THR:HG22	1:B:398:ASN:N	2.17	0.60
1:A:711:LEU:CD2	1:A:714:LEU:HB2	2.32	0.60
1:C:397:THR:HG22	1:C:398:ASN:N	2.17	0.60
1:B:688:VAL:HG13	1:C:369:TRP:CZ3	2.37	0.60
1:A:614:GLU:HG3	1:A:627:ARG:CZ	2.31	0.60
1:B:614:GLU:HG3	1:B:627:ARG:CZ	2.31	0.60
1:B:299:PRO:HA	1:B:354:TRP:HE1	1.66	0.60
1:A:658:GLN:C	1:A:659:LEU:HD12	2.23	0.60
1:B:711:LEU:HD11	1:C:242:ARG:HB3	1.84	0.59
1:A:156:PRO:HD2	1:C:700:LEU:CD2	2.31	0.59
1:B:658:GLN:C	1:B:659:LEU:HD12	2.23	0.59
1:A:312:THR:HG23	1:A:314:TYR:CG	2.37	0.59
1:B:688:VAL:CG1	1:C:448:PHE:HE2	2.12	0.59
1:C:456:LEU:HD23	1:C:457:SER:O	2.01	0.59
1:B:189:ARG:HD3	1:B:349:LYS:CE	2.33	0.59
1:C:208:ARG:HG2	1:C:210:THR:H	1.66	0.59
1:C:156:PRO:HG2	1:C:158:LYS:HZ2	1.66	0.59
1:C:115:VAL:HG22	1:C:623:LEU:HB2	1.85	0.59
1:B:297:MET:O	1:B:298:SER:HB2	2.03	0.59
1:C:189:ARG:HD3	1:C:349:LYS:CE	2.33	0.59
1:B:502:GLU:HG2	1:C:502:GLU:HG2	1.84	0.59
1:A:189:ARG:NH1	1:A:349:LYS:HD3	2.16	0.59
1:B:281:VAL:CG1	1:B:282:TYR:HD1	2.13	0.59
1:B:664:ILE:HG22	1:B:665:THR:O	2.02	0.59
1:B:706:GLN:HE21	1:C:699:LEU:HD21	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:VAL:HA	1:C:217:ASN:HD22	1.67	0.59
1:A:603:SER:HB3	1:A:612:LEU:CD2	2.33	0.59
1:A:502:GLU:HG2	1:C:502:GLU:HG2	1.84	0.59
1:B:715:ARG:HG3	1:C:243:THR:HG22	1.85	0.59
1:B:280:SER:HB2	1:B:287:PHE:HB3	1.83	0.59
1:C:129:GLN:HB3	1:C:130:PRO:HD2	1.85	0.59
1:C:256:PRO:HG3	1:C:265:TYR:C	2.23	0.59
1:B:129:GLN:HB3	1:B:130:PRO:HD2	1.85	0.59
1:A:154:ILE:HG13	1:A:155:ALA:CA	2.25	0.59
1:C:224:HIS:HE1	1:C:268:THR:HG22	1.67	0.59
1:A:502:GLU:HG2	1:B:502:GLU:HG2	1.84	0.59
1:A:115:VAL:HG22	1:A:623:LEU:HB2	1.85	0.58
1:A:289:LEU:CD2	1:A:290:ALA:H	2.15	0.58
1:A:664:ILE:HG22	1:A:665:THR:O	2.02	0.58
1:A:714:LEU:HG	1:C:286:GLU:OE2	2.01	0.58
1:B:688:VAL:HA	1:C:369:TRP:CE2	2.37	0.58
1:C:701:ASP:HB2	1:C:704:GLU:CB	2.33	0.58
1:C:288:VAL:HG12	1:C:289:LEU:N	2.18	0.58
1:C:316:ALA:HB3	1:C:317:ASP:HA	1.85	0.58
1:A:344:LEU:HD12	1:A:344:LEU:N	2.16	0.58
1:A:148:VAL:HG13	1:A:370:GLN:O	2.04	0.58
1:A:189:ARG:HD3	1:A:349:LYS:CE	2.33	0.58
1:C:200:LYS:HE3	1:C:208:ARG:HH21	1.69	0.58
1:A:129:GLN:HB3	1:A:130:PRO:HD2	1.84	0.58
1:A:696:ASP:HA	1:A:701:ASP:OD1	2.04	0.58
1:A:701:ASP:N	1:B:158:LYS:HE2	2.00	0.58
1:A:719:ILE:HG23	1:A:720:ASP:N	2.18	0.58
1:A:290:ALA:HB2	1:C:715:ARG:NH1	2.18	0.58
1:A:711:LEU:HD23	1:A:714:LEU:HB2	1.85	0.58
1:A:714:LEU:HG	1:C:286:GLU:CD	2.23	0.58
1:B:699:LEU:CB	1:C:156:PRO:HB3	2.33	0.58
1:B:163:MET:SD	1:B:276:VAL:HG21	2.44	0.58
1:A:232:MET:O	1:A:233:GLU:HG2	2.03	0.58
1:C:189:ARG:HD3	1:C:349:LYS:HD3	1.86	0.58
1:B:276:VAL:HG13	1:B:290:ALA:HB3	1.86	0.58
1:C:658:GLN:C	1:C:659:LEU:HD12	2.23	0.58
1:B:695:LYS:HE3	1:B:703:THR:OG1	2.03	0.58
1:B:326:TYR:CZ	1:B:339:PRO:HG3	2.39	0.58
1:B:147:ALA:HA	1:B:451:ALA:O	2.04	0.58
1:C:300:PHE:HB3	1:C:359:LYS:HB2	1.85	0.58
1:C:638:ARG:HG3	1:C:649:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:VAL:HG13	1:B:370:GLN:O	2.03	0.57
1:B:701:ASP:OD1	1:B:704:GLU:HB2	2.04	0.57
1:A:207:CYS:HB2	1:A:234:LEU:CD1	2.34	0.57
1:A:147:ALA:HA	1:A:451:ALA:O	2.04	0.57
1:C:148:VAL:HG13	1:C:370:GLN:O	2.04	0.57
1:B:711:LEU:HD13	1:C:242:ARG:O	2.03	0.57
1:B:115:VAL:HG22	1:B:623:LEU:HB2	1.85	0.57
1:A:189:ARG:HD3	1:A:349:LYS:HD3	1.86	0.57
1:A:221:THR:HG22	1:A:222:ALA:N	2.19	0.57
1:A:326:TYR:CZ	1:A:339:PRO:HG3	2.39	0.57
1:A:700:LEU:HD11	1:B:156:PRO:CG	2.35	0.57
1:B:302:GLY:O	1:B:305:GLU:HB2	2.05	0.57
1:A:638:ARG:HG3	1:A:649:TYR:CE1	2.39	0.57
1:B:189:ARG:HD3	1:B:349:LYS:HD3	1.86	0.57
1:B:288:VAL:CG1	1:B:292:GLY:HA2	2.34	0.57
1:C:221:THR:HG22	1:C:222:ALA:N	2.19	0.57
1:C:147:ALA:HA	1:C:451:ALA:O	2.05	0.57
1:A:711:LEU:HD12	1:B:242:ARG:O	2.04	0.57
1:A:108:ASN:HB2	1:A:645:GLY:H	1.69	0.57
1:A:151:LYS:HD2	1:C:688:VAL:HG13	1.86	0.57
1:A:368:LYS:HG2	1:A:368:LYS:O	2.05	0.57
1:C:108:ASN:HB2	1:C:645:GLY:H	1.70	0.57
1:A:723:ILE:HB	1:C:217:ASN:CB	2.25	0.57
1:A:706:GLN:O	1:A:710:GLN:HG3	2.05	0.57
1:B:343:ASN:C	1:B:344:LEU:HD12	2.25	0.57
1:C:326:TYR:CZ	1:C:339:PRO:HG3	2.39	0.57
1:B:221:THR:HG22	1:B:222:ALA:N	2.19	0.57
1:A:391:ILE:CG2	1:A:393:THR:HG23	2.27	0.56
1:C:605:ARG:NH1	1:C:607:GLU:HB3	2.20	0.56
1:B:287:PHE:HE1	1:B:297:MET:HB3	1.69	0.56
1:B:391:ILE:CG2	1:B:393:THR:HG23	2.27	0.56
1:A:209:SER:O	1:A:269:VAL:HG11	2.05	0.56
1:A:711:LEU:CD1	1:B:240:ALA:HB3	2.23	0.56
1:B:276:VAL:HG12	1:B:277:ASP:N	2.20	0.56
1:A:708:ARG:HD2	1:B:244:SER:OG	2.06	0.56
1:B:286:GLU:HG2	1:B:296:TYR:CE2	2.41	0.56
1:B:281:VAL:HG13	1:B:282:TYR:N	2.20	0.56
1:B:638:ARG:HG3	1:B:649:TYR:CE1	2.39	0.56
1:B:347:THR:HB	1:B:348:PRO:HD2	1.87	0.56
1:A:572:THR:HG22	1:A:573:CYS:H	1.71	0.56
1:C:343:ASN:C	1:C:344:LEU:HD12	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:CD1	1:A:290:ALA:H	2.18	0.56
1:A:541:GLU:O	1:A:544:LYS:HB3	2.06	0.56
1:A:400:THR:HG22	1:A:401:GLU:N	2.20	0.56
1:B:108:ASN:HB2	1:B:645:GLY:CA	2.35	0.56
1:A:699:LEU:HD13	1:C:702:TYR:CE2	2.40	0.56
1:B:541:GLU:O	1:B:544:LYS:HB3	2.06	0.56
1:B:400:THR:HG22	1:B:401:GLU:N	2.20	0.56
1:A:343:ASN:C	1:A:344:LEU:HD12	2.25	0.56
1:B:715:ARG:CG	1:C:243:THR:HG22	2.35	0.56
1:A:291:THR:HG23	1:C:712:HIS:HE1	1.71	0.56
1:C:541:GLU:O	1:C:544:LYS:HB3	2.06	0.56
1:B:288:VAL:HG12	1:B:289:LEU:N	2.21	0.56
1:A:291:THR:HB	1:A:293:ASP:H	1.70	0.56
1:C:696:ASP:HA	1:C:701:ASP:OD1	2.05	0.56
1:B:108:ASN:HB2	1:B:645:GLY:H	1.70	0.56
1:A:290:ALA:CB	1:C:716:PHE:HE2	2.19	0.56
1:C:347:THR:HB	1:C:348:PRO:HD2	1.87	0.56
1:A:587:MET:HE1	1:A:597:TYR:O	2.06	0.55
1:C:400:THR:HG22	1:C:401:GLU:N	2.20	0.55
1:C:108:ASN:HB2	1:C:645:GLY:N	2.21	0.55
1:C:108:ASN:HB2	1:C:645:GLY:CA	2.35	0.55
1:B:108:ASN:HB2	1:B:645:GLY:N	2.21	0.55
1:A:347:THR:HB	1:A:348:PRO:HD2	1.87	0.55
1:A:582:ILE:HG22	1:A:583:VAL:N	2.21	0.55
1:A:108:ASN:HB2	1:A:645:GLY:N	2.21	0.55
1:A:360:ARG:CB	1:A:361:PRO:HD3	2.36	0.55
1:B:605:ARG:NH1	1:B:607:GLU:HB3	2.21	0.55
1:B:607:GLU:HG2	1:B:608:ASP:N	2.22	0.55
1:A:605:ARG:NH1	1:A:607:GLU:HB3	2.21	0.55
1:C:420:ALA:O	1:C:424:ILE:HG13	2.06	0.55
1:B:283:PRO:HA	1:B:300:PHE:CD2	2.41	0.55
1:B:587:MET:HE1	1:B:597:TYR:O	2.06	0.55
1:C:601:LEU:HD23	1:C:627:ARG:NE	2.22	0.55
1:C:543:ARG:CA	1:C:550:ILE:HG12	2.36	0.55
1:C:192:VAL:HG13	1:C:193:PRO:HD2	1.88	0.55
1:B:572:THR:HG22	1:B:573:CYS:H	1.71	0.55
1:C:360:ARG:CB	1:C:361:PRO:HD3	2.35	0.55
1:A:204:LYS:HB3	1:A:206:VAL:HG22	1.86	0.55
1:B:420:ALA:O	1:B:424:ILE:HG13	2.06	0.55
1:B:719:ILE:N	1:B:720:ASP:HA	2.21	0.55
1:B:217:ASN:ND2	1:C:723:ILE:HG22	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:PHE:HD2	1:C:258:ARG:HH11	1.53	0.55
1:A:711:LEU:HD22	1:A:715:ARG:HG3	1.89	0.55
1:A:420:ALA:O	1:A:424:ILE:HG13	2.06	0.55
1:B:192:VAL:HG13	1:B:193:PRO:HD2	1.88	0.55
1:A:108:ASN:HB2	1:A:645:GLY:CA	2.37	0.55
1:B:360:ARG:CB	1:B:361:PRO:HD3	2.36	0.55
1:A:541:GLU:OE2	1:B:546:ASN:HB2	2.07	0.55
1:B:649:TYR:CD2	1:B:656:SER:HB3	2.42	0.55
1:A:326:TYR:HE1	1:A:337:THR:O	1.90	0.55
1:B:388:SER:CB	1:B:391:ILE:HB	2.33	0.55
1:B:541:GLU:OE2	1:C:546:ASN:HB2	2.07	0.55
1:B:157:TYR:CE2	1:B:159:PHE:CD1	2.95	0.55
1:A:597:TYR:HD1	1:A:599:ARG:N	2.05	0.55
1:C:649:TYR:CD2	1:C:656:SER:HB3	2.42	0.55
1:C:175:PHE:CD2	1:C:258:ARG:HG2	2.41	0.55
1:C:388:SER:CB	1:C:391:ILE:HB	2.33	0.55
1:C:603:SER:HB3	1:C:612:LEU:CD2	2.32	0.55
1:B:689:TYR:HD2	1:B:694:ILE:CD1	2.16	0.55
1:A:649:TYR:CD2	1:A:656:SER:HB3	2.42	0.55
1:C:520:MET:CE	1:C:520:MET:HA	2.37	0.55
1:B:391:ILE:HG22	1:B:393:THR:CG2	2.28	0.54
1:A:429:TYR:CE2	1:A:455:LEU:HD13	2.43	0.54
1:C:326:TYR:HE1	1:C:337:THR:O	1.90	0.54
1:B:367:THR:HG22	1:B:368:LYS:N	2.22	0.54
1:C:297:MET:HG2	1:C:354:TRP:HH2	1.72	0.54
1:C:607:GLU:HG2	1:C:608:ASP:N	2.22	0.54
1:A:299:PRO:HB3	1:A:354:TRP:NE1	2.23	0.54
1:B:600:PRO:HD3	1:B:641:PHE:CE2	2.43	0.54
1:A:711:LEU:HD12	1:B:243:THR:CA	2.38	0.54
1:C:163:MET:CG	1:C:276:VAL:HG21	2.37	0.54
1:B:242:ARG:NH1	1:C:284:TYR:HD2	1.98	0.54
1:B:543:ARG:CA	1:B:550:ILE:HG12	2.36	0.54
1:B:157:TYR:CD2	1:B:300:PHE:CE1	2.95	0.54
1:C:587:MET:HE1	1:C:597:TYR:O	2.07	0.54
1:A:652:GLU:OE1	1:A:652:GLU:HA	2.07	0.54
1:B:652:GLU:OE1	1:B:652:GLU:HA	2.07	0.54
1:A:192:VAL:HG13	1:A:193:PRO:HD2	1.88	0.54
1:A:275:GLU:C	1:A:276:VAL:HG23	2.28	0.54
1:C:553:VAL:HG13	1:C:554:THR:N	2.23	0.54
1:C:600:PRO:HD3	1:C:641:PHE:CE2	2.43	0.54
1:C:124:VAL:HG12	1:C:125:VAL:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:652:GLU:HA	1:C:652:GLU:OE1	2.07	0.54
1:C:391:ILE:CG2	1:C:393:THR:HG23	2.27	0.54
1:C:429:TYR:CE2	1:C:455:LEU:HD13	2.43	0.54
1:B:204:LYS:HB3	1:B:206:VAL:HG13	1.89	0.54
1:A:124:VAL:HG12	1:A:125:VAL:N	2.23	0.54
1:A:259:VAL:HG23	1:A:264:ARG:HH11	1.73	0.54
1:C:582:ILE:HG22	1:C:583:VAL:N	2.22	0.54
1:B:363:VAL:HG23	1:B:364:CYS:HA	1.89	0.54
1:A:607:GLU:HG2	1:A:608:ASP:N	2.22	0.54
1:B:288:VAL:HG12	1:B:292:GLY:HA2	1.89	0.54
1:A:283:PRO:HB3	1:A:300:PHE:HD2	1.73	0.54
1:B:432:THR:HG22	1:B:433:HIS:ND1	2.23	0.54
1:A:601:LEU:HD23	1:A:627:ARG:NE	2.22	0.54
1:B:326:TYR:HE1	1:B:337:THR:O	1.90	0.54
1:A:697:SER:CB	1:B:154:ILE:HG13	2.38	0.54
1:B:601:LEU:HD23	1:B:627:ARG:NE	2.22	0.54
1:B:299:PRO:HG3	1:B:354:TRP:CD1	2.42	0.54
1:C:224:HIS:CE1	1:C:268:THR:HG22	2.43	0.54
1:B:603:SER:HB3	1:B:612:LEU:CD2	2.32	0.54
1:C:701:ASP:HB2	1:C:704:GLU:HB3	1.89	0.54
1:B:582:ILE:HG22	1:B:583:VAL:N	2.21	0.54
1:A:156:PRO:HD2	1:C:700:LEU:HD23	1.89	0.54
1:A:275:GLU:O	1:A:276:VAL:HG23	2.08	0.54
1:A:543:ARG:CA	1:A:550:ILE:HG12	2.36	0.54
1:A:297:MET:CG	1:A:345:LEU:HD22	2.38	0.54
1:B:429:TYR:CE2	1:B:455:LEU:HD13	2.43	0.53
1:B:520:MET:HA	1:B:520:MET:CE	2.37	0.53
1:B:124:VAL:HG12	1:B:125:VAL:N	2.23	0.53
1:A:432:THR:HG22	1:A:433:HIS:ND1	2.23	0.53
1:A:553:VAL:HG13	1:A:554:THR:N	2.22	0.53
1:C:666:THR:HG22	1:C:667:VAL:N	2.22	0.53
1:A:666:THR:HG22	1:A:667:VAL:N	2.22	0.53
1:A:128:GLU:HG2	1:A:129:GLN:O	2.08	0.53
1:B:666:THR:HG22	1:B:667:VAL:N	2.22	0.53
1:A:520:MET:HA	1:A:520:MET:CE	2.37	0.53
1:A:162:THR:HG23	1:A:274:GLU:O	2.08	0.53
1:C:367:THR:HG22	1:C:368:LYS:N	2.24	0.53
1:A:276:VAL:HG12	1:A:277:ASP:N	2.23	0.53
1:B:162:THR:HG22	1:B:163:MET:N	2.24	0.53
1:A:546:ASN:HB2	1:C:541:GLU:OE2	2.07	0.53
1:B:283:PRO:HA	1:B:300:PHE:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:GLU:HG2	1:C:294:PHE:HB3	1.90	0.53
1:A:600:PRO:HD3	1:A:641:PHE:CE2	2.43	0.53
1:A:376:LEU:O	1:A:386:PHE:HA	2.09	0.53
1:B:376:LEU:O	1:B:386:PHE:HA	2.09	0.53
1:C:289:LEU:CD1	1:C:291:THR:HG22	2.39	0.53
1:C:572:THR:HG22	1:C:573:CYS:H	1.71	0.53
1:B:128:GLU:HG2	1:B:129:GLN:O	2.09	0.53
1:C:432:THR:HG22	1:C:433:HIS:ND1	2.23	0.53
1:A:388:SER:CB	1:A:391:ILE:HB	2.33	0.53
1:A:321:GLN:HE21	1:A:341:THR:CG2	2.22	0.53
1:A:699:LEU:HB2	1:C:702:TYR:CE2	2.44	0.52
1:C:254:TYR:CB	1:C:268:THR:HG23	2.39	0.52
1:A:290:ALA:HB3	1:C:716:PHE:CZ	2.44	0.52
1:B:553:VAL:HG13	1:B:554:THR:N	2.23	0.52
1:C:425:PHE:CD1	1:C:429:TYR:HB3	2.45	0.52
1:A:295:VAL:CG1	1:A:345:LEU:HD23	2.39	0.52
1:C:561:ALA:HB1	1:C:569:ALA:O	2.10	0.52
1:B:368:LYS:HG2	1:B:368:LYS:O	2.09	0.52
1:B:429:TYR:CZ	1:B:455:LEU:HD13	2.44	0.52
1:A:561:ALA:HB1	1:A:569:ALA:O	2.10	0.52
1:C:429:TYR:CZ	1:C:455:LEU:HD13	2.44	0.52
1:A:715:ARG:HD2	1:B:243:THR:HG21	1.90	0.52
1:B:597:TYR:HD1	1:B:599:ARG:N	2.05	0.52
1:C:701:ASP:HB3	1:C:704:GLU:H	1.74	0.52
1:C:376:LEU:O	1:C:386:PHE:HA	2.09	0.52
1:A:360:ARG:NH2	1:A:409:LEU:HD23	2.25	0.52
1:A:158:LYS:HZ1	1:C:700:LEU:HD22	1.74	0.52
1:B:217:ASN:CB	1:C:723:ILE:HG22	2.39	0.52
1:B:561:ALA:HB2	1:B:570:VAL:HG12	1.91	0.52
1:A:191:PRO:HG3	1:A:348:PRO:O	2.10	0.52
1:A:157:TYR:HB3	1:A:280:SER:O	2.09	0.52
1:A:576:VAL:HG12	1:A:577:ALA:N	2.25	0.52
1:A:497:THR:HG22	1:A:498:THR:N	2.25	0.52
1:A:299:PRO:HB3	1:A:354:TRP:CD1	2.45	0.52
1:A:429:TYR:CZ	1:A:455:LEU:HD13	2.44	0.52
1:B:561:ALA:HB1	1:B:569:ALA:O	2.10	0.52
1:A:699:LEU:CD1	1:A:699:LEU:H	2.23	0.52
1:B:217:ASN:ND2	1:C:723:ILE:H	2.07	0.52
1:C:561:ALA:HB2	1:C:570:VAL:HG12	1.91	0.52
1:C:276:VAL:HG11	1:C:289:LEU:HD23	1.92	0.52
1:B:601:LEU:HD23	1:B:627:ARG:CZ	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:TYR:HB2	1:B:659:LEU:HD11	1.92	0.52
1:C:227:ASP:HB3	1:C:228:HIS:O	2.10	0.52
1:B:701:ASP:CG	1:B:704:GLU:HB2	2.30	0.52
1:B:329:ASP:O	1:B:333:LYS:HA	2.10	0.52
1:A:711:LEU:HD13	1:A:715:ARG:HD2	1.92	0.51
1:C:605:ARG:HD3	1:C:607:GLU:N	2.10	0.51
1:B:297:MET:HG3	1:B:298:SER:H	1.76	0.51
1:B:299:PRO:HB3	1:B:354:TRP:CD1	2.45	0.51
1:A:391:ILE:HG22	1:A:393:THR:CG2	2.28	0.51
1:C:329:ASP:O	1:C:333:LYS:HA	2.11	0.51
1:A:244:SER:HB2	1:A:276:VAL:HG22	1.91	0.51
1:B:425:PHE:CD1	1:B:429:TYR:HB3	2.45	0.51
1:A:234:LEU:HD23	1:A:247:TRP:CB	2.40	0.51
1:A:561:ALA:HB2	1:A:570:VAL:HG12	1.91	0.51
1:C:128:GLU:HG2	1:C:129:GLN:O	2.09	0.51
1:A:425:PHE:CD1	1:A:429:TYR:HB3	2.44	0.51
1:A:208:ARG:HA	1:A:231:ASP:CB	2.41	0.51
1:A:649:TYR:HB2	1:A:659:LEU:HD11	1.92	0.51
1:B:108:ASN:HB2	1:B:645:GLY:HA3	1.92	0.51
1:B:152:GLU:HG2	1:B:153:ASN:N	2.25	0.51
1:C:576:VAL:HG12	1:C:577:ALA:N	2.25	0.51
1:C:601:LEU:HD23	1:C:627:ARG:CZ	2.40	0.51
1:A:297:MET:HE3	1:A:319:PHE:HB2	1.92	0.51
1:C:689:TYR:CD2	1:C:694:ILE:HD13	2.44	0.51
1:B:321:GLN:HE21	1:B:341:THR:CG2	2.22	0.51
1:A:640:TYR:HB2	1:C:567:VAL:HG22	1.93	0.51
1:A:567:VAL:HG22	1:B:640:TYR:HB2	1.92	0.51
1:A:670:PHE:HD2	1:C:131:ARG:NH2	2.08	0.51
1:B:701:ASP:OD2	1:B:704:GLU:HB2	2.11	0.51
1:A:601:LEU:HD23	1:A:627:ARG:CZ	2.40	0.51
1:A:641:PHE:HB2	1:A:648:VAL:CG1	2.40	0.51
1:C:641:PHE:HB2	1:C:648:VAL:CG1	2.40	0.51
1:C:497:THR:HG22	1:C:498:THR:N	2.24	0.51
1:A:329:ASP:O	1:A:333:LYS:HA	2.10	0.51
1:B:175:PHE:CE2	1:B:258:ARG:HA	2.46	0.51
1:B:217:ASN:HB3	1:C:723:ILE:HG22	1.91	0.51
1:A:713:ASP:HB2	1:C:294:PHE:HB2	1.92	0.51
1:B:148:VAL:HG12	1:B:149:VAL:N	2.26	0.51
1:B:576:VAL:HG12	1:B:577:ALA:N	2.25	0.51
1:B:317:ASP:O	1:B:320:LYS:HE3	2.11	0.51
1:B:641:PHE:HB2	1:B:648:VAL:CG1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:631:GLU:HB2	1:C:632:PRO:HD2	1.93	0.51
1:B:191:PRO:HG3	1:B:348:PRO:O	2.10	0.51
1:C:191:PRO:HG3	1:C:348:PRO:O	2.10	0.51
1:C:175:PHE:CE2	1:C:258:ARG:HG2	2.45	0.51
1:C:286:GLU:CG	1:C:294:PHE:HD2	2.11	0.51
1:C:145:GLY:HA2	1:C:455:LEU:HG	1.93	0.51
1:B:719:ILE:HB	1:B:720:ASP:CA	2.41	0.51
1:A:131:ARG:NH2	1:B:670:PHE:HD2	2.08	0.51
1:A:471:GLU:OE1	1:A:471:GLU:HA	2.11	0.51
1:A:605:ARG:HD3	1:A:607:GLU:N	2.14	0.50
1:A:708:ARG:NH2	1:B:276:VAL:HG22	2.27	0.50
1:A:282:TYR:HB2	1:A:283:PRO:CD	2.41	0.50
1:B:172:GLN:CB	1:B:183:MET:HB2	2.40	0.50
1:C:649:TYR:HB2	1:C:659:LEU:HD11	1.92	0.50
1:B:360:ARG:NE	1:B:409:LEU:HD21	2.26	0.50
1:A:711:LEU:HD21	1:B:240:ALA:CB	2.27	0.50
1:B:605:ARG:HD3	1:B:607:GLU:N	2.14	0.50
1:B:224:HIS:C	1:B:226:ASP:H	2.15	0.50
1:C:321:GLN:HE21	1:C:341:THR:CG2	2.23	0.50
1:B:131:ARG:NH2	1:C:670:PHE:HD2	2.08	0.50
1:C:471:GLU:OE1	1:C:471:GLU:HA	2.11	0.50
1:A:156:PRO:HB3	1:A:281:VAL:HA	1.94	0.50
1:C:429:TYR:CE2	1:C:455:LEU:CD1	2.95	0.50
1:C:119:PRO:CG	1:C:561:ALA:HA	2.42	0.50
1:C:150:PHE:CE2	1:C:368:LYS:HB2	2.46	0.50
1:C:596:CYS:HB3	1:C:653:TYR:CD1	2.47	0.50
1:B:156:PRO:HG2	1:B:158:LYS:NZ	2.27	0.50
1:B:429:TYR:CE2	1:B:455:LEU:CD1	2.95	0.50
1:C:597:TYR:HD1	1:C:599:ARG:N	2.05	0.50
1:A:596:CYS:HB3	1:A:653:TYR:CD1	2.47	0.50
1:B:497:THR:HG22	1:B:498:THR:N	2.25	0.50
1:C:286:GLU:HA	1:C:295:VAL:O	2.12	0.50
1:C:159:PHE:CZ	1:C:278:ALA:CB	2.95	0.50
1:C:626:THR:HG22	1:C:627:ARG:N	2.27	0.50
1:A:425:PHE:CD1	1:A:429:TYR:CB	2.95	0.50
1:B:145:GLY:HA2	1:B:455:LEU:HG	1.93	0.50
1:B:567:VAL:HG22	1:C:640:TYR:HB2	1.93	0.50
1:C:649:TYR:CD2	1:C:656:SER:CB	2.95	0.50
1:B:204:LYS:HB3	1:B:206:VAL:HG22	1.93	0.50
1:B:631:GLU:HB2	1:B:632:PRO:HD2	1.93	0.50
1:A:502:GLU:CG	1:B:502:GLU:HG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:VAL:HG12	1:A:149:VAL:N	2.27	0.50
1:C:108:ASN:HB2	1:C:645:GLY:HA3	1.92	0.50
1:C:152:GLU:HG2	1:C:153:ASN:N	2.25	0.50
1:B:706:GLN:HE21	1:C:699:LEU:CD2	2.25	0.50
1:B:397:THR:HG22	1:B:398:ASN:O	2.12	0.50
1:A:707:ARG:C	1:B:242:ARG:HB3	2.31	0.50
1:A:290:ALA:HB2	1:C:715:ARG:HH22	1.75	0.50
1:C:425:PHE:CD1	1:C:429:TYR:CB	2.95	0.50
1:A:502:GLU:HG2	1:C:502:GLU:CG	2.42	0.50
1:B:467:GLU:O	1:B:471:GLU:HG2	2.12	0.50
1:B:681:HIS:HE1	1:C:389:ASP:O	1.95	0.50
1:C:162:THR:HG22	1:C:163:MET:N	2.27	0.50
1:B:626:THR:HG22	1:B:627:ARG:N	2.27	0.50
1:A:119:PRO:CG	1:A:561:ALA:HA	2.42	0.50
1:B:201:ILE:O	1:B:205:GLY:HA2	2.12	0.50
1:B:596:CYS:HB3	1:B:653:TYR:CD1	2.47	0.50
1:B:700:LEU:HD12	1:C:158:LYS:CB	2.42	0.50
1:A:162:THR:HG22	1:A:163:MET:N	2.27	0.50
1:B:471:GLU:HA	1:B:471:GLU:OE1	2.12	0.50
1:C:201:ILE:O	1:C:205:GLY:HA2	2.12	0.50
1:B:699:LEU:HB3	1:C:156:PRO:CA	2.42	0.49
1:A:397:THR:HG22	1:A:398:ASN:O	2.12	0.49
1:A:605:ARG:HD3	1:A:606:TYR:N	2.27	0.49
1:B:276:VAL:HG12	1:B:277:ASP:O	2.12	0.49
1:A:146:ILE:HG13	1:A:455:LEU:HD11	1.94	0.49
1:B:119:PRO:CG	1:B:561:ALA:HA	2.42	0.49
1:A:252:LEU:HD23	1:C:721:THR:HG21	1.94	0.49
1:A:699:LEU:HB3	1:A:700:LEU:CD2	2.33	0.49
1:B:425:PHE:CD1	1:B:429:TYR:CB	2.95	0.49
1:B:649:TYR:CD2	1:B:656:SER:CB	2.95	0.49
1:A:631:GLU:HB2	1:A:632:PRO:HD2	1.93	0.49
1:A:364:CYS:CB	1:A:409:LEU:HB3	2.41	0.49
1:C:397:THR:HG22	1:C:398:ASN:O	2.12	0.49
1:A:429:TYR:CE2	1:A:455:LEU:CD1	2.95	0.49
1:C:467:GLU:O	1:C:471:GLU:HG2	2.12	0.49
1:A:145:GLY:HA2	1:A:455:LEU:HG	1.93	0.49
1:A:467:GLU:O	1:A:471:GLU:HG2	2.12	0.49
1:C:689:TYR:CD2	1:C:694:ILE:CD1	2.95	0.49
1:A:212:LYS:HE2	1:A:219:GLU:OE2	2.12	0.49
1:A:719:ILE:HG23	1:A:720:ASP:OD1	2.12	0.49
1:B:297:MET:CE	1:B:319:PHE:CD1	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ILE:HG13	1:B:455:LEU:HD11	1.94	0.49
1:B:363:VAL:HG23	1:B:364:CYS:CA	2.42	0.49
1:B:543:ARG:HA	1:B:550:ILE:CG1	2.40	0.49
1:C:148:VAL:HG12	1:C:149:VAL:N	2.27	0.49
1:C:205:GLY:O	1:C:234:LEU:HD12	2.12	0.49
1:A:707:ARG:CA	1:B:242:ARG:HB3	2.43	0.49
1:C:298:SER:HB3	1:C:300:PHE:CE2	2.48	0.49
1:A:230:THR:HG22	1:A:231:ASP:N	2.28	0.49
1:A:649:TYR:CD2	1:A:656:SER:CB	2.95	0.49
1:A:201:ILE:O	1:A:205:GLY:HA2	2.13	0.49
1:A:626:THR:HG22	1:A:627:ARG:N	2.27	0.49
1:B:233:GLU:HG2	1:B:234:LEU:N	2.28	0.49
1:A:299:PRO:CB	1:A:354:TRP:HE1	2.26	0.49
1:B:501:ILE:HG23	1:B:502:GLU:HA	1.95	0.49
1:A:215:ARG:HG3	1:A:216:ASN:OD1	2.13	0.49
1:B:699:LEU:HB3	1:C:156:PRO:CB	2.42	0.48
1:C:456:LEU:HD21	1:C:461:ALA:CA	2.36	0.48
1:A:235:LYS:HB2	1:A:236:PRO:HD2	1.95	0.48
1:B:288:VAL:HG12	1:B:289:LEU:O	2.13	0.48
1:C:254:TYR:N	1:C:268:THR:HG23	2.28	0.48
1:A:286:GLU:H	1:A:286:GLU:CD	2.17	0.48
1:A:108:ASN:HB2	1:A:645:GLY:HA3	1.95	0.48
1:A:389:ASP:O	1:C:681:HIS:HE1	1.95	0.48
1:B:699:LEU:CD1	1:C:281:VAL:HG13	2.19	0.48
1:C:291:THR:CG2	1:C:293:ASP:H	2.10	0.48
1:C:146:ILE:HG13	1:C:455:LEU:HD11	1.94	0.48
1:A:193:PRO:HD2	1:A:196:GLU:OE1	2.13	0.48
1:C:193:PRO:HD2	1:C:196:GLU:OE1	2.13	0.48
1:C:591:SER:C	1:C:593:PRO:HD3	2.34	0.48
1:B:123:THR:HB	1:B:570:VAL:O	2.14	0.48
1:C:501:ILE:HG23	1:C:502:GLU:HA	1.95	0.48
1:B:502:GLU:CG	1:C:502:GLU:HG2	2.42	0.48
1:A:722:VAL:HG12	1:A:723:ILE:N	2.28	0.48
1:C:543:ARG:HA	1:C:550:ILE:CG1	2.40	0.48
1:A:286:GLU:HA	1:A:296:TYR:HA	1.94	0.48
1:B:193:PRO:HD2	1:B:196:GLU:OE1	2.13	0.48
1:C:630:ILE:HG22	1:C:631:GLU:N	2.28	0.48
1:C:599:ARG:HB3	1:C:600:PRO:HD2	1.95	0.48
1:A:681:HIS:HE1	1:B:389:ASP:O	1.95	0.48
1:B:225:ARG:HG3	1:B:254:TYR:HE2	1.77	0.48
1:A:591:SER:C	1:A:593:PRO:HD3	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ARG:HG3	1:C:216:ASN:OD1	2.13	0.48
1:B:700:LEU:H	1:C:279:ARG:NH2	2.10	0.48
1:C:159:PHE:CZ	1:C:278:ALA:HB3	2.48	0.48
1:B:298:SER:OG	1:B:299:PRO:HD2	2.14	0.48
1:B:157:TYR:CE2	1:B:300:PHE:CE1	2.95	0.48
1:B:198:ILE:HD12	1:B:198:ILE:N	2.29	0.48
1:B:700:LEU:O	1:B:701:ASP:HB3	2.14	0.48
1:B:605:ARG:HD3	1:B:606:TYR:N	2.28	0.48
1:C:123:THR:HB	1:C:570:VAL:O	2.14	0.48
1:B:568:MET:HG2	1:B:569:ALA:O	2.14	0.48
1:B:173:VAL:HG12	1:B:174:TRP:N	2.29	0.48
1:A:711:LEU:HD12	1:B:242:ARG:C	2.34	0.48
1:A:123:THR:HB	1:A:570:VAL:O	2.14	0.48
1:C:297:MET:HG2	1:C:354:TRP:CH2	2.49	0.48
1:B:287:PHE:CE1	1:B:297:MET:HB3	2.47	0.48
1:B:295:VAL:HG13	1:B:345:LEU:HD23	1.96	0.48
1:B:630:ILE:HG22	1:B:631:GLU:N	2.28	0.48
1:B:591:SER:C	1:B:593:PRO:HD3	2.34	0.48
1:A:501:ILE:HG23	1:A:502:GLU:HA	1.96	0.48
1:C:260:GLU:O	1:C:262:PHE:HD1	1.97	0.48
1:B:706:GLN:NE2	1:C:699:LEU:HD21	2.27	0.47
1:A:198:ILE:HD12	1:A:198:ILE:N	2.29	0.47
1:A:568:MET:HG2	1:A:569:ALA:O	2.14	0.47
1:C:265:TYR:N	1:C:265:TYR:CD1	2.82	0.47
1:A:116:CYS:CB	1:A:560:SER:HB2	2.39	0.47
1:B:354:TRP:N	1:B:354:TRP:CE3	2.82	0.47
1:A:630:ILE:HG22	1:A:631:GLU:N	2.28	0.47
1:C:116:CYS:CB	1:C:560:SER:HB2	2.39	0.47
1:B:599:ARG:HB3	1:B:600:PRO:HD2	1.95	0.47
1:A:173:VAL:HG12	1:A:174:TRP:N	2.29	0.47
1:B:604:PHE:CD1	1:B:604:PHE:N	2.83	0.47
1:A:240:ALA:CB	1:A:243:THR:HG21	2.26	0.47
1:A:605:ARG:CZ	1:A:611:PRO:HD2	2.45	0.47
1:A:543:ARG:HA	1:A:550:ILE:CG1	2.40	0.47
1:A:286:GLU:HB3	1:A:295:VAL:O	2.15	0.47
1:C:259:VAL:HG23	1:C:264:ARG:HH11	1.80	0.47
1:B:314:TYR:HA	1:B:314:TYR:HD1	1.37	0.47
1:B:708:ARG:CZ	1:C:277:ASP:HB2	2.44	0.47
1:B:605:ARG:CZ	1:B:611:PRO:HD2	2.44	0.47
1:A:289:LEU:CG	1:A:290:ALA:H	2.26	0.47
1:B:265:TYR:N	1:B:265:TYR:CD1	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:ILE:N	1:C:198:ILE:HD12	2.29	0.47
1:C:247:TRP:CE3	1:C:330:LEU:HD12	2.50	0.47
1:B:215:ARG:HG3	1:B:216:ASN:OD1	2.14	0.47
1:C:695:LYS:HZ2	1:C:702:TYR:HB3	1.76	0.47
1:B:687:GLU:HG2	1:B:689:TYR:O	2.14	0.47
1:A:597:TYR:CD1	1:A:598:SER:N	2.83	0.47
1:A:265:TYR:CD1	1:A:265:TYR:N	2.81	0.47
1:A:442:TYR:N	1:A:442:TYR:CD1	2.83	0.47
1:B:295:VAL:CG1	1:B:345:LEU:HD23	2.44	0.47
1:C:225:ARG:HD2	1:C:254:TYR:CD1	2.49	0.47
1:A:599:ARG:HB3	1:A:600:PRO:HD2	1.95	0.47
1:A:296:TYR:N	1:A:296:TYR:CD1	2.82	0.47
1:B:438:GLN:HB3	1:B:439:PRO:CD	2.45	0.47
1:C:568:MET:HG2	1:C:569:ALA:O	2.14	0.47
1:A:165:TYR:CD1	1:A:165:TYR:N	2.83	0.47
1:B:365:THR:HG22	1:B:366:MET:N	2.29	0.47
1:C:276:VAL:HG22	1:C:289:LEU:HD21	1.97	0.47
1:C:159:PHE:N	1:C:159:PHE:CD1	2.82	0.47
1:A:670:PHE:CD1	1:C:532:GLN:HB3	2.50	0.47
1:B:532:GLN:HB3	1:C:670:PHE:CD1	2.50	0.47
1:B:303:TYR:CD1	1:B:304:ARG:N	2.82	0.47
1:C:403:PRO:HG2	1:C:406:ARG:HH21	1.80	0.47
1:C:354:TRP:N	1:C:354:TRP:CE3	2.83	0.47
1:C:605:ARG:CZ	1:C:611:PRO:HD2	2.44	0.47
1:B:363:VAL:HG23	1:B:409:LEU:HD13	1.89	0.47
1:C:240:ALA:CB	1:C:243:THR:HG21	2.27	0.47
1:B:295:VAL:HG12	1:B:296:TYR:N	2.30	0.47
1:C:550:ILE:HD12	1:C:550:ILE:N	2.30	0.47
1:B:508:PHE:CE1	1:B:512:HIS:CE1	3.03	0.47
1:B:697:SER:CA	1:C:154:ILE:HG21	2.39	0.46
1:A:403:PRO:HG2	1:A:406:ARG:HH21	1.80	0.46
1:A:713:ASP:CB	1:C:294:PHE:CD1	2.96	0.46
1:A:532:GLN:HB3	1:B:670:PHE:CD1	2.50	0.46
1:C:391:ILE:HG22	1:C:393:THR:CG2	2.28	0.46
1:B:690:THR:OG1	1:B:693:GLU:HG3	2.16	0.46
1:C:119:PRO:HG3	1:C:561:ALA:HA	1.97	0.46
1:A:386:PHE:CD1	1:A:386:PHE:N	2.84	0.46
1:C:442:TYR:CD1	1:C:442:TYR:N	2.83	0.46
1:B:116:CYS:CB	1:B:560:SER:HB2	2.39	0.46
1:B:401:GLU:OE2	1:B:475:LYS:HD3	2.16	0.46
1:A:401:GLU:OE2	1:A:475:LYS:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:TYR:N	1:B:165:TYR:CD1	2.83	0.46
1:B:212:LYS:HE2	1:B:219:GLU:OE2	2.15	0.46
1:C:407:VAL:HG12	1:C:408:ASP:N	2.30	0.46
1:C:408:ASP:OD1	1:C:409:LEU:HG	2.16	0.46
1:A:279:ARG:CZ	1:C:700:LEU:HD12	2.44	0.46
1:A:354:TRP:N	1:A:354:TRP:CE3	2.83	0.46
1:A:290:ALA:CA	1:C:708:ARG:HH21	2.27	0.46
1:A:531:LEU:HD12	1:C:671:ILE:HD13	1.97	0.46
1:A:574:VAL:HG12	1:A:575:PRO:O	2.16	0.46
1:B:213:TYR:CD1	1:B:213:TYR:N	2.84	0.46
1:A:604:PHE:N	1:A:604:PHE:CD1	2.83	0.46
1:C:574:VAL:HG12	1:C:575:PRO:O	2.16	0.46
1:A:508:PHE:CE1	1:A:512:HIS:CE1	3.03	0.46
1:B:700:LEU:HD11	1:C:158:LYS:HE3	1.95	0.46
1:A:711:LEU:HD23	1:A:714:LEU:HD12	1.98	0.46
1:C:605:ARG:HD3	1:C:606:TYR:N	2.30	0.46
1:B:297:MET:SD	1:B:345:LEU:HD13	2.56	0.46
1:C:189:ARG:HD3	1:C:349:LYS:CD	2.45	0.46
1:C:175:PHE:HD2	1:C:258:ARG:NH1	2.12	0.46
1:C:508:PHE:CE1	1:C:512:HIS:CE1	3.03	0.46
1:A:214:VAL:O	1:A:214:VAL:HG13	2.15	0.46
1:C:212:LYS:HE2	1:C:219:GLU:OE2	2.16	0.46
1:C:555:VAL:HG23	1:C:556:GLY:N	2.30	0.46
1:C:597:TYR:CD1	1:C:598:SER:N	2.83	0.46
1:A:196:GLU:OE2	1:A:208:ARG:HG2	2.15	0.46
1:B:247:TRP:CE3	1:B:330:LEU:HD12	2.51	0.46
1:A:159:PHE:N	1:A:159:PHE:CD1	2.82	0.46
1:C:165:TYR:CD1	1:C:165:TYR:N	2.83	0.46
1:A:291:THR:HA	1:C:712:HIS:CE1	2.51	0.46
1:A:119:PRO:HG3	1:A:561:ALA:HA	1.97	0.46
1:B:463:LEU:HD22	1:B:467:GLU:HG2	1.98	0.46
1:C:604:PHE:CD1	1:C:604:PHE:N	2.83	0.46
1:B:441:TYR:CD1	1:B:441:TYR:N	2.83	0.46
1:C:699:LEU:HG	1:C:699:LEU:O	2.16	0.46
1:C:360:ARG:NH2	1:C:409:LEU:HD23	2.30	0.46
1:B:403:PRO:HG2	1:B:406:ARG:HH21	1.81	0.46
1:A:299:PRO:HB3	1:A:354:TRP:HE1	1.81	0.46
1:B:555:VAL:HG23	1:B:556:GLY:N	2.30	0.46
1:B:597:TYR:CD1	1:B:598:SER:N	2.83	0.46
1:A:438:GLN:HB3	1:A:439:PRO:CD	2.45	0.46
1:B:386:PHE:N	1:B:386:PHE:CD1	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:TRP:CD1	1:A:263:HIS:CE1	3.04	0.46
1:B:574:VAL:HG12	1:B:575:PRO:O	2.16	0.46
1:C:214:VAL:HG13	1:C:214:VAL:O	2.15	0.46
1:A:441:TYR:CD1	1:A:441:TYR:N	2.83	0.46
1:B:407:VAL:HG12	1:B:408:ASP:N	2.30	0.46
1:A:555:VAL:HG23	1:A:556:GLY:N	2.30	0.46
1:A:671:ILE:HD13	1:B:531:LEU:HD12	1.97	0.46
1:C:173:VAL:HG12	1:C:174:TRP:N	2.30	0.46
1:B:363:VAL:HG23	1:B:364:CYS:N	2.31	0.46
1:C:276:VAL:CG1	1:C:289:LEU:CD2	2.94	0.46
1:B:159:PHE:CD1	1:B:159:PHE:N	2.82	0.46
1:B:214:VAL:HG13	1:B:214:VAL:O	2.15	0.46
1:A:699:LEU:HD13	1:C:702:TYR:CD2	2.51	0.45
1:A:713:ASP:CG	1:C:294:PHE:HD1	2.19	0.45
1:A:550:ILE:HD12	1:A:550:ILE:N	2.30	0.45
1:A:247:TRP:CE3	1:A:330:LEU:HD12	2.50	0.45
1:C:438:GLN:HB3	1:C:439:PRO:CD	2.45	0.45
1:C:386:PHE:N	1:C:386:PHE:CD1	2.84	0.45
1:A:290:ALA:HA	1:C:708:ARG:NH2	2.31	0.45
1:A:290:ALA:HA	1:C:708:ARG:HH21	1.81	0.45
1:A:189:ARG:HD3	1:A:349:LYS:CD	2.46	0.45
1:C:129:GLN:HB3	1:C:130:PRO:CD	2.47	0.45
1:B:174:TRP:CD1	1:B:263:HIS:CE1	3.03	0.45
1:A:352:VAL:HG22	1:A:353:ALA:N	2.31	0.45
1:A:688:VAL:HG13	1:B:151:LYS:HD2	1.99	0.45
1:C:605:ARG:HH11	1:C:607:GLU:C	2.20	0.45
1:A:300:PHE:N	1:A:300:PHE:CD1	2.82	0.45
1:B:301:TYR:HB3	1:B:307:SER:OG	2.17	0.45
1:B:189:ARG:HD3	1:B:349:LYS:CD	2.46	0.45
1:A:386:PHE:O	1:A:394:THR:HA	2.16	0.45
1:B:386:PHE:O	1:B:394:THR:HA	2.16	0.45
1:C:352:VAL:HG22	1:C:353:ALA:N	2.30	0.45
1:A:288:VAL:HG12	1:A:289:LEU:N	2.30	0.45
1:B:671:ILE:HD13	1:C:531:LEU:HD12	1.98	0.45
1:A:213:TYR:CD1	1:A:213:TYR:N	2.84	0.45
1:B:550:ILE:N	1:B:550:ILE:HD12	2.30	0.45
1:B:705:VAL:HG23	1:C:279:ARG:NH1	2.31	0.45
1:B:442:TYR:CD1	1:B:442:TYR:N	2.83	0.45
1:C:291:THR:CG2	1:C:293:ASP:HB2	2.46	0.45
1:A:289:LEU:CD1	1:C:716:PHE:HZ	2.30	0.45
1:A:200:LYS:O	1:A:204:LYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:MET:HG3	1:A:650:PHE:CE2	2.52	0.45
1:A:349:LYS:HB2	1:A:350:PHE:CD1	2.52	0.45
1:A:475:LYS:HA	1:A:476:PRO:HD3	1.77	0.45
1:A:407:VAL:HG12	1:A:408:ASP:N	2.31	0.45
1:C:284:TYR:HA	1:C:284:TYR:HD1	1.31	0.45
1:B:607:GLU:HG2	1:B:608:ASP:H	1.82	0.45
1:B:456:LEU:HD21	1:B:461:ALA:CA	2.36	0.45
1:B:300:PHE:CD2	1:B:359:LYS:HG3	2.52	0.45
1:C:706:GLN:O	1:C:710:GLN:HG3	2.17	0.45
1:B:587:MET:HG3	1:B:650:PHE:CE2	2.52	0.45
1:A:520:MET:CA	1:A:520:MET:CE	2.95	0.45
1:C:401:GLU:CD	1:C:475:LYS:HD3	2.37	0.45
1:B:174:TRP:HD1	1:B:263:HIS:CE1	2.35	0.45
1:B:503:PHE:CG	1:B:504:ALA:N	2.85	0.45
1:C:276:VAL:CG2	1:C:289:LEU:HD21	2.46	0.45
1:C:116:CYS:SG	1:C:622:GLU:HG3	2.57	0.45
1:C:209:SER:O	1:C:269:VAL:HG11	2.17	0.45
1:B:256:PRO:HG3	1:B:265:TYR:O	2.17	0.45
1:C:597:TYR:HD1	1:C:598:SER:N	2.14	0.45
1:A:150:PHE:CE2	1:A:368:LYS:HB2	2.52	0.45
1:C:698:GLY:HA2	1:C:699:LEU:HA	1.31	0.45
1:C:159:PHE:CE1	1:C:278:ALA:HB3	2.52	0.45
1:B:614:GLU:CG	1:B:627:ARG:CZ	2.95	0.45
1:A:689:TYR:CD2	1:A:694:ILE:CD1	2.96	0.45
1:B:589:ILE:CD1	1:B:630:ILE:HD13	2.46	0.45
1:B:129:GLN:HB3	1:B:130:PRO:CD	2.47	0.45
1:A:463:LEU:HD22	1:A:467:GLU:HG2	1.98	0.45
1:C:463:LEU:HD22	1:C:467:GLU:HG2	1.98	0.45
1:C:289:LEU:HD12	1:C:291:THR:HG22	1.98	0.45
1:C:297:MET:HE3	1:C:298:SER:H	1.80	0.45
1:B:605:ARG:HH11	1:B:607:GLU:C	2.20	0.45
1:C:614:GLU:CG	1:C:627:ARG:CZ	2.95	0.45
1:B:157:TYR:CG	1:B:300:PHE:CZ	3.05	0.45
1:C:401:GLU:OE2	1:C:475:LYS:HD3	2.16	0.45
1:A:129:GLN:HB3	1:A:130:PRO:CD	2.47	0.45
1:C:291:THR:CG2	1:C:293:ASP:CB	2.94	0.44
1:C:520:MET:CA	1:C:520:MET:CE	2.95	0.44
1:C:189:ARG:HB2	1:C:349:LYS:HE2	1.99	0.44
1:A:326:TYR:OH	1:A:339:PRO:HG3	2.17	0.44
1:A:700:LEU:CB	1:B:279:ARG:CZ	2.95	0.44
1:B:686:LEU:HD11	1:C:369:TRP:CZ2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:CYS:SG	1:A:622:GLU:HG3	2.57	0.44
1:B:200:LYS:HB3	1:B:206:VAL:O	2.17	0.44
1:A:343:ASN:OD1	1:A:356:TRP:HB2	2.17	0.44
1:C:386:PHE:O	1:C:394:THR:HA	2.16	0.44
1:C:446:GLY:O	1:C:497:THR:HG23	2.17	0.44
1:C:213:TYR:CD1	1:C:213:TYR:N	2.85	0.44
1:A:711:LEU:CD2	1:B:240:ALA:HB1	2.31	0.44
1:A:268:THR:HG22	1:A:269:VAL:N	2.33	0.44
1:A:301:TYR:N	1:A:301:TYR:CD1	2.83	0.44
1:A:597:TYR:HD1	1:A:598:SER:N	2.15	0.44
1:C:687:GLU:HB3	1:C:689:TYR:O	2.18	0.44
1:B:520:MET:CA	1:B:520:MET:CE	2.95	0.44
1:C:349:LYS:HB2	1:C:350:PHE:CD1	2.52	0.44
1:B:567:VAL:HG21	1:C:640:TYR:CD1	2.53	0.44
1:C:363:VAL:HG13	1:C:364:CYS:N	2.30	0.44
1:B:360:ARG:NH2	1:B:409:LEU:HG	2.32	0.44
1:A:241:THR:O	1:A:243:THR:HG23	2.17	0.44
1:A:314:TYR:HD1	1:A:314:TYR:HA	1.47	0.44
1:A:267:THR:HG22	1:A:268:THR:N	2.32	0.44
1:A:242:ARG:HA	1:C:707:ARG:HH21	1.82	0.44
1:B:597:TYR:HD1	1:B:598:SER:N	2.14	0.44
1:C:587:MET:HG3	1:C:650:PHE:CE2	2.52	0.44
1:A:649:TYR:HB3	1:A:657:HIS:O	2.18	0.44
1:B:189:ARG:HB2	1:B:349:LYS:HE2	1.99	0.44
1:B:532:GLN:NE2	1:B:532:GLN:HA	2.33	0.44
1:B:700:LEU:HD21	1:B:704:GLU:OE2	2.17	0.44
1:B:360:ARG:O	1:B:363:VAL:HG22	2.18	0.44
1:A:713:ASP:CB	1:C:294:PHE:HB2	2.48	0.44
1:A:605:ARG:CZ	1:A:607:GLU:HB3	2.48	0.44
1:B:116:CYS:SG	1:B:622:GLU:HG3	2.57	0.44
1:A:189:ARG:HB2	1:A:349:LYS:HE2	1.99	0.44
1:A:401:GLU:CD	1:A:475:LYS:HD3	2.37	0.44
1:B:352:VAL:HG22	1:B:353:ALA:N	2.32	0.44
1:C:441:TYR:CD1	1:C:441:TYR:N	2.83	0.44
1:B:700:LEU:CD1	1:C:158:LYS:CG	2.95	0.44
1:B:605:ARG:HH12	1:B:610:GLY:H	1.61	0.44
1:A:367:THR:HG22	1:A:368:LYS:N	2.33	0.44
1:B:700:LEU:CD1	1:C:158:LYS:CB	2.96	0.44
1:C:605:ARG:HB2	1:C:611:PRO:O	2.17	0.44
1:B:688:VAL:HA	1:C:369:TRP:CZ2	2.53	0.44
1:B:605:ARG:CZ	1:B:607:GLU:HB3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:VAL:CG1	1:A:277:ASP:N	2.80	0.44
1:A:599:ARG:HA	1:A:600:PRO:HD3	1.76	0.44
1:C:701:ASP:CB	1:C:704:GLU:H	2.30	0.44
1:B:349:LYS:HB2	1:B:350:PHE:CD1	2.52	0.44
1:C:108:ASN:CB	1:C:645:GLY:HA3	2.48	0.44
1:C:174:TRP:HD1	1:C:263:HIS:CE1	2.36	0.44
1:A:503:PHE:CG	1:A:504:ALA:N	2.85	0.44
1:B:700:LEU:CD2	1:B:704:GLU:CB	2.95	0.44
1:C:605:ARG:CZ	1:C:607:GLU:HB3	2.48	0.44
1:B:649:TYR:HB3	1:B:657:HIS:O	2.17	0.44
1:C:649:TYR:HB3	1:C:657:HIS:O	2.17	0.44
1:B:538:LEU:HD21	1:C:539:TRP:CE3	2.53	0.44
1:A:589:ILE:CD1	1:A:630:ILE:HD13	2.46	0.44
1:C:503:PHE:CG	1:C:504:ALA:N	2.85	0.44
1:B:155:ALA:HA	1:B:156:PRO:HD3	1.63	0.44
1:A:301:TYR:HA	1:A:302:GLY:HA3	1.78	0.44
1:B:606:TYR:CD1	1:B:606:TYR:N	2.86	0.44
1:A:605:ARG:HH12	1:A:610:GLY:H	1.60	0.44
1:B:689:TYR:CD2	1:B:694:ILE:CD1	2.95	0.44
1:B:119:PRO:HG3	1:B:561:ALA:HA	1.97	0.44
1:B:708:ARG:NH2	1:C:277:ASP:H	2.15	0.43
1:A:313:SER:CB	1:A:314:TYR:CA	2.93	0.43
1:B:605:ARG:HB2	1:B:611:PRO:O	2.18	0.43
1:B:299:PRO:CB	1:B:354:TRP:HE1	2.30	0.43
1:A:125:VAL:HG12	1:B:665:THR:OG1	2.18	0.43
1:C:394:THR:HG22	1:C:395:PHE:N	2.33	0.43
1:B:688:VAL:HG23	1:C:499:SER:O	2.18	0.43
1:B:688:VAL:CG1	1:C:369:TRP:CZ2	2.97	0.43
1:A:605:ARG:HB2	1:A:611:PRO:O	2.18	0.43
1:A:607:GLU:HG2	1:A:608:ASP:H	1.82	0.43
1:A:610:GLY:HA3	1:A:611:PRO:HD3	1.44	0.43
1:C:253:LYS:CA	1:C:268:THR:HG21	2.43	0.43
1:C:338:ALA:HA	1:C:339:PRO:HD3	1.76	0.43
1:A:567:VAL:HG21	1:B:640:TYR:CD1	2.53	0.43
1:C:305:GLU:HA	1:C:305:GLU:OE1	2.19	0.43
1:A:408:ASP:OD1	1:A:409:LEU:HG	2.18	0.43
1:A:156:PRO:HB2	1:C:700:LEU:HD11	1.99	0.43
1:A:294:PHE:N	1:A:294:PHE:CD1	2.85	0.43
1:B:543:ARG:HB3	1:B:550:ILE:HG21	2.00	0.43
1:A:501:ILE:HG23	1:A:502:GLU:N	2.33	0.43
1:C:326:TYR:OH	1:C:339:PRO:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:TYR:CD1	1:C:567:VAL:HG21	2.53	0.43
1:A:686:LEU:HD11	1:B:369:TRP:CZ2	2.54	0.43
1:B:257:SER:HB3	1:B:264:ARG:HH12	1.83	0.43
1:B:397:THR:CG2	1:B:398:ASN:N	2.82	0.43
1:C:610:GLY:HA3	1:C:611:PRO:HD3	1.43	0.43
1:A:614:GLU:CG	1:A:627:ARG:CZ	2.95	0.43
1:A:605:ARG:HH11	1:A:607:GLU:C	2.21	0.43
1:A:156:PRO:CD	1:C:700:LEU:HD21	2.48	0.43
1:B:401:GLU:CD	1:B:475:LYS:HD3	2.38	0.43
1:B:125:VAL:HG12	1:C:665:THR:OG1	2.18	0.43
1:B:108:ASN:CB	1:B:645:GLY:HA3	2.48	0.43
1:A:713:ASP:HB2	1:C:294:PHE:CG	2.53	0.43
1:C:607:GLU:HG2	1:C:608:ASP:H	1.83	0.43
1:C:543:ARG:HB3	1:C:550:ILE:HG21	2.00	0.43
1:A:394:THR:HG22	1:A:395:PHE:N	2.33	0.43
1:C:532:GLN:NE2	1:C:532:GLN:HA	2.33	0.43
1:A:532:GLN:NE2	1:A:532:GLN:HA	2.33	0.43
1:A:152:GLU:HB2	1:A:495:ILE:O	2.19	0.43
1:A:456:LEU:HD21	1:A:461:ALA:CA	2.36	0.43
1:B:146:ILE:HG21	1:B:424:ILE:HD12	2.01	0.43
1:A:665:THR:OG1	1:C:125:VAL:HG12	2.18	0.43
1:C:207:CYS:HB2	1:C:234:LEU:HD11	2.00	0.43
1:B:434:ILE:HG22	1:B:435:LYS:N	2.34	0.43
1:A:313:SER:HB2	1:A:314:TYR:CD1	2.43	0.43
1:A:224:HIS:HB2	1:A:269:VAL:CB	2.37	0.43
1:A:156:PRO:HD2	1:C:700:LEU:HD21	1.99	0.43
1:A:543:ARG:HB3	1:A:550:ILE:HG21	2.00	0.43
1:B:200:LYS:O	1:B:204:LYS:HB2	2.18	0.43
1:B:326:TYR:OH	1:B:339:PRO:HG3	2.17	0.43
1:A:284:TYR:HD1	1:A:284:TYR:N	2.16	0.43
1:B:705:VAL:HG12	1:B:706:GLN:N	2.29	0.43
1:B:553:VAL:CG1	1:B:554:THR:N	2.82	0.43
1:C:501:ILE:HG23	1:C:502:GLU:N	2.33	0.43
1:C:291:THR:HG21	1:C:293:ASP:CB	2.48	0.43
1:A:597:TYR:CZ	1:A:629:ALA:O	2.72	0.43
1:C:589:ILE:CD1	1:C:630:ILE:HD13	2.46	0.43
1:B:501:ILE:HG23	1:B:502:GLU:N	2.33	0.43
1:A:434:ILE:HG22	1:A:435:LYS:N	2.34	0.43
1:C:404:LEU:HA	1:C:404:LEU:HD12	1.85	0.43
1:A:699:LEU:CB	1:C:702:TYR:HE2	2.30	0.43
1:C:288:VAL:HG12	1:C:289:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:THR:HG22	1:B:505:ARG:HG2	2.01	0.43
1:A:538:LEU:HD21	1:B:539:TRP:CE3	2.53	0.43
1:A:497:THR:HG22	1:A:498:THR:O	2.19	0.43
1:C:218:LEU:HD23	1:C:219:GLU:C	2.39	0.43
1:C:384:PHE:HA	1:C:384:PHE:HD1	1.75	0.43
1:A:312:THR:HG23	1:A:313:SER:N	2.34	0.42
1:C:605:ARG:HH12	1:C:610:GLY:H	1.65	0.42
1:A:401:GLU:OE1	1:A:475:LYS:HD3	2.19	0.42
1:B:218:LEU:HD23	1:B:219:GLU:C	2.40	0.42
1:C:254:TYR:N	1:C:268:THR:CG2	2.82	0.42
1:C:553:VAL:CG1	1:C:554:THR:N	2.82	0.42
1:A:286:GLU:HG2	1:B:714:LEU:HD21	2.01	0.42
1:B:640:TYR:N	1:B:640:TYR:CD1	2.88	0.42
1:A:218:LEU:HD23	1:A:219:GLU:C	2.39	0.42
1:A:701:ASP:HB2	1:B:158:LYS:HZ3	1.84	0.42
1:A:707:ARG:CZ	1:B:242:ARG:H	2.33	0.42
1:B:297:MET:HE2	1:B:319:PHE:CE1	2.54	0.42
1:B:649:TYR:CD2	1:B:657:HIS:CE1	3.07	0.42
1:A:640:TYR:CD1	1:A:640:TYR:N	2.88	0.42
1:C:117:PRO:HA	1:C:118:PRO:HD3	1.90	0.42
1:C:312:THR:CG2	1:C:314:TYR:HB2	2.30	0.42
1:B:688:VAL:N	1:C:369:TRP:CZ2	2.88	0.42
1:B:288:VAL:CG1	1:B:289:LEU:N	2.82	0.42
1:B:297:MET:HE1	1:B:319:PHE:CD1	2.55	0.42
1:B:597:TYR:CZ	1:B:629:ALA:O	2.72	0.42
1:A:217:ASN:HB3	1:B:723:ILE:O	2.19	0.42
1:A:539:TRP:CE3	1:C:538:LEU:HD21	2.53	0.42
1:B:475:LYS:HA	1:B:476:PRO:HD3	1.77	0.42
1:B:394:THR:HG22	1:B:395:PHE:N	2.33	0.42
1:B:360:ARG:CZ	1:B:409:LEU:HD21	2.49	0.42
1:A:711:LEU:HD13	1:A:715:ARG:CD	2.49	0.42
1:C:666:THR:CG2	1:C:667:VAL:N	2.83	0.42
1:C:649:TYR:CD2	1:C:657:HIS:CE1	3.07	0.42
1:B:446:GLY:O	1:B:497:THR:HG23	2.20	0.42
1:C:434:ILE:HG22	1:C:435:LYS:N	2.34	0.42
1:A:715:ARG:CD	1:B:243:THR:HG23	2.46	0.42
1:A:301:TYR:O	1:A:301:TYR:CD1	2.73	0.42
1:A:553:VAL:CG1	1:A:554:THR:N	2.82	0.42
1:B:401:GLU:OE1	1:B:475:LYS:HD3	2.20	0.42
1:C:572:THR:CG2	1:C:573:CYS:N	2.82	0.42
1:B:118:PRO:HA	1:B:119:PRO:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:PHE:CE2	1:B:368:LYS:HB2	2.54	0.42
1:C:640:TYR:CD1	1:C:640:TYR:N	2.88	0.42
1:B:596:CYS:CB	1:B:653:TYR:CE1	3.03	0.42
1:C:301:TYR:HA	1:C:302:GLY:HA3	1.64	0.42
1:B:400:THR:CG2	1:B:401:GLU:N	2.83	0.42
1:C:401:GLU:OE1	1:C:475:LYS:HD3	2.19	0.42
1:B:536:LEU:HD13	1:C:669:THR:HG21	2.02	0.42
1:A:118:PRO:HA	1:A:119:PRO:HD3	1.83	0.42
1:A:124:VAL:CG1	1:A:125:VAL:N	2.83	0.42
1:A:273:VAL:HG12	1:A:274:GLU:N	2.34	0.42
1:A:397:THR:CG2	1:A:398:ASN:N	2.82	0.42
1:A:265:TYR:HD1	1:A:265:TYR:N	2.17	0.42
1:A:284:TYR:N	1:A:284:TYR:CD1	2.87	0.42
1:B:378:SER:HB2	1:B:385:ARG:HB2	2.02	0.42
1:A:164:TYR:N	1:A:164:TYR:CD1	2.88	0.42
1:C:363:VAL:HG13	1:C:364:CYS:SG	2.60	0.42
1:C:276:VAL:HG13	1:C:289:LEU:CD2	2.50	0.42
1:A:279:ARG:HH22	1:C:700:LEU:H	1.67	0.42
1:C:146:ILE:HG21	1:C:424:ILE:HD12	2.01	0.42
1:C:550:ILE:CD1	1:C:550:ILE:N	2.83	0.42
1:C:367:THR:CG2	1:C:368:LYS:N	2.83	0.42
1:A:576:VAL:CG1	1:A:577:ALA:N	2.83	0.42
1:B:469:LEU:HA	1:B:469:LEU:HD22	1.90	0.42
1:B:700:LEU:HD11	1:C:158:LYS:HB3	1.98	0.41
1:C:276:VAL:CG1	1:C:277:ASP:N	2.83	0.41
1:B:550:ILE:N	1:B:550:ILE:CD1	2.83	0.41
1:B:301:TYR:HA	1:B:359:LYS:HB2	2.02	0.41
1:A:649:TYR:CD2	1:A:657:HIS:CE1	3.07	0.41
1:A:655:TYR:CE2	1:A:656:SER:O	2.74	0.41
1:A:369:TRP:CZ2	1:C:686:LEU:HD11	2.54	0.41
1:A:446:GLY:O	1:A:497:THR:HG23	2.19	0.41
1:B:497:THR:HG22	1:B:498:THR:O	2.19	0.41
1:C:276:VAL:HG12	1:C:277:ASP:N	2.35	0.41
1:C:289:LEU:HD13	1:C:291:THR:HG22	2.02	0.41
1:C:393:THR:HG22	1:C:505:ARG:HG2	2.01	0.41
1:A:723:ILE:H	1:C:217:ASN:HB3	1.84	0.41
1:B:610:GLY:HA3	1:B:611:PRO:HD3	1.44	0.41
1:B:666:THR:CG2	1:B:667:VAL:N	2.83	0.41
1:C:597:TYR:C	1:C:597:TYR:CD1	2.94	0.41
1:B:124:VAL:CG1	1:B:125:VAL:N	2.83	0.41
1:A:536:LEU:CD1	1:B:669:THR:HG21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:SER:HB2	1:A:385:ARG:HB2	2.02	0.41
1:A:318:ARG:HD2	1:A:346:THR:O	2.20	0.41
1:A:707:ARG:NH2	1:B:242:ARG:H	2.18	0.41
1:A:711:LEU:CD1	1:B:243:THR:CG2	2.95	0.41
1:C:296:TYR:N	1:C:296:TYR:HD1	2.10	0.41
1:C:606:TYR:N	1:C:606:TYR:CD1	2.86	0.41
1:B:281:VAL:CG1	1:B:282:TYR:N	2.82	0.41
1:A:108:ASN:CB	1:A:645:GLY:HA3	2.49	0.41
1:C:576:VAL:CG1	1:C:577:ALA:N	2.83	0.41
1:A:688:VAL:HA	1:B:369:TRP:CZ2	2.56	0.41
1:A:536:LEU:HD13	1:B:669:THR:HG21	2.02	0.41
1:C:288:VAL:CG1	1:C:289:LEU:N	2.82	0.41
1:A:146:ILE:HG21	1:A:424:ILE:HD12	2.01	0.41
1:B:157:TYR:CD1	1:B:300:PHE:CZ	3.08	0.41
1:B:283:PRO:O	1:B:300:PHE:HD2	2.02	0.41
1:B:536:LEU:CD1	1:C:669:THR:HG21	2.50	0.41
1:B:601:LEU:HD12	1:B:601:LEU:N	2.36	0.41
1:B:276:VAL:CG1	1:B:277:ASP:N	2.82	0.41
1:C:597:TYR:CZ	1:C:629:ALA:O	2.73	0.41
1:A:256:PRO:HG3	1:A:265:TYR:O	2.20	0.41
1:C:124:VAL:CG1	1:C:125:VAL:N	2.83	0.41
1:B:582:ILE:CG2	1:B:583:VAL:N	2.83	0.41
1:C:174:TRP:CD1	1:C:263:HIS:CE1	3.08	0.41
1:B:164:TYR:N	1:B:164:TYR:CD1	2.88	0.41
1:A:697:SER:OG	1:B:154:ILE:HG13	2.20	0.41
1:A:229:GLU:HG2	1:A:230:THR:N	2.36	0.41
1:B:638:ARG:HD2	1:B:638:ARG:HH11	1.75	0.41
1:B:221:THR:CG2	1:B:222:ALA:N	2.83	0.41
1:C:596:CYS:CB	1:C:653:TYR:CE1	3.03	0.41
1:A:596:CYS:CB	1:A:653:TYR:CE1	3.03	0.41
1:A:699:LEU:CD1	1:A:699:LEU:N	2.82	0.41
1:B:154:ILE:HB	1:B:155:ALA:HA	2.02	0.41
1:A:288:VAL:CG1	1:A:289:LEU:N	2.83	0.41
1:A:666:THR:CG2	1:A:667:VAL:N	2.83	0.41
1:B:157:TYR:CG	1:B:300:PHE:CE1	3.09	0.41
1:C:172:GLN:CB	1:C:183:MET:HB2	2.48	0.41
1:A:106:ALA:HB2	1:A:643:PHE:CZ	2.55	0.41
1:A:223:PHE:N	1:A:223:PHE:CD1	2.89	0.41
1:A:550:ILE:CD1	1:A:550:ILE:N	2.83	0.41
1:A:667:VAL:HB	1:C:554:THR:CG2	2.51	0.41
1:C:597:TYR:CE2	1:C:629:ALA:O	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:LEU:N	1:A:659:LEU:CD1	2.83	0.41
1:B:576:VAL:CG1	1:B:577:ALA:N	2.83	0.41
1:A:669:THR:HG21	1:C:536:LEU:CD1	2.50	0.41
1:C:287:PHE:CD1	1:C:297:MET:O	2.74	0.41
1:A:708:ARG:HD2	1:B:244:SER:CB	2.51	0.41
1:B:276:VAL:CG1	1:B:290:ALA:H	2.33	0.41
1:B:332:THR:O	1:B:333:LYS:HB2	2.21	0.41
1:B:554:THR:CG2	1:C:667:VAL:HB	2.51	0.41
1:B:283:PRO:O	1:B:300:PHE:CD2	2.74	0.41
1:A:400:THR:CG2	1:A:401:GLU:N	2.83	0.41
1:B:572:THR:CG2	1:B:573:CYS:N	2.82	0.41
1:A:221:THR:CG2	1:A:222:ALA:N	2.83	0.41
1:C:221:THR:CG2	1:C:222:ALA:N	2.83	0.41
1:A:582:ILE:CG2	1:A:583:VAL:N	2.83	0.41
1:B:248:HIS:HA	1:B:271:CYS:O	2.20	0.41
1:C:378:SER:HB2	1:C:385:ARG:HB2	2.02	0.41
1:C:133:CYS:HA	1:C:134:PRO:HD3	1.86	0.41
1:C:332:THR:O	1:C:333:LYS:HB2	2.21	0.41
1:B:597:TYR:CD1	1:B:597:TYR:C	2.94	0.41
1:C:600:PRO:HG3	1:C:641:PHE:CD2	2.56	0.41
1:C:400:THR:CG2	1:C:401:GLU:N	2.83	0.41
1:B:365:THR:CG2	1:B:366:MET:N	2.84	0.41
1:B:267:THR:HG22	1:B:268:THR:N	2.36	0.41
1:A:393:THR:HG22	1:A:505:ARG:HG2	2.01	0.40
1:C:283:PRO:HB3	1:C:300:PHE:CZ	2.56	0.40
1:A:332:THR:O	1:A:333:LYS:HB2	2.21	0.40
1:A:293:ASP:C	1:A:294:PHE:HD1	2.24	0.40
1:C:655:TYR:CE2	1:C:656:SER:O	2.74	0.40
1:A:194:PHE:C	1:A:194:PHE:CD1	2.95	0.40
1:A:700:LEU:HD12	1:B:158:LYS:HZ1	1.86	0.40
1:A:713:ASP:CB	1:C:294:PHE:HD1	2.35	0.40
1:C:275:GLU:HG2	1:C:276:VAL:N	2.36	0.40
1:B:297:MET:HE2	1:B:319:PHE:CD1	2.56	0.40
1:A:276:VAL:HG21	1:C:715:ARG:CZ	2.52	0.40
1:C:175:PHE:CD1	1:C:259:VAL:O	2.74	0.40
1:C:497:THR:HG22	1:C:498:THR:O	2.21	0.40
1:B:707:ARG:CZ	1:C:242:ARG:HB3	2.51	0.40
1:A:715:ARG:CD	1:B:243:THR:CG2	2.96	0.40
1:A:554:THR:CG2	1:B:667:VAL:HB	2.51	0.40
1:A:597:TYR:CE2	1:A:629:ALA:O	2.74	0.40
1:B:600:PRO:HG3	1:B:641:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:TYR:CE2	1:B:629:ALA:O	2.74	0.40
1:C:587:MET:HE1	1:C:598:SER:O	2.21	0.40
1:C:641:PHE:HB2	1:C:648:VAL:HG12	2.03	0.40
1:B:194:PHE:C	1:B:194:PHE:CD1	2.95	0.40
1:B:198:ILE:CD1	1:B:198:ILE:N	2.85	0.40
1:A:369:TRP:CE2	1:C:688:VAL:HA	2.56	0.40
1:C:582:ILE:CG2	1:C:583:VAL:N	2.83	0.40
1:B:408:ASP:OD1	1:B:409:LEU:HG	2.21	0.40
1:A:601:LEU:N	1:A:601:LEU:HD12	2.36	0.40
1:B:341:THR:HB	1:B:356:TRP:HE3	1.87	0.40
1:A:669:THR:HG21	1:C:536:LEU:HD13	2.02	0.40
1:A:510:TYR:C	1:A:510:TYR:CD1	2.95	0.40
1:A:469:LEU:HA	1:A:469:LEU:HD22	1.90	0.40
1:C:224:HIS:HB2	1:C:269:VAL:HB	2.04	0.40
1:A:245:ARG:HG3	1:A:275:GLU:OE1	2.22	0.40
1:A:297:MET:HB2	1:A:345:LEU:HD22	2.04	0.40
1:A:117:PRO:HA	1:A:118:PRO:HD3	1.90	0.40
1:C:377:ARG:HA	1:C:385:ARG:O	2.22	0.40
1:C:510:TYR:C	1:C:510:TYR:CD1	2.95	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	604/622 (97%)	585 (97%)	14 (2%)	5 (1%)	24	69
1	B	604/622 (97%)	581 (96%)	19 (3%)	4 (1%)	26	71
1	C	604/622 (97%)	588 (97%)	13 (2%)	3 (0%)	34	77
All	All	1812/1866 (97%)	1754 (97%)	46 (2%)	12 (1%)	31	71

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	VAL
1	A	409	LEU
1	B	276	VAL
1	B	409	LEU
1	C	226	ASP
1	C	409	LEU
1	A	226	ASP
1	A	233	GLU
1	A	410	GLY
1	B	228	HIS
1	B	410	GLY
1	C	410	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	530/541 (98%)	493 (93%)	37 (7%)	19	56
1	B	530/541 (98%)	495 (93%)	35 (7%)	21	57
1	C	530/541 (98%)	494 (93%)	36 (7%)	20	57
All	All	1590/1623 (98%)	1482 (93%)	108 (7%)	24	57

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	140	GLN
1	A	154	ILE
1	A	195	GLU
1	A	227	ASP
1	A	232	MET
1	A	234	LEU
1	A	235	LYS
1	A	255	ASN
1	A	265	TYR
1	A	286	GLU

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Mol	Chain	Res	Type
1	A	289	LEU
1	A	296	TYR
1	A	297	MET
1	A	301	TYR
1	A	304	ARG
1	A	312	THR
1	A	314	TYR
1	A	380	TYR
1	A	384	PHE
1	A	392	SER
1	A	404	LEU
1	A	415	LYS
1	A	463	LEU
1	A	502	GLU
1	A	584	GLN
1	A	588	ARG
1	A	597	TYR
1	A	605	ARG
1	A	628	ASP
1	A	689	TYR
1	A	700	LEU
1	A	701	ASP
1	A	702	TYR
1	A	707	ARG
1	A	711	LEU
1	A	719	ILE
1	B	110	ASP
1	B	140	GLN
1	B	195	GLU
1	B	226	ASP
1	B	228	HIS
1	B	232	MET
1	B	235	LYS
1	B	243	THR
1	B	254	TYR
1	B	255	ASN
1	B	265	TYR
1	B	285	ASP
1	B	300	PHE
1	B	301	TYR
1	B	303	TYR
1	B	304	ARG

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Mol	Chain	Res	Type
1	B	312	THR
1	B	314	TYR
1	B	380	TYR
1	B	384	PHE
1	B	392	SER
1	B	404	LEU
1	B	415	LYS
1	B	463	LEU
1	B	502	GLU
1	B	584	GLN
1	B	588	ARG
1	B	597	TYR
1	B	605	ARG
1	B	628	ASP
1	B	687	GLU
1	B	688	VAL
1	B	699	LEU
1	B	700	LEU
1	B	718	ASP
1	C	110	ASP
1	C	140	GLN
1	C	154	ILE
1	C	158	LYS
1	C	195	GLU
1	C	225	ARG
1	C	227	ASP
1	C	234	LEU
1	C	235	LYS
1	C	255	ASN
1	C	258	ARG
1	C	265	TYR
1	C	268	THR
1	C	282	TYR
1	C	284	TYR
1	C	286	GLU
1	C	289	LEU
1	C	291	THR
1	C	296	TYR
1	C	304	ARG
1	C	307	SER
1	C	310	GLU
1	C	314	TYR

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Mol	Chain	Res	Type
1	C	380	TYR
1	C	384	PHE
1	C	392	SER
1	C	404	LEU
1	C	415	LYS
1	C	463	LEU
1	C	502	GLU
1	C	584	GLN
1	C	588	ARG
1	C	597	TYR
1	C	605	ARG
1	C	628	ASP
1	C	700	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	217	ASN
1	A	248	HIS
1	A	321	GLN
1	A	516	HIS
1	A	580	ASN
1	B	217	ASN
1	B	248	HIS
1	B	311	HIS
1	B	321	GLN
1	B	516	HIS
1	B	580	ASN
1	B	706	GLN
1	C	217	ASN
1	C	248	HIS
1	C	321	GLN
1	C	516	HIS
1	C	580	ASN
1	C	712	HIS

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.