



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:51 AM GMT

PDB ID : 3CF3
Title : Structure of P97/vcp in complex with ADP
Authors : Davies, J.M.; Delabarre, B.; Brunger, A.T.; Weis, W.I.
Deposited on : 2008-03-01
Resolution : 4.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

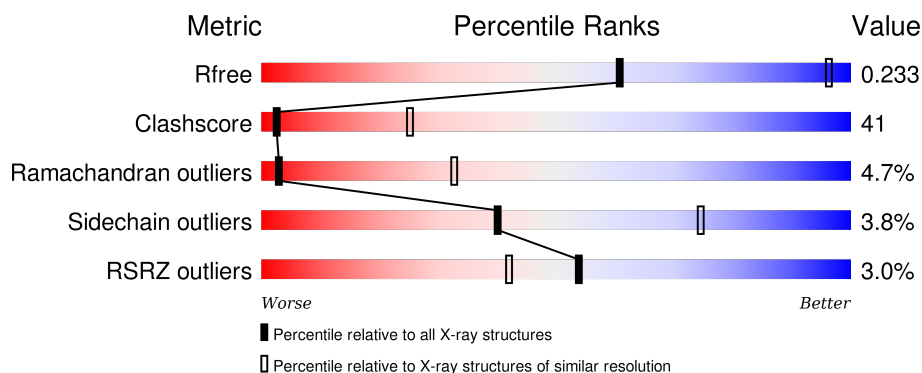
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.25 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1043 (4.92-3.60)
Clashscore	102246	1145 (4.92-3.60)
Ramachandran outliers	100387	1088 (4.92-3.60)
Sidechain outliers	100360	1072 (4.92-3.60)
RSRZ outliers	91569	1047 (4.92-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	806	<div> <div>3%</div> <div> <div></div> <div>37%</div> <div>48%</div> <div>5%</div> <div>10%</div> </div> </div>
1	B	806	<div> <div>2%</div> <div> <div></div> <div>37%</div> <div>49%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	806	<div> <div>2%</div> <div> <div></div> <div>37%</div> <div>47%</div> <div>5%</div> <div>10%</div> </div> </div>

2 Entry composition [i](#)

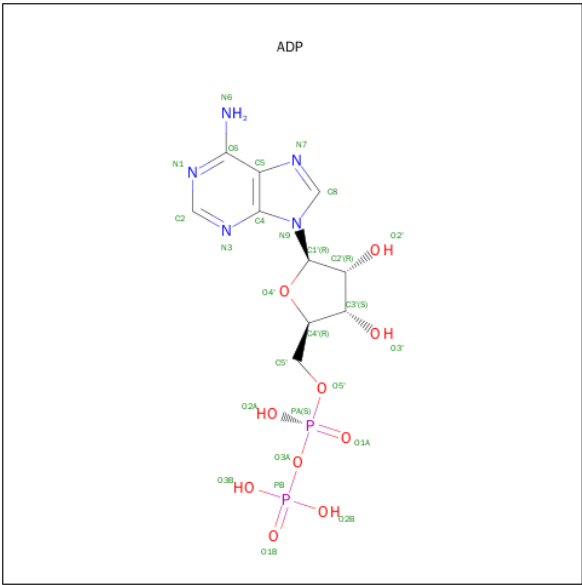
There are 2 unique types of molecules in this entry. The entry contains 17139 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	723	Total	C	N	O	S	0	0	0
			5659	3561	996	1072	30			
1	B	723	Total	C	N	O	S	0	0	0
			5659	3561	996	1072	30			
1	C	723	Total	C	N	O	S	0	0	0
			5659	3561	996	1072	30			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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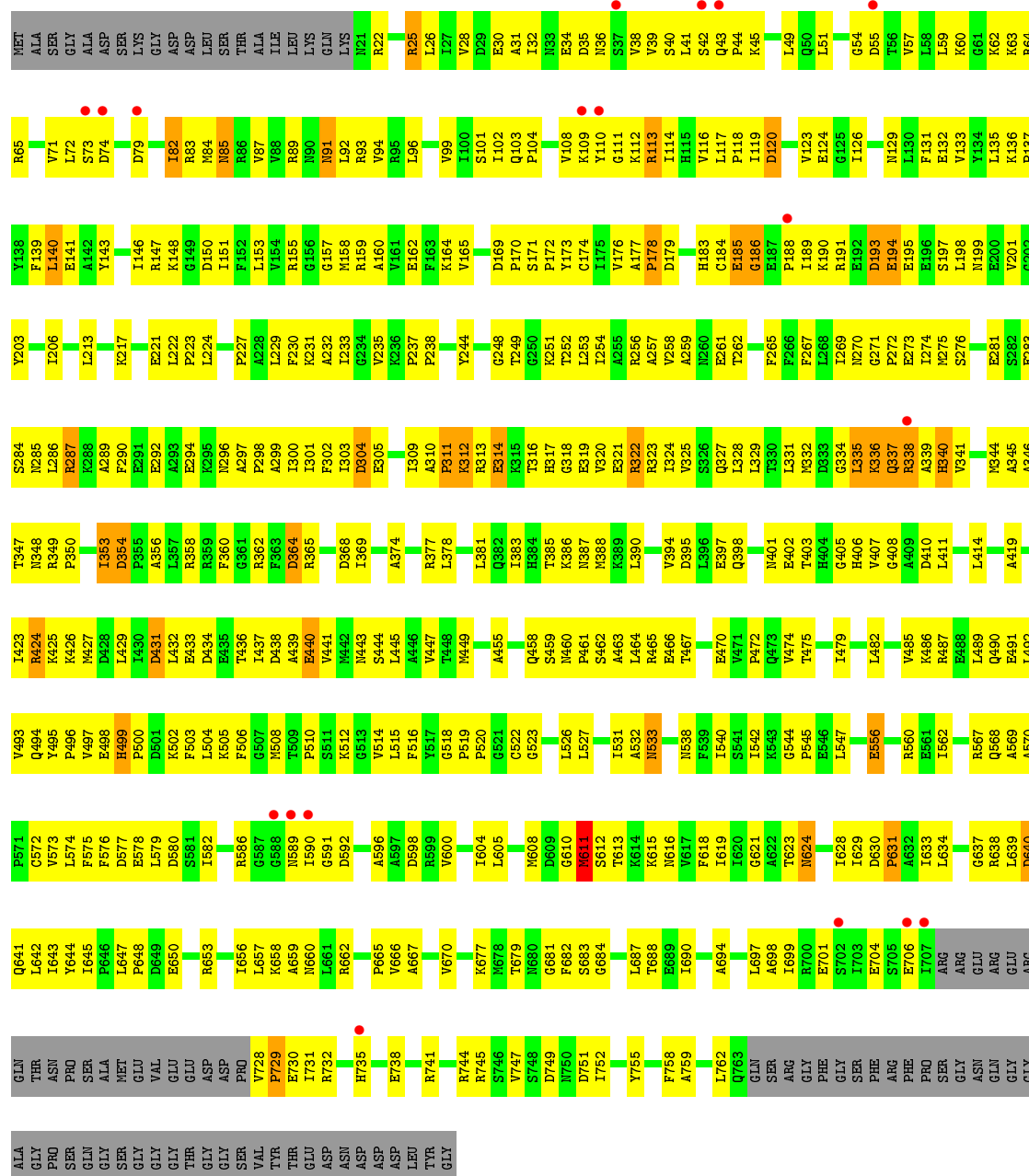
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

GLY
PRO
SER
GLN
GLY
SER
GLY
GLY
GLY
THR
GLY
THR
GLY
SER
SER
VAL
THR
THR
GLU
LEU
ASP
ASN
ASP
ASP
LEU
TYR
GLY

• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain B: 



• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C: 





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	163.97Å 178.93Å 320.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.25 29.94 – 4.25	Depositor EDS
% Data completeness (in resolution range)	86.4 (40.00-4.25) 92.9 (29.94-4.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 4.26Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.198 , 0.226 0.208 , 0.233	Depositor DCC
R_{free} test set	2167 reflections (7.41%)	DCC
Wilson B-factor (Å ²)	143.2	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 188.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 63665 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17139	wwPDB-VP
Average B, all atoms (Å ²)	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.38	0/5751	0.87	9/7767 (0.1%)
1	B	0.37	0/5751	0.87	9/7767 (0.1%)
1	C	0.38	0/5751	0.88	9/7767 (0.1%)
All	All	0.38	0/17253	0.87	27/23301 (0.1%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	322	ARG	NE-CZ-NH2	-29.67	105.46	120.30
1	A	338	ARG	NE-CZ-NH1	-29.13	105.74	120.30
1	B	287	ARG	NE-CZ-NH2	-28.38	106.11	120.30
1	A	338	ARG	NE-CZ-NH2	27.38	133.99	120.30
1	B	287	ARG	NE-CZ-NH1	27.28	133.94	120.30
1	C	322	ARG	NE-CZ-NH1	27.22	133.91	120.30
1	C	322	ARG	CD-NE-CZ	18.81	149.94	123.60
1	B	287	ARG	CD-NE-CZ	18.44	149.41	123.60
1	A	338	ARG	CD-NE-CZ	18.30	149.23	123.60
1	C	287	ARG	NE-CZ-NH1	-14.83	112.89	120.30
1	B	322	ARG	NE-CZ-NH1	-14.75	112.92	120.30
1	C	338	ARG	NE-CZ-NH2	-14.54	113.03	120.30
1	B	338	ARG	NE-CZ-NH2	-14.37	113.12	120.30
1	A	322	ARG	NE-CZ-NH1	-14.28	113.16	120.30
1	A	287	ARG	NE-CZ-NH1	-14.04	113.28	120.30
1	A	287	ARG	NE-CZ-NH2	13.90	127.25	120.30
1	C	287	ARG	NE-CZ-NH2	13.86	127.23	120.30
1	C	338	ARG	NE-CZ-NH1	13.63	127.12	120.30
1	B	322	ARG	NE-CZ-NH2	13.51	127.05	120.30
1	B	338	ARG	NE-CZ-NH1	13.43	127.02	120.30
1	A	322	ARG	NE-CZ-NH2	13.11	126.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	287	ARG	CD-NE-CZ	10.69	138.56	123.60
1	A	287	ARG	CD-NE-CZ	10.58	138.41	123.60
1	B	322	ARG	CD-NE-CZ	10.14	137.80	123.60
1	A	322	ARG	CD-NE-CZ	10.02	137.63	123.60
1	C	338	ARG	CD-NE-CZ	9.89	137.45	123.60
1	B	338	ARG	CD-NE-CZ	9.82	137.35	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5659	0	5731	495	0
1	B	5659	0	5731	491	0
1	C	5659	0	5731	466	0
2	A	54	0	24	6	0
2	B	54	0	24	4	0
2	C	54	0	24	3	0
All	All	17139	0	17265	1421	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 41.

All (1421) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:CD1	1:A:213:LEU:HD11	1.25	1.64
1:B:206:ILE:CD1	1:B:213:LEU:HD11	1.24	1.61
1:C:206:ILE:CD1	1:C:213:LEU:HD11	1.25	1.59
1:A:206:ILE:HD11	1:A:213:LEU:CD1	1.55	1.34
1:C:206:ILE:HD11	1:C:213:LEU:CD1	1.55	1.34
1:B:206:ILE:HD11	1:B:213:LEU:CD1	1.56	1.33
1:B:206:ILE:CD1	1:B:213:LEU:CD1	2.15	1.23
1:A:206:ILE:CD1	1:A:213:LEU:CD1	2.15	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:HD12	1:B:213:LEU:HD11	1.22	1.16
1:C:206:ILE:CD1	1:C:213:LEU:CD1	2.15	1.15
1:C:206:ILE:HD12	1:C:213:LEU:HD11	1.25	1.12
1:A:206:ILE:HD12	1:A:213:LEU:HD11	1.26	1.11
1:C:51:LEU:HD21	1:C:104:PRO:HB3	1.35	1.09
1:B:51:LEU:HD21	1:B:104:PRO:HB3	1.35	1.08
1:A:51:LEU:HD21	1:A:104:PRO:HB3	1.34	1.07
1:B:353:ILE:HG22	1:B:354:ASP:H	1.22	1.04
1:C:353:ILE:HG22	1:C:354:ASP:H	1.21	1.04
1:A:259:ALA:HB2	1:A:300:ILE:HD12	1.38	1.04
1:C:337:GLN:HE21	1:C:337:GLN:HA	1.24	1.03
1:A:353:ILE:HG22	1:A:354:ASP:H	1.22	1.03
1:B:169:ASP:HB3	1:B:170:PRO:HD3	1.39	1.02
1:A:337:GLN:HA	1:A:337:GLN:HE21	1.24	1.01
1:B:337:GLN:HA	1:B:337:GLN:HE21	1.24	1.01
1:A:169:ASP:HB3	1:A:170:PRO:HD3	1.41	1.01
1:C:111:GLY:HA2	1:C:170:PRO:HG2	1.43	1.00
1:C:169:ASP:HB3	1:C:170:PRO:HD3	1.42	0.98
1:A:111:GLY:HA2	1:A:170:PRO:HG2	1.39	0.98
1:B:111:GLY:HA2	1:B:170:PRO:HG2	1.45	0.98
1:C:397:GLU:HG2	1:C:401:ASN:HD21	1.29	0.98
1:B:397:GLU:HG2	1:B:401:ASN:HD21	1.29	0.97
1:B:466:GLU:HG2	1:B:467:THR:H	1.27	0.96
1:A:397:GLU:HG2	1:A:401:ASN:HD21	1.29	0.96
1:C:313:ARG:O	1:C:316:THR:HG22	1.65	0.95
1:A:133:VAL:HG13	1:A:443:ASN:ND2	1.83	0.94
1:A:164:LYS:HE2	1:A:189:ILE:HD12	1.50	0.94
1:A:126:ILE:HB	1:A:439:ALA:HB2	1.47	0.93
1:A:611:MET:HE1	1:A:619:ILE:HD11	1.48	0.93
1:B:313:ARG:O	1:B:316:THR:HG22	1.69	0.92
1:C:164:LYS:HE2	1:C:189:ILE:HD12	1.52	0.92
1:C:113:ARG:HH11	1:C:113:ARG:HG2	1.33	0.91
1:B:164:LYS:HE2	1:B:189:ILE:HD12	1.52	0.91
1:B:611:MET:HE1	1:B:619:ILE:HD11	1.50	0.91
1:C:611:MET:HE1	1:C:619:ILE:HD11	1.52	0.90
1:A:313:ARG:O	1:A:316:THR:HG22	1.72	0.90
1:C:313:ARG:HG2	1:C:314:GLU:H	1.36	0.88
1:B:113:ARG:HG2	1:B:113:ARG:HH11	1.38	0.87
1:A:113:ARG:HG2	1:A:113:ARG:HH11	1.37	0.87
1:A:614:LYS:HD3	1:B:402:GLU:HB2	1.55	0.86
1:B:206:ILE:HD11	1:B:213:LEU:HD11	0.88	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:TYR:CE1	1:A:178:PRO:HD2	2.10	0.85
1:C:206:ILE:HD11	1:C:213:LEU:HD11	0.86	0.85
1:A:133:VAL:HG13	1:A:443:ASN:HD22	1.38	0.85
1:B:329:LEU:HD22	1:B:362:ARG:NH1	1.92	0.85
1:A:329:LEU:HD22	1:A:362:ARG:NH1	1.92	0.84
1:B:665:PRO:O	1:B:731:ILE:HG22	1.75	0.84
1:A:472:PRO:HG2	1:A:532:ALA:HB3	1.60	0.84
1:A:206:ILE:HD11	1:A:213:LEU:HD11	0.86	0.84
1:C:329:LEU:HD22	1:C:362:ARG:NH1	1.93	0.84
1:A:499:HIS:N	1:A:500:PRO:HD3	1.93	0.84
1:C:499:HIS:N	1:C:500:PRO:HD3	1.93	0.84
1:B:129:ASN:ND2	1:B:132:GLU:HB2	1.94	0.83
1:C:665:PRO:O	1:C:731:ILE:HG22	1.77	0.83
1:A:129:ASN:ND2	1:A:132:GLU:HB2	1.94	0.82
1:A:460:ASN:N	1:A:461:PRO:HD2	1.93	0.82
1:B:499:HIS:N	1:B:500:PRO:HD3	1.94	0.82
1:C:143:TYR:CE1	1:C:178:PRO:HD2	2.15	0.81
1:C:31:ALA:HA	1:C:83:ARG:HB3	1.63	0.81
1:C:129:ASN:ND2	1:C:132:GLU:HB2	1.95	0.81
1:B:143:TYR:CE1	1:B:178:PRO:HD2	2.15	0.80
1:B:514:VAL:HG11	1:B:643:ILE:HD12	1.63	0.80
1:A:514:VAL:HG11	1:A:643:ILE:HD12	1.62	0.80
1:C:514:VAL:HG11	1:C:643:ILE:HD12	1.63	0.80
1:A:31:ALA:HA	1:A:83:ARG:HB3	1.64	0.80
1:C:749:ASP:HA	1:C:752:ILE:HD12	1.63	0.80
1:A:749:ASP:HA	1:A:752:ILE:HD12	1.64	0.80
1:B:749:ASP:HA	1:B:752:ILE:HD12	1.62	0.80
1:C:337:GLN:NE2	1:C:337:GLN:HA	1.97	0.79
1:B:337:GLN:HA	1:B:337:GLN:NE2	1.98	0.79
1:B:31:ALA:HA	1:B:83:ARG:HB3	1.65	0.79
1:B:65:ARG:NH1	1:B:93:ARG:HH12	1.81	0.79
1:C:472:PRO:HG2	1:C:532:ALA:HB3	1.65	0.79
1:A:337:GLN:HA	1:A:337:GLN:NE2	1.98	0.79
1:A:267:PHE:HE2	1:A:289:ALA:HB1	1.48	0.78
1:A:313:ARG:HG2	1:A:314:GLU:H	1.49	0.78
1:B:206:ILE:HD12	1:B:213:LEU:CD1	1.99	0.78
1:C:318:GLY:O	1:C:322:ARG:HG3	1.85	0.77
1:C:491:GLU:HG2	1:C:495:TYR:CE2	2.19	0.77
1:B:500:PRO:O	1:B:504:LEU:HD13	1.83	0.77
1:A:500:PRO:O	1:A:504:LEU:HD13	1.83	0.77
1:B:491:GLU:HG2	1:B:495:TYR:CE2	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:PHE:HE2	1:B:289:ALA:HB1	1.49	0.77
1:A:62:LYS:O	1:A:64:ARG:N	2.17	0.77
1:B:230:PHE:HA	1:B:233:ILE:HG22	1.67	0.77
1:B:405:GLY:HA3	1:B:465:ARG:HD3	1.67	0.77
1:A:491:GLU:HG2	1:A:495:TYR:CE2	2.19	0.77
1:C:267:PHE:HE2	1:C:289:ALA:HB1	1.50	0.77
1:B:329:LEU:HD22	1:B:362:ARG:HH11	1.50	0.77
1:C:658:LYS:O	1:C:662:ARG:HG3	1.86	0.76
1:A:329:LEU:HD22	1:A:362:ARG:HH11	1.51	0.76
1:B:490:GLN:HB3	1:B:494:GLN:HG3	1.68	0.76
1:B:136:LYS:HB3	1:B:137:PRO:HD3	1.67	0.76
1:A:506:PHE:CD2	1:B:699:ILE:HG12	2.20	0.76
1:A:512:LYS:HD3	1:A:637:GLY:O	1.86	0.76
1:C:259:ALA:HB2	1:C:300:ILE:HD12	1.66	0.76
1:C:519:PRO:HG2	1:C:522:CYS:SG	2.26	0.76
1:B:658:LYS:O	1:B:662:ARG:HG3	1.86	0.76
1:C:60:LYS:NZ	1:C:103:GLN:NE2	2.33	0.75
1:C:230:PHE:HA	1:C:233:ILE:HG22	1.68	0.75
1:C:500:PRO:O	1:C:504:LEU:HD13	1.85	0.75
1:A:560:ARG:HG3	1:A:560:ARG:HH11	1.51	0.75
1:C:206:ILE:HD12	1:C:213:LEU:CD1	2.02	0.75
1:A:353:ILE:HG22	1:A:354:ASP:N	2.00	0.75
1:B:353:ILE:HG22	1:B:354:ASP:N	1.99	0.75
1:A:133:VAL:CG1	1:A:443:ASN:HD22	1.99	0.75
1:B:313:ARG:HG2	1:B:314:GLU:H	1.52	0.75
1:A:658:LYS:O	1:A:662:ARG:HG3	1.86	0.75
1:A:490:GLN:HB3	1:A:494:GLN:HG3	1.69	0.75
1:B:323:ARG:HH22	1:C:279:ALA:HB2	1.50	0.75
1:C:353:ILE:HG22	1:C:354:ASP:N	1.99	0.74
1:B:519:PRO:HG2	1:B:522:CYS:SG	2.27	0.74
1:A:328:LEU:HD11	1:A:332:MET:HG2	1.69	0.74
1:C:499:HIS:H	1:C:500:PRO:HD3	1.51	0.74
1:B:328:LEU:HD11	1:B:332:MET:HG2	1.69	0.74
1:C:336:LYS:C	1:C:338:ARG:H	1.90	0.74
1:C:394:VAL:HA	1:C:449:MET:HB2	1.68	0.74
1:A:230:PHE:HA	1:A:233:ILE:HG22	1.69	0.74
1:C:136:LYS:HB3	1:C:137:PRO:HD3	1.69	0.74
1:B:336:LYS:C	1:B:338:ARG:H	1.90	0.74
1:C:570:ALA:HB1	1:C:616:ASN:HB3	1.68	0.74
1:A:222:LEU:HD21	1:B:424:ARG:HG2	1.70	0.73
1:A:665:PRO:O	1:A:731:ILE:HG22	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:ARG:HH11	1:B:560:ARG:HG3	1.51	0.73
1:A:336:LYS:C	1:A:338:ARG:H	1.91	0.73
1:A:394:VAL:HA	1:A:449:MET:HB2	1.68	0.73
1:B:377:ARG:HD2	1:B:403:THR:OG1	1.87	0.73
1:A:499:HIS:H	1:A:500:PRO:HD3	1.51	0.73
1:A:377:ARG:HD2	1:A:403:THR:OG1	1.88	0.73
1:C:490:GLN:HB3	1:C:494:GLN:HG3	1.71	0.73
1:C:51:LEU:CD2	1:C:104:PRO:HB3	2.16	0.72
1:B:570:ALA:HB1	1:B:616:ASN:HB3	1.69	0.72
1:A:110:TYR:CD1	1:A:177:ALA:HB2	2.25	0.72
1:C:329:LEU:HD22	1:C:362:ARG:HH11	1.51	0.72
1:A:158:MET:HE2	1:A:388:MET:HB3	1.70	0.72
1:C:423:ILE:HG12	1:C:445:LEU:HD11	1.72	0.72
1:C:560:ARG:HG3	1:C:560:ARG:HH11	1.52	0.72
1:A:427:MET:HG3	1:A:432:LEU:HG	1.71	0.72
1:B:423:ILE:HG12	1:B:445:LEU:HD11	1.71	0.72
1:A:519:PRO:HG2	1:A:522:CYS:SG	2.29	0.72
1:B:394:VAL:HA	1:B:449:MET:HB2	1.70	0.72
1:A:113:ARG:NH2	1:A:183:HIS:NE2	2.38	0.72
1:A:51:LEU:CD2	1:A:104:PRO:HB3	2.16	0.72
1:B:460:ASN:N	1:B:461:PRO:HD2	2.05	0.72
1:B:51:LEU:CD2	1:B:104:PRO:HB3	2.17	0.71
1:B:170:PRO:HB2	1:B:174:CYS:HB3	1.73	0.71
1:B:259:ALA:HB2	1:B:300:ILE:HD12	1.70	0.71
1:C:110:TYR:CD1	1:C:177:ALA:HB2	2.25	0.71
1:B:499:HIS:H	1:B:500:PRO:HD3	1.52	0.71
1:C:34:GLU:N	1:C:34:GLU:OE1	2.22	0.71
1:B:466:GLU:HG2	1:B:467:THR:N	2.04	0.71
1:C:206:ILE:HD11	1:C:213:LEU:HD13	1.67	0.71
1:A:206:ILE:HD12	1:A:213:LEU:CD1	2.02	0.70
1:A:253:LEU:HD12	2:A:807:ADP:H2'	1.73	0.70
1:A:170:PRO:HB2	1:A:174:CYS:HB3	1.73	0.70
1:B:117:LEU:HD21	1:B:185:GLU:HG2	1.73	0.70
1:B:110:TYR:CD1	1:B:177:ALA:HB2	2.26	0.70
1:A:136:LYS:HB3	1:A:137:PRO:HD3	1.72	0.70
1:B:427:MET:HG3	1:B:432:LEU:HG	1.74	0.70
1:A:206:ILE:HD11	1:A:213:LEU:HD13	1.68	0.70
1:B:383:ILE:O	1:B:386:LYS:HG2	1.91	0.70
1:C:377:ARG:HD2	1:C:403:THR:OG1	1.91	0.70
1:B:512:LYS:HD3	1:B:637:GLY:O	1.92	0.69
1:C:608:MET:HG3	1:C:619:ILE:CD1	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLY:HA2	1:A:170:PRO:CG	2.20	0.69
1:A:383:ILE:O	1:A:386:LYS:HG2	1.93	0.69
1:C:113:ARG:HH11	1:C:113:ARG:CG	2.05	0.69
1:B:608:MET:HG3	1:B:619:ILE:CD1	2.22	0.69
1:B:113:ARG:NH2	1:B:183:HIS:NE2	2.41	0.69
1:C:328:LEU:HD11	1:C:332:MET:HG2	1.73	0.69
1:C:512:LYS:HD3	1:C:637:GLY:O	1.92	0.69
1:C:203:TYR:CE2	1:C:261:GLU:HG2	2.27	0.69
1:C:518:GLY:C	1:C:755:TYR:HE2	1.97	0.69
1:B:206:ILE:HD11	1:B:213:LEU:HD13	1.67	0.68
1:C:87:VAL:HG22	1:C:198:LEU:HD13	1.74	0.68
1:A:475:THR:HG22	1:A:533:ASN:HD21	1.56	0.68
1:B:270:ASN:HB3	1:B:273:GLU:HB2	1.75	0.68
1:C:491:GLU:HG2	1:C:495:TYR:HE2	1.58	0.68
1:C:158:MET:HE2	1:C:388:MET:HB3	1.73	0.68
1:A:95:ARG:HB2	1:A:225:ARG:CZ	2.23	0.68
1:B:87:VAL:HG22	1:B:198:LEU:HD13	1.75	0.68
1:C:170:PRO:HB2	1:C:174:CYS:HB3	1.74	0.68
1:C:461:PRO:O	1:C:463:ALA:N	2.26	0.68
1:B:34:GLU:N	1:B:34:GLU:OE1	2.24	0.68
1:C:482:LEU:O	1:C:486:LYS:HG3	1.94	0.68
1:C:514:VAL:HG12	1:C:515:LEU:N	2.09	0.67
1:A:151:ILE:HD11	1:A:195:GLU:OE2	1.93	0.67
1:A:203:TYR:O	1:A:206:ILE:HG12	1.95	0.67
1:B:514:VAL:HG12	1:B:515:LEU:N	2.09	0.67
1:A:267:PHE:HE2	1:A:289:ALA:CB	2.07	0.67
1:C:490:GLN:O	1:C:494:GLN:HB2	1.95	0.67
1:C:270:ASN:HB3	1:C:273:GLU:HB2	1.75	0.67
1:C:612:SER:HB3	1:C:615:LYS:HG2	1.76	0.67
1:B:169:ASP:HB3	1:B:170:PRO:CD	2.21	0.67
1:C:320:VAL:O	1:C:324:ILE:HG13	1.94	0.67
1:B:490:GLN:O	1:B:494:GLN:HB2	1.94	0.67
1:B:133:VAL:HG13	1:B:443:ASN:HD22	1.60	0.67
1:A:423:ILE:HG12	1:A:445:LEU:HD11	1.75	0.67
1:A:270:ASN:HB3	1:A:273:GLU:HB2	1.75	0.67
1:A:251:LYS:HG3	2:A:807:ADP:O2B	1.95	0.67
1:A:608:MET:HG3	1:A:619:ILE:CD1	2.23	0.67
1:A:117:LEU:HD21	1:A:185:GLU:HG2	1.76	0.67
1:C:667:ALA:HB3	1:C:670:VAL:HG23	1.77	0.67
1:A:437:ILE:HG22	1:A:438:ASP:N	2.09	0.67
1:A:34:GLU:OE1	1:A:34:GLU:N	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:ALA:HB3	1:A:670:VAL:HG23	1.77	0.67
1:A:482:LEU:O	1:A:486:LYS:HG3	1.94	0.67
1:A:30:GLU:OE2	1:A:217:LYS:NZ	2.28	0.67
1:A:490:GLN:O	1:A:494:GLN:HB2	1.94	0.67
1:B:612:SER:HB3	1:B:615:LYS:HG2	1.75	0.67
1:A:169:ASP:HB3	1:A:170:PRO:CD	2.22	0.66
1:A:611:MET:CE	1:A:619:ILE:HD11	2.22	0.66
1:A:612:SER:HB3	1:A:615:LYS:HG2	1.76	0.66
1:C:206:ILE:CD1	1:C:213:LEU:HD21	2.26	0.66
1:C:383:ILE:O	1:C:386:LYS:HG2	1.95	0.66
1:C:466:GLU:HG2	1:C:467:THR:H	1.60	0.66
1:B:667:ALA:HB3	1:B:670:VAL:HG23	1.78	0.66
1:B:267:PHE:HE2	1:B:289:ALA:CB	2.09	0.66
1:B:482:LEU:O	1:B:486:LYS:HG3	1.96	0.66
1:A:489:LEU:O	1:A:493:VAL:HG22	1.95	0.66
1:A:259:ALA:CB	1:A:300:ILE:HD12	2.23	0.66
1:C:749:ASP:HA	1:C:752:ILE:CD1	2.27	0.65
1:A:206:ILE:CD1	1:A:213:LEU:HD21	2.26	0.65
1:A:405:GLY:O	1:A:463:ALA:HB3	1.96	0.65
1:B:491:GLU:HG2	1:B:495:TYR:HE2	1.59	0.65
1:C:169:ASP:HB3	1:C:170:PRO:CD	2.22	0.65
1:A:460:ASN:OD1	1:A:461:PRO:HD3	1.96	0.65
1:B:203:TYR:CE2	1:B:261:GLU:HG2	2.32	0.65
1:B:611:MET:CE	1:B:619:ILE:HD11	2.26	0.65
1:A:567:ARG:NH2	1:A:611:MET:HG3	2.10	0.65
1:A:113:ARG:HH11	1:A:113:ARG:CG	2.09	0.65
1:A:728:VAL:N	1:A:729:PRO:HD2	2.11	0.65
1:A:353:ILE:CG2	1:A:354:ASP:H	2.05	0.65
1:A:201:VAL:HG21	1:A:256:ARG:HD2	1.78	0.65
1:A:43:GLN:N	1:A:44:PRO:HD2	2.11	0.65
1:B:311:PRO:O	1:B:313:ARG:N	2.30	0.65
1:B:65:ARG:NH1	1:B:93:ARG:NH1	2.45	0.65
1:B:749:ASP:HA	1:B:752:ILE:CD1	2.26	0.65
1:C:151:ILE:HD11	1:C:195:GLU:OE2	1.95	0.65
1:A:87:VAL:HG22	1:A:198:LEU:HD13	1.78	0.65
1:C:460:ASN:N	1:C:461:PRO:HD2	2.11	0.64
1:C:43:GLN:N	1:C:44:PRO:HD2	2.12	0.64
1:B:43:GLN:N	1:B:44:PRO:HD2	2.12	0.64
1:A:614:LYS:CD	1:B:402:GLU:HB2	2.27	0.64
1:A:491:GLU:HG2	1:A:495:TYR:HE2	1.59	0.64
1:A:514:VAL:HG12	1:A:515:LEU:N	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ASN:HB3	1:C:273:GLU:CB	2.28	0.64
1:B:151:ILE:HD11	1:B:195:GLU:OE2	1.96	0.64
1:B:113:ARG:CG	1:B:113:ARG:HH11	2.09	0.64
1:B:177:ALA:O	1:B:179:ASP:N	2.29	0.64
1:A:489:LEU:HB3	1:A:531:ILE:HD13	1.80	0.64
1:C:117:LEU:HD21	1:C:185:GLU:HG2	1.78	0.64
1:C:22:ARG:HB3	1:C:24:ASN:OD1	1.96	0.64
1:B:274:ILE:HG21	1:B:286:LEU:HD21	1.79	0.64
1:B:206:ILE:CD1	1:B:213:LEU:HD21	2.28	0.64
1:A:311:PRO:O	1:A:313:ARG:N	2.31	0.64
1:B:353:ILE:CG2	1:B:354:ASP:H	2.04	0.64
1:A:432:LEU:HD12	1:A:441:VAL:HG11	1.79	0.64
1:B:489:LEU:O	1:B:493:VAL:HG22	1.97	0.64
1:A:438:ASP:HB3	1:A:441:VAL:HG23	1.80	0.64
1:B:270:ASN:HB3	1:B:273:GLU:CB	2.28	0.64
1:B:320:VAL:O	1:B:324:ILE:HG13	1.97	0.64
1:C:605:LEU:HD22	1:C:638:ARG:HD3	1.80	0.64
1:B:438:ASP:HB3	1:B:441:VAL:HG23	1.80	0.63
1:B:489:LEU:HB3	1:B:531:ILE:HD13	1.80	0.63
1:C:427:MET:SD	1:C:432:LEU:HD12	2.38	0.63
1:C:489:LEU:O	1:C:493:VAL:HG22	1.98	0.63
1:C:489:LEU:HB3	1:C:531:ILE:HD13	1.79	0.63
1:C:335:LEU:O	1:C:337:GLN:N	2.32	0.63
1:A:614:LYS:HE2	1:B:402:GLU:OE1	1.97	0.63
1:A:499:HIS:N	1:A:500:PRO:CD	2.61	0.63
1:C:499:HIS:N	1:C:500:PRO:CD	2.61	0.63
1:A:267:PHE:CE2	1:A:289:ALA:HB1	2.31	0.63
1:C:267:PHE:HE2	1:C:289:ALA:CB	2.10	0.63
1:B:158:MET:HE1	1:B:419:ALA:HB1	1.80	0.63
1:B:358:ARG:HH11	1:B:358:ARG:HG3	1.64	0.63
1:A:335:LEU:O	1:A:337:GLN:N	2.32	0.63
1:A:749:ASP:HA	1:A:752:ILE:CD1	2.27	0.63
1:A:328:LEU:CD1	1:A:332:MET:HG2	2.29	0.63
1:B:335:LEU:O	1:B:337:GLN:N	2.32	0.63
1:C:111:GLY:HA2	1:C:170:PRO:CG	2.24	0.63
1:A:177:ALA:O	1:A:179:ASP:N	2.32	0.63
1:B:153:LEU:HD11	1:B:160:ALA:HB1	1.80	0.63
1:A:274:ILE:HG21	1:A:286:LEU:HD21	1.79	0.63
1:C:113:ARG:NH2	1:C:183:HIS:NE2	2.46	0.63
1:B:328:LEU:CD1	1:B:332:MET:HG2	2.29	0.62
1:B:605:LEU:HD22	1:B:638:ARG:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:HIS:N	1:B:500:PRO:CD	2.61	0.62
1:C:177:ALA:O	1:C:179:ASP:N	2.32	0.62
1:C:438:ASP:HB3	1:C:441:VAL:HG23	1.79	0.62
1:A:203:TYR:CE2	1:A:217:LYS:HE2	2.34	0.62
1:B:492:LEU:O	1:B:496:PRO:HG3	1.99	0.62
1:A:65:ARG:NH1	1:A:93:ARG:HH12	1.97	0.62
1:B:458:GLN:HB3	1:B:460:ASN:OD1	2.00	0.62
1:B:111:GLY:HA2	1:B:170:PRO:CG	2.26	0.62
1:A:102:ILE:HG12	1:A:103:GLN:N	2.14	0.62
1:C:271:GLY:HA2	1:C:309:ILE:HD11	1.82	0.62
1:A:458:GLN:HB3	1:A:460:ASN:OD1	1.99	0.62
1:A:270:ASN:HB3	1:A:273:GLU:CB	2.28	0.62
1:B:267:PHE:CE2	1:B:289:ALA:HB1	2.32	0.62
1:B:119:ILE:HD12	1:B:162:GLU:HB2	1.82	0.62
1:B:253:LEU:HD23	1:B:253:LEU:C	2.20	0.62
1:C:102:ILE:HG12	1:C:103:GLN:N	2.15	0.62
1:A:431:ASP:OD1	1:A:433:GLU:HG3	2.00	0.62
1:A:728:VAL:N	1:A:729:PRO:CD	2.63	0.62
1:A:91:ASN:HD22	1:A:91:ASN:N	1.97	0.62
1:A:143:TYR:HA	1:A:176:VAL:O	2.00	0.62
1:B:458:GLN:O	1:B:461:PRO:HD2	1.99	0.62
1:C:274:ILE:HG21	1:C:286:LEU:HD21	1.80	0.62
1:C:567:ARG:HH21	1:C:611:MET:HA	1.64	0.62
1:A:310:ALA:HA	1:A:325:VAL:HG22	1.81	0.62
1:A:567:ARG:HH21	1:A:611:MET:CG	2.13	0.61
1:C:267:PHE:CE2	1:C:289:ALA:HB1	2.33	0.61
1:A:650:GLU:HG2	1:A:677:LYS:HZ3	1.65	0.61
1:C:503:PHE:CD1	1:C:510:PRO:HG3	2.35	0.61
1:C:458:GLN:HB3	1:C:460:ASN:OD1	2.00	0.61
1:B:503:PHE:CD1	1:B:510:PRO:HG3	2.36	0.61
1:A:347:THR:HB	1:A:353:ILE:HD11	1.82	0.61
1:A:335:LEU:C	1:A:337:GLN:H	2.03	0.61
1:B:232:ALA:HB2	1:C:125:GLY:O	2.01	0.61
1:C:153:LEU:HD11	1:C:160:ALA:HB1	1.82	0.61
1:C:470:GLU:O	1:C:538:ASN:HA	2.00	0.61
1:B:91:ASN:HD22	1:B:91:ASN:N	1.96	0.61
1:C:358:ARG:HH11	1:C:358:ARG:HG3	1.65	0.61
1:C:119:ILE:HD12	1:C:162:GLU:HB2	1.83	0.61
1:A:492:LEU:O	1:A:496:PRO:HG3	2.00	0.61
1:A:460:ASN:N	1:A:461:PRO:CD	2.63	0.61
1:C:353:ILE:CG2	1:C:354:ASP:H	2.04	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LYS:HZ1	1:C:103:GLN:HE21	1.46	0.61
1:C:514:VAL:HG12	1:C:515:LEU:H	1.65	0.61
1:C:502:LYS:O	1:C:505:LYS:HB2	2.00	0.61
1:A:503:PHE:CD1	1:A:510:PRO:HG3	2.36	0.61
1:C:492:LEU:O	1:C:496:PRO:HG3	2.01	0.61
1:A:459:SER:C	1:A:461:PRO:HD2	2.21	0.61
1:B:251:LYS:HD2	1:B:346:ALA:HB1	1.83	0.61
1:A:358:ARG:HH11	1:A:358:ARG:HG3	1.65	0.61
1:C:611:MET:CE	1:C:619:ILE:HD11	2.27	0.60
1:A:432:LEU:O	1:A:437:ILE:CD1	2.49	0.60
1:A:437:ILE:CG2	1:A:438:ASP:N	2.63	0.60
1:B:582:ILE:HD13	1:B:600:VAL:HB	1.83	0.60
1:A:605:LEU:HD22	1:A:638:ARG:HD3	1.81	0.60
1:B:472:PRO:HB2	1:B:533:ASN:HB2	1.83	0.60
1:B:573:VAL:HG23	1:B:573:VAL:O	2.00	0.60
1:B:514:VAL:HG12	1:B:515:LEU:H	1.65	0.60
1:B:749:ASP:HA	1:B:752:ILE:CG1	2.31	0.60
1:A:283:GLU:HB3	1:A:327:GLN:HE21	1.66	0.60
1:B:322:ARG:HD3	1:C:321:GLU:OE2	2.02	0.60
1:A:253:LEU:HD23	1:A:253:LEU:C	2.21	0.60
1:B:518:GLY:C	1:B:755:TYR:HE2	2.04	0.60
1:A:502:LYS:O	1:A:505:LYS:HB2	2.02	0.60
1:A:271:GLY:HA2	1:A:309:ILE:HD11	1.84	0.60
1:B:580:ASP:HB2	1:B:628:ILE:HD11	1.83	0.60
1:C:251:LYS:HD2	1:C:346:ALA:HB1	1.82	0.60
1:B:313:ARG:HH21	1:B:313:ARG:HG3	1.65	0.60
1:C:143:TYR:HA	1:C:176:VAL:O	2.02	0.60
1:C:335:LEU:C	1:C:337:GLN:H	2.04	0.60
1:B:335:LEU:C	1:B:337:GLN:H	2.04	0.60
1:A:407:VAL:HG22	1:A:410:ASP:OD2	2.02	0.60
1:A:65:ARG:NH1	1:A:93:ARG:HH22	2.00	0.60
1:A:518:GLY:C	1:A:755:TYR:HE2	2.04	0.60
1:B:502:LYS:O	1:B:505:LYS:HB2	2.01	0.60
1:A:251:LYS:HD2	1:A:346:ALA:HB1	1.83	0.60
1:B:347:THR:HB	1:B:353:ILE:HD11	1.83	0.60
1:A:201:VAL:HG12	1:A:257:ALA:HB2	1.84	0.60
1:C:92:LEU:O	1:C:93:ARG:HB2	2.02	0.60
1:A:96:LEU:HD22	1:A:96:LEU:H	1.66	0.60
1:B:407:VAL:HG22	1:B:410:ASP:OD2	2.02	0.60
1:B:133:VAL:HG13	1:B:443:ASN:ND2	2.17	0.60
1:A:102:ILE:HG12	1:A:103:GLN:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:HD11	1:A:160:ALA:HB1	1.83	0.60
1:A:496:PRO:O	1:A:500:PRO:HG3	2.02	0.59
1:A:514:VAL:HG12	1:A:515:LEU:H	1.68	0.59
1:C:60:LYS:NZ	1:C:103:GLN:HE21	1.98	0.59
1:C:466:GLU:O	1:C:468:VAL:HG23	2.02	0.59
1:C:63:LYS:HD2	1:C:93:ARG:HB3	1.83	0.59
1:C:310:ALA:HA	1:C:325:VAL:HG22	1.84	0.59
1:C:253:LEU:HD23	1:C:253:LEU:C	2.21	0.59
1:C:347:THR:HB	1:C:353:ILE:HD11	1.83	0.59
1:A:475:THR:HG22	1:A:533:ASN:ND2	2.18	0.59
1:A:96:LEU:HD22	1:A:96:LEU:N	2.17	0.59
1:C:650:GLU:HG2	1:C:677:LYS:HZ3	1.66	0.59
1:B:378:LEU:C	1:B:378:LEU:HD13	2.23	0.59
1:C:515:LEU:HB3	1:C:642:LEU:HD13	1.85	0.59
1:C:749:ASP:HA	1:C:752:ILE:CG1	2.32	0.59
1:B:283:GLU:HB3	1:B:327:GLN:HE21	1.67	0.59
1:B:206:ILE:HD12	1:B:213:LEU:CG	2.33	0.59
1:B:515:LEU:HB3	1:B:642:LEU:HD13	1.85	0.59
1:A:749:ASP:HA	1:A:752:ILE:CG1	2.32	0.59
1:A:679:THR:HB	1:A:682:PHE:CD2	2.38	0.59
1:C:311:PRO:O	1:C:313:ARG:N	2.35	0.59
1:B:143:TYR:HA	1:B:176:VAL:O	2.02	0.59
1:C:472:PRO:HB2	1:C:533:ASN:HB2	1.84	0.59
1:C:407:VAL:HG22	1:C:410:ASP:OD2	2.03	0.59
1:A:155:ARG:HD3	1:A:386:LYS:O	2.02	0.59
1:A:119:ILE:HD12	1:A:162:GLU:HB2	1.85	0.59
1:C:244:TYR:CZ	1:C:350:PRO:HG3	2.38	0.59
1:C:458:GLN:O	1:C:461:PRO:HD2	2.03	0.59
1:A:313:ARG:HG3	1:A:313:ARG:HH21	1.68	0.59
1:C:91:ASN:N	1:C:91:ASN:HD22	2.00	0.59
1:A:244:TYR:CZ	1:A:350:PRO:HG3	2.38	0.59
1:B:92:LEU:O	1:B:93:ARG:HB2	2.03	0.58
1:C:336:LYS:C	1:C:338:ARG:N	2.57	0.58
1:C:283:GLU:HB3	1:C:327:GLN:HE21	1.68	0.58
1:B:472:PRO:HG2	1:B:532:ALA:HB3	1.85	0.58
1:A:89:ARG:HG2	1:A:94:VAL:O	2.03	0.58
1:C:378:LEU:HD13	1:C:378:LEU:C	2.24	0.58
1:A:731:ILE:O	1:A:731:ILE:HG23	2.04	0.58
1:C:411:LEU:O	1:C:414:LEU:HB3	2.03	0.58
1:C:135:LEU:H	1:C:135:LEU:HD22	1.69	0.58
1:A:206:ILE:HD12	1:A:213:LEU:CG	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:LEU:HD12	1:A:455:ALA:HB1	1.85	0.58
1:A:432:LEU:O	1:A:434:ASP:OD2	2.20	0.58
1:B:244:TYR:CZ	1:B:350:PRO:HG3	2.38	0.58
1:A:378:LEU:HD13	1:A:378:LEU:C	2.23	0.58
1:A:514:VAL:HG11	1:A:643:ILE:CD1	2.33	0.58
1:B:667:ALA:HB2	1:B:731:ILE:O	2.03	0.58
1:A:697:LEU:O	1:A:701:GLU:HG2	2.02	0.58
1:B:414:LEU:HD12	1:B:455:ALA:HB1	1.86	0.58
1:C:479:ILE:HD13	1:C:527:LEU:HD23	1.85	0.58
1:C:337:GLN:HE21	1:C:337:GLN:CA	2.08	0.58
1:B:496:PRO:O	1:B:500:PRO:HG3	2.03	0.58
1:B:650:GLU:HB3	1:B:677:LYS:HZ1	1.69	0.58
1:B:697:LEU:O	1:B:701:GLU:HG2	2.03	0.58
1:C:697:LEU:O	1:C:701:GLU:HG2	2.02	0.58
1:C:206:ILE:HD12	1:C:213:LEU:CG	2.34	0.58
1:A:164:LYS:HE2	1:A:189:ILE:CD1	2.29	0.58
1:A:65:ARG:NH1	1:A:93:ARG:NH1	2.52	0.58
1:C:414:LEU:HD12	1:C:455:ALA:HB1	1.86	0.58
1:A:62:LYS:C	1:A:64:ARG:N	2.51	0.58
1:B:679:THR:HB	1:B:682:PHE:CD2	2.39	0.58
1:C:582:ILE:HD13	1:C:600:VAL:HB	1.86	0.58
1:B:337:GLN:CA	1:B:337:GLN:HE21	2.08	0.57
1:B:117:LEU:HD21	1:B:185:GLU:CG	2.34	0.57
1:B:65:ARG:HH11	1:B:93:ARG:NH1	2.02	0.57
1:A:411:LEU:O	1:A:414:LEU:HB3	2.03	0.57
1:C:102:ILE:HG12	1:C:103:GLN:H	1.67	0.57
1:A:249:THR:HG21	1:A:369:ILE:HB	1.85	0.57
1:C:206:ILE:HG22	1:C:253:LEU:CD2	2.35	0.57
1:C:206:ILE:HG22	1:C:253:LEU:HD22	1.86	0.57
1:A:95:ARG:HB2	1:A:225:ARG:NH1	2.20	0.57
1:B:96:LEU:H	1:B:96:LEU:HD22	1.69	0.57
1:B:96:LEU:N	1:B:96:LEU:HD22	2.19	0.57
1:C:328:LEU:CD1	1:C:332:MET:HG2	2.34	0.57
1:C:113:ARG:NH1	1:C:113:ARG:HG2	2.12	0.57
1:C:679:THR:HB	1:C:682:PHE:CD2	2.39	0.57
1:C:313:ARG:HH21	1:C:313:ARG:HG3	1.69	0.57
1:B:158:MET:HE2	1:B:388:MET:HB3	1.86	0.57
1:A:523:GLY:HA2	1:A:526:LEU:HG	1.87	0.57
1:A:129:ASN:CG	1:A:132:GLU:HB2	2.26	0.57
1:C:129:ASN:OD1	1:C:132:GLU:N	2.37	0.57
1:B:336:LYS:C	1:B:338:ARG:N	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:650:GLU:HB3	1:C:677:LYS:HZ1	1.70	0.57
1:B:249:THR:HG21	1:B:369:ILE:HB	1.86	0.57
1:C:222:LEU:N	1:C:223:PRO:HD2	2.20	0.57
1:A:580:ASP:HB2	1:A:628:ILE:HD11	1.86	0.57
1:C:316:THR:O	1:C:316:THR:HG23	2.04	0.56
1:B:129:ASN:CG	1:B:132:GLU:HB2	2.25	0.56
1:B:560:ARG:NH1	1:B:560:ARG:HG3	2.20	0.56
1:A:336:LYS:C	1:A:338:ARG:N	2.57	0.56
1:B:102:ILE:HG12	1:B:103:GLN:N	2.20	0.56
1:C:253:LEU:HD12	2:C:807:ADP:H2'	1.87	0.56
1:B:411:LEU:O	1:B:414:LEU:HB3	2.05	0.56
1:A:445:LEU:HD23	1:A:445:LEU:C	2.26	0.56
1:A:275:MET:HG2	1:A:309:ILE:HG12	1.85	0.56
1:A:466:GLU:HG2	1:A:467:THR:H	1.69	0.56
1:B:312:LYS:HB3	1:B:354:ASP:CG	2.25	0.56
1:A:133:VAL:CG1	1:A:443:ASN:ND2	2.62	0.56
1:C:496:PRO:O	1:C:500:PRO:HG3	2.05	0.56
1:B:129:ASN:OD1	1:B:132:GLU:N	2.34	0.56
1:A:129:ASN:OD1	1:A:132:GLU:N	2.37	0.56
1:A:96:LEU:CD2	1:A:96:LEU:H	2.18	0.56
1:C:96:LEU:HD22	1:C:96:LEU:N	2.20	0.56
1:C:249:THR:HG21	1:C:369:ILE:HB	1.86	0.56
1:C:611:MET:HE1	1:C:619:ILE:CD1	2.32	0.56
1:A:32:ILE:HG12	1:A:83:ARG:HD3	1.88	0.56
1:B:410:ASP:CG	1:B:463:ALA:HB2	2.25	0.56
1:B:738:GLU:OE2	1:B:741:ARG:HG3	2.05	0.56
1:A:611:MET:HE1	1:A:619:ILE:CD1	2.28	0.56
1:A:283:GLU:HB3	1:A:327:GLN:NE2	2.21	0.56
1:A:62:LYS:C	1:A:64:ARG:H	2.09	0.56
1:C:729:PRO:C	1:C:730:GLU:CD	2.64	0.56
1:B:650:GLU:HG2	1:B:677:LYS:HZ3	1.70	0.56
1:A:35:ASP:O	1:A:38:VAL:HG12	2.04	0.56
1:A:427:MET:SD	1:A:432:LEU:HD12	2.45	0.56
1:A:647:LEU:HD12	1:A:647:LEU:H	1.70	0.56
1:C:518:GLY:C	1:C:755:TYR:CE2	2.79	0.56
1:B:135:LEU:HD22	1:B:135:LEU:H	1.71	0.56
1:A:515:LEU:HB3	1:A:642:LEU:HD13	1.87	0.56
1:A:65:ARG:NH1	1:A:93:ARG:NH2	2.54	0.56
1:C:96:LEU:HD22	1:C:96:LEU:H	1.70	0.56
1:A:582:ILE:HD13	1:A:600:VAL:HB	1.87	0.56
1:B:749:ASP:O	1:B:752:ILE:HB	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:O	1:A:93:ARG:HB2	2.06	0.56
1:C:458:GLN:HG3	1:C:459:SER:H	1.71	0.56
1:A:423:ILE:C	1:A:425:LYS:H	2.10	0.55
1:A:515:LEU:HD21	1:A:623:THR:HG22	1.88	0.55
1:B:60:LYS:HB2	1:B:101:SER:OG	2.05	0.55
1:B:201:VAL:HG12	1:B:257:ALA:HB2	1.88	0.55
1:C:87:VAL:HG22	1:C:198:LEU:CD1	2.36	0.55
1:B:96:LEU:H	1:B:96:LEU:CD2	2.19	0.55
1:C:523:GLY:HA2	1:C:526:LEU:HG	1.87	0.55
1:B:728:VAL:N	1:B:729:PRO:CD	2.69	0.55
1:A:206:ILE:CD1	1:A:213:LEU:CD2	2.85	0.55
1:A:458:GLN:HG3	1:A:459:SER:H	1.71	0.55
1:B:445:LEU:HD23	1:B:445:LEU:C	2.27	0.55
1:A:738:GLU:OE2	1:A:741:ARG:HG3	2.06	0.55
1:C:423:ILE:C	1:C:425:LYS:H	2.08	0.55
1:B:423:ILE:C	1:B:425:LYS:H	2.09	0.55
1:C:28:VAL:HG23	1:C:84:MET:HG2	1.88	0.55
1:A:681:GLY:HA3	1:A:745:ARG:NH2	2.21	0.55
1:B:35:ASP:O	1:B:38:VAL:HG12	2.07	0.55
1:A:28:VAL:HG23	1:A:84:MET:HG2	1.89	0.55
1:C:312:LYS:HB3	1:C:354:ASP:CG	2.26	0.55
1:B:133:VAL:CG1	1:B:443:ASN:HD22	2.19	0.55
1:A:741:ARG:HE	1:A:741:ARG:HA	1.71	0.55
1:B:523:GLY:HA2	1:B:526:LEU:HG	1.89	0.55
1:C:118:PRO:HG2	1:C:188:PRO:HG3	1.89	0.55
1:C:35:ASP:O	1:C:38:VAL:HG12	2.07	0.55
1:C:164:LYS:HE2	1:C:189:ILE:CD1	2.32	0.55
1:A:640:ASP:HB2	1:A:641:GLN:HE21	1.72	0.55
1:A:650:GLU:HB3	1:A:677:LYS:HZ1	1.71	0.55
1:C:206:ILE:CD1	1:C:213:LEU:CD2	2.85	0.55
1:A:336:LYS:O	1:A:338:ARG:N	2.37	0.55
1:A:438:ASP:OD2	1:A:440:GLU:HB2	2.07	0.55
1:B:741:ARG:HA	1:B:741:ARG:HE	1.72	0.55
1:C:738:GLU:OE2	1:C:741:ARG:HG3	2.07	0.55
1:A:117:LEU:HD21	1:A:185:GLU:CG	2.37	0.55
1:B:640:ASP:HB2	1:B:641:GLN:HE21	1.72	0.55
1:A:118:PRO:HG2	1:A:188:PRO:HG3	1.87	0.55
1:B:45:LYS:O	1:B:49:LEU:HD13	2.07	0.55
1:C:129:ASN:CG	1:C:132:GLU:HB2	2.27	0.54
1:B:283:GLU:HB3	1:B:327:GLN:NE2	2.22	0.54
1:B:438:ASP:OD2	1:B:440:GLU:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HG22	1:A:253:LEU:HD22	1.88	0.54
1:C:640:ASP:HB2	1:C:641:GLN:HE21	1.72	0.54
1:C:741:ARG:HE	1:C:741:ARG:HA	1.72	0.54
1:A:45:LYS:O	1:A:49:LEU:HD13	2.07	0.54
1:A:459:SER:O	1:A:462:SER:OG	2.24	0.54
1:C:624:ASN:ND2	1:C:624:ASN:H	2.06	0.54
1:C:60:LYS:HG2	1:C:66:GLU:HG2	1.90	0.54
1:B:624:ASN:ND2	1:B:624:ASN:H	2.06	0.54
1:B:32:ILE:HG12	1:B:83:ARG:HD3	1.89	0.54
1:B:458:GLN:HG3	1:B:459:SER:H	1.72	0.54
1:B:303:ILE:HD12	1:B:345:ALA:HB2	1.90	0.54
1:B:574:LEU:HG	1:B:576:PHE:HE1	1.72	0.54
1:B:310:ALA:HA	1:B:325:VAL:HG22	1.89	0.54
1:B:694:ALA:HB1	1:B:731:ILE:HD11	1.89	0.54
1:C:445:LEU:C	1:C:445:LEU:HD23	2.27	0.54
1:A:647:LEU:HD21	1:A:747:VAL:HB	1.90	0.54
1:A:600:VAL:O	1:A:604:ILE:HG13	2.07	0.54
1:A:206:ILE:HG22	1:A:253:LEU:CD2	2.38	0.54
1:C:567:ARG:NH2	1:C:611:MET:HA	2.21	0.54
1:B:514:VAL:HG11	1:B:643:ILE:CD1	2.35	0.54
1:B:89:ARG:HG2	1:B:94:VAL:O	2.08	0.54
1:A:570:ALA:HB1	1:A:616:ASN:HB3	1.88	0.54
1:A:57:VAL:CG2	1:A:59:LEU:HD21	2.36	0.54
1:B:164:LYS:HE2	1:B:189:ILE:CD1	2.32	0.54
1:C:749:ASP:O	1:C:752:ILE:HB	2.07	0.54
1:B:63:LYS:HD2	1:B:93:ARG:HB3	1.90	0.54
1:C:438:ASP:OD2	1:C:440:GLU:HB2	2.08	0.54
1:A:119:ILE:HG13	1:A:162:GLU:O	2.08	0.54
1:C:96:LEU:CD2	1:C:96:LEU:H	2.21	0.54
1:B:729:PRO:O	1:B:730:GLU:OE2	2.25	0.54
1:C:114:ILE:CD1	1:C:176:VAL:HG22	2.37	0.54
1:C:283:GLU:HB3	1:C:327:GLN:NE2	2.23	0.54
1:B:87:VAL:HG22	1:B:198:LEU:CD1	2.37	0.54
1:A:87:VAL:HG22	1:A:198:LEU:CD1	2.37	0.54
1:B:55:ASP:O	1:B:71:VAL:HG12	2.08	0.54
1:B:206:ILE:HG22	1:B:253:LEU:CD2	2.38	0.54
1:A:113:ARG:NH1	1:A:113:ARG:CG	2.70	0.54
1:A:502:LYS:HE2	1:B:706:GLU:OE2	2.08	0.54
1:B:206:ILE:CD1	1:B:213:LEU:CD2	2.86	0.54
1:C:514:VAL:HG11	1:C:643:ILE:CD1	2.34	0.54
1:B:155:ARG:HD3	1:B:386:LYS:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ARG:CZ	1:B:96:LEU:HD21	2.38	0.54
1:C:89:ARG:HG2	1:C:94:VAL:O	2.08	0.54
1:B:254:ILE:O	1:B:258:VAL:HG23	2.08	0.54
1:B:184:CYS:C	1:B:186:GLY:H	2.11	0.54
1:A:55:ASP:O	1:A:71:VAL:HG12	2.08	0.54
1:B:206:ILE:HG22	1:B:253:LEU:HD22	1.89	0.53
1:B:113:ARG:CG	1:B:113:ARG:NH1	2.70	0.53
1:C:731:ILE:HG23	1:C:731:ILE:O	2.07	0.53
1:A:749:ASP:O	1:A:752:ILE:HB	2.08	0.53
1:B:647:LEU:H	1:B:647:LEU:HD12	1.73	0.53
1:C:437:ILE:HG22	1:C:438:ASP:N	2.22	0.53
1:C:244:TYR:HB2	1:C:368:ASP:HA	1.90	0.53
1:C:237:PRO:O	1:C:238:PRO:C	2.46	0.53
1:C:313:ARG:CG	1:C:314:GLU:H	2.10	0.53
1:B:647:LEU:HD21	1:B:747:VAL:HB	1.90	0.53
1:A:489:LEU:HD13	1:A:531:ILE:HB	1.90	0.53
1:B:158:MET:CE	1:B:419:ALA:HB1	2.38	0.53
1:B:600:VAL:O	1:B:604:ILE:HG13	2.08	0.53
1:C:184:CYS:C	1:C:186:GLY:H	2.11	0.53
1:A:347:THR:CB	1:A:353:ILE:HD11	2.38	0.53
1:B:701:GLU:O	1:B:704:GLU:N	2.37	0.53
1:B:119:ILE:HD12	1:B:162:GLU:CB	2.38	0.53
1:B:201:VAL:HG21	1:B:256:ARG:HD2	1.90	0.53
1:A:254:ILE:O	1:A:258:VAL:HG23	2.08	0.53
1:B:222:LEU:N	1:B:223:PRO:HD2	2.23	0.53
1:A:252:THR:HA	1:A:302:PHE:CZ	2.44	0.53
1:B:169:ASP:O	1:B:171:SER:N	2.38	0.53
1:A:567:ARG:NH2	1:A:611:MET:CG	2.71	0.53
1:A:490:GLN:CB	1:A:494:GLN:HG3	2.38	0.53
1:A:89:ARG:CZ	1:A:96:LEU:HD21	2.38	0.53
1:B:102:ILE:HG12	1:B:103:GLN:H	1.72	0.53
1:C:647:LEU:HD12	1:C:647:LEU:H	1.73	0.53
1:C:89:ARG:CZ	1:C:96:LEU:HD21	2.39	0.53
1:B:302:PHE:HA	1:B:344:MET:O	2.09	0.53
1:C:169:ASP:O	1:C:171:SER:N	2.35	0.53
1:B:506:PHE:CD2	1:C:699:ILE:HG12	2.43	0.53
1:C:532:ALA:HB2	1:C:573:VAL:HG21	1.91	0.53
1:C:254:ILE:O	1:C:258:VAL:HG23	2.08	0.53
1:A:758:PHE:O	1:A:762:LEU:HB2	2.09	0.53
1:B:118:PRO:HG2	1:B:188:PRO:HG3	1.89	0.53
1:A:337:GLN:CA	1:A:337:GLN:HE21	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLY:O	1:A:159:ARG:HG2	2.08	0.53
1:C:139:PHE:O	1:C:141:GLU:N	2.42	0.53
1:C:32:ILE:HG12	1:C:83:ARG:HD3	1.91	0.53
1:B:158:MET:HE1	1:B:419:ALA:CB	2.39	0.53
1:A:237:PRO:O	1:A:238:PRO:C	2.46	0.53
1:A:222:LEU:N	1:A:223:PRO:HD2	2.24	0.53
1:A:95:ARG:HB2	1:A:225:ARG:NH2	2.23	0.53
1:A:518:GLY:HA2	1:A:755:TYR:HD2	1.73	0.53
1:B:28:VAL:HG23	1:B:84:MET:HG2	1.89	0.53
1:A:458:GLN:O	1:A:461:PRO:HD2	2.08	0.53
1:A:244:TYR:HB2	1:A:368:ASP:HA	1.90	0.53
1:C:666:VAL:O	1:C:666:VAL:HG23	2.09	0.53
1:C:117:LEU:HD21	1:C:185:GLU:CG	2.39	0.52
1:C:640:ASP:HB2	1:C:641:GLN:NE2	2.24	0.52
1:C:560:ARG:HG3	1:C:560:ARG:NH1	2.21	0.52
1:C:518:GLY:HA2	1:C:755:TYR:HD2	1.74	0.52
1:C:728:VAL:N	1:C:729:PRO:CD	2.72	0.52
1:A:466:GLU:HG2	1:A:467:THR:N	2.24	0.52
1:B:728:VAL:N	1:B:729:PRO:HD2	2.24	0.52
1:B:237:PRO:O	1:B:238:PRO:C	2.47	0.52
1:C:568:GLN:O	1:C:568:GLN:HG2	2.08	0.52
1:B:269:ILE:HD11	1:B:301:ILE:HG22	1.90	0.52
1:A:119:ILE:HD12	1:A:162:GLU:CB	2.39	0.52
1:A:515:LEU:HA	1:A:621:GLY:O	2.09	0.52
1:A:395:ASP:O	1:A:398:GLN:HB3	2.09	0.52
1:C:158:MET:CE	1:C:419:ALA:HB1	2.39	0.52
1:B:395:ASP:O	1:B:398:GLN:HB3	2.10	0.52
1:B:347:THR:CB	1:B:353:ILE:HD11	2.39	0.52
1:A:184:CYS:C	1:A:186:GLY:H	2.13	0.52
1:A:135:LEU:HD22	1:A:135:LEU:H	1.74	0.52
1:C:312:LYS:HB3	1:C:354:ASP:HB2	1.91	0.52
1:C:347:THR:CB	1:C:353:ILE:HD11	2.40	0.52
1:A:614:LYS:HD3	1:B:402:GLU:CB	2.33	0.52
1:C:336:LYS:O	1:C:338:ARG:N	2.37	0.52
1:A:269:ILE:HD11	1:A:301:ILE:CG2	2.39	0.52
1:A:666:VAL:O	1:A:666:VAL:HG23	2.09	0.52
1:B:656:ILE:HG21	1:B:687:LEU:HD12	1.89	0.52
1:C:403:THR:HB	1:C:406:HIS:CG	2.45	0.52
1:A:540:ILE:HD12	1:A:572:CYS:SG	2.50	0.52
1:A:112:LYS:HB2	1:A:169:ASP:CB	2.39	0.52
1:C:313:ARG:O	1:C:316:THR:CG2	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:THR:HB	1:A:406:HIS:CG	2.44	0.52
1:A:640:ASP:HB2	1:A:641:GLN:NE2	2.24	0.52
1:B:323:ARG:NH1	1:C:278:LEU:HA	2.24	0.52
1:A:36:ASN:OD1	1:A:87:VAL:HG21	2.10	0.52
1:C:577:ASP:O	1:C:578:GLU:C	2.48	0.52
1:B:233:ILE:HD13	1:C:442:MET:CE	2.40	0.52
1:B:490:GLN:CB	1:B:494:GLN:HG3	2.37	0.52
1:B:336:LYS:O	1:B:338:ARG:N	2.37	0.52
1:C:65:ARG:NH1	1:C:93:ARG:HH12	2.07	0.52
1:C:299:ALA:HB3	1:C:341:VAL:HG12	1.91	0.52
1:A:318:GLY:O	1:A:322:ARG:HG3	2.10	0.52
1:B:403:THR:HB	1:B:406:HIS:CG	2.44	0.52
1:B:432:LEU:O	1:B:437:ILE:CD1	2.58	0.52
1:B:489:LEU:HD13	1:B:531:ILE:HB	1.91	0.52
1:C:728:VAL:N	1:C:729:PRO:HD2	2.25	0.52
1:A:299:ALA:HB3	1:A:341:VAL:HG12	1.92	0.52
1:C:269:ILE:HD12	1:C:303:ILE:HG12	1.92	0.52
1:A:624:ASN:ND2	1:A:624:ASN:H	2.06	0.52
1:C:108:VAL:HG22	1:C:173:TYR:CD1	2.45	0.52
1:A:169:ASP:O	1:A:171:SER:N	2.38	0.51
1:C:648:PRO:HD2	1:C:682:PHE:O	2.10	0.51
1:B:157:GLY:O	1:B:159:ARG:HG2	2.10	0.51
1:C:55:ASP:O	1:C:71:VAL:HG12	2.09	0.51
1:B:139:PHE:CD1	1:B:176:VAL:HG11	2.45	0.51
1:C:395:ASP:O	1:C:398:GLN:HB3	2.10	0.51
1:B:108:VAL:HG22	1:B:173:TYR:CD1	2.46	0.51
1:A:139:PHE:CD1	1:A:176:VAL:HG11	2.46	0.51
1:B:299:ALA:HB3	1:B:341:VAL:HG12	1.91	0.51
1:B:611:MET:HE1	1:B:619:ILE:CD1	2.31	0.51
1:A:614:LYS:CD	1:B:402:GLU:CB	2.88	0.51
1:B:139:PHE:O	1:B:141:GLU:N	2.43	0.51
1:A:63:LYS:HD2	1:A:93:ARG:HB3	1.92	0.51
1:B:410:ASP:OD2	1:B:463:ALA:CB	2.58	0.51
1:B:647:LEU:HB3	1:B:648:PRO:HD2	1.93	0.51
1:A:479:ILE:HD13	1:A:527:LEU:HD23	1.91	0.51
1:A:495:TYR:N	1:A:496:PRO:HD2	2.25	0.51
1:B:640:ASP:HB2	1:B:641:GLN:NE2	2.25	0.51
1:B:437:ILE:HG22	1:B:438:ASP:N	2.24	0.51
1:B:505:LYS:HZ3	1:C:729:PRO:HG3	1.75	0.51
1:B:244:TYR:HB2	1:B:368:ASP:HA	1.92	0.51
1:C:269:ILE:HD11	1:C:301:ILE:CG2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:VAL:HG12	1:C:257:ALA:HB2	1.92	0.51
1:C:157:GLY:O	1:C:159:ARG:HG2	2.10	0.51
1:A:656:ILE:HG21	1:A:687:LEU:HD12	1.92	0.51
1:A:560:ARG:HG3	1:A:560:ARG:NH1	2.20	0.51
1:A:433:GLU:O	1:A:434:ASP:CG	2.49	0.51
1:A:648:PRO:HD2	1:A:682:PHE:O	2.11	0.51
1:A:732:ARG:HD2	1:A:734:ASP:OD1	2.11	0.51
1:A:587:GLY:HA3	1:A:591:GLY:HA2	1.93	0.51
1:B:206:ILE:O	1:B:206:ILE:HG13	2.10	0.51
1:B:335:LEU:C	1:B:337:GLN:N	2.64	0.51
1:C:229:LEU:O	1:C:233:ILE:HG22	2.11	0.51
1:B:648:PRO:HD2	1:B:682:PHE:O	2.11	0.51
1:B:666:VAL:O	1:B:666:VAL:HG23	2.11	0.51
1:A:410:ASP:CG	1:A:463:ALA:HB2	2.31	0.51
1:B:431:ASP:O	1:B:432:LEU:HD23	2.11	0.51
1:C:290:PHE:CE2	1:C:331:LEU:HB3	2.46	0.51
1:C:119:ILE:HD12	1:C:162:GLU:CB	2.40	0.51
1:C:647:LEU:HB3	1:C:648:PRO:HD2	1.93	0.51
1:A:40:SER:HB3	1:A:74:ASP:HB2	1.92	0.51
1:A:252:THR:HB	2:A:807:ADP:O1A	2.11	0.51
1:B:410:ASP:OD2	1:B:463:ALA:HB1	2.10	0.51
1:C:60:LYS:HZ3	1:C:103:GLN:NE2	2.06	0.51
1:C:518:GLY:HA2	1:C:755:TYR:CD2	2.46	0.51
1:C:65:ARG:NH1	1:C:93:ARG:NH1	2.59	0.51
1:A:139:PHE:O	1:A:141:GLU:N	2.44	0.50
1:B:495:TYR:N	1:B:496:PRO:HD2	2.25	0.50
1:A:290:PHE:CE2	1:A:331:LEU:HB3	2.45	0.50
1:B:582:ILE:CD1	1:B:600:VAL:HB	2.42	0.50
1:C:732:ARG:HG3	1:C:734:ASP:OD1	2.11	0.50
1:B:408:GLY:HA3	2:B:807:ADP:N7	2.26	0.50
1:B:290:PHE:CE2	1:B:331:LEU:HB3	2.47	0.50
1:A:647:LEU:HB3	1:A:648:PRO:HD2	1.93	0.50
1:B:489:LEU:HD21	1:B:516:PHE:CZ	2.47	0.50
1:C:656:ILE:HG21	1:C:687:LEU:HD12	1.93	0.50
1:A:65:ARG:HH11	1:A:93:ARG:NH2	2.09	0.50
1:A:437:ILE:CG2	1:A:438:ASP:H	2.25	0.50
1:A:95:ARG:HG3	1:A:225:ARG:NH1	2.26	0.50
1:B:489:LEU:HD21	1:B:516:PHE:HZ	1.76	0.50
1:C:564:ASP:C	1:C:566:ALA:H	2.14	0.50
1:B:113:ARG:HG2	1:B:113:ARG:NH1	2.16	0.50
1:B:681:GLY:HA3	1:B:745:ARG:NH2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LEU:HD21	1:A:516:PHE:HZ	1.77	0.50
1:A:89:ARG:HD3	1:A:96:LEU:HD22	1.93	0.50
1:B:575:PHE:HE2	1:B:577:ASP:HB2	1.75	0.50
1:C:302:PHE:HA	1:C:344:MET:O	2.12	0.50
1:C:489:LEU:HD13	1:C:531:ILE:HB	1.91	0.50
1:A:524:LYS:HZ2	1:A:524:LYS:HB2	1.77	0.50
1:C:126:ILE:HG21	1:C:159:ARG:HD2	1.94	0.50
1:C:40:SER:HB3	1:C:74:ASP:HB2	1.92	0.50
1:A:131:PHE:O	1:A:136:LYS:HB2	2.11	0.50
1:B:232:ALA:HB2	1:C:125:GLY:C	2.31	0.50
1:B:574:LEU:HG	1:B:576:PHE:CE1	2.47	0.50
1:C:45:LYS:O	1:C:49:LEU:HD13	2.12	0.50
1:A:335:LEU:C	1:A:337:GLN:N	2.64	0.50
1:B:608:MET:HG3	1:B:619:ILE:HD12	1.94	0.50
1:B:36:ASN:OD1	1:B:87:VAL:HG21	2.11	0.50
1:C:335:LEU:C	1:C:337:GLN:N	2.65	0.50
1:B:63:LYS:HD2	1:B:93:ARG:CG	2.41	0.50
1:B:460:ASN:N	1:B:461:PRO:CD	2.75	0.50
1:C:508:MET:HG3	1:C:508:MET:O	2.09	0.50
1:A:206:ILE:HD13	1:A:213:LEU:HD21	1.93	0.49
1:A:126:ILE:HG21	1:A:159:ARG:HD2	1.94	0.49
1:C:667:ALA:HB2	1:C:731:ILE:O	2.12	0.49
1:B:232:ALA:HA	1:C:125:GLY:HA3	1.94	0.49
1:C:119:ILE:HG13	1:C:162:GLU:O	2.11	0.49
1:A:147:ARG:HB3	1:A:150:ASP:OD2	2.12	0.49
1:C:681:GLY:HA3	1:C:745:ARG:NH2	2.27	0.49
1:A:206:ILE:O	1:A:206:ILE:HG13	2.11	0.49
1:B:183:HIS:HB3	1:B:185:GLU:OE2	2.12	0.49
1:C:495:TYR:N	1:C:496:PRO:HD2	2.26	0.49
1:B:408:GLY:HA3	2:B:807:ADP:C8	2.47	0.49
1:B:112:LYS:HB2	1:B:169:ASP:CB	2.42	0.49
1:C:112:LYS:HB2	1:C:169:ASP:CB	2.43	0.49
1:B:647:LEU:HD21	1:B:747:VAL:CB	2.43	0.49
1:C:682:PHE:CE1	1:C:690:ILE:HD11	2.48	0.49
1:A:57:VAL:HG23	1:A:59:LEU:HD21	1.94	0.49
1:C:184:CYS:O	1:C:186:GLY:N	2.45	0.49
1:A:540:ILE:CG2	1:A:574:LEU:HD12	2.42	0.49
1:B:575:PHE:CE2	1:B:577:ASP:HB2	2.47	0.49
1:B:304:ASP:OD2	1:B:305:GLU:HG3	2.12	0.49
1:B:694:ALA:CB	1:B:731:ILE:HD11	2.43	0.49
1:A:62:LYS:O	1:A:63:LYS:C	2.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:THR:HG22	1:A:438:ASP:HA	1.93	0.49
1:B:684:GLY:HA3	2:B:900:ADP:C8	2.46	0.49
1:A:108:VAL:HG22	1:A:173:TYR:CD1	2.48	0.49
1:B:297:ALA:HA	1:B:298:PRO:C	2.33	0.49
1:B:519:PRO:HG3	1:B:647:LEU:HD12	1.92	0.49
1:B:147:ARG:HB3	1:B:150:ASP:OD2	2.13	0.49
1:C:608:MET:HG3	1:C:619:ILE:HD12	1.95	0.49
1:A:158:MET:HE1	1:A:419:ALA:HB1	1.94	0.49
1:A:518:GLY:HA2	1:A:755:TYR:CD2	2.47	0.49
1:A:368:ASP:HB2	1:A:568:GLN:CD	2.33	0.49
1:C:647:LEU:HD21	1:C:747:VAL:HB	1.93	0.49
1:C:542:ILE:N	1:C:542:ILE:HD12	2.27	0.49
1:C:758:PHE:O	1:C:762:LEU:HB2	2.12	0.49
1:B:229:LEU:O	1:B:233:ILE:HG22	2.12	0.49
1:B:381:LEU:HD21	1:B:411:LEU:HD22	1.95	0.49
1:B:438:ASP:HB3	1:B:441:VAL:CG2	2.42	0.49
1:A:489:LEU:HD21	1:A:516:PHE:CZ	2.47	0.49
1:A:633:ILE:HG22	1:A:639:LEU:HD12	1.94	0.49
1:A:281:GLU:O	1:A:284:SER:HB3	2.13	0.49
1:C:206:ILE:HG13	1:C:206:ILE:O	2.11	0.49
1:B:567:ARG:CZ	1:B:567:ARG:HB2	2.43	0.49
1:A:183:HIS:HB3	1:A:185:GLU:OE2	2.12	0.49
1:A:614:LYS:HE2	1:B:402:GLU:CD	2.32	0.49
1:C:644:TYR:C	1:C:645:ILE:HD12	2.32	0.49
1:C:755:TYR:N	1:C:755:TYR:HD1	2.11	0.49
1:A:265:PHE:CD2	1:A:296:ASN:HB2	2.48	0.49
1:B:542:ILE:N	1:B:542:ILE:HD12	2.27	0.49
1:A:542:ILE:HD12	1:A:542:ILE:N	2.27	0.49
1:B:253:LEU:CD2	1:B:253:LEU:C	2.81	0.49
1:C:206:ILE:CD1	1:C:213:LEU:CG	2.86	0.49
1:C:472:PRO:HG2	1:C:532:ALA:CB	2.39	0.49
1:B:43:GLN:N	1:B:44:PRO:CD	2.76	0.48
1:A:297:ALA:HA	1:A:298:PRO:C	2.33	0.48
1:B:508:MET:HG3	1:B:508:MET:O	2.12	0.48
1:B:608:MET:HG3	1:B:619:ILE:HD13	1.95	0.48
1:A:644:TYR:C	1:A:645:ILE:HD12	2.34	0.48
1:B:755:TYR:N	1:B:755:TYR:CD1	2.81	0.48
1:C:93:ARG:HG2	1:C:93:ARG:HH11	1.78	0.48
1:C:227:PRO:HA	1:C:340:HIS:CE1	2.48	0.48
1:B:567:ARG:HH21	1:B:611:MET:CG	2.26	0.48
1:B:755:TYR:N	1:B:755:TYR:HD1	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ARG:NH1	1:B:96:LEU:HD21	2.28	0.48
1:A:348:ASN:O	1:A:349:ARG:HB3	2.14	0.48
1:C:431:ASP:OD1	1:C:433:GLU:HG3	2.12	0.48
1:A:503:PHE:HA	1:B:699:ILE:HD13	1.95	0.48
1:B:177:ALA:C	1:B:179:ASP:H	2.16	0.48
1:B:633:ILE:HG22	1:B:639:LEU:HD12	1.95	0.48
1:B:281:GLU:O	1:B:284:SER:HB3	2.13	0.48
1:A:458:GLN:O	1:A:461:PRO:CD	2.61	0.48
1:B:114:ILE:HD13	1:B:146:ILE:HD11	1.95	0.48
1:B:93:ARG:HG2	1:B:93:ARG:HH11	1.79	0.48
1:A:290:PHE:CD2	1:A:331:LEU:HB3	2.48	0.48
1:A:682:PHE:CE1	1:A:690:ILE:HD11	2.48	0.48
1:C:432:LEU:CD1	1:C:441:VAL:HG21	2.44	0.48
1:A:253:LEU:C	1:A:253:LEU:CD2	2.82	0.48
1:B:567:ARG:HH21	1:B:611:MET:HG3	1.78	0.48
1:B:515:LEU:HA	1:B:621:GLY:O	2.13	0.48
1:C:459:SER:O	1:C:462:SER:OG	2.14	0.48
1:C:755:TYR:N	1:C:755:TYR:CD1	2.81	0.48
1:C:206:ILE:HD12	1:C:213:LEU:HD21	1.95	0.48
1:C:253:LEU:CD2	1:C:253:LEU:C	2.82	0.48
1:B:169:ASP:CB	1:B:170:PRO:HD3	2.27	0.48
1:C:113:ARG:NH1	1:C:113:ARG:CG	2.67	0.48
1:C:183:HIS:HB3	1:C:185:GLU:OE2	2.14	0.48
1:B:644:TYR:C	1:B:645:ILE:HD12	2.33	0.48
1:A:44:PRO:HG2	1:A:79:ASP:OD1	2.13	0.48
1:C:133:VAL:HG22	1:C:440:GLU:HA	1.96	0.48
1:A:89:ARG:HG3	1:A:94:VAL:HG23	1.95	0.48
1:B:540:ILE:HD12	1:B:572:CYS:SG	2.53	0.48
1:A:487:ARG:CZ	1:A:487:ARG:HB3	2.44	0.48
1:B:758:PHE:O	1:B:762:LEU:HB2	2.13	0.48
1:B:41:LEU:O	1:B:73:SER:HA	2.14	0.48
1:B:590:ILE:HG13	1:B:591:GLY:H	1.78	0.48
1:B:203:TYR:CE2	1:B:217:LYS:HE2	2.48	0.48
1:A:313:ARG:NH2	1:A:313:ARG:HG3	2.28	0.48
1:C:36:ASN:OD1	1:C:87:VAL:HG21	2.13	0.48
1:C:438:ASP:HB3	1:C:441:VAL:CG2	2.42	0.48
1:B:518:GLY:HA2	1:B:755:TYR:HD2	1.79	0.48
1:B:89:ARG:HD3	1:B:96:LEU:HD22	1.94	0.48
1:B:57:VAL:CG2	1:B:59:LEU:HD21	2.44	0.48
1:C:265:PHE:CD2	1:C:296:ASN:HB2	2.49	0.48
1:C:112:LYS:H	1:C:170:PRO:HD3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LEU:HD21	1:A:411:LEU:HD22	1.95	0.48
1:B:515:LEU:HD13	1:B:634:LEU:HD21	1.95	0.48
1:B:427:MET:O	1:B:431:ASP:N	2.46	0.48
1:C:432:LEU:O	1:C:437:ILE:CD1	2.61	0.48
1:B:25:ARG:HH12	1:B:99:VAL:HG21	1.79	0.48
1:A:508:MET:O	1:A:508:MET:HG3	2.14	0.48
1:B:313:ARG:NH2	1:B:313:ARG:HG3	2.29	0.48
1:C:701:GLU:O	1:C:704:GLU:N	2.42	0.48
1:B:328:LEU:O	1:B:331:LEU:N	2.45	0.48
1:A:647:LEU:N	1:A:647:LEU:HD12	2.28	0.48
1:B:44:PRO:HG2	1:B:79:ASP:OD1	2.14	0.48
1:C:38:VAL:HG21	1:C:72:LEU:HD12	1.96	0.48
1:A:26:LEU:HD13	1:A:41:LEU:HD21	1.95	0.48
1:B:269:ILE:HD11	1:B:301:ILE:CG2	2.44	0.48
1:B:227:PRO:HA	1:B:340:HIS:CE1	2.49	0.48
1:C:147:ARG:HB3	1:C:150:ASP:OD2	2.13	0.48
1:B:40:SER:HB3	1:B:74:ASP:HB2	1.95	0.48
1:C:297:ALA:HA	1:C:298:PRO:C	2.34	0.48
1:B:206:ILE:HD13	1:B:213:LEU:HD21	1.96	0.47
1:C:206:ILE:HD13	1:C:213:LEU:HD21	1.96	0.47
1:A:112:LYS:H	1:A:170:PRO:HD3	1.78	0.47
1:A:608:MET:HG3	1:A:619:ILE:HD13	1.95	0.47
1:A:472:PRO:HG2	1:A:532:ALA:CB	2.39	0.47
1:B:515:LEU:HD21	1:B:623:THR:HG22	1.96	0.47
1:B:119:ILE:HG13	1:B:162:GLU:O	2.13	0.47
1:A:608:MET:HG3	1:A:619:ILE:HD12	1.95	0.47
1:A:532:ALA:HB2	1:A:573:VAL:HG21	1.96	0.47
1:C:131:PHE:O	1:C:136:LYS:HB2	2.14	0.47
1:C:490:GLN:CB	1:C:494:GLN:HG3	2.40	0.47
1:A:438:ASP:HB3	1:A:441:VAL:CG2	2.44	0.47
1:A:755:TYR:N	1:A:755:TYR:HD1	2.11	0.47
1:A:35:ASP:O	1:A:85:ASN:ND2	2.48	0.47
1:C:281:GLU:O	1:C:284:SER:HB3	2.14	0.47
1:A:313:ARG:O	1:A:316:THR:CG2	2.53	0.47
1:A:515:LEU:HD13	1:A:634:LEU:HD21	1.95	0.47
1:C:489:LEU:HD21	1:C:516:PHE:CZ	2.50	0.47
1:C:729:PRO:O	1:C:730:GLU:OE2	2.32	0.47
1:B:82:ILE:HD13	1:B:84:MET:CE	2.44	0.47
1:C:269:ILE:HD11	1:C:301:ILE:HG22	1.94	0.47
1:C:197:SER:OG	1:C:199:ASN:HB3	2.14	0.47
1:B:131:PHE:O	1:B:136:LYS:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:PHE:HA	1:C:699:ILE:HD13	1.95	0.47
1:A:93:ARG:HG2	1:A:93:ARG:HH11	1.80	0.47
1:A:378:LEU:O	1:A:378:LEU:HD22	2.15	0.47
1:A:114:ILE:CD1	1:A:176:VAL:HG22	2.44	0.47
1:B:233:ILE:HD13	1:C:442:MET:HE1	1.96	0.47
1:B:290:PHE:CD2	1:B:331:LEU:HB3	2.50	0.47
1:B:437:ILE:CG2	1:B:438:ASP:N	2.76	0.47
1:C:410:ASP:OD2	1:C:463:ALA:CB	2.62	0.47
1:A:42:SER:HB2	1:A:44:PRO:HD2	1.96	0.47
1:B:193:ASP:O	1:B:195:GLU:N	2.48	0.47
1:A:615:LYS:NZ	1:B:461:PRO:HG2	2.29	0.47
1:B:431:ASP:OD1	1:B:433:GLU:HG3	2.14	0.47
1:C:729:PRO:O	1:C:730:GLU:CD	2.53	0.47
1:B:265:PHE:CD2	1:B:296:ASN:HB2	2.49	0.47
1:B:206:ILE:CD1	1:B:213:LEU:CG	2.87	0.47
1:B:114:ILE:CD1	1:B:176:VAL:HG22	2.44	0.47
1:C:290:PHE:CD2	1:C:331:LEU:HB3	2.49	0.47
1:A:43:GLN:N	1:A:44:PRO:CD	2.76	0.47
1:B:42:SER:HB2	1:B:44:PRO:HD2	1.96	0.47
1:A:89:ARG:NH1	1:A:96:LEU:HD21	2.28	0.47
1:B:348:ASN:O	1:B:349:ARG:HB3	2.14	0.47
1:A:191:ARG:NH1	1:A:197:SER:HA	2.29	0.47
1:A:197:SER:OG	1:A:199:ASN:HB3	2.15	0.47
1:C:348:ASN:O	1:C:349:ARG:HB3	2.14	0.47
1:B:544:GLY:O	1:B:547:LEU:HB2	2.14	0.47
1:B:197:SER:OG	1:B:199:ASN:HB3	2.15	0.47
1:B:568:GLN:HG2	1:B:568:GLN:O	2.15	0.47
1:A:573:VAL:HG23	1:A:573:VAL:O	2.15	0.47
1:B:641:GLN:C	1:B:642:LEU:HD22	2.35	0.47
1:B:410:ASP:CG	1:B:463:ALA:CB	2.83	0.47
1:C:600:VAL:O	1:C:604:ILE:HG13	2.14	0.47
1:C:647:LEU:HD12	1:C:647:LEU:N	2.30	0.47
1:B:184:CYS:O	1:B:186:GLY:N	2.48	0.47
1:C:227:PRO:HA	1:C:340:HIS:HE1	1.78	0.47
1:C:556:GLU:N	1:C:556:GLU:OE1	2.46	0.47
1:A:206:ILE:CD1	1:A:213:LEU:CG	2.85	0.47
1:A:316:THR:HG23	1:A:316:THR:O	2.15	0.47
1:C:489:LEU:HD21	1:C:516:PHE:HZ	1.79	0.47
1:B:60:LYS:CE	1:B:103:GLN:HE21	2.28	0.47
1:C:89:ARG:HD3	1:C:96:LEU:HD22	1.96	0.47
1:C:491:GLU:HA	1:C:495:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:624:ASN:HD22	1:C:624:ASN:C	2.18	0.47
1:B:323:ARG:HH22	1:C:279:ALA:CB	2.25	0.47
1:C:390:LEU:HD22	1:C:394:VAL:HG11	1.96	0.47
1:C:381:LEU:HD21	1:C:411:LEU:HD22	1.96	0.47
1:C:42:SER:HB2	1:C:44:PRO:HD2	1.96	0.47
1:C:44:PRO:HG2	1:C:79:ASP:OD1	2.14	0.47
1:B:126:ILE:HB	1:B:439:ALA:HB2	1.96	0.47
1:A:544:GLY:O	1:A:547:LEU:HB2	2.13	0.47
1:C:544:GLY:O	1:C:547:LEU:HB2	2.14	0.47
1:B:682:PHE:CE1	1:B:690:ILE:HD11	2.50	0.46
1:A:390:LEU:HD22	1:A:394:VAL:HG11	1.96	0.46
1:B:427:MET:O	1:B:427:MET:HG2	2.15	0.46
1:A:703:ILE:O	1:A:707:ILE:HG12	2.15	0.46
1:C:134:TYR:HB3	1:C:154:VAL:HG11	1.97	0.46
1:B:487:ARG:CZ	1:B:487:ARG:HB3	2.45	0.46
1:A:556:GLU:N	1:A:556:GLU:OE1	2.44	0.46
1:C:60:LYS:HZ3	1:C:103:GLN:HE22	1.62	0.46
1:B:390:LEU:HD22	1:B:394:VAL:HG11	1.96	0.46
1:C:427:MET:HE1	1:C:437:ILE:HG21	1.97	0.46
1:A:518:GLY:C	1:A:755:TYR:CE2	2.86	0.46
1:A:82:ILE:HD13	1:A:84:MET:CE	2.45	0.46
1:B:577:ASP:O	1:B:578:GLU:C	2.53	0.46
1:C:587:GLY:HA3	1:C:591:GLY:HA2	1.97	0.46
1:B:596:ALA:HB1	1:B:630:ASP:HA	1.98	0.46
1:C:487:ARG:HB3	1:C:487:ARG:CZ	2.45	0.46
1:C:519:PRO:HD2	1:C:645:ILE:O	2.15	0.46
1:C:60:LYS:HZ1	1:C:103:GLN:NE2	2.03	0.46
1:A:647:LEU:HD21	1:A:747:VAL:CB	2.44	0.46
1:B:116:VAL:HG12	1:B:165:VAL:HA	1.97	0.46
1:C:629:ILE:O	1:C:631:PRO:HD3	2.15	0.46
1:B:567:ARG:NH2	1:B:611:MET:HG3	2.31	0.46
1:A:634:LEU:HD22	1:A:642:LEU:HD11	1.98	0.46
1:B:624:ASN:C	1:B:624:ASN:HD22	2.18	0.46
1:A:177:ALA:C	1:A:179:ASP:H	2.18	0.46
1:C:633:ILE:HG22	1:C:639:LEU:HD12	1.96	0.46
1:C:122:THR:O	1:C:161:VAL:HG22	2.16	0.46
1:A:755:TYR:N	1:A:755:TYR:CD1	2.81	0.46
1:C:135:LEU:H	1:C:135:LEU:CD2	2.28	0.46
1:B:629:ILE:O	1:B:631:PRO:HD3	2.16	0.46
1:C:515:LEU:HD13	1:C:634:LEU:HD21	1.97	0.46
1:C:474:VAL:HG22	1:C:475:THR:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:ASN:HD22	1:A:624:ASN:C	2.18	0.46
1:A:227:PRO:HA	1:A:340:HIS:CE1	2.50	0.46
1:B:203:TYR:O	1:B:206:ILE:HG12	2.16	0.46
1:B:112:LYS:H	1:B:170:PRO:HD3	1.81	0.46
1:A:229:LEU:O	1:A:233:ILE:HG22	2.16	0.46
1:B:485:VAL:HG23	1:B:486:LYS:N	2.30	0.46
1:C:43:GLN:N	1:C:44:PRO:CD	2.77	0.46
1:A:526:LEU:HD21	2:A:900:ADP:H3'	1.97	0.46
1:B:227:PRO:HA	1:B:340:HIS:HE1	1.79	0.46
1:C:706:GLU:O	1:C:707:ILE:O	2.33	0.46
1:A:313:ARG:NE	1:A:351:ASN:O	2.49	0.46
1:C:641:GLN:C	1:C:642:LEU:HD22	2.36	0.46
1:B:647:LEU:N	1:B:647:LEU:HD12	2.30	0.46
1:A:427:MET:O	1:A:427:MET:HG2	2.16	0.46
1:B:441:VAL:O	1:B:444:SER:OG	2.27	0.46
1:C:63:LYS:HD2	1:C:93:ARG:CB	2.46	0.46
1:C:580:ASP:HB2	1:C:628:ILE:HD11	1.97	0.46
1:A:432:LEU:CD1	1:A:441:VAL:HG11	2.44	0.46
1:C:327:GLN:O	1:C:331:LEU:HG	2.15	0.46
1:A:193:ASP:O	1:A:195:GLU:N	2.48	0.46
1:A:482:LEU:HB3	1:A:485:VAL:CG2	2.46	0.46
1:C:437:ILE:CG2	1:C:438:ASP:N	2.78	0.46
1:B:518:GLY:C	1:B:755:TYR:CE2	2.86	0.46
1:A:41:LEU:O	1:A:73:SER:HA	2.15	0.46
1:B:317:HIS:CE1	1:C:317:HIS:NE2	2.83	0.46
1:C:116:VAL:HG12	1:C:165:VAL:HA	1.98	0.46
1:A:206:ILE:HD12	1:A:213:LEU:HD21	1.97	0.46
1:B:491:GLU:HA	1:B:495:TYR:CD2	2.51	0.46
1:A:641:GLN:C	1:A:642:LEU:HD22	2.35	0.46
1:C:515:LEU:HA	1:C:621:GLY:O	2.15	0.46
1:A:93:ARG:HH21	1:A:194:GLU:HG2	1.81	0.46
1:C:378:LEU:HD22	1:C:378:LEU:O	2.15	0.46
1:B:592:ASP:OD1	1:B:592:ASP:N	2.49	0.46
1:C:410:ASP:OD2	1:C:463:ALA:HB1	2.16	0.46
1:B:519:PRO:HD2	1:B:645:ILE:O	2.16	0.45
1:A:441:VAL:O	1:A:444:SER:OG	2.27	0.45
1:C:177:ALA:C	1:C:179:ASP:H	2.18	0.45
1:A:485:VAL:HG23	1:A:486:LYS:N	2.31	0.45
1:B:378:LEU:O	1:B:378:LEU:HD22	2.16	0.45
1:A:524:LYS:HB2	2:A:900:ADP:O1B	2.16	0.45
1:C:577:ASP:O	1:C:579:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:GLU:O	1:A:538:ASN:HA	2.16	0.45
1:C:313:ARG:HG3	1:C:313:ARG:NH2	2.31	0.45
1:B:316:THR:HG23	1:B:316:THR:O	2.15	0.45
1:A:491:GLU:HA	1:A:495:TYR:CD2	2.51	0.45
1:C:139:PHE:CD1	1:C:176:VAL:HG11	2.51	0.45
1:B:327:GLN:O	1:B:331:LEU:HG	2.16	0.45
1:C:482:LEU:HB3	1:C:485:VAL:CG2	2.46	0.45
1:C:485:VAL:HG23	1:C:486:LYS:N	2.31	0.45
1:A:585:ALA:O	1:A:587:GLY:N	2.49	0.45
1:A:629:ILE:O	1:A:631:PRO:HD3	2.16	0.45
1:C:524:LYS:HB2	2:C:900:ADP:O1B	2.16	0.45
1:A:116:VAL:HG12	1:A:165:VAL:HA	1.97	0.45
1:A:377:ARG:O	1:A:381:LEU:HG	2.16	0.45
1:C:640:ASP:O	1:C:642:LEU:CD2	2.65	0.45
1:C:89:ARG:NH1	1:C:96:LEU:HD21	2.31	0.45
1:C:82:ILE:HD13	1:C:84:MET:CE	2.46	0.45
1:B:126:ILE:HG21	1:B:159:ARG:HD2	1.99	0.45
1:A:169:ASP:CB	1:A:170:PRO:HD3	2.29	0.45
1:B:206:ILE:HD12	1:B:213:LEU:HD21	1.97	0.45
1:C:312:LYS:HB3	1:C:354:ASP:CB	2.46	0.45
1:A:38:VAL:HG21	1:A:72:LEU:HD12	1.99	0.45
1:B:354:ASP:OD2	1:B:356:ALA:HB3	2.17	0.45
1:A:472:PRO:HB2	1:A:533:ASN:HB2	1.98	0.45
1:B:230:PHE:HA	1:B:233:ILE:CG2	2.43	0.45
1:B:377:ARG:O	1:B:381:LEU:HG	2.16	0.45
1:B:463:ALA:O	1:B:464:LEU:C	2.55	0.45
1:A:327:GLN:O	1:A:331:LEU:HG	2.17	0.45
1:A:184:CYS:O	1:A:186:GLY:N	2.49	0.45
1:C:114:ILE:HD13	1:C:146:ILE:HD11	1.98	0.45
1:B:640:ASP:O	1:B:642:LEU:CD2	2.65	0.45
1:A:328:LEU:O	1:A:331:LEU:N	2.45	0.45
1:C:377:ARG:O	1:C:381:LEU:HG	2.16	0.45
1:B:270:ASN:OD1	1:B:272:PRO:HD2	2.17	0.45
1:A:139:PHE:CG	1:A:176:VAL:HG11	2.52	0.45
1:B:682:PHE:CZ	1:B:744:ARG:O	2.70	0.45
1:A:270:ASN:OD1	1:A:272:PRO:HD2	2.17	0.45
1:B:482:LEU:HB3	1:B:485:VAL:CG2	2.47	0.45
1:B:505:LYS:NZ	1:C:729:PRO:HG3	2.31	0.45
1:A:585:ALA:C	1:A:587:GLY:H	2.20	0.45
1:C:41:LEU:O	1:C:73:SER:HA	2.16	0.45
1:B:586:ARG:NH1	1:B:598:ASP:HB3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:ASP:OD2	1:C:356:ALA:HB3	2.17	0.45
1:A:311:PRO:O	1:A:312:LYS:C	2.54	0.45
1:C:496:PRO:HA	1:C:503:PHE:CE2	2.52	0.45
1:A:731:ILE:O	1:A:731:ILE:CG2	2.64	0.45
1:A:258:VAL:O	1:A:262:THR:HG23	2.16	0.45
1:A:322:ARG:HD3	1:B:321:GLU:OE2	2.17	0.45
1:A:227:PRO:HA	1:A:340:HIS:HE1	1.80	0.45
1:A:275:MET:CG	1:A:309:ILE:HG12	2.47	0.44
1:A:248:GLY:O	1:A:249:THR:C	2.55	0.44
1:B:172:PRO:HG2	1:B:173:TYR:CD2	2.52	0.44
1:A:306:LEU:HD22	1:A:345:ALA:HB1	1.97	0.44
1:B:385:THR:C	1:B:387:ASN:H	2.21	0.44
1:C:608:MET:HG3	1:C:619:ILE:HD13	1.96	0.44
1:C:539:PHE:HD1	1:C:573:VAL:HG23	1.82	0.44
1:B:425:LYS:O	1:B:429:LEU:HB2	2.17	0.44
1:A:519:PRO:HD2	1:A:645:ILE:O	2.18	0.44
1:C:203:TYR:CE2	1:C:217:LYS:HE2	2.52	0.44
1:B:758:PHE:O	1:B:762:LEU:HG	2.16	0.44
1:B:474:VAL:HG22	1:B:475:THR:N	2.31	0.44
1:C:385:THR:C	1:C:387:ASN:H	2.21	0.44
1:A:112:LYS:HB2	1:A:169:ASP:HB3	1.99	0.44
1:A:640:ASP:O	1:A:642:LEU:CD2	2.65	0.44
1:A:91:ASN:ND2	1:A:91:ASN:N	2.65	0.44
1:C:248:GLY:O	1:C:249:THR:C	2.55	0.44
1:B:732:ARG:O	1:B:735:HIS:HB2	2.17	0.44
1:B:634:LEU:HD22	1:B:642:LEU:HD11	1.99	0.44
1:A:653:ARG:O	1:A:657:LEU:HG	2.17	0.44
1:C:109:LYS:O	1:C:110:TYR:C	2.56	0.44
1:C:270:ASN:OD1	1:C:272:PRO:HD2	2.18	0.44
1:C:427:MET:SD	1:C:441:VAL:HG11	2.57	0.44
1:C:153:LEU:HD12	1:C:161:VAL:O	2.17	0.44
1:B:518:GLY:HA2	1:B:755:TYR:CD2	2.52	0.44
1:C:63:LYS:HD2	1:C:93:ARG:CG	2.47	0.44
1:C:648:PRO:HD2	1:C:683:SER:HA	2.00	0.44
1:A:172:PRO:HG2	1:A:173:TYR:CD2	2.52	0.44
1:C:364:ASP:OD1	1:C:365:ARG:HG2	2.17	0.44
1:C:464:LEU:HA	1:C:464:LEU:HD23	1.84	0.44
1:A:425:LYS:O	1:A:429:LEU:HB2	2.18	0.44
1:B:135:LEU:CD2	1:B:135:LEU:H	2.30	0.44
1:B:729:PRO:C	1:B:730:GLU:CD	2.76	0.44
1:B:35:ASP:O	1:B:85:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ILE:N	1:A:707:ILE:HD13	2.31	0.44
1:A:231:LYS:O	1:A:231:LYS:HG2	2.18	0.44
1:C:540:ILE:HD12	1:C:572:CYS:SG	2.58	0.44
1:C:313:ARG:CG	1:C:314:GLU:N	2.77	0.44
1:A:614:LYS:CE	1:B:402:GLU:OE1	2.64	0.44
1:C:425:LYS:O	1:C:429:LEU:HB2	2.17	0.44
1:A:682:PHE:HE1	1:A:690:ILE:HD11	1.82	0.44
1:B:91:ASN:N	1:B:91:ASN:ND2	2.66	0.44
1:A:275:MET:SD	1:A:324:ILE:HD13	2.58	0.44
1:B:545:PRO:HD3	1:B:578:GLU:OE1	2.17	0.44
1:C:684:GLY:HA3	2:C:900:ADP:C8	2.53	0.44
1:B:271:GLY:HA2	1:B:309:ILE:HD11	1.98	0.44
1:A:294:GLU:CD	1:A:339:ALA:HB2	2.38	0.44
1:A:354:ASP:OD2	1:A:356:ALA:HB3	2.18	0.44
1:A:514:VAL:CG1	1:A:515:LEU:N	2.80	0.44
1:C:634:LEU:HD22	1:C:642:LEU:HD11	1.99	0.44
1:B:65:ARG:HH11	1:B:93:ARG:CZ	2.31	0.44
1:C:520:PRO:HG3	1:C:624:ASN:HB2	2.00	0.44
1:C:22:ARG:C	1:C:24:ASN:H	2.21	0.44
1:B:605:LEU:HD21	1:B:633:ILE:HG12	2.00	0.44
1:A:650:GLU:CG	1:A:677:LYS:HZ3	2.30	0.44
1:A:96:LEU:CD2	1:A:96:LEU:N	2.79	0.44
1:A:82:ILE:O	1:A:82:ILE:HG23	2.18	0.44
1:C:758:PHE:HB3	1:C:762:LEU:HD12	2.00	0.44
1:B:665:PRO:C	1:B:731:ILE:HG22	2.37	0.44
1:A:132:GLU:OE2	1:A:136:LYS:HD3	2.18	0.44
1:C:410:ASP:CG	1:C:463:ALA:HB2	2.38	0.44
1:C:682:PHE:HE1	1:C:690:ILE:HD11	1.83	0.44
1:C:84:MET:O	1:C:84:MET:HG3	2.18	0.44
1:A:385:THR:C	1:A:387:ASN:H	2.22	0.44
1:B:312:LYS:HB3	1:B:354:ASP:HB2	2.00	0.44
1:B:496:PRO:HA	1:B:503:PHE:CE2	2.53	0.44
1:B:405:GLY:CA	1:B:465:ARG:HD3	2.41	0.44
1:B:358:ARG:NH1	1:B:358:ARG:HG3	2.28	0.44
1:C:65:ARG:NH1	1:C:93:ARG:HH22	2.16	0.44
1:C:514:VAL:CG1	1:C:515:LEU:N	2.78	0.43
1:C:515:LEU:HD21	1:C:623:THR:HG22	2.00	0.43
1:C:230:PHE:HA	1:C:233:ILE:CG2	2.44	0.43
1:A:648:PRO:HD2	1:A:683:SER:HA	1.98	0.43
1:C:455:ALA:O	1:C:460:ASN:OD1	2.36	0.43
1:A:405:GLY:HA3	1:A:465:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:HD21	1:A:623:THR:CG2	2.48	0.43
1:B:89:ARG:HG3	1:B:94:VAL:HG23	2.00	0.43
1:C:647:LEU:HD21	1:C:747:VAL:CB	2.48	0.43
1:C:89:ARG:HG3	1:C:94:VAL:HG23	1.98	0.43
1:B:540:ILE:CG2	1:B:574:LEU:HD12	2.48	0.43
1:B:519:PRO:HG3	1:B:647:LEU:CD1	2.49	0.43
1:B:248:GLY:O	1:B:249:THR:C	2.56	0.43
1:B:60:LYS:CE	1:B:103:GLN:NE2	2.81	0.43
1:C:89:ARG:NH2	1:C:96:LEU:HD11	2.34	0.43
1:C:96:LEU:N	1:C:96:LEU:CD2	2.81	0.43
1:A:26:LEU:HD21	1:A:45:LYS:HE2	2.00	0.43
1:A:496:PRO:HA	1:A:503:PHE:CE2	2.52	0.43
1:B:132:GLU:OE2	1:B:136:LYS:HD3	2.18	0.43
1:B:233:ILE:HG13	1:B:235:VAL:HG23	2.00	0.43
1:A:615:LYS:HZ3	1:B:461:PRO:CG	2.30	0.43
1:A:432:LEU:O	1:A:437:ILE:HD13	2.18	0.43
1:A:45:LYS:HD2	1:A:45:LYS:HA	1.80	0.43
1:B:540:ILE:HG22	1:B:574:LEU:HD12	2.01	0.43
1:A:540:ILE:HG22	1:A:574:LEU:HD12	1.99	0.43
1:A:123:VAL:O	1:A:124:GLU:C	2.57	0.43
1:B:364:ASP:OD1	1:B:365:ARG:HG2	2.19	0.43
1:B:231:LYS:HG2	1:B:231:LYS:O	2.19	0.43
1:A:615:LYS:NZ	1:B:461:PRO:CG	2.82	0.43
1:C:193:ASP:O	1:C:195:GLU:N	2.50	0.43
1:A:102:ILE:CG1	1:A:103:GLN:H	2.31	0.43
1:C:358:ARG:HG3	1:C:358:ARG:NH1	2.29	0.43
1:B:318:GLY:O	1:B:322:ARG:HG3	2.19	0.43
1:B:294:GLU:CD	1:B:339:ALA:HB2	2.38	0.43
1:A:143:TYR:CE1	1:A:178:PRO:CD	2.93	0.43
1:B:229:LEU:O	1:B:229:LEU:HD12	2.19	0.43
1:B:252:THR:HB	2:B:807:ADP:O1A	2.18	0.43
1:A:633:ILE:O	1:A:639:LEU:HB2	2.18	0.43
1:B:89:ARG:NH2	1:B:96:LEU:HD11	2.34	0.43
1:C:139:PHE:O	1:C:140:LEU:C	2.57	0.43
1:B:139:PHE:CG	1:B:176:VAL:HG11	2.53	0.43
1:B:63:LYS:HD2	1:B:93:ARG:CB	2.48	0.43
1:B:275:MET:SD	1:B:324:ILE:HD13	2.59	0.43
1:A:84:MET:HG3	1:A:84:MET:O	2.19	0.43
1:C:258:VAL:O	1:C:262:THR:HG23	2.18	0.43
1:C:285:ASN:HD22	1:C:285:ASN:N	2.16	0.43
1:A:539:PHE:HD1	1:A:573:VAL:CG2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:GLY:O	1:B:463:ALA:HB3	2.19	0.43
1:B:455:ALA:O	1:B:460:ASN:OD1	2.37	0.43
1:B:519:PRO:HA	1:B:520:PRO:HD3	1.78	0.43
1:B:648:PRO:HD2	1:B:683:SER:HA	2.00	0.43
1:B:272:PRO:O	1:B:276:SER:HB3	2.19	0.43
1:C:158:MET:HE3	1:C:419:ALA:HB1	2.01	0.43
1:C:272:PRO:O	1:C:276:SER:HB3	2.19	0.43
1:C:93:ARG:HH21	1:C:194:GLU:HG2	1.83	0.43
1:A:28:VAL:HG23	1:A:84:MET:CG	2.49	0.43
1:B:82:ILE:HG23	1:B:82:ILE:O	2.18	0.43
1:C:191:ARG:NH1	1:C:197:SER:HA	2.34	0.43
1:C:294:GLU:CD	1:C:339:ALA:HB2	2.38	0.43
1:B:653:ARG:O	1:B:657:LEU:HG	2.19	0.43
1:A:65:ARG:HH12	1:A:93:ARG:HH22	1.66	0.43
1:A:109:LYS:O	1:A:110:TYR:C	2.57	0.43
1:A:89:ARG:NH2	1:A:96:LEU:HD11	2.34	0.43
1:C:82:ILE:O	1:C:82:ILE:HG23	2.18	0.43
1:C:172:PRO:HG2	1:C:173:TYR:CD2	2.54	0.43
1:B:120:ASP:OD2	1:B:190:LYS:HA	2.19	0.43
1:A:65:ARG:HH11	1:A:93:ARG:CZ	2.31	0.43
1:C:427:MET:O	1:C:427:MET:HG2	2.19	0.43
1:C:65:ARG:NH1	1:C:93:ARG:NH2	2.66	0.43
1:C:650:GLU:CG	1:C:677:LYS:HZ3	2.32	0.43
1:B:96:LEU:N	1:B:96:LEU:CD2	2.81	0.43
1:C:653:ARG:O	1:C:657:LEU:HG	2.19	0.43
1:B:258:VAL:O	1:B:262:THR:HG23	2.18	0.43
1:B:191:ARG:NH1	1:B:197:SER:HA	2.33	0.43
1:A:21:ASN:O	1:A:22:ARG:HB2	2.19	0.43
1:A:114:ILE:HD13	1:A:146:ILE:HD11	2.00	0.42
1:B:514:VAL:CG1	1:B:515:LEU:N	2.77	0.42
1:C:659:ALA:HA	1:C:662:ARG:CD	2.49	0.42
1:A:648:PRO:CD	1:A:683:SER:HA	2.49	0.42
1:A:364:ASP:OD1	1:A:365:ARG:HG2	2.19	0.42
1:C:231:LYS:O	1:C:231:LYS:HG2	2.18	0.42
1:A:407:VAL:HG23	1:A:408:GLY:N	2.34	0.42
1:A:460:ASN:OD1	1:A:461:PRO:CD	2.65	0.42
1:A:358:ARG:NH1	1:A:358:ARG:HG3	2.29	0.42
1:A:759:ALA:HA	1:A:762:LEU:HB2	2.02	0.42
1:B:759:ALA:HA	1:B:762:LEU:HB2	2.01	0.42
1:C:120:ASP:OD2	1:C:190:LYS:HA	2.19	0.42
1:B:433:GLU:O	1:B:434:ASP:OD1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ASP:O	1:A:583:ALA:N	2.52	0.42
1:A:384:HIS:HE1	2:A:807:ADP:N3	2.17	0.42
1:C:665:PRO:C	1:C:731:ILE:HG22	2.39	0.42
1:C:102:ILE:CG1	1:C:103:GLN:N	2.83	0.42
1:A:519:PRO:HG3	1:A:647:LEU:HD12	2.00	0.42
1:B:437:ILE:HG22	1:B:438:ASP:O	2.20	0.42
1:C:575:PHE:CE2	1:C:577:ASP:HB2	2.53	0.42
1:A:732:ARG:CD	1:A:734:ASP:OD1	2.67	0.42
1:B:556:GLU:N	1:B:556:GLU:OE1	2.47	0.42
1:C:169:ASP:CB	1:C:170:PRO:HD3	2.30	0.42
1:C:694:ALA:O	1:C:697:LEU:HB2	2.19	0.42
1:C:515:LEU:C	1:C:515:LEU:HD23	2.40	0.42
1:C:751:ASP:O	1:C:752:ILE:C	2.58	0.42
1:C:233:ILE:HG13	1:C:235:VAL:HG23	2.01	0.42
1:A:233:ILE:HG13	1:A:235:VAL:HG23	2.00	0.42
1:B:109:LYS:O	1:B:110:TYR:C	2.58	0.42
1:C:290:PHE:HE2	1:C:331:LEU:O	2.02	0.42
1:B:193:ASP:C	1:B:195:GLU:H	2.23	0.42
1:B:26:LEU:CD1	1:B:41:LEU:HD21	2.49	0.42
1:B:624:ASN:ND2	1:B:624:ASN:N	2.66	0.42
1:A:664:SER:HA	1:A:665:PRO:HD3	1.87	0.42
1:C:519:PRO:HA	1:C:520:PRO:HD3	1.79	0.42
1:A:758:PHE:C	1:A:762:LEU:HD12	2.39	0.42
1:B:515:LEU:CD1	1:B:634:LEU:HD21	2.50	0.42
1:A:659:ALA:HA	1:A:662:ARG:CD	2.49	0.42
1:C:21:ASN:O	1:C:22:ARG:HB2	2.20	0.42
1:B:388:MET:HE1	1:B:447:VAL:HG21	2.02	0.42
1:A:416:SER:O	1:A:420:LEU:HG	2.19	0.42
1:C:664:SER:HA	1:C:665:PRO:HD3	1.88	0.42
1:A:455:ALA:O	1:A:460:ASN:OD1	2.38	0.42
1:B:139:PHE:O	1:B:140:LEU:C	2.58	0.42
1:C:515:LEU:CD1	1:C:634:LEU:HD21	2.50	0.42
1:C:520:PRO:HG3	1:C:624:ASN:CB	2.50	0.42
1:C:423:ILE:C	1:C:425:LYS:N	2.73	0.42
1:A:431:ASP:O	1:A:432:LEU:HD23	2.19	0.42
1:C:328:LEU:O	1:C:331:LEU:N	2.44	0.42
1:C:605:LEU:HD21	1:C:633:ILE:HG12	2.02	0.42
1:C:648:PRO:CD	1:C:683:SER:HA	2.50	0.42
1:B:610:GLY:O	1:B:611:MET:C	2.58	0.42
1:A:461:PRO:O	1:A:463:ALA:N	2.51	0.42
1:A:515:LEU:CD1	1:A:634:LEU:HD21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:LEU:HD13	1:C:642:LEU:HA	1.88	0.42
1:A:285:ASN:HD22	1:A:285:ASN:N	2.18	0.42
1:B:731:ILE:O	1:B:731:ILE:HG23	2.20	0.41
1:A:65:ARG:NH1	1:A:93:ARG:CZ	2.83	0.41
1:C:466:GLU:HG2	1:C:467:THR:N	2.32	0.41
1:A:269:ILE:HD11	1:A:301:ILE:HG22	2.00	0.41
1:C:524:LYS:HB2	1:C:524:LYS:HZ2	1.85	0.41
1:C:497:VAL:HG13	1:C:498:GLU:HG3	2.02	0.41
1:B:479:ILE:HD13	1:B:527:LEU:HD23	2.02	0.41
1:A:292:GLU:O	1:A:292:GLU:HG2	2.20	0.41
1:B:461:PRO:O	1:B:463:ALA:N	2.46	0.41
1:B:520:PRO:HG3	1:B:624:ASN:HB2	2.03	0.41
1:C:193:ASP:C	1:C:195:GLU:H	2.24	0.41
1:A:134:TYR:HB3	1:A:154:VAL:HG11	2.01	0.41
1:C:416:SER:O	1:C:420:LEU:HG	2.20	0.41
1:B:694:ALA:O	1:B:697:LEU:HB2	2.20	0.41
1:A:410:ASP:OD2	1:A:463:ALA:HB1	2.20	0.41
1:C:460:ASN:N	1:C:461:PRO:CD	2.80	0.41
1:A:270:ASN:O	1:A:273:GLU:HB3	2.21	0.41
1:A:605:LEU:HD21	1:A:633:ILE:HG12	2.01	0.41
1:B:45:LYS:HD2	1:B:45:LYS:HA	1.82	0.41
1:B:466:GLU:CG	1:B:467:THR:H	2.12	0.41
1:B:642:LEU:HA	1:B:642:LEU:HD13	1.88	0.41
1:A:427:MET:SD	1:A:441:VAL:HG11	2.61	0.41
1:B:427:MET:SD	1:B:441:VAL:HG11	2.61	0.41
1:B:383:ILE:O	1:B:386:LYS:HE3	2.20	0.41
1:C:441:VAL:O	1:C:444:SER:OG	2.28	0.41
1:B:39:VAL:HG12	1:B:84:MET:HB3	2.02	0.41
1:C:590:ILE:HG12	1:C:590:ILE:H	1.66	0.41
1:B:63:LYS:HD2	1:B:93:ARG:HD2	2.01	0.41
1:B:648:PRO:CD	1:B:683:SER:HA	2.50	0.41
1:B:177:ALA:C	1:B:179:ASP:N	2.73	0.41
1:C:407:VAL:HG23	1:C:408:GLY:N	2.35	0.41
1:A:272:PRO:O	1:A:276:SER:HB3	2.20	0.41
1:B:532:ALA:HB2	1:B:573:VAL:HG21	2.02	0.41
1:C:430:ILE:HD13	1:C:430:ILE:HA	1.92	0.41
1:C:624:ASN:N	1:C:624:ASN:ND2	2.66	0.41
1:B:659:ALA:HA	1:B:662:ARG:CD	2.50	0.41
1:C:458:GLN:HG3	1:C:459:SER:N	2.36	0.41
1:A:580:ASP:O	1:A:581:SER:C	2.58	0.41
1:B:147:ARG:CG	1:B:148:LYS:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:ASN:ND2	1:C:688:THR:OG1	2.54	0.41
1:B:667:ALA:HB3	1:B:670:VAL:CG2	2.50	0.41
1:C:514:VAL:CG1	1:C:515:LEU:H	2.33	0.41
1:A:230:PHE:HA	1:A:233:ILE:CG2	2.46	0.41
1:B:633:ILE:O	1:B:639:LEU:HB2	2.21	0.41
1:A:135:LEU:CD2	1:A:135:LEU:H	2.33	0.41
1:C:108:VAL:HG22	1:C:173:TYR:CE1	2.55	0.41
1:B:470:GLU:O	1:B:538:ASN:HA	2.20	0.41
1:A:610:GLY:O	1:A:611:MET:C	2.59	0.41
1:A:474:VAL:HG22	1:A:475:THR:N	2.34	0.41
1:B:460:ASN:OD1	1:B:461:PRO:HD3	2.21	0.41
1:A:221:GLU:HG3	1:A:222:LEU:HD23	2.02	0.41
1:A:519:PRO:HA	1:A:520:PRO:HD3	1.77	0.41
1:B:133:VAL:HG13	1:B:443:ASN:HB2	2.03	0.41
1:C:354:ASP:HA	1:C:355:PRO:HD3	1.92	0.41
1:A:351:ASN:N	1:A:351:ASN:OD1	2.54	0.41
1:B:112:LYS:HB2	1:B:169:ASP:HB3	2.01	0.41
1:A:112:LYS:H	1:A:170:PRO:CD	2.34	0.41
1:A:539:PHE:HD1	1:A:573:VAL:HG23	1.85	0.41
1:A:410:ASP:OD2	1:A:463:ALA:CB	2.69	0.41
1:C:129:ASN:HD21	1:C:132:GLU:HB2	1.82	0.41
1:B:751:ASP:O	1:B:752:ILE:C	2.59	0.41
1:B:93:ARG:HH21	1:B:194:GLU:HG2	1.86	0.41
1:B:407:VAL:HG23	1:B:408:GLY:N	2.35	0.41
1:C:645:ILE:N	1:C:645:ILE:HD12	2.36	0.41
1:B:682:PHE:HE1	1:B:690:ILE:HD11	1.85	0.41
1:A:391:ALA:HB3	1:A:394:VAL:HG23	2.02	0.41
1:A:644:TYR:CE2	1:A:646:PRO:HB3	2.56	0.41
1:B:270:ASN:O	1:B:273:GLU:HB3	2.21	0.41
1:C:275:MET:SD	1:C:324:ILE:HD13	2.60	0.41
1:A:650:GLU:HG2	1:A:677:LYS:NZ	2.36	0.41
1:A:694:ALA:O	1:A:697:LEU:HB2	2.21	0.41
1:A:197:SER:C	1:A:199:ASN:H	2.24	0.41
1:A:751:ASP:O	1:A:754:LYS:HB2	2.20	0.41
1:C:292:GLU:O	1:C:292:GLU:HG2	2.21	0.41
1:C:123:VAL:O	1:C:124:GLU:C	2.57	0.41
1:A:448:THR:C	1:A:450:ASP:N	2.74	0.41
1:A:660:ASN:ND2	1:A:688:THR:OG1	2.53	0.41
1:A:320:VAL:O	1:A:321:GLU:C	2.58	0.41
1:B:514:VAL:CG1	1:B:515:LEU:H	2.33	0.41
1:C:229:LEU:HD12	1:C:229:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:PHE:CE2	1:B:745:ARG:HG2	2.56	0.41
1:C:432:LEU:HD12	1:C:441:VAL:HG11	2.03	0.41
1:B:388:MET:CE	1:B:447:VAL:HG21	2.51	0.41
1:B:322:ARG:HD3	1:C:321:GLU:CD	2.41	0.41
1:C:39:VAL:HG12	1:C:84:MET:HB3	2.03	0.41
1:B:108:VAL:HG22	1:B:173:TYR:CE1	2.56	0.41
1:B:285:ASN:HD22	1:B:285:ASN:N	2.17	0.41
1:A:313:ARG:CG	1:A:314:GLU:H	2.20	0.40
1:B:515:LEU:HD23	1:B:515:LEU:C	2.42	0.40
1:B:432:LEU:O	1:B:437:ILE:HD11	2.20	0.40
1:C:270:ASN:O	1:C:273:GLU:HB3	2.21	0.40
1:C:653:ARG:HD2	1:C:679:THR:OG1	2.21	0.40
1:C:35:ASP:O	1:C:85:ASN:ND2	2.54	0.40
1:B:542:ILE:HG12	1:B:562:ILE:HD13	2.03	0.40
1:A:303:ILE:HG13	1:A:303:ILE:H	1.66	0.40
1:B:292:GLU:HG2	1:B:292:GLU:O	2.21	0.40
1:A:139:PHE:O	1:A:140:LEU:C	2.60	0.40
1:C:694:ALA:HB1	1:C:731:ILE:HD11	2.03	0.40
1:C:102:ILE:CG1	1:C:103:GLN:H	2.33	0.40
1:A:102:ILE:CG1	1:A:103:GLN:N	2.82	0.40
1:B:573:VAL:HA	1:B:618:PHE:O	2.21	0.40
1:B:502:LYS:HE3	1:B:505:LYS:HZ1	1.85	0.40
1:A:26:LEU:CD1	1:A:41:LEU:HD21	2.52	0.40
1:B:118:PRO:HB2	1:B:123:VAL:HG11	2.02	0.40
1:C:147:ARG:CG	1:C:148:LYS:N	2.84	0.40
1:C:703:ILE:O	1:C:707:ILE:HG12	2.22	0.40
1:B:497:VAL:HG13	1:B:498:GLU:HG3	2.03	0.40
1:C:206:ILE:CG2	1:C:253:LEU:CD2	3.00	0.40
1:C:397:GLU:O	1:C:401:ASN:ND2	2.54	0.40
1:C:514:VAL:HG13	1:C:641:GLN:HB2	2.04	0.40
1:B:749:ASP:CA	1:B:752:ILE:HD12	2.42	0.40
1:C:475:THR:HG22	1:C:533:ASN:HD21	1.87	0.40
1:B:290:PHE:HE2	1:B:331:LEU:O	2.05	0.40
1:A:334:GLY:O	1:A:336:LYS:N	2.55	0.40
1:A:398:GLN:HG2	1:A:449:MET:CE	2.51	0.40
1:A:437:ILE:HG22	1:A:438:ASP:O	2.21	0.40
1:A:95:ARG:HG3	1:A:225:ARG:HH12	1.86	0.40
1:B:38:VAL:HG21	1:B:72:LEU:HD12	2.03	0.40
1:C:564:ASP:C	1:C:566:ALA:N	2.74	0.40
1:C:26:LEU:HD13	1:C:41:LEU:HD21	2.02	0.40
1:A:122:THR:O	1:A:161:VAL:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:HD12	1:B:213:LEU:CD2	2.52	0.40
1:A:312:LYS:HB3	1:A:354:ASP:CG	2.42	0.40
1:C:610:GLY:O	1:C:611:MET:C	2.58	0.40
1:A:506:PHE:CE1	1:B:698:ALA:HB1	2.57	0.40
1:A:463:ALA:O	1:A:464:LEU:C	2.59	0.40
1:A:642:LEU:HA	1:A:642:LEU:HD13	1.89	0.40
1:C:391:ALA:HB3	1:C:394:VAL:HG23	2.02	0.40
1:A:653:ARG:HD2	1:A:679:THR:OG1	2.21	0.40
1:A:680:ASN:C	1:A:682:PHE:H	2.24	0.40
1:C:177:ALA:C	1:C:179:ASP:N	2.75	0.40
1:A:568:GLN:HG2	1:A:568:GLN:O	2.21	0.40
1:B:123:VAL:O	1:B:124:GLU:C	2.60	0.40
1:A:147:ARG:CG	1:A:148:LYS:N	2.84	0.40
1:C:542:ILE:HG12	1:C:562:ILE:HD13	2.02	0.40
1:B:660:ASN:ND2	1:B:688:THR:OG1	2.55	0.40
1:A:497:VAL:HG13	1:A:498:GLU:HG3	2.03	0.40
1:C:514:VAL:HG23	1:C:618:PHE:CE2	2.57	0.40
1:A:177:ALA:C	1:A:179:ASP:N	2.75	0.40
1:A:632:ALA:HA	1:A:635:ARG:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	719/806 (89%)	566 (79%)	119 (17%)	34 (5%)	3	33
1	B	719/806 (89%)	564 (78%)	123 (17%)	32 (4%)	3	34
1	C	719/806 (89%)	561 (78%)	122 (17%)	36 (5%)	3	31
All	All	2157/2418 (89%)	1691 (78%)	364 (17%)	102 (5%)	3	33

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	85	ASN
1	A	140	LEU
1	A	185	GLU
1	A	312	LYS
1	A	426	LYS
1	B	85	ASN
1	B	140	LEU
1	B	185	GLU
1	B	194	GLU
1	B	312	LYS
1	B	426	LYS
1	C	140	LEU
1	C	185	GLU
1	C	304	ASP
1	C	312	LYS
1	C	426	LYS
1	C	462	SER
1	A	62	LYS
1	A	178	PRO
1	A	194	GLU
1	A	221	GLU
1	A	336	LYS
1	A	360	PHE
1	A	431	ASP
1	A	464	LEU
1	A	586	ARG
1	B	62	LYS
1	B	178	PRO
1	B	221	GLU
1	B	336	LYS
1	B	360	PHE
1	B	431	ASP
1	C	62	LYS
1	C	85	ASN
1	C	178	PRO
1	C	194	GLU
1	C	221	GLU
1	C	336	LYS
1	C	360	PHE
1	C	431	ASP
1	C	467	THR
1	C	569	ALA

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Mol	Chain	Res	Type
1	C	578	GLU
1	C	589	ASN
1	A	193	ASP
1	A	335	LEU
1	A	353	ILE
1	A	374	ALA
1	A	424	ARG
1	A	462	SER
1	A	585	ALA
1	A	589	ASN
1	B	30	GLU
1	B	193	ASP
1	B	304	ASP
1	B	335	LEU
1	B	353	ILE
1	B	374	ALA
1	B	424	ARG
1	B	462	SER
1	B	569	ALA
1	C	63	LYS
1	C	353	ILE
1	C	424	ARG
1	C	586	ARG
1	A	22	ARG
1	A	30	GLU
1	A	304	ASP
1	B	22	ARG
1	B	311	PRO
1	B	589	ASN
1	B	729	PRO
1	C	22	ARG
1	C	30	GLU
1	C	193	ASP
1	C	335	LEU
1	C	374	ALA
1	A	611	MET
1	B	120	ASP
1	B	186	GLY
1	B	499	HIS
1	B	611	MET
1	C	120	ASP
1	C	463	ALA

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Mol	Chain	Res	Type
1	C	499	HIS
1	C	611	MET
1	C	729	PRO
1	A	186	GLY
1	A	499	HIS
1	A	631	PRO
1	C	631	PRO
1	A	334	GLY
1	B	334	GLY
1	B	631	PRO
1	C	334	GLY
1	A	729	PRO
1	B	54	GLY
1	C	54	GLY
1	C	186	GLY
1	A	54	GLY
1	A	311	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	615/678 (91%)	590 (96%)	25 (4%)	37	73
1	B	615/678 (91%)	593 (96%)	22 (4%)	42	76
1	C	615/678 (91%)	592 (96%)	23 (4%)	41	75
All	All	1845/2034 (91%)	1775 (96%)	70 (4%)	40	74

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	64	ARG
1	A	82	ILE
1	A	91	ASN
1	A	113	ARG

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Mol	Chain	Res	Type
1	A	224	LEU
1	A	307	ASP
1	A	314	GLU
1	A	319	GLU
1	A	337	GLN
1	A	340	HIS
1	A	354	ASP
1	A	364	ASP
1	A	433	GLU
1	A	436	THR
1	A	440	GLU
1	A	462	SER
1	A	533	ASN
1	A	556	GLU
1	A	579	LEU
1	A	590	ILE
1	A	611	MET
1	A	613	THR
1	A	624	ASN
1	A	640	ASP
1	B	25	ARG
1	B	64	ARG
1	B	82	ILE
1	B	91	ASN
1	B	113	ARG
1	B	224	LEU
1	B	287	ARG
1	B	314	GLU
1	B	319	GLU
1	B	337	GLN
1	B	340	HIS
1	B	354	ASP
1	B	364	ASP
1	B	436	THR
1	B	440	GLU
1	B	533	ASN
1	B	556	GLU
1	B	579	LEU
1	B	611	MET
1	B	613	THR
1	B	624	ASN
1	B	640	ASP

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Mol	Chain	Res	Type
1	C	25	ARG
1	C	82	ILE
1	C	91	ASN
1	C	113	ARG
1	C	224	LEU
1	C	314	GLU
1	C	319	GLU
1	C	322	ARG
1	C	337	GLN
1	C	340	HIS
1	C	354	ASP
1	C	364	ASP
1	C	436	THR
1	C	440	GLU
1	C	464	LEU
1	C	533	ASN
1	C	556	GLU
1	C	579	LEU
1	C	611	MET
1	C	613	THR
1	C	624	ASN
1	C	640	ASP
1	C	728	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	91	ASN
1	A	103	GLN
1	A	260	ASN
1	A	285	ASN
1	A	317	HIS
1	A	327	GLN
1	A	337	GLN
1	A	340	HIS
1	A	348	ASN
1	A	384	HIS
1	A	401	ASN
1	A	443	ASN
1	A	490	GLN
1	A	533	ASN

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Mol	Chain	Res	Type
1	A	616	ASN
1	A	624	ASN
1	A	641	GLN
1	A	660	ASN
1	B	91	ASN
1	B	103	GLN
1	B	285	ASN
1	B	317	HIS
1	B	327	GLN
1	B	337	GLN
1	B	340	HIS
1	B	348	ASN
1	B	401	ASN
1	B	443	ASN
1	B	616	ASN
1	B	624	ASN
1	B	641	GLN
1	B	660	ASN
1	C	91	ASN
1	C	103	GLN
1	C	285	ASN
1	C	327	GLN
1	C	337	GLN
1	C	340	HIS
1	C	348	ASN
1	C	384	HIS
1	C	401	ASN
1	C	533	ASN
1	C	616	ASN
1	C	624	ASN
1	C	641	GLN
1	C	660	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ADP	A	807	-	22,29,29	1.73	7 (31%)	27,45,45	3.30	6 (22%)
2	ADP	A	900	-	22,29,29	1.90	5 (22%)	27,45,45	3.08	1 (3%)
2	ADP	B	807	-	22,29,29	1.74	5 (22%)	27,45,45	3.11	4 (14%)
2	ADP	B	900	-	22,29,29	1.57	3 (13%)	27,45,45	2.88	3 (11%)
2	ADP	C	807	-	22,29,29	1.45	2 (9%)	27,45,45	3.16	5 (18%)
2	ADP	C	900	-	22,29,29	1.78	4 (18%)	27,45,45	3.15	4 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	807	-	-	0/12/32/32	0/3/3/3
2	ADP	A	900	-	-	0/12/32/32	0/3/3/3
2	ADP	B	807	-	-	0/12/32/32	0/3/3/3
2	ADP	B	900	-	-	0/12/32/32	0/3/3/3
2	ADP	C	807	-	-	0/12/32/32	0/3/3/3
2	ADP	C	900	-	-	0/12/32/32	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	807	ADP	C5-N7	-3.13	1.28	1.39
2	C	900	ADP	C5-N7	-2.89	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	ADP	C5-N7	-2.62	1.30	1.39
2	A	807	ADP	C5-N7	-2.55	1.30	1.39
2	B	900	ADP	C5-N7	-2.52	1.30	1.39
2	B	807	ADP	C5-N7	-2.46	1.31	1.39
2	C	807	ADP	PB-O1B	-2.28	1.43	1.51
2	B	807	ADP	PA-O2A	-2.04	1.46	1.54
2	A	807	ADP	PA-O2A	-2.01	1.46	1.54
2	B	807	ADP	C4-N3	2.11	1.38	1.35
2	C	900	ADP	PB-O2B	2.14	1.62	1.54
2	A	807	ADP	C2-N1	2.18	1.38	1.33
2	A	807	ADP	PB-O2B	2.22	1.62	1.54
2	A	900	ADP	C5'-C4'	2.27	1.59	1.51
2	A	807	ADP	C4-N3	2.39	1.39	1.35
2	C	900	ADP	C2-N3	2.71	1.37	1.32
2	B	900	ADP	C2-N3	2.71	1.37	1.32
2	A	900	ADP	PB-O2B	2.74	1.64	1.54
2	A	807	ADP	C2-N3	3.31	1.38	1.32
2	A	900	ADP	C2-N3	3.40	1.38	1.32
2	B	807	ADP	C2-N3	3.68	1.38	1.32
2	A	807	ADP	O4'-C1'	3.87	1.46	1.41
2	B	900	ADP	O4'-C1'	3.93	1.46	1.41
2	B	807	ADP	O4'-C1'	3.95	1.46	1.41
2	C	900	ADP	O4'-C1'	4.86	1.47	1.41
2	A	900	ADP	O4'-C1'	4.97	1.47	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	807	ADP	N3-C2-N1	-15.67	116.89	128.89
2	C	900	ADP	N3-C2-N1	-15.24	117.22	128.89
2	A	900	ADP	N3-C2-N1	-15.08	117.35	128.89
2	B	807	ADP	N3-C2-N1	-14.95	117.45	128.89
2	C	807	ADP	N3-C2-N1	-14.94	117.45	128.89
2	B	900	ADP	N3-C2-N1	-14.02	118.16	128.89
2	A	807	ADP	O5'-C5'-C4'	-2.92	98.36	109.12
2	B	807	ADP	O5'-C5'-C4'	-2.49	99.94	109.12
2	B	900	ADP	C4-C5-N7	-2.40	107.27	109.48
2	B	807	ADP	O3A-PA-O5'	2.01	108.27	102.94
2	C	807	ADP	C2-N1-C6	2.03	122.39	118.77
2	A	807	ADP	O3A-PA-O5'	2.03	108.33	102.94
2	C	900	ADP	C2-N1-C6	2.06	122.46	118.77
2	B	900	ADP	C2'-C3'-C4'	2.10	106.93	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	807	ADP	C2'-C3'-C4'	2.12	106.96	102.61
2	A	807	ADP	C2-N1-C6	2.18	122.67	118.77
2	B	807	ADP	C2'-C3'-C4'	2.22	107.18	102.61
2	C	900	ADP	O3A-PA-O5'	2.28	108.97	102.94
2	C	900	ADP	C4'-O4'-C1'	2.65	112.64	109.72
2	C	807	ADP	C2'-C3'-C4'	2.90	108.58	102.61
2	C	807	ADP	O3A-PA-O5'	2.92	110.68	102.94
2	A	807	ADP	C4'-O4'-C1'	3.26	113.31	109.72
2	C	807	ADP	C4'-O4'-C1'	3.39	113.44	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	807	ADP	4	0
2	A	900	ADP	2	0
2	B	807	ADP	3	0
2	B	900	ADP	1	0
2	C	807	ADP	1	0
2	C	900	ADP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	723/806 (89%)	-0.02	26 (3%)	46 36	40, 202, 284, 353	0
1	B	723/806 (89%)	-0.07	18 (2%)	61 50	39, 200, 282, 352	0
1	C	723/806 (89%)	-0.06	20 (2%)	56 46	38, 202, 283, 352	0
All	All	2169/2418 (89%)	-0.05	64 (2%)	54 42	38, 201, 283, 353	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	435	GLU	5.2
1	A	589	ASN	4.8
1	B	589	ASN	4.5
1	B	590	ILE	3.9
1	A	73	SER	3.8
1	B	79	ASP	3.7
1	A	74	ASP	3.5
1	A	588	GLY	3.5
1	C	446	ALA	3.5
1	A	446	ALA	3.4
1	C	590	ILE	3.3
1	A	590	ILE	3.2
1	A	447	VAL	3.1
1	C	141	GLU	3.1
1	B	706	GLU	3.0
1	A	113	ARG	2.9
1	C	81	LYS	2.9
1	A	109	LYS	2.9
1	B	74	ASP	2.9
1	C	588	GLY	2.7
1	C	196	GLU	2.7
1	C	589	ASN	2.7
1	A	43	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	588	GLY	2.7
1	C	757	MET	2.7
1	B	702	SER	2.7
1	B	42	SER	2.6
1	A	426	LYS	2.6
1	B	735	HIS	2.6
1	C	314	GLU	2.6
1	B	109	LYS	2.6
1	A	763	GLN	2.6
1	C	79	ASP	2.5
1	C	706	GLU	2.5
1	A	191	ARG	2.5
1	C	75	ASP	2.5
1	A	107	ASP	2.4
1	A	25	ARG	2.4
1	C	436	THR	2.4
1	A	595	GLY	2.4
1	A	75	ASP	2.3
1	C	190	LYS	2.3
1	A	108	VAL	2.3
1	A	340	HIS	2.3
1	B	188	PRO	2.3
1	C	731	ILE	2.3
1	A	76	THR	2.2
1	A	190	LYS	2.2
1	B	110	TYR	2.2
1	A	389	LYS	2.2
1	C	162	GLU	2.2
1	B	707	ILE	2.1
1	A	81	LYS	2.1
1	A	591	GLY	2.1
1	B	55	ASP	2.1
1	A	79	ASP	2.1
1	B	338	ARG	2.1
1	A	23	PRO	2.1
1	C	340	HIS	2.1
1	B	37	SER	2.1
1	C	41	LEU	2.1
1	B	73	SER	2.0
1	B	43	GLN	2.0
1	C	195	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ADP	A	900	27/27	0.84	0.32	0.83	122,174,209,218	0
2	ADP	C	807	27/27	0.89	0.31	0.52	144,177,268,273	0
2	ADP	B	900	27/27	0.84	0.29	0.21	106,157,202,277	0
2	ADP	C	900	27/27	0.82	0.32	0.17	118,157,187,206	0
2	ADP	B	807	27/27	0.88	0.26	0.03	139,163,218,268	0
2	ADP	A	807	27/27	0.91	0.26	-0.24	133,149,222,335	0

6.5 Other polymers [i](#)

There are no such residues in this entry.