



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:25 AM GMT

PDB ID : 3AOB
Title : Structures of the multidrug exporter AcrB reveal a proximal multisite drug-binding pocket
Authors : Nakashima, R.; Sakurai, K.; Yamaguchi, A.
Deposited on : 2010-09-23
Resolution : 3.35 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

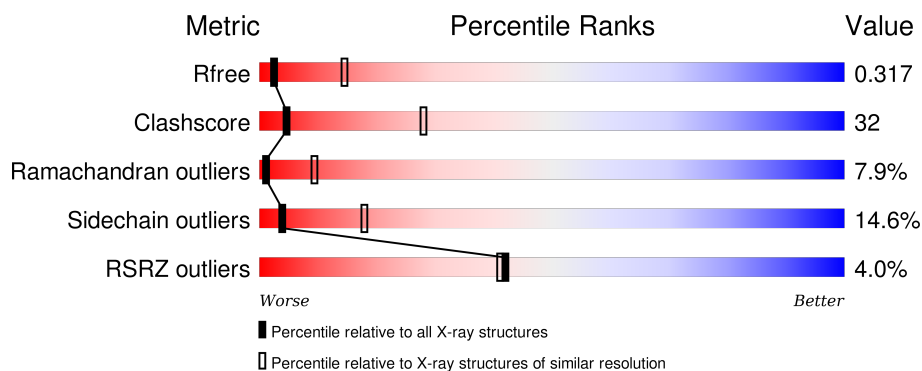
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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	1053	<div> <div>3%</div> <div>44%</div> <div>42%</div> <div>10%</div> <div>..</div> </div>
1	B	1053	<div> <div>5%</div> <div>39%</div> <div>47%</div> <div>11%</div> <div>.</div> </div>
1	C	1053	<div> <div>4%</div> <div>42%</div> <div>43%</div> <div>11%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	RFP	C	2002	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23385 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.

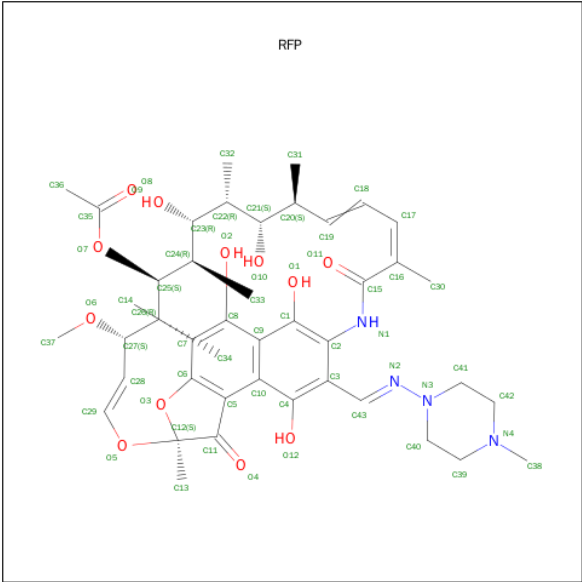
- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	B	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	C	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	EXPRESSION TAG	UNP P31224
A	1051	HIS	-	EXPRESSION TAG	UNP P31224
A	1052	HIS	-	EXPRESSION TAG	UNP P31224
A	1053	HIS	-	EXPRESSION TAG	UNP P31224
B	1050	HIS	-	EXPRESSION TAG	UNP P31224
B	1051	HIS	-	EXPRESSION TAG	UNP P31224
B	1052	HIS	-	EXPRESSION TAG	UNP P31224
B	1053	HIS	-	EXPRESSION TAG	UNP P31224
C	1050	HIS	-	EXPRESSION TAG	UNP P31224
C	1051	HIS	-	EXPRESSION TAG	UNP P31224
C	1052	HIS	-	EXPRESSION TAG	UNP P31224
C	1053	HIS	-	EXPRESSION TAG	UNP P31224

- Molecule 2 is RIFAMPICIN (three-letter code: RFP) (formula: C₄₃H₅₈N₄O₁₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			59	43	4	12		

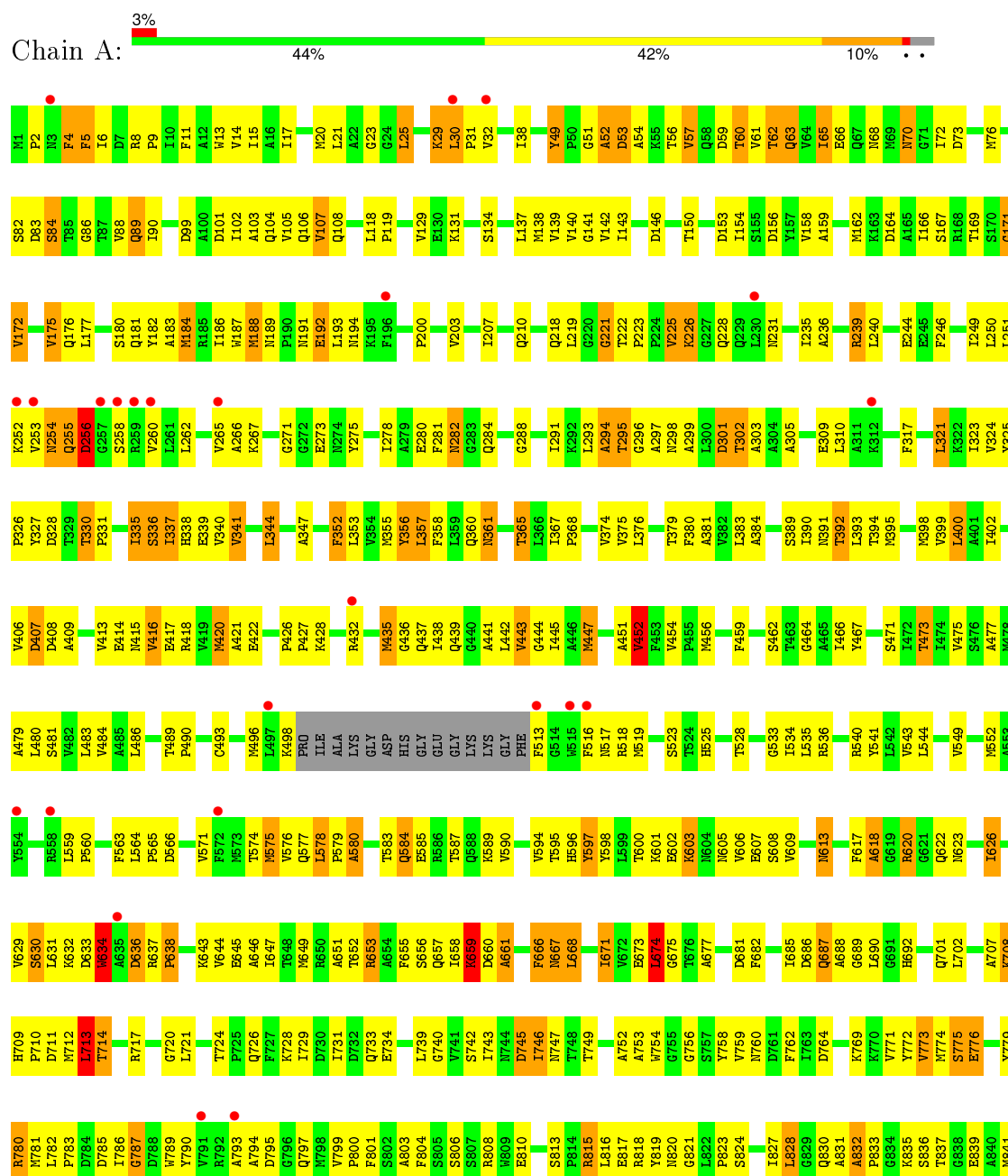
- Molecule 3 is water.

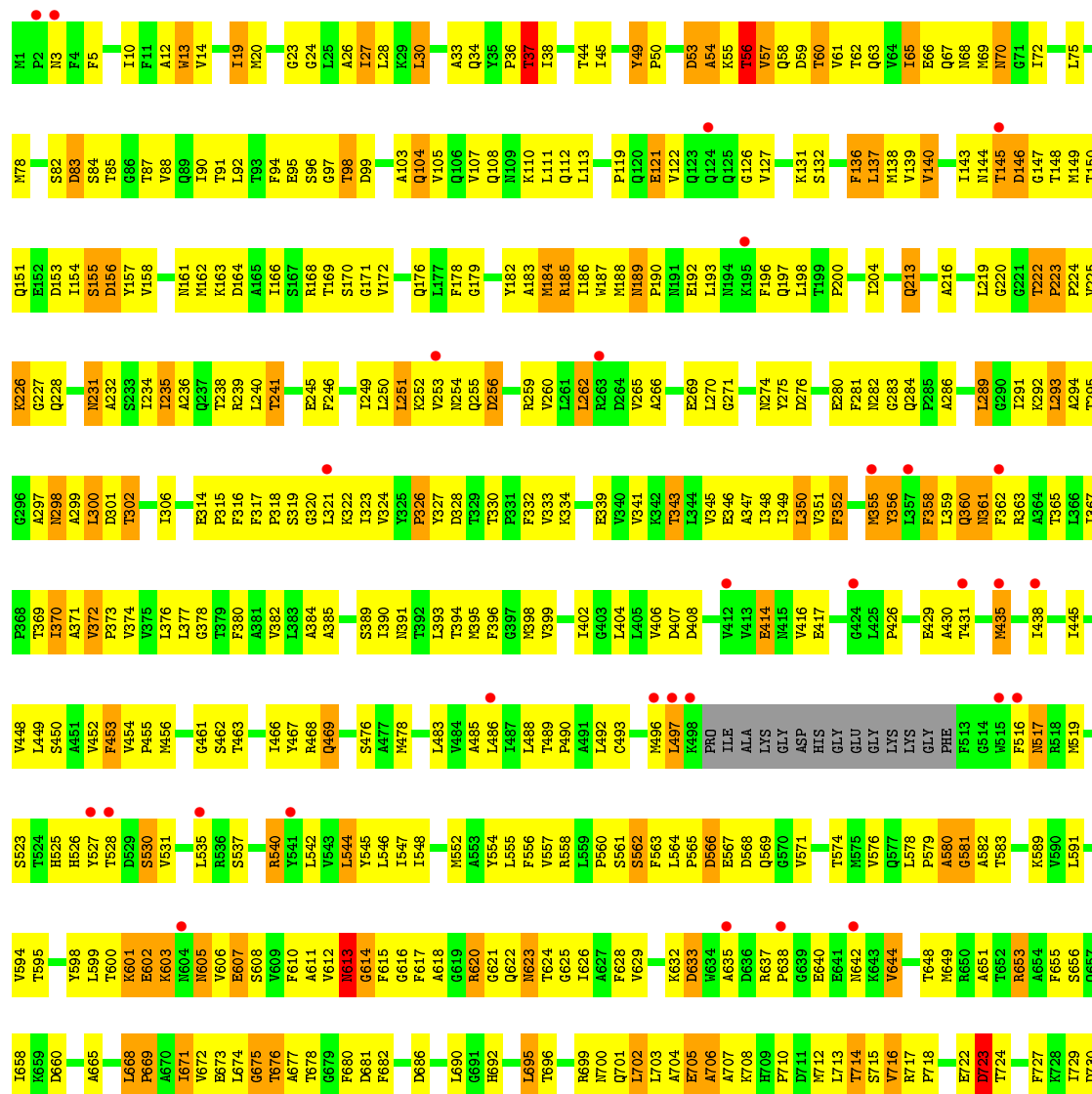
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	2	Total	O	0	0
			2	2		
3	C	1	Total	O	0	0
			1	1		

3 Residue-property plots

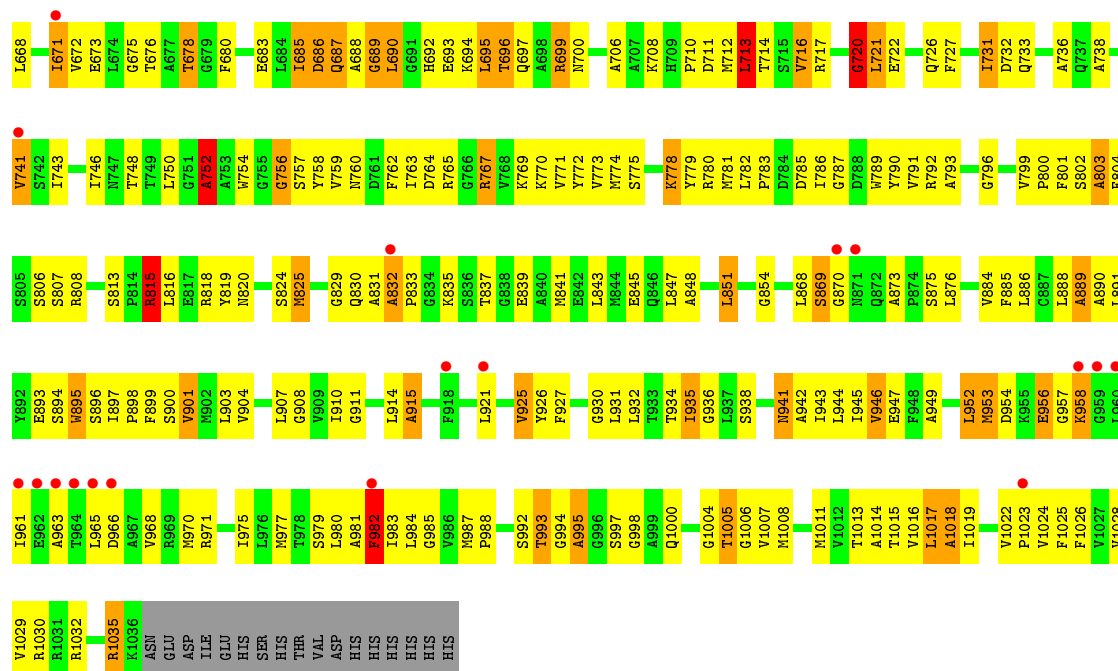
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Acriflavine resistance protein B









4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.90Å 134.31Å 161.77Å 90.00° 98.10° 90.00°	Depositor
Resolution (Å)	48.91 – 3.35 48.91 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.91-3.35) 97.7 (48.91-3.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.64 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.261 , 0.326 0.256 , 0.317	Depositor DCC
R_{free} test set	3350 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 71.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 66713 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23385	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: RFP

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	0.62	0/7920	0.75	2/10756 (0.0%)
1	B	0.58	0/7920	0.76	4/10756 (0.0%)
1	C	0.62	0/7920	0.76	5/10756 (0.0%)
All	All	0.61	0/23760	0.76	11/32268 (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	C	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	356	TYR	N-CA-CB	-12.26	88.53	110.60
1	B	355	MET	CB-CA-C	10.91	132.23	110.40
1	C	321	LEU	CA-CB-CG	8.34	134.48	115.30
1	B	960	LEU	CA-CB-CG	6.20	129.56	115.30
1	B	352	PHE	CB-CA-C	6.12	122.65	110.40
1	C	425	LEU	CA-CB-CG	5.95	128.98	115.30
1	C	752	ALA	N-CA-C	-5.36	96.53	111.00
1	C	720	GLY	N-CA-C	5.34	126.45	113.10
1	A	828	LEU	CA-CB-CG	5.27	127.42	115.30
1	C	578	LEU	CA-CB-CG	5.21	127.27	115.30
1	A	674	LEU	CA-CB-CG	5.19	127.24	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	221	GLY	Peptide
1	C	222	THR	Peptide

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	7774	0	7931	460	0
1	B	7774	0	7931	536	0
1	C	7774	0	7931	577	0
2	C	59	0	57	10	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	23385	0	23850	1518	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 32.

All (1518) 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:447:MET:HB3	1:A:887:CYS:SG	1.82	1.20
1:C:222:THR:HG23	1:C:223:PRO:CD	1.73	1.17
1:C:815:ARG:HH11	1:C:815:ARG:HG2	1.09	1.17
1:C:146:ASP:HB3	1:C:148:THR:HG23	1.31	1.12
1:A:379:THR:HG21	1:A:477:ALA:HA	1.27	1.12
1:B:200:PRO:HD2	1:B:749:THR:HG22	1.32	1.11
1:C:222:THR:HG23	1:C:223:PRO:HD2	1.07	1.06
1:A:275:TYR:HB3	1:C:223:PRO:HD3	1.38	1.06
1:B:456:MET:HG3	1:B:467:TYR:HB3	1.29	1.05
1:B:367:ILE:HG13	1:B:492:LEU:HB3	1.37	1.03
1:C:564:LEU:HD13	1:C:671:ILE:HD12	1.38	1.01
1:B:219:LEU:HG	1:B:234:ILE:HD11	1.40	0.99
1:C:222:THR:CG2	1:C:223:PRO:HD2	1.93	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:860:THR:HG22	1:B:861:GLY:H	1.24	0.99
1:A:400:LEU:HD11	1:A:930:GLY:HA2	1.41	0.98
1:A:414:GLU:HG2	1:A:974:PRO:HG3	1.47	0.97
1:C:1:MET:HB2	1:C:2:PRO:HD2	1.44	0.97
1:B:95:GLU:O	1:B:98:THR:HG22	1.64	0.96
1:B:222:THR:HB	1:B:223:PRO:CD	1.95	0.95
1:A:139:VAL:HG12	1:A:327:TYR:HB3	1.48	0.95
1:A:167:SER:OG	1:A:175:VAL:HG21	1.64	0.95
1:A:674:LEU:HD22	1:A:675:GLY:H	1.33	0.93
1:C:367:ILE:HD11	1:C:492:LEU:HB3	1.50	0.93
1:C:911:GLY:HA3	1:C:1013:THR:HG21	1.47	0.93
1:C:832:ALA:HB3	1:C:833:PRO:HD3	1.49	0.92
1:C:267:LYS:HE3	1:C:269:GLU:HG2	1.52	0.92
1:A:713:LEU:HD23	1:A:833:PRO:HD3	1.50	0.92
1:B:255:GLN:HG3	1:B:256:ASP:OD1	1.70	0.91
1:B:65:ILE:HG22	1:B:69:MET:HE1	1.48	0.91
1:C:372:VAL:HG12	1:C:373:PRO:HD3	1.50	0.91
1:A:221:GLY:HA2	1:B:622:GLN:NE2	1.86	0.91
1:A:383:LEU:HD21	1:A:473:THR:HG23	1.53	0.90
1:B:136:PHE:HE1	1:B:617:PHE:CZ	1.90	0.90
1:A:407:ASP:OD2	1:A:978:THR:HG21	1.71	0.90
1:C:146:ASP:CB	1:C:148:THR:HG23	2.01	0.90
1:B:222:THR:HB	1:B:223:PRO:HD3	1.53	0.90
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.55	0.89
1:A:221:GLY:HA2	1:B:622:GLN:HE22	1.37	0.89
1:A:901:VAL:O	1:A:904:VAL:HG23	1.74	0.88
1:A:993:THR:HB	1:A:997:SER:HB3	1.54	0.88
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.54	0.88
1:B:355:MET:O	1:B:359:LEU:CB	2.22	0.88
1:C:55:LYS:HE2	1:C:59:ASP:OD1	1.74	0.88
1:B:185:ARG:HH11	1:B:185:ARG:HG3	1.36	0.88
1:A:275:TYR:CB	1:C:223:PRO:HD3	2.02	0.88
1:B:463:THR:HG21	1:B:869:SER:HB2	1.56	0.87
1:B:867:ARG:HG2	1:B:868:LEU:HD22	1.57	0.87
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.54	0.87
1:C:713:LEU:HD23	1:C:831:ALA:HA	1.57	0.86
1:B:876:LEU:O	1:B:880:SER:HB2	1.74	0.86
1:C:815:ARG:NH1	1:C:815:ARG:HG2	1.90	0.86
1:C:146:ASP:HB3	1:C:148:THR:CG2	2.05	0.85
1:B:139:VAL:HG12	1:B:139:VAL:O	1.74	0.85
1:C:345:VAL:O	1:C:348:ILE:HG22	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:PHE:O	1:C:249:ILE:HG13	1.76	0.84
1:C:131:LYS:HB2	1:C:295:THR:HG21	1.59	0.84
1:C:911:GLY:HA3	1:C:1013:THR:CG2	2.07	0.84
1:C:968:VAL:HG11	1:C:1023:PRO:HG3	1.57	0.84
1:C:53:ASP:O	1:C:84:SER:HA	1.75	0.84
1:C:953:MET:SD	1:C:963:ALA:HB2	2.18	0.84
1:B:918:PHE:HD1	1:B:919:ARG:HD3	1.41	0.84
1:B:200:PRO:HD2	1:B:749:THR:CG2	2.08	0.84
1:C:190:PRO:HG3	1:C:789:TRP:CZ2	2.13	0.84
1:B:171:GLY:HA3	1:B:302:THR:HB	1.59	0.84
1:B:729:ILE:HG13	1:B:730:ASP:H	1.44	0.83
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.58	0.83
1:B:274:ASN:HD22	1:B:276:ASP:HB2	1.43	0.83
1:C:131:LYS:HB2	1:C:295:THR:CG2	2.09	0.82
1:B:835:LYS:HB2	1:B:839:GLU:OE2	1.77	0.82
1:B:226:LYS:HA	1:B:226:LYS:NZ	1.95	0.82
1:B:552:MET:SD	1:B:909:VAL:HG23	2.20	0.81
1:C:375:VAL:HG11	1:C:405:LEU:HD22	1.61	0.81
1:B:892:TYR:HB2	1:B:897:ILE:HD11	1.61	0.81
1:A:961:ILE:HD11	1:A:1031:ARG:NH1	1.95	0.81
1:B:355:MET:O	1:B:359:LEU:HB2	1.80	0.81
1:C:889:ALA:HB2	1:C:898:PRO:HG3	1.61	0.81
1:A:389:SER:O	1:A:394:THR:HG21	1.80	0.81
1:A:60:THR:HG23	1:A:119:PRO:HG3	1.62	0.81
1:A:993:THR:HG21	1:A:1000:GLN:OE1	1.80	0.81
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.61	0.81
1:C:568:ASP:OD2	1:C:644:VAL:HG23	1.80	0.81
1:A:781:MET:HE2	1:C:225:VAL:H	1.46	0.81
1:A:728:LYS:HD3	1:C:235:ILE:HG22	1.62	0.81
1:A:180:SER:O	1:A:181:GLN:HB3	1.81	0.81
1:B:298:ASN:HB2	1:B:301:ASP:HB2	1.62	0.80
1:B:94:PHE:HB3	1:B:98:THR:HG21	1.62	0.80
1:B:226:LYS:HZ3	1:B:226:LYS:HA	1.46	0.80
1:A:60:THR:CG2	1:A:119:PRO:HG3	2.10	0.80
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.63	0.80
1:C:355:MET:CE	1:C:355:MET:HA	2.10	0.80
1:C:190:PRO:HD2	1:C:779:TYR:CD1	2.17	0.80
1:A:713:LEU:HD12	1:A:830:GLN:HB2	1.64	0.79
1:C:31:PRO:O	1:C:389:SER:HB2	1.81	0.79
1:C:459:PHE:N	1:C:459:PHE:HD1	1.81	0.79
1:B:831:ALA:HB2	1:B:840:ALA:HB2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ILE:HD11	1:B:110:LYS:HG3	1.65	0.79
1:A:379:THR:CG2	1:A:477:ALA:HA	2.09	0.79
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.63	0.79
1:A:108:GLN:NE2	1:B:112:GLN:HB3	1.97	0.79
1:A:267:LYS:HE2	1:A:776:GLU:OE2	1.83	0.79
1:B:668:LEU:HB3	1:B:676:THR:HG23	1.65	0.78
1:A:375:VAL:O	1:A:379:THR:HG23	1.83	0.78
1:C:355:MET:SD	1:C:410:ILE:HD11	2.23	0.78
1:B:250:LEU:HD12	1:B:259:ARG:HH21	1.48	0.78
1:B:23:GLY:HA3	1:B:377:LEU:O	1.83	0.78
1:B:1026:PHE:O	1:B:1030:ARG:HB2	1.83	0.78
1:B:905:VAL:HG13	1:B:906:PRO:HD3	1.63	0.77
1:A:437:GLN:HB3	1:A:948:PHE:HE2	1.50	0.77
1:C:246:PHE:O	1:C:249:ILE:CG1	2.32	0.77
1:B:919:ARG:HG3	1:B:1005:THR:HG21	1.67	0.77
1:A:720:GLY:O	1:A:721:LEU:HD23	1.85	0.77
1:B:910:ILE:O	1:B:914:LEU:HB2	1.84	0.76
1:B:416:VAL:CG2	1:B:431:THR:HA	2.15	0.76
1:B:252:LYS:HB3	1:B:260:VAL:CG1	2.15	0.76
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.66	0.76
1:C:767:ARG:HH11	1:C:767:ARG:HG3	1.49	0.76
1:C:186:ILE:HG12	1:C:262:LEU:HD21	1.68	0.76
1:B:394:THR:HG23	1:B:469:GLN:HG3	1.68	0.76
1:A:418:ARG:HH12	1:A:973:ARG:HB3	1.49	0.76
1:A:56:THR:O	1:A:60:THR:HB	1.85	0.76
1:B:780:ARG:O	1:B:781:MET:HE2	1.86	0.76
1:A:961:ILE:HD11	1:A:1031:ARG:HH12	1.51	0.76
1:B:327:TYR:HB2	1:B:628:PHE:HB3	1.68	0.76
1:B:360:GLN:O	1:B:361:ASN:HB3	1.86	0.76
1:A:52:ALA:HB3	1:A:86:GLY:HA2	1.68	0.75
1:A:435:MET:SD	1:A:490:PRO:HB3	2.26	0.75
1:B:1021:PHE:O	1:B:1024:VAL:HB	1.86	0.75
1:A:733:GLN:HE21	1:C:210:GLN:HG2	1.50	0.75
1:A:13:TRP:O	1:A:17:ILE:HG13	1.86	0.75
1:C:712:MET:O	1:C:714:THR:HG23	1.85	0.75
1:C:34:GLN:HE21	1:C:34:GLN:H	1.35	0.74
1:B:574:THR:HG23	1:B:665:ALA:HB2	1.67	0.74
1:C:459:PHE:CD1	1:C:459:PHE:N	2.54	0.74
1:B:324:VAL:HG23	1:B:326:PRO:HD3	1.68	0.74
1:B:722:GLU:O	1:B:723:ASP:O	2.04	0.74
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ILE:HD12	1:C:893:GLU:O	1.86	0.74
1:C:767:ARG:HH11	1:C:767:ARG:CG	1.99	0.74
1:C:242:SER:HB3	1:C:245:GLU:HG3	1.70	0.74
1:B:225:VAL:H	1:C:781:MET:HE3	1.53	0.74
1:B:314:GLU:HG2	1:B:317:PHE:CE2	2.23	0.74
1:A:464:GLY:HA2	1:A:467:TYR:HB2	1.69	0.74
1:B:241:THR:HG22	1:B:763:ILE:O	1.88	0.74
1:C:202:ASP:OD2	1:C:792:ARG:NH2	2.21	0.74
1:B:699:ARG:HB3	1:B:699:ARG:HH11	1.52	0.74
1:A:73:ASP:H	1:A:106:GLN:HE22	1.36	0.74
1:A:14:VAL:HG21	1:B:890:ALA:HB2	1.70	0.73
1:A:574:THR:HG21	1:A:594:VAL:HG11	1.69	0.73
1:B:370:ILE:O	1:B:370:ILE:HG22	1.87	0.73
1:C:414:GLU:HA	1:C:417:GLU:HG2	1.67	0.73
1:C:575:MET:SD	1:C:575:MET:N	2.61	0.73
1:B:185:ARG:CG	1:B:185:ARG:HH11	2.01	0.73
1:B:730:ASP:HB3	1:B:806:SER:HB3	1.71	0.73
1:B:26:ALA:O	1:B:30:LEU:HB2	1.88	0.73
1:B:355:MET:O	1:B:359:LEU:HB3	1.88	0.73
1:C:38:ILE:HG21	1:C:466:ILE:HD11	1.71	0.73
1:C:345:VAL:O	1:C:348:ILE:CG2	2.37	0.73
1:A:317:PHE:HB3	1:A:321:LEU:CD2	2.17	0.73
1:C:686:ASP:OD1	1:C:690:LEU:HB2	1.89	0.73
1:C:425:LEU:HB2	1:C:426:PRO:HD3	1.70	0.73
1:B:188:MET:HB2	1:B:775:SER:HA	1.70	0.73
1:A:2:PRO:O	1:A:6:ILE:HG23	1.89	0.72
1:A:945:ILE:HG13	1:A:971:ARG:HG2	1.71	0.72
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.24	0.72
1:A:447:MET:CB	1:A:887:CYS:SG	2.72	0.72
1:A:101:ASP:O	1:A:105:VAL:HG23	1.88	0.72
1:A:393:LEU:CD1	1:A:466:ILE:HG23	2.19	0.72
1:A:471:SER:O	1:A:475:VAL:HG12	1.87	0.72
1:B:274:ASN:ND2	1:B:276:ASP:HB2	2.03	0.72
1:C:945:ILE:C	1:C:947:GLU:H	1.93	0.72
1:C:983:ILE:HG23	1:C:1008:MET:HG3	1.69	0.72
1:C:420:MET:HB2	1:C:498:LYS:HE2	1.71	0.72
1:B:452:VAL:O	1:B:453:PHE:HB2	1.89	0.72
1:A:923:ASN:HD22	1:A:923:ASN:C	1.92	0.72
1:A:4:PHE:O	1:A:8:ARG:NH2	2.23	0.72
1:C:463:THR:HG23	1:C:563:PHE:HE1	1.54	0.72
1:B:416:VAL:HG22	1:B:431:THR:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:VAL:O	1:B:402:ILE:HG22	1.89	0.71
1:C:643:LYS:O	1:C:647:ILE:HG12	1.88	0.71
1:C:832:ALA:CB	1:C:833:PRO:HD3	2.21	0.71
1:B:197:GLN:O	1:B:792:ARG:NH2	2.22	0.71
1:A:375:VAL:HG21	1:A:481:SER:HA	1.73	0.71
1:C:456:MET:HA	1:C:459:PHE:CE1	2.25	0.71
1:C:456:MET:HA	1:C:459:PHE:HE1	1.55	0.71
1:C:694:LYS:O	1:C:697:GLN:HB2	1.91	0.71
1:C:5:PHE:HE2	1:C:11:PHE:CD2	2.08	0.71
1:C:350:LEU:HD12	1:C:985:GLY:HA2	1.73	0.71
1:C:815:ARG:HH11	1:C:815:ARG:CG	1.94	0.71
1:A:139:VAL:HG12	1:A:327:TYR:CB	2.21	0.71
1:B:904:VAL:HG21	1:B:942:ALA:HB2	1.71	0.71
1:C:351:VAL:HG13	1:C:981:ALA:HB1	1.73	0.71
1:B:136:PHE:CE1	1:B:617:PHE:CZ	2.77	0.71
1:B:328:ASP:OD2	1:B:330:THR:HG22	1.90	0.71
1:B:171:GLY:HA3	1:B:302:THR:CB	2.20	0.70
1:A:707:ALA:O	1:A:710:PRO:HD3	1.91	0.70
1:B:36:PRO:O	1:B:38:ILE:HG12	1.90	0.70
1:C:534:ILE:O	1:C:539:GLY:HA3	1.90	0.70
1:A:383:LEU:HD21	1:A:473:THR:CG2	2.20	0.70
1:B:911:GLY:HA3	1:B:1013:THR:HG21	1.74	0.70
1:C:601:LYS:O	1:C:602:GLU:HG2	1.91	0.70
1:C:713:LEU:O	1:C:713:LEU:HD22	1.92	0.70
1:A:337:ILE:HD11	1:A:395:MET:HG3	1.73	0.70
1:C:713:LEU:HD23	1:C:830:GLN:O	1.91	0.70
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.26	0.70
1:B:911:GLY:CA	1:B:1013:THR:HG21	2.22	0.70
1:C:1:MET:HB2	1:C:2:PRO:CD	2.22	0.70
1:C:952:LEU:HA	1:C:956:GLU:HB3	1.73	0.70
1:B:445:ILE:HG23	1:B:940:LYS:HG3	1.74	0.69
1:C:911:GLY:CA	1:C:1013:THR:HG21	2.21	0.69
1:C:265:VAL:HG23	1:C:265:VAL:O	1.92	0.69
1:A:418:ARG:NH1	1:A:973:ARG:HB3	2.06	0.69
1:A:360:GLN:HB2	1:A:513:PHE:HB2	1.72	0.69
1:C:65:ILE:HD13	1:C:111:LEU:HD21	1.73	0.69
1:B:851:LEU:N	1:B:852:PRO:HD3	2.08	0.69
1:B:291:ILE:HG21	1:B:306:ILE:CD1	2.23	0.69
2:C:2002:RFP:H323	2:C:2002:RFP:H311	1.75	0.69
1:A:904:VAL:HG21	1:A:942:ALA:CB	2.23	0.69
1:B:68:ASN:O	1:B:110:LYS:HE3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:722:GLU:HA	1:C:722:GLU:OE1	1.91	0.69
1:C:380:PHE:CE1	1:C:398:MET:SD	2.86	0.69
1:A:888:LEU:HB3	1:A:898:PRO:HB3	1.75	0.69
1:C:155:SER:OG	1:C:179:GLY:HA3	1.93	0.69
1:B:860:THR:HG22	1:B:861:GLY:N	2.03	0.68
1:A:753:ALA:O	1:A:775:SER:HB3	1.94	0.68
1:C:756:GLY:CA	1:C:774:MET:HG3	2.23	0.68
1:A:658:ILE:HG22	1:A:659:LYS:HD2	1.74	0.68
1:C:762:PHE:CE2	1:C:764:ASP:HB2	2.29	0.68
1:C:34:GLN:HG3	1:C:333:VAL:HG11	1.74	0.68
1:B:680:PHE:HD1	1:B:859:TRP:HZ3	1.41	0.68
1:B:699:ARG:HB3	1:B:699:ARG:NH1	2.09	0.68
1:C:523:SER:HA	1:C:526:HIS:HB2	1.75	0.68
1:A:579:PRO:HG3	1:A:660:ASP:HB2	1.75	0.68
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.28	0.68
1:B:136:PHE:CE1	1:B:617:PHE:HZ	2.12	0.68
1:B:372:VAL:HB	1:B:402:ILE:HD11	1.76	0.68
1:A:51:GLY:O	1:C:215:ALA:HB1	1.93	0.68
1:C:459:PHE:H	1:C:459:PHE:HD1	1.42	0.68
1:C:244:GLU:HA	1:C:263:ARG:NH2	2.09	0.68
1:B:1024:VAL:O	1:B:1028:VAL:HG23	1.94	0.68
1:B:222:THR:CB	1:B:223:PRO:HD3	2.23	0.67
1:B:84:SER:HB3	1:B:814:PRO:HA	1.74	0.67
1:B:314:GLU:HG2	1:B:317:PHE:HE2	1.56	0.67
1:A:924:ASP:O	1:A:928:GLN:HG3	1.94	0.67
1:C:476:SER:O	1:C:477:ALA:HB3	1.94	0.67
1:B:252:LYS:HB3	1:B:260:VAL:HG12	1.76	0.67
1:B:343:THR:HG21	1:B:1000:GLN:OE1	1.93	0.67
1:A:418:ARG:HH12	1:A:973:ARG:CB	2.08	0.67
1:B:171:GLY:HA3	1:B:302:THR:CG2	2.24	0.67
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.30	0.67
1:A:1025:PHE:O	1:A:1029:VAL:HG23	1.95	0.67
1:A:613:ASN:C	1:A:613:ASN:HD22	1.98	0.67
1:A:138:MET:HB2	1:A:327:TYR:O	1.95	0.67
1:B:14:VAL:HG21	1:C:890:ALA:HB2	1.77	0.67
1:C:824:SER:OG	1:C:825:MET:N	2.26	0.67
1:B:298:ASN:CB	1:B:301:ASP:HB2	2.25	0.67
1:B:778:LYS:H	1:B:778:LYS:HD3	1.59	0.67
1:C:56:THR:O	1:C:60:THR:HB	1.93	0.67
1:C:210:GLN:HE22	1:C:250:LEU:H	1.42	0.67
1:B:706:ALA:C	1:B:708:LYS:H	1.97	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:GLU:OE2	1:C:995:ALA:HB3	1.95	0.67
1:A:795:ASP:OD1	1:A:797:GLN:HG2	1.95	0.66
1:C:200:PRO:O	1:C:204:ILE:HG12	1.95	0.66
1:A:880:SER:O	1:A:884:VAL:HG23	1.94	0.66
1:A:780:ARG:HG2	1:A:780:ARG:HH11	1.61	0.66
1:C:521:GLU:HA	1:C:524:THR:OG1	1.95	0.66
1:C:355:MET:HB3	1:C:365:THR:HG23	1.77	0.66
1:B:961:ILE:HD11	1:B:1031:ARG:HH12	1.60	0.66
1:A:781:MET:HE2	1:C:225:VAL:N	2.09	0.66
1:C:824:SER:O	1:C:825:MET:HB2	1.95	0.66
1:B:860:THR:CG2	1:B:861:GLY:H	2.05	0.66
1:B:880:SER:O	1:B:884:VAL:HG23	1.96	0.66
1:A:1029:VAL:HG12	1:A:1030:ARG:H	1.60	0.66
1:B:144:ASN:HD21	1:B:148:THR:H	1.44	0.66
1:C:252:LYS:O	1:C:260:VAL:HG12	1.95	0.66
1:B:736:ALA:HB1	1:B:741:VAL:HG12	1.77	0.66
1:B:225:VAL:H	1:C:781:MET:CE	2.08	0.66
1:A:188:MET:HA	1:A:266:ALA:HB2	1.76	0.66
1:C:367:ILE:CD1	1:C:492:LEU:HB3	2.26	0.66
1:B:65:ILE:HG22	1:B:69:MET:CE	2.23	0.66
1:C:39:ALA:CB	1:C:673:GLU:HG2	2.25	0.66
1:A:707:ALA:C	1:A:709:HIS:H	1.97	0.65
1:B:727:PHE:HE1	1:B:786:ILE:HD11	1.61	0.65
1:B:818:ARG:HG3	1:B:818:ARG:HH11	1.60	0.65
1:B:734:GLU:C	1:B:736:ALA:H	1.99	0.65
1:A:445:ILE:HG21	1:A:940:LYS:HD2	1.78	0.65
1:A:782:LEU:O	1:A:785:ASP:HB2	1.97	0.65
1:C:9:PRO:HD2	1:C:10:ILE:HD13	1.78	0.65
1:A:886:LEU:HD21	1:C:17:ILE:HG22	1.77	0.65
1:A:57:VAL:HG13	1:A:88:VAL:HG22	1.77	0.65
1:B:326:PRO:HG3	1:B:610:PHE:CD1	2.32	0.65
1:B:213:GLN:HE21	1:B:239:ARG:HD2	1.60	0.65
1:A:979:SER:O	1:A:983:ILE:HG23	1.97	0.65
1:B:601:LYS:O	1:B:602:GLU:HG2	1.97	0.65
1:A:911:GLY:HA2	1:A:914:LEU:HB2	1.77	0.65
1:C:355:MET:HE3	1:C:355:MET:HA	1.76	0.65
1:B:57:VAL:HG13	1:B:82:SER:OG	1.97	0.65
1:C:518:ARG:HH21	1:C:518:ARG:HA	1.62	0.65
1:A:584:GLN:N	1:A:622:GLN:HB3	2.11	0.64
1:B:103:ALA:O	1:B:107:VAL:HG23	1.97	0.64
1:C:848:ALA:HA	1:C:851:LEU:CD2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:THR:CB	1:B:223:PRO:CD	2.74	0.64
1:A:221:GLY:CA	1:B:622:GLN:HE22	2.10	0.64
1:A:989:LEU:HB3	1:A:993:THR:HG23	1.79	0.64
1:A:335:ILE:HG13	1:A:336:SER:N	2.12	0.64
1:C:448:VAL:HG22	1:C:884:VAL:HG22	1.79	0.64
1:B:613:ASN:O	1:B:615:PHE:N	2.30	0.64
1:C:57:VAL:CG2	1:C:86:GLY:HA2	2.26	0.64
1:B:905:VAL:CG1	1:B:906:PRO:HD3	2.27	0.64
1:B:314:GLU:N	1:B:315:PRO:CD	2.61	0.64
1:B:879:ILE:O	1:B:883:VAL:HG23	1.96	0.64
1:C:956:GLU:CD	1:C:957:GLY:H	2.00	0.64
1:A:330:THR:H	1:A:331:PRO:HD2	1.63	0.64
1:B:231:ASN:ND2	1:B:231:ASN:C	2.51	0.64
1:C:137:LEU:O	1:C:329:THR:HG22	1.98	0.64
1:C:1025:PHE:O	1:C:1029:VAL:HG23	1.97	0.64
1:B:904:VAL:HG13	1:B:907:LEU:HD12	1.80	0.64
1:A:632:LYS:O	1:A:637:ARG:HD3	1.98	0.64
1:A:154:ILE:O	1:A:158:VAL:HG23	1.97	0.64
1:B:527:TYR:HA	1:B:530:SER:HB2	1.80	0.63
1:B:699:ARG:HG2	1:B:700:ASN:H	1.63	0.63
1:A:597:TYR:C	1:A:597:TYR:CD1	2.71	0.63
1:A:317:PHE:HB3	1:A:321:LEU:HD21	1.79	0.63
1:C:1032:ARG:O	1:C:1035:ARG:HG2	1.97	0.63
1:C:144:ASN:ND2	1:C:148:THR:H	1.95	0.63
1:C:911:GLY:HA3	1:C:1013:THR:CB	2.27	0.63
1:A:712:MET:HA	1:A:832:ALA:HB2	1.81	0.63
1:C:188:MET:HE1	1:C:193:LEU:HD11	1.78	0.63
1:B:918:PHE:CD1	1:B:919:ARG:HD3	2.30	0.63
1:B:754:TRP:CZ3	1:B:780:ARG:HA	2.33	0.63
1:A:11:PHE:CD1	1:B:890:ALA:HB1	2.32	0.63
1:B:294:ALA:HB3	1:B:297:ALA:HB2	1.79	0.63
1:C:720:GLY:HA3	2:C:2002:RFP:H17C	1.81	0.63
1:C:925:VAL:O	1:C:927:PHE:N	2.32	0.63
1:B:1025:PHE:O	1:B:1029:VAL:HG12	1.98	0.63
1:C:897:ILE:N	1:C:898:PRO:HD2	2.13	0.63
1:C:646:ALA:HA	1:C:649:MET:HB2	1.81	0.63
1:C:435:MET:HA	1:C:438:ILE:HG22	1.81	0.63
1:C:406:VAL:C	1:C:408:ASP:H	2.02	0.63
1:A:218:GLN:O	1:A:219:LEU:HG	1.98	0.63
1:A:552:MET:HE1	1:A:906:PRO:CA	2.28	0.63
1:B:62:THR:O	1:B:66:GLU:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASN:ND2	1:A:258:SER:OG	2.31	0.62
1:C:265:VAL:O	1:C:266:ALA:HB2	1.99	0.62
1:A:781:MET:HB3	1:C:228:GLN:OE1	1.99	0.62
1:C:394:THR:HG22	1:C:395:MET:HE2	1.80	0.62
1:B:605:ASN:HD22	1:B:605:ASN:H	1.47	0.62
1:C:34:GLN:HG3	1:C:333:VAL:CG1	2.29	0.62
1:C:1035:ARG:HA	1:C:1035:ARG:HE	1.64	0.62
1:C:1030:ARG:HG2	1:C:1030:ARG:HH11	1.65	0.62
1:C:688:ALA:O	1:C:689:GLY:O	2.16	0.62
1:C:23:GLY:HA3	1:C:377:LEU:O	1.99	0.62
1:C:26:ALA:O	1:C:30:LEU:HB2	1.99	0.62
1:A:686:ASP:HB3	1:A:823:PRO:HG2	1.81	0.62
1:B:136:PHE:H	1:B:136:PHE:HD1	1.47	0.62
1:C:901:VAL:O	1:C:904:VAL:HG23	1.98	0.62
1:C:712:MET:SD	1:C:843:LEU:HD22	2.40	0.62
1:C:204:ILE:CD1	1:C:773:VAL:HG21	2.30	0.62
1:B:137:LEU:HD13	1:B:293:LEU:HG	1.81	0.62
1:B:249:ILE:HB	1:B:262:LEU:HB2	1.82	0.62
1:B:456:MET:HG3	1:B:467:TYR:CB	2.19	0.62
1:A:391:ASN:H	1:A:394:THR:HG22	1.64	0.62
1:B:155:SER:OG	1:B:179:GLY:HA3	1.99	0.62
1:A:883:VAL:O	1:A:887:CYS:HB2	1.99	0.61
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.80	0.61
1:C:756:GLY:HA2	1:C:774:MET:HG3	1.81	0.61
1:B:729:ILE:HG13	1:B:730:ASP:N	2.16	0.61
1:B:778:LYS:C	1:B:780:ARG:H	2.04	0.61
1:A:713:LEU:HD22	1:A:714:THR:H	1.64	0.61
1:B:921:LEU:HD22	1:B:1005:THR:HB	1.82	0.61
1:C:327:TYR:HB2	1:C:628:PHE:HB3	1.82	0.61
1:A:1013:THR:O	1:A:1017:LEU:HB3	1.99	0.61
1:C:692:HIS:CE1	1:C:721:LEU:HD21	2.34	0.61
1:A:83:ASP:HB3	1:A:815:ARG:HG3	1.82	0.61
1:A:643:LYS:O	1:A:647:ILE:HG13	2.00	0.61
1:A:667:ASN:HD22	1:A:668:LEU:N	1.99	0.61
1:B:906:PRO:HA	1:B:909:VAL:HG22	1.83	0.61
1:B:251:LEU:HD12	1:B:262:LEU:HA	1.82	0.61
1:C:39:ALA:HB1	1:C:673:GLU:HG2	1.82	0.61
1:B:790:TYR:CD1	1:B:800:PRO:HA	2.36	0.61
1:B:925:VAL:HA	1:B:928:GLN:OE1	2.00	0.61
1:C:1004:GLY:O	1:C:1006:GLY:N	2.33	0.61
1:A:620:ARG:H	1:A:620:ARG:HD2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:736:ALA:HB1	1:C:741:VAL:HG23	1.83	0.61
1:B:651:ALA:HB1	1:B:655:PHE:HE2	1.65	0.61
1:C:309:GLU:HG3	1:C:313:MET:CE	2.31	0.61
1:B:300:LEU:HD11	1:B:334:LYS:HE2	1.82	0.61
1:C:1:MET:HG3	1:C:3:ASN:H	1.66	0.60
1:A:317:PHE:HB3	1:A:321:LEU:HD23	1.82	0.60
1:C:423:GLU:HB3	1:C:426:PRO:HD2	1.82	0.60
1:B:291:ILE:HG21	1:B:306:ILE:HD11	1.80	0.60
1:B:736:ALA:HB2	1:B:804:PHE:CB	2.31	0.60
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.83	0.60
1:C:144:ASN:ND2	1:C:148:THR:N	2.48	0.60
1:A:280:GLU:HB2	1:A:284:GLN:O	2.01	0.60
1:C:790:TYR:CE1	1:C:800:PRO:HB3	2.36	0.60
1:C:57:VAL:HG21	1:C:86:GLY:CA	2.29	0.60
1:B:598:TYR:HB3	1:B:606:VAL:HG21	1.83	0.60
1:C:298:ASN:HB3	1:C:301:ASP:HB2	1.83	0.60
1:A:108:GLN:HG2	1:A:129:VAL:HB	1.84	0.60
1:B:911:GLY:HA3	1:B:1013:THR:CG2	2.31	0.60
1:C:99:ASP:OD2	1:C:102:ILE:HG12	2.02	0.60
1:C:176:GLN:HE22	1:C:620:ARG:HH12	1.49	0.60
1:B:591:LEU:O	1:B:595:THR:HG22	2.02	0.60
1:B:616:GLY:HA3	1:B:624:THR:CG2	2.32	0.60
1:A:6:ILE:CG2	1:A:490:PRO:HB2	2.31	0.60
1:B:741:VAL:HG21	1:B:791:VAL:HG23	1.83	0.60
1:B:911:GLY:HA2	1:B:914:LEU:HB3	1.84	0.59
1:A:1018:ALA:O	1:A:1022:VAL:HG22	2.01	0.59
1:B:736:ALA:HB2	1:B:804:PHE:HB3	1.83	0.59
1:C:592:ASN:O	1:C:593:GLU:HB2	2.01	0.59
1:C:415:ASN:CG	1:C:434:SER:HB2	2.23	0.59
1:B:919:ARG:CG	1:B:1005:THR:HG21	2.30	0.59
1:A:443:VAL:HG22	1:A:486:LEU:HD11	1.84	0.59
1:C:365:THR:HG22	1:C:365:THR:O	2.02	0.59
1:C:9:PRO:HB3	1:C:491:ALA:HB1	1.84	0.59
1:A:57:VAL:HG13	1:A:88:VAL:CG2	2.32	0.59
1:B:921:LEU:CD2	1:B:1005:THR:HB	2.32	0.59
1:C:835:LYS:HB3	1:C:839:GLU:OE2	2.01	0.59
1:B:850:LYS:C	1:B:852:PRO:HD3	2.23	0.59
1:B:213:GLN:HB2	1:B:239:ARG:HD2	1.84	0.59
1:C:326:PRO:HG3	1:C:610:PHE:CD1	2.38	0.59
1:A:671:ILE:HB	1:A:674:LEU:HB3	1.84	0.59
1:B:144:ASN:HD21	1:B:148:THR:N	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:THR:HG23	1:A:601:LYS:N	2.18	0.59
1:C:367:ILE:N	1:C:368:PRO:CD	2.66	0.59
1:A:713:LEU:HB2	1:A:832:ALA:HA	1.83	0.59
1:C:713:LEU:HD12	1:C:835:LYS:H	1.66	0.59
1:B:276:ASP:O	1:B:614:GLY:HA3	2.03	0.59
1:C:547:ILE:HA	1:C:550:VAL:HG12	1.85	0.59
1:B:362:PHE:HA	1:B:365:THR:HG22	1.84	0.59
1:C:375:VAL:HG13	1:C:480:LEU:HB2	1.82	0.59
1:C:379:THR:HG21	1:C:398:MET:HE3	1.84	0.59
1:B:552:MET:SD	1:B:909:VAL:CG2	2.88	0.58
1:C:220:GLY:HA3	1:C:231:ASN:ND2	2.18	0.58
1:C:938:SER:O	1:C:941:ASN:ND2	2.36	0.58
1:C:914:LEU:O	1:C:915:ALA:HB3	2.03	0.58
1:C:401:ALA:O	1:C:405:LEU:HG	2.03	0.58
1:A:441:ALA:O	1:A:445:ILE:HG23	2.02	0.58
1:A:667:ASN:C	1:A:667:ASN:HD22	2.06	0.58
1:B:104:GLN:HE22	1:B:108:GLN:NE2	2.01	0.58
1:B:523:SER:HA	1:B:526:HIS:HD2	1.67	0.58
1:C:340:VAL:O	1:C:340:VAL:HG12	2.04	0.58
1:C:945:ILE:O	1:C:947:GLU:N	2.35	0.58
1:A:1015:THR:C	1:A:1017:LEU:H	2.05	0.58
1:A:6:ILE:HD11	1:A:432:ARG:HG2	1.85	0.58
1:A:668:LEU:H	1:A:668:LEU:CD2	2.15	0.58
1:A:108:GLN:HE22	1:B:112:GLN:HB3	1.67	0.58
1:A:776:GLU:HB3	1:A:779:TYR:HD1	1.68	0.58
1:A:415:ASN:HD21	1:A:948:PHE:HZ	1.50	0.58
1:B:680:PHE:CD1	1:B:859:TRP:HZ3	2.20	0.58
1:B:651:ALA:O	1:B:655:PHE:CD2	2.57	0.58
1:C:746:ILE:HD13	1:C:791:VAL:HG11	1.86	0.58
1:B:326:PRO:HG3	1:B:610:PHE:HD1	1.68	0.58
1:A:578:LEU:CD2	1:A:587:THR:HG23	2.34	0.58
1:A:38:ILE:HD11	1:A:674:LEU:HG	1.85	0.58
1:C:378:GLY:O	1:C:382:VAL:HG23	2.04	0.58
1:A:578:LEU:HB3	1:A:579:PRO:HD2	1.86	0.58
1:C:497:LEU:HD12	1:C:498:LYS:HG3	1.85	0.58
1:A:360:GLN:HB2	1:A:513:PHE:CB	2.33	0.58
1:A:210:GLN:HE22	1:A:250:LEU:H	1.51	0.58
1:A:813:SER:HB3	1:A:816:LEU:CD2	2.33	0.58
1:B:200:PRO:CD	1:B:749:THR:HG22	2.22	0.58
1:C:564:LEU:HD13	1:C:671:ILE:CD1	2.23	0.58
1:A:400:LEU:HD22	1:A:1003:VAL:HG13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LEU:HD23	1:C:31:PRO:HD2	1.84	0.58
1:C:186:ILE:O	1:C:186:ILE:HG22	2.03	0.58
1:C:946:VAL:O	1:C:946:VAL:HG12	2.04	0.58
1:A:253:VAL:HG13	1:A:253:VAL:O	2.04	0.58
1:B:69:MET:HG2	1:B:92:LEU:HD11	1.86	0.58
1:B:346:GLU:O	1:B:350:LEU:HB2	2.04	0.58
1:B:231:ASN:HD22	1:B:231:ASN:C	2.06	0.58
1:B:1022:VAL:HA	1:B:1025:PHE:CD1	2.38	0.58
1:C:713:LEU:HD23	1:C:831:ALA:CA	2.32	0.58
1:B:911:GLY:N	1:B:1013:THR:HG21	2.19	0.58
1:B:528:THR:OG1	1:B:969:ARG:HB2	2.04	0.58
1:B:897:ILE:HD13	1:B:898:PRO:HD3	1.86	0.57
1:B:888:LEU:C	1:B:890:ALA:H	2.06	0.57
1:B:445:ILE:CG2	1:B:940:LYS:HG3	2.33	0.57
1:A:707:ALA:O	1:A:709:HIS:N	2.36	0.57
1:C:695:LEU:HD22	1:C:825:MET:SD	2.44	0.57
1:A:740:GLY:CA	1:A:793:ALA:HB1	2.34	0.57
1:C:485:ALA:O	1:C:490:PRO:HD3	2.04	0.57
1:B:143:ILE:CG2	1:B:286:ALA:HB2	2.34	0.57
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.84	0.57
1:B:166:ILE:HG21	1:B:291:ILE:HD12	1.86	0.57
1:C:713:LEU:CD2	1:C:831:ALA:HA	2.31	0.57
1:B:911:GLY:H	1:B:1013:THR:HG21	1.68	0.57
1:B:416:VAL:HG21	1:B:431:THR:HA	1.86	0.57
1:B:934:THR:HA	1:B:937:LEU:HD12	1.86	0.57
1:B:523:SER:HA	1:B:526:HIS:CD2	2.39	0.57
1:B:53:ASP:HB2	1:B:56:THR:OG1	2.04	0.57
1:C:1018:ALA:O	1:C:1022:VAL:HG23	2.04	0.57
1:C:406:VAL:O	1:C:408:ASP:N	2.37	0.57
1:B:104:GLN:HE22	1:B:108:GLN:HE21	1.50	0.57
1:A:418:ARG:HH21	1:A:970:MET:C	2.07	0.57
1:B:158:VAL:HA	1:B:162:MET:CG	2.34	0.57
1:B:449:LEU:HD23	1:B:478:MET:CE	2.34	0.57
1:A:297:ALA:HB1	1:A:302:THR:HG21	1.87	0.57
1:C:143:ILE:HD11	1:C:281:PHE:HB3	1.85	0.57
1:B:271:GLY:HA3	1:B:275:TYR:OH	2.05	0.57
1:C:952:LEU:O	1:C:953:MET:HG3	2.04	0.57
1:A:775:SER:O	1:A:780:ARG:NH1	2.38	0.57
1:A:800:PRO:O	1:A:803:ALA:HB3	2.04	0.57
1:C:894:SER:O	1:C:898:PRO:HD3	2.04	0.56
1:C:10:ILE:HD13	1:C:10:ILE:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ALA:HB1	1:A:816:LEU:HG	1.87	0.56
1:B:24:GLY:H	1:B:27:ILE:HG23	1.69	0.56
1:C:144:ASN:ND2	1:C:149:MET:H	2.04	0.56
1:C:395:MET:O	1:C:398:MET:N	2.38	0.56
1:B:914:LEU:O	1:B:917:THR:HB	2.05	0.56
1:B:699:ARG:O	1:B:701:GLN:N	2.34	0.56
1:C:686:ASP:C	1:C:686:ASP:OD2	2.43	0.56
1:C:137:LEU:HD13	1:C:293:LEU:HD13	1.86	0.56
1:A:872:GLN:O	1:A:876:LEU:HB2	2.06	0.56
1:B:332:PHE:CD1	1:B:569:GLN:HA	2.39	0.56
1:C:463:THR:HG22	1:C:464:GLY:H	1.71	0.56
1:B:300:LEU:O	1:B:300:LEU:HD12	2.06	0.56
1:C:3:ASN:HD21	1:C:432:ARG:HG3	1.70	0.56
1:B:391:ASN:O	1:B:395:MET:HG2	2.04	0.56
1:B:10:ILE:CD1	1:C:893:GLU:O	2.53	0.56
1:A:746:ILE:HG12	1:A:804:PHE:CE1	2.41	0.56
1:A:991:ILE:HD11	1:A:1005:THR:N	2.21	0.56
1:C:888:LEU:C	1:C:890:ALA:H	2.09	0.56
1:B:736:ALA:HB1	1:B:741:VAL:CG1	2.35	0.56
1:C:680:PHE:CZ	1:C:829:GLY:HA3	2.40	0.56
1:B:57:VAL:O	1:B:61:VAL:HG12	2.05	0.56
1:B:67:GLN:O	1:B:70:ASN:ND2	2.34	0.56
1:A:65:ILE:HD11	1:A:90:ILE:HD13	1.88	0.56
1:C:643:LYS:O	1:C:647:ILE:CG1	2.54	0.56
1:C:444:GLY:HA3	1:C:891:LEU:HD13	1.86	0.56
1:B:435:MET:HA	1:B:435:MET:CE	2.36	0.56
1:C:641:GLU:O	1:C:650:ARG:NH1	2.38	0.56
1:C:294:ALA:HB3	1:C:297:ALA:HB2	1.87	0.56
1:A:379:THR:HG21	1:A:477:ALA:CA	2.18	0.56
1:B:30:LEU:HD22	1:B:390:ILE:HG13	1.87	0.56
1:B:404:LEU:HD22	1:B:449:LEU:HD21	1.88	0.56
1:A:552:MET:HE1	1:A:906:PRO:HB3	1.87	0.56
1:B:281:PHE:CE1	1:B:608:SER:HB2	2.41	0.56
1:C:379:THR:OG1	1:C:477:ALA:HB2	2.06	0.56
1:A:740:GLY:HA3	1:A:793:ALA:HB1	1.88	0.56
1:A:246:PHE:O	1:A:249:ILE:HG13	2.05	0.56
1:A:62:THR:O	1:A:66:GLU:HG2	2.05	0.56
1:C:134:SER:O	1:C:292:LYS:HE2	2.06	0.56
1:C:888:LEU:O	1:C:890:ALA:N	2.33	0.55
1:B:1009:GLY:O	1:B:1012:VAL:HG22	2.06	0.55
1:A:584:GLN:H	1:A:622:GLN:HB3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:979:SER:O	1:C:983:ILE:HG13	2.07	0.55
1:B:59:ASP:HA	1:B:63:GLN:HG2	1.88	0.55
1:C:199:THR:OG1	1:C:201:VAL:N	2.39	0.55
1:B:282:ASN:O	1:B:284:GLN:N	2.39	0.55
1:B:742:SER:HB3	1:B:745:ASP:OD2	2.05	0.55
1:C:228:GLN:HG3	1:C:229:GLN:O	2.06	0.55
1:C:379:THR:HG21	1:C:398:MET:CE	2.36	0.55
1:C:477:ALA:C	1:C:479:ALA:H	2.10	0.55
1:B:360:GLN:O	1:B:361:ASN:CB	2.53	0.55
1:B:734:GLU:C	1:B:736:ALA:N	2.59	0.55
1:C:166:ILE:HG21	1:C:291:ILE:HD11	1.88	0.55
1:C:242:SER:OG	1:C:244:GLU:HB3	2.06	0.55
1:A:775:SER:HB2	1:A:789:TRP:CZ2	2.42	0.55
1:A:552:MET:HB2	1:A:910:ILE:HG23	1.86	0.55
1:C:692:HIS:HE1	1:C:721:LEU:HD21	1.70	0.55
1:B:370:ILE:CG2	1:B:370:ILE:O	2.55	0.55
1:B:448:VAL:O	1:B:452:VAL:HG23	2.05	0.55
1:B:193:LEU:HG	1:B:265:VAL:HG22	1.88	0.55
1:A:668:LEU:H	1:A:668:LEU:HD23	1.71	0.55
1:B:1012:VAL:HG23	1:B:1013:THR:N	2.22	0.55
1:C:1024:VAL:O	1:C:1028:VAL:HG23	2.06	0.55
1:C:350:LEU:C	1:C:352:PHE:H	2.10	0.55
1:C:746:ILE:HD12	1:C:804:PHE:CZ	2.42	0.55
1:B:87:THR:HG21	1:B:620:ARG:NH1	2.21	0.55
1:C:818:ARG:HA	1:C:824:SER:H	1.70	0.55
1:C:953:MET:SD	1:C:963:ALA:CB	2.92	0.55
1:B:53:ASP:O	1:B:54:ALA:HB2	2.06	0.55
1:B:219:LEU:HG	1:B:234:ILE:CD1	2.26	0.55
1:C:908:GLY:CA	1:C:1014:ALA:HB2	2.34	0.55
1:B:986:VAL:O	1:B:990:VAL:HG23	2.07	0.55
1:C:65:ILE:HD13	1:C:111:LEU:CD2	2.37	0.55
1:B:239:ARG:NH2	1:B:761:ASP:HB2	2.22	0.55
1:B:790:TYR:HE1	1:B:800:PRO:HB3	1.71	0.55
1:B:649:MET:O	1:B:653:ARG:HB2	2.07	0.55
1:A:278:ILE:HB	1:A:613:ASN:HB3	1.88	0.54
1:A:451:ALA:O	1:A:452:VAL:HG22	2.06	0.54
1:A:159:ALA:HB2	1:A:177:LEU:CD2	2.37	0.54
1:B:808:ARG:HH21	1:B:808:ARG:HB2	1.71	0.54
1:C:38:ILE:CG2	1:C:466:ILE:HD11	2.37	0.54
1:C:727:PHE:CZ	1:C:807:SER:CB	2.90	0.54
1:B:997:SER:C	1:B:999:ALA:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:731:ILE:HG21	1:B:746:ILE:HG21	1.89	0.54
1:B:1012:VAL:HG23	1:B:1013:THR:H	1.73	0.54
1:A:894:SER:OG	1:A:897:ILE:HB	2.07	0.54
1:C:1013:THR:O	1:C:1017:LEU:HB3	2.06	0.54
1:C:188:MET:HE1	1:C:200:PRO:HA	1.89	0.54
1:A:1022:VAL:HG23	1:A:1023:PRO:HD3	1.89	0.54
1:A:1029:VAL:O	1:A:1030:ARG:HB2	2.07	0.54
1:B:605:ASN:ND2	1:B:605:ASN:H	2.05	0.54
1:C:775:SER:HG	1:C:789:TRP:HZ2	1.56	0.54
1:B:859:TRP:HB3	1:B:863:SER:HB3	1.90	0.54
1:A:688:ALA:C	1:A:690:LEU:H	2.10	0.54
1:B:139:VAL:O	1:B:140:VAL:C	2.44	0.54
1:B:544:LEU:O	1:B:548:ILE:HG12	2.07	0.54
1:A:659:LYS:HG2	1:A:660:ASP:N	2.23	0.54
1:B:404:LEU:HD21	1:B:937:LEU:HD23	1.89	0.54
1:C:895:TRP:HA	1:C:895:TRP:CE3	2.43	0.54
1:B:185:ARG:NH1	1:B:185:ARG:CG	2.66	0.54
1:C:131:LYS:HB2	1:C:295:THR:HG22	1.90	0.54
1:B:416:VAL:HG11	1:B:431:THR:HG22	1.90	0.54
1:B:452:VAL:O	1:B:453:PHE:CB	2.56	0.54
1:A:442:LEU:C	1:A:444:GLY:H	2.12	0.54
1:B:613:ASN:O	1:B:625:GLY:HA2	2.08	0.54
1:B:1022:VAL:HG23	1:B:1023:PRO:CD	2.37	0.54
1:A:606:VAL:HA	1:A:631:LEU:HD23	1.90	0.54
1:C:782:LEU:HB3	1:C:783:PRO:HD2	1.90	0.54
1:C:904:VAL:HA	1:C:907:LEU:HD23	1.90	0.54
1:B:945:ILE:HG13	1:B:946:VAL:N	2.23	0.54
1:C:741:VAL:HG13	1:C:793:ALA:HB2	1.90	0.54
1:A:340:VAL:HG13	1:A:399:VAL:CG2	2.38	0.54
1:B:578:LEU:HB3	1:B:579:PRO:HD2	1.89	0.54
1:A:563:PHE:O	1:A:564:LEU:HD23	2.08	0.54
1:A:685:ILE:HG22	1:A:687:GLN:NE2	2.23	0.54
1:B:916:ALA:HA	1:B:919:ARG:HG2	1.90	0.53
1:A:210:GLN:O	1:A:240:LEU:HD11	2.08	0.53
1:A:172:VAL:HG23	1:A:172:VAL:O	2.08	0.53
1:A:479:ALA:O	1:A:483:LEU:HD23	2.07	0.53
1:A:634:TRP:HD1	1:A:634:TRP:H	1.50	0.53
1:C:158:VAL:HG12	1:C:177:LEU:HD21	1.91	0.53
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.90	0.53
1:C:188:MET:HG3	1:C:774:MET:O	2.09	0.53
1:C:190:PRO:CD	1:C:779:TYR:CD1	2.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:VAL:HG13	1:B:906:PRO:CD	2.36	0.53
1:A:552:MET:HE1	1:A:906:PRO:CB	2.38	0.53
1:C:605:ASN:ND2	1:C:637:ARG:HG2	2.24	0.53
1:A:552:MET:HE1	1:A:906:PRO:HA	1.90	0.53
1:C:801:PHE:O	1:C:803:ALA:N	2.40	0.53
1:C:319:SER:OG	1:C:320:GLY:N	2.39	0.53
1:A:31:PRO:HB3	1:A:296:GLY:HA2	1.90	0.53
1:A:783:PRO:HD3	1:C:219:LEU:HD13	1.90	0.53
1:C:452:VAL:HG12	1:C:932:LEU:HD22	1.89	0.53
1:B:158:VAL:HA	1:B:162:MET:HG2	1.89	0.53
1:B:841:MET:SD	1:B:866:GLU:OE2	2.66	0.53
1:C:590:VAL:O	1:C:594:VAL:HG23	2.09	0.53
1:B:671:ILE:C	1:B:673:GLU:N	2.61	0.53
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.90	0.53
1:C:361:ASN:HB3	1:C:364:ALA:HB3	1.89	0.53
1:B:220:GLY:HA2	1:C:781:MET:SD	2.49	0.53
1:B:314:GLU:HA	1:B:317:PHE:CE2	2.42	0.53
1:A:709:HIS:N	1:A:710:PRO:HD3	2.24	0.53
1:C:371:ALA:HB2	1:C:488:LEU:HD23	1.91	0.53
1:B:178:PHE:CD1	1:B:612:VAL:HG11	2.43	0.53
2:C:2002:RFP:C18	2:C:2002:RFP:H401	2.39	0.53
1:C:246:PHE:O	1:C:249:ILE:HG12	2.09	0.53
1:C:1026:PHE:CE1	1:C:1030:ARG:HD2	2.44	0.53
1:C:837:THR:O	1:C:841:MET:HB2	2.09	0.53
1:B:485:ALA:HA	1:B:489:THR:OG1	2.08	0.53
1:B:985:GLY:O	1:B:988:PRO:HD2	2.09	0.53
1:B:983:ILE:HD12	1:B:1012:VAL:HG13	1.89	0.53
1:A:708:LYS:O	1:A:709:HIS:CD2	2.62	0.53
1:C:49:TYR:HE1	1:C:60:THR:HG21	1.74	0.53
1:C:225:VAL:O	1:C:226:LYS:C	2.46	0.53
1:B:291:ILE:HG21	1:B:306:ILE:HD13	1.90	0.53
1:B:732:ASP:O	1:B:734:GLU:N	2.42	0.53
1:B:600:THR:OG1	1:B:601:LYS:N	2.42	0.53
1:C:317:PHE:CD1	1:C:321:LEU:HD12	2.44	0.53
1:B:426:PRO:HB3	1:B:430:ALA:CB	2.39	0.53
1:B:924:ASP:HB3	1:B:926:TYR:H	1.75	0.53
1:C:204:ILE:HD13	1:C:773:VAL:HG21	1.90	0.52
1:C:442:LEU:O	1:C:445:ILE:HG13	2.09	0.52
1:A:1021:PHE:O	1:A:1024:VAL:HB	2.10	0.52
1:C:2:PRO:HB2	1:C:6:ILE:HD11	1.91	0.52
1:C:176:GLN:HE22	1:C:620:ARG:NH1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ALA:HB2	1:A:177:LEU:HD22	1.92	0.52
1:A:688:ALA:O	1:A:690:LEU:N	2.42	0.52
1:C:514:GLY:C	1:C:516:PHE:H	2.12	0.52
1:C:351:VAL:HG11	1:C:406:VAL:HG21	1.91	0.52
1:C:351:VAL:HG22	1:C:981:ALA:O	2.09	0.52
1:C:767:ARG:HD3	1:C:769:LYS:HE3	1.91	0.52
1:A:105:VAL:CG2	1:B:105:VAL:HG13	2.39	0.52
1:B:316:PHE:HD1	1:C:854:GLY:HA2	1.74	0.52
1:A:352:PHE:HA	1:A:365:THR:HB	1.92	0.52
1:C:157:TYR:O	1:C:161:ASN:HB2	2.09	0.52
1:A:139:VAL:HG13	1:A:139:VAL:O	2.09	0.52
1:A:923:ASN:ND2	1:A:923:ASN:C	2.61	0.52
1:A:172:VAL:HG12	1:A:291:ILE:HG21	1.91	0.52
1:A:575:MET:HA	1:A:626:ILE:HD13	1.91	0.52
1:C:966:ASP:O	1:C:970:MET:HG3	2.09	0.52
1:C:222:THR:CG2	1:C:223:PRO:CD	2.66	0.52
1:A:832:ALA:O	1:A:833:PRO:C	2.48	0.52
1:C:192:GLU:HB3	1:C:265:VAL:HB	1.91	0.52
1:A:194:ASN:ND2	1:A:790:TYR:CD2	2.77	0.52
1:B:183:ALA:O	1:B:185:ARG:N	2.42	0.52
1:A:560:PRO:HB2	1:A:922:THR:HG22	1.92	0.52
1:B:356:TYR:O	1:B:360:GLN:N	2.38	0.52
1:B:682:PHE:HD1	1:B:859:TRP:CH2	2.28	0.52
1:A:337:ILE:CD1	1:A:395:MET:HG3	2.39	0.52
1:A:746:ILE:HG22	1:A:747:ASN:N	2.24	0.52
1:C:308:ALA:O	1:C:312:LYS:HG3	2.10	0.52
1:B:675:GLY:O	1:B:677:ALA:N	2.43	0.52
1:C:249:ILE:O	1:C:261:LEU:HA	2.10	0.52
1:C:230:LEU:C	1:C:230:LEU:HD13	2.30	0.52
1:B:404:LEU:HD21	1:B:937:LEU:CD2	2.39	0.52
1:C:415:ASN:HA	1:C:418:ARG:HH21	1.73	0.52
1:A:919:ARG:HG3	1:A:920:GLY:N	2.24	0.52
1:C:592:ASN:HA	1:C:595:THR:OG1	2.10	0.52
1:A:240:LEU:N	1:A:240:LEU:HD12	2.25	0.52
1:A:299:ALA:O	1:A:303:ALA:HB2	2.10	0.52
1:A:790:TYR:CE1	1:A:800:PRO:HB3	2.44	0.52
1:A:23:GLY:HA2	1:A:381:ALA:HB2	1.92	0.52
1:B:699:ARG:HH11	1:B:699:ARG:CB	2.19	0.52
1:C:945:ILE:C	1:C:947:GLU:N	2.62	0.52
1:C:531:VAL:O	1:C:533:GLY:N	2.42	0.52
1:B:78:MET:HA	1:B:91:THR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:THR:HA	1:C:466:ILE:HG12	1.91	0.52
1:A:890:ALA:HB1	1:C:11:PHE:CD1	2.45	0.52
1:B:282:ASN:C	1:B:284:GLN:H	2.12	0.52
1:C:760:ASN:O	1:C:771:VAL:HG23	2.09	0.51
1:A:65:ILE:HG22	1:A:118:LEU:HD11	1.92	0.51
1:A:600:THR:O	1:A:603:LYS:HD3	2.09	0.51
1:C:482:VAL:O	1:C:486:LEU:HG	2.10	0.51
1:B:973:ARG:HB3	1:B:974:PRO:HD3	1.93	0.51
1:A:525:HIS:HA	1:A:528:THR:HG22	1.91	0.51
1:C:400:LEU:HD11	1:C:930:GLY:HA2	1.92	0.51
1:C:527:TYR:OH	1:C:968:VAL:HG12	2.09	0.51
1:B:919:ARG:HB2	1:B:921:LEU:HD13	1.91	0.51
1:B:189:ASN:HD22	1:B:190:PRO:HD2	1.76	0.51
1:B:462:SER:OG	1:B:865:GLN:HG2	2.10	0.51
1:A:911:GLY:CA	1:A:914:LEU:HB2	2.41	0.51
1:A:909:VAL:O	1:A:912:ALA:HB3	2.10	0.51
1:A:30:LEU:HD21	1:A:384:ALA:HB2	1.90	0.51
1:C:574:THR:HG23	1:C:665:ALA:HB2	1.92	0.51
1:A:1010:GLY:O	1:A:1014:ALA:HB2	2.11	0.51
1:C:368:PRO:HD2	1:C:369:THR:H	1.75	0.51
1:C:193:LEU:HB3	1:C:198:LEU:O	2.10	0.51
1:C:420:MET:SD	1:C:498:LYS:HD3	2.51	0.51
1:C:983:ILE:CG2	1:C:1008:MET:HG3	2.38	0.51
1:A:158:VAL:HA	1:A:162:MET:HG2	1.92	0.51
1:B:525:HIS:O	1:B:528:THR:HG22	2.09	0.51
1:C:361:ASN:HD22	1:C:362:PHE:N	2.08	0.51
1:A:862:MET:HA	1:A:865:GLN:HB3	1.93	0.51
1:C:564:LEU:HD23	1:C:565:PRO:HD2	1.93	0.51
1:A:38:ILE:CD1	1:A:674:LEU:HG	2.40	0.51
1:C:944:LEU:HB3	1:C:971:ARG:HD2	1.92	0.51
1:B:146:ASP:O	1:B:148:THR:N	2.44	0.51
1:C:415:ASN:HA	1:C:418:ARG:NH2	2.25	0.51
1:C:400:LEU:CD1	1:C:930:GLY:HA2	2.41	0.51
1:C:1013:THR:HG23	1:C:1014:ALA:N	2.26	0.51
1:B:166:ILE:HG21	1:B:291:ILE:CD1	2.41	0.51
1:A:649:MET:HB3	1:A:653:ARG:HH22	1.75	0.51
1:C:1016:VAL:O	1:C:1018:ALA:N	2.42	0.51
1:B:171:GLY:HA3	1:B:302:THR:HG21	1.93	0.51
1:C:946:VAL:HG13	1:C:1026:PHE:CD1	2.46	0.51
1:A:298:ASN:HB2	1:A:301:ASP:H	1.76	0.51
1:C:819:TYR:N	1:C:824:SER:HB3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASP:OD1	1:A:330:THR:HB	2.11	0.51
1:C:143:ILE:HD11	1:C:281:PHE:CB	2.40	0.51
1:C:832:ALA:HB3	1:C:833:PRO:CD	2.33	0.51
1:A:776:GLU:HB3	1:A:779:TYR:CD1	2.46	0.51
1:B:10:ILE:HD12	1:C:893:GLU:HG3	1.92	0.51
1:C:520:PHE:O	1:C:524:THR:HG23	2.10	0.51
1:B:651:ALA:HB1	1:B:655:PHE:CE2	2.45	0.51
1:A:282:ASN:ND2	1:A:609:VAL:H	2.09	0.51
1:C:662:MET:H	1:C:662:MET:CE	2.24	0.51
1:B:768:VAL:HG23	1:C:63:GLN:NE2	2.25	0.51
1:A:959:GLY:HA3	1:A:962:GLU:HB3	1.92	0.51
1:C:144:ASN:HD21	1:C:148:THR:H	1.57	0.51
1:C:131:LYS:O	1:C:295:THR:HG22	2.11	0.51
1:B:250:LEU:HD12	1:B:259:ARG:NH2	2.21	0.51
1:C:615:PHE:C	1:C:615:PHE:CD2	2.85	0.51
1:C:624:THR:HB	2:C:2002:RFP:H381	1.92	0.50
1:A:400:LEU:HD11	1:A:930:GLY:CA	2.28	0.50
1:C:184:MET:HG2	1:C:246:PHE:CE1	2.46	0.50
1:C:474:ILE:O	1:C:478:MET:HB2	2.11	0.50
1:B:1028:VAL:O	1:B:1032:ARG:HB2	2.11	0.50
1:A:454:VAL:O	1:A:456:MET:N	2.44	0.50
1:B:818:ARG:NH1	1:B:818:ARG:HG3	2.25	0.50
1:C:176:GLN:NE2	1:C:620:ARG:NH1	2.58	0.50
1:A:813:SER:HB3	1:A:816:LEU:HD21	1.93	0.50
1:C:713:LEU:O	1:C:713:LEU:CD2	2.59	0.50
1:A:418:ARG:NH2	1:A:970:MET:O	2.44	0.50
1:B:708:LYS:C	1:B:710:PRO:HD3	2.31	0.50
1:A:102:ILE:O	1:A:106:GLN:HG3	2.11	0.50
1:B:213:GLN:HG2	1:C:56:THR:HG23	1.94	0.50
1:A:987:MET:N	1:A:988:PRO:CD	2.74	0.50
1:A:251:LEU:CD1	1:A:265:VAL:HG21	2.41	0.50
1:C:193:LEU:HD23	1:C:265:VAL:HG21	1.93	0.50
1:C:204:ILE:HD11	1:C:773:VAL:HG21	1.92	0.50
1:C:459:PHE:O	1:C:464:GLY:HA3	2.11	0.50
1:C:643:LYS:HE2	1:C:645:GLU:HB3	1.92	0.50
1:B:166:ILE:C	1:B:168:ARG:H	2.14	0.50
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.92	0.50
1:A:252:LYS:HE3	1:A:254:ASN:HB3	1.93	0.50
1:C:732:ASP:N	1:C:804:PHE:O	2.36	0.50
1:C:140:VAL:O	1:C:288:GLY:HA3	2.10	0.50
1:B:13:TRP:CE3	1:B:13:TRP:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:541:TYR:C	1:C:543:VAL:H	2.13	0.50
1:A:104:GLN:OE1	1:A:131:LYS:HE3	2.11	0.50
1:C:188:MET:CE	1:C:200:PRO:HA	2.42	0.50
1:C:391:ASN:H	1:C:394:THR:HB	1.77	0.50
1:A:574:THR:HG21	1:A:594:VAL:CG1	2.39	0.50
1:A:235:ILE:CD1	1:B:53:ASP:HB3	2.42	0.50
1:B:414:GLU:CD	1:B:974:PRO:HG3	2.32	0.50
1:C:655:PHE:C	1:C:657:GLN:N	2.65	0.50
1:C:1007:VAL:O	1:C:1011:MET:HB2	2.11	0.50
1:A:1019:ILE:HG12	1:A:1020:PHE:CD1	2.46	0.50
1:C:204:ILE:HG22	1:C:208:LYS:HD2	1.92	0.50
1:C:941:ASN:HD22	1:C:942:ALA:N	2.10	0.50
1:B:198:LEU:HD23	1:B:792:ARG:HH22	1.76	0.50
1:C:688:ALA:O	1:C:689:GLY:C	2.50	0.50
1:A:481:SER:O	1:A:484:VAL:HG22	2.11	0.50
1:C:352:PHE:HA	1:C:369:THR:HG21	1.92	0.50
1:A:713:LEU:HB2	1:A:832:ALA:CA	2.42	0.50
1:B:560:PRO:HB3	1:B:839:GLU:OE1	2.12	0.50
1:B:376:LEU:HD11	1:B:402:ILE:HD13	1.94	0.50
1:A:59:ASP:HB3	1:C:763:ILE:HD11	1.94	0.50
1:B:987:MET:HB3	1:B:988:PRO:CD	2.37	0.50
1:A:6:ILE:HG22	1:A:490:PRO:HB2	1.93	0.50
1:B:143:ILE:HG23	1:B:286:ALA:HB2	1.93	0.50
1:A:780:ARG:HG2	1:A:780:ARG:NH1	2.26	0.50
1:A:235:ILE:HD13	1:B:53:ASP:HB3	1.93	0.50
1:C:786:ILE:HD12	1:C:786:ILE:H	1.77	0.50
1:C:476:SER:O	1:C:477:ALA:CB	2.59	0.49
1:A:108:GLN:NE2	1:B:112:GLN:CB	2.70	0.49
1:B:1013:THR:HA	1:B:1017:LEU:HD13	1.93	0.49
1:A:897:ILE:N	1:A:898:PRO:HD2	2.27	0.49
1:C:949:ALA:HB1	1:C:1026:PHE:CZ	2.47	0.49
1:B:616:GLY:HA3	1:B:624:THR:HG21	1.93	0.49
1:C:156:ASP:O	1:C:157:TYR:C	2.51	0.49
1:C:489:THR:N	1:C:490:PRO:HD2	2.27	0.49
1:C:199:THR:OG1	1:C:201:VAL:HB	2.12	0.49
1:C:158:VAL:HG13	1:C:289:LEU:HD21	1.93	0.49
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.92	0.49
1:C:190:PRO:HG3	1:C:789:TRP:CH2	2.46	0.49
1:C:380:PHE:HE1	1:C:398:MET:SD	2.32	0.49
1:A:707:ALA:C	1:A:709:HIS:N	2.65	0.49
1:A:442:LEU:O	1:A:445:ILE:HG13	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ASP:C	1:A:303:ALA:H	2.16	0.49
1:C:757:SER:O	1:C:772:TYR:HA	2.12	0.49
1:B:138:MET:HG2	1:B:139:VAL:N	2.27	0.49
1:A:585:GLU:OE2	1:C:227:GLY:HA2	2.12	0.49
1:A:590:VAL:O	1:A:594:VAL:HG23	2.13	0.49
1:C:945:ILE:HG13	1:C:971:ARG:HG3	1.93	0.49
1:B:55:LYS:O	1:B:57:VAL:N	2.37	0.49
1:C:115:MET:HA	1:C:118:LEU:HD22	1.95	0.49
1:B:669:PRO:HG3	1:B:678:THR:HA	1.94	0.49
1:C:349:ILE:O	1:C:352:PHE:HB3	2.13	0.49
1:C:382:VAL:HG11	1:C:476:SER:HB2	1.94	0.49
1:A:228:GLN:HG2	1:B:781:MET:HG3	1.94	0.49
1:A:240:LEU:N	1:A:240:LEU:CD1	2.76	0.49
1:A:171:GLY:HA3	1:A:302:THR:HG21	1.95	0.49
1:C:314:GLU:HB2	1:C:315:PRO:HD3	1.94	0.49
1:B:493:CYS:HA	1:B:497:LEU:HB2	1.94	0.49
1:A:447:MET:HB3	1:A:887:CYS:HG	1.73	0.49
1:A:713:LEU:HD13	1:A:714:THR:N	2.27	0.49
1:A:578:LEU:HD21	1:A:587:THR:HG23	1.95	0.49
1:B:450:SER:O	1:B:452:VAL:O	2.31	0.49
1:C:332:PHE:CD2	1:C:569:GLN:HA	2.47	0.49
1:C:437:GLN:O	1:C:438:ILE:HB	2.13	0.49
1:A:53:ASP:HA	1:A:84:SER:HA	1.93	0.49
1:C:985:GLY:O	1:C:988:PRO:HD2	2.12	0.49
1:A:634:TRP:N	1:A:634:TRP:CD1	2.66	0.49
1:A:70:ASN:HB3	1:C:167:SER:HB3	1.95	0.49
1:C:586:ARG:O	1:C:590:VAL:HG23	2.13	0.49
1:C:752:ALA:O	1:C:774:MET:HA	2.13	0.49
1:A:578:LEU:HD23	1:A:587:THR:HG23	1.94	0.49
1:C:150:THR:O	1:C:154:ILE:HG13	2.12	0.49
1:B:555:LEU:HA	1:B:558:ARG:HE	1.77	0.49
1:C:685:ILE:CG1	1:C:685:ILE:O	2.61	0.49
1:C:564:LEU:CD1	1:C:671:ILE:HD12	2.27	0.49
1:C:355:MET:HG2	1:C:368:PRO:HG2	1.94	0.49
1:C:847:LEU:H	1:C:847:LEU:HD23	1.78	0.49
1:B:139:VAL:CG1	1:B:139:VAL:O	2.47	0.49
1:C:345:VAL:O	1:C:348:ILE:N	2.40	0.49
1:A:780:ARG:O	1:A:780:ARG:HD2	2.13	0.49
1:A:813:SER:CB	1:A:816:LEU:HD23	2.42	0.49
1:A:899:PHE:HA	1:A:902:MET:HG3	1.94	0.49
1:C:815:ARG:NH1	1:C:815:ARG:CG	2.62	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ASN:N	1:B:605:ASN:ND2	2.60	0.49
1:A:843:LEU:HD22	1:A:843:LEU:O	2.13	0.49
1:A:786:ILE:O	1:A:787:GLY:C	2.52	0.49
1:C:655:PHE:O	1:C:657:GLN:N	2.46	0.48
1:C:40:PRO:HB2	1:C:94:PHE:O	2.12	0.48
1:B:922:THR:OG1	1:B:923:ASN:N	2.45	0.48
1:B:382:VAL:HG11	1:B:476:SER:OG	2.13	0.48
1:C:577:GLN:HG2	2:C:2002:RFP:C39	2.44	0.48
1:B:184:MET:H	1:B:762:PHE:HE2	1.59	0.48
1:C:53:ASP:O	1:C:54:ALA:HB2	2.13	0.48
1:A:61:VAL:HG22	1:A:118:LEU:HD22	1.93	0.48
1:B:339:GLU:HG3	1:B:996:GLY:H	1.77	0.48
1:C:344:LEU:HD23	1:C:399:VAL:HG22	1.94	0.48
1:B:780:ARG:O	1:B:781:MET:HB2	2.13	0.48
1:A:713:LEU:HD13	1:A:714:THR:H	1.78	0.48
1:C:399:VAL:O	1:C:402:ILE:HB	2.13	0.48
1:C:404:LEU:HD23	1:C:449:LEU:HD13	1.96	0.48
1:A:239:ARG:HD3	1:A:762:PHE:HA	1.95	0.48
1:B:776:GLU:OE1	1:B:778:LYS:HE2	2.13	0.48
1:A:1015:THR:O	1:A:1017:LEU:N	2.47	0.48
1:C:419:VAL:HG23	1:C:430:ALA:HB1	1.94	0.48
1:C:841:MET:O	1:C:845:GLU:HG3	2.13	0.48
1:C:907:LEU:HD12	1:C:1017:LEU:HG	1.95	0.48
1:B:723:ASP:HA	1:B:814:PRO:HD3	1.95	0.48
1:B:449:LEU:HD23	1:B:478:MET:HE2	1.96	0.48
1:B:940:LYS:NZ	1:B:978:THR:HG22	2.29	0.48
1:B:531:VAL:O	1:B:535:LEU:HD23	2.13	0.48
1:A:188:MET:SD	1:A:200:PRO:HB3	2.53	0.48
1:C:801:PHE:CD1	1:C:804:PHE:HE1	2.32	0.48
1:A:301:ASP:N	1:A:301:ASP:OD2	2.46	0.48
1:A:340:VAL:HG13	1:A:399:VAL:HG23	1.96	0.48
1:C:672:VAL:HG13	1:C:676:THR:H	1.78	0.48
1:B:947:GLU:HG3	1:B:947:GLU:O	2.14	0.48
1:C:624:THR:CB	2:C:2002:RFP:H381	2.44	0.48
1:C:184:MET:HG2	1:C:246:PHE:CD1	2.49	0.48
1:B:888:LEU:O	1:B:890:ALA:N	2.47	0.48
1:B:348:ILE:HG23	1:B:372:VAL:HG21	1.96	0.48
1:B:600:THR:C	1:B:602:GLU:H	2.17	0.48
1:C:968:VAL:HG11	1:C:1023:PRO:CG	2.38	0.48
1:A:142:VAL:CG1	1:A:321:LEU:HD12	2.43	0.48
1:A:605:ASN:OD1	1:A:637:ARG:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:HIS:CE1	1:A:813:SER:HB2	2.49	0.48
1:C:158:VAL:CG1	1:C:177:LEU:HD21	2.43	0.48
1:A:21:LEU:O	1:A:25:LEU:HB2	2.14	0.48
1:C:402:ILE:O	1:C:406:VAL:HG23	2.13	0.48
1:C:192:GLU:HG2	1:C:264:ASP:O	2.13	0.48
1:C:265:VAL:O	1:C:265:VAL:CG2	2.62	0.48
1:C:644:VAL:CG1	1:C:667:ASN:HB2	2.43	0.48
1:A:108:GLN:HB3	1:B:112:GLN:HE22	1.79	0.48
1:B:1017:LEU:H	1:B:1017:LEU:HD12	1.79	0.48
1:C:968:VAL:CG1	1:C:1023:PRO:HG3	2.36	0.47
1:B:224:PRO:HA	1:C:781:MET:HE3	1.95	0.47
1:C:216:ALA:HB3	1:C:234:ILE:O	2.14	0.47
1:C:409:ALA:O	1:C:413:VAL:HG22	2.14	0.47
1:C:997:SER:HA	1:C:1000:GLN:OE1	2.14	0.47
1:A:674:LEU:HD22	1:A:675:GLY:N	2.15	0.47
1:B:136:PHE:N	1:B:136:PHE:CD1	2.78	0.47
1:A:108:GLN:HB3	1:B:112:GLN:NE2	2.29	0.47
1:B:676:THR:HG22	1:B:676:THR:O	2.15	0.47
1:B:58:GLN:NE2	1:B:818:ARG:NH1	2.62	0.47
1:C:326:PRO:O	1:C:327:TYR:C	2.52	0.47
1:C:895:TRP:HA	1:C:895:TRP:HE3	1.77	0.47
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.79	0.47
1:B:556:PHE:C	1:B:558:ARG:H	2.17	0.47
1:B:19:ILE:HG22	1:B:378:GLY:HA3	1.97	0.47
1:B:222:THR:HB	1:B:223:PRO:HD2	1.90	0.47
1:C:210:GLN:NE2	1:C:250:LEU:H	2.11	0.47
1:B:225:VAL:N	1:C:781:MET:HE3	2.25	0.47
1:B:715:SER:O	1:B:716:VAL:C	2.53	0.47
1:B:372:VAL:HB	1:B:402:ILE:CD1	2.41	0.47
1:B:1022:VAL:HG23	1:B:1023:PRO:HD3	1.95	0.47
1:A:668:LEU:HD23	1:A:668:LEU:N	2.29	0.47
1:C:801:PHE:HA	1:C:804:PHE:CZ	2.49	0.47
1:A:30:LEU:CD2	1:A:384:ALA:HB2	2.45	0.47
1:C:873:ALA:C	1:C:875:SER:H	2.18	0.47
1:C:708:LYS:C	1:C:710:PRO:HD3	2.35	0.47
1:A:275:TYR:CB	1:C:223:PRO:CD	2.86	0.47
1:B:860:THR:O	1:B:861:GLY:C	2.52	0.47
1:C:467:TYR:CE2	1:C:925:VAL:HG12	2.50	0.47
1:C:655:PHE:C	1:C:657:GLN:H	2.16	0.47
1:C:303:ALA:O	1:C:307:ARG:HG2	2.14	0.47
1:C:195:LYS:HE3	1:C:196:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ASP:OD2	1:B:182:TYR:HB2	2.15	0.47
1:B:568:ASP:HA	1:B:644:VAL:HG21	1.96	0.47
1:B:75:LEU:HA	1:B:75:LEU:HD12	1.75	0.47
1:B:915:ALA:O	1:B:917:THR:N	2.44	0.47
1:A:6:ILE:HD11	1:A:432:ARG:CG	2.44	0.47
1:B:696:THR:HA	1:B:699:ARG:NH1	2.30	0.47
1:B:713:LEU:HD23	1:B:716:VAL:HG21	1.96	0.47
1:B:852:PRO:HB2	1:B:853:THR:H	1.54	0.47
1:C:692:HIS:NE2	1:C:813:SER:HB2	2.30	0.47
1:C:785:ASP:C	1:C:787:GLY:H	2.18	0.47
1:B:240:LEU:HB2	1:B:246:PHE:CE2	2.50	0.47
1:B:219:LEU:CG	1:B:234:ILE:HD11	2.30	0.47
1:B:256:ASP:OD1	1:B:256:ASP:N	2.44	0.47
1:B:858:ASP:OD1	1:B:867:ARG:NH2	2.48	0.47
1:C:465:ALA:O	1:C:469:GLN:HG2	2.14	0.47
1:B:23:GLY:HA2	1:B:26:ALA:HB3	1.97	0.47
1:A:192:GLU:O	1:A:265:VAL:HG12	2.15	0.47
1:A:843:LEU:HD22	1:A:847:LEU:HG	1.96	0.47
1:B:225:VAL:HG22	1:C:781:MET:CE	2.44	0.47
1:B:873:ALA:HB2	1:B:928:GLN:HE21	1.80	0.47
1:B:528:THR:O	1:B:531:VAL:HG12	2.15	0.47
1:A:324:VAL:HG12	1:A:325:TYR:H	1.80	0.47
1:B:782:LEU:O	1:B:784:ASP:N	2.47	0.47
1:C:83:ASP:HB2	1:C:87:THR:HB	1.97	0.47
1:A:435:MET:HE2	1:A:438:ILE:HD11	1.96	0.47
1:A:813:SER:HB3	1:A:816:LEU:HD23	1.96	0.47
1:A:747:ASN:HD21	1:C:237:GLN:NE2	2.13	0.47
1:C:672:VAL:HG13	1:C:675:GLY:H	1.79	0.47
1:A:543:VAL:O	1:A:544:LEU:HB3	2.14	0.47
1:C:706:ALA:HB3	1:C:716:VAL:HG21	1.97	0.47
1:B:764:ASP:O	1:B:766:GLY:N	2.48	0.47
1:C:188:MET:CE	1:C:193:LEU:HD11	2.44	0.47
1:C:748:THR:O	1:C:752:ALA:HB2	2.15	0.47
1:C:463:THR:O	1:C:465:ALA:N	2.41	0.47
1:A:73:ASP:H	1:A:106:GLN:NE2	2.09	0.47
1:C:764:ASP:OD1	1:C:765:ARG:HG3	2.14	0.47
1:C:329:THR:C	1:C:331:PRO:HD2	2.35	0.47
1:C:992:SER:HB3	1:C:997:SER:HB2	1.97	0.47
1:A:752:ALA:O	1:A:756:GLY:HA2	2.15	0.47
1:B:582:ALA:HB3	1:B:623:ASN:HB3	1.97	0.47
1:B:367:ILE:CG2	1:B:489:THR:HG23	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:LEU:O	1:C:230:LEU:HD13	2.15	0.46
1:C:379:THR:CG2	1:C:398:MET:HE3	2.45	0.46
1:C:30:LEU:HD11	1:C:380:PHE:O	2.15	0.46
1:A:682:PHE:HD1	1:A:859:TRP:CH2	2.33	0.46
1:C:915:ALA:HB1	1:C:1005:THR:HG22	1.96	0.46
1:A:729:ILE:HD11	1:A:786:ILE:HD11	1.97	0.46
1:B:566:ASP:C	1:B:567:GLU:HG2	2.35	0.46
1:B:762:PHE:HD2	1:B:771:VAL:HG22	1.79	0.46
1:B:193:LEU:HG	1:B:265:VAL:CG2	2.45	0.46
1:B:143:ILE:HD12	1:B:322:LYS:HB3	1.97	0.46
1:B:49:TYR:O	1:B:50:PRO:C	2.54	0.46
1:C:410:ILE:HG23	1:C:977:MET:HE3	1.98	0.46
1:C:911:GLY:HA3	1:C:1013:THR:HB	1.97	0.46
1:A:231:ASN:OD1	1:B:622:GLN:NE2	2.49	0.46
1:B:704:ALA:O	1:B:705:GLU:HB2	2.14	0.46
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.51	0.46
1:A:281:PHE:O	1:A:282:ASN:C	2.54	0.46
1:C:958:LYS:N	1:C:958:LYS:HD2	2.31	0.46
1:B:198:LEU:HD13	1:B:251:LEU:HD22	1.97	0.46
1:C:813:SER:HB3	1:C:816:LEU:HD21	1.96	0.46
1:A:598:TYR:O	1:A:602:GLU:HB2	2.15	0.46
1:A:153:ASP:HA	1:A:182:TYR:OH	2.16	0.46
1:B:561:SER:O	1:B:838:GLY:HA3	2.16	0.46
1:B:235:ILE:N	1:B:235:ILE:HD12	2.30	0.46
1:C:897:ILE:N	1:C:898:PRO:CD	2.79	0.46
1:B:36:PRO:O	1:B:37:THR:C	2.53	0.46
1:B:137:LEU:O	1:B:137:LEU:HG	2.14	0.46
1:A:600:THR:HG23	1:A:601:LYS:H	1.78	0.46
1:A:740:GLY:O	1:A:794:ALA:N	2.41	0.46
1:C:174:ASP:HB3	1:C:292:LYS:HB2	1.96	0.46
1:C:577:GLN:CD	1:C:578:LEU:H	2.18	0.46
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.98	0.46
1:B:892:TYR:HB2	1:B:897:ILE:CD1	2.41	0.46
1:A:726:GLN:HB2	1:C:235:ILE:HD13	1.98	0.46
1:C:38:ILE:HG21	1:C:466:ILE:CD1	2.42	0.46
1:B:648:THR:HG23	1:B:665:ALA:O	2.15	0.46
1:B:706:ALA:C	1:B:708:LYS:N	2.66	0.46
1:B:937:LEU:HD22	1:B:1011:MET:HE2	1.97	0.46
1:B:398:MET:O	1:B:402:ILE:HB	2.15	0.46
1:B:435:MET:HE2	1:B:435:MET:HA	1.96	0.46
1:B:964:THR:O	1:B:968:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLN:O	1:A:256:ASP:HB3	2.15	0.46
1:C:712:MET:O	1:C:713:LEU:C	2.54	0.46
1:A:781:MET:HE3	1:C:228:GLN:OE1	2.16	0.46
1:A:99:ASP:OD1	1:A:101:ASP:N	2.46	0.46
1:B:61:VAL:HG13	1:B:88:VAL:HG21	1.98	0.46
1:B:316:PHE:CD1	1:C:854:GLY:HA2	2.51	0.46
1:C:758:TYR:CE1	1:C:770:LYS:HD3	2.51	0.46
1:A:186:ILE:HB	1:A:773:VAL:HG23	1.97	0.46
1:C:160:ALA:HB1	1:C:767:ARG:HD2	1.98	0.46
1:C:263:ARG:HD3	1:C:268:ILE:HD12	1.98	0.46
1:A:584:GLN:H	1:A:622:GLN:HE21	1.62	0.46
1:B:345:VAL:HA	1:B:348:ILE:HD12	1.97	0.46
1:A:253:VAL:O	1:A:253:VAL:CG1	2.64	0.46
1:C:142:VAL:C	1:C:143:ILE:HD12	2.36	0.46
1:A:324:VAL:HG12	1:A:325:TYR:N	2.30	0.46
1:C:213:GLN:NE2	1:C:238:THR:HA	2.31	0.46
1:B:927:PHE:CE2	1:B:931:LEU:HD11	2.51	0.46
1:A:180:SER:HB3	1:A:273:GLU:H	1.81	0.46
1:B:224:PRO:HA	1:C:781:MET:CE	2.45	0.46
1:B:700:ASN:C	1:B:702:LEU:H	2.19	0.46
1:A:454:VAL:C	1:A:456:MET:H	2.19	0.46
1:A:330:THR:N	1:A:331:PRO:HD2	2.31	0.46
1:B:695:LEU:HD12	1:B:825:MET:CE	2.46	0.46
1:B:111:LEU:O	1:B:113:LEU:N	2.49	0.46
1:A:406:VAL:C	1:A:408:ASP:H	2.19	0.46
1:C:367:ILE:H	1:C:368:PRO:HD3	1.81	0.46
1:C:261:LEU:O	1:C:264:ASP:HB2	2.16	0.46
1:C:780:ARG:HG3	1:C:780:ARG:O	2.16	0.46
1:C:415:ASN:O	1:C:419:VAL:HG22	2.16	0.46
1:A:540:ARG:HD2	1:A:541:TYR:CZ	2.51	0.46
1:B:343:THR:HA	1:B:346:GLU:HG2	1.98	0.45
1:A:894:SER:CB	1:A:897:ILE:HD13	2.45	0.45
1:C:786:ILE:HD12	1:C:786:ILE:N	2.31	0.45
1:C:183:ALA:O	1:C:185:ARG:HG2	2.16	0.45
1:C:894:SER:O	1:C:898:PRO:CD	2.64	0.45
1:A:742:SER:O	1:A:743:ILE:C	2.54	0.45
1:B:775:SER:OG	1:B:789:TRP:HZ2	1.99	0.45
1:C:518:ARG:NH2	1:C:518:ARG:HA	2.30	0.45
1:B:27:ILE:HG13	1:B:28:LEU:N	2.31	0.45
1:A:917:THR:O	1:A:919:ARG:N	2.49	0.45
1:C:706:ALA:CB	1:C:716:VAL:HG21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:PRO:HB3	1:A:409:ALA:HB1	1.98	0.45
1:A:189:ASN:O	1:A:191:ASN:N	2.50	0.45
1:B:78:MET:HB3	1:B:92:LEU:HD13	1.98	0.45
1:C:344:LEU:HD23	1:C:399:VAL:CG2	2.47	0.45
1:A:799:VAL:HG13	1:A:800:PRO:HD2	1.97	0.45
1:A:626:ILE:HA	1:A:626:ILE:HD13	1.77	0.45
1:B:235:ILE:N	1:B:235:ILE:CD1	2.78	0.45
1:C:342:LYS:C	1:C:344:LEU:H	2.18	0.45
1:C:713:LEU:HD12	1:C:835:LYS:N	2.31	0.45
1:C:843:LEU:O	1:C:847:LEU:HD23	2.17	0.45
1:C:189:ASN:ND2	1:C:191:ASN:H	2.14	0.45
1:B:930:GLY:O	1:B:934:THR:HG23	2.17	0.45
1:C:39:ALA:HB2	1:C:673:GLU:HG2	1.97	0.45
1:B:70:ASN:N	1:B:70:ASN:ND2	2.65	0.45
1:B:537:SER:HA	1:B:540:ARG:NH2	2.31	0.45
1:A:841:MET:O	1:A:845:GLU:HG3	2.17	0.45
1:C:888:LEU:HD13	1:C:901:VAL:HG23	1.99	0.45
1:A:713:LEU:CD2	1:A:714:THR:H	2.30	0.45
1:A:105:VAL:HG21	1:B:105:VAL:HG13	1.98	0.45
1:B:49:TYR:HE1	1:B:60:THR:HG21	1.82	0.45
1:C:934:THR:O	1:C:936:GLY:N	2.50	0.45
1:B:454:VAL:O	1:B:455:PRO:C	2.54	0.45
1:B:318:PRO:HD2	1:B:321:LEU:HD22	1.99	0.45
1:B:193:LEU:HD22	1:B:198:LEU:O	2.17	0.45
1:B:462:SER:OG	1:B:865:GLN:CG	2.64	0.45
1:A:395:MET:HA	1:A:395:MET:HE2	1.98	0.45
1:A:298:ASN:O	1:A:302:THR:HG23	2.16	0.45
1:A:355:MET:HB3	1:A:365:THR:HB	1.97	0.45
1:C:666:PHE:CZ	2:C:2002:RFP:H28C	2.52	0.45
1:B:463:THR:HG21	1:B:869:SER:CB	2.39	0.45
1:C:160:ALA:HA	1:C:767:ARG:NE	2.32	0.45
1:A:579:PRO:O	1:A:580:ALA:O	2.34	0.45
1:B:945:ILE:HD11	1:B:1022:VAL:HB	1.99	0.45
1:B:966:ASP:O	1:B:970:MET:CG	2.65	0.45
1:B:516:PHE:CG	1:B:517:ASN:N	2.84	0.45
1:C:77:TYR:CD2	1:C:77:TYR:N	2.85	0.45
1:A:713:LEU:HB2	1:A:832:ALA:N	2.31	0.45
1:B:326:PRO:HB2	1:B:327:TYR:H	1.63	0.45
1:A:682:PHE:CZ	1:A:857:TYR:CB	2.98	0.45
1:B:169:THR:HG22	1:B:170:SER:N	2.31	0.45
1:A:252:LYS:HB3	1:A:260:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:THR:OG1	1:B:132:SER:CB	2.65	0.45
1:C:577:GLN:HG2	2:C:2002:RFP:H391	1.99	0.45
1:C:35:TYR:CE1	1:C:671:ILE:HG12	2.51	0.45
1:C:548:ILE:HD13	1:C:1017:LEU:HD21	1.98	0.45
1:A:219:LEU:HD23	1:B:754:TRP:CZ3	2.52	0.45
1:B:680:PHE:O	1:B:828:LEU:HD23	2.17	0.45
1:B:651:ALA:O	1:B:655:PHE:HD2	1.99	0.45
1:C:914:LEU:O	1:C:915:ALA:CB	2.64	0.45
1:B:13:TRP:CE3	1:B:488:LEU:HD21	2.52	0.45
1:C:591:LEU:HD23	1:C:613:ASN:HB2	1.98	0.45
1:A:681:ASP:HB3	1:A:860:THR:O	2.16	0.45
1:C:354:VAL:HG21	1:C:980:LEU:O	2.17	0.45
1:C:44:THR:HB	1:C:91:THR:HB	1.99	0.45
1:C:78:MET:HG3	1:C:78:MET:O	2.16	0.45
1:C:365:THR:CG2	1:C:365:THR:O	2.66	0.45
1:B:455:PRO:HG3	1:B:880:SER:HA	1.99	0.45
1:A:380:PHE:CZ	1:A:398:MET:HE1	2.52	0.45
1:B:185:ARG:HH22	1:B:774:MET:CE	2.29	0.44
1:C:53:ASP:O	1:C:54:ALA:CB	2.65	0.44
1:B:983:ILE:CD1	1:B:1012:VAL:HG13	2.47	0.44
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.51	0.44
1:B:240:LEU:HD22	1:B:245:GLU:OE1	2.16	0.44
1:A:103:ALA:O	1:A:107:VAL:HG23	2.17	0.44
1:A:808:ARG:HG2	1:A:808:ARG:HH11	1.83	0.44
1:C:894:SER:C	1:C:896:SER:H	2.20	0.44
1:B:680:PHE:CD1	1:B:859:TRP:CZ3	3.03	0.44
1:C:971:ARG:HB3	1:C:975:ILE:HD13	2.00	0.44
1:B:213:GLN:HB2	1:B:213:GLN:HE21	1.69	0.44
1:B:561:SER:HB3	1:B:563:PHE:CE1	2.52	0.44
1:B:966:ASP:O	1:B:970:MET:HG2	2.17	0.44
1:C:454:VAL:N	1:C:455:PRO:HD2	2.32	0.44
1:C:172:VAL:O	1:C:172:VAL:HG12	2.18	0.44
1:B:671:ILE:C	1:B:673:GLU:H	2.20	0.44
1:C:10:ILE:HG12	1:C:11:PHE:H	1.82	0.44
1:A:1022:VAL:HA	1:A:1025:PHE:CD1	2.52	0.44
1:C:415:ASN:OD1	1:C:418:ARG:NE	2.42	0.44
1:B:83:ASP:OD1	1:B:87:THR:HB	2.17	0.44
1:C:314:GLU:N	1:C:315:PRO:CD	2.80	0.44
1:A:416:VAL:O	1:A:420:MET:HB2	2.17	0.44
1:B:314:GLU:OE2	1:B:323:ILE:HD12	2.18	0.44
1:A:339:GLU:O	1:A:341:VAL:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:696:THR:O	1:C:699:ARG:HG3	2.17	0.44
1:B:187:TRP:O	1:B:266:ALA:HB1	2.17	0.44
1:A:413:VAL:HG23	1:A:493:CYS:SG	2.57	0.44
1:A:901:VAL:HG13	1:A:942:ALA:HB3	1.99	0.44
1:C:203:VAL:HG13	1:C:262:LEU:HD11	1.98	0.44
1:A:587:THR:OG1	1:A:622:GLN:O	2.26	0.44
1:A:884:VAL:O	1:A:888:LEU:HB2	2.17	0.44
1:B:231:ASN:HD22	1:B:232:ALA:N	2.15	0.44
1:A:166:ILE:O	1:A:172:VAL:HG21	2.17	0.44
1:C:653:ARG:O	1:C:655:PHE:O	2.36	0.44
1:B:49:TYR:CE1	1:B:60:THR:HG21	2.52	0.44
1:B:673:GLU:HG2	1:B:861:GLY:HA2	2.00	0.44
1:B:356:TYR:O	1:B:358:PHE:N	2.47	0.44
1:B:402:ILE:HA	1:B:402:ILE:HD12	1.80	0.44
1:B:166:ILE:HA	1:B:169:THR:OG1	2.17	0.44
1:A:171:GLY:O	1:A:172:VAL:C	2.56	0.44
1:B:332:PHE:HB2	1:B:569:GLN:O	2.18	0.44
1:C:307:ARG:HE	1:C:307:ARG:HB3	1.57	0.44
1:A:926:TYR:CE1	1:A:999:ALA:HB1	2.52	0.44
1:B:192:GLU:OE1	1:B:196:PHE:HE2	1.99	0.44
1:C:92:LEU:HD12	1:C:92:LEU:H	1.83	0.44
1:B:289:LEU:CD1	1:B:289:LEU:N	2.79	0.44
1:C:406:VAL:C	1:C:408:ASP:N	2.69	0.44
1:C:394:THR:HG22	1:C:395:MET:CE	2.47	0.44
1:C:5:PHE:CE2	1:C:11:PHE:CD2	2.96	0.44
1:C:415:ASN:ND2	1:C:434:SER:HB2	2.33	0.44
1:A:255:GLN:O	1:A:256:ASP:CB	2.65	0.44
1:A:375:VAL:CG2	1:A:481:SER:HA	2.45	0.44
1:A:225:VAL:HB	1:B:781:MET:HE3	2.00	0.44
1:A:1015:THR:C	1:A:1017:LEU:N	2.71	0.44
1:A:731:ILE:HG12	1:A:746:ILE:HG21	2.00	0.44
1:A:525:HIS:O	1:A:528:THR:HG22	2.18	0.44
1:B:20:MET:CG	1:B:374:VAL:HA	2.48	0.44
1:C:687:GLN:HE21	1:C:687:GLN:HB3	1.48	0.44
1:C:220:GLY:HA3	1:C:231:ASN:HD22	1.82	0.44
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.53	0.44
1:C:427:PRO:HB3	1:C:498:LYS:HD2	1.99	0.44
1:A:907:LEU:HG	1:A:1017:LEU:HD22	2.00	0.44
1:A:235:ILE:O	1:A:235:ILE:HG22	2.16	0.44
1:B:878:ALA:O	1:B:882:ILE:HG12	2.18	0.44
1:B:33:ALA:O	1:B:391:ASN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:ALA:HA	1:B:713:LEU:HD22	2.00	0.43
1:B:190:PRO:HB3	1:B:789:TRP:CD2	2.53	0.43
1:B:143:ILE:CD1	1:B:322:LYS:HB3	2.48	0.43
1:B:562:SER:O	1:B:924:ASP:HA	2.18	0.43
1:C:579:PRO:O	1:C:580:ALA:O	2.36	0.43
1:B:5:PHE:HB3	1:B:12:ALA:HB2	2.00	0.43
1:B:674:LEU:HD23	1:B:674:LEU:HA	1.83	0.43
1:C:368:PRO:CD	1:C:369:THR:H	2.30	0.43
1:C:372:VAL:HG12	1:C:373:PRO:CD	2.34	0.43
1:A:882:ILE:O	1:A:886:LEU:HB2	2.18	0.43
1:C:662:MET:H	1:C:662:MET:HE2	1.83	0.43
1:C:931:LEU:O	1:C:935:ILE:HD13	2.18	0.43
1:B:932:LEU:HA	1:B:935:ILE:HD12	2.00	0.43
1:A:347:ALA:HB3	1:A:402:ILE:HD13	2.00	0.43
1:C:265:VAL:O	1:C:266:ALA:CB	2.63	0.43
1:A:225:VAL:O	1:A:226:LYS:C	2.56	0.43
1:C:445:ILE:O	1:C:448:VAL:N	2.51	0.43
1:A:747:ASN:HD21	1:C:237:GLN:HE22	1.66	0.43
1:C:815:ARG:NH2	2:C:2002:RFP:H302	2.34	0.43
1:B:367:ILE:HD11	1:B:496:MET:HB2	2.00	0.43
1:B:222:THR:CG2	1:B:223:PRO:HD3	2.48	0.43
1:A:578:LEU:HD11	1:A:590:VAL:HG21	1.99	0.43
1:C:683:GLU:HG3	1:C:819:TYR:CD2	2.52	0.43
1:A:184:MET:HB3	1:A:771:VAL:HG13	2.00	0.43
1:C:982:PHE:HD2	1:C:982:PHE:HA	1.77	0.43
1:B:97:GLY:O	1:B:98:THR:O	2.37	0.43
1:B:144:ASN:ND2	1:B:149:MET:H	2.16	0.43
1:A:338:HIS:O	1:A:341:VAL:HG12	2.18	0.43
1:A:406:VAL:O	1:A:408:ASP:N	2.51	0.43
1:A:156:ASP:OD1	1:A:769:LYS:NZ	2.49	0.43
1:B:703:LEU:HD21	1:B:718:PRO:HD3	2.01	0.43
1:A:644:VAL:C	1:A:646:ALA:H	2.21	0.43
1:C:367:ILE:N	1:C:368:PRO:HD3	2.33	0.43
1:A:742:SER:OG	1:A:745:ASP:HB2	2.19	0.43
1:A:894:SER:OG	1:A:898:PRO:HD2	2.19	0.43
1:A:754:TRP:CE3	1:A:780:ARG:HB2	2.53	0.43
1:A:328:ASP:CG	1:A:330:THR:HB	2.39	0.43
1:A:817:GLU:HB2	1:A:824:SER:O	2.18	0.43
1:A:934:THR:C	1:A:936:GLY:N	2.72	0.43
1:C:713:LEU:O	1:C:830:GLN:O	2.37	0.43
1:A:60:THR:HG23	1:A:119:PRO:CG	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:GLN:O	1:C:230:LEU:HB3	2.17	0.43
1:B:225:VAL:HG11	1:C:778:LYS:HB3	2.00	0.43
1:C:792:ARG:HG3	1:C:796:GLY:HA2	2.00	0.43
1:B:606:VAL:CG1	1:B:607:GLU:N	2.82	0.43
1:A:819:TYR:H	1:A:824:SER:HB3	1.83	0.43
1:C:34:GLN:CG	1:C:333:VAL:HG21	2.48	0.43
1:B:544:LEU:HB3	1:B:1021:PHE:HZ	1.82	0.43
1:B:449:LEU:HD23	1:B:478:MET:SD	2.59	0.43
1:A:187:TRP:O	1:A:188:MET:O	2.37	0.43
1:A:848:ALA:HA	1:A:851:LEU:HD12	2.01	0.43
1:B:145:THR:HG23	1:B:320:GLY:CA	2.48	0.43
1:A:356:TYR:C	1:A:358:PHE:H	2.22	0.43
1:A:636:ASP:O	1:A:638:PRO:HD3	2.18	0.43
1:B:183:ALA:N	1:B:271:GLY:O	2.48	0.43
1:C:713:LEU:CD2	1:C:830:GLN:O	2.65	0.43
1:C:247:GLY:CA	1:C:263:ARG:HD3	2.49	0.43
1:A:29:LYS:CG	1:A:30:LEU:H	2.32	0.43
1:A:899:PHE:O	1:A:903:LEU:HG	2.19	0.43
1:B:119:PRO:HB2	1:B:122:VAL:HG23	2.01	0.43
1:B:952:LEU:HG	1:B:956:GLU:OE1	2.18	0.43
1:C:577:GLN:CD	1:C:578:LEU:N	2.72	0.43
1:A:352:PHE:HD1	1:A:353:LEU:HD12	1.84	0.43
1:B:768:VAL:HG23	1:C:63:GLN:CD	2.39	0.43
1:B:94:PHE:CB	1:B:98:THR:HG21	2.41	0.42
1:C:341:VAL:O	1:C:344:LEU:HB3	2.19	0.42
1:C:186:ILE:CG2	1:C:186:ILE:O	2.66	0.42
1:C:241:THR:HG22	1:C:245:GLU:OE2	2.19	0.42
1:C:697:GLN:O	1:C:700:ASN:HB2	2.19	0.42
1:B:169:THR:HB	1:B:172:VAL:HG21	2.00	0.42
1:C:569:GLN:C	1:C:634:TRP:HZ2	2.23	0.42
1:C:736:ALA:C	1:C:738:ALA:H	2.22	0.42
1:A:166:ILE:HD13	1:A:166:ILE:N	2.34	0.42
1:B:962:GLU:O	1:B:966:ASP:HB2	2.18	0.42
1:C:66:GLU:HA	1:C:69:MET:HB2	2.00	0.42
1:B:157:TYR:HA	1:B:161:ASN:ND2	2.34	0.42
1:C:331:PRO:O	1:C:332:PHE:C	2.57	0.42
1:B:790:TYR:HD1	1:B:800:PRO:HA	1.84	0.42
1:C:731:ILE:HG12	1:C:746:ILE:HG21	2.01	0.42
1:C:785:ASP:C	1:C:787:GLY:N	2.72	0.42
1:B:351:VAL:O	1:B:352:PHE:C	2.57	0.42
1:A:758:TYR:HB2	1:A:772:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:886:LEU:O	1:C:890:ALA:HB2	2.19	0.42
1:C:131:LYS:HG3	1:C:131:LYS:O	2.18	0.42
1:B:314:GLU:N	1:B:315:PRO:HD3	2.34	0.42
1:B:708:LYS:O	1:B:708:LYS:HG2	2.19	0.42
1:B:828:LEU:HB3	1:B:829:GLY:H	1.76	0.42
1:A:660:ASP:O	1:A:661:ALA:HB2	2.18	0.42
1:B:393:LEU:HD13	1:B:466:ILE:HG23	2.01	0.42
1:B:961:ILE:HG22	1:B:961:ILE:O	2.19	0.42
1:A:335:ILE:O	1:A:339:GLU:HG3	2.19	0.42
1:A:426:PRO:HB3	1:A:427:PRO:HD2	2.00	0.42
1:B:897:ILE:N	1:B:898:PRO:CD	2.83	0.42
1:C:767:ARG:CG	1:C:767:ARG:NH1	2.69	0.42
1:A:655:PHE:O	1:A:658:ILE:HG13	2.19	0.42
1:B:372:VAL:HG22	1:B:373:PRO:HD3	2.00	0.42
1:A:596:HIS:O	1:A:597:TYR:C	2.58	0.42
1:B:669:PRO:HB2	1:B:862:MET:CE	2.50	0.42
1:C:591:LEU:HD13	1:C:591:LEU:HA	1.90	0.42
1:A:617:PHE:O	1:A:618:ALA:HB3	2.20	0.42
1:A:571:VAL:HG12	1:A:630:SER:HB3	2.00	0.42
1:C:328:ASP:OD1	1:C:328:ASP:C	2.58	0.42
1:B:250:LEU:HD11	1:B:253:VAL:HG23	2.01	0.42
1:B:780:ARG:HG2	1:B:780:ARG:O	2.19	0.42
1:C:331:PRO:HG2	1:C:332:PHE:H	1.85	0.42
1:A:355:MET:HG2	1:A:365:THR:HA	2.02	0.42
1:B:99:ASP:OD2	1:B:99:ASP:C	2.57	0.42
1:C:355:MET:HE2	1:C:355:MET:HA	1.96	0.42
1:C:372:VAL:HG21	1:C:406:VAL:HG22	2.02	0.42
1:B:990:VAL:HG13	1:B:1005:THR:OG1	2.19	0.42
1:C:30:LEU:HD21	1:C:384:ALA:HA	2.01	0.42
1:C:466:ILE:N	1:C:466:ILE:HD13	2.35	0.42
1:A:655:PHE:O	1:A:657:GLN:N	2.41	0.42
1:A:702:LEU:HB2	1:A:851:LEU:HD11	2.01	0.42
1:A:323:ILE:O	1:A:323:ILE:HG13	2.20	0.42
1:A:400:LEU:HD12	1:A:400:LEU:O	2.20	0.42
1:C:644:VAL:HG12	1:C:667:ASN:HB2	2.02	0.42
1:B:343:THR:O	1:B:347:ALA:HB2	2.20	0.42
1:A:780:ARG:NH1	1:A:780:ARG:CG	2.82	0.42
1:A:187:TRP:HA	1:A:774:MET:O	2.19	0.42
1:A:141:GLY:N	1:A:324:VAL:O	2.46	0.42
1:B:848:ALA:C	1:B:850:LYS:H	2.23	0.42
1:B:701:GLN:HB3	1:B:851:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:941:ASN:HA	1:C:944:LEU:HD12	2.02	0.42
1:C:672:VAL:HG13	1:C:675:GLY:N	2.34	0.42
1:B:568:ASP:HA	1:B:644:VAL:CG2	2.49	0.42
1:A:565:PRO:HG2	1:A:999:ALA:HA	2.01	0.42
1:B:972:LEU:HD21	1:B:1019:ILE:HD12	2.02	0.42
1:C:869:SER:HB2	1:C:870:GLY:H	1.71	0.42
1:A:1007:VAL:O	1:A:1011:MET:HB2	2.20	0.42
1:B:692:HIS:ND1	1:B:692:HIS:O	2.53	0.42
1:A:701:GLN:HE21	1:A:701:GLN:HB2	1.61	0.42
1:C:577:GLN:O	1:C:661:ALA:HB1	2.19	0.42
1:B:204:ILE:HG23	1:B:759:VAL:HG13	2.02	0.42
1:B:216:ALA:HB2	1:B:236:ALA:HB2	2.02	0.42
1:A:395:MET:HA	1:A:395:MET:CE	2.48	0.42
1:A:897:ILE:HD11	1:A:1030:ARG:HD3	2.01	0.42
1:C:137:LEU:N	1:C:291:ILE:O	2.52	0.42
1:A:552:MET:CE	1:A:906:PRO:HB3	2.50	0.42
1:A:203:VAL:O	1:A:207:ILE:HG13	2.20	0.42
1:C:897:ILE:O	1:C:900:SER:OG	2.31	0.42
1:A:49:TYR:O	1:A:52:ALA:HB2	2.20	0.42
1:B:704:ALA:O	1:B:705:GLU:CB	2.68	0.42
1:C:574:THR:HB	1:C:627:ALA:HB3	2.02	0.42
1:A:367:ILE:HG13	1:A:368:PRO:HD3	2.02	0.42
1:B:970:MET:HA	1:B:970:MET:CE	2.50	0.42
1:B:970:MET:HE2	1:B:970:MET:HA	2.02	0.42
1:A:295:THR:O	1:A:295:THR:HG22	2.20	0.42
1:C:668:LEU:H	1:C:668:LEU:HD23	1.85	0.42
1:A:589:LYS:HA	1:A:589:LYS:HD3	1.81	0.42
1:C:35:TYR:CD1	1:C:671:ILE:HG12	2.55	0.41
1:A:713:LEU:CG	1:A:714:THR:H	2.33	0.41
1:C:189:ASN:C	1:C:189:ASN:HD22	2.23	0.41
1:A:63:GLN:OE1	1:C:767:ARG:HA	2.20	0.41
1:C:240:LEU:HB3	1:C:245:GLU:HB2	2.02	0.41
1:B:391:ASN:OD1	1:B:394:THR:N	2.35	0.41
1:C:426:PRO:HA	1:C:427:PRO:HD3	1.64	0.41
1:A:20:MET:HG3	1:A:374:VAL:HG22	2.02	0.41
1:B:580:ALA:O	1:B:581:GLY:C	2.58	0.41
1:B:204:ILE:H	1:B:204:ILE:HG12	1.74	0.41
1:B:367:ILE:HG13	1:B:492:LEU:CB	2.28	0.41
1:B:983:ILE:HD12	1:B:1012:VAL:CG1	2.50	0.41
1:B:700:ASN:O	1:B:704:ALA:CB	2.68	0.41
1:B:852:PRO:HA	1:B:855:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:HG23	1:A:106:GLN:HE21	1.84	0.41
1:A:578:LEU:O	1:A:623:ASN:ND2	2.53	0.41
1:B:186:ILE:HD13	1:B:262:LEU:HD11	2.02	0.41
1:B:38:ILE:HG23	1:B:462:SER:HB2	2.01	0.41
1:B:34:GLN:HE21	1:B:332:PHE:HE2	1.68	0.41
1:A:282:ASN:HD22	1:A:282:ASN:HA	1.62	0.41
1:B:280:GLU:HG2	1:B:611:ALA:HB3	2.01	0.41
1:A:895:TRP:HZ2	1:C:13:TRP:HE3	1.67	0.41
1:C:284:GLN:HB2	1:C:284:GLN:HE21	1.65	0.41
1:C:388:PHE:CD1	1:C:388:PHE:N	2.87	0.41
1:C:222:THR:O	1:C:223:PRO:C	2.58	0.41
1:A:1029:VAL:HG12	1:A:1030:ARG:N	2.33	0.41
1:B:58:GLN:HE22	1:B:818:ARG:NH1	2.18	0.41
1:A:983:ILE:HG13	1:A:984:LEU:N	2.35	0.41
1:B:55:LYS:C	1:B:57:VAL:H	2.20	0.41
1:C:445:ILE:O	1:C:448:VAL:HG12	2.19	0.41
1:A:340:VAL:O	1:A:344:LEU:HB2	2.20	0.41
1:A:575:MET:HG2	1:A:626:ILE:HD11	2.02	0.41
1:A:533:GLY:C	1:A:535:LEU:H	2.24	0.41
1:A:818:ARG:NH2	1:A:821:GLY:O	2.52	0.41
2:C:2002:RFP:O4	2:C:2002:RFP:O12	2.35	0.41
1:C:34:GLN:HA	1:C:333:VAL:HG13	2.01	0.41
1:B:216:ALA:HB3	1:B:234:ILE:O	2.21	0.41
1:B:10:ILE:H	1:B:10:ILE:HG13	1.62	0.41
1:B:154:ILE:HD11	1:B:286:ALA:HA	2.02	0.41
1:A:194:ASN:ND2	1:A:790:TYR:CE2	2.88	0.41
1:C:873:ALA:C	1:C:875:SER:N	2.74	0.41
1:B:396:PHE:CD2	1:B:1003:VAL:HG21	2.54	0.41
1:C:2:PRO:O	1:C:6:ILE:HG12	2.21	0.41
1:C:901:VAL:HG11	1:C:943:ILE:HA	2.01	0.41
1:C:748:THR:O	1:C:752:ALA:CB	2.69	0.41
1:C:456:MET:CA	1:C:459:PHE:HE1	2.28	0.41
1:B:1017:LEU:N	1:B:1017:LEU:HD12	2.35	0.41
1:A:6:ILE:HG21	1:A:490:PRO:HB2	2.02	0.41
1:B:680:PHE:HZ	1:B:716:VAL:HG22	1.84	0.41
1:C:467:TYR:CZ	1:C:925:VAL:HG12	2.56	0.41
1:A:301:ASP:O	1:A:305:ALA:N	2.49	0.41
1:A:895:TRP:HZ2	1:C:13:TRP:CE3	2.38	0.41
1:B:545:TYR:C	1:B:547:ILE:H	2.24	0.41
1:A:836:SER:O	1:A:839:GLU:HG2	2.21	0.41
1:B:564:LEU:HA	1:B:565:PRO:HD3	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLN:HB2	1:A:89:GLN:HE21	1.62	0.41
1:C:21:LEU:HA	1:C:21:LEU:HD23	1.83	0.41
1:C:34:GLN:O	1:C:392:THR:HG23	2.20	0.41
1:B:14:VAL:HG21	1:C:886:LEU:O	2.21	0.41
1:C:189:ASN:HA	1:C:190:PRO:HD3	1.80	0.41
1:A:733:GLN:O	1:A:734:GLU:C	2.59	0.41
1:B:317:PHE:HB3	1:B:321:LEU:HB3	2.03	0.41
1:B:462:SER:O	1:B:466:ILE:HG12	2.20	0.41
1:A:200:PRO:CD	1:A:749:THR:HG23	2.51	0.41
1:B:613:ASN:C	1:B:615:PHE:H	2.23	0.41
1:C:592:ASN:O	1:C:593:GLU:CB	2.65	0.41
1:A:685:ILE:HD11	1:A:819:TYR:HD1	1.86	0.41
1:C:92:LEU:HD12	1:C:92:LEU:N	2.35	0.41
1:A:183:ALA:N	1:A:271:GLY:O	2.53	0.41
1:B:369:THR:C	1:B:371:ALA:H	2.24	0.41
1:B:121:GLU:HG2	1:B:121:GLU:H	1.42	0.41
1:B:200:PRO:O	1:B:204:ILE:HG12	2.20	0.41
1:A:733:GLN:HE22	1:A:743:ILE:HG12	1.85	0.41
1:A:655:PHE:C	1:A:657:GLN:H	2.22	0.41
1:A:579:PRO:CG	1:A:660:ASP:HB2	2.47	0.41
1:A:600:THR:C	1:A:602:GLU:H	2.23	0.41
1:A:66:GLU:C	1:A:68:ASN:H	2.24	0.41
1:B:997:SER:C	1:B:999:ALA:N	2.73	0.41
1:B:695:LEU:HD12	1:B:825:MET:HE3	2.01	0.41
1:B:406:VAL:O	1:B:407:ASP:C	2.59	0.41
1:A:222:THR:O	1:A:223:PRO:C	2.59	0.41
1:C:262:LEU:HD23	1:C:268:ILE:HD11	2.03	0.41
1:B:190:PRO:HB3	1:B:789:TRP:CE3	2.55	0.41
1:B:213:GLN:HE21	1:B:239:ARG:CD	2.30	0.41
1:B:527:TYR:HA	1:B:530:SER:CB	2.49	0.41
1:B:790:TYR:CE1	1:B:800:PRO:HB3	2.55	0.41
1:C:801:PHE:CD1	1:C:804:PHE:CE1	3.09	0.41
1:B:34:GLN:HB2	1:B:333:VAL:HG22	2.03	0.41
1:C:83:ASP:HB3	1:C:85:THR:H	1.86	0.41
1:A:186:ILE:HD13	1:A:262:LEU:HD21	2.02	0.41
1:A:845:GLU:O	1:A:848:ALA:HB3	2.21	0.41
1:A:895:TRP:HA	1:A:895:TRP:CE3	2.55	0.41
1:B:899:PHE:O	1:B:903:LEU:HG	2.21	0.41
1:B:45:ILE:HB	1:B:90:ILE:HB	2.03	0.41
1:C:1:MET:CB	1:C:2:PRO:CD	2.97	0.41
1:C:832:ALA:CB	1:C:833:PRO:CD	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ASN:O	1:A:392:THR:C	2.58	0.41
1:A:467:TYR:CE1	1:A:925:VAL:HG13	2.56	0.41
1:C:5:PHE:HE2	1:C:11:PHE:HD2	1.60	0.41
1:B:973:ARG:O	1:B:977:MET:HG2	2.21	0.41
1:C:934:THR:O	1:C:935:ILE:C	2.59	0.41
1:A:607:GLU:HB3	1:A:630:SER:O	2.20	0.41
1:A:294:ALA:O	1:A:295:THR:CB	2.69	0.41
1:A:516:PHE:O	1:A:519:MET:N	2.50	0.41
1:A:519:MET:O	1:A:523:SER:HB2	2.20	0.41
1:C:218:GLN:HG3	1:C:233:SER:HA	2.03	0.41
1:C:474:ILE:O	1:C:476:SER:O	2.38	0.41
1:B:723:ASP:O	1:B:724:THR:HB	2.21	0.41
1:B:686:ASP:HB3	1:B:823:PRO:HG2	2.01	0.41
1:B:948:PHE:HB2	1:B:971:ARG:NH2	2.36	0.41
1:B:908:GLY:CA	1:B:1014:ALA:HB2	2.50	0.41
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	2.03	0.41
1:A:651:ALA:O	1:A:652:THR:C	2.58	0.41
1:C:144:ASN:HD22	1:C:149:MET:H	1.66	0.40
1:C:34:GLN:HB2	1:C:35:TYR:CD1	2.55	0.40
1:A:139:VAL:O	1:A:326:PRO:HD2	2.21	0.40
1:C:888:LEU:C	1:C:890:ALA:N	2.72	0.40
1:B:356:TYR:CD2	1:B:365:THR:HG21	2.56	0.40
1:C:325:TYR:O	1:C:326:PRO:O	2.39	0.40
1:A:83:ASP:HA	1:A:815:ARG:HA	2.03	0.40
1:A:66:GLU:C	1:A:68:ASN:N	2.74	0.40
1:A:516:PHE:O	1:A:518:ARG:N	2.54	0.40
1:A:659:LYS:CG	1:A:660:ASP:N	2.83	0.40
1:A:150:THR:O	1:A:154:ILE:HG13	2.21	0.40
1:C:541:TYR:C	1:C:543:VAL:N	2.73	0.40
1:A:633:ASP:O	1:A:636:ASP:N	2.46	0.40
1:A:617:PHE:O	1:A:618:ALA:CB	2.69	0.40
1:A:951:ASP:C	1:A:953:MET:H	2.25	0.40
1:B:635:ALA:C	1:B:637:ARG:H	2.24	0.40
1:C:658:ILE:C	1:C:659:LYS:HD2	2.42	0.40
1:A:559:LEU:HA	1:A:560:PRO:HD3	1.92	0.40
1:C:220:GLY:HA2	1:C:228:GLN:HE21	1.84	0.40
1:B:346:GLU:HG3	1:B:988:PRO:HG3	2.03	0.40
1:C:203:VAL:HG13	1:C:262:LEU:CD1	2.51	0.40
1:B:705:GLU:O	1:B:708:LYS:N	2.55	0.40
1:C:610:PHE:HB3	1:C:628:PHE:HB2	2.04	0.40
1:B:598:TYR:HH	1:B:655:PHE:HE2	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:885:PHE:CE2	1:C:899:PHE:CE1	3.09	0.40
1:B:632:LYS:O	1:B:633:ASP:O	2.40	0.40
1:A:759:VAL:HG12	1:A:760:ASN:N	2.37	0.40
1:A:666:PHE:N	1:A:666:PHE:CD1	2.90	0.40
1:C:1016:VAL:HG23	1:C:1017:LEU:H	1.86	0.40
1:C:226:LYS:HB3	1:C:227:GLY:H	1.74	0.40
1:C:398:MET:HA	1:C:398:MET:HE2	2.03	0.40
1:B:110:LYS:HA	1:B:110:LYS:HD2	1.92	0.40
1:A:456:MET:HG2	1:A:471:SER:HB2	2.04	0.40
1:B:197:GLN:HB3	1:B:798:MET:HE3	2.03	0.40
1:A:707:ALA:O	1:A:710:PRO:CD	2.66	0.40
1:B:445:ILE:HD11	1:B:944:LEU:HD21	2.01	0.40
1:C:754:TRP:CE3	1:C:780:ARG:HB2	2.57	0.40
1:A:281:PHE:CZ	1:A:608:SER:HB2	2.57	0.40
1:A:140:VAL:HG12	1:A:141:GLY:N	2.37	0.40
1:B:703:LEU:HD12	1:B:703:LEU:H	1.85	0.40
1:A:169:THR:CG2	1:A:309:GLU:HG3	2.52	0.40
1:B:183:ALA:O	1:B:184:MET:C	2.59	0.40
1:B:185:ARG:HH22	1:B:774:MET:HE2	1.87	0.40
1:A:658:ILE:HG22	1:A:659:LYS:H	1.86	0.40
1:C:425:LEU:CB	1:C:426:PRO:HD3	2.47	0.40
1:B:450:SER:OG	1:B:478:MET:HB2	2.20	0.40
1:B:594:VAL:HA	1:B:655:PHE:CE1	2.56	0.40
1:B:576:VAL:HG11	1:B:591:LEU:HD22	2.02	0.40
1:C:732:ASP:O	1:C:733:GLN:C	2.58	0.40
1:C:314:GLU:HA	1:C:317:PHE:CE2	2.57	0.40
1:B:192:GLU:OE1	1:B:196:PHE:CE2	2.74	0.40
1:C:388:PHE:HD1	1:C:388:PHE:N	2.19	0.40
1:C:1015:THR:O	1:C:1019:ILE:HB	2.21	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	1018/1053 (97%)	769 (76%)	174 (17%)	75 (7%)	1	11
1	B	1018/1053 (97%)	742 (73%)	193 (19%)	83 (8%)	1	9
1	C	1018/1053 (97%)	754 (74%)	182 (18%)	82 (8%)	1	9
All	All	3054/3159 (97%)	2265 (74%)	549 (18%)	240 (8%)	1	9

All (240) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	VAL
1	A	188	MET
1	A	239	ARG
1	A	256	ASP
1	A	293	LEU
1	A	295	THR
1	A	357	LEU
1	A	421	ALA
1	A	517	ASN
1	A	534	ILE
1	A	580	ALA
1	A	618	ALA
1	A	659	LYS
1	A	677	ALA
1	A	713	LEU
1	A	832	ALA
1	A	998	GLY
1	A	1008	MET
1	A	1016	VAL
1	B	98	THR
1	B	147	GLY
1	B	184	MET
1	B	222	THR
1	B	270	LEU
1	B	326	PRO
1	B	358	PHE
1	B	517	ASN
1	B	519	MET
1	B	633	ASP
1	B	669	PRO
1	B	676	THR
1	B	705	GLU
1	B	716	VAL
1	B	723	ASP

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Mol	Chain	Res	Type
1	B	733	GLN
1	B	781	MET
1	B	871	ASN
1	C	54	ALA
1	C	223	PRO
1	C	226	LYS
1	C	258	SER
1	C	266	ALA
1	C	319	SER
1	C	326	PRO
1	C	407	ASP
1	C	425	LEU
1	C	427	PRO
1	C	438	ILE
1	C	457	ALA
1	C	463	THR
1	C	532	GLY
1	C	580	ALA
1	C	656	SER
1	C	678	THR
1	C	820	ASN
1	C	825	MET
1	C	869	SER
1	C	946	VAL
1	C	1018	ALA
1	A	5	PHE
1	A	134	SER
1	A	146	ASP
1	A	221	GLY
1	A	236	ALA
1	A	288	GLY
1	A	352	PHE
1	A	407	ASP
1	A	452	VAL
1	A	462	SER
1	A	496	MET
1	A	566	ASP
1	A	634	TRP
1	A	656	SER
1	A	689	GLY
1	A	708	LYS
1	A	787	GLY

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Mol	Chain	Res	Type
1	A	831	ALA
1	A	918	PHE
1	A	951	ASP
1	A	960	LEU
1	A	991	ILE
1	B	37	THR
1	B	53	ASP
1	B	54	ALA
1	B	56	THR
1	B	57	VAL
1	B	227	GLY
1	B	228	GLN
1	B	283	GLY
1	B	361	ASN
1	B	370	ILE
1	B	384	ALA
1	B	453	PHE
1	B	461	GLY
1	B	486	LEU
1	B	557	VAL
1	B	580	ALA
1	B	581	GLY
1	B	613	ASN
1	B	614	GLY
1	B	638	PRO
1	B	656	SER
1	B	671	ILE
1	B	675	GLY
1	B	706	ALA
1	B	765	ARG
1	B	849	SER
1	B	852	PRO
1	B	889	ALA
1	B	953	MET
1	C	216	ALA
1	C	689	GLY
1	C	713	LEU
1	C	720	GLY
1	C	752	ALA
1	C	802	SER
1	C	815	ARG
1	C	832	ALA

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Mol	Chain	Res	Type
1	C	889	ALA
1	C	926	TYR
1	C	935	ILE
1	C	953	MET
1	C	958	LYS
1	C	961	ILE
1	C	993	THR
1	C	1017	LEU
1	A	30	LEU
1	A	53	ASP
1	A	171	GLY
1	A	226	LYS
1	A	282	ASN
1	A	330	THR
1	A	392	THR
1	A	436	GLY
1	A	439	GLN
1	A	443	VAL
1	A	638	PRO
1	A	661	ALA
1	A	914	LEU
1	A	917	THR
1	A	988	PRO
1	A	997	SER
1	B	140	VAL
1	B	269	GLU
1	B	299	ALA
1	B	319	SER
1	B	363	ARG
1	B	385	ALA
1	B	583	THR
1	B	601	LYS
1	B	602	GLU
1	B	672	VAL
1	B	707	ALA
1	B	779	TYR
1	B	851	LEU
1	B	893	GLU
1	B	909	VAL
1	B	921	LEU
1	B	959	GLY
1	C	243	THR

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Mol	Chain	Res	Type
1	C	255	GLN
1	C	368	PRO
1	C	478	MET
1	C	520	PHE
1	C	530	SER
1	C	579	PRO
1	C	602	GLU
1	C	690	LEU
1	C	711	ASP
1	C	721	LEU
1	C	778	LYS
1	C	806	SER
1	C	925	VAL
1	C	994	GLY
1	A	9	PRO
1	A	52	ALA
1	A	184	MET
1	A	193	LEU
1	A	294	ALA
1	A	992	SER
1	B	153	ASP
1	B	618	ALA
1	B	690	LEU
1	B	820	ASN
1	B	997	SER
1	B	1016	VAL
1	C	69	MET
1	C	257	GLY
1	C	351	VAL
1	C	422	GLU
1	C	514	GLY
1	C	516	PHE
1	C	554	TYR
1	C	601	LYS
1	C	671	ILE
1	C	915	ALA
1	C	952	LEU
1	C	965	LEU
1	A	361	ASN
1	A	459	PHE
1	B	126	GLY
1	B	127	VAL

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Mol	Chain	Res	Type
1	B	360	GLN
1	B	603	LYS
1	B	640	GLU
1	C	230	LEU
1	C	372	VAL
1	C	464	GLY
1	C	803	ALA
1	C	982	PHE
1	C	995	ALA
1	A	29	LYS
1	A	192	GLU
1	A	584	GLN
1	A	806	SER
1	A	994	GLY
1	A	1004	GLY
1	B	490	PRO
1	B	542	LEU
1	B	621	GLY
1	B	861	GLY
1	C	86	GLY
1	C	534	ILE
1	C	1005	THR
1	A	15	ILE
1	A	746	ILE
1	A	975	ILE
1	B	783	PRO
1	B	834	GLY
1	B	974	PRO
1	C	539	GLY
1	C	998	GLY
1	A	107	VAL
1	C	743	ILE
1	B	223	PRO
1	C	658	ILE
1	C	756	GLY
1	C	759	VAL
1	C	411	VAL
1	C	716	VAL

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	833/859 (97%)	712 (86%)	121 (14%)	4	18
1	B	833/859 (97%)	705 (85%)	128 (15%)	3	16
1	C	833/859 (97%)	718 (86%)	115 (14%)	4	20
All	All	2499/2577 (97%)	2135 (85%)	364 (15%)	4	18

All (364) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	5	PHE
1	A	25	LEU
1	A	49	TYR
1	A	57	VAL
1	A	60	THR
1	A	62	THR
1	A	63	GLN
1	A	65	ILE
1	A	70	ASN
1	A	76	MET
1	A	82	SER
1	A	84	SER
1	A	89	GLN
1	A	137	LEU
1	A	164	ASP
1	A	175	VAL
1	A	176	GLN
1	A	225	VAL
1	A	244	GLU
1	A	254	ASN
1	A	255	GLN
1	A	256	ASP
1	A	301	ASP
1	A	302	THR
1	A	310	LEU

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Mol	Chain	Res	Type
1	A	321	LEU
1	A	335	ILE
1	A	336	SER
1	A	337	ILE
1	A	341	VAL
1	A	344	LEU
1	A	356	TYR
1	A	357	LEU
1	A	361	ASN
1	A	365	THR
1	A	376	LEU
1	A	400	LEU
1	A	416	VAL
1	A	417	GLU
1	A	420	MET
1	A	422	GLU
1	A	428	LYS
1	A	435	MET
1	A	447	MET
1	A	452	VAL
1	A	473	THR
1	A	480	LEU
1	A	489	THR
1	A	498	LYS
1	A	536	ARG
1	A	549	VAL
1	A	575	MET
1	A	576	VAL
1	A	577	GLN
1	A	578	LEU
1	A	583	THR
1	A	595	THR
1	A	597	TYR
1	A	603	LYS
1	A	613	ASN
1	A	620	ARG
1	A	626	ILE
1	A	629	VAL
1	A	630	SER
1	A	634	TRP
1	A	636	ASP
1	A	645	GLU

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Mol	Chain	Res	Type
1	A	653	ARG
1	A	659	LYS
1	A	666	PHE
1	A	667	ASN
1	A	668	LEU
1	A	671	ILE
1	A	673	GLU
1	A	674	LEU
1	A	687	GLN
1	A	711	ASP
1	A	713	LEU
1	A	714	THR
1	A	717	ARG
1	A	724	THR
1	A	739	LEU
1	A	745	ASP
1	A	773	VAL
1	A	775	SER
1	A	776	GLU
1	A	780	ARG
1	A	801	PHE
1	A	810	GLU
1	A	815	ARG
1	A	820	ASN
1	A	827	ILE
1	A	828	LEU
1	A	837	THR
1	A	843	LEU
1	A	863	SER
1	A	868	LEU
1	A	876	LEU
1	A	881	LEU
1	A	887	CYS
1	A	895	TRP
1	A	899	PHE
1	A	902	MET
1	A	904	VAL
1	A	923	ASN
1	A	924	ASP
1	A	948	PHE
1	A	954	ASP
1	A	960	LEU

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Mol	Chain	Res	Type
1	A	968	VAL
1	A	971	ARG
1	A	982	PHE
1	A	983	ILE
1	A	986	VAL
1	A	993	THR
1	A	997	SER
1	A	1005	THR
1	A	1011	MET
1	A	1017	LEU
1	A	1019	ILE
1	B	3	ASN
1	B	13	TRP
1	B	19	ILE
1	B	27	ILE
1	B	30	LEU
1	B	37	THR
1	B	49	TYR
1	B	56	THR
1	B	60	THR
1	B	65	ILE
1	B	70	ASN
1	B	83	ASP
1	B	85	THR
1	B	96	SER
1	B	104	GLN
1	B	121	GLU
1	B	131	LYS
1	B	136	PHE
1	B	137	LEU
1	B	145	THR
1	B	146	ASP
1	B	150	THR
1	B	151	GLN
1	B	155	SER
1	B	156	ASP
1	B	163	LYS
1	B	164	ASP
1	B	176	GLN
1	B	185	ARG
1	B	189	ASN
1	B	213	GLN

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Mol	Chain	Res	Type
1	B	226	LYS
1	B	231	ASN
1	B	235	ILE
1	B	238	THR
1	B	241	THR
1	B	251	LEU
1	B	254	ASN
1	B	256	ASP
1	B	262	LEU
1	B	289	LEU
1	B	292	LYS
1	B	293	LEU
1	B	295	THR
1	B	298	ASN
1	B	300	LEU
1	B	302	THR
1	B	341	VAL
1	B	343	THR
1	B	349	ILE
1	B	350	LEU
1	B	372	VAL
1	B	380	PHE
1	B	389	SER
1	B	408	ASP
1	B	414	GLU
1	B	417	GLU
1	B	429	GLU
1	B	435	MET
1	B	438	ILE
1	B	468	ARG
1	B	469	GLN
1	B	483	LEU
1	B	497	LEU
1	B	530	SER
1	B	540	ARG
1	B	544	LEU
1	B	546	LEU
1	B	554	TYR
1	B	562	SER
1	B	566	ASP
1	B	571	VAL
1	B	589	LYS

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Mol	Chain	Res	Type
1	B	599	LEU
1	B	603	LYS
1	B	605	ASN
1	B	607	GLU
1	B	613	ASN
1	B	620	ARG
1	B	623	ASN
1	B	626	ILE
1	B	629	VAL
1	B	642	ASN
1	B	644	VAL
1	B	653	ARG
1	B	658	ILE
1	B	660	ASP
1	B	668	LEU
1	B	681	ASP
1	B	695	LEU
1	B	702	LEU
1	B	712	MET
1	B	714	THR
1	B	717	ARG
1	B	723	ASP
1	B	741	VAL
1	B	744	ASN
1	B	750	LEU
1	B	758	TYR
1	B	770	LYS
1	B	776	GLU
1	B	778	LYS
1	B	779	TYR
1	B	799	VAL
1	B	801	PHE
1	B	808	ARG
1	B	817	GLU
1	B	825	MET
1	B	867	ARG
1	B	871	ASN
1	B	876	LEU
1	B	879	ILE
1	B	897	ILE
1	B	900	SER
1	B	910	ILE

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Mol	Chain	Res	Type
1	B	919	ARG
1	B	922	THR
1	B	925	VAL
1	B	948	PHE
1	B	950	LYS
1	B	958	LYS
1	B	966	ASP
1	B	972	LEU
1	B	973	ARG
1	B	993	THR
1	B	1007	VAL
1	B	1022	VAL
1	B	1030	ARG
1	C	10	ILE
1	C	13	TRP
1	C	34	GLN
1	C	35	TYR
1	C	38	ILE
1	C	44	THR
1	C	46	SER
1	C	48	SER
1	C	49	TYR
1	C	63	GLN
1	C	69	MET
1	C	75	LEU
1	C	84	SER
1	C	91	THR
1	C	108	GLN
1	C	111	LEU
1	C	118	LEU
1	C	123	GLN
1	C	128	SER
1	C	131	LYS
1	C	134	SER
1	C	135	SER
1	C	137	LEU
1	C	152	GLU
1	C	155	SER
1	C	177	LEU
1	C	186	ILE
1	C	189	ASN
1	C	192	GLU

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Mol	Chain	Res	Type
1	C	204	ILE
1	C	205	THR
1	C	208	LYS
1	C	222	THR
1	C	226	LYS
1	C	230	LEU
1	C	233	SER
1	C	238	THR
1	C	255	GLN
1	C	263	ARG
1	C	269	GLU
1	C	274	ASN
1	C	275	TYR
1	C	284	GLN
1	C	295	THR
1	C	302	THR
1	C	307	ARG
1	C	330	THR
1	C	339	GLU
1	C	348	ILE
1	C	355	MET
1	C	356	TYR
1	C	361	ASN
1	C	362	PHE
1	C	369	THR
1	C	372	VAL
1	C	377	LEU
1	C	386	PHE
1	C	394	THR
1	C	410	ILE
1	C	422	GLU
1	C	438	ILE
1	C	454	VAL
1	C	456	MET
1	C	459	PHE
1	C	463	THR
1	C	483	LEU
1	C	496	MET
1	C	497	LEU
1	C	515	TRP
1	C	520	PHE
1	C	544	LEU

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Mol	Chain	Res	Type
1	C	555	LEU
1	C	571	VAL
1	C	575	MET
1	C	578	LEU
1	C	588	GLN
1	C	591	LEU
1	C	596	HIS
1	C	624	THR
1	C	652	THR
1	C	659	LYS
1	C	662	MET
1	C	678	THR
1	C	685	ILE
1	C	686	ASP
1	C	687	GLN
1	C	693	GLU
1	C	695	LEU
1	C	696	THR
1	C	699	ARG
1	C	713	LEU
1	C	717	ARG
1	C	726	GLN
1	C	731	ILE
1	C	741	VAL
1	C	750	LEU
1	C	767	ARG
1	C	799	VAL
1	C	808	ARG
1	C	815	ARG
1	C	851	LEU
1	C	868	LEU
1	C	876	LEU
1	C	895	TRP
1	C	901	VAL
1	C	903	LEU
1	C	910	ILE
1	C	921	LEU
1	C	941	ASN
1	C	954	ASP
1	C	956	GLU
1	C	982	PHE
1	C	984	LEU

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Mol	Chain	Res	Type
1	C	993	THR
1	C	1035	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	106	GLN
1	A	108	GLN
1	A	109	ASN
1	A	125	GLN
1	A	191	ASN
1	A	210	GLN
1	A	229	GLN
1	A	254	ASN
1	A	282	ASN
1	A	361	ASN
1	A	415	ASN
1	A	577	GLN
1	A	584	GLN
1	A	588	GLN
1	A	592	ASN
1	A	613	ASN
1	A	622	GLN
1	A	667	ASN
1	A	687	GLN
1	A	692	HIS
1	A	701	GLN
1	A	709	HIS
1	A	719	ASN
1	A	733	GLN
1	A	846	GLN
1	A	923	ASN
1	B	58	GLN
1	B	67	GLN
1	B	74	ASN
1	B	106	GLN
1	B	108	GLN
1	B	109	ASN
1	B	112	GLN
1	B	144	ASN
1	B	151	GLN

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Mol	Chain	Res	Type
1	B	161	ASN
1	B	189	ASN
1	B	210	GLN
1	B	213	GLN
1	B	231	ASN
1	B	274	ASN
1	B	437	GLN
1	B	526	HIS
1	B	605	ASN
1	B	613	ASN
1	B	622	GLN
1	B	700	ASN
1	B	744	ASN
1	B	846	GLN
1	B	865	GLN
1	B	923	ASN
1	C	3	ASN
1	C	34	GLN
1	C	58	GLN
1	C	63	GLN
1	C	144	ASN
1	C	151	GLN
1	C	176	GLN
1	C	189	ASN
1	C	197	GLN
1	C	210	GLN
1	C	211	ASN
1	C	213	GLN
1	C	231	ASN
1	C	237	GLN
1	C	274	ASN
1	C	284	GLN
1	C	338	HIS
1	C	360	GLN
1	C	361	ASN
1	C	588	GLN
1	C	700	ASN
1	C	846	GLN
1	C	865	GLN
1	C	872	GLN
1	C	941	ASN
1	C	1001	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	RFP	C	2002	-	63,63,63	1.75	3 (4%)	82,94,94	1.95	16 (19%)

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	RFP	C	2002	-	-	0/60/85/85	0/1/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2002	RFP	O5-C29	2.86	1.48	1.39
2	C	2002	RFP	O7-C35	5.39	1.47	1.35
2	C	2002	RFP	O4-C11	11.34	1.43	1.21

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2002	RFP	O4-C11-C5	-8.13	115.09	132.02
2	C	2002	RFP	O4-C11-C12	-3.12	112.25	119.93
2	C	2002	RFP	C30-C16-C17	-2.89	116.36	123.22
2	C	2002	RFP	C12-C11-C5	-2.78	101.03	107.53
2	C	2002	RFP	C32-C22-C21	2.01	115.38	111.24
2	C	2002	RFP	C39-C40-N3	2.30	113.41	110.39
2	C	2002	RFP	O7-C25-C26	2.32	113.96	107.56
2	C	2002	RFP	C3-C43-N2	2.87	125.64	120.77
2	C	2002	RFP	C42-C41-N3	3.01	114.34	110.39
2	C	2002	RFP	O3-C6-C7	3.22	127.95	121.29
2	C	2002	RFP	C40-C39-N4	3.28	114.25	110.79
2	C	2002	RFP	C42-N4-C39	3.53	114.17	109.53
2	C	2002	RFP	C20-C21-C22	3.86	120.56	114.24
2	C	2002	RFP	C12-O5-C29	4.05	127.07	116.58
2	C	2002	RFP	O7-C35-C36	4.37	119.35	111.10
2	C	2002	RFP	C41-C42-N4	5.84	116.96	110.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2002	RFP	10	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	1022/1053 (97%)	0.09	30 (2%) 55 56	40, 90, 124, 144	0
1	B	1022/1053 (97%)	0.24	53 (5%) 31 30	57, 97, 133, 162	0
1	C	1022/1053 (97%)	0.11	41 (4%) 42 41	35, 89, 138, 167	0
All	All	3066/3159 (97%)	0.15	124 (4%) 42 41	35, 92, 134, 167	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1036	LYS	6.3
1	C	538	THR	5.9
1	B	1034	SER	5.1
1	A	515	TRP	5.1
1	C	870	GLY	5.1
1	C	965	LEU	4.6
1	C	871	ASN	4.5
1	A	497	LEU	4.4
1	B	1035	ARG	4.2
1	B	791	VAL	3.9
1	C	964	THR	3.8
1	B	516	PHE	3.8
1	A	259	ARG	3.6
1	B	355	MET	3.5
1	B	604	ASN	3.5
1	B	438	ILE	3.5
1	C	516	PHE	3.5
1	A	432	ARG	3.4
1	C	962	GLU	3.4
1	C	497	LEU	3.3
1	B	948	PHE	3.3
1	C	7	ASP	3.3
1	B	993	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	638	PRO	3.3
1	B	541	TYR	3.3
1	B	1033	PHE	3.2
1	A	1036	LYS	3.2
1	C	671	ILE	3.2
1	C	966	ASP	3.2
1	B	635	ALA	3.2
1	C	515	TRP	3.1
1	C	425	LEU	3.1
1	B	949	ALA	3.1
1	A	253	VAL	3.0
1	B	991	ILE	3.0
1	B	528	THR	3.0
1	C	351	VAL	3.0
1	B	497	LEU	2.9
1	B	498	LYS	2.9
1	C	963	ALA	2.9
1	C	424	GLY	2.9
1	A	258	SER	2.9
1	B	253	VAL	2.9
1	A	572	PHE	2.8
1	B	902	MET	2.8
1	C	959	GLY	2.8
1	C	539	GLY	2.8
1	B	833	PRO	2.8
1	A	32	VAL	2.7
1	C	537	SER	2.7
1	C	960	LEU	2.7
1	C	413	VAL	2.7
1	C	921	LEU	2.6
1	A	196	PHE	2.6
1	A	3	ASN	2.6
1	A	966	ASP	2.6
1	B	362	PHE	2.6
1	A	793	ALA	2.6
1	A	952	LEU	2.6
1	A	257	GLY	2.6
1	B	790	TYR	2.5
1	B	2	PRO	2.5
1	B	527	TYR	2.5
1	C	9	PRO	2.5
1	B	321	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	535	LEU	2.5
1	B	435	MET	2.5
1	B	964	THR	2.5
1	C	961	ILE	2.4
1	A	312	LYS	2.4
1	A	516	PHE	2.4
1	C	252	LYS	2.4
1	A	260	VAL	2.4
1	A	1035	ARG	2.4
1	A	558	ARG	2.4
1	B	945	ILE	2.4
1	A	635	ALA	2.4
1	C	741	VAL	2.4
1	C	918	PHE	2.4
1	C	6	ILE	2.3
1	C	496	MET	2.3
1	B	515	TRP	2.3
1	B	124	GLN	2.3
1	A	252	LYS	2.3
1	C	982	PHE	2.3
1	B	195	LYS	2.3
1	A	30	LEU	2.3
1	C	958	LYS	2.3
1	B	889	ALA	2.3
1	C	542	LEU	2.3
1	A	265	VAL	2.2
1	C	253	VAL	2.2
1	B	412	VAL	2.2
1	C	832	ALA	2.2
1	A	918	PHE	2.2
1	A	230	LEU	2.2
1	C	1023	PRO	2.2
1	C	543	VAL	2.2
1	B	145	THR	2.2
1	B	989	LEU	2.2
1	A	513	PHE	2.2
1	B	1026	PHE	2.2
1	C	255	GLN	2.1
1	B	799	VAL	2.1
1	B	895	TRP	2.1
1	B	855	VAL	2.1
1	B	992	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	554	TYR	2.1
1	B	431	THR	2.1
1	B	798	MET	2.1
1	A	791	VAL	2.1
1	A	964	THR	2.1
1	C	34	GLN	2.1
1	B	486	LEU	2.1
1	B	496	MET	2.1
1	B	3	ASN	2.1
1	C	522	LYS	2.1
1	B	357	LEU	2.1
1	B	424	GLY	2.1
1	B	263	ARG	2.0
1	C	8	ARG	2.0
1	B	944	LEU	2.0
1	B	642	ASN	2.0
1	C	365	THR	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	RFP	C	2002	59/59	0.83	0.34	2.22	100,104,105,105	59

6.5 Other polymers

There are no such residues in this entry.