



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2017 – 01:34 PM EDT

PDB ID : 4ZIT
Title : Crystal structure of AcrB in P21 space group
Authors : Ababou, A.; Koronakis, V.
Deposited on : unknown
Resolution : 3.30 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029824

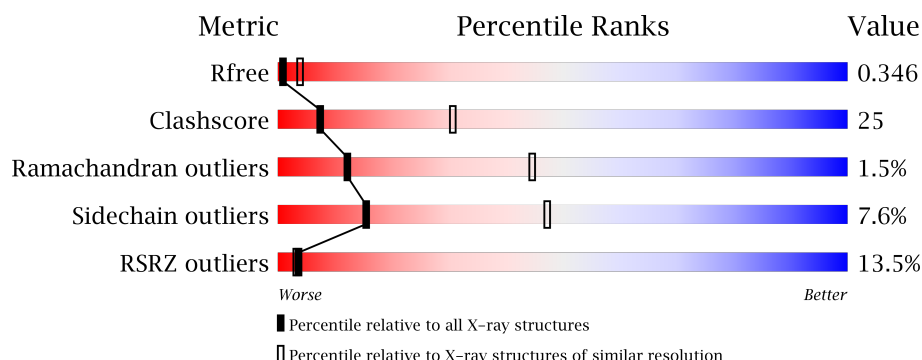
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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	1049	<div> <div>12%</div> <div>50%</div> <div>45%</div> <div>...</div> </div>
1	B	1049	<div> <div>11%</div> <div>54%</div> <div>41%</div> <div>...</div> </div>
1	C	1049	<div> <div>11%</div> <div>51%</div> <div>44%</div> <div>...</div> </div>
1	D	1049	<div> <div>14%</div> <div>48%</div> <div>47%</div> <div>...</div> </div>
1	E	1049	<div> <div>16%</div> <div>49%</div> <div>46%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	1049	

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	LMT	A	1101	-	-	-	X
2	LMT	B	1101	-	-	-	X
2	LMT	C	1101	X	-	-	-
2	LMT	E	1101	-	-	-	X
2	LMT	F	1101	-	-	-	X

2 Entry composition ⓘ

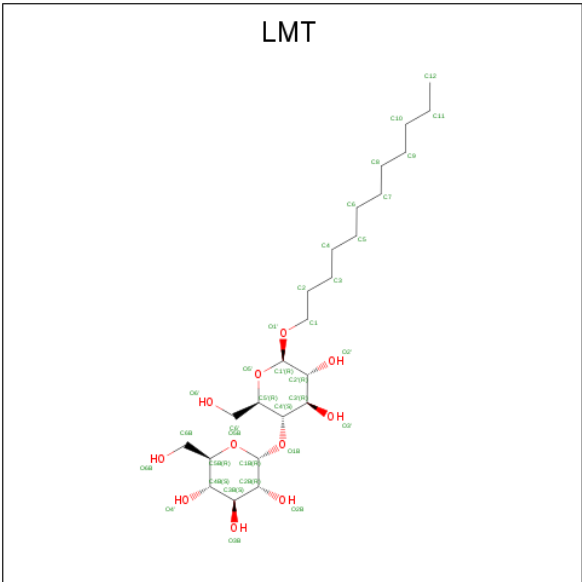
There are 3 unique types of molecules in this entry. The entry contains 47773 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	B	1043	Total	C	N	O	S	0	0	0
			7935	5101	1314	1477	43			
1	C	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	D	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	E	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	F	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			

- Molecule 2 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	F	1	Total C O 35 24 11	0	0

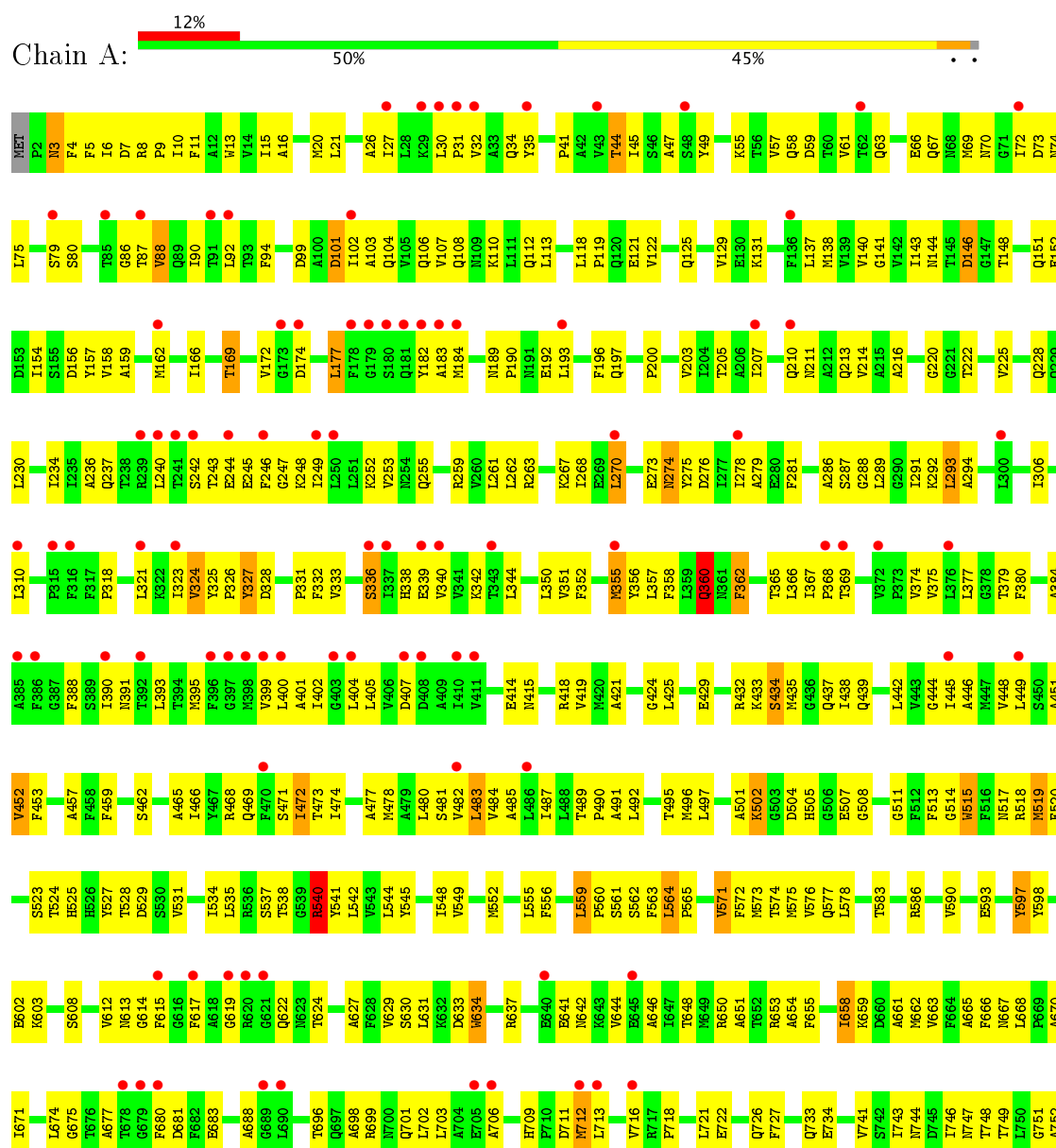
- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

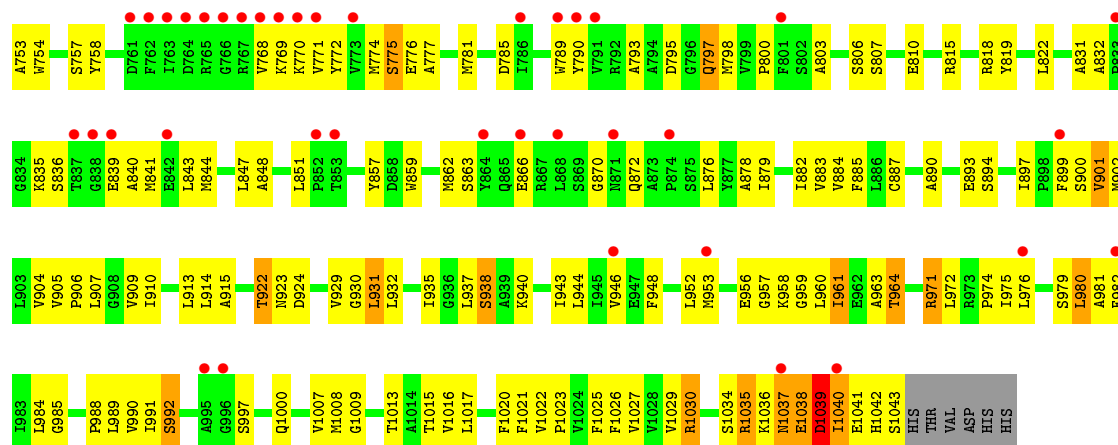
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0
3	C	1	Total Ni 1 1	0	0
3	E	1	Total Ni 1 1	0	0

3 Residue-property plots

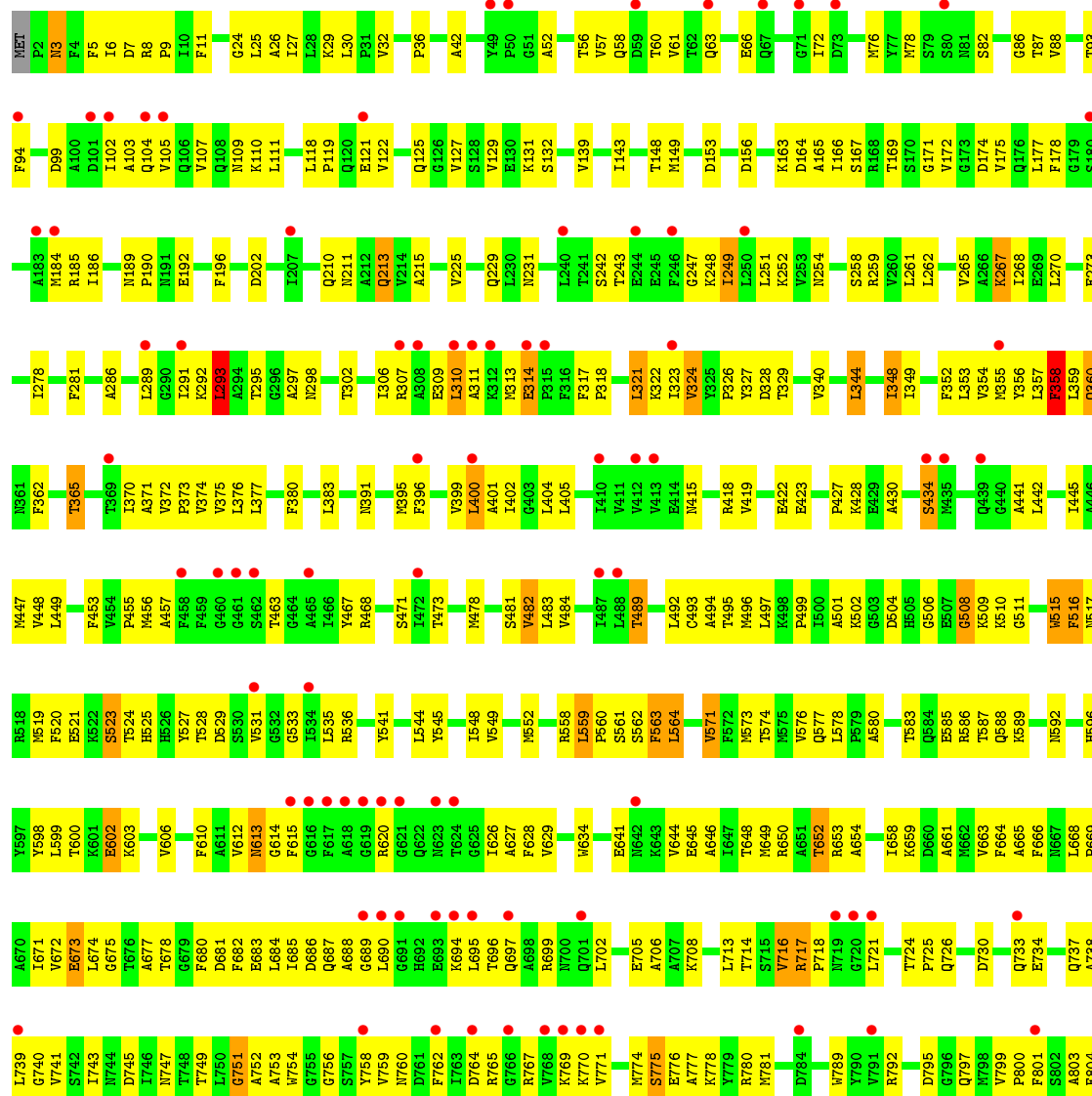
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

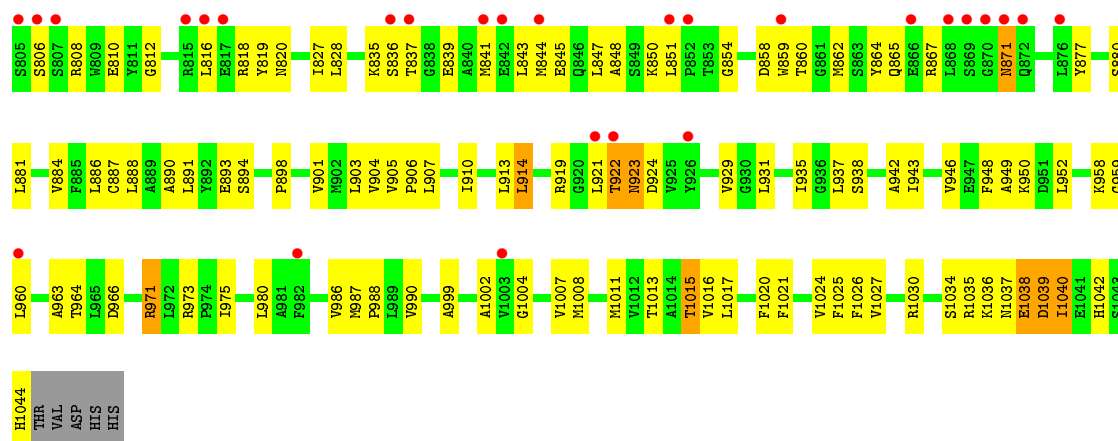
- Molecule 1: Multidrug efflux pump subunit AcrB



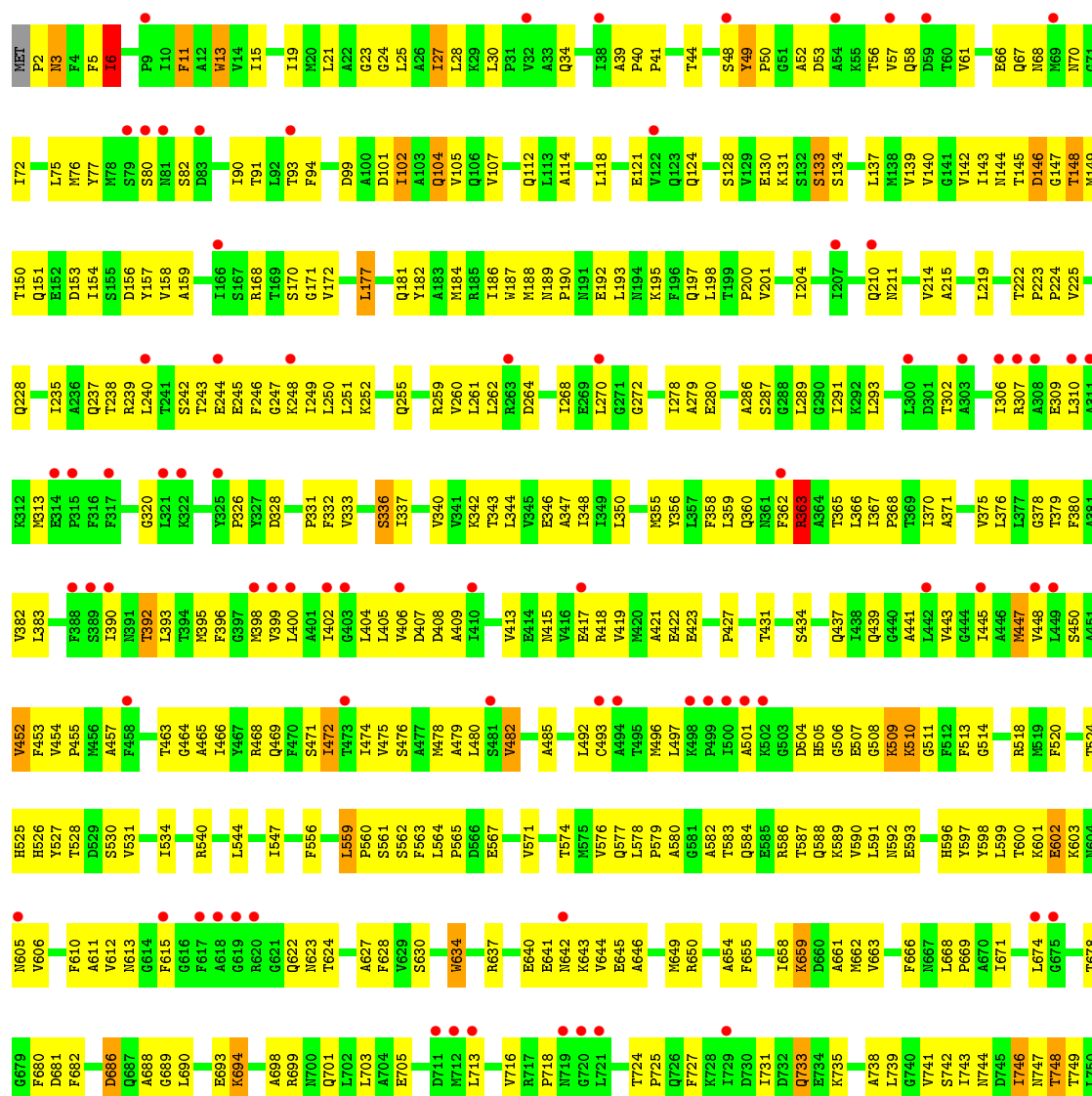


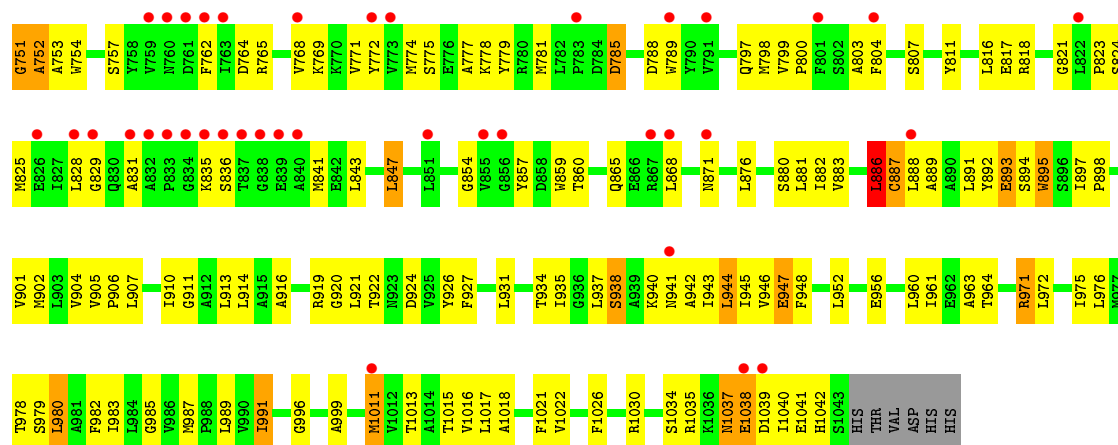
• Molecule 1: Multidrug efflux pump subunit AcrB



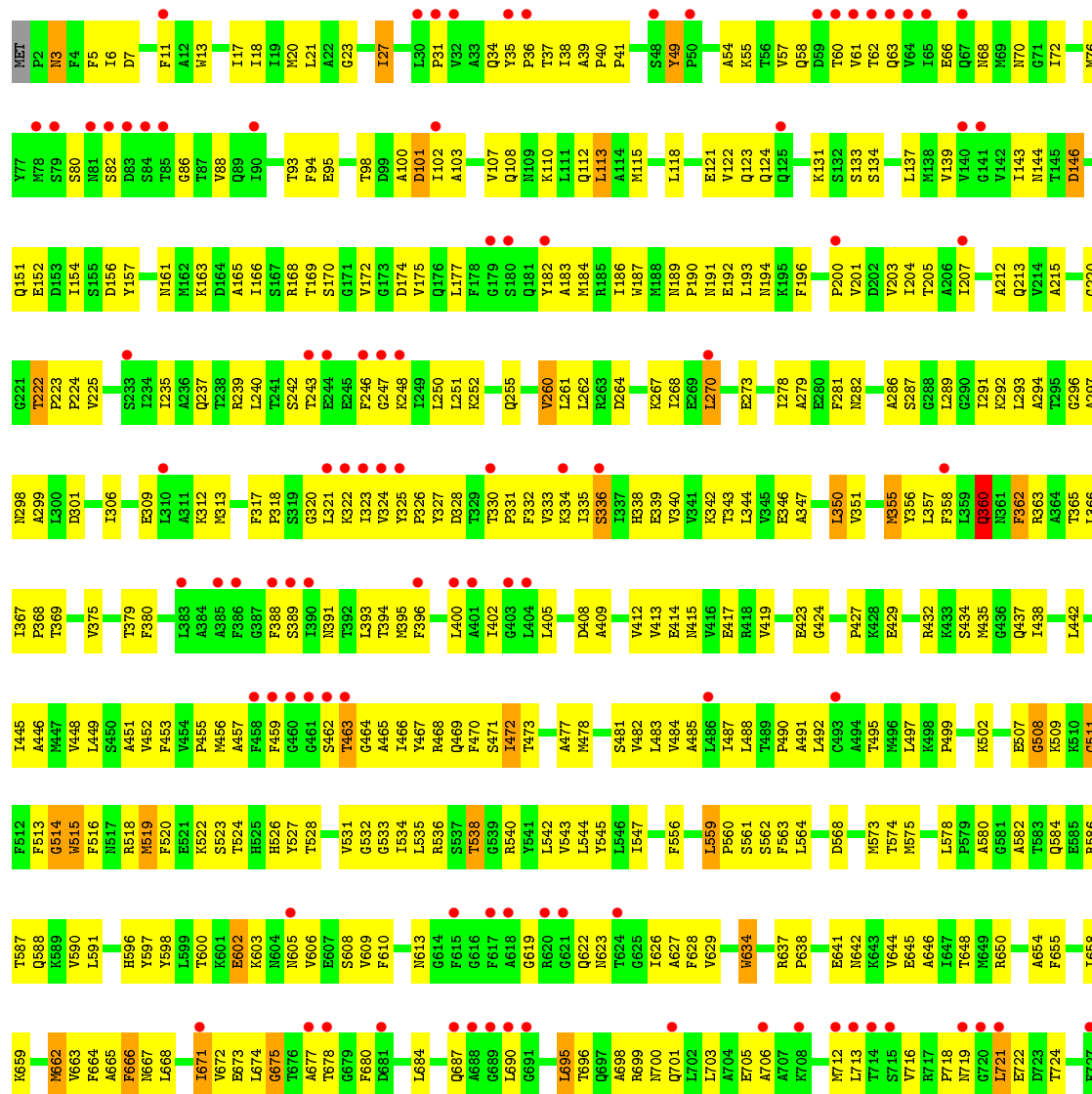
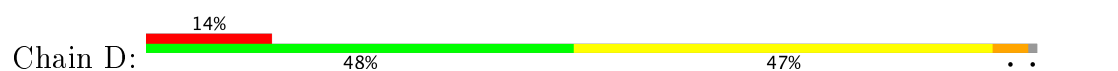


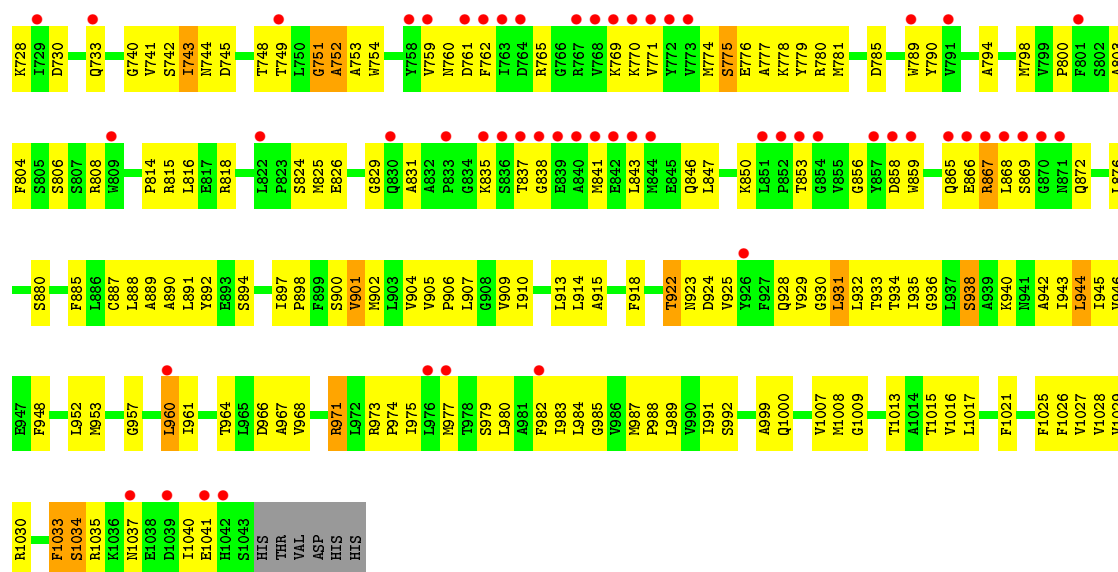
• Molecule 1: Multidrug efflux pump subunit AcrB



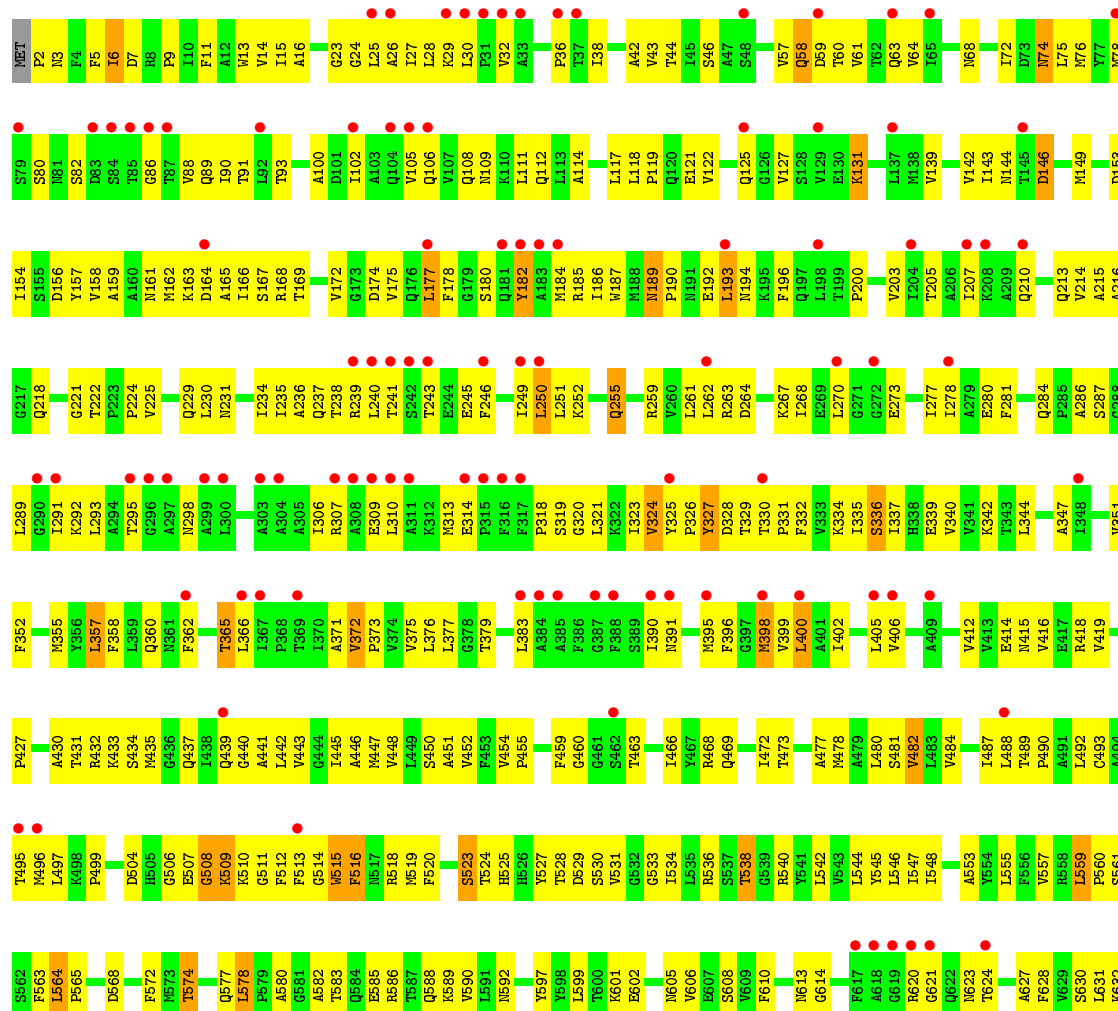


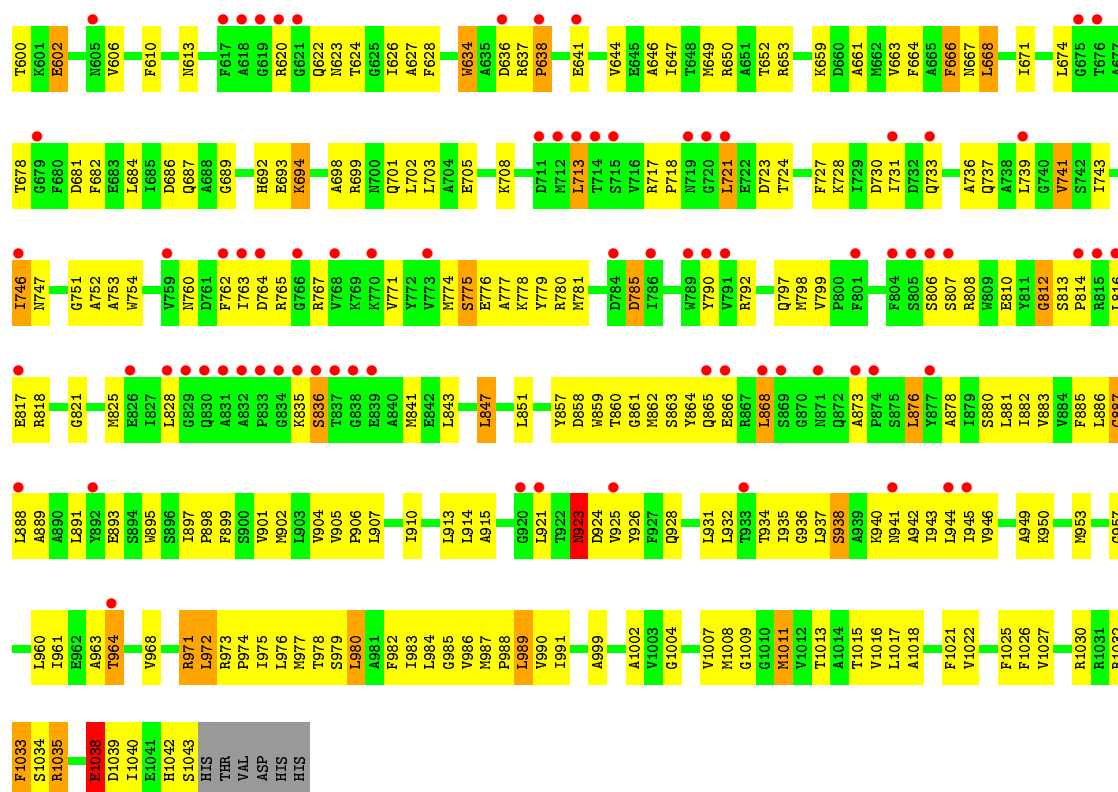
• Molecule 1: Multidrug efflux pump subunit AcrB





• Molecule 1: Multidrug efflux pump subunit AcrB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.84Å 156.86Å 218.58Å 90.00° 92.70° 90.00°	Depositor
Resolution (Å)	19.95 – 3.30 127.41 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.95-3.30) 97.3 (127.41-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.268 , 0.339 0.275 , 0.346	Depositor DCC
R_{free} test set	7509 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	90.9	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.097 for -k,-h,-l 0.108 for k,h,-l 0.107 for h,-k,-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	47773	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.50 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.8396e-05.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: NI, LMT

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	0.61	1/8076 (0.0%)	0.85	6/10965 (0.1%)
1	B	0.62	1/8087 (0.0%)	0.86	5/10980 (0.0%)
1	C	0.62	0/8076	0.86	6/10965 (0.1%)
1	D	0.56	1/8076 (0.0%)	0.82	8/10965 (0.1%)
1	E	0.58	2/8076 (0.0%)	0.83	6/10965 (0.1%)
1	F	0.58	1/8076 (0.0%)	0.85	10/10965 (0.1%)
All	All	0.60	6/48467 (0.0%)	0.84	41/65805 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	2
1	E	0	1
1	F	0	2
All	All	0	8

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	515	TRP	CB-CG	7.59	1.64	1.50
1	B	515	TRP	CB-CG	6.22	1.61	1.50
1	D	515	TRP	CB-CG	6.04	1.61	1.50
1	E	515	TRP	CB-CG	5.75	1.60	1.50
1	E	493	CYS	CB-SG	-5.49	1.72	1.81
1	F	887	CYS	CB-SG	5.43	1.91	1.82

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	529	ASP	CB-CG-OD1	10.05	127.35	118.30
1	B	483	LEU	CA-CB-CG	8.63	135.14	115.30
1	A	972	LEU	CA-CB-CG	7.07	131.55	115.30
1	B	529	ASP	CB-CG-OD1	6.99	124.59	118.30
1	B	357	LEU	CA-CB-CG	6.93	131.25	115.30
1	E	888	LEU	CA-CB-CG	-6.90	99.44	115.30
1	A	529	ASP	CB-CG-OD1	6.89	124.50	118.30
1	E	250	LEU	CA-CB-CG	6.75	130.82	115.30
1	F	529	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	C	75	LEU	CA-CB-CG	6.49	130.22	115.30
1	D	944	LEU	CA-CB-CG	-6.45	100.47	115.30
1	A	483	LEU	CA-CB-CG	6.22	129.60	115.30
1	F	989	LEU	CA-CB-CG	6.18	129.52	115.30
1	D	113	LEU	CA-CB-CG	6.01	129.12	115.30
1	D	350	LEU	CA-CB-CG	-6.00	101.49	115.30
1	D	483	LEU	CA-CB-CG	6.00	129.11	115.30
1	C	363	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	293	LEU	CA-CB-CG	5.88	128.83	115.30
1	A	519	MET	CB-CG-SD	5.87	130.01	112.40
1	C	980	LEU	CA-CB-CG	-5.75	102.06	115.30
1	F	49	TYR	CA-CB-CG	5.75	124.32	113.40
1	D	519	MET	CB-CG-SD	5.74	129.63	112.40
1	A	1030	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	F	721	LEU	CA-CB-CG	5.59	128.15	115.30
1	D	673	GLU	N-CA-C	5.48	125.79	111.00
1	C	886	LEU	CA-CB-CG	5.47	127.88	115.30
1	E	357	LEU	CA-CB-CG	5.38	127.69	115.30
1	E	193	LEU	CA-CB-CG	5.36	127.62	115.30
1	F	812	GLY	N-CA-C	-5.35	99.72	113.10
1	E	599	LEU	CA-CB-CG	5.29	127.47	115.30
1	F	847	LEU	CA-CB-CG	5.26	127.39	115.30
1	D	721	LEU	CA-CB-CG	5.25	127.37	115.30
1	E	529	ASP	CB-CG-OD1	5.22	123.00	118.30
1	F	921	LEU	CA-CB-CG	-5.21	103.33	115.30
1	C	944	LEU	CA-CB-CG	5.19	127.25	115.30
1	A	932	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	344	LEU	CA-CB-CG	5.19	127.24	115.30
1	F	363	ARG	CG-CD-NE	5.17	122.65	111.80
1	F	972	LEU	CA-CB-CG	5.09	127.02	115.30
1	D	488	LEU	CA-CB-CG	-5.09	103.59	115.30
1	C	270	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1038	GLU	Peptide
1	A	540	ARG	Sidechain
1	B	1039	ASP	Peptide
1	C	540	ARG	Sidechain
1	C	6	ILE	Peptide
1	E	1039	ASP	Peptide
1	F	6	ILE	Peptide
1	F	812	GLY	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	7925	0	8066	432	0
1	B	7935	0	8073	340	0
1	C	7925	0	8066	397	1
1	D	7925	0	8066	418	1
1	E	7925	0	8066	425	0
1	F	7925	0	8066	439	0
2	A	35	0	46	3	0
2	B	35	0	46	7	0
2	C	35	0	46	0	0
2	D	35	0	46	7	0
2	E	35	0	46	9	0
2	F	35	0	46	3	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
All	All	47773	0	48679	2382	1

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 25.

All (2382) 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:781:MET:HE1	1:C:225:VAL:H	1.22	1.04
1:D:781:MET:HE1	1:F:225:VAL:H	1.19	1.03
1:A:971:ARG:HG2	1:A:974:PRO:HG2	1.44	0.96
1:B:1035:ARG:HG3	1:B:1036:LYS:HG3	1.49	0.95
1:B:959:GLY:HA2	1:B:1040:ILE:HB	1.46	0.95
1:B:541:TYR:HH	2:B:1101:LMT:H6'	1.00	0.93
1:C:944:LEU:HB3	1:C:971:ARG:HD2	1.50	0.93
1:D:41:PRO:HG2	1:D:94:PHE:HB2	1.48	0.92
1:A:1034:SER:HB3	1:A:1035:ARG:HA	1.50	0.92
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.52	0.90
1:D:344:LEU:HD22	1:D:402:ILE:HD11	1.53	0.90
1:B:225:VAL:HG12	1:C:777:ALA:HB1	1.52	0.89
2:E:1101:LMT:H6D	2:E:1101:LMT:H5B	1.54	0.89
1:F:559:LEU:HD22	1:F:560:PRO:HD2	1.53	0.89
1:A:619:GLY:HA3	1:A:815:ARG:HH22	1.36	0.88
1:E:415:ASN:HD22	1:E:434:SER:HB2	1.37	0.88
1:F:731:ILE:HD13	1:F:746:ILE:HD11	1.54	0.87
1:E:733:GLN:HE22	1:E:743:ILE:HG21	1.39	0.87
1:E:699:ARG:NH2	1:E:722:GLU:OE2	2.08	0.86
1:B:562:SER:HB3	1:B:924:ASP:HB3	1.57	0.86
1:C:919:ARG:O	1:C:921:LEU:N	2.09	0.86
1:D:57:VAL:HG21	1:D:86:GLY:HA2	1.55	0.86
1:E:146:ASP:OD2	1:E:146:ASP:N	2.07	0.86
1:D:696:THR:HG23	1:D:699:ARG:HH12	1.41	0.86
1:E:196:PHE:O	1:E:252:LYS:NZ	2.09	0.85
1:F:35:TYR:HB3	1:F:38:ILE:HD12	1.58	0.85
1:A:445:ILE:HD13	1:A:940:LYS:HE3	1.58	0.85
1:B:1037:ASN:HA	1:B:1038:GLU:HG2	1.59	0.84
1:F:897:ILE:HG23	1:F:946:VAL:HG11	1.59	0.84
1:A:957:GLY:HA2	1:A:1042:HIS:HB3	1.59	0.84
1:C:892:TYR:O	1:C:894:SER:N	2.11	0.84
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.59	0.84
1:F:901:VAL:HG23	1:F:942:ALA:HB3	1.60	0.84
1:E:950:LYS:HA	1:E:953:MET:HE3	1.58	0.83
1:A:537:SER:OG	1:A:540:ARG:HD2	1.78	0.83
1:E:507:GLU:HG2	1:E:518:ARG:HA	1.61	0.82
1:D:360:GLN:NE2	1:D:513:PHE:O	2.12	0.82
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.60	0.82
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.15	0.81
1:C:901:VAL:HG23	1:C:942:ALA:HB3	1.62	0.81
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.62	0.81
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:LEU:HD22	1:C:293:LEU:HD23	1.61	0.81
1:B:652:THR:HG23	1:B:665:ALA:H	1.46	0.80
1:C:577:GLN:HG3	1:C:624:THR:HG22	1.63	0.80
1:C:151:GLN:NE2	1:C:279:ALA:O	2.13	0.80
1:D:400:LEU:HD23	1:D:929:VAL:HG12	1.64	0.80
1:F:41:PRO:HG2	1:F:94:PHE:HB2	1.61	0.80
1:B:422:GLU:O	1:B:502:LYS:NZ	2.15	0.80
1:E:441:ALA:HA	1:E:891:LEU:HD21	1.64	0.79
1:E:156:ASP:OD2	1:E:769:LYS:NZ	2.14	0.79
1:F:82:SER:HB2	1:F:816:LEU:HB2	1.65	0.79
1:D:596:HIS:O	1:D:600:THR:OG1	2.01	0.79
1:A:243:THR:HG23	1:A:268:ILE:HG22	1.64	0.78
1:D:564:LEU:HB2	1:D:671:ILE:HD11	1.65	0.78
1:A:196:PHE:O	1:A:252:LYS:NZ	2.17	0.78
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.17	0.78
1:C:641:GLU:HB2	1:C:650:ARG:HH22	1.49	0.78
1:A:703:LEU:HD21	1:A:718:PRO:HD3	1.66	0.77
1:B:668:LEU:HD23	1:B:668:LEU:H	1.48	0.77
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.63	0.77
1:A:129:VAL:O	1:B:110:LYS:NZ	2.17	0.77
1:C:53:ASP:OD1	1:C:56:THR:OG1	2.01	0.77
1:F:358:PHE:HD1	1:F:977:MET:HG3	1.47	0.77
1:D:55:LYS:NZ	1:F:238:THR:OG1	2.16	0.77
1:E:530:SER:CB	2:E:1101:LMT:H2O2	1.97	0.77
1:E:699:ARG:HE	1:E:718:PRO:HG3	1.49	0.77
1:F:307:ARG:NH2	1:F:314:GLU:OE2	2.18	0.77
1:C:578:LEU:HG	1:C:587:THR:HG22	1.66	0.76
1:F:248:LYS:HA	1:F:261:LEU:HD13	1.67	0.76
1:D:536:ARG:NH2	2:D:1101:LMT:O3B	2.18	0.76
1:E:641:GLU:HA	1:E:646:ALA:HB3	1.66	0.76
1:E:976:LEU:HD21	2:E:1101:LMT:H111	1.68	0.76
1:A:1041:GLU:HB3	1:A:1042:HIS:HA	1.67	0.76
1:B:9:PRO:HB3	1:B:495:THR:HG21	1.68	0.76
1:F:910:ILE:O	1:F:914:LEU:HB2	1.85	0.76
1:A:451:ALA:HB1	1:A:883:VAL:HG12	1.67	0.76
1:D:82:SER:HB2	1:D:816:LEU:HB2	1.67	0.76
1:F:596:HIS:O	1:F:600:THR:OG1	2.04	0.75
1:A:225:VAL:H	1:B:781:MET:HE1	1.49	0.75
1:F:733:GLN:HE22	1:F:743:ILE:HG21	1.50	0.75
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.69	0.75
1:A:70:ASN:O	1:A:110:LYS:NZ	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LEU:HB2	1:C:246:PHE:HE1	1.49	0.75
1:E:326:PRO:O	1:E:630:SER:OG	2.04	0.75
1:A:146:ASP:HB2	1:A:148:THR:HG23	1.69	0.75
1:C:159:ALA:HB2	1:C:177:LEU:HD11	1.67	0.75
1:E:508:GLY:HA3	1:E:518:ARG:HE	1.52	0.75
1:A:400:LEU:HD21	1:A:930:GLY:HA2	1.69	0.74
1:A:57:VAL:HG21	1:A:86:GLY:HA2	1.67	0.74
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.69	0.74
1:C:587:THR:HG21	1:C:622:GLN:O	1.86	0.74
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.69	0.74
1:C:356:TYR:HA	1:C:365:THR:HG21	1.68	0.74
1:D:133:SER:OG	1:D:134:SER:N	2.20	0.74
1:D:156:ASP:OD2	1:D:769:LYS:NZ	2.20	0.74
1:D:225:VAL:H	1:E:781:MET:HE1	1.51	0.74
1:E:174:ASP:HB3	1:E:292:LYS:HB2	1.69	0.74
1:A:713:LEU:HD21	1:A:843:LEU:HD12	1.67	0.74
1:B:598:TYR:HB3	1:B:606:VAL:HG21	1.70	0.74
1:F:343:THR:HG21	1:F:989:LEU:HD23	1.67	0.74
1:A:1040:ILE:HG13	1:A:1041:GLU:H	1.51	0.74
1:A:144:ASN:HD22	1:A:321:LEU:HD23	1.50	0.74
1:B:508:GLY:O	1:B:510:LYS:N	2.21	0.74
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.70	0.74
1:F:664:PHE:HD2	1:F:717:ARG:HD3	1.50	0.74
1:F:298:ASN:ND2	1:F:301:ASP:OD2	2.21	0.74
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.21	0.73
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.70	0.73
1:C:3:ASN:N	1:C:3:ASN:OD1	2.21	0.73
1:E:559:LEU:HD23	1:E:560:PRO:HD2	1.71	0.73
1:F:61:VAL:HA	1:F:118:LEU:HD22	1.69	0.73
1:B:362:PHE:O	1:B:365:THR:HG22	1.89	0.73
1:D:137:LEU:HD13	1:D:293:LEU:HD12	1.71	0.73
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.71	0.72
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.71	0.72
1:B:213:GLN:HE22	1:C:52:ALA:HA	1.54	0.72
1:B:658:ILE:O	1:B:659:LYS:HD2	1.89	0.72
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.69	0.72
1:B:536:ARG:NH2	2:B:1101:LMT:O2B	2.20	0.72
1:B:423:GLU:HA	1:B:502:LYS:HZ3	1.53	0.72
1:C:61:VAL:HA	1:C:118:LEU:HD22	1.71	0.72
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.72	0.72
1:D:777:ALA:HB1	1:F:225:VAL:HG12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:VAL:HG11	1:E:395:MET:HB3	1.71	0.72
1:A:655:PHE:HB3	1:A:663:VAL:HB	1.71	0.72
1:C:201:VAL:HA	1:C:204:ILE:HD12	1.71	0.72
1:D:712:MET:HB3	1:D:713:LEU:HD22	1.70	0.72
1:C:598:TYR:HB3	1:C:606:VAL:HG21	1.72	0.72
1:D:427:PRO:HD3	1:D:499:PRO:HB3	1.72	0.72
1:F:537:SER:OG	1:F:540:ARG:NH2	2.23	0.72
1:F:58:GLN:OE1	1:F:818:ARG:NH1	2.23	0.72
1:F:668:LEU:H	1:F:668:LEU:HD23	1.54	0.72
1:E:156:ASP:OD1	1:E:765:ARG:NH2	2.22	0.71
1:E:508:GLY:O	1:E:510:LYS:N	2.23	0.71
1:B:24:GLY:O	1:B:27:ILE:HG22	1.89	0.71
1:E:7:ASP:OD1	1:E:432:ARG:NH2	2.23	0.71
1:C:450:SER:HB2	1:C:475:VAL:HG22	1.72	0.71
1:C:746:ILE:HG13	1:C:747:ASN:N	2.06	0.71
1:F:133:SER:OG	1:F:293:LEU:O	2.07	0.71
1:C:596:HIS:O	1:C:600:THR:OG1	2.08	0.71
1:C:588:GLN:O	1:C:592:ASN:ND2	2.23	0.71
1:D:982:PHE:O	1:D:985:GLY:N	2.24	0.71
1:E:971:ARG:O	1:E:975:ILE:HG12	1.91	0.71
1:F:360:GLN:NE2	1:F:513:PHE:O	2.16	0.71
1:E:743:ILE:HA	1:E:746:ILE:HD12	1.72	0.71
1:D:225:VAL:HG22	1:E:781:MET:HE2	1.71	0.71
1:D:335:ILE:O	1:D:339:GLU:HG2	1.91	0.71
1:E:540:ARG:NH1	2:E:1101:LMT:O6B	2.19	0.71
1:F:510:LYS:HA	1:F:518:ARG:HH12	1.54	0.71
1:C:668:LEU:H	1:C:668:LEU:HD23	1.56	0.70
1:F:187:TRP:HB3	1:F:776:GLU:HG2	1.73	0.70
1:A:259:ARG:HH21	1:A:261:LEU:HD11	1.55	0.70
1:D:170:SER:HB2	1:E:75:LEU:H	1.56	0.70
1:E:1013:THR:O	1:E:1017:LEU:HB2	1.92	0.70
1:A:1016:VAL:HG13	2:A:1101:LMT:H112	1.74	0.70
1:C:564:LEU:HG	1:C:565:PRO:HD2	1.73	0.70
1:B:172:VAL:HG13	1:B:291:ILE:HG23	1.72	0.70
1:D:540:ARG:NH2	2:D:1101:LMT:O6B	2.24	0.70
1:C:960:LEU:HB3	1:C:1040:ILE:HG23	1.74	0.70
1:D:6:ILE:HG13	1:D:7:ASP:N	2.06	0.70
1:D:66:GLU:OE2	1:D:80:SER:OG	2.07	0.69
1:F:340:VAL:HG11	1:F:395:MET:HB3	1.75	0.69
1:F:456:MET:HB3	1:F:876:LEU:HD21	1.73	0.69
1:A:61:VAL:HG22	1:A:118:LEU:HD22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:VAL:HG22	1:A:887:CYS:HB3	1.74	0.69
1:E:637:ARG:HB3	1:E:642:ASN:HB3	1.74	0.69
1:F:352:PHE:HA	1:F:355:MET:HE2	1.73	0.69
1:A:400:LEU:HD11	1:A:1007:VAL:HG21	1.74	0.69
1:B:423:GLU:HA	1:B:502:LYS:NZ	2.07	0.69
1:C:897:ILE:HG23	1:C:946:VAL:HG11	1.74	0.69
1:E:589:LYS:HA	1:E:592:ASN:HD22	1.57	0.69
1:E:901:VAL:HG21	1:E:943:ILE:HG13	1.73	0.69
1:B:372:VAL:HG23	1:B:373:PRO:HD3	1.75	0.69
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.28	0.69
1:D:298:ASN:HB3	1:D:301:ASP:HB2	1.75	0.69
1:B:907:LEU:HG	1:B:1017:LEU:HD23	1.75	0.69
1:D:1040:ILE:HG12	1:D:1041:GLU:H	1.58	0.69
1:E:139:VAL:HG13	1:E:178:PHE:HE1	1.57	0.69
1:E:149:MET:HB2	1:E:153:ASP:HB3	1.74	0.69
1:C:982:PHE:O	1:C:985:GLY:N	2.25	0.69
1:D:491:ALA:O	1:D:495:THR:OG1	2.09	0.69
1:E:959:GLY:HA2	1:E:1040:ILE:HB	1.75	0.69
1:E:157:TYR:O	1:E:161:ASN:ND2	2.21	0.69
1:F:428:LYS:HG2	1:F:494:ALA:HB1	1.75	0.69
1:A:712:MET:HB3	1:A:713:LEU:HD22	1.73	0.69
1:C:904:VAL:HG21	1:C:942:ALA:HB2	1.73	0.69
1:D:196:PHE:HB3	1:D:252:LYS:NZ	2.07	0.69
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.74	0.69
1:E:588:GLN:O	1:E:592:ASN:ND2	2.26	0.69
1:E:57:VAL:HG11	1:E:86:GLY:HA2	1.74	0.69
1:A:654:ALA:O	1:A:658:ILE:HG12	1.92	0.69
1:E:1037:ASN:H	1:E:1038:GLU:HA	1.58	0.69
1:E:169:THR:HG21	1:E:306:ILE:HG13	1.74	0.69
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.73	0.69
1:A:415:ASN:HB3	1:A:434:SER:HB2	1.74	0.69
1:B:196:PHE:O	1:B:252:LYS:NZ	2.24	0.69
1:A:747:ASN:ND2	1:C:237:GLN:OE1	2.25	0.69
1:D:598:TYR:HB3	1:D:606:VAL:HG21	1.74	0.69
1:D:70:ASN:O	1:D:110:LYS:NZ	2.25	0.69
1:E:362:PHE:O	1:E:365:THR:HG22	1.92	0.68
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.74	0.68
1:F:509:LYS:O	1:F:518:ARG:NH1	2.26	0.68
1:F:739:LEU:HD13	1:F:799:VAL:HG11	1.75	0.68
1:D:115:MET:O	1:D:123:GLN:NE2	2.26	0.68
1:D:49:TYR:HB3	1:D:57:VAL:HG22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:702:LEU:HD12	1:F:851:LEU:HD11	1.76	0.68
1:F:3:ASN:OD1	1:F:3:ASN:N	2.26	0.68
1:A:158:VAL:HG22	1:A:162:MET:HE2	1.75	0.68
1:F:73:ASP:OD2	1:F:106:GLN:NE2	2.24	0.68
1:F:667:ASN:O	1:F:678:THR:OG1	2.11	0.68
1:A:564:LEU:HD23	1:A:565:PRO:HD2	1.75	0.68
1:E:146:ASP:OD2	1:E:320:GLY:HA3	1.94	0.68
1:F:577:GLN:HG3	1:F:624:THR:HG22	1.76	0.68
1:D:393:LEU:HD11	1:D:466:ILE:HD13	1.76	0.68
1:E:949:ALA:HB3	1:E:1026:PHE:HE1	1.59	0.68
1:A:768:VAL:HG12	1:B:63:GLN:HE21	1.58	0.68
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.74	0.68
1:C:363:ARG:HH11	1:C:363:ARG:HB3	1.59	0.68
1:D:170:SER:OG	1:E:74:ASN:N	2.22	0.68
1:F:452:VAL:HG12	1:F:880:SER:HB3	1.76	0.68
1:A:491:ALA:O	1:A:495:THR:OG1	2.06	0.67
1:E:675:GLY:HA2	1:E:862:MET:SD	2.34	0.67
1:A:393:LEU:HD12	1:A:469:GLN:HG3	1.76	0.67
1:B:26:ALA:O	1:B:30:LEU:HB2	1.94	0.67
1:C:72:ILE:HD13	1:C:107:VAL:HG22	1.76	0.67
1:E:9:PRO:HB3	1:E:495:THR:HG21	1.76	0.67
1:F:24:GLY:O	1:F:27:ILE:HG12	1.94	0.67
1:A:156:ASP:OD2	1:A:769:LYS:NZ	2.28	0.67
1:C:186:ILE:HG12	1:C:268:ILE:HG12	1.77	0.67
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.29	0.67
1:F:527:TYR:HB2	2:F:1101:LMT:H101	1.77	0.67
1:A:350:LEU:HD22	1:A:984:LEU:HB3	1.76	0.67
1:D:562:SER:HB2	1:D:924:ASP:HB3	1.77	0.67
1:B:775:SER:OG	1:B:776:GLU:O	2.13	0.67
1:D:113:LEU:HD11	1:F:128:SER:HB3	1.77	0.67
1:E:376:LEU:O	1:E:379:THR:N	2.27	0.67
1:E:531:VAL:O	1:E:534:ILE:HG13	1.93	0.67
1:E:858:ASP:OD1	1:E:859:TRP:N	2.27	0.67
1:B:267:LYS:HD3	1:B:776:GLU:OE2	1.95	0.67
1:F:251:LEU:HD11	1:F:262:LEU:HA	1.74	0.67
1:A:531:VAL:O	1:A:534:ILE:HG13	1.94	0.67
1:E:213:GLN:HE22	1:F:52:ALA:HA	1.60	0.67
1:F:180:SER:OG	1:F:274:ASN:O	2.07	0.67
1:F:578:LEU:HG	1:F:587:THR:HG22	1.75	0.67
1:C:889:ALA:HB1	1:C:895:TRP:HZ3	1.59	0.67
1:E:237:GLN:OE1	1:F:747:ASN:ND2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:LEU:HD13	1:B:799:VAL:HG11	1.77	0.66
1:F:358:PHE:CD1	1:F:977:MET:HG3	2.30	0.66
1:B:111:LEU:HD21	1:B:127:VAL:HG11	1.77	0.66
1:B:167:SER:CB	1:B:175:VAL:HG21	2.25	0.66
1:F:808:ARG:NH1	1:F:810:GLU:OE2	2.28	0.66
1:A:957:GLY:CA	1:A:1042:HIS:HB3	2.25	0.66
1:D:330:THR:HG23	1:D:334:LYS:HD2	1.75	0.66
1:D:448:VAL:HG22	1:D:887:CYS:HB3	1.76	0.66
1:D:904:VAL:HG21	1:D:942:ALA:HB2	1.77	0.66
1:F:885:PHE:HD2	1:F:886:LEU:HD22	1.60	0.66
1:D:641:GLU:HB2	1:D:650:ARG:HH22	1.60	0.66
1:A:405:LEU:HD22	1:A:481:SER:HB3	1.77	0.66
1:A:421:ALA:HB1	1:A:505:HIS:CE1	2.30	0.66
1:E:901:VAL:HG23	1:E:942:ALA:HB3	1.78	0.66
1:E:931:LEU:O	1:E:935:ILE:HG13	1.96	0.66
1:A:415:ASN:OD1	1:A:418:ARG:NH2	2.29	0.66
1:A:573:MET:HG3	1:A:666:PHE:CE2	2.31	0.66
1:B:559:LEU:HD22	1:B:560:PRO:HD2	1.78	0.66
1:B:58:GLN:O	1:B:63:GLN:HG3	1.95	0.66
1:A:971:ARG:C	1:A:974:PRO:HD2	2.16	0.65
1:A:571:VAL:HG22	1:A:630:SER:HA	1.77	0.65
1:D:897:ILE:HA	1:D:1029:VAL:HG11	1.78	0.65
1:F:365:THR:O	1:F:368:PRO:HD2	1.95	0.65
1:C:686:ASP:OD1	1:C:690:LEU:HB2	1.96	0.65
1:A:137:LEU:HB2	1:A:293:LEU:HB2	1.79	0.65
1:A:362:PHE:O	1:A:365:THR:HG22	1.96	0.65
1:A:540:ARG:HG3	1:A:541:TYR:HD1	1.62	0.65
1:A:540:ARG:HG3	1:A:541:TYR:CD1	2.31	0.65
1:D:184:MET:HB3	1:D:771:VAL:HG13	1.79	0.65
1:D:967:ALA:O	1:D:971:ARG:NH1	2.28	0.65
1:E:658:ILE:O	1:E:659:LYS:HD2	1.96	0.65
1:B:610:PHE:HB3	1:B:628:PHE:HB3	1.77	0.65
1:C:947:GLU:HG3	1:C:948:PHE:HD1	1.61	0.65
1:A:923:ASN:ND2	1:A:923:ASN:O	2.30	0.65
1:E:189:ASN:HB3	1:E:192:GLU:HB2	1.79	0.65
1:E:702:LEU:HD13	1:E:851:LEU:HD21	1.79	0.65
1:C:744:ASN:O	1:C:748:THR:HG23	1.97	0.65
1:B:139:VAL:O	1:B:326:PRO:HD2	1.96	0.64
1:D:174:ASP:HB3	1:D:292:LYS:HB2	1.79	0.64
1:A:781:MET:HE1	1:C:225:VAL:N	2.05	0.64
1:B:511:GLY:HA2	1:B:515:TRP:CD1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:971:ARG:O	1:B:975:ILE:HG12	1.98	0.64
1:D:453:PHE:O	1:D:471:SER:OG	2.12	0.64
1:D:655:PHE:HB3	1:D:663:VAL:HB	1.80	0.64
1:E:511:GLY:HA2	1:E:515:TRP:CD1	2.32	0.64
1:F:452:VAL:O	1:F:455:PRO:HD2	1.97	0.64
1:A:960:LEU:HD21	1:A:1027:VAL:HG13	1.78	0.64
1:B:1013:THR:O	1:B:1017:LEU:HB2	1.96	0.64
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.80	0.64
1:B:536:ARG:NE	2:B:1101:LMT:O3B	2.30	0.64
1:D:243:THR:HG23	1:D:268:ILE:HG22	1.80	0.64
1:D:568:ASP:O	1:D:634:TRP:HZ3	1.81	0.64
1:E:261:LEU:HD12	1:E:263:ARG:HH12	1.63	0.64
1:B:156:ASP:OD1	1:B:765:ARG:NH2	2.30	0.64
1:D:318:PRO:HD2	1:D:321:LEU:HD12	1.78	0.64
1:F:424:GLY:HA3	1:F:502:LYS:HB2	1.79	0.64
1:A:73:ASP:OD2	1:A:106:GLN:NE2	2.30	0.64
1:E:907:LEU:HG	1:E:1017:LEU:HD23	1.80	0.64
1:C:944:LEU:HB3	1:C:971:ARG:CD	2.27	0.64
1:C:682:PHE:CE1	1:C:857:TYR:HB2	2.33	0.64
1:E:14:VAL:HG22	1:F:886:LEU:HD12	1.78	0.64
1:D:894:SER:HB3	1:D:897:ILE:HB	1.79	0.64
1:C:41:PRO:HG2	1:C:94:PHE:HB2	1.80	0.64
1:D:931:LEU:O	1:D:935:ILE:HG13	1.98	0.64
1:D:168:ARG:HB3	1:E:75:LEU:HD22	1.80	0.64
1:D:869:SER:OG	1:D:872:GLN:NE2	2.31	0.63
1:D:971:ARG:HH11	1:D:971:ARG:HB3	1.63	0.63
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.80	0.63
1:F:671:ILE:HD13	1:F:674:LEU:HD12	1.81	0.63
1:D:388:PHE:CE1	1:D:472:ILE:HG21	2.34	0.63
1:D:713:LEU:HD21	1:D:843:LEU:HD12	1.79	0.63
1:C:376:LEU:HD22	1:C:398:MET:HE3	1.80	0.63
1:C:671:ILE:HD13	1:C:674:LEU:HD12	1.80	0.63
1:E:108:GLN:HE22	1:F:109:ASN:HA	1.64	0.63
1:F:379:THR:HG23	1:F:476:SER:OG	1.97	0.63
1:F:479:ALA:O	1:F:482:VAL:HG23	1.99	0.63
1:A:94:PHE:CE1	1:A:103:ALA:HB1	2.34	0.63
1:B:400:LEU:HG	1:B:929:VAL:HG12	1.80	0.63
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.80	0.63
1:D:507:GLU:O	1:D:509:LYS:N	2.29	0.63
1:E:318:PRO:HD2	1:E:321:LEU:HD22	1.80	0.63
1:E:445:ILE:HG21	1:E:940:LYS:HD2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:919:ARG:HB3	1:B:921:LEU:HD23	1.80	0.63
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.80	0.63
1:C:559:LEU:HD23	1:C:560:PRO:HD2	1.79	0.63
1:D:358:PHE:CD1	1:D:977:MET:HG2	2.33	0.63
1:A:668:LEU:H	1:A:668:LEU:HD23	1.62	0.63
1:A:696:THR:HG23	1:A:699:ARG:HH12	1.64	0.63
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.80	0.63
1:E:776:GLU:HG2	1:E:777:ALA:H	1.63	0.63
1:A:457:ALA:HB1	1:A:468:ARG:HG3	1.81	0.63
1:D:971:ARG:NH1	1:D:971:ARG:HB3	2.13	0.63
1:E:415:ASN:ND2	1:E:437:GLN:OE1	2.28	0.63
1:A:520:PHE:O	1:A:524:THR:HG23	1.98	0.63
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.81	0.63
1:F:971:ARG:O	1:F:971:ARG:NE	2.31	0.63
1:A:832:ALA:HB3	1:A:835:LYS:HD3	1.82	0.62
1:D:644:VAL:HG11	1:D:667:ASN:HB2	1.80	0.62
1:D:72:ILE:HD13	1:D:107:VAL:HG22	1.79	0.62
1:E:484:VAL:HG12	1:E:489:THR:HG23	1.80	0.62
1:F:358:PHE:HE2	1:F:516:PHE:HZ	1.45	0.62
1:A:357:LEU:HD23	1:A:358:PHE:CD1	2.34	0.62
1:B:1011:MET:O	1:B:1015:THR:HG23	1.99	0.62
1:D:412:VAL:HG22	1:D:438:ILE:HD12	1.81	0.62
1:D:728:LYS:HG2	1:D:808:ARG:NH1	2.14	0.62
1:B:682:PHE:HE2	1:B:684:LEU:HB2	1.63	0.62
1:E:64:VAL:HG11	1:E:117:LEU:HB2	1.80	0.62
1:E:149:MET:HB2	1:E:153:ASP:CB	2.29	0.62
1:A:174:ASP:HB3	1:A:292:LYS:HB2	1.80	0.62
1:C:493:CYS:O	1:C:497:LEU:HB2	1.99	0.62
1:C:694:LYS:HE3	1:C:694:LYS:H	1.65	0.62
1:D:580:ALA:HB1	1:D:724:THR:HG22	1.80	0.62
1:F:146:ASP:O	1:F:148:THR:N	2.33	0.62
1:F:713:LEU:HD21	1:F:843:LEU:HD12	1.80	0.62
1:B:441:ALA:HA	1:B:891:LEU:HD21	1.79	0.62
1:C:261:LEU:N	1:C:264:ASP:OD2	2.32	0.62
1:C:597:TYR:HE1	1:C:601:LYS:HD2	1.63	0.62
1:C:960:LEU:O	1:C:964:THR:HG23	1.99	0.62
1:D:282:ASN:HD21	1:D:608:SER:HA	1.63	0.62
1:F:506:GLY:C	1:F:508:GLY:H	2.01	0.62
1:B:428:LYS:HG2	1:B:494:ALA:HB1	1.80	0.62
1:C:937:LEU:HD13	1:C:1011:MET:HE1	1.80	0.62
1:F:578:LEU:HB2	1:F:623:ASN:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:LYS:O	1:A:1040:ILE:HG12	2.00	0.62
1:C:171:GLY:HA3	1:C:302:THR:OG1	1.99	0.62
1:B:950:LYS:HZ1	1:B:1030:ARG:HH21	1.48	0.62
1:F:971:ARG:HB3	1:F:971:ARG:CZ	2.30	0.62
1:A:276:ASP:HA	1:C:222:THR:HG21	1.82	0.62
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.82	0.62
1:E:165:ALA:HB3	1:E:313:MET:CE	2.29	0.62
1:F:154:ILE:HG22	1:F:287:SER:HB3	1.81	0.62
1:A:733:GLN:NE2	1:A:743:ILE:HG21	2.15	0.62
1:D:674:LEU:HD23	1:D:675:GLY:N	2.14	0.62
1:F:372:VAL:HG22	1:F:405:LEU:HD11	1.81	0.62
1:C:101:ASP:OD1	1:C:131:LYS:NZ	2.33	0.61
1:C:520:PHE:O	1:C:524:THR:HG23	2.00	0.61
1:D:144:ASN:HA	1:D:320:GLY:O	2.00	0.61
1:D:700:ASN:HA	1:D:703:LEU:HD12	1.81	0.61
1:F:363:ARG:HG2	1:F:363:ARG:HH11	1.65	0.61
1:A:184:MET:HG2	1:A:246:PHE:CE2	2.36	0.61
1:B:759:VAL:HG12	1:B:760:ASN:HB2	1.81	0.61
1:F:674:LEU:HD22	1:F:861:GLY:HA2	1.83	0.61
1:A:574:THR:HG21	1:A:598:TYR:HE2	1.65	0.61
1:E:680:PHE:HB2	1:E:863:SER:OG	2.00	0.61
1:F:120:GLN:HA	1:F:123:GLN:HB2	1.81	0.61
1:A:225:VAL:HG12	1:B:777:ALA:HB1	1.82	0.61
1:A:415:ASN:HD22	1:A:434:SER:HB2	1.66	0.61
1:B:484:VAL:O	1:B:489:THR:HG23	2.00	0.61
1:C:187:TRP:HA	1:C:774:MET:O	2.00	0.61
1:C:944:LEU:HD13	1:C:975:ILE:HG12	1.82	0.61
1:D:578:LEU:HD21	1:D:590:VAL:HG21	1.81	0.61
1:D:641:GLU:HA	1:D:646:ALA:HB3	1.82	0.61
1:F:139:VAL:HG22	1:F:290:GLY:HA2	1.81	0.61
1:F:429:GLU:O	1:F:433:LYS:HB2	2.01	0.61
1:F:610:PHE:HB3	1:F:628:PHE:HB2	1.82	0.61
1:D:225:VAL:HG12	1:E:777:ALA:HB1	1.82	0.61
1:F:408:ASP:N	1:F:408:ASP:OD2	2.32	0.61
1:F:897:ILE:HG23	1:F:946:VAL:CG1	2.30	0.61
1:F:1021:PHE:HB3	1:F:1025:PHE:CE1	2.35	0.61
1:A:559:LEU:HD13	1:A:923:ASN:HB2	1.82	0.61
1:B:648:THR:O	1:B:652:THR:OG1	2.19	0.61
1:C:198:LEU:HD11	1:C:252:LYS:HB2	1.83	0.61
1:B:1037:ASN:HA	1:B:1038:GLU:CG	2.29	0.61
1:C:326:PRO:O	1:C:630:SER:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:795:ASP:OD2	1:E:797:GLN:HG3	2.00	0.61
1:F:455:PRO:HG3	1:F:883:VAL:HG21	1.83	0.61
1:A:244:GLU:O	1:A:247:GLY:N	2.34	0.60
1:A:795:ASP:OD2	1:A:797:GLN:HG3	2.00	0.60
1:A:768:VAL:HG12	1:B:63:GLN:NE2	2.16	0.60
1:B:82:SER:HB2	1:B:816:LEU:HB2	1.82	0.60
1:A:944:LEU:HB3	1:A:971:ARG:CZ	2.31	0.60
1:B:52:ALA:HB1	1:B:56:THR:HB	1.83	0.60
1:B:596:HIS:O	1:B:600:THR:OG1	2.09	0.60
1:C:479:ALA:O	1:C:482:VAL:HG23	2.02	0.60
1:D:368:PRO:HG3	1:D:413:VAL:HG21	1.82	0.60
1:E:583:THR:HG22	1:E:585:GLU:H	1.66	0.60
1:D:900:SER:HA	1:D:1025:PHE:HB3	1.83	0.60
1:D:247:GLY:O	1:D:261:LEU:HB3	2.01	0.60
1:E:165:ALA:HB3	1:E:313:MET:HE3	1.82	0.60
1:D:18:ILE:HG13	1:E:886:LEU:HD23	1.83	0.60
1:A:514:GLY:HA2	1:A:517:ASN:HD22	1.66	0.60
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.82	0.60
1:C:576:VAL:HG21	1:C:591:LEU:HD23	1.83	0.60
1:C:889:ALA:HB1	1:C:895:TRP:CZ3	2.35	0.60
1:D:251:LEU:HD11	1:D:262:LEU:HA	1.83	0.60
1:A:959:GLY:HA2	1:A:1040:ILE:HB	1.84	0.60
1:A:515:TRP:O	1:A:519:MET:HG3	2.01	0.60
1:A:326:PRO:HA	1:A:630:SER:OG	2.00	0.60
1:D:514:GLY:HA2	1:D:516:PHE:HB3	1.83	0.60
1:F:979:SER:CB	1:F:1015:THR:HG21	2.32	0.60
1:C:15:ILE:O	1:C:19:ILE:HG13	2.02	0.60
1:D:531:VAL:O	1:D:534:ILE:HG13	2.01	0.60
1:E:26:ALA:O	1:E:30:LEU:HB2	2.01	0.60
1:E:525:HIS:HA	1:E:528:THR:HG22	1.84	0.60
1:F:351:VAL:HG11	1:F:406:VAL:HG11	1.84	0.60
1:F:519:MET:O	1:F:523:SER:OG	2.18	0.60
1:A:549:VAL:O	1:A:552:MET:HB3	2.00	0.60
1:A:6:ILE:HG13	1:A:7:ASP:N	2.16	0.60
1:C:359:LEU:HB2	1:C:365:THR:HG22	1.84	0.60
1:C:556:PHE:HD1	1:C:913:LEU:HD21	1.66	0.60
1:D:429:GLU:OE1	1:D:432:ARG:NH1	2.34	0.60
1:E:1037:ASN:N	1:E:1038:GLU:HA	2.16	0.60
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.37	0.60
1:A:9:PRO:HG2	1:A:10:ILE:HD12	1.82	0.60
1:E:166:ILE:O	1:E:169:THR:HB	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:559:LEU:HD12	1:F:923:ASN:HB2	1.83	0.60
1:A:445:ILE:CD1	1:A:940:LYS:HE3	2.30	0.60
1:B:493:CYS:O	1:B:497:LEU:HB2	2.00	0.60
1:D:910:ILE:O	1:D:914:LEU:HB2	2.01	0.60
1:E:733:GLN:NE2	1:E:743:ILE:HG21	2.13	0.60
1:A:193:LEU:HD13	1:A:200:PRO:HD3	1.83	0.60
1:A:360:GLN:NE2	1:A:513:PHE:HB3	2.16	0.60
1:A:47:ALA:HB3	1:A:88:VAL:HG13	1.82	0.60
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.84	0.60
1:B:652:THR:HG22	1:B:664:PHE:HD1	1.66	0.59
1:E:154:ILE:HG22	1:E:287:SER:HB3	1.83	0.59
1:F:598:TYR:HB3	1:F:606:VAL:HG21	1.83	0.59
1:A:248:LYS:HA	1:A:261:LEU:HD13	1.83	0.59
1:A:355:MET:HE3	1:A:355:MET:HA	1.84	0.59
1:B:990:VAL:HG22	1:B:1004:GLY:HA3	1.85	0.59
1:D:400:LEU:HD11	1:D:1007:VAL:HG21	1.84	0.59
1:D:578:LEU:HB2	1:D:623:ASN:HB2	1.85	0.59
1:E:544:LEU:O	1:E:548:ILE:HG13	2.01	0.59
1:F:762:PHE:CE1	1:F:764:ASP:HB2	2.37	0.59
1:C:189:ASN:HB3	1:C:192:GLU:HB2	1.85	0.59
1:D:157:TYR:O	1:D:161:ASN:ND2	2.26	0.59
1:D:375:VAL:HG11	1:D:405:LEU:HD22	1.85	0.59
1:A:859:TRP:HE3	1:A:863:SER:HG	1.48	0.59
1:B:60:THR:HG22	1:B:119:PRO:HD3	1.83	0.59
1:C:393:LEU:HD12	1:C:469:GLN:HG3	1.82	0.59
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.38	0.59
1:E:653:ARG:O	1:E:656:SER:OG	2.19	0.59
1:F:1035:ARG:HD3	1:F:1038:GLU:OE1	2.03	0.59
1:B:166:ILE:O	1:B:169:THR:HB	2.02	0.59
1:D:201:VAL:HA	1:D:204:ILE:HD12	1.84	0.59
1:E:520:PHE:O	1:E:523:SER:OG	2.20	0.59
1:A:699:ARG:NH2	1:A:722:GLU:OE2	2.35	0.59
1:D:442:LEU:O	1:D:445:ILE:HG13	2.02	0.59
1:D:60:THR:HG23	1:D:61:VAL:HG23	1.84	0.59
1:D:733:GLN:OE1	1:D:743:ILE:HG21	2.02	0.59
2:B:1101:LMT:H5B	2:B:1101:LMT:H6D	1.84	0.59
1:D:457:ALA:O	1:D:468:ARG:NE	2.30	0.59
1:F:671:ILE:HD12	1:F:862:MET:SD	2.43	0.59
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.02	0.59
1:C:945:ILE:HA	1:C:971:ARG:NH1	2.18	0.59
1:D:1013:THR:O	1:D:1017:LEU:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:VAL:HG21	1:E:158:VAL:HG21	1.84	0.59
1:E:76:MET:HB2	1:E:93:THR:O	2.03	0.59
1:C:733:GLN:OE1	1:C:743:ILE:HG21	2.03	0.59
1:D:699:ARG:NH2	1:D:722:GLU:OE2	2.36	0.59
1:E:200:PRO:HB2	1:E:749:THR:HG22	1.85	0.59
1:E:213:GLN:HA	1:E:237:GLN:O	2.02	0.59
1:E:43:VAL:HG22	1:E:131:LYS:HG3	1.85	0.59
1:E:702:LEU:HD11	1:E:847:LEU:HB3	1.84	0.59
1:F:859:TRP:HE3	1:F:863:SER:HG	1.50	0.59
1:B:519:MET:O	1:B:523:SER:OG	2.21	0.59
1:B:278:ILE:HG13	1:B:613:ASN:HB3	1.85	0.59
1:B:910:ILE:O	1:B:914:LEU:HB2	2.03	0.59
1:D:366:LEU:HA	1:D:369:THR:HB	1.85	0.59
1:E:932:LEU:HA	1:E:935:ILE:HD12	1.84	0.59
1:F:172:VAL:HG13	1:F:291:ILE:HG23	1.85	0.59
1:F:455:PRO:HG2	1:F:880:SER:HA	1.84	0.59
1:B:167:SER:HB2	1:B:175:VAL:HG21	1.84	0.58
1:B:184:MET:HB3	1:B:771:VAL:HG13	1.85	0.58
1:C:139:VAL:HG21	1:C:628:PHE:CE2	2.38	0.58
1:F:267:LYS:HB2	1:F:776:GLU:OE1	2.02	0.58
1:B:696:THR:HG23	1:B:699:ARG:HH12	1.67	0.58
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.84	0.58
1:C:743:ILE:HD12	1:C:743:ILE:H	1.69	0.58
1:D:154:ILE:O	1:D:157:TYR:N	2.37	0.58
1:E:960:LEU:O	1:E:964:THR:HG23	2.03	0.58
1:A:332:PHE:O	1:A:336:SER:HB3	2.03	0.58
1:A:66:GLU:OE2	1:A:80:SER:OG	2.21	0.58
1:B:448:VAL:HG13	1:B:884:VAL:HG13	1.85	0.58
1:C:941:ASN:ND2	1:C:1015:THR:HG22	2.18	0.58
1:C:249:ILE:HB	1:C:262:LEU:HB2	1.85	0.58
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.39	0.58
1:C:881:LEU:HB3	1:C:902:MET:HE1	1.85	0.58
1:D:932:LEU:HA	1:D:935:ILE:HD12	1.85	0.58
1:F:987:MET:HG3	1:F:1008:MET:HE1	1.85	0.58
1:B:545:TYR:HB2	1:B:1021:PHE:HE2	1.69	0.58
1:B:167:SER:HB2	1:C:70:ASN:ND2	2.18	0.58
1:B:359:LEU:C	1:B:360:GLN:HG2	2.21	0.58
1:D:223:PRO:O	1:E:780:ARG:NH2	2.36	0.58
1:A:1040:ILE:HG13	1:A:1041:GLU:N	2.18	0.58
1:C:347:ALA:HB3	1:C:402:ILE:HD12	1.84	0.58
1:F:527:TYR:CE2	1:F:968:VAL:HG13	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:ALA:HB2	1:E:488:LEU:HD13	1.85	0.58
1:E:435:MET:SD	1:E:490:PRO:HB3	2.44	0.58
1:F:520:PHE:O	1:F:524:THR:HG22	2.03	0.58
1:F:664:PHE:CD2	1:F:717:ARG:HD3	2.35	0.58
1:A:253:VAL:HG12	1:A:259:ARG:HG2	1.86	0.58
1:A:644:VAL:HG11	1:A:667:ASN:HB2	1.84	0.58
1:B:415:ASN:ND2	1:B:418:ARG:HH12	2.02	0.58
1:F:817:GLU:OE2	1:F:825:MET:HA	2.03	0.58
1:B:905:VAL:HG13	1:B:935:ILE:HG23	1.85	0.58
1:D:375:VAL:HB	1:D:405:LEU:HD13	1.85	0.58
1:D:721:LEU:HB2	1:D:814:PRO:HG2	1.86	0.58
1:F:465:ALA:HA	1:F:468:ARG:NH1	2.18	0.58
1:A:375:VAL:HG21	1:A:481:SER:HA	1.86	0.58
1:A:562:SER:HB2	1:A:924:ASP:HB3	1.85	0.58
1:B:535:LEU:HD13	1:B:1027:VAL:HG21	1.86	0.58
1:B:511:GLY:HA2	1:B:515:TRP:NE1	2.19	0.58
1:C:197:GLN:HA	1:C:798:MET:SD	2.43	0.58
1:D:17:ILE:HA	1:D:20:MET:HE2	1.85	0.58
1:D:776:GLU:HB3	1:D:779:TYR:CE1	2.39	0.58
1:E:210:GLN:HE22	1:E:250:LEU:HB3	1.69	0.58
1:F:462:SER:O	1:F:466:ILE:HG12	2.03	0.58
1:F:278:ILE:HG13	1:F:613:ASN:HB3	1.84	0.58
1:A:680:PHE:HB2	1:A:859:TRP:HZ3	1.68	0.57
1:C:363:ARG:H	1:C:363:ARG:NH1	2.01	0.57
1:E:1019:ILE:HG13	1:E:1020:PHE:CD1	2.39	0.57
1:F:11:PHE:O	1:F:15:ILE:HG13	2.03	0.57
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.86	0.57
1:B:688:ALA:O	1:B:690:LEU:HG	2.04	0.57
1:C:971:ARG:HB3	1:C:971:ARG:CZ	2.34	0.57
1:E:310:LEU:HD23	1:E:325:TYR:OH	2.04	0.57
1:E:919:ARG:HB3	1:E:921:LEU:HD23	1.85	0.57
1:F:937:LEU:HD13	1:F:1011:MET:SD	2.44	0.57
1:C:971:ARG:O	1:C:971:ARG:NE	2.37	0.57
1:B:72:ILE:HD13	1:B:107:VAL:HA	1.86	0.57
1:E:44:THR:OG1	1:E:91:THR:OG1	2.22	0.57
1:F:858:ASP:OD2	1:F:859:TRP:N	2.37	0.57
1:A:424:GLY:HA3	1:A:502:LYS:CG	2.35	0.57
1:C:452:VAL:HG12	1:C:880:SER:HB3	1.85	0.57
1:D:137:LEU:HB2	1:D:293:LEU:HB2	1.87	0.57
1:E:144:ASN:ND2	1:E:319:SER:O	2.37	0.57
1:E:318:PRO:HG2	1:E:321:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:LEU:HD21	1:E:477:ALA:HB1	1.87	0.57
1:F:239:ARG:HB2	1:F:763:ILE:HD12	1.85	0.57
1:C:66:GLU:OE2	1:C:80:SER:OG	2.09	0.57
1:F:949:ALA:HB3	1:F:1026:PHE:HE2	1.70	0.57
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.87	0.57
1:C:492:LEU:O	1:C:496:MET:HG2	2.05	0.57
1:D:201:VAL:HG23	1:D:749:THR:HG23	1.86	0.57
1:F:888:LEU:HD21	1:F:943:ILE:HD11	1.87	0.57
1:F:915:ALA:HB2	1:F:1009:GLY:HA3	1.85	0.57
1:B:907:LEU:HD21	1:B:1021:PHE:HB2	1.87	0.57
1:E:932:LEU:HD23	1:E:935:ILE:HD12	1.86	0.57
1:F:979:SER:HB3	1:F:1015:THR:HG21	1.87	0.57
1:F:380:PHE:HA	1:F:383:LEU:HD12	1.87	0.57
1:F:940:LYS:NZ	1:F:978:THR:HG21	2.18	0.57
1:D:240:LEU:HB2	1:D:246:PHE:CE1	2.40	0.57
1:E:38:ILE:HD13	1:E:466:ILE:HG12	1.87	0.57
1:C:450:SER:O	1:C:454:VAL:HG23	2.04	0.57
1:F:507:GLU:HG2	1:F:518:ARG:HA	1.86	0.57
1:A:709:HIS:HB2	1:A:713:LEU:HD23	1.87	0.56
1:B:66:GLU:OE2	1:B:818:ARG:HD3	2.04	0.56
1:B:57:VAL:HG11	1:B:86:GLY:O	2.05	0.56
1:D:242:SER:O	1:D:246:PHE:HD1	1.87	0.56
1:F:409:ALA:O	1:F:413:VAL:HG23	2.05	0.56
1:F:976:LEU:O	1:F:980:LEU:HB2	2.05	0.56
1:A:140:VAL:N	1:A:289:LEU:O	2.36	0.56
1:C:393:LEU:HD13	1:C:466:ILE:HA	1.86	0.56
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.04	0.56
1:F:907:LEU:HD23	1:F:1017:LEU:HB3	1.87	0.56
1:C:713:LEU:HD21	1:C:843:LEU:HD12	1.88	0.56
1:D:412:VAL:HG22	1:D:438:ILE:CD1	2.35	0.56
1:F:144:ASN:HB3	1:F:148:THR:HG23	1.86	0.56
1:A:743:ILE:HA	1:A:746:ILE:HD12	1.87	0.56
1:B:186:ILE:HG12	1:B:268:ILE:HG12	1.86	0.56
1:B:189:ASN:OD1	1:B:190:PRO:HD2	2.06	0.56
1:B:696:THR:HG23	1:B:699:ARG:NH1	2.21	0.56
1:D:405:LEU:HD22	1:D:481:SER:HB3	1.88	0.56
1:F:69:MET:HG3	1:F:92:LEU:HD11	1.86	0.56
1:A:492:LEU:O	1:A:496:MET:HG2	2.06	0.56
1:A:4:PHE:HB3	1:A:8:ARG:NH1	2.20	0.56
1:A:519:MET:O	1:A:523:SER:OG	2.15	0.56
1:A:597:TYR:HB3	1:A:655:PHE:HZ	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:GLN:OE1	1:A:624:THR:HG22	2.05	0.56
1:B:535:LEU:HD21	1:B:1024:VAL:HA	1.87	0.56
1:C:3:ASN:O	1:C:6:ILE:N	2.38	0.56
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.87	0.56
1:D:934:THR:O	1:D:938:SER:OG	2.20	0.56
1:E:375:VAL:HG22	1:E:484:VAL:HG21	1.86	0.56
1:E:327:TYR:HB2	1:E:628:PHE:CZ	2.40	0.56
1:A:157:TYR:CZ	1:A:318:PRO:HD3	2.41	0.56
1:A:57:VAL:HG21	1:A:86:GLY:CA	2.35	0.56
1:B:251:LEU:HD11	1:B:262:LEU:HA	1.86	0.56
1:C:380:PHE:HA	1:C:383:LEU:HD12	1.88	0.56
1:C:681:ASP:HB2	1:C:828:LEU:HD23	1.86	0.56
1:D:100:ALA:HB1	1:D:131:LYS:HD2	1.87	0.56
1:E:186:ILE:HG12	1:E:268:ILE:HG12	1.86	0.56
1:F:968:VAL:O	1:F:972:LEU:HB2	2.05	0.56
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.05	0.56
1:B:950:LYS:NZ	1:B:1030:ARG:HH21	2.03	0.56
1:D:248:LYS:HA	1:D:261:LEU:HD13	1.86	0.56
1:D:556:PHE:HD1	1:D:913:LEU:HD21	1.71	0.56
1:E:752:ALA:O	1:E:774:MET:HA	2.05	0.56
1:F:404:LEU:HB3	1:F:478:MET:SD	2.45	0.56
1:F:160:ALA:HA	1:F:767:ARG:HE	1.71	0.56
1:A:259:ARG:NH1	1:B:734:GLU:OE1	2.36	0.56
1:A:393:LEU:HD11	1:A:466:ILE:HD13	1.88	0.56
1:A:344:LEU:HD21	1:A:399:VAL:HA	1.87	0.56
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.86	0.56
1:E:911:GLY:HA3	1:E:1013:THR:OG1	2.05	0.56
1:E:175:VAL:HG23	1:F:70:ASN:ND2	2.20	0.56
1:B:455:PRO:HG2	1:B:880:SER:OG	2.04	0.56
1:D:605:ASN:HD21	1:D:642:ASN:CG	2.09	0.56
1:D:751:GLY:O	1:D:753:ALA:N	2.39	0.56
1:A:35:TYR:CE2	1:A:564:LEU:HD21	2.41	0.56
1:C:688:ALA:O	1:C:690:LEU:N	2.39	0.56
1:D:239:ARG:NH1	1:D:761:ASP:O	2.38	0.56
1:E:415:ASN:O	1:E:419:VAL:HG23	2.06	0.56
1:F:298:ASN:HB3	1:F:301:ASP:HB2	1.87	0.56
1:C:11:PHE:O	1:C:11:PHE:HD2	1.88	0.55
1:E:979:SER:HB3	1:E:1015:THR:HG21	1.88	0.55
1:B:211:ASN:O	1:B:760:ASN:ND2	2.39	0.55
1:B:745:ASP:O	1:B:749:THR:OG1	2.14	0.55
1:B:717:ARG:NE	1:B:828:LEU:HB2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:ALA:HA	1:F:314:GLU:CD	2.27	0.55
1:F:780:ARG:O	1:F:781:MET:HE2	2.06	0.55
1:A:99:ASP:HB3	1:A:102:ILE:HB	1.88	0.55
1:B:888:LEU:HD21	1:B:943:ILE:HD11	1.89	0.55
1:C:1026:PHE:O	1:C:1030:ARG:HG2	2.06	0.55
1:C:407:ASP:OD2	1:C:940:LYS:HD2	2.06	0.55
1:D:559:LEU:HD23	1:D:560:PRO:HD2	1.89	0.55
1:D:989:LEU:HB3	1:D:1000:GLN:O	2.06	0.55
1:E:58:GLN:O	1:E:63:GLN:HG3	2.06	0.55
1:F:186:ILE:HD13	1:F:262:LEU:HD21	1.87	0.55
1:F:414:GLU:OE1	1:F:973:ARG:HD3	2.07	0.55
1:F:443:VAL:O	1:F:447:MET:HB3	2.06	0.55
1:F:945:ILE:HA	1:F:971:ARG:NH1	2.20	0.55
1:A:753:ALA:O	1:A:775:SER:HB3	2.06	0.55
1:D:196:PHE:HB3	1:D:252:LYS:HZ3	1.71	0.55
1:D:261:LEU:N	1:D:264:ASP:OD2	2.40	0.55
1:F:187:TRP:HA	1:F:774:MET:O	2.06	0.55
1:E:241:THR:N	1:E:245:GLU:OE1	2.36	0.55
1:E:261:LEU:HD12	1:E:263:ARG:NH1	2.21	0.55
1:E:261:LEU:N	1:E:264:ASP:OD2	2.38	0.55
1:D:733:GLN:NE2	1:F:210:GLN:HG2	2.21	0.55
1:F:506:GLY:O	1:F:508:GLY:N	2.32	0.55
1:A:1037:ASN:N	1:A:1038:GLU:HB2	2.22	0.55
1:B:293:LEU:HD22	1:B:297:ALA:HB3	1.87	0.55
1:C:501:ALA:O	1:C:504:ASP:HB2	2.06	0.55
1:C:762:PHE:CE1	1:C:764:ASP:HB2	2.42	0.55
1:D:154:ILE:HG22	1:D:287:SER:HB3	1.88	0.55
1:E:934:THR:O	1:E:938:SER:OG	2.23	0.55
1:C:421:ALA:HB1	1:C:505:HIS:H	1.71	0.55
1:C:888:LEU:HD21	1:C:943:ILE:HD11	1.88	0.55
1:D:186:ILE:HG12	1:D:268:ILE:HG12	1.89	0.55
2:E:1101:LMT:H6D	2:E:1101:LMT:C5B	2.34	0.55
1:F:57:VAL:HG23	1:F:82:SER:HB3	1.89	0.55
1:A:58:GLN:NE2	1:A:59:ASP:OD1	2.36	0.55
1:D:58:GLN:OE1	1:D:818:ARG:NH1	2.38	0.55
1:E:524:THR:O	1:E:527:TYR:HB3	2.07	0.55
1:E:577:GLN:NE2	1:E:721:LEU:HD11	2.21	0.55
1:A:622:GLN:HE21	1:C:222:THR:HG22	1.72	0.55
1:B:699:ARG:HD2	1:B:718:PRO:HB3	1.89	0.55
1:D:1016:VAL:HG12	2:D:1101:LMT:H91	1.89	0.55
1:F:65:ILE:HB	1:F:90:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:O	1:A:157:TYR:N	2.40	0.55
1:A:424:GLY:HA3	1:A:502:LYS:CB	2.37	0.55
1:B:327:TYR:HB2	1:B:628:PHE:CE2	2.41	0.55
1:B:583:THR:HG22	1:B:585:GLU:H	1.71	0.55
1:B:752:ALA:O	1:B:774:MET:HA	2.07	0.55
1:B:76:MET:SD	1:B:864:TYR:HE2	2.30	0.55
1:C:343:THR:HA	1:C:346:GLU:OE1	2.07	0.55
1:E:23:GLY:HA3	1:E:377:LEU:HB3	1.88	0.55
1:E:430:ALA:O	1:E:433:LYS:HB3	2.07	0.55
1:F:112:GLN:HA	1:F:115:MET:HB2	1.87	0.55
1:F:214:VAL:HG23	1:F:237:GLN:HB2	1.89	0.55
1:A:982:PHE:O	1:A:985:GLY:N	2.40	0.54
1:B:248:LYS:HA	1:B:261:LEU:HD13	1.90	0.54
1:B:356:TYR:C	1:B:358:PHE:H	2.11	0.54
1:B:573:MET:HA	1:B:629:VAL:HG23	1.89	0.54
1:C:278:ILE:HG13	1:C:613:ASN:HB3	1.88	0.54
1:C:599:LEU:O	1:C:603:LYS:HG2	2.07	0.54
1:E:559:LEU:HD13	1:E:923:ASN:HB2	1.89	0.54
1:F:414:GLU:HG2	1:F:973:ARG:NH1	2.21	0.54
1:A:101:ASP:OD1	1:A:101:ASP:N	2.41	0.54
1:A:121:GLU:O	1:A:125:GLN:HB2	2.07	0.54
1:A:573:MET:HA	1:A:629:VAL:HG23	1.88	0.54
1:A:976:LEU:O	1:A:980:LEU:HB2	2.07	0.54
1:B:442:LEU:O	1:B:445:ILE:HG13	2.06	0.54
1:B:492:LEU:O	1:B:496:MET:HG2	2.07	0.54
1:D:408:ASP:OD2	1:D:940:LYS:NZ	2.28	0.54
1:D:745:ASP:O	1:D:749:THR:OG1	2.22	0.54
1:E:355:MET:SD	1:E:365:THR:HA	2.47	0.54
1:E:405:LEU:HD22	1:E:481:SER:HB3	1.89	0.54
1:E:910:ILE:O	1:E:914:LEU:HB2	2.07	0.54
1:F:776:GLU:HB2	1:F:779:TYR:CE1	2.43	0.54
1:F:960:LEU:HD21	1:F:1027:VAL:HA	1.89	0.54
1:F:982:PHE:O	1:F:985:GLY:N	2.41	0.54
1:F:1042:HIS:CG	1:F:1043:SER:H	2.24	0.54
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.90	0.54
1:C:210:GLN:OE1	1:C:249:ILE:HG23	2.08	0.54
1:E:335:ILE:O	1:E:339:GLU:HG2	2.08	0.54
1:A:702:LEU:HD12	1:A:851:LEU:HD21	1.89	0.54
1:B:588:GLN:O	1:B:592:ASN:ND2	2.40	0.54
1:C:725:PRO:HG3	1:C:811:TYR:CE1	2.43	0.54
1:D:139:VAL:HB	1:D:327:TYR:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:945:ILE:HG12	1:D:971:ARG:CZ	2.37	0.54
1:E:175:VAL:HG23	1:F:70:ASN:HD22	1.73	0.54
1:E:448:VAL:HG13	1:E:884:VAL:HG22	1.89	0.54
1:F:420:MET:HB3	1:F:500:ILE:HB	1.88	0.54
1:F:568:ASP:OD1	1:F:637:ARG:NH1	2.31	0.54
1:A:901:VAL:HG21	1:A:943:ILE:HG13	1.88	0.54
1:B:318:PRO:HD2	1:B:321:LEU:HD22	1.88	0.54
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.89	0.54
1:D:448:VAL:HG22	1:D:887:CYS:CB	2.37	0.54
1:E:157:TYR:CZ	1:E:318:PRO:HD3	2.42	0.54
1:E:7:ASP:CG	1:E:432:ARG:HH21	2.09	0.54
1:F:422:GLU:HB3	1:F:423:GLU:HG3	1.90	0.54
1:F:775:SER:OG	1:F:776:GLU:O	2.25	0.54
1:B:986:VAL:HG21	1:B:1007:VAL:HG11	1.89	0.54
1:C:893:GLU:HG3	1:C:893:GLU:O	2.06	0.54
1:E:121:GLU:O	1:E:125:GLN:HB2	2.08	0.54
1:F:284:GLN:HG3	1:F:285:PRO:HD2	1.90	0.54
1:F:13:TRP:CH2	1:F:370:ILE:HD13	2.42	0.54
1:F:926:TYR:HD1	1:F:1002:ALA:HB3	1.73	0.54
1:C:193:LEU:HD13	1:C:200:PRO:HD3	1.89	0.54
1:C:248:LYS:HA	1:C:261:LEU:HD13	1.90	0.54
1:C:895:TRP:HA	1:C:895:TRP:CE3	2.42	0.54
1:C:941:ASN:HD21	1:C:1015:THR:HG22	1.72	0.54
1:A:27:ILE:HD11	1:A:380:PHE:CD1	2.43	0.54
1:B:415:ASN:OD1	1:B:434:SER:HB2	2.08	0.54
1:B:730:ASP:OD1	1:B:808:ARG:NH2	2.40	0.54
1:A:11:PHE:CD2	1:B:890:ALA:HB1	2.43	0.54
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.90	0.54
1:C:907:LEU:HD21	1:C:1021:PHE:CB	2.38	0.54
1:E:111:LEU:HD21	1:E:127:VAL:HG11	1.90	0.54
1:E:785:ASP:OD1	1:E:785:ASP:N	2.41	0.54
1:B:901:VAL:HG21	1:B:943:ILE:HG13	1.89	0.54
1:C:894:SER:HB3	1:C:897:ILE:HG12	1.88	0.54
1:C:44:THR:OG1	1:C:91:THR:OG1	2.25	0.54
1:E:751:GLY:O	1:E:753:ALA:N	2.41	0.54
1:E:375:VAL:O	1:E:379:THR:OG1	2.24	0.53
1:E:460:GLY:O	1:E:463:THR:OG1	2.25	0.53
1:E:281:PHE:HD1	1:E:610:PHE:HD1	1.55	0.53
1:A:73:ASP:CG	1:A:106:GLN:HE22	2.12	0.53
1:B:668:LEU:CD2	1:B:668:LEU:H	2.21	0.53
1:B:705:GLU:HA	1:B:708:LYS:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:TYR:CD1	1:D:60:THR:HG21	2.44	0.53
1:D:584:GLN:N	1:D:622:GLN:HB3	2.24	0.53
1:D:699:ARG:NE	1:D:718:PRO:HB3	2.24	0.53
1:E:1040:ILE:O	1:E:1041:GLU:HG3	2.07	0.53
1:E:218:GLN:HG3	1:E:221:GLY:HA3	1.90	0.53
1:A:279:ALA:HB3	1:A:286:ALA:O	2.09	0.53
1:B:356:TYR:O	1:B:358:PHE:N	2.34	0.53
1:B:602:GLU:OE2	1:B:650:ARG:HD2	2.09	0.53
1:D:156:ASP:OD1	1:D:765:ARG:NH2	2.41	0.53
1:D:563:PHE:O	1:D:564:LEU:HD12	2.09	0.53
1:F:587:THR:HG21	1:F:622:GLN:O	2.07	0.53
1:F:686:ASP:OD1	1:F:687:GLN:N	2.41	0.53
1:A:210:GLN:HE21	1:B:733:GLN:HE21	1.56	0.53
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.90	0.53
1:C:34:GLN:O	1:C:392:THR:OG1	2.26	0.53
1:C:453:PHE:HB3	1:C:471:SER:HA	1.88	0.53
1:C:979:SER:HB3	1:C:1015:THR:HG21	1.90	0.53
1:D:419:VAL:HG13	1:D:423:GLU:OE2	2.09	0.53
1:D:72:ILE:HD13	1:D:107:VAL:HA	1.91	0.53
1:E:262:LEU:HG	1:E:268:ILE:HD11	1.90	0.53
1:F:376:LEU:O	1:F:379:THR:N	2.41	0.53
1:F:375:VAL:HB	1:F:405:LEU:HD22	1.89	0.53
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.43	0.53
1:D:564:LEU:HD22	1:D:671:ILE:HG12	1.90	0.53
1:E:214:VAL:HG21	1:F:747:ASN:ND2	2.23	0.53
1:F:699:ARG:HE	1:F:718:PRO:HB3	1.72	0.53
1:A:108:GLN:NE2	1:B:109:ASN:O	2.41	0.53
1:A:465:ALA:O	1:A:469:GLN:HG2	2.09	0.53
1:C:654:ALA:O	1:C:658:ILE:HG12	2.08	0.53
1:C:731:ILE:HD13	1:C:746:ILE:HD11	1.90	0.53
1:D:68:ASN:O	1:D:110:LYS:HB3	2.08	0.53
1:D:151:GLN:HG3	1:D:152:GLU:N	2.24	0.53
1:E:240:LEU:HB2	1:E:246:PHE:CE1	2.44	0.53
1:E:448:VAL:HG13	1:E:884:VAL:HG13	1.90	0.53
1:E:492:LEU:O	1:E:496:MET:HG2	2.09	0.53
1:E:606:VAL:HA	1:E:631:LEU:HD23	1.89	0.53
1:F:462:SER:HB3	1:F:865:GLN:HG2	1.91	0.53
1:A:434:SER:O	1:A:438:ILE:HG12	2.09	0.53
1:B:174:ASP:HB3	1:B:292:LYS:HD2	1.90	0.53
1:E:172:VAL:HG22	1:E:306:ILE:HD11	1.90	0.53
1:E:506:GLY:HA2	1:E:509:LYS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:578:LEU:HD13	1:E:661:ALA:HB2	1.91	0.53
1:E:555:LEU:HD11	1:E:914:LEU:HD12	1.89	0.53
1:A:448:VAL:O	1:A:451:ALA:HB3	2.08	0.53
1:B:726:GLN:CD	1:B:812:GLY:HA3	2.29	0.53
1:B:789:TRP:O	1:B:801:PHE:HD2	1.92	0.53
1:C:57:VAL:HG23	1:C:82:SER:HB3	1.90	0.53
1:C:882:ILE:O	1:C:886:LEU:HD22	2.08	0.53
1:E:632:LYS:O	1:E:637:ARG:NE	2.42	0.53
1:E:753:ALA:O	1:E:775:SER:HB3	2.08	0.53
1:F:396:PHE:O	1:F:400:LEU:HB2	2.09	0.53
1:A:242:SER:OG	1:A:245:GLU:HG2	2.08	0.53
1:B:139:VAL:HG13	1:B:178:PHE:HE1	1.73	0.53
1:B:340:VAL:HG11	1:B:395:MET:HB3	1.91	0.53
1:B:396:PHE:O	1:B:400:LEU:HB2	2.08	0.53
1:C:363:ARG:CB	1:C:363:ARG:HH11	2.21	0.53
1:C:686:ASP:HB3	1:C:823:PRO:O	2.09	0.53
2:D:1101:LMT:H6D	2:D:1101:LMT:H5B	1.91	0.53
1:D:58:GLN:O	1:D:62:THR:HB	2.08	0.53
1:D:582:ALA:HB3	1:D:623:ASN:HB3	1.91	0.53
1:E:705:GLU:HB3	1:E:847:LEU:HD22	1.89	0.53
1:F:212:ALA:HA	1:F:239:ARG:HG2	1.90	0.53
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.91	0.53
1:B:169:THR:HG21	1:B:306:ILE:HG13	1.90	0.53
1:D:298:ASN:OD1	1:D:301:ASP:N	2.40	0.53
1:E:189:ASN:ND2	1:E:190:PRO:HD2	2.24	0.53
1:E:445:ILE:HG12	1:E:940:LYS:HE3	1.90	0.53
1:A:744:ASN:O	1:A:748:THR:HG23	2.09	0.52
1:A:952:LEU:O	1:A:956:GLU:HB2	2.08	0.52
1:B:281:PHE:CZ	1:B:324:VAL:HG11	2.44	0.52
1:D:166:ILE:HD12	1:D:306:ILE:HG23	1.91	0.52
1:D:587:THR:HB	1:D:613:ASN:HD21	1.74	0.52
1:D:95:GLU:HB2	1:D:98:THR:OG1	2.09	0.52
1:E:60:THR:HG22	1:E:119:PRO:HD3	1.92	0.52
1:E:57:VAL:HG11	1:E:86:GLY:CA	2.39	0.52
1:F:137:LEU:HB2	1:F:293:LEU:HB2	1.91	0.52
1:F:143:ILE:HG22	1:F:286:ALA:HB2	1.90	0.52
1:A:26:ALA:O	1:A:30:LEU:HB2	2.09	0.52
1:B:3:ASN:HA	1:B:6:ILE:HD12	1.90	0.52
1:B:800:PRO:HG2	1:B:803:ALA:HB2	1.91	0.52
1:C:525:HIS:HA	1:C:528:THR:HG22	1.91	0.52
1:D:344:LEU:CD2	1:D:402:ILE:HD11	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:775:SER:HB2	1:D:789:TRP:HZ2	1.74	0.52
1:D:235:ILE:HD11	1:E:726:GLN:NE2	2.24	0.52
1:F:753:ALA:O	1:F:775:SER:HB3	2.09	0.52
1:B:354:VAL:O	1:B:358:PHE:HB2	2.10	0.52
1:B:457:ALA:HB2	1:B:471:SER:OG	2.10	0.52
1:B:456:MET:O	1:B:467:TYR:HB3	2.09	0.52
1:B:987:MET:HA	1:B:1008:MET:HE3	1.90	0.52
1:C:937:LEU:HD13	1:C:1011:MET:CE	2.40	0.52
1:D:451:ALA:O	1:D:880:SER:OG	2.22	0.52
1:E:544:LEU:HA	1:E:547:ILE:HD12	1.90	0.52
1:F:247:GLY:O	1:F:261:LEU:HB3	2.09	0.52
1:A:401:ALA:O	1:A:405:LEU:HG	2.10	0.52
1:A:902:MET:O	1:A:905:VAL:HG23	2.09	0.52
1:C:137:LEU:HB2	1:C:293:LEU:HB2	1.91	0.52
1:C:452:VAL:O	1:C:455:PRO:HD2	2.08	0.52
1:C:916:ALA:HB2	1:C:927:PHE:CE1	2.43	0.52
1:E:1039:ASP:N	1:E:1040:ILE:HG13	2.24	0.52
1:E:447:MET:HB3	1:E:887:CYS:SG	2.49	0.52
1:F:986:VAL:HG21	1:F:1007:VAL:HG11	1.90	0.52
1:F:580:ALA:HB1	1:F:724:THR:HG22	1.91	0.52
1:A:776:GLU:HG2	1:A:777:ALA:H	1.75	0.52
1:C:940:LYS:NZ	1:C:978:THR:HG21	2.25	0.52
1:D:456:MET:HG3	1:D:471:SER:HB2	1.92	0.52
1:D:987:MET:HA	1:D:1008:MET:HE3	1.92	0.52
1:F:1015:THR:OG1	1:F:1016:VAL:N	2.43	0.52
1:F:451:ALA:HB1	1:F:883:VAL:HG12	1.90	0.52
1:A:650:ARG:O	1:A:653:ARG:HB3	2.08	0.52
1:E:278:ILE:CG1	1:E:613:ASN:HB3	2.40	0.52
1:F:187:TRP:CB	1:F:776:GLU:HG2	2.40	0.52
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.45	0.52
1:F:985:GLY:O	1:F:988:PRO:HD2	2.09	0.52
1:A:958:LYS:C	1:A:1040:ILE:HG12	2.30	0.52
1:A:971:ARG:O	1:A:974:PRO:HD2	2.10	0.52
1:B:586:ARG:O	1:B:589:LYS:HB3	2.09	0.52
1:B:87:THR:HG21	1:B:620:ARG:NH2	2.25	0.52
1:C:188:MET:HB3	1:C:193:LEU:HD11	1.92	0.52
1:D:375:VAL:HG22	1:D:484:VAL:HG21	1.92	0.52
1:D:678:THR:HA	1:D:837:THR:OG1	2.10	0.52
1:D:905:VAL:HB	1:D:906:PRO:HD3	1.91	0.52
1:E:533:GLY:HA2	1:E:536:ARG:HD3	1.92	0.52
1:E:80:SER:HB3	1:E:90:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:778:LYS:HG3	1:F:779:TYR:CZ	2.45	0.52
1:F:971:ARG:HH21	1:F:975:ILE:HD11	1.75	0.52
1:A:574:THR:HG21	1:A:598:TYR:CE2	2.44	0.52
1:A:407:ASP:HB3	1:A:940:LYS:HZ3	1.74	0.52
1:C:901:VAL:HG23	1:C:942:ALA:CB	2.36	0.52
1:D:892:TYR:CD2	1:D:897:ILE:HG22	2.45	0.52
1:E:225:VAL:HG12	1:F:777:ALA:HB1	1.90	0.52
1:F:698:ALA:O	1:F:701:GLN:HB3	2.10	0.52
1:A:485:ALA:O	1:A:490:PRO:HD3	2.10	0.52
1:B:267:LYS:N	1:B:267:LYS:HD2	2.24	0.52
1:B:669:PRO:HB3	1:B:674:LEU:HD12	1.91	0.52
1:C:82:SER:HB2	1:C:816:LEU:HB2	1.92	0.52
1:E:42:ALA:HB2	1:E:93:THR:HG23	1.91	0.52
1:F:250:LEU:HD11	1:F:259:ARG:HB3	1.92	0.52
1:F:682:PHE:CE1	1:F:857:TYR:HB2	2.44	0.52
1:A:11:PHE:HE1	1:A:15:ILE:HD11	1.75	0.52
1:A:836:SER:HB3	1:A:839:GLU:HG3	1.92	0.52
1:A:841:MET:HG2	1:A:859:TRP:CH2	2.45	0.52
1:E:59:ASP:OD1	1:E:63:GLN:NE2	2.43	0.52
1:E:904:VAL:HG21	1:E:942:ALA:HB2	1.92	0.52
1:A:1020:PHE:CZ	2:A:1101:LMT:H32	2.46	0.51
1:A:216:ALA:HB2	1:A:236:ALA:HB2	1.92	0.51
1:A:711:ASP:O	1:A:835:LYS:NZ	2.36	0.51
1:B:580:ALA:HB1	1:B:724:THR:HG22	1.92	0.51
1:C:336:SER:O	1:C:340:VAL:HG23	2.09	0.51
1:D:332:PHE:O	1:D:336:SER:HB3	2.10	0.51
1:E:1038:GLU:OE1	1:E:1040:ILE:HG12	2.10	0.51
1:E:339:GLU:OE1	1:E:342:LYS:HD3	2.11	0.51
1:E:184:MET:HB2	1:E:762:PHE:CE2	2.46	0.51
1:F:521:GLU:O	1:F:524:THR:HG23	2.10	0.51
1:F:841:MET:HG2	1:F:859:TRP:CH2	2.45	0.51
2:A:1101:LMT:H6D	2:A:1101:LMT:O5B	2.09	0.51
1:B:172:VAL:HG22	1:B:306:ILE:HD11	1.92	0.51
1:B:82:SER:HA	1:B:88:VAL:HG22	1.92	0.51
1:C:247:GLY:O	1:C:261:LEU:HB3	2.11	0.51
1:C:940:LYS:HE2	1:C:941:ASN:OD1	2.10	0.51
1:D:163:LYS:HD2	1:D:289:LEU:HD21	1.91	0.51
1:D:362:PHE:HE2	1:D:363:ARG:HH21	1.59	0.51
1:D:775:SER:OG	1:D:780:ARG:HG2	2.10	0.51
1:D:971:ARG:O	1:D:975:ILE:HG12	2.11	0.51
1:E:897:ILE:N	1:E:898:PRO:HD2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:527:TYR:CE2	1:E:972:LEU:HG	2.45	0.51
1:F:754:TRP:CH2	1:F:780:ARG:HA	2.45	0.51
1:F:760:ASN:O	1:F:771:VAL:HB	2.11	0.51
1:F:83:ASP:HB2	1:F:87:THR:O	2.10	0.51
1:C:1038:GLU:HA	1:C:1039:ASP:CB	2.40	0.51
1:C:149:MET:HG3	1:C:154:ILE:HG13	1.92	0.51
1:D:143:ILE:HG22	1:D:286:ALA:HB2	1.93	0.51
1:D:637:ARG:HB3	1:D:642:ASN:HB3	1.92	0.51
1:D:776:GLU:HB3	1:D:779:TYR:CD1	2.45	0.51
1:F:733:GLN:NE2	1:F:743:ILE:HG21	2.22	0.51
1:A:11:PHE:CE1	1:A:15:ILE:HD11	2.45	0.51
1:A:3:ASN:O	1:A:6:ILE:HG12	2.10	0.51
1:A:790:TYR:HB3	1:A:798:MET:HB3	1.92	0.51
1:D:586:ARG:O	1:D:590:VAL:HG23	2.11	0.51
1:D:182:TYR:HD2	1:D:765:ARG:HH22	1.59	0.51
1:F:340:VAL:HG22	1:F:396:PHE:CE2	2.46	0.51
1:F:905:VAL:HB	1:F:906:PRO:HD3	1.93	0.51
1:A:992:SER:OG	1:A:1000:GLN:OE1	2.26	0.51
1:B:61:VAL:HG22	1:B:118:LEU:HD22	1.91	0.51
1:C:751:GLY:O	1:C:753:ALA:N	2.43	0.51
1:C:739:LEU:HD13	1:C:799:VAL:HG11	1.92	0.51
1:D:212:ALA:HA	1:D:239:ARG:HD3	1.92	0.51
1:D:690:LEU:HD21	1:D:853:THR:O	2.09	0.51
1:E:441:ALA:O	1:E:445:ILE:HG23	2.10	0.51
1:E:578:LEU:HD21	1:E:590:VAL:HG21	1.93	0.51
1:F:431:THR:HG21	1:F:490:PRO:O	2.11	0.51
1:F:650:ARG:O	1:F:653:ARG:HB3	2.10	0.51
1:A:905:VAL:HG13	1:A:935:ILE:HD13	1.93	0.51
1:B:415:ASN:O	1:B:419:VAL:HG23	2.10	0.51
1:B:654:ALA:O	1:B:658:ILE:HG12	2.11	0.51
1:C:686:ASP:OD2	1:C:823:PRO:HD2	2.11	0.51
1:E:102:ILE:O	1:E:106:GLN:HG3	2.10	0.51
1:E:139:VAL:O	1:E:326:PRO:HD2	2.10	0.51
1:E:904:VAL:HG21	1:E:942:ALA:CB	2.40	0.51
1:D:728:LYS:HA	1:F:235:ILE:HB	1.92	0.51
1:F:261:LEU:N	1:F:264:ASP:OD2	2.43	0.51
1:F:340:VAL:CG1	1:F:395:MET:HB3	2.40	0.51
1:F:524:THR:O	1:F:528:THR:HG22	2.11	0.51
1:F:937:LEU:HD11	1:F:982:PHE:HE2	1.76	0.51
1:F:944:LEU:HD13	1:F:975:ILE:HG12	1.91	0.51
1:A:612:VAL:HG12	1:A:615:PHE:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:PHE:CE1	1:A:899:PHE:CE2	2.98	0.51
1:C:979:SER:HA	1:C:1011:MET:HE3	1.93	0.51
1:D:169:THR:HG21	1:D:306:ILE:HG13	1.92	0.51
1:E:184:MET:HG2	1:E:246:PHE:CD2	2.46	0.51
1:E:597:TYR:CD2	1:E:655:PHE:HZ	2.29	0.51
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.93	0.51
1:A:459:PHE:CE2	1:A:876:LEU:HD12	2.45	0.51
1:A:424:GLY:HA3	1:A:502:LYS:HB3	1.93	0.51
1:A:424:GLY:HA3	1:A:502:LYS:HG2	1.91	0.51
1:C:693:GLU:HB3	1:C:694:LYS:HE2	1.93	0.51
1:D:800:PRO:HG2	1:D:803:ALA:HB2	1.93	0.51
1:A:213:GLN:HA	1:A:237:GLN:O	2.11	0.51
1:C:396:PHE:O	1:C:400:LEU:HB2	2.11	0.51
1:C:400:LEU:O	1:C:404:LEU:HD13	2.10	0.51
1:D:328:ASP:O	1:D:331:PRO:HD2	2.11	0.51
1:D:728:LYS:HG2	1:D:808:ARG:CZ	2.41	0.51
1:D:953:MET:SD	1:D:960:LEU:HA	2.51	0.51
1:E:165:ALA:HA	1:E:168:ARG:HB2	1.93	0.51
1:E:251:LEU:HD11	1:E:262:LEU:HA	1.91	0.51
1:E:643:LYS:NZ	1:E:993:THR:HG23	2.26	0.51
1:F:63:GLN:OE1	1:F:818:ARG:NH2	2.44	0.51
1:A:971:ARG:HB3	1:A:971:ARG:CZ	2.41	0.51
1:B:254:ASN:HB2	1:B:258:SER:O	2.11	0.51
1:B:3:ASN:O	1:B:6:ILE:HB	2.11	0.51
1:C:156:ASP:OD2	1:C:769:LYS:NZ	2.41	0.51
1:C:214:VAL:HG23	1:C:237:GLN:HB2	1.93	0.51
1:E:58:GLN:HE21	1:E:816:LEU:HD13	1.76	0.51
1:F:23:GLY:O	1:F:27:ILE:HG23	2.11	0.51
1:F:404:LEU:HG	1:F:449:LEU:HD13	1.92	0.51
1:A:151:GLN:HE22	1:A:278:ILE:HG22	1.76	0.50
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.41	0.50
1:C:531:VAL:O	1:C:534:ILE:HG13	2.11	0.50
1:C:49:TYR:HD1	1:C:57:VAL:HG12	1.76	0.50
1:D:23:GLY:O	1:D:27:ILE:HB	2.11	0.50
1:D:336:SER:O	1:D:340:VAL:HG23	2.11	0.50
1:D:544:LEU:O	1:D:547:ILE:HB	2.11	0.50
1:D:58:GLN:O	1:D:63:GLN:HG3	2.12	0.50
1:F:380:PHE:HD2	1:F:383:LEU:HD12	1.75	0.50
1:F:901:VAL:HG23	1:F:942:ALA:CB	2.37	0.50
1:B:5:PHE:HE2	1:B:11:PHE:CD2	2.29	0.50
1:C:222:THR:HA	1:C:224:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:602:GLU:HG3	1:C:605:ASN:HD22	1.77	0.50
1:D:112:GLN:HG3	1:E:112:GLN:OE1	2.10	0.50
1:D:393:LEU:HB3	1:D:470:PHE:CE1	2.46	0.50
1:D:602:GLU:HB3	1:D:606:VAL:HG23	1.93	0.50
1:D:730:ASP:HB2	1:D:808:ARG:NH2	2.26	0.50
1:E:166:ILE:HG23	1:E:306:ILE:HG12	1.92	0.50
1:E:696:THR:HG23	1:E:699:ARG:HH12	1.75	0.50
1:A:151:GLN:HG3	1:A:152:GLU:N	2.27	0.50
1:C:343:THR:HG21	1:C:989:LEU:HD21	1.92	0.50
1:E:357:LEU:O	1:E:358:PHE:HD1	1.94	0.50
1:F:694:LYS:H	1:F:694:LYS:HD2	1.77	0.50
1:F:898:PRO:O	1:F:902:MET:HG2	2.10	0.50
1:B:57:VAL:HG23	1:B:82:SER:HB3	1.92	0.50
1:C:578:LEU:HD12	1:C:582:ALA:HB1	1.92	0.50
1:C:934:THR:O	1:C:938:SER:OG	2.28	0.50
1:D:971:ARG:C	1:D:974:PRO:HD2	2.32	0.50
1:E:442:LEU:O	1:E:445:ILE:HG13	2.11	0.50
1:E:6:ILE:HD11	1:E:431:THR:HG22	1.92	0.50
1:E:82:SER:HB2	1:E:816:LEU:HB2	1.94	0.50
1:E:901:VAL:HG23	1:E:942:ALA:CB	2.42	0.50
1:F:310:LEU:O	1:F:314:GLU:HG3	2.12	0.50
1:F:428:LYS:O	1:F:432:ARG:HG3	2.11	0.50
1:F:923:ASN:ND2	1:F:923:ASN:O	2.36	0.50
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.93	0.50
1:A:293:LEU:HD22	1:A:294:ALA:H	1.76	0.50
1:A:360:GLN:HE22	1:A:513:PHE:HB3	1.76	0.50
1:D:379:THR:HG21	1:D:477:ALA:HB2	1.93	0.50
1:E:216:ALA:HB1	1:E:234:ILE:HG22	1.92	0.50
1:A:572:PHE:HB2	1:A:666:PHE:O	2.11	0.50
1:A:971:ARG:O	1:A:975:ILE:HG12	2.11	0.50
1:B:210:GLN:HG2	1:C:733:GLN:NE2	2.27	0.50
1:B:588:GLN:HG3	1:B:592:ASN:HD21	1.76	0.50
1:C:952:LEU:HD23	1:C:956:GLU:HG3	1.93	0.50
1:D:915:ALA:HB2	1:D:1009:GLY:HA3	1.93	0.50
1:D:400:LEU:HD21	1:D:930:GLY:HA2	1.93	0.50
1:E:222:THR:HA	1:E:224:PRO:HD3	1.93	0.50
1:E:340:VAL:HG22	1:E:396:PHE:CE2	2.47	0.50
1:E:379:THR:HA	1:E:480:LEU:HD12	1.94	0.50
1:E:46:SER:OG	1:E:89:GLN:HG2	2.11	0.50
1:A:907:LEU:HD21	1:A:1021:PHE:CD1	2.47	0.50
1:A:909:VAL:HG22	1:A:931:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:HD23	1:B:178:PHE:N	2.26	0.50
1:B:401:ALA:O	1:B:405:LEU:HG	2.11	0.50
1:B:894:SER:HB3	1:B:898:PRO:HD3	1.92	0.50
1:A:734:GLU:HG2	1:C:250:LEU:HD22	1.93	0.50
1:C:634:TRP:CD1	1:C:634:TRP:N	2.72	0.50
1:E:177:LEU:HG	1:E:289:LEU:HD21	1.93	0.50
1:E:396:PHE:O	1:E:400:LEU:HB2	2.12	0.50
1:E:564:LEU:HD13	1:E:674:LEU:HD21	1.94	0.50
1:E:892:TYR:O	1:E:893:GLU:HB2	2.11	0.50
1:F:431:THR:HG22	1:F:435:MET:CE	2.41	0.50
1:F:66:GLU:OE1	1:F:821:GLY:HA2	2.11	0.50
1:F:445:ILE:HG12	1:F:940:LYS:HG3	1.94	0.50
1:A:13:TRP:NE1	1:A:492:LEU:HD21	2.27	0.50
1:A:197:GLN:HA	1:A:798:MET:SD	2.52	0.50
1:C:658:ILE:O	1:C:659:LYS:NZ	2.37	0.50
1:D:609:VAL:HG22	1:D:629:VAL:HG13	1.94	0.50
1:D:909:VAL:HG22	1:D:931:LEU:HD21	1.94	0.50
1:E:184:MET:HG2	1:E:246:PHE:CE2	2.46	0.50
1:F:189:ASN:OD1	1:F:190:PRO:HD2	2.12	0.50
1:F:527:TYR:O	1:F:531:VAL:HG23	2.11	0.50
1:F:590:VAL:O	1:F:593:GLU:HB2	2.11	0.50
1:F:723:ASP:HA	1:F:813:SER:HA	1.94	0.50
1:F:69:MET:SD	1:F:72:ILE:HD11	2.52	0.50
1:F:746:ILE:HG13	1:F:747:ASN:N	2.26	0.50
1:A:140:VAL:HG11	1:A:310:LEU:HD21	1.93	0.50
1:A:350:LEU:HD13	1:A:985:GLY:HA2	1.93	0.50
1:C:946:VAL:HG13	1:C:1026:PHE:CE1	2.47	0.50
1:C:144:ASN:O	1:C:148:THR:HG23	2.11	0.50
1:C:27:ILE:HG13	1:C:28:LEU:N	2.27	0.50
1:C:612:VAL:HG12	1:C:615:PHE:HB3	1.94	0.50
1:D:222:THR:HA	1:D:224:PRO:HD3	1.93	0.50
1:D:668:LEU:H	1:D:668:LEU:HD23	1.77	0.50
1:E:580:ALA:HB1	1:E:724:THR:HG22	1.92	0.50
1:F:121:GLU:O	1:F:124:GLN:HG2	2.11	0.50
1:F:413:VAL:O	1:F:417:GLU:HG2	2.12	0.50
1:F:485:ALA:O	1:F:490:PRO:HD3	2.11	0.50
1:F:764:ASP:OD2	1:F:765:ARG:NH2	2.45	0.50
1:A:352:PHE:HD1	1:A:369:THR:HG21	1.77	0.49
1:B:249:ILE:HG12	1:B:262:LEU:HB2	1.94	0.49
1:B:527:TYR:O	1:B:531:VAL:HG23	2.12	0.49
1:B:871:ASN:N	1:B:871:ASN:OD1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.93	0.49
1:C:379:THR:HG23	1:C:476:SER:OG	2.11	0.49
1:D:415:ASN:HB3	1:D:434:SER:HB2	1.94	0.49
1:D:778:LYS:HG3	1:D:779:TYR:CE2	2.47	0.49
1:E:440:GLY:C	1:E:891:LEU:HD11	2.32	0.49
1:E:58:GLN:OE1	1:E:818:ARG:NH1	2.45	0.49
1:E:602:GLU:HG3	1:E:605:ASN:HB2	1.94	0.49
1:F:332:PHE:HD1	1:F:634:TRP:CH2	2.30	0.49
1:F:587:THR:OG1	1:F:588:GLN:N	2.45	0.49
1:F:64:VAL:HG12	1:F:114:ALA:HB1	1.93	0.49
1:A:577:GLN:O	1:A:661:ALA:HB1	2.12	0.49
1:A:887:CYS:O	1:A:890:ALA:HB3	2.12	0.49
1:A:915:ALA:HB2	1:A:1009:GLY:HA3	1.94	0.49
1:C:817:GLU:HB2	1:C:824:SER:O	2.12	0.49
1:D:267:LYS:HD2	1:D:776:GLU:CD	2.33	0.49
1:D:957:GLY:O	1:D:1040:ILE:HG21	2.11	0.49
1:E:358:PHE:CD2	1:E:977:MET:HG3	2.47	0.49
1:E:574:THR:HG23	1:E:627:ALA:HB3	1.94	0.49
1:E:671:ILE:HB	1:E:674:LEU:HG	1.94	0.49
1:F:426:PRO:O	1:F:430:ALA:N	2.42	0.49
1:F:457:ALA:HB1	1:F:468:ARG:HG3	1.94	0.49
1:A:444:GLY:O	1:A:448:VAL:HG23	2.12	0.49
1:B:354:VAL:HG21	1:B:980:LEU:HB3	1.93	0.49
1:B:478:MET:O	1:B:482:VAL:HG12	2.12	0.49
1:B:563:PHE:O	1:B:564:LEU:HD12	2.11	0.49
1:E:339:GLU:O	1:E:342:LYS:HB3	2.13	0.49
1:E:415:ASN:HD22	1:E:434:SER:CB	2.17	0.49
1:E:583:THR:H	1:E:586:ARG:HG3	1.77	0.49
1:F:352:PHE:HA	1:F:355:MET:CE	2.39	0.49
1:B:1020:PHE:HZ	2:B:1101:LMT:H62	1.76	0.49
1:B:139:VAL:HG13	1:B:178:PHE:CE1	2.47	0.49
1:B:525:HIS:HA	1:B:528:THR:HG22	1.93	0.49
1:B:877:TYR:HA	1:B:880:SER:HB2	1.93	0.49
1:C:393:LEU:HD11	1:C:466:ILE:HD13	1.94	0.49
1:D:445:ILE:HG12	1:D:940:LYS:HE3	1.94	0.49
1:F:184:MET:HB3	1:F:771:VAL:HG13	1.95	0.49
1:F:904:VAL:O	1:F:907:LEU:N	2.45	0.49
1:A:177:LEU:HD23	1:A:288:GLY:O	2.13	0.49
1:A:501:ALA:O	1:A:504:ASP:HB2	2.13	0.49
1:B:671:ILE:O	1:B:673:GLU:N	2.40	0.49
1:C:455:PRO:HG2	1:C:880:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:THR:O	1:C:603:LYS:HG3	2.11	0.49
1:D:175:VAL:HG12	1:D:289:LEU:HD22	1.94	0.49
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.92	0.49
1:D:5:PHE:HE2	1:D:11:PHE:HD1	1.59	0.49
1:D:575:MET:HA	1:D:626:ILE:HD12	1.93	0.49
1:D:626:ILE:HG13	1:D:627:ALA:N	2.28	0.49
1:D:678:THR:HB	1:D:831:ALA:HB3	1.95	0.49
1:E:162:MET:HA	1:E:313:MET:CE	2.43	0.49
1:F:937:LEU:HD22	1:F:1011:MET:HE2	1.94	0.49
1:B:559:LEU:HD12	1:B:923:ASN:HB2	1.95	0.49
1:C:201:VAL:O	1:C:204:ILE:HB	2.13	0.49
1:C:668:LEU:HB2	1:C:669:PRO:HD2	1.93	0.49
1:D:1034:SER:OG	1:D:1035:ARG:N	2.46	0.49
1:D:449:LEU:HB3	1:D:478:MET:SD	2.53	0.49
1:D:459:PHE:CB	1:D:464:GLY:HA2	2.43	0.49
1:E:154:ILE:CG2	1:E:287:SER:HB3	2.42	0.49
1:E:46:SER:HA	1:E:88:VAL:O	2.13	0.49
1:F:587:THR:HG21	1:F:623:ASN:HA	1.94	0.49
1:F:923:ASN:HD22	1:F:923:ASN:C	2.14	0.49
1:A:544:LEU:O	1:A:548:ILE:HG13	2.13	0.49
1:B:405:LEU:HD22	1:B:481:SER:HB3	1.93	0.49
1:B:87:THR:HG21	1:B:620:ARG:HH22	1.78	0.49
1:F:344:LEU:HD13	1:F:402:ILE:HD11	1.95	0.49
1:A:800:PRO:HG2	1:A:803:ALA:HB2	1.94	0.49
1:C:291:ILE:HG21	1:C:306:ILE:HD11	1.94	0.49
1:D:520:PHE:O	1:D:524:THR:HG23	2.13	0.49
1:F:623:ASN:OD1	1:F:623:ASN:N	2.45	0.49
1:F:65:ILE:HD11	1:F:118:LEU:HD11	1.95	0.49
1:A:442:LEU:O	1:A:445:ILE:HG13	2.12	0.49
1:A:831:ALA:HB2	1:A:840:ALA:HB2	1.93	0.49
1:A:900:SER:HB3	1:A:1029:VAL:HG21	1.93	0.49
1:B:577:GLN:O	1:B:661:ALA:HB1	2.13	0.49
1:C:150:THR:HG23	1:C:153:ASP:OD1	2.12	0.49
1:C:405:LEU:HD12	1:C:406:VAL:N	2.27	0.49
1:C:544:LEU:O	1:C:547:ILE:HB	2.13	0.49
1:C:578:LEU:CG	1:C:587:THR:HG22	2.39	0.49
1:D:262:LEU:HG	1:D:268:ILE:HD11	1.95	0.49
1:D:394:THR:HG23	1:D:469:GLN:HB3	1.95	0.49
1:E:177:LEU:HA	1:E:289:LEU:HD23	1.95	0.49
1:E:362:PHE:HA	1:E:365:THR:HG22	1.94	0.49
1:F:415:ASN:OD1	1:F:434:SER:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:623:ASN:N	1:C:623:ASN:OD1	2.46	0.49
1:C:907:LEU:HD21	1:C:1021:PHE:HB2	1.95	0.49
1:C:567:GLU:OE1	1:C:996:GLY:HA2	2.12	0.49
1:D:108:GLN:NE2	1:E:109:ASN:O	2.46	0.49
1:E:530:SER:OG	2:E:1101:LMT:H1'	2.12	0.49
1:E:717:ARG:HD2	1:E:828:LEU:HB2	1.94	0.49
1:F:507:GLU:HG2	1:F:518:ARG:HG3	1.94	0.49
1:F:983:ILE:HG23	1:F:1008:MET:HE2	1.95	0.49
1:B:516:PHE:O	1:B:520:PHE:N	2.37	0.48
1:B:463:THR:HG22	1:B:563:PHE:HE2	1.78	0.48
1:C:343:THR:HG21	1:C:989:LEU:CD2	2.43	0.48
1:C:742:SER:O	1:C:746:ILE:HG23	2.13	0.48
1:D:455:PRO:HG2	1:D:880:SER:OG	2.13	0.48
1:D:527:TYR:O	1:D:531:VAL:HG23	2.13	0.48
1:F:427:PRO:O	1:F:431:THR:OG1	2.26	0.48
1:F:451:ALA:O	1:F:883:VAL:HG11	2.13	0.48
1:A:583:THR:H	1:A:586:ARG:HG3	1.78	0.48
1:B:251:LEU:HD21	1:B:262:LEU:HB2	1.95	0.48
1:C:332:PHE:O	1:C:336:SER:HB3	2.13	0.48
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.94	0.48
1:D:452:VAL:HA	1:D:880:SER:OG	2.12	0.48
1:D:532:GLY:O	1:D:536:ARG:HG3	2.13	0.48
1:D:744:ASN:O	1:D:748:THR:HG23	2.12	0.48
1:F:80:SER:OG	1:F:818:ARG:HB2	2.13	0.48
1:F:971:ARG:HB3	1:F:971:ARG:NH1	2.28	0.48
1:B:166:ILE:HD12	1:B:309:GLU:HG3	1.95	0.48
1:C:13:TRP:HH2	1:C:370:ILE:HD13	1.78	0.48
1:E:327:TYR:CD2	1:E:327:TYR:C	2.87	0.48
1:E:602:GLU:OE2	1:E:650:ARG:NH1	2.46	0.48
1:F:562:SER:HB2	1:F:924:ASP:HB3	1.95	0.48
1:A:1037:ASN:CA	1:A:1038:GLU:HB2	2.43	0.48
1:A:391:ASN:O	1:A:395:MET:HG2	2.12	0.48
1:A:574:THR:HG23	1:A:627:ALA:HB3	1.94	0.48
1:B:427:PRO:CD	1:B:499:PRO:HB3	2.41	0.48
1:C:590:VAL:HA	1:C:593:GLU:OE1	2.14	0.48
1:D:889:ALA:HA	1:D:894:SER:O	2.14	0.48
1:E:324:VAL:O	1:E:326:PRO:HD3	2.14	0.48
1:E:399:VAL:O	1:E:402:ILE:HG13	2.13	0.48
1:F:49:TYR:CD1	1:F:57:VAL:HA	2.48	0.48
1:A:138:MET:O	1:A:291:ILE:N	2.41	0.48
1:A:79:SER:HA	1:A:818:ARG:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:VAL:HA	1:A:931:LEU:HD21	1.95	0.48
1:B:121:GLU:O	1:B:125:GLN:HB2	2.14	0.48
1:B:371:ALA:O	1:B:375:VAL:HG23	2.13	0.48
1:E:36:PRO:HG3	1:E:469:GLN:HG3	1.95	0.48
1:F:363:ARG:HH11	1:F:363:ARG:CG	2.26	0.48
1:B:1020:PHE:CZ	2:B:1101:LMT:H62	2.48	0.48
1:B:383:LEU:HD11	1:B:473:THR:HG23	1.96	0.48
1:B:682:PHE:HB3	1:B:827:ILE:O	2.14	0.48
1:D:838:GLY:O	1:D:841:MET:HB2	2.14	0.48
1:E:520:PHE:O	1:E:524:THR:HG23	2.13	0.48
1:E:832:ALA:HB3	1:E:835:LYS:HD2	1.95	0.48
1:F:343:THR:HG21	1:F:989:LEU:CD2	2.39	0.48
1:F:375:VAL:O	1:F:379:THR:OG1	2.15	0.48
1:F:776:GLU:HB2	1:F:779:TYR:HE1	1.78	0.48
1:A:593:GLU:OE2	1:A:659:LYS:NZ	2.36	0.48
1:B:36:PRO:HD3	1:B:391:ASN:CG	2.34	0.48
1:B:327:TYR:CD1	1:B:571:VAL:HG11	2.48	0.48
1:F:11:PHE:CE2	1:F:15:ILE:HD11	2.49	0.48
1:F:120:GLN:HG3	1:F:123:GLN:CD	2.34	0.48
1:F:133:SER:O	1:F:134:SER:HB2	2.14	0.48
1:F:340:VAL:HG11	1:F:395:MET:CB	2.43	0.48
1:F:602:GLU:HB3	1:F:606:VAL:HG23	1.96	0.48
1:A:108:GLN:O	1:A:112:GLN:HG2	2.14	0.48
1:A:58:GLN:O	1:A:63:GLN:HG3	2.13	0.48
1:A:326:PRO:HA	1:A:630:SER:HG	1.78	0.48
1:B:327:TYR:HD1	1:B:571:VAL:HG11	1.79	0.48
1:C:443:VAL:HG11	1:C:891:LEU:HD11	1.95	0.48
1:D:281:PHE:CZ	1:D:608:SER:HB2	2.49	0.48
1:D:901:VAL:HG21	1:D:943:ILE:HG13	1.95	0.48
1:F:242:SER:HB2	1:F:244:GLU:HB3	1.95	0.48
1:F:412:VAL:HA	1:F:438:ILE:CD1	2.43	0.48
1:F:2:PRO:O	1:F:5:PHE:HB3	2.14	0.48
1:A:421:ALA:HB1	1:A:505:HIS:HE1	1.78	0.48
1:A:979:SER:CB	1:A:1015:THR:HG21	2.44	0.48
1:B:960:LEU:HD13	1:B:1030:ARG:HG2	1.96	0.48
1:B:717:ARG:CD	1:B:828:LEU:HB2	2.44	0.48
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.96	0.48
1:D:193:LEU:HD13	1:D:200:PRO:HD3	1.96	0.48
1:D:293:LEU:HD11	1:D:299:ALA:HA	1.94	0.48
1:D:960:LEU:O	1:D:964:THR:HG23	2.13	0.48
1:E:351:VAL:HG21	1:E:406:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:676:THR:O	1:E:679:GLY:N	2.47	0.48
1:E:699:ARG:HE	1:E:718:PRO:CG	2.24	0.48
1:E:903:LEU:O	1:E:906:PRO:HD2	2.13	0.48
1:F:949:ALA:HB3	1:F:1026:PHE:CE2	2.49	0.48
1:A:16:ALA:O	1:A:20:MET:HG3	2.14	0.48
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.95	0.48
1:A:435:MET:HE3	1:A:439:GLN:HB2	1.95	0.48
1:B:904:VAL:HG21	1:B:942:ALA:CB	2.43	0.48
1:D:27:ILE:HD11	1:D:380:PHE:CE1	2.48	0.48
1:D:705:GLU:HB3	1:D:847:LEU:HD22	1.96	0.48
1:D:719:ASN:HB3	1:D:826:GLU:HG2	1.95	0.48
1:E:327:TYR:HD2	1:E:327:TYR:C	2.16	0.48
1:E:680:PHE:HB2	1:E:863:SER:HG	1.77	0.48
1:F:383:LEU:HD23	1:F:472:ILE:HD13	1.96	0.48
1:C:527:TYR:O	1:C:531:VAL:HG23	2.14	0.47
1:C:66:GLU:OE1	1:C:821:GLY:HA2	2.14	0.47
1:D:740:GLY:O	1:D:794:ALA:N	2.40	0.47
1:D:985:GLY:O	1:D:988:PRO:HD2	2.14	0.47
1:A:979:SER:HB2	1:A:1015:THR:HG21	1.96	0.47
1:A:1021:PHE:HB3	1:A:1025:PHE:CE1	2.48	0.47
1:A:152:GLU:HB2	1:A:182:TYR:HE1	1.79	0.47
1:A:425:LEU:HB3	1:A:429:GLU:HB2	1.96	0.47
1:A:63:GLN:O	1:A:67:GLN:HG3	2.15	0.47
1:A:757:SER:O	1:A:772:TYR:HA	2.14	0.47
1:B:743:ILE:H	1:B:743:ILE:HD12	1.78	0.47
1:C:690:LEU:HD11	1:C:854:GLY:O	2.14	0.47
1:D:391:ASN:O	1:D:395:MET:HG2	2.14	0.47
1:E:440:GLY:O	1:E:891:LEU:HD11	2.15	0.47
1:E:776:GLU:HG2	1:E:777:ALA:N	2.29	0.47
1:F:350:LEU:HD23	1:F:984:LEU:HB3	1.96	0.47
1:A:511:GLY:HA2	1:A:515:TRP:CD1	2.49	0.47
1:A:681:ASP:HB2	1:A:862:MET:HE3	1.96	0.47
1:B:717:ARG:HE	1:B:828:LEU:HB2	1.78	0.47
1:C:39:ALA:HA	1:C:40:PRO:HD2	1.67	0.47
1:D:34:GLN:HB2	1:D:333:VAL:HG22	1.94	0.47
1:E:281:PHE:CE1	1:E:608:SER:HB2	2.49	0.47
1:F:149:MET:HG3	1:F:154:ILE:HG13	1.97	0.47
1:F:746:ILE:HG13	1:F:747:ASN:H	1.78	0.47
1:A:960:LEU:O	1:A:964:THR:HG23	2.15	0.47
1:B:678:THR:HA	1:B:837:THR:OG1	2.15	0.47
1:B:877:TYR:O	1:B:881:LEU:HG	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:VAL:HG13	1:C:781:MET:SD	2.54	0.47
1:D:455:PRO:HG2	1:D:880:SER:CB	2.44	0.47
1:E:1037:ASN:HB2	1:E:1038:GLU:O	2.15	0.47
1:E:572:PHE:CD1	1:E:648:THR:HG22	2.49	0.47
1:E:992:SER:O	1:E:997:SER:HB2	2.14	0.47
1:F:202:ASP:OD1	1:F:792:ARG:NH2	2.47	0.47
1:F:368:PRO:O	1:F:371:ALA:HB3	2.13	0.47
1:F:885:PHE:HE1	1:F:899:PHE:CE2	2.32	0.47
1:A:67:GLN:NE2	1:C:768:VAL:HG13	2.29	0.47
1:B:32:VAL:HG22	1:B:298:ASN:ND2	2.29	0.47
1:C:146:ASP:O	1:C:148:THR:N	2.47	0.47
1:D:343:THR:O	1:D:346:GLU:N	2.47	0.47
1:D:634:TRP:CD1	1:D:634:TRP:N	2.82	0.47
1:E:61:VAL:HG21	1:E:122:VAL:HG21	1.96	0.47
1:E:246:PHE:HA	1:E:249:ILE:HG23	1.97	0.47
1:F:361:ASN:HB3	1:F:364:ALA:HB3	1.95	0.47
1:F:405:LEU:HD12	1:F:406:VAL:N	2.29	0.47
1:A:72:ILE:HD13	1:A:107:VAL:HG22	1.95	0.47
1:A:535:LEU:HA	1:A:535:LEU:HD23	1.65	0.47
1:A:637:ARG:HB3	1:A:642:ASN:HB3	1.96	0.47
1:A:937:LEU:O	1:A:940:LYS:HB3	2.15	0.47
1:B:574:THR:HA	1:B:665:ALA:HA	1.96	0.47
1:B:685:ILE:HD11	1:B:819:TYR:CD2	2.49	0.47
1:D:610:PHE:HB3	1:D:628:PHE:HB2	1.97	0.47
1:E:158:VAL:HB	1:E:177:LEU:HD11	1.96	0.47
1:E:61:VAL:HA	1:E:118:LEU:HD22	1.97	0.47
1:F:345:VAL:O	1:F:348:ILE:HB	2.14	0.47
1:A:220:GLY:HA3	1:A:230:LEU:O	2.14	0.47
1:A:671:ILE:HG21	1:A:674:LEU:HB3	1.95	0.47
1:B:501:ALA:O	1:B:504:ASP:HB2	2.15	0.47
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.80	0.47
1:C:133:SER:OG	1:C:293:LEU:O	2.31	0.47
1:C:375:VAL:HA	1:C:480:LEU:HD13	1.96	0.47
1:D:559:LEU:CD2	1:D:922:THR:HA	2.44	0.47
1:E:238:THR:HG22	1:E:239:ARG:O	2.13	0.47
1:E:525:HIS:HA	1:E:528:THR:CG2	2.44	0.47
1:A:641:GLU:HA	1:A:646:ALA:HB3	1.96	0.47
1:B:645:GLU:O	1:B:649:MET:HB2	2.15	0.47
1:C:139:VAL:HA	1:C:289:LEU:O	2.14	0.47
1:C:383:LEU:HD23	1:C:472:ILE:HD12	1.97	0.47
1:B:164:ASP:OD2	1:C:67:GLN:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:778:LYS:HG3	1:C:779:TYR:CZ	2.50	0.47
1:D:191:ASN:O	1:D:194:ASN:N	2.48	0.47
1:D:574:THR:HG23	1:D:627:ALA:HB3	1.96	0.47
1:E:538:THR:HG22	1:E:1024:VAL:HG13	1.97	0.47
1:E:987:MET:HB3	1:E:988:PRO:HD3	1.96	0.47
1:F:253:VAL:HG13	1:F:259:ARG:HG2	1.96	0.47
1:F:588:GLN:O	1:F:592:ASN:ND2	2.48	0.47
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.63	0.47
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.35	0.47
1:A:44:THR:HA	1:A:90:ILE:O	2.13	0.47
1:A:514:GLY:HA2	1:A:517:ASN:ND2	2.29	0.47
1:B:273:GLU:CD	1:B:770:LYS:HD2	2.35	0.47
1:C:30:LEU:HD23	1:C:390:ILE:HD11	1.97	0.47
1:C:831:ALA:HB3	1:C:835:LYS:HG2	1.97	0.47
1:D:196:PHE:HB3	1:D:252:LYS:HZ1	1.77	0.47
1:D:21:LEU:HA	1:D:21:LEU:HD13	1.63	0.47
1:D:183:ALA:HB2	1:D:273:GLU:HG3	1.97	0.47
1:D:573:MET:HG3	1:D:666:PHE:HE2	1.80	0.47
1:D:888:LEU:HD11	1:D:901:VAL:HG22	1.96	0.47
1:E:621:GLY:O	1:E:624:THR:HG22	2.14	0.47
1:F:453:PHE:HE1	1:F:474:ILE:HG21	1.80	0.47
1:A:578:LEU:CD2	1:A:590:VAL:HG21	2.40	0.47
1:A:69:MET:SD	1:A:72:ILE:HD11	2.55	0.47
1:A:75:LEU:HD23	1:C:168:ARG:HD3	1.97	0.47
1:B:725:PRO:HA	1:B:810:GLU:O	2.15	0.47
1:B:795:ASP:OD2	1:B:797:GLN:HG2	2.15	0.47
1:B:888:LEU:HD23	1:B:888:LEU:HA	1.65	0.47
1:B:231:ASN:HB2	1:C:583:THR:HG22	1.97	0.47
1:D:907:LEU:HD21	1:D:1021:PHE:CB	2.45	0.47
1:D:538:THR:HG21	1:D:1028:VAL:HG22	1.97	0.47
1:D:121:GLU:O	1:D:124:GLN:HG2	2.15	0.47
1:D:907:LEU:HD21	1:D:1021:PHE:HB2	1.96	0.47
1:E:371:ALA:O	1:E:375:VAL:HG23	2.15	0.47
1:E:751:GLY:O	1:E:754:TRP:N	2.48	0.47
1:E:888:LEU:HD23	1:E:888:LEU:HA	1.49	0.47
1:A:613:ASN:OD1	1:A:614:GLY:N	2.48	0.47
1:A:793:ALA:HB3	1:A:795:ASP:OD2	2.14	0.47
1:C:457:ALA:HB2	1:C:471:SER:OG	2.15	0.47
1:C:895:TRP:HA	1:C:895:TRP:HE3	1.78	0.47
1:D:888:LEU:HD12	1:D:902:MET:HG3	1.97	0.47
1:D:948:PHE:O	1:D:952:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:732:ASP:OD1	1:E:735:LYS:HG3	2.14	0.47
1:F:382:VAL:HG11	1:F:476:SER:CB	2.45	0.47
1:F:347:ALA:HB3	1:F:402:ILE:HD12	1.97	0.47
1:F:736:ALA:O	1:F:741:VAL:HG23	2.15	0.47
1:A:146:ASP:OD2	1:A:146:ASP:N	2.29	0.46
1:A:169:THR:HG22	1:A:172:VAL:HG23	1.97	0.46
1:A:563:PHE:CD2	1:A:671:ILE:HD11	2.50	0.46
1:B:399:VAL:O	1:B:402:ILE:HG13	2.15	0.46
1:B:404:LEU:HD21	1:B:449:LEU:HD22	1.97	0.46
1:C:154:ILE:HG22	1:C:287:SER:HB3	1.96	0.46
1:C:504:ASP:C	1:C:506:GLY:H	2.18	0.46
1:C:641:GLU:HA	1:C:646:ALA:HB3	1.96	0.46
1:E:249:ILE:CG1	1:E:262:LEU:HB2	2.45	0.46
1:E:568:ASP:O	1:E:634:TRP:HZ3	1.98	0.46
1:E:841:MET:O	1:E:845:GLU:HG3	2.14	0.46
1:F:602:GLU:OE2	1:F:650:ARG:HD2	2.16	0.46
1:F:682:PHE:HE1	1:F:857:TYR:HB2	1.80	0.46
1:A:648:THR:HB	1:A:665:ALA:O	2.15	0.46
1:B:42:ALA:HB3	1:B:132:SER:HB3	1.96	0.46
1:B:447:MET:HB3	1:B:887:CYS:SG	2.56	0.46
1:C:371:ALA:O	1:C:375:VAL:HG23	2.15	0.46
1:C:524:THR:O	1:C:528:THR:HG22	2.14	0.46
1:B:213:GLN:NE2	1:C:52:ALA:HA	2.28	0.46
1:C:888:LEU:CD1	1:C:901:VAL:HG11	2.45	0.46
1:D:163:LYS:HE3	1:D:177:LEU:HB2	1.97	0.46
1:D:776:GLU:HG2	1:D:777:ALA:H	1.81	0.46
1:E:330:THR:HG22	1:E:334:LYS:HE2	1.97	0.46
1:E:332:PHE:O	1:E:336:SER:HB2	2.15	0.46
1:F:36:PRO:HD3	1:F:391:ASN:ND2	2.30	0.46
1:F:578:LEU:HD21	1:F:590:VAL:HG21	1.97	0.46
1:F:743:ILE:HD12	1:F:743:ILE:H	1.80	0.46
1:F:835:LYS:HG2	1:F:836:SER:H	1.80	0.46
1:B:706:ALA:HB1	1:B:713:LEU:HD13	1.97	0.46
1:C:375:VAL:HB	1:C:405:LEU:HD22	1.97	0.46
1:C:725:PRO:HG3	1:C:811:TYR:HE1	1.81	0.46
1:C:944:LEU:CD1	1:C:975:ILE:HG12	2.45	0.46
1:D:347:ALA:O	1:D:351:VAL:HG23	2.16	0.46
1:D:540:ARG:O	1:D:543:VAL:HB	2.16	0.46
1:E:527:TYR:O	1:E:530:SER:HB3	2.14	0.46
1:F:566:ASP:OD1	1:F:678:THR:HG23	2.16	0.46
1:A:583:THR:HA	1:A:622:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:PHE:HD1	1:A:913:LEU:HD21	1.80	0.46
1:B:143:ILE:HG12	1:B:322:LYS:O	2.16	0.46
1:B:578:LEU:HD21	1:B:587:THR:HA	1.97	0.46
1:B:753:ALA:O	1:B:775:SER:HB3	2.16	0.46
1:C:562:SER:HB2	1:C:924:ASP:HB3	1.96	0.46
1:C:735:LYS:O	1:C:738:ALA:HB3	2.15	0.46
1:D:184:MET:HB3	1:D:771:VAL:HG22	1.98	0.46
1:D:485:ALA:O	1:D:490:PRO:HD3	2.15	0.46
1:D:545:TYR:HB2	1:D:1021:PHE:HE2	1.81	0.46
1:E:450:SER:HB2	1:E:454:VAL:HG23	1.97	0.46
1:E:508:GLY:HA3	1:E:518:ARG:NE	2.25	0.46
1:E:652:THR:OG1	1:E:665:ALA:HB3	2.15	0.46
1:F:151:GLN:NE2	1:F:279:ALA:H	2.14	0.46
1:A:69:MET:HE1	1:A:107:VAL:O	2.14	0.46
1:B:310:LEU:HG	1:B:323:ILE:HG13	1.98	0.46
1:B:713:LEU:HD11	1:B:843:LEU:HD12	1.97	0.46
1:C:170:SER:O	1:C:302:THR:HA	2.14	0.46
1:C:841:MET:HG2	1:C:859:TRP:CH2	2.51	0.46
1:C:76:MET:N	1:C:93:THR:O	2.46	0.46
1:D:250:LEU:HD23	1:E:737:GLN:NE2	2.30	0.46
1:D:417:GLU:OE1	1:D:497:LEU:HD11	2.16	0.46
1:D:55:LYS:HZ1	1:F:238:THR:HG1	1.56	0.46
1:E:13:TRP:HA	1:E:13:TRP:CE3	2.49	0.46
1:F:152:GLU:HB3	1:F:182:TYR:HE1	1.80	0.46
1:F:278:ILE:CG1	1:F:613:ASN:HB3	2.45	0.46
1:F:368:PRO:HG3	1:F:413:VAL:HG21	1.97	0.46
1:F:382:VAL:HG21	1:F:476:SER:HB2	1.96	0.46
1:F:549:VAL:O	1:F:552:MET:HB3	2.15	0.46
1:F:873:ALA:HB2	1:F:928:GLN:NE2	2.29	0.46
1:A:659:LYS:HD3	1:A:659:LYS:HA	1.67	0.46
1:B:104:GLN:HG3	1:B:129:VAL:HG12	1.98	0.46
1:B:758:TYR:CE1	1:B:770:LYS:HD3	2.50	0.46
1:C:121:GLU:O	1:C:124:GLN:HG2	2.15	0.46
1:C:144:ASN:HA	1:C:320:GLY:O	2.16	0.46
1:C:366:LEU:O	1:C:370:ILE:HG13	2.16	0.46
1:D:449:LEU:HD13	1:D:478:MET:SD	2.55	0.46
1:D:712:MET:HE3	1:D:835:LYS:HG2	1.96	0.46
1:E:162:MET:O	1:E:164:ASP:N	2.48	0.46
1:E:255:GLN:HG3	1:E:255:GLN:H	1.21	0.46
1:E:310:LEU:CD2	1:E:323:ILE:HG21	2.45	0.46
1:F:393:LEU:HD12	1:F:469:GLN:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:895:TRP:HA	1:F:895:TRP:CE3	2.50	0.46
1:A:1039:ASP:H	1:A:1040:ILE:HB	1.80	0.46
1:A:449:LEU:HB3	1:A:478:MET:SD	2.56	0.46
1:A:457:ALA:HB2	1:A:471:SER:CB	2.46	0.46
1:A:597:TYR:CG	1:A:655:PHE:CZ	3.04	0.46
1:B:600:THR:O	1:B:603:LYS:HB2	2.15	0.46
1:B:683:GLU:HG2	1:B:819:TYR:CG	2.50	0.46
1:C:427:PRO:O	1:C:431:THR:OG1	2.30	0.46
1:C:611:ALA:HA	1:C:627:ALA:HA	1.97	0.46
1:C:947:GLU:HG3	1:C:948:PHE:CD1	2.47	0.46
1:D:189:ASN:HB3	1:D:192:GLU:HB2	1.97	0.46
1:D:423:GLU:O	1:D:502:LYS:HB3	2.16	0.46
1:D:562:SER:OG	1:D:922:THR:HG21	2.16	0.46
1:D:957:GLY:O	1:D:1040:ILE:HD13	2.16	0.46
1:E:727:PHE:CE1	1:E:807:SER:HB2	2.51	0.46
1:F:574:THR:HG23	1:F:627:ALA:HB3	1.97	0.46
1:F:971:ARG:C	1:F:974:PRO:HD2	2.36	0.46
1:A:375:VAL:HG13	1:A:480:LEU:HB3	1.98	0.46
1:B:166:ILE:HG12	1:B:310:LEU:HD13	1.97	0.46
1:B:517:ASN:O	1:B:521:GLU:N	2.45	0.46
1:B:702:LEU:HD22	1:B:851:LEU:HD11	1.97	0.46
1:C:2:PRO:O	1:C:5:PHE:HB3	2.16	0.46
1:D:463:THR:HG23	1:D:467:TYR:CD1	2.51	0.46
1:D:57:VAL:HG21	1:D:86:GLY:CA	2.36	0.46
1:D:897:ILE:HA	1:D:1029:VAL:CG1	2.43	0.46
1:D:987:MET:HB3	1:D:988:PRO:HD3	1.98	0.46
1:E:32:VAL:HG12	1:E:390:ILE:HB	1.97	0.46
1:E:478:MET:O	1:E:482:VAL:HG12	2.15	0.46
1:E:741:VAL:HB	1:E:746:ILE:HD11	1.97	0.46
1:F:366:LEU:HA	1:F:369:THR:HB	1.97	0.46
1:F:534:ILE:HB	1:F:541:TYR:CZ	2.51	0.46
1:F:652:THR:HG23	1:F:664:PHE:HD1	1.80	0.46
1:F:885:PHE:CD2	1:F:886:LEU:HD22	2.47	0.46
1:F:449:LEU:HD23	1:F:936:GLY:HA3	1.96	0.46
1:B:559:LEU:HA	1:B:560:PRO:HD2	1.61	0.46
1:B:641:GLU:HA	1:B:646:ALA:HB3	1.98	0.46
1:C:238:THR:HG22	1:C:239:ARG:O	2.16	0.46
1:C:641:GLU:OE2	1:C:641:GLU:N	2.37	0.46
1:C:445:ILE:HG12	1:C:940:LYS:HG3	1.98	0.46
1:C:972:LEU:O	1:C:975:ILE:HB	2.16	0.46
1:D:139:VAL:HA	1:D:289:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:ILE:HG12	1:E:262:LEU:HB2	1.98	0.46
1:E:344:LEU:HD23	1:E:402:ILE:HD11	1.98	0.46
1:F:447:MET:SD	1:F:891:LEU:HD22	2.56	0.46
1:A:375:VAL:HG22	1:A:484:VAL:HG21	1.98	0.46
1:B:903:LEU:HB3	1:B:1025:PHE:CE2	2.51	0.46
1:C:211:ASN:OD1	1:C:240:LEU:HG	2.16	0.46
1:C:698:ALA:O	1:C:701:GLN:HB3	2.16	0.46
1:C:785:ASP:O	1:C:789:TRP:HD1	1.98	0.46
1:D:165:ALA:HB3	1:D:313:MET:HE1	1.97	0.46
1:D:252:LYS:HE2	1:D:260:VAL:HG21	1.98	0.46
1:D:346:GLU:O	1:D:350:LEU:HD12	2.16	0.46
1:D:424:GLY:HA3	1:D:502:LYS:HB3	1.97	0.46
1:D:515:TRP:O	1:D:519:MET:HG3	2.16	0.46
1:D:752:ALA:O	1:D:774:MET:HA	2.15	0.46
1:D:459:PHE:CE2	1:D:876:LEU:HD12	2.51	0.46
1:E:185:ARG:HH12	1:E:774:MET:HE3	1.81	0.46
1:E:184:MET:HB3	1:E:771:VAL:HG13	1.98	0.46
1:F:73:ASP:CG	1:F:106:GLN:HE22	2.19	0.46
1:F:564:LEU:HD12	1:F:564:LEU:HA	1.85	0.46
1:B:149:MET:HB2	1:B:153:ASP:CB	2.45	0.45
1:B:247:GLY:O	1:B:261:LEU:HB3	2.16	0.45
1:B:310:LEU:CD2	1:B:323:ILE:HG21	2.46	0.45
1:B:702:LEU:HD13	1:B:848:ALA:HA	1.97	0.45
1:C:562:SER:OG	1:C:922:THR:HG21	2.16	0.45
1:C:584:GLN:N	1:C:622:GLN:HB3	2.31	0.45
1:D:445:ILE:O	1:D:449:LEU:HB2	2.16	0.45
1:E:193:LEU:HD13	1:E:200:PRO:HD3	1.97	0.45
1:E:597:TYR:CD1	1:E:601:LYS:HD2	2.51	0.45
1:E:680:PHE:CE1	1:E:682:PHE:HB2	2.50	0.45
1:E:682:PHE:CE1	1:E:857:TYR:HB2	2.52	0.45
1:A:110:LYS:O	1:A:113:LEU:N	2.45	0.45
1:A:377:LEU:O	1:A:380:PHE:HB2	2.16	0.45
1:A:404:LEU:HD23	1:A:449:LEU:HD13	1.98	0.45
1:A:5:PHE:HE2	1:A:11:PHE:CD1	2.33	0.45
1:A:758:TYR:CD1	1:A:770:LYS:HD3	2.51	0.45
1:B:558:ARG:HA	1:B:558:ARG:HD3	1.77	0.45
1:B:847:LEU:O	1:B:850:LYS:HB2	2.15	0.45
1:C:48:SER:O	1:C:50:PRO:HD3	2.17	0.45
1:D:535:LEU:HD22	1:D:1027:VAL:HG21	1.98	0.45
1:D:172:VAL:HG13	1:D:291:ILE:HG23	1.98	0.45
1:D:400:LEU:HA	1:D:400:LEU:HD12	1.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:MET:HB3	1:D:435:MET:HE3	1.75	0.45
1:D:713:LEU:CD2	1:D:843:LEU:HD12	2.46	0.45
1:E:414:GLU:HG3	1:E:974:PRO:HB3	1.98	0.45
1:E:468:ARG:HG2	1:E:472:ILE:HD13	1.98	0.45
1:A:293:LEU:HD22	1:A:294:ALA:N	2.32	0.45
1:A:819:TYR:N	1:A:822:LEU:O	2.48	0.45
1:C:346:GLU:O	1:C:350:LEU:HD13	2.17	0.45
1:C:818:ARG:NH2	1:C:821:GLY:O	2.49	0.45
1:C:817:GLU:OE2	1:C:825:MET:HA	2.16	0.45
1:C:947:GLU:HG3	1:C:948:PHE:N	2.30	0.45
1:E:158:VAL:HG13	1:E:162:MET:HE2	1.97	0.45
1:E:445:ILE:CG2	1:E:940:LYS:HD2	2.46	0.45
1:E:972:LEU:HD22	1:E:972:LEU:HA	1.67	0.45
1:F:398:MET:HE3	1:F:398:MET:HB3	1.81	0.45
1:F:460:GLY:O	1:F:868:LEU:HD21	2.16	0.45
1:A:964:THR:HG21	1:A:1027:VAL:HG23	1.99	0.45
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.97	0.45
1:A:597:TYR:CB	1:A:655:PHE:HZ	2.30	0.45
1:B:310:LEU:HD23	1:B:323:ILE:HG21	1.98	0.45
1:C:434:SER:O	1:C:437:GLN:N	2.45	0.45
1:D:237:GLN:OE1	1:E:747:ASN:ND2	2.40	0.45
1:D:293:LEU:HD23	1:D:294:ALA:N	2.30	0.45
1:D:933:THR:O	1:D:936:GLY:N	2.49	0.45
1:E:545:TYR:O	1:E:548:ILE:N	2.50	0.45
1:E:597:TYR:HD1	1:E:601:LYS:HD2	1.81	0.45
1:F:69:MET:HA	1:F:72:ILE:HD11	1.98	0.45
1:A:325:TYR:HA	1:A:326:PRO:HD2	1.85	0.45
1:A:910:ILE:O	1:A:914:LEU:HB2	2.17	0.45
1:C:408:ASP:HB3	1:C:485:ALA:HB2	1.99	0.45
1:C:400:LEU:HD23	1:C:474:ILE:HD11	1.99	0.45
1:C:644:VAL:HG12	1:C:645:GLU:N	2.31	0.45
1:D:609:VAL:HG13	1:D:629:VAL:HG22	1.99	0.45
1:D:654:ALA:O	1:D:658:ILE:HG12	2.16	0.45
1:E:443:VAL:O	1:E:446:ALA:HB3	2.16	0.45
1:D:781:MET:SD	1:F:225:VAL:HG13	2.56	0.45
1:F:291:ILE:HD13	1:F:306:ILE:HD13	1.99	0.45
1:F:527:TYR:CZ	1:F:968:VAL:HG13	2.51	0.45
1:A:156:ASP:OD2	1:A:182:TYR:HB2	2.16	0.45
1:A:69:MET:HE1	1:A:107:VAL:HG13	1.99	0.45
1:B:419:VAL:HG13	1:B:423:GLU:OE1	2.16	0.45
1:B:544:LEU:O	1:B:548:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:VAL:HG21	1:C:158:VAL:HG22	1.99	0.45
1:C:443:VAL:O	1:C:447:MET:HB3	2.16	0.45
1:D:644:VAL:CG1	1:D:667:ASN:HB2	2.45	0.45
1:E:512:PHE:HB3	1:E:513:PHE:CD1	2.51	0.45
1:E:572:PHE:CE1	1:E:648:THR:HG22	2.51	0.45
1:F:228:GLN:NE2	1:F:230:LEU:O	2.41	0.45
1:A:848:ALA:HA	1:A:851:LEU:HG	1.99	0.45
1:B:545:TYR:CE2	1:B:1025:PHE:HZ	2.34	0.45
1:C:24:GLY:HA2	1:C:27:ILE:HG23	1.98	0.45
1:C:637:ARG:HD2	1:C:642:ASN:O	2.16	0.45
1:C:682:PHE:CZ	1:C:857:TYR:HB2	2.52	0.45
1:D:362:PHE:O	1:D:365:THR:HG22	2.16	0.45
1:D:434:SER:O	1:D:438:ILE:HG12	2.17	0.45
1:E:516:PHE:HA	1:E:519:MET:HG3	1.98	0.45
1:E:564:LEU:CD1	1:E:671:ILE:HD12	2.47	0.45
1:E:680:PHE:HE1	1:E:682:PHE:HB2	1.81	0.45
1:E:836:SER:OG	1:E:839:GLU:HG3	2.16	0.45
1:E:894:SER:HB3	1:E:897:ILE:H	1.82	0.45
1:F:466:ILE:HG21	1:F:925:VAL:HG11	1.98	0.45
1:F:705:GLU:HA	1:F:708:LYS:HE3	1.99	0.45
1:F:960:LEU:O	1:F:963:ALA:N	2.49	0.45
1:A:727:PHE:CZ	1:A:807:SER:HB2	2.52	0.45
1:A:953:MET:HE2	1:A:963:ALA:HB3	1.99	0.45
1:C:578:LEU:HD22	1:C:661:ALA:CB	2.47	0.45
1:D:182:TYR:O	1:D:769:LYS:HD3	2.17	0.45
1:D:325:TYR:HA	1:D:326:PRO:HD2	1.93	0.45
1:D:591:LEU:HD12	1:D:613:ASN:HB2	1.99	0.45
1:E:1011:MET:O	1:E:1015:THR:HG23	2.17	0.45
1:E:216:ALA:HB1	1:E:234:ILE:CG2	2.47	0.45
1:E:949:ALA:HB3	1:E:1026:PHE:CE1	2.45	0.45
1:F:336:SER:O	1:F:340:VAL:HG23	2.17	0.45
1:A:1043:SER:OG	1:A:1043:SER:O	2.34	0.45
1:A:45:ILE:HD12	1:A:90:ILE:HB	1.98	0.45
1:A:575:MET:O	1:A:575:MET:HG3	2.17	0.45
1:B:999:ALA:O	1:B:1002:ALA:N	2.50	0.45
1:C:800:PRO:HG2	1:C:803:ALA:HB2	1.99	0.45
1:D:979:SER:CB	1:D:1015:THR:HG21	2.46	0.45
1:D:101:ASP:N	1:D:101:ASP:OD1	2.49	0.45
1:D:1030:ARG:HA	1:D:1030:ARG:HD2	1.63	0.45
1:D:775:SER:HB2	1:D:789:TRP:CZ2	2.51	0.45
1:E:240:LEU:HB2	1:E:246:PHE:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:GLU:HG2	1:E:284:GLN:O	2.17	0.45
1:E:466:ILE:HD13	1:E:564:LEU:HD11	1.99	0.45
1:F:94:PHE:CE1	1:F:103:ALA:HB1	2.52	0.45
1:F:307:ARG:NH1	1:F:325:TYR:OH	2.48	0.45
1:F:659:LYS:HG3	1:F:661:ALA:H	1.81	0.45
1:A:544:LEU:HG	1:A:544:LEU:O	2.17	0.45
1:C:378:GLY:O	1:C:382:VAL:HG23	2.16	0.45
1:D:309:GLU:O	1:D:312:LYS:HB2	2.17	0.45
1:D:508:GLY:H	1:D:518:ARG:HG3	1.82	0.45
1:E:167:SER:HB3	1:E:175:VAL:HG21	1.99	0.45
1:E:186:ILE:HD13	1:E:262:LEU:HD21	1.99	0.45
1:F:251:LEU:HD21	1:F:262:LEU:HB2	1.98	0.45
1:F:497:LEU:HD12	1:F:497:LEU:HA	1.56	0.45
1:F:61:VAL:HG11	1:F:88:VAL:HG11	1.99	0.45
1:F:641:GLU:HA	1:F:646:ALA:HB3	1.99	0.45
1:A:259:ARG:NH2	1:A:261:LEU:HD11	2.27	0.44
1:A:350:LEU:HD13	1:A:984:LEU:O	2.17	0.44
1:B:377:LEU:O	1:B:380:PHE:HB2	2.17	0.44
1:C:150:THR:N	1:C:153:ASP:HB2	2.32	0.44
1:C:574:THR:HG21	1:C:598:TYR:HE2	1.81	0.44
2:D:1101:LMT:H72	2:D:1101:LMT:H102	1.66	0.44
1:D:13:TRP:CZ2	1:D:492:LEU:HD21	2.52	0.44
1:D:751:GLY:O	1:D:754:TRP:N	2.49	0.44
1:D:759:VAL:HG12	1:D:760:ASN:HB2	1.99	0.44
1:E:291:ILE:HD13	1:E:306:ILE:HD13	1.99	0.44
1:F:987:MET:HE2	1:F:987:MET:HB3	1.93	0.44
1:A:203:VAL:HG12	1:A:207:ILE:HD11	1.97	0.44
1:B:102:ILE:O	1:B:105:VAL:HG12	2.18	0.44
1:B:171:GLY:HA3	1:B:302:THR:OG1	2.17	0.44
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.53	0.44
1:D:343:THR:O	1:D:344:LEU:C	2.55	0.44
1:D:3:ASN:O	1:D:6:ILE:HG12	2.16	0.44
1:D:891:LEU:HA	1:D:891:LEU:HD12	1.82	0.44
1:E:399:VAL:HA	1:E:402:ILE:HG13	1.98	0.44
1:E:6:ILE:HD13	1:E:432:ARG:HG2	1.98	0.44
1:E:455:PRO:O	1:E:876:LEU:HD13	2.16	0.44
1:E:68:ASN:HB2	1:E:114:ALA:HB2	1.99	0.44
1:E:159:ALA:O	1:E:767:ARG:NH2	2.50	0.44
1:F:563:PHE:HB2	1:F:866:GLU:HB2	1.99	0.44
1:A:261:LEU:HD12	1:A:263:ARG:NH1	2.31	0.44
1:A:32:VAL:HG13	1:A:390:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:PHE:CZ	1:A:844:MET:HG3	2.53	0.44
1:A:753:ALA:HB3	1:A:754:TRP:HD1	1.82	0.44
1:A:879:ILE:HD13	1:C:25:LEU:HD21	1.99	0.44
1:B:27:ILE:HD13	1:B:380:PHE:CD1	2.53	0.44
1:C:356:TYR:CD1	1:C:365:THR:HG21	2.52	0.44
1:F:144:ASN:O	1:F:148:THR:HG23	2.17	0.44
1:F:730:ASP:OD1	1:F:808:ARG:NH2	2.51	0.44
1:F:5:PHE:CE2	1:F:8:ARG:HD2	2.52	0.44
1:A:211:ASN:OD1	1:A:240:LEU:HG	2.16	0.44
1:A:21:LEU:HA	1:A:21:LEU:HD13	1.76	0.44
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.86	0.44
1:A:774:MET:HG2	1:A:775:SER:N	2.33	0.44
1:A:58:GLN:OE1	1:A:818:ARG:NH1	2.49	0.44
1:A:885:PHE:HD1	1:A:902:MET:HE1	1.83	0.44
1:B:682:PHE:CD2	1:B:827:ILE:HD12	2.52	0.44
1:B:99:ASP:HB3	1:B:102:ILE:HB	1.99	0.44
1:C:242:SER:HB2	1:C:245:GLU:H	1.81	0.44
1:C:699:ARG:HD3	1:C:825:MET:SD	2.56	0.44
1:C:184:MET:HB2	1:C:762:PHE:CE2	2.52	0.44
1:D:220:GLY:O	1:D:224:PRO:HB3	2.18	0.44
1:E:80:SER:CB	1:E:90:ILE:HG12	2.48	0.44
1:A:183:ALA:HB2	1:A:273:GLU:HG3	1.99	0.44
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.77	0.44
1:B:524:THR:O	1:B:527:TYR:HB3	2.18	0.44
1:B:901:VAL:HG23	1:B:942:ALA:HB3	1.99	0.44
1:D:703:LEU:HD21	1:D:718:PRO:HD3	1.98	0.44
1:E:68:ASN:CB	1:E:114:ALA:HB2	2.48	0.44
1:E:448:VAL:O	1:E:452:VAL:HG13	2.17	0.44
1:E:744:ASN:O	1:E:748:THR:HG23	2.17	0.44
1:F:185:ARG:HB3	1:F:187:TRP:NE1	2.33	0.44
1:F:587:THR:CG2	1:F:623:ASN:HA	2.46	0.44
1:F:65:ILE:O	1:F:69:MET:HG2	2.18	0.44
1:F:990:VAL:HG22	1:F:1004:GLY:HA3	2.00	0.44
1:A:159:ALA:HB2	1:A:177:LEU:HD11	1.98	0.44
1:A:452:VAL:HG12	1:A:884:VAL:CG2	2.48	0.44
1:A:743:ILE:HD12	1:A:743:ILE:H	1.82	0.44
1:A:781:MET:SD	1:C:225:VAL:HG13	2.58	0.44
1:A:190:PRO:HG3	1:A:789:TRP:CZ2	2.52	0.44
1:A:961:ILE:HG13	1:A:961:ILE:H	1.33	0.44
1:B:767:ARG:HH22	1:C:67:GLN:NE2	2.15	0.44
1:B:78:MET:N	1:B:820:ASN:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLU:HA	1:C:195:LYS:HE3	1.99	0.44
1:C:508:GLY:O	1:C:509:LYS:HB2	2.17	0.44
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.98	0.44
1:C:952:LEU:HB2	1:C:963:ALA:HB1	1.99	0.44
1:C:987:MET:O	1:C:991:ILE:HG22	2.18	0.44
1:D:270:LEU:HA	1:D:270:LEU:HD12	1.89	0.44
1:D:34:GLN:HG3	1:D:332:PHE:HE2	1.82	0.44
1:D:465:ALA:O	1:D:469:GLN:HG2	2.17	0.44
1:E:658:ILE:C	1:E:659:LYS:HD2	2.37	0.44
1:E:105:VAL:HG23	1:F:109:ASN:OD1	2.18	0.44
1:F:149:MET:HB2	1:F:153:ASP:CB	2.47	0.44
1:F:859:TRP:O	1:F:864:TYR:HD1	2.01	0.44
1:A:275:TYR:CD1	1:C:223:PRO:HD3	2.53	0.44
1:A:20:MET:SD	1:A:374:VAL:HG22	2.58	0.44
1:A:726:GLN:O	1:A:810:GLU:HG2	2.18	0.44
1:A:562:SER:OG	1:A:922:THR:HG21	2.17	0.44
1:A:400:LEU:CD2	1:A:929:VAL:HG12	2.48	0.44
1:A:74:ASN:O	1:A:94:PHE:HD2	2.00	0.44
1:B:937:LEU:HD23	1:B:937:LEU:HA	1.80	0.44
1:C:587:THR:HG21	1:C:623:ASN:HA	2.00	0.44
1:E:990:VAL:HG22	1:E:1004:GLY:HA3	2.00	0.44
1:F:151:GLN:HB3	1:F:152:GLU:OE2	2.17	0.44
1:F:506:GLY:C	1:F:508:GLY:N	2.71	0.44
1:F:727:PHE:CZ	1:F:807:SER:HB2	2.52	0.44
1:F:889:ALA:HB1	1:F:895:TRP:CZ3	2.51	0.44
1:A:508:GLY:N	1:A:518:ARG:HG3	2.32	0.44
1:C:587:THR:HA	1:C:590:VAL:HG23	2.00	0.44
1:C:889:ALA:HB2	1:C:898:PRO:HG2	2.00	0.44
1:D:680:PHE:CZ	1:D:829:GLY:HA3	2.53	0.44
1:E:72:ILE:HG23	1:E:106:GLN:OE1	2.18	0.44
1:E:544:LEU:O	1:E:547:ILE:HB	2.17	0.44
1:F:544:LEU:O	1:F:547:ILE:HB	2.18	0.44
1:F:564:LEU:HD12	1:F:565:PRO:HD2	2.00	0.44
1:A:644:VAL:HG11	1:A:667:ASN:CB	2.48	0.44
1:B:289:LEU:HA	1:B:289:LEU:HD23	1.79	0.44
1:B:549:VAL:O	1:B:552:MET:HB3	2.18	0.44
1:C:904:VAL:O	1:C:907:LEU:HB2	2.17	0.44
1:D:239:ARG:HD2	1:D:761:ASP:O	2.18	0.44
1:D:184:MET:HB2	1:D:762:PHE:CE2	2.53	0.44
1:E:695:LEU:HB3	1:E:825:MET:SD	2.58	0.44
1:E:984:LEU:HA	1:E:984:LEU:HD23	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:507:GLU:HG2	1:F:518:ARG:CG	2.47	0.44
1:F:63:GLN:O	1:F:67:GLN:HG3	2.18	0.44
1:F:84:SER:HB3	1:F:814:PRO:O	2.18	0.44
1:A:339:GLU:HB2	1:A:1000:GLN:HE22	1.83	0.43
1:A:30:LEU:HD11	1:A:384:ALA:HA	2.00	0.43
1:A:726:GLN:OE1	1:C:235:ILE:HD11	2.18	0.43
1:A:992:SER:O	1:A:997:SER:HB2	2.18	0.43
1:B:61:VAL:HG21	1:B:122:VAL:HG21	2.00	0.43
1:C:368:PRO:HA	1:C:409:ALA:HB1	2.00	0.43
1:C:727:PHE:HZ	1:C:807:SER:HB2	1.76	0.43
1:D:402:ILE:HG21	1:D:402:ILE:HD13	1.77	0.43
1:E:100:ALA:HB1	1:E:131:LYS:HE3	2.00	0.43
1:E:32:VAL:HG22	1:E:298:ASN:ND2	2.33	0.43
1:F:937:LEU:HD11	1:F:982:PHE:CE2	2.53	0.43
1:A:646:ALA:O	1:A:650:ARG:HG2	2.18	0.43
1:B:427:PRO:O	1:B:430:ALA:HB3	2.18	0.43
1:B:613:ASN:HD22	1:B:614:GLY:N	2.15	0.43
1:C:1038:GLU:HA	1:C:1039:ASP:HB2	2.00	0.43
2:D:1101:LMT:H31	2:D:1101:LMT:H62	1.59	0.43
1:D:61:VAL:HA	1:D:118:LEU:HD22	1.99	0.43
1:E:166:ILE:HD12	1:E:309:GLU:HG3	2.00	0.43
1:E:200:PRO:HA	1:E:203:VAL:HG23	1.99	0.43
1:E:36:PRO:HD3	1:E:391:ASN:CG	2.38	0.43
1:E:459:PHE:CE1	1:E:876:LEU:HD12	2.53	0.43
1:E:754:TRP:CH2	1:E:780:ARG:HA	2.53	0.43
1:F:692:HIS:NE2	1:F:723:ASP:OD1	2.49	0.43
1:B:610:PHE:O	1:B:628:PHE:N	2.45	0.43
1:B:901:VAL:HG23	1:B:942:ALA:CB	2.49	0.43
1:C:465:ALA:O	1:C:469:GLN:HG2	2.18	0.43
1:C:504:ASP:C	1:C:506:GLY:N	2.72	0.43
1:C:509:LYS:HD2	1:C:509:LYS:HA	1.77	0.43
1:C:883:VAL:O	1:C:887:CYS:HB2	2.19	0.43
1:D:31:PRO:O	1:D:389:SER:HB2	2.18	0.43
1:D:761:ASP:OD1	1:D:770:LYS:HA	2.17	0.43
1:D:470:PHE:CD2	1:D:929:VAL:HG21	2.52	0.43
1:E:1020:PHE:CZ	2:E:1101:LMT:H41	2.54	0.43
1:E:352:PHE:HE1	1:E:366:LEU:HD23	1.83	0.43
1:E:415:ASN:CG	1:E:418:ARG:HH12	2.15	0.43
1:E:497:LEU:HD12	1:E:497:LEU:HA	1.48	0.43
1:E:542:LEU:O	1:E:546:LEU:HG	2.17	0.43
1:E:652:THR:HG23	1:E:665:ALA:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:931:LEU:HD23	1:E:931:LEU:HA	1.84	0.43
1:F:647:ILE:O	1:F:650:ARG:HG2	2.18	0.43
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.53	0.43
1:A:400:LEU:HA	1:A:400:LEU:HD12	1.50	0.43
1:A:379:THR:HG21	1:A:477:ALA:HB2	2.00	0.43
1:A:47:ALA:O	1:A:87:THR:HA	2.19	0.43
1:B:36:PRO:HD3	1:B:391:ASN:OD1	2.18	0.43
1:A:225:VAL:HG11	1:B:778:LYS:HA	2.00	0.43
1:B:847:LEU:HA	1:B:847:LEU:HD23	1.83	0.43
1:B:913:LEU:HD23	1:B:913:LEU:HA	1.85	0.43
1:C:751:GLY:O	1:C:754:TRP:N	2.51	0.43
1:D:396:PHE:HE1	1:D:999:ALA:HB1	1.81	0.43
1:D:790:TYR:HB3	1:D:798:MET:HB3	1.99	0.43
1:D:967:ALA:C	1:D:971:ARG:HH12	2.21	0.43
1:E:588:GLN:HG3	1:E:592:ASN:HD21	1.83	0.43
1:E:908:GLY:O	1:E:1010:GLY:HA2	2.18	0.43
1:F:1015:THR:O	1:F:1017:LEU:N	2.51	0.43
1:F:340:VAL:HG22	1:F:396:PHE:HE2	1.82	0.43
1:F:560:PRO:HB2	1:F:836:SER:OG	2.18	0.43
1:A:1038:GLU:HB3	1:A:1039:ASP:C	2.39	0.43
1:A:344:LEU:HD22	1:A:402:ILE:HD11	1.98	0.43
1:A:893:GLU:OE1	1:C:11:PHE:HB2	2.18	0.43
1:B:149:MET:HB2	1:B:153:ASP:HB3	2.01	0.43
1:B:192:GLU:HB3	1:B:265:VAL:HA	2.01	0.43
1:B:504:ASP:C	1:B:506:GLY:H	2.21	0.43
1:B:950:LYS:HZ1	1:B:1030:ARG:NH2	2.14	0.43
1:C:144:ASN:ND2	1:C:149:MET:SD	2.92	0.43
1:C:187:TRP:HZ3	1:C:774:MET:CE	2.32	0.43
1:C:21:LEU:HA	1:C:21:LEU:HD23	1.80	0.43
1:C:139:VAL:O	1:C:326:PRO:HD2	2.18	0.43
1:C:509:LYS:HG2	1:C:513:PHE:HB2	1.99	0.43
1:D:165:ALA:HA	1:D:168:ARG:NH1	2.34	0.43
1:D:619:GLY:HA3	1:D:815:ARG:HH22	1.82	0.43
1:D:659:LYS:HD3	1:D:659:LYS:HA	1.71	0.43
1:E:182:TYR:HD1	1:E:182:TYR:HA	1.74	0.43
1:F:412:VAL:HA	1:F:438:ILE:HD12	2.00	0.43
1:E:238:THR:OG1	1:F:728:LYS:NZ	2.51	0.43
1:E:214:VAL:HG11	1:F:747:ASN:HB3	2.00	0.43
1:A:104:GLN:OE1	1:A:131:LYS:HD3	2.19	0.43
1:A:118:LEU:HA	1:A:119:PRO:HD3	1.78	0.43
1:A:61:VAL:HG21	1:A:122:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:LEU:O	1:A:452:VAL:HG22	2.19	0.43
1:A:944:LEU:CB	1:A:971:ARG:NH2	2.81	0.43
1:B:682:PHE:HB3	1:B:827:ILE:HB	2.00	0.43
1:C:189:ASN:OD1	1:C:190:PRO:HD2	2.18	0.43
1:C:775:SER:HB2	1:C:789:TRP:CZ2	2.53	0.43
1:D:457:ALA:HB1	1:D:468:ARG:HG3	1.99	0.43
1:D:394:THR:HG22	1:D:473:THR:OG1	2.18	0.43
1:D:887:CYS:O	1:D:890:ALA:HB3	2.19	0.43
1:E:180:SER:HB3	1:E:273:GLU:H	1.83	0.43
1:E:778:LYS:H	1:E:778:LYS:HG2	1.64	0.43
1:F:893:GLU:O	1:F:893:GLU:HG3	2.18	0.43
1:F:984:LEU:HD23	1:F:984:LEU:HA	1.69	0.43
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.54	0.43
1:A:270:LEU:HA	1:A:270:LEU:HD12	1.73	0.43
1:A:34:GLN:HB2	1:A:333:VAL:HG22	2.01	0.43
1:A:379:THR:OG1	1:A:477:ALA:HA	2.19	0.43
1:A:400:LEU:HD23	1:A:929:VAL:HG12	2.01	0.43
1:A:555:LEU:HA	1:A:555:LEU:HD23	1.78	0.43
1:A:683:GLU:HG2	1:A:819:TYR:CG	2.53	0.43
1:B:754:TRP:CH2	1:B:780:ARG:HA	2.54	0.43
1:B:952:LEU:HD23	1:B:952:LEU:HA	1.78	0.43
1:C:182:TYR:O	1:C:769:LYS:HD3	2.19	0.43
1:C:674:LEU:HA	1:C:674:LEU:HD23	1.84	0.43
1:D:393:LEU:CD1	1:D:466:ILE:HA	2.49	0.43
1:D:559:LEU:HD23	1:D:560:PRO:CD	2.49	0.43
1:D:58:GLN:HA	1:D:62:THR:HB	2.00	0.43
1:E:668:LEU:H	1:E:668:LEU:HD23	1.83	0.43
1:E:905:VAL:HG13	1:E:935:ILE:HG23	2.00	0.43
1:F:940:LYS:HZ2	1:F:978:THR:HG21	1.83	0.43
1:A:246:PHE:HB3	1:A:268:ILE:HD13	2.00	0.43
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.79	0.43
1:B:9:PRO:CB	1:B:495:THR:HG21	2.45	0.43
1:B:6:ILE:O	1:B:428:LYS:NZ	2.49	0.43
1:B:858:ASP:OD1	1:B:859:TRP:N	2.44	0.43
1:C:328:ASP:O	1:C:331:PRO:HD2	2.19	0.43
1:C:415:ASN:O	1:C:419:VAL:HG23	2.18	0.43
1:D:706:ALA:HB3	1:D:716:VAL:HG21	2.00	0.43
1:D:194:ASN:OD1	1:D:798:MET:HG3	2.18	0.43
1:D:414:GLU:HG3	1:D:974:PRO:HG3	2.01	0.43
1:E:230:LEU:HG	1:E:231:ASN:N	2.33	0.43
1:E:564:LEU:HD23	1:E:565:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:ARG:HH12	1:E:774:MET:CE	2.32	0.43
1:F:1038:GLU:HA	1:F:1039:ASP:HA	1.81	0.43
1:F:11:PHE:HE2	1:F:15:ILE:HD11	1.84	0.43
1:F:380:PHE:O	1:F:383:LEU:HB2	2.19	0.43
1:A:267:LYS:HD2	1:A:776:GLU:CD	2.39	0.43
2:B:1101:LMT:H6D	2:B:1101:LMT:C5B	2.48	0.43
1:B:578:LEU:HD13	1:B:661:ALA:HB2	2.01	0.43
1:C:982:PHE:O	1:C:983:ILE:C	2.57	0.43
1:D:278:ILE:HG13	1:D:613:ASN:HB3	2.00	0.43
1:D:858:ASP:OD2	1:D:859:TRP:N	2.49	0.43
1:E:589:LYS:O	1:E:592:ASN:HB2	2.19	0.43
1:E:682:PHE:CD2	1:E:827:ILE:HD12	2.53	0.43
1:F:192:GLU:HB3	1:F:265:VAL:HA	2.00	0.43
1:A:228:GLN:NE2	1:A:230:LEU:O	2.43	0.43
1:A:344:LEU:CD2	1:A:399:VAL:HG22	2.49	0.43
1:A:75:LEU:HD11	1:A:92:LEU:HB3	2.01	0.43
1:B:510:LYS:O	1:B:515:TRP:HD1	2.02	0.43
1:C:757:SER:O	1:C:772:TYR:HA	2.18	0.43
1:C:898:PRO:HA	1:C:901:VAL:HG12	2.01	0.43
1:C:945:ILE:HG12	1:C:971:ARG:NH2	2.34	0.43
1:D:35:TYR:HB3	1:D:36:PRO:HD2	2.01	0.43
1:D:37:THR:OG1	1:D:296:GLY:HA2	2.18	0.43
1:D:415:ASN:O	1:D:419:VAL:HG23	2.19	0.43
1:D:644:VAL:HG12	1:D:645:GLU:N	2.33	0.43
1:D:742:SER:HG	1:D:744:ASN:HD22	1.64	0.43
1:D:54:ALA:HB1	1:D:816:LEU:HG	2.00	0.43
1:D:973:ARG:HB3	1:D:974:PRO:HD3	2.01	0.43
1:E:1021:PHE:O	1:E:1024:VAL:HB	2.19	0.43
1:E:504:ASP:C	1:E:506:GLY:H	2.23	0.43
1:E:555:LEU:HB3	1:E:913:LEU:HB3	2.00	0.43
1:F:216:ALA:HB1	1:F:234:ILE:CG2	2.49	0.43
1:F:733:GLN:O	1:F:737:GLN:HG3	2.18	0.43
1:A:216:ALA:HB1	1:A:234:ILE:HG22	2.01	0.42
1:A:400:LEU:HD11	1:A:1007:VAL:CG2	2.46	0.42
1:A:572:PHE:HD1	1:A:666:PHE:O	2.02	0.42
1:A:847:LEU:HA	1:A:847:LEU:HD23	1.83	0.42
1:B:348:ILE:HG22	1:B:349:ILE:N	2.34	0.42
1:B:801:PHE:HA	1:B:804:PHE:CZ	2.53	0.42
1:C:143:ILE:HG22	1:C:286:ALA:CB	2.46	0.42
1:C:398:MET:HE3	1:C:398:MET:HB3	1.82	0.42
1:C:418:ARG:HH11	1:C:422:GLU:CD	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:LYS:HG2	1:C:511:GLY:N	2.34	0.42
1:C:610:PHE:HB3	1:C:628:PHE:HB2	2.00	0.42
1:C:659:LYS:HD3	1:C:659:LYS:HA	1.64	0.42
1:C:44:THR:HA	1:C:90:ILE:O	2.17	0.42
1:D:187:TRP:HA	1:D:774:MET:O	2.19	0.42
1:E:578:LEU:HB2	1:E:623:ASN:OD1	2.19	0.42
1:F:139:VAL:HA	1:F:289:LEU:O	2.19	0.42
1:F:293:LEU:HD22	1:F:294:ALA:H	1.84	0.42
1:F:828:LEU:HA	1:F:828:LEU:HD23	1.84	0.42
1:F:84:SER:C	1:F:86:GLY:H	2.22	0.42
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	2.01	0.42
1:A:542:LEU:HD12	1:A:542:LEU:HA	1.78	0.42
1:A:703:LEU:CD2	1:A:718:PRO:HD3	2.44	0.42
1:B:165:ALA:HB3	1:B:313:MET:HE1	2.01	0.42
1:B:317:PHE:HE2	1:B:323:ILE:HG12	1.84	0.42
1:B:453:PHE:O	1:B:456:MET:HG2	2.19	0.42
1:B:497:LEU:HA	1:B:497:LEU:HD12	1.77	0.42
1:B:612:VAL:HG12	1:B:615:PHE:HB3	2.01	0.42
1:D:252:LYS:HE2	1:D:252:LYS:HB3	1.72	0.42
1:D:357:LEU:HD23	1:D:357:LEU:O	2.18	0.42
1:D:984:LEU:HD23	1:D:984:LEU:HA	1.81	0.42
1:E:553:ALA:O	1:E:557:VAL:HG23	2.19	0.42
1:E:793:ALA:HB3	1:E:795:ASP:OD2	2.19	0.42
1:F:277:ILE:HD11	1:F:620:ARG:NH1	2.34	0.42
1:F:425:LEU:HD22	1:F:429:GLU:HG2	2.01	0.42
1:F:897:ILE:HD11	1:F:950:LYS:HE2	2.01	0.42
1:F:953:MET:SD	1:F:960:LEU:HA	2.59	0.42
1:A:166:ILE:HD13	1:A:166:ILE:HA	1.76	0.42
1:A:545:TYR:O	1:A:548:ILE:N	2.53	0.42
1:A:80:SER:HB3	1:A:90:ILE:HA	2.01	0.42
1:B:602:GLU:OE2	1:B:650:ARG:NH1	2.52	0.42
1:B:958:LYS:HB3	1:B:963:ALA:HB2	2.01	0.42
1:C:376:LEU:HD22	1:C:398:MET:CE	2.49	0.42
1:C:393:LEU:CD1	1:C:466:ILE:HD13	2.49	0.42
1:C:404:LEU:HB3	1:C:478:MET:SD	2.59	0.42
1:C:187:TRP:HZ3	1:C:774:MET:HE3	1.84	0.42
1:C:931:LEU:O	1:C:935:ILE:HG13	2.19	0.42
1:D:414:GLU:CG	1:D:974:PRO:HG3	2.48	0.42
1:D:574:THR:HG21	1:D:598:TYR:HE2	1.84	0.42
1:E:194:ASN:OD1	1:E:798:MET:HG3	2.18	0.42
1:E:330:THR:O	1:E:334:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:VAL:O	1:E:416:VAL:HG23	2.19	0.42
1:E:564:LEU:CD1	1:E:674:LEU:HD21	2.49	0.42
1:F:181:GLN:HG2	1:F:182:TYR:N	2.34	0.42
1:F:34:GLN:HB2	1:F:333:VAL:HG22	2.00	0.42
1:F:534:ILE:HG22	2:F:1101:LMT:H5'	2.00	0.42
1:F:536:ARG:HD2	2:F:1101:LMT:O4'	2.19	0.42
1:F:58:GLN:O	1:F:62:THR:HB	2.19	0.42
1:F:898:PRO:HA	1:F:901:VAL:HG12	2.01	0.42
1:A:327:TYR:CD2	1:A:327:TYR:C	2.93	0.42
1:A:388:PHE:CZ	1:A:472:ILE:HG21	2.54	0.42
1:A:375:VAL:CG2	1:A:481:SER:HA	2.49	0.42
1:A:948:PHE:CE2	1:A:971:ARG:HD3	2.55	0.42
1:B:511:GLY:HA2	1:B:515:TRP:HE1	1.82	0.42
1:B:733:GLN:O	1:B:737:GLN:HG3	2.18	0.42
1:A:781:MET:HE2	1:C:225:VAL:HG22	2.00	0.42
1:C:640:GLU:O	1:C:643:LYS:HB3	2.20	0.42
1:C:655:PHE:HB3	1:C:663:VAL:HB	2.02	0.42
1:C:847:LEU:HA	1:C:847:LEU:HD12	1.90	0.42
1:D:39:ALA:HA	1:D:40:PRO:HD2	1.90	0.42
1:D:684:LEU:O	1:D:824:SER:HB2	2.20	0.42
1:E:578:LEU:HA	1:E:661:ALA:HB1	2.00	0.42
1:E:682:PHE:CZ	1:E:857:TYR:HB2	2.54	0.42
1:E:57:VAL:HG11	1:E:86:GLY:O	2.19	0.42
1:E:902:MET:O	1:E:905:VAL:HG23	2.19	0.42
1:F:941:ASN:HD21	1:F:1015:THR:HG22	1.84	0.42
1:A:462:SER:O	1:A:466:ILE:HG12	2.19	0.42
1:A:572:PHE:HE2	1:A:631:LEU:HD21	1.83	0.42
1:A:6:ILE:HD11	1:A:432:ARG:HE	1.85	0.42
1:A:835:LYS:HG3	1:A:839:GLU:OE2	2.20	0.42
1:B:143:ILE:HG22	1:B:286:ALA:HB2	2.02	0.42
1:B:167:SER:HB3	1:B:175:VAL:HG21	2.00	0.42
1:B:887:CYS:O	1:B:890:ALA:HB3	2.18	0.42
1:B:76:MET:HB2	1:B:93:THR:O	2.20	0.42
1:C:356:TYR:HA	1:C:365:THR:CG2	2.43	0.42
1:C:559:LEU:HA	1:C:560:PRO:HD2	1.84	0.42
1:D:137:LEU:HD22	1:D:293:LEU:HG	2.01	0.42
1:D:365:THR:O	1:D:368:PRO:HD2	2.18	0.42
1:D:578:LEU:HG	1:D:623:ASN:O	2.19	0.42
1:E:281:PHE:CD1	1:E:610:PHE:HD1	2.36	0.42
1:E:58:GLN:NE2	1:E:816:LEU:HD13	2.34	0.42
1:F:957:GLY:HA3	1:F:1043:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:504:ASP:C	1:F:506:GLY:H	2.22	0.42
1:F:563:PHE:CD2	1:F:564:LEU:HB2	2.54	0.42
1:F:576:VAL:HG13	1:F:663:VAL:HG22	2.01	0.42
1:F:941:ASN:CG	1:F:975:ILE:HG23	2.40	0.42
1:A:207:ILE:O	1:A:211:ASN:HB3	2.19	0.42
1:A:55:LYS:HE2	1:A:55:LYS:HB3	1.92	0.42
1:A:57:VAL:HG21	1:A:86:GLY:O	2.19	0.42
1:A:878:ALA:O	1:A:882:ILE:HG12	2.19	0.42
1:B:1037:ASN:HA	1:B:1038:GLU:CB	2.49	0.42
1:B:344:LEU:HD23	1:B:402:ILE:HD11	2.02	0.42
1:A:583:THR:HG21	1:C:228:GLN:HG3	2.02	0.42
1:D:445:ILE:HG21	1:D:940:LYS:HD2	2.01	0.42
1:D:753:ALA:O	1:D:775:SER:HB3	2.18	0.42
1:D:946:VAL:HG13	1:D:1026:PHE:CD1	2.55	0.42
1:E:43:VAL:HG22	1:E:131:LYS:HD2	2.02	0.42
1:E:602:GLU:OE1	1:E:650:ARG:HD2	2.20	0.42
1:E:726:GLN:NE2	1:E:812:GLY:HA3	2.35	0.42
1:E:923:ASN:OD1	1:E:928:GLN:NE2	2.49	0.42
1:F:30:LEU:HA	1:F:30:LEU:HD12	1.93	0.42
1:F:931:LEU:HA	1:F:931:LEU:HD23	1.79	0.42
1:A:1030:ARG:HA	1:A:1030:ARG:HD2	1.64	0.42
1:A:419:VAL:HG11	1:A:433:LYS:HG2	2.02	0.42
1:A:633:ASP:OD2	1:A:634:TRP:HD1	2.02	0.42
1:A:576:VAL:HG22	1:A:663:VAL:HG22	2.02	0.42
1:B:599:LEU:HA	1:B:599:LEU:HD23	1.86	0.42
1:C:752:ALA:O	1:C:774:MET:HA	2.20	0.42
1:D:213:GLN:HA	1:D:237:GLN:O	2.19	0.42
1:D:338:HIS:NE2	1:D:342:LYS:HE3	2.35	0.42
1:E:1030:ARG:HA	1:E:1030:ARG:HD2	1.77	0.42
1:E:891:LEU:HA	1:E:891:LEU:HD12	1.80	0.42
1:E:972:LEU:HD13	1:E:976:LEU:HD13	2.01	0.42
1:F:881:LEU:HD23	1:F:935:ILE:HG21	2.01	0.42
1:A:525:HIS:HA	1:A:528:THR:HG22	2.01	0.42
1:B:1038:GLU:C	1:B:1040:ILE:HG13	2.40	0.42
1:B:370:ILE:O	1:B:374:VAL:HG23	2.19	0.42
1:B:510:LYS:O	1:B:515:TRP:CD1	2.72	0.42
1:A:214:VAL:HG21	1:B:747:ASN:CG	2.39	0.42
1:C:102:ILE:HD13	1:C:102:ILE:HA	1.87	0.42
1:C:289:LEU:HD23	1:C:289:LEU:HA	1.74	0.42
1:C:464:GLY:O	1:C:468:ARG:HB2	2.20	0.42
1:C:716:VAL:HA	1:C:829:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:ALA:HB2	1:C:948:PHE:HE1	1.85	0.42
1:D:317:PHE:HA	1:D:318:PRO:HD3	1.83	0.42
1:D:533:GLY:O	1:D:536:ARG:HB2	2.19	0.42
1:D:865:GLN:HA	1:D:868:LEU:HD12	2.01	0.42
1:E:760:ASN:O	1:E:771:VAL:HB	2.20	0.42
1:E:919:ARG:HB3	1:E:921:LEU:CD2	2.50	0.42
1:F:110:LYS:O	1:F:113:LEU:HB2	2.19	0.42
1:F:328:ASP:O	1:F:331:PRO:HD2	2.19	0.42
1:F:376:LEU:HD22	1:F:398:MET:HE3	2.02	0.42
1:F:895:TRP:HA	1:F:895:TRP:HE3	1.85	0.42
1:A:247:GLY:O	1:A:261:LEU:HB3	2.20	0.42
1:A:375:VAL:HG11	1:A:481:SER:HB3	2.01	0.42
1:B:175:VAL:HG23	1:C:70:ASN:HD21	1.85	0.42
1:B:415:ASN:HD21	1:B:948:PHE:HZ	1.67	0.42
1:C:979:SER:CB	1:C:1015:THR:HG21	2.50	0.42
1:C:507:GLU:HG2	1:C:518:ARG:HG3	2.01	0.42
1:C:591:LEU:HD12	1:C:613:ASN:HB2	2.02	0.42
1:C:61:VAL:HG13	1:C:118:LEU:HD13	2.02	0.42
1:D:459:PHE:HB3	1:D:464:GLY:HA2	2.01	0.42
1:D:49:TYR:CB	1:D:57:VAL:HG22	2.47	0.42
1:D:5:PHE:CD2	1:D:487:ILE:HG23	2.54	0.42
1:D:885:PHE:CE1	1:D:898:PRO:HB2	2.55	0.42
1:E:215:ALA:HA	1:F:51:GLY:HA3	2.02	0.42
1:E:235:ILE:HB	1:F:728:LYS:HA	2.02	0.42
1:E:143:ILE:HG22	1:E:286:ALA:HB2	2.01	0.42
1:E:347:ALA:CB	1:E:402:ILE:HG21	2.49	0.42
1:E:613:ASN:OD1	1:E:614:GLY:N	2.53	0.42
1:F:907:LEU:CD2	1:F:1017:LEU:HB3	2.50	0.42
1:F:382:VAL:HG11	1:F:476:SER:HB3	2.02	0.42
1:F:775:SER:OG	1:F:780:ARG:HG2	2.20	0.42
1:A:989:LEU:HD22	1:A:1000:GLN:HB3	2.01	0.42
1:B:706:ALA:HB1	1:B:716:VAL:HG11	2.01	0.42
1:C:68:ASN:OD1	1:C:114:ALA:HB2	2.19	0.42
1:C:252:LYS:HB3	1:C:260:VAL:CG2	2.50	0.42
1:C:355:MET:SD	1:C:368:PRO:HB2	2.60	0.42
1:D:322:LYS:HG2	1:D:323:ILE:O	2.20	0.42
1:D:61:VAL:CG2	1:D:122:VAL:HG21	2.49	0.42
1:D:867:ARG:HA	1:D:867:ARG:HD3	1.87	0.42
1:D:76:MET:HB2	1:D:93:THR:O	2.19	0.42
1:E:530:SER:OG	2:E:1101:LMT:C1'	2.68	0.42
1:E:582:ALA:HA	1:E:586:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:ILE:HD11	1:F:497:LEU:HD13	2.01	0.42
1:F:555:LEU:HB3	1:F:913:LEU:HB3	2.02	0.42
1:A:41:PRO:HG2	1:A:94:PHE:CB	2.40	0.41
1:A:511:GLY:HA2	1:A:515:TRP:HD1	1.85	0.41
1:A:698:ALA:O	1:A:701:GLN:HB3	2.20	0.41
1:A:712:MET:HG3	1:A:835:LYS:HE2	2.02	0.41
1:A:562:SER:CB	1:A:924:ASP:HB3	2.50	0.41
1:B:652:THR:HG22	1:B:664:PHE:CD1	2.52	0.41
1:B:686:ASP:HA	1:B:854:GLY:O	2.20	0.41
1:C:144:ASN:HB3	1:C:148:THR:HG23	2.02	0.41
1:D:523:SER:O	1:D:526:HIS:HB2	2.20	0.41
1:D:925:VAL:HA	1:D:928:GLN:OE1	2.20	0.41
1:D:909:VAL:HG22	1:D:931:LEU:CD2	2.50	0.41
1:D:94:PHE:CE2	1:D:103:ALA:HB1	2.56	0.41
1:E:15:ILE:HD12	1:E:487:ILE:HG21	2.01	0.41
1:F:99:ASP:HB3	1:F:102:ILE:HB	2.02	0.41
1:F:1038:GLU:HG2	1:F:1038:GLU:O	2.19	0.41
1:F:400:LEU:HD11	1:F:1007:VAL:HG21	2.02	0.41
1:F:407:ASP:OD1	1:F:978:THR:HG23	2.20	0.41
1:F:49:TYR:CE1	1:F:57:VAL:HA	2.55	0.41
1:F:693:GLU:HB3	1:F:694:LYS:HD2	2.02	0.41
1:A:971:ARG:CB	1:A:971:ARG:CZ	2.98	0.41
1:B:165:ALA:HB3	1:B:313:MET:CE	2.50	0.41
1:B:751:GLY:O	1:B:753:ALA:N	2.53	0.41
1:C:244:GLU:O	1:C:247:GLY:N	2.53	0.41
1:C:252:LYS:HB3	1:C:260:VAL:HG21	2.02	0.41
1:C:563:PHE:CD2	1:C:564:LEU:HB2	2.56	0.41
1:C:911:GLY:HA3	1:C:1013:THR:OG1	2.20	0.41
1:D:415:ASN:OD1	1:D:434:SER:HB2	2.21	0.41
1:E:352:PHE:HE1	1:E:366:LEU:CD2	2.33	0.41
1:F:213:GLN:HA	1:F:237:GLN:O	2.19	0.41
1:F:375:VAL:HG13	1:F:480:LEU:HB2	2.02	0.41
1:E:214:VAL:HG21	1:F:747:ASN:CG	2.39	0.41
1:F:841:MET:SD	1:F:863:SER:HB2	2.60	0.41
1:F:934:THR:O	1:F:938:SER:OG	2.38	0.41
1:A:200:PRO:HB2	1:A:749:THR:HG22	2.01	0.41
1:A:34:GLN:NE2	1:A:35:TYR:HE1	2.19	0.41
1:A:492:LEU:HA	1:A:492:LEU:HD23	1.73	0.41
1:A:597:TYR:CZ	1:A:651:ALA:HA	2.54	0.41
1:B:311:ALA:O	1:B:314:GLU:HB2	2.21	0.41
1:B:468:ARG:HB2	1:B:468:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:681:ASP:O	1:B:860:THR:HG22	2.20	0.41
1:B:738:ALA:O	1:B:740:GLY:N	2.54	0.41
1:B:7:ASP:C	1:B:8:ARG:HG3	2.41	0.41
1:C:250:LEU:HD11	1:C:259:ARG:HB3	2.01	0.41
1:C:578:LEU:HB3	1:C:579:PRO:HD2	2.02	0.41
1:C:910:ILE:O	1:C:914:LEU:HB2	2.20	0.41
1:D:293:LEU:CD2	1:D:297:ALA:HB3	2.50	0.41
1:D:544:LEU:HA	1:D:547:ILE:HD12	2.02	0.41
1:D:58:GLN:HA	1:D:62:THR:OG1	2.20	0.41
1:E:277:ILE:HG23	1:E:620:ARG:HH21	1.84	0.41
1:E:602:GLU:HB3	1:E:606:VAL:HG23	2.02	0.41
1:F:358:PHE:HD1	1:F:977:MET:CG	2.26	0.41
1:F:531:VAL:HG11	1:F:968:VAL:HG11	2.03	0.41
1:A:565:PRO:O	1:A:670:ALA:HB2	2.20	0.41
1:B:562:SER:HB2	1:B:922:THR:CG2	2.51	0.41
1:B:717:ARG:HD2	1:B:828:LEU:HB2	2.01	0.41
1:C:1016:VAL:HG12	1:C:1016:VAL:O	2.20	0.41
1:C:184:MET:HG2	1:C:246:PHE:CD2	2.55	0.41
1:C:340:VAL:HG11	1:C:395:MET:HB3	2.02	0.41
1:C:413:VAL:O	1:C:417:GLU:HG2	2.21	0.41
1:C:586:ARG:O	1:C:590:VAL:HG23	2.20	0.41
1:C:693:GLU:HB3	1:C:694:LYS:CE	2.50	0.41
1:D:27:ILE:HD11	1:D:380:PHE:CD1	2.55	0.41
1:D:695:LEU:HD13	1:D:825:MET:SD	2.61	0.41
1:D:974:PRO:O	1:D:975:ILE:C	2.59	0.41
1:E:166:ILE:HD12	1:E:309:GLU:CG	2.49	0.41
1:E:252:LYS:HE2	1:E:252:LYS:HB3	1.61	0.41
1:E:508:GLY:CA	1:E:518:ARG:HE	2.26	0.41
1:F:559:LEU:HA	1:F:560:PRO:HD2	1.81	0.41
1:F:49:TYR:N	1:F:86:GLY:O	2.42	0.41
1:A:140:VAL:O	1:A:289:LEU:N	2.44	0.41
1:A:328:ASP:O	1:A:331:PRO:HD2	2.20	0.41
1:A:524:THR:O	1:A:527:TYR:HB3	2.20	0.41
1:A:75:LEU:CD2	1:C:168:ARG:HD3	2.50	0.41
1:B:680:PHE:HB2	1:B:859:TRP:CZ3	2.55	0.41
1:B:904:VAL:HA	1:B:1025:PHE:HE1	1.86	0.41
1:C:23:GLY:O	1:C:27:ILE:HG23	2.20	0.41
1:C:309:GLU:HG3	1:C:313:MET:CE	2.51	0.41
1:C:713:LEU:CD2	1:C:843:LEU:HD12	2.50	0.41
1:D:355:MET:HA	1:D:355:MET:HE2	2.02	0.41
1:D:34:GLN:NE2	1:D:35:TYR:HE1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:ALA:O	1:D:413:VAL:HG23	2.19	0.41
1:E:24:GLY:O	1:E:27:ILE:HG22	2.21	0.41
1:E:347:ALA:HB1	1:E:402:ILE:HG21	2.02	0.41
1:E:937:LEU:HA	1:E:937:LEU:HD23	1.88	0.41
1:F:566:ASP:CG	1:F:678:THR:HG23	2.40	0.41
1:F:878:ALA:O	1:F:882:ILE:HG13	2.21	0.41
1:A:141:GLY:O	1:A:323:ILE:HA	2.21	0.41
1:A:377:LEU:HA	1:A:377:LEU:HD23	1.84	0.41
1:A:492:LEU:HD22	1:A:496:MET:SD	2.60	0.41
1:A:904:VAL:HG12	1:A:938:SER:HB3	2.03	0.41
1:C:1040:ILE:O	1:C:1040:ILE:HG22	2.20	0.41
1:C:154:ILE:O	1:C:157:TYR:N	2.54	0.41
1:C:181:GLN:O	1:C:272:GLY:HA2	2.20	0.41
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.50	0.41
1:C:422:GLU:HB3	1:C:423:GLU:HG3	2.01	0.41
1:C:703:LEU:CD1	1:C:718:PRO:HD3	2.51	0.41
1:D:113:LEU:HD21	1:F:128:SER:HB3	2.02	0.41
1:D:137:LEU:HD23	1:D:291:ILE:HG22	2.02	0.41
1:D:38:ILE:HD11	1:D:466:ILE:HD11	2.02	0.41
1:F:459:PHE:CE1	1:F:876:LEU:HG	2.56	0.41
1:A:1035:ARG:HG2	1:A:1036:LYS:H	1.85	0.41
1:A:1040:ILE:HG13	1:A:1042:HIS:HB2	2.02	0.41
1:A:252:LYS:HE2	1:A:252:LYS:HB3	1.75	0.41
1:A:274:ASN:OD1	1:A:276:ASP:HB2	2.20	0.41
1:A:27:ILE:HD11	1:A:380:PHE:CE1	2.56	0.41
1:A:472:ILE:HG22	1:A:473:THR:N	2.35	0.41
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.87	0.41
1:A:507:GLU:HG3	1:A:518:ARG:HA	2.03	0.41
1:B:1015:THR:O	1:B:1017:LEU:N	2.54	0.41
1:B:278:ILE:CG1	1:B:613:ASN:HB3	2.49	0.41
1:C:365:THR:O	1:C:368:PRO:HD2	2.20	0.41
1:C:586:ARG:O	1:C:589:LYS:HB2	2.21	0.41
1:D:203:VAL:O	1:D:207:ILE:HG13	2.20	0.41
1:D:524:THR:O	1:D:528:THR:HG22	2.19	0.41
1:D:888:LEU:HD13	1:D:901:VAL:HG13	2.02	0.41
1:D:944:LEU:HA	1:D:944:LEU:HD23	1.78	0.41
1:E:5:PHE:HE2	1:E:11:PHE:CD2	2.39	0.41
1:E:185:ARG:CD	1:E:772:TYR:HB2	2.51	0.41
1:E:78:MET:HE3	1:E:821:GLY:N	2.35	0.41
1:F:392:THR:O	1:F:395:MET:HB2	2.20	0.41
1:F:684:LEU:HB3	1:F:825:MET:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:971:ARG:NH2	1:F:975:ILE:HD11	2.36	0.41
1:A:351:VAL:HG22	1:A:981:ALA:HB1	2.03	0.41
1:A:699:ARG:HE	1:A:718:PRO:HG3	1.85	0.41
1:B:675:GLY:HA2	1:B:862:MET:SD	2.61	0.41
1:B:716:VAL:HG23	1:B:827:ILE:CG2	2.51	0.41
1:B:836:SER:OG	1:B:839:GLU:HG3	2.21	0.41
1:C:48:SER:C	1:C:50:PRO:HD3	2.41	0.41
1:C:80:SER:OG	1:C:818:ARG:HD3	2.20	0.41
1:D:72:ILE:HG21	1:D:107:VAL:HG23	2.03	0.41
1:D:544:LEU:HG	1:D:544:LEU:O	2.21	0.41
1:D:648:THR:HB	1:D:665:ALA:O	2.20	0.41
1:D:597:TYR:CD2	1:D:655:PHE:CZ	3.09	0.41
1:E:310:LEU:HD21	1:E:323:ILE:HG21	2.03	0.41
1:E:639:GLY:O	1:E:643:LYS:HG3	2.20	0.41
1:E:565:PRO:HG2	1:E:999:ALA:HA	2.02	0.41
1:F:1018:ALA:O	1:F:1022:VAL:HG23	2.21	0.41
1:F:356:TYR:CE1	1:F:362:PHE:HD1	2.38	0.41
1:A:154:ILE:HG22	1:A:287:SER:HB3	2.02	0.41
1:B:576:VAL:HG22	1:B:663:VAL:HG13	2.03	0.41
1:C:926:TYR:HE1	1:C:999:ALA:HB1	1.86	0.41
1:D:143:ILE:O	1:D:321:LEU:HA	2.21	0.41
1:D:671:ILE:H	1:D:671:ILE:HG13	1.70	0.41
1:E:738:ALA:C	1:E:740:GLY:H	2.23	0.41
1:E:885:PHE:HD2	1:E:886:LEU:HD13	1.85	0.41
1:F:465:ALA:HA	1:F:468:ARG:CZ	2.51	0.41
1:F:542:LEU:O	1:F:545:TYR:HB3	2.21	0.41
1:A:11:PHE:CE2	1:B:890:ALA:HB1	2.56	0.41
1:A:216:ALA:HB3	1:A:234:ILE:O	2.21	0.41
1:A:172:VAL:HG22	1:A:306:ILE:HD11	2.03	0.41
1:A:30:LEU:HA	1:A:31:PRO:HD3	1.92	0.41
1:A:366:LEU:HA	1:A:366:LEU:HD23	1.62	0.41
1:A:278:ILE:HG13	1:A:613:ASN:HB3	2.02	0.41
1:A:985:GLY:O	1:A:988:PRO:HD2	2.20	0.41
1:B:949:ALA:HB3	1:B:1026:PHE:CE1	2.55	0.41
1:B:94:PHE:CE1	1:B:103:ALA:HB1	2.56	0.41
1:B:706:ALA:HB2	1:B:844:MET:HE1	2.03	0.41
1:C:1034:SER:OG	1:C:1037:ASN:HB3	2.21	0.41
1:C:150:THR:H	1:C:153:ASP:HB2	1.85	0.41
1:C:151:GLN:NE2	1:C:286:ALA:O	2.54	0.41
1:C:77:TYR:CZ	1:C:93:THR:HG21	2.56	0.41
1:D:172:VAL:CG2	1:D:306:ILE:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:478:MET:HB3	1:D:478:MET:HE2	1.95	0.41
1:D:278:ILE:HD13	1:D:584:GLN:HE21	1.85	0.41
1:D:588:GLN:N	1:D:613:ASN:ND2	2.69	0.41
1:D:698:ALA:O	1:D:701:GLN:HB3	2.21	0.41
1:D:687:GLN:OE1	1:D:856:GLY:HA3	2.21	0.41
1:E:538:THR:CG2	1:E:1024:VAL:HG13	2.51	0.41
1:E:187:TRP:HA	1:E:774:MET:O	2.21	0.41
1:E:511:GLY:HA2	1:E:515:TRP:HD1	1.82	0.41
1:E:545:TYR:OH	1:E:906:PRO:HG2	2.20	0.41
1:E:844:MET:CE	1:E:844:MET:HA	2.50	0.41
1:F:1032:ARG:O	1:F:1033:PHE:HB2	2.21	0.41
1:F:578:LEU:HB2	1:F:623:ASN:CB	2.51	0.41
1:F:447:MET:HE1	1:F:887:CYS:O	2.21	0.41
1:A:478:MET:HE2	1:A:478:MET:HB3	1.91	0.41
1:B:946:VAL:HG22	1:B:1026:PHE:HD1	1.86	0.41
1:B:1026:PHE:O	1:B:1030:ARG:HB2	2.21	0.41
1:B:177:LEU:HA	1:B:289:LEU:HD23	2.03	0.41
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.54	0.41
1:B:533:GLY:HA2	1:B:536:ARG:HB2	2.03	0.41
1:B:888:LEU:HD13	1:B:901:VAL:HG11	2.03	0.41
1:B:960:LEU:O	1:B:964:THR:HG23	2.21	0.41
1:C:104:GLN:HG3	1:C:105:VAL:N	2.35	0.41
1:D:542:LEU:HD12	1:D:542:LEU:HA	1.71	0.41
1:D:662:MET:HG2	1:D:664:PHE:CZ	2.56	0.41
1:E:692:HIS:NE2	1:E:813:SER:HB2	2.35	0.41
1:F:907:LEU:HG	1:F:1017:LEU:HD23	2.03	0.41
1:F:926:TYR:HE1	1:F:999:ALA:HB1	1.86	0.41
1:A:897:ILE:HG12	1:A:1030:ARG:HD3	2.03	0.40
1:A:1040:ILE:CG1	1:A:1041:GLU:H	2.26	0.40
1:A:453:PHE:CE2	1:A:474:ILE:HG21	2.56	0.40
1:A:870:GLY:O	1:A:872:GLN:HG3	2.21	0.40
1:A:990:VAL:HG21	1:A:1008:MET:HE3	2.02	0.40
1:B:352:PHE:HD2	1:B:353:LEU:HD23	1.86	0.40
1:B:841:MET:O	1:B:845:GLU:HG3	2.22	0.40
1:C:987:MET:HB3	1:C:987:MET:HE2	1.94	0.40
1:D:393:LEU:HD12	1:D:469:GLN:HG3	2.03	0.40
1:D:514:GLY:C	1:D:516:PHE:N	2.72	0.40
1:E:448:VAL:HA	1:E:451:ALA:HB3	2.03	0.40
1:E:586:ARG:O	1:E:589:LYS:HB3	2.21	0.40
1:F:160:ALA:HA	1:F:767:ARG:NE	2.34	0.40
1:F:47:ALA:HB2	1:F:127:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:LYS:HA	1:F:816:LEU:CD1	2.51	0.40
1:F:563:PHE:CE2	1:F:564:LEU:HD22	2.56	0.40
1:F:565:PRO:HG2	1:F:567:GLU:OE2	2.21	0.40
1:F:572:PHE:HB2	1:F:666:PHE:O	2.22	0.40
1:F:6:ILE:HG12	1:F:6:ILE:H	1.41	0.40
1:A:210:GLN:OE1	1:A:249:ILE:HG23	2.22	0.40
1:A:338:HIS:NE2	1:A:342:LYS:HD2	2.37	0.40
1:A:344:LEU:HD21	1:A:399:VAL:HG22	2.04	0.40
1:A:356:TYR:HE2	1:A:513:PHE:HE2	1.68	0.40
1:B:442:LEU:HD23	1:B:442:LEU:HA	1.79	0.40
1:B:760:ASN:O	1:B:771:VAL:HB	2.21	0.40
1:C:1018:ALA:O	1:C:1022:VAL:HG23	2.21	0.40
1:C:182:TYR:HD2	1:C:765:ARG:HH22	1.68	0.40
1:D:146:ASP:OD2	1:D:146:ASP:N	2.44	0.40
1:D:151:GLN:CG	1:D:152:GLU:N	2.84	0.40
1:D:189:ASN:HA	1:D:190:PRO:HD3	1.91	0.40
1:D:251:LEU:HD21	1:D:262:LEU:HD13	2.02	0.40
1:D:279:ALA:HB3	1:D:286:ALA:O	2.20	0.40
1:E:1042:HIS:HB3	1:E:1043:SER:H	1.59	0.40
1:E:203:VAL:O	1:E:207:ILE:HG13	2.21	0.40
1:E:383:LEU:HD23	1:E:383:LEU:HA	1.92	0.40
1:F:752:ALA:O	1:F:774:MET:HA	2.21	0.40
1:F:790:TYR:HB3	1:F:798:MET:HB3	2.01	0.40
1:A:577:GLN:HE22	1:A:624:THR:HG22	1.86	0.40
1:A:752:ALA:O	1:A:774:MET:HA	2.22	0.40
1:A:706:ALA:HB2	1:A:844:MET:HE3	2.02	0.40
1:A:894:SER:HB3	1:A:897:ILE:HB	2.03	0.40
1:B:1015:THR:OG1	1:B:1016:VAL:N	2.53	0.40
1:B:756:GLY:CA	1:B:774:MET:HG3	2.52	0.40
1:B:185:ARG:HH12	1:B:774:MET:CE	2.35	0.40
1:B:448:VAL:HG13	1:B:884:VAL:HG22	2.03	0.40
1:B:931:LEU:O	1:B:935:ILE:HG13	2.21	0.40
1:C:466:ILE:H	1:C:466:ILE:HG12	1.77	0.40
1:C:668:LEU:H	1:C:668:LEU:CD2	2.30	0.40
1:C:701:GLN:HG2	1:C:705:GLU:OE2	2.20	0.40
1:C:940:LYS:O	1:C:943:ILE:HB	2.21	0.40
1:D:356:TYR:O	1:D:360:GLN:N	2.48	0.40
1:D:846:GLN:O	1:D:850:LYS:HD3	2.21	0.40
1:E:2:PRO:HB2	1:E:439:GLN:OE1	2.21	0.40
1:F:238:THR:HG22	1:F:239:ARG:O	2.21	0.40
1:F:453:PHE:CE1	1:F:474:ILE:HG21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:666:PHE:CD1	1:F:666:PHE:N	2.88	0.40
1:A:152:GLU:HB2	1:A:182:TYR:CE1	2.56	0.40
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.56	0.40
1:B:163:LYS:HD2	1:B:177:LEU:HD12	2.03	0.40
1:B:348:ILE:HD13	1:B:348:ILE:HG21	1.80	0.40
1:B:650:ARG:O	1:B:653:ARG:HB3	2.21	0.40
1:C:1037:ASN:HB3	1:C:1038:GLU:H	1.81	0.40
1:C:344:LEU:HA	1:C:399:VAL:HG22	2.03	0.40
1:C:368:PRO:O	1:C:371:ALA:HB3	2.21	0.40
1:C:699:ARG:HE	1:C:718:PRO:HB3	1.87	0.40
2:D:1101:LMT:C5B	2:D:1101:LMT:H6D	2.52	0.40
1:D:112:GLN:OE1	1:D:115:MET:HG3	2.22	0.40
1:D:706:ALA:HB1	1:D:716:VAL:HG11	2.03	0.40
1:D:982:PHE:O	1:D:983:ILE:C	2.59	0.40
1:E:167:SER:CB	1:E:175:VAL:HG21	2.52	0.40
1:E:216:ALA:HB2	1:E:236:ALA:HB2	2.04	0.40
1:E:291:ILE:HG21	1:E:306:ILE:HD11	2.02	0.40
1:E:328:ASP:O	1:E:331:PRO:HD2	2.21	0.40
1:E:398:MET:HG2	1:E:473:THR:CG2	2.52	0.40
1:F:149:MET:HB2	1:F:153:ASP:HB3	2.03	0.40
1:D:777:ALA:CB	1:F:225:VAL:HG12	2.44	0.40
1:F:30:LEU:HA	1:F:31:PRO:HD3	1.89	0.40
1:F:355:MET:HG2	1:F:410:ILE:HD11	2.04	0.40
1:F:636:ASP:O	1:F:638:PRO:HD3	2.22	0.40
1:F:778:LYS:HG2	1:F:778:LYS:H	1.58	0.40
1:F:964:THR:O	1:F:968:VAL:HB	2.21	0.40
1:A:261:LEU:HD12	1:A:263:ARG:CZ	2.51	0.40
1:A:483:LEU:HD13	1:A:487:ILE:HD12	2.04	0.40
1:A:944:LEU:HB3	1:A:971:ARG:NH2	2.37	0.40
1:B:156:ASP:OD2	1:B:769:LYS:NZ	2.31	0.40
1:C:1015:THR:OG1	1:C:1016:VAL:N	2.55	0.40
1:A:110:LYS:HE2	1:C:130:GLU:OE2	2.21	0.40
1:C:520:PHE:HE1	1:C:976:LEU:HD22	1.87	0.40
1:C:931:LEU:HA	1:C:931:LEU:HD23	1.82	0.40
1:D:586:ARG:HD2	1:D:586:ARG:HH11	1.78	0.40
1:E:157:TYR:CE1	1:E:318:PRO:HD3	2.57	0.40
1:E:158:VAL:HG11	1:E:289:LEU:HD11	2.03	0.40
1:E:189:ASN:HD22	1:E:190:PRO:HD2	1.85	0.40
1:E:527:TYR:HB2	2:E:1101:LMT:H82	2.04	0.40
1:E:848:ALA:HA	1:E:851:LEU:HG	2.04	0.40
1:F:1035:ARG:HH11	1:F:1038:GLU:CD	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:462:SER:HB3	1:F:865:GLN:CG	2.50	0.40
1:F:785:ASP:N	1:F:785:ASP:OD1	2.55	0.40
1:F:932:LEU:O	1:F:935:ILE:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:GLU:OE2	1:D:522:LYS:NZ[1_556]	2.16	0.04

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	1040/1049 (99%)	940 (90%)	89 (9%)	11 (1%)	17	52
1	B	1041/1049 (99%)	950 (91%)	75 (7%)	16 (2%)	12	44
1	C	1040/1049 (99%)	946 (91%)	77 (7%)	17 (2%)	11	43
1	D	1040/1049 (99%)	954 (92%)	70 (7%)	16 (2%)	12	44
1	E	1040/1049 (99%)	946 (91%)	77 (7%)	17 (2%)	11	43
1	F	1040/1049 (99%)	946 (91%)	76 (7%)	18 (2%)	11	42
All	All	6241/6294 (99%)	5682 (91%)	464 (7%)	95 (2%)	12	44

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	677	ALA
1	A	991	ILE
1	A	1037	ASN
1	A	1040	ILE
1	B	509	LYS

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Mol	Chain	Res	Type
1	B	516	PHE
1	B	673	GLU
1	B	677	ALA
1	B	689	GLY
1	B	1038	GLU
1	C	133	SER
1	C	360	GLN
1	C	509	LYS
1	C	689	GLY
1	C	836	SER
1	C	893	GLU
1	C	920	GLY
1	C	1037	ASN
1	D	508	GLY
1	D	511	GLY
1	D	992	SER
1	E	509	LYS
1	E	893	GLU
1	E	1042	HIS
1	F	133	SER
1	F	134	SER
1	F	146	ASP
1	F	360	GLN
1	F	836	SER
1	F	1035	ARG
1	F	1040	ILE
1	A	360	GLN
1	A	675	GLY
1	A	688	ALA
1	A	992	SER
1	A	1039	ASP
1	B	672	VAL
1	B	751	GLY
1	C	134	SER
1	C	146	ASP
1	C	147	GLY
1	C	751	GLY
1	C	871	ASN
1	D	360	GLN
1	D	675	GLY
1	D	751	GLY
1	D	991	ILE

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Mol	Chain	Res	Type
1	D	1033	PHE
1	E	508	GLY
1	E	672	VAL
1	E	674	LEU
1	E	677	ALA
1	E	1039	ASP
1	F	147	GLY
1	F	507	GLU
1	F	1033	PHE
1	A	751	GLY
1	B	1034	SER
1	B	1040	ILE
1	C	514	GLY
1	C	752	ALA
1	C	1042	HIS
1	D	215	ALA
1	D	752	ALA
1	E	516	PHE
1	E	751	GLY
1	F	514	GLY
1	F	1038	GLU
1	D	514	GLY
1	D	677	ALA
1	D	1034	SER
1	E	163	LYS
1	E	514	GLY
1	E	1034	SER
1	F	689	GLY
1	F	751	GLY
1	F	923	ASN
1	B	358	PHE
1	B	923	ASN
1	C	215	ALA
1	D	923	ASN
1	D	960	LEU
1	E	638	PRO
1	E	1040	ILE
1	B	215	ALA
1	B	893	GLU
1	E	74	ASN
1	F	638	PRO
1	A	658	ILE

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Mol	Chain	Res	Type
1	B	508	GLY
1	B	644	VAL
1	D	638	PRO
1	E	658	ILE
1	F	204	ILE
1	F	644	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	848/855 (99%)	790 (93%)	58 (7%)	18	53
1	B	849/855 (99%)	782 (92%)	67 (8%)	14	45
1	C	848/855 (99%)	775 (91%)	73 (9%)	12	42
1	D	848/855 (99%)	796 (94%)	52 (6%)	22	57
1	E	848/855 (99%)	779 (92%)	69 (8%)	14	44
1	F	848/855 (99%)	780 (92%)	68 (8%)	14	45
All	All	5089/5130 (99%)	4702 (92%)	387 (8%)	15	47

All (387) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	44	THR
1	A	49	TYR
1	A	88	VAL
1	A	101	ASP
1	A	146	ASP
1	A	169	THR
1	A	177	LEU
1	A	205	THR
1	A	222	THR
1	A	255	GLN
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	274	ASN
1	A	293	LEU
1	A	324	VAL
1	A	327	TYR
1	A	336	SER
1	A	355	MET
1	A	360	GLN
1	A	362	PHE
1	A	434	SER
1	A	437	GLN
1	A	452	VAL
1	A	472	ILE
1	A	489	THR
1	A	502	LYS
1	A	538	THR
1	A	540	ARG
1	A	559	LEU
1	A	561	SER
1	A	564	LEU
1	A	571	VAL
1	A	597	TYR
1	A	602	GLU
1	A	603	LYS
1	A	617	PHE
1	A	634	TRP
1	A	662	MET
1	A	712	MET
1	A	716	VAL
1	A	721	LEU
1	A	741	VAL
1	A	775	SER
1	A	785	ASP
1	A	797	GLN
1	A	806	SER
1	A	857	TYR
1	A	866	GLU
1	A	901	VAL
1	A	922	THR
1	A	931	LEU
1	A	938	SER
1	A	961	ILE
1	A	964	THR

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Mol	Chain	Res	Type
1	A	971	ARG
1	A	980	LEU
1	A	1035	ARG
1	A	1039	ASP
1	B	3	ASN
1	B	25	LEU
1	B	29	LYS
1	B	131	LYS
1	B	148	THR
1	B	213	GLN
1	B	229	GLN
1	B	242	SER
1	B	243	THR
1	B	249	ILE
1	B	259	ARG
1	B	267	LYS
1	B	270	LEU
1	B	293	LEU
1	B	295	THR
1	B	310	LEU
1	B	314	GLU
1	B	321	LEU
1	B	324	VAL
1	B	329	THR
1	B	348	ILE
1	B	355	MET
1	B	358	PHE
1	B	360	GLN
1	B	365	THR
1	B	400	LEU
1	B	434	SER
1	B	482	VAL
1	B	489	THR
1	B	523	SER
1	B	559	LEU
1	B	561	SER
1	B	563	PHE
1	B	564	LEU
1	B	571	VAL
1	B	602	GLU
1	B	613	ASN
1	B	626	ILE

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Mol	Chain	Res	Type
1	B	634	TRP
1	B	652	THR
1	B	666	PHE
1	B	687	GLN
1	B	694	LYS
1	B	695	LEU
1	B	697	GLN
1	B	714	THR
1	B	716	VAL
1	B	717	ARG
1	B	721	LEU
1	B	741	VAL
1	B	775	SER
1	B	806	SER
1	B	835	LYS
1	B	865	GLN
1	B	867	ARG
1	B	871	ASN
1	B	886	LEU
1	B	914	LEU
1	B	922	THR
1	B	938	SER
1	B	966	ASP
1	B	971	ARG
1	B	973	ARG
1	B	1015	THR
1	B	1039	ASP
1	B	1042	HIS
1	B	1044	HIS
1	C	3	ASN
1	C	6	ILE
1	C	11	PHE
1	C	13	TRP
1	C	27	ILE
1	C	49	TYR
1	C	58	GLN
1	C	102	ILE
1	C	104	GLN
1	C	112	GLN
1	C	145	THR
1	C	148	THR
1	C	177	LEU

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Mol	Chain	Res	Type
1	C	243	THR
1	C	255	GLN
1	C	280	GLU
1	C	307	ARG
1	C	336	SER
1	C	337	ILE
1	C	342	LYS
1	C	358	PHE
1	C	362	PHE
1	C	363	ARG
1	C	392	THR
1	C	439	GLN
1	C	447	MET
1	C	448	VAL
1	C	452	VAL
1	C	463	THR
1	C	472	ILE
1	C	482	VAL
1	C	510	LYS
1	C	526	HIS
1	C	530	SER
1	C	559	LEU
1	C	561	SER
1	C	571	VAL
1	C	602	GLU
1	C	634	TRP
1	C	649	MET
1	C	659	LYS
1	C	662	MET
1	C	666	PHE
1	C	678	THR
1	C	686	ASP
1	C	694	LYS
1	C	733	GLN
1	C	741	VAL
1	C	746	ILE
1	C	748	THR
1	C	749	THR
1	C	785	ASP
1	C	788	ASP
1	C	797	GLN
1	C	804	PHE

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Mol	Chain	Res	Type
1	C	847	LEU
1	C	860	THR
1	C	865	GLN
1	C	868	LEU
1	C	876	LEU
1	C	886	LEU
1	C	887	CYS
1	C	895	TRP
1	C	938	SER
1	C	947	GLU
1	C	961	ILE
1	C	971	ARG
1	C	980	LEU
1	C	991	ILE
1	C	1011	MET
1	C	1035	ARG
1	C	1038	GLU
1	C	1041	GLU
1	D	3	ASN
1	D	27	ILE
1	D	49	TYR
1	D	88	VAL
1	D	101	ASP
1	D	102	ILE
1	D	146	ASP
1	D	205	THR
1	D	222	THR
1	D	255	GLN
1	D	260	VAL
1	D	270	LEU
1	D	324	VAL
1	D	336	SER
1	D	355	MET
1	D	360	GLN
1	D	362	PHE
1	D	437	GLN
1	D	462	SER
1	D	463	THR
1	D	472	ILE
1	D	538	THR
1	D	559	LEU
1	D	561	SER

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Mol	Chain	Res	Type
1	D	602	GLU
1	D	603	LYS
1	D	634	TRP
1	D	662	MET
1	D	666	PHE
1	D	671	ILE
1	D	672	VAL
1	D	695	LEU
1	D	741	VAL
1	D	743	ILE
1	D	775	SER
1	D	785	ASP
1	D	804	PHE
1	D	806	SER
1	D	866	GLU
1	D	867	ARG
1	D	901	VAL
1	D	918	PHE
1	D	922	THR
1	D	931	LEU
1	D	938	SER
1	D	961	ILE
1	D	966	ASP
1	D	968	VAL
1	D	971	ARG
1	D	980	LEU
1	D	1033	PHE
1	D	1037	ASN
1	E	3	ASN
1	E	6	ILE
1	E	25	LEU
1	E	28	LEU
1	E	29	LYS
1	E	58	GLN
1	E	131	LYS
1	E	146	ASP
1	E	177	LEU
1	E	182	TYR
1	E	189	ASN
1	E	205	THR
1	E	229	GLN
1	E	243	THR

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Mol	Chain	Res	Type
1	E	255	GLN
1	E	259	ARG
1	E	267	LYS
1	E	270	LEU
1	E	293	LEU
1	E	295	THR
1	E	314	GLU
1	E	324	VAL
1	E	327	TYR
1	E	329	THR
1	E	336	SER
1	E	337	ILE
1	E	360	GLN
1	E	365	THR
1	E	372	VAL
1	E	398	MET
1	E	400	LEU
1	E	482	VAL
1	E	523	SER
1	E	538	THR
1	E	559	LEU
1	E	561	SER
1	E	563	PHE
1	E	564	LEU
1	E	574	THR
1	E	578	LEU
1	E	634	TRP
1	E	652	THR
1	E	653	ARG
1	E	672	VAL
1	E	673	GLU
1	E	690	LEU
1	E	694	LYS
1	E	697	GLN
1	E	714	THR
1	E	717	ARG
1	E	721	LEU
1	E	741	VAL
1	E	785	ASP
1	E	797	GLN
1	E	804	PHE
1	E	835	LYS

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Mol	Chain	Res	Type
1	E	865	GLN
1	E	867	ARG
1	E	871	ASN
1	E	886	LEU
1	E	938	SER
1	E	966	ASP
1	E	968	VAL
1	E	971	ARG
1	E	972	LEU
1	E	980	LEU
1	E	1021	PHE
1	E	1036	LYS
1	E	1043	SER
1	F	3	ASN
1	F	6	ILE
1	F	13	TRP
1	F	21	LEU
1	F	34	GLN
1	F	49	TYR
1	F	59	ASP
1	F	104	GLN
1	F	176	GLN
1	F	177	LEU
1	F	242	SER
1	F	280	GLU
1	F	293	LEU
1	F	327	TYR
1	F	335	ILE
1	F	337	ILE
1	F	357	LEU
1	F	358	PHE
1	F	362	PHE
1	F	363	ARG
1	F	408	ASP
1	F	447	MET
1	F	448	VAL
1	F	452	VAL
1	F	472	ILE
1	F	482	VAL
1	F	510	LYS
1	F	515	TRP
1	F	523	SER

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Mol	Chain	Res	Type
1	F	524	THR
1	F	526	HIS
1	F	538	THR
1	F	540	ARG
1	F	542	LEU
1	F	559	LEU
1	F	564	LEU
1	F	602	GLU
1	F	626	ILE
1	F	634	TRP
1	F	649	MET
1	F	666	PHE
1	F	668	LEU
1	F	681	ASP
1	F	694	LYS
1	F	703	LEU
1	F	713	LEU
1	F	721	LEU
1	F	741	VAL
1	F	746	ILE
1	F	775	SER
1	F	785	ASP
1	F	797	GLN
1	F	806	SER
1	F	847	LEU
1	F	860	THR
1	F	868	LEU
1	F	876	LEU
1	F	923	ASN
1	F	938	SER
1	F	961	ILE
1	F	964	THR
1	F	971	ARG
1	F	980	LEU
1	F	991	ILE
1	F	1011	MET
1	F	1030	ARG
1	F	1034	SER
1	F	1038	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	151	GLN
1	A	181	GLN
1	A	505	HIS
1	A	517	ASN
1	A	605	ASN
1	A	928	GLN
1	B	63	GLN
1	B	189	ASN
1	B	231	ASN
1	B	588	GLN
1	B	592	ASN
1	B	613	ASN
1	B	642	ASN
1	B	733	GLN
1	B	1037	ASN
1	C	70	ASN
1	D	34	GLN
1	D	605	ASN
1	D	744	ASN
1	E	67	GLN
1	E	108	GLN
1	E	189	ASN
1	E	588	GLN
1	E	592	ASN
1	E	733	GLN
1	E	737	GLN
1	F	89	GLN
1	F	588	GLN
1	F	592	ASN
1	F	733	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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	LMT	A	1101	-	36,36,36	1.80	10 (27%)	47,47,47	1.15	4 (8%)
2	LMT	B	1101	-	36,36,36	1.77	10 (27%)	47,47,47	1.48	8 (17%)
2	LMT	C	1101	-	36,36,36	1.93	8 (22%)	47,47,47	1.67	10 (21%)
2	LMT	D	1101	-	36,36,36	1.77	7 (19%)	47,47,47	1.35	8 (17%)
2	LMT	E	1101	-	36,36,36	1.84	10 (27%)	47,47,47	1.16	6 (12%)
2	LMT	F	1101	-	36,36,36	1.78	8 (22%)	47,47,47	1.07	1 (2%)

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	LMT	A	1101	-	-	0/21/61/61	0/2/2/2
2	LMT	B	1101	-	-	0/21/61/61	0/2/2/2
2	LMT	C	1101	-	1/1/10/10	0/21/61/61	0/2/2/2
2	LMT	D	1101	-	-	0/21/61/61	0/2/2/2
2	LMT	E	1101	-	-	0/21/61/61	0/2/2/2
2	LMT	F	1101	-	-	0/21/61/61	0/2/2/2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1101	LMT	C6'-C5'	-3.45	1.40	1.51
2	E	1101	LMT	C6'-C5'	-3.27	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	LMT	C6'-C5'	-3.19	1.41	1.51
2	D	1101	LMT	C6'-C5'	-3.07	1.41	1.51
2	A	1101	LMT	C6'-C5'	-3.06	1.41	1.51
2	C	1101	LMT	C6'-C5'	-2.88	1.42	1.51
2	F	1101	LMT	C3'-C2'	-2.87	1.45	1.52
2	C	1101	LMT	C3'-C2'	-2.68	1.45	1.52
2	A	1101	LMT	C3'-C2'	-2.52	1.45	1.52
2	B	1101	LMT	C3B-C2B	-2.37	1.46	1.52
2	B	1101	LMT	C3'-C2'	-2.23	1.46	1.52
2	A	1101	LMT	C3B-C2B	-2.22	1.46	1.52
2	E	1101	LMT	C3B-C2B	-2.19	1.46	1.52
2	E	1101	LMT	C3'-C2'	-2.04	1.47	1.52
2	B	1101	LMT	O2'-C2'	2.03	1.47	1.43
2	F	1101	LMT	O2'-C2'	2.13	1.47	1.43
2	A	1101	LMT	O3'-C3'	2.26	1.48	1.43
2	E	1101	LMT	O3'-C3'	2.31	1.48	1.43
2	A	1101	LMT	O2'-C2'	2.37	1.48	1.43
2	E	1101	LMT	O3B-C3B	2.39	1.48	1.43
2	B	1101	LMT	O3'-C3'	2.39	1.48	1.43
2	D	1101	LMT	O2'-C2'	2.42	1.48	1.43
2	E	1101	LMT	O2'-C2'	2.51	1.48	1.43
2	B	1101	LMT	O5'-C1'	2.63	1.48	1.41
2	C	1101	LMT	O2'-C2'	2.63	1.49	1.43
2	A	1101	LMT	O3B-C3B	2.70	1.49	1.43
2	C	1101	LMT	O3B-C3B	2.71	1.49	1.43
2	B	1101	LMT	O3B-C3B	2.84	1.49	1.43
2	F	1101	LMT	O3B-C3B	2.92	1.49	1.43
2	A	1101	LMT	O1'-C1'	3.01	1.45	1.40
2	E	1101	LMT	O5'-C1'	3.20	1.49	1.41
2	D	1101	LMT	O3B-C3B	3.22	1.50	1.43
2	D	1101	LMT	O5'-C1'	3.25	1.49	1.41
2	A	1101	LMT	O5'-C1'	3.26	1.49	1.41
2	B	1101	LMT	O1'-C1'	3.31	1.46	1.40
2	B	1101	LMT	O5'-C5'	3.33	1.52	1.44
2	F	1101	LMT	O5'-C1'	3.36	1.50	1.41
2	F	1101	LMT	O1'-C1'	3.55	1.46	1.40
2	D	1101	LMT	O1'-C1'	3.60	1.46	1.40
2	D	1101	LMT	O5B-C1B	3.60	1.50	1.41
2	F	1101	LMT	O5'-C5'	3.64	1.53	1.44
2	F	1101	LMT	O5B-C1B	3.67	1.50	1.41
2	C	1101	LMT	O5B-C1B	3.73	1.51	1.41
2	E	1101	LMT	O5'-C5'	3.82	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	LMT	O5'-C1'	3.84	1.51	1.41
2	D	1101	LMT	O5'-C5'	3.86	1.53	1.44
2	E	1101	LMT	O5B-C1B	3.87	1.51	1.41
2	A	1101	LMT	O5B-C1B	3.93	1.51	1.41
2	A	1101	LMT	O5'-C5'	3.99	1.54	1.44
2	C	1101	LMT	O1'-C1'	4.04	1.47	1.40
2	E	1101	LMT	O1'-C1'	4.04	1.47	1.40
2	B	1101	LMT	O5B-C1B	4.06	1.51	1.41
2	C	1101	LMT	O5'-C5'	4.66	1.55	1.44

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	LMT	C1'-O5'-C5'	-4.19	105.82	113.72
2	E	1101	LMT	C3B-C4B-C5B	-3.62	103.84	110.22
2	A	1101	LMT	C1B-O1B-C4'	-3.35	109.83	118.00
2	C	1101	LMT	C1B-O1B-C4'	-3.27	110.03	118.00
2	C	1101	LMT	O3B-C3B-C4B	-2.99	103.86	110.36
2	D	1101	LMT	C1B-O1B-C4'	-2.41	112.11	118.00
2	F	1101	LMT	O4'-C4B-C3B	-2.41	105.12	110.36
2	A	1101	LMT	C1'-C2'-C3'	-2.28	105.74	109.98
2	B	1101	LMT	O2'-C2'-C3'	-2.27	105.41	110.36
2	B	1101	LMT	O5'-C5'-C4'	-2.22	105.21	109.75
2	C	1101	LMT	O4'-C4B-C3B	-2.21	105.55	110.36
2	E	1101	LMT	C1B-O1B-C4'	-2.19	112.65	118.00
2	E	1101	LMT	C4B-C3B-C2B	-2.18	107.00	110.84
2	D	1101	LMT	O3'-C3'-C2'	-2.17	105.64	110.36
2	C	1101	LMT	O3B-C3B-C2B	-2.16	105.65	110.36
2	D	1101	LMT	C6B-C5B-C4B	-2.02	108.28	113.00
2	A	1101	LMT	O3B-C3B-C2B	-2.00	106.00	110.36
2	E	1101	LMT	O5B-C5B-C6B	2.07	111.38	106.41
2	E	1101	LMT	C1-O1'-C1'	2.20	117.64	113.87
2	D	1101	LMT	O5B-C5B-C6B	2.25	111.79	106.41
2	B	1101	LMT	O5'-C5'-C6'	2.38	112.11	106.41
2	E	1101	LMT	O1'-C1'-C2'	2.40	112.14	108.23
2	C	1101	LMT	O1B-C1B-C2B	2.42	113.57	108.11
2	D	1101	LMT	C1'-C2'-C3'	2.46	114.55	109.98
2	C	1101	LMT	O5'-C5'-C6'	2.46	112.31	106.41
2	D	1101	LMT	C1B-C2B-C3B	2.68	114.97	109.98
2	B	1101	LMT	O1'-C1'-C2'	2.71	112.66	108.23
2	B	1101	LMT	C1'-C2'-C3'	2.72	115.04	109.98
2	D	1101	LMT	O1B-C1B-C2B	2.88	114.60	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	LMT	O5'-C5'-C6'	2.99	113.56	106.41
2	D	1101	LMT	C2'-C3'-C4'	3.10	116.03	109.61
2	C	1101	LMT	C1-O1'-C1'	3.29	119.51	113.87
2	C	1101	LMT	C1B-C2B-C3B	3.42	116.34	109.98
2	B	1101	LMT	O5B-C5B-C4B	3.47	116.06	109.66
2	B	1101	LMT	C1B-O5B-C5B	3.65	120.59	113.72
2	C	1101	LMT	C3B-C4B-C5B	3.97	117.21	110.22
2	C	1101	LMT	C4B-C3B-C2B	4.09	118.05	110.84

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1101	LMT	C3B

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	LMT	3	0
2	B	1101	LMT	7	0
2	D	1101	LMT	7	0
2	E	1101	LMT	9	0
2	F	1101	LMT	3	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	1042/1049 (99%)	0.64	131 (12%) 4 4	48, 78, 110, 142	0
1	B	1043/1049 (99%)	0.59	113 (10%) 6 5	36, 72, 102, 149	0
1	C	1042/1049 (99%)	0.58	115 (11%) 6 5	34, 72, 100, 155	0
1	D	1042/1049 (99%)	0.71	152 (14%) 3 2	40, 89, 116, 145	0
1	E	1042/1049 (99%)	0.85	168 (16%) 2 2	57, 90, 113, 158	0
1	F	1042/1049 (99%)	0.83	164 (15%) 2 2	51, 86, 112, 144	0
All	All	6253/6294 (99%)	0.70	843 (13%) 3 3	34, 82, 111, 158	0

All (843) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	869	SER	19.1
1	F	836	SER	18.1
1	E	314	GLU	11.6
1	D	869	SER	11.6
1	E	315	PRO	11.6
1	F	837	THR	11.2
1	F	442	LEU	11.1
1	E	311	ALA	10.1
1	E	296	GLY	10.0
1	D	868	LEU	9.7
1	F	835	LYS	9.5
1	D	870	GLY	9.4
1	E	869	SER	9.2
1	C	836	SER	8.6
1	F	834	GLY	8.6
1	E	33	ALA	8.5
1	F	831	ALA	8.3
1	C	835	LYS	8.2
1	D	386	PHE	8.1

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Mol	Chain	Res	Type	RSRZ
1	F	815	ARG	8.0
1	C	712	MET	7.9
1	F	59	ASP	7.9
1	E	32	VAL	7.6
1	F	403	GLY	7.6
1	B	868	LEU	7.5
1	F	618	ALA	7.4
1	F	441	ALA	7.2
1	E	922	THR	7.2
1	F	80	SER	7.1
1	D	837	THR	7.1
1	E	242	SER	7.1
1	F	620	ARG	7.1
1	C	720	GLY	7.1
1	D	839	GLU	7.1
1	E	769	LYS	7.0
1	C	719	ASN	6.8
1	C	310	LEU	6.8
1	C	307	ARG	6.7
1	C	721	LEU	6.6
1	D	720	GLY	6.6
1	E	765	ARG	6.6
1	C	314	GLU	6.6
1	E	390	ILE	6.5
1	F	619	GLY	6.5
1	E	307	ARG	6.5
1	A	396	PHE	6.4
1	D	719	ASN	6.4
1	F	402	ILE	6.4
1	D	322	LYS	6.2
1	B	314	GLU	6.2
1	B	315	PRO	6.1
1	D	841	MET	6.1
1	D	690	LEU	6.1
1	C	837	THR	6.1
1	D	840	ALA	6.0
1	F	721	LEU	6.0
1	F	675	GLY	6.0
1	B	620	ARG	5.9
1	D	461	GLY	5.9
1	F	240	LEU	5.9
1	D	836	SER	5.9

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Mol	Chain	Res	Type	RSRZ
1	E	933	THR	5.9
1	F	833	PRO	5.9
1	F	711	ASP	5.9
1	E	105	VAL	5.9
1	D	867	ARG	5.8
1	F	720	GLY	5.8
1	E	764	ASP	5.8
1	E	303	ALA	5.8
1	E	291	ILE	5.7
1	E	290	GLY	5.7
1	D	859	TRP	5.6
1	E	310	LEU	5.6
1	E	297	ALA	5.5
1	C	79	SER	5.5
1	F	873	ALA	5.5
1	E	78	MET	5.5
1	B	619	GLY	5.5
1	C	713	LEU	5.5
1	A	400	LEU	5.5
1	A	765	ARG	5.4
1	D	853	THR	5.4
1	F	481	SER	5.4
1	F	719	ASN	5.4
1	F	117	LEU	5.3
1	B	871	ASN	5.3
1	E	31	PRO	5.3
1	C	834	GLY	5.3
1	E	210	GLN	5.3
1	A	761	ASP	5.2
1	D	459	PHE	5.2
1	F	676	THR	5.2
1	C	501	ALA	5.2
1	E	678	THR	5.1
1	C	403	GLY	5.1
1	C	711	ASP	5.1
1	E	770	LYS	5.0
1	E	783	PRO	5.0
1	E	102	ILE	5.0
1	F	60	THR	5.0
1	F	62	THR	5.0
1	E	929	VAL	5.0
1	F	81	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	842	GLU	5.0
1	A	801	PHE	5.0
1	E	30	LEU	5.0
1	E	366	LEU	5.0
1	F	832	ALA	4.9
1	F	763	ILE	4.9
1	A	766	GLY	4.9
1	A	640	GLU	4.9
1	D	460	GLY	4.9
1	D	400	LEU	4.9
1	E	868	LEU	4.9
1	B	618	ALA	4.9
1	A	620	ARG	4.9
1	A	1040	ILE	4.9
1	B	617	PHE	4.9
1	B	866	GLU	4.9
1	B	73	ASP	4.8
1	A	621	GLY	4.8
1	E	79	SER	4.8
1	F	801	PHE	4.8
1	B	870	GLY	4.7
1	E	762	PHE	4.7
1	A	767	ARG	4.7
1	A	30	LEU	4.7
1	F	826	GLU	4.7
1	B	764	ASP	4.7
1	E	243	THR	4.7
1	F	410	ILE	4.7
1	E	387	GLY	4.7
1	F	58	GLN	4.6
1	C	1039	ASP	4.6
1	D	768	VAL	4.6
1	A	615	PHE	4.6
1	A	240	LEU	4.6
1	D	323	ILE	4.6
1	D	620	ARG	4.6
1	F	406	VAL	4.5
1	D	31	PRO	4.5
1	E	308	ALA	4.5
1	A	768	VAL	4.5
1	F	791	VAL	4.5
1	B	246	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	768	VAL	4.5
1	B	624	THR	4.5
1	C	494	ALA	4.5
1	B	720	GLY	4.4
1	D	50	PRO	4.4
1	A	102	ILE	4.4
1	D	84	SER	4.4
1	F	941	ASN	4.4
1	D	59	ASP	4.4
1	A	239	ARG	4.4
1	A	397	GLY	4.4
1	C	402	ILE	4.4
1	D	851	LEU	4.3
1	D	180	SER	4.3
1	A	321	LEU	4.3
1	E	944	LEU	4.3
1	A	769	LYS	4.3
1	D	835	LYS	4.3
1	F	828	LEU	4.3
1	D	843	LEU	4.3
1	E	400	LEU	4.3
1	A	32	VAL	4.3
1	F	399	VAL	4.3
1	B	102	ILE	4.3
1	B	311	ALA	4.3
1	F	109	ASN	4.3
1	F	816	LEU	4.2
1	F	57	VAL	4.2
1	E	181	GLN	4.2
1	D	396	PHE	4.2
1	C	642	ASN	4.2
1	C	838	GLY	4.2
1	E	25	LEU	4.2
1	D	389	SER	4.2
1	C	833	PRO	4.2
1	F	805	SER	4.2
1	C	856	GLY	4.2
1	D	388	PHE	4.2
1	A	390	ILE	4.2
1	D	866	GLU	4.2
1	E	620	ARG	4.1
1	D	330	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	943	ILE	4.1
1	E	241	THR	4.1
1	D	36	PRO	4.1
1	E	619	GLY	4.1
1	C	868	LEU	4.1
1	A	369	THR	4.1
1	F	713	LEU	4.1
1	A	866	GLU	4.1
1	F	865	GLN	4.1
1	F	714	THR	4.1
1	E	761	ASP	4.1
1	D	244	GLU	4.0
1	A	174	ASP	4.0
1	D	871	ASN	4.0
1	E	362	PHE	4.0
1	A	705	GLU	4.0
1	E	513	PHE	4.0
1	E	937	LEU	4.0
1	C	826	GLU	4.0
1	F	501	ALA	4.0
1	E	104	GLN	4.0
1	E	164	ASP	4.0
1	C	804	PHE	3.9
1	F	786	ILE	3.9
1	A	35	TYR	3.9
1	D	772	TYR	3.9
1	B	308	ALA	3.9
1	C	500	ILE	3.9
1	D	791	VAL	3.9
1	D	32	VAL	3.9
1	F	79	SER	3.9
1	C	32	VAL	3.9
1	B	721	LEU	3.9
1	B	180	SER	3.9
1	E	681	ASP	3.9
1	E	921	LEU	3.8
1	A	789	TRP	3.8
1	D	1041	GLU	3.8
1	A	336	SER	3.8
1	E	409	ALA	3.8
1	E	183	ALA	3.8
1	F	830	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	458	PHE	3.8
1	F	804	PHE	3.8
1	D	844	MET	3.8
1	E	801	PHE	3.8
1	B	693	GLU	3.8
1	E	84	SER	3.8
1	E	398	MET	3.8
1	F	448	VAL	3.8
1	A	340	VAL	3.7
1	B	59	ASP	3.7
1	A	871	ASN	3.7
1	D	689	GLY	3.7
1	B	101	ASP	3.7
1	C	122	VAL	3.7
1	F	54	ALA	3.7
1	B	71	GLY	3.7
1	A	995	ALA	3.7
1	A	337	ILE	3.7
1	F	838	GLY	3.7
1	C	48	SER	3.7
1	C	311	ALA	3.7
1	F	762	PHE	3.7
1	F	617	PHE	3.7
1	B	872	GLN	3.7
1	D	63	GLN	3.7
1	A	193	LEU	3.7
1	D	83	ASP	3.7
1	D	141	GLY	3.7
1	E	866	GLU	3.7
1	A	868	LEU	3.6
1	B	766	GLY	3.6
1	A	92	LEU	3.6
1	D	458	PHE	3.6
1	F	362	PHE	3.6
1	D	688	ALA	3.6
1	A	407	ASP	3.6
1	B	770	LYS	3.6
1	A	486	LEU	3.6
1	D	764	ASP	3.6
1	F	712	MET	3.6
1	D	852	PRO	3.6
1	C	69	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	488	LEU	3.6
1	A	242	SER	3.6
1	D	1042	HIS	3.6
1	A	679	GLY	3.6
1	A	372	VAL	3.5
1	D	767	ARG	3.5
1	F	770	LYS	3.5
1	D	404	LEU	3.5
1	A	210	GLN	3.5
1	E	405	LEU	3.5
1	E	867	ARG	3.5
1	F	103	ALA	3.5
1	D	390	ILE	3.5
1	E	182	TYR	3.5
1	B	291	ILE	3.5
1	B	701	GLN	3.5
1	B	733	GLN	3.5
1	B	801	PHE	3.5
1	B	462	SER	3.5
1	F	807	SER	3.5
1	C	388	PHE	3.5
1	E	37	THR	3.5
1	C	59	ASP	3.5
1	F	3	ASN	3.5
1	D	833	PRO	3.5
1	E	789	TRP	3.5
1	B	691	GLY	3.5
1	F	621	GLY	3.5
1	A	470	PHE	3.5
1	C	801	PHE	3.5
1	A	181	GLN	3.4
1	F	306	ILE	3.4
1	F	445	ILE	3.4
1	E	367	ILE	3.4
1	F	96	SER	3.4
1	F	83	ASP	3.4
1	F	638	PRO	3.4
1	E	29	LYS	3.4
1	E	720	GLY	3.4
1	A	376	LEU	3.4
1	E	250	LEU	3.4
1	A	79	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	731	ILE	3.4
1	A	762	PHE	3.4
1	E	87	THR	3.4
1	B	791	VAL	3.4
1	E	177	LEU	3.4
1	B	719	ASN	3.4
1	A	770	LYS	3.4
1	E	926	TYR	3.3
1	C	791	VAL	3.3
1	D	729	ILE	3.3
1	A	339	GLU	3.3
1	C	244	GLU	3.3
1	F	259	ARG	3.3
1	A	180	SER	3.3
1	A	403	GLY	3.3
1	E	791	VAL	3.3
1	F	871	ASN	3.3
1	D	35	TYR	3.3
1	A	183	ALA	3.3
1	D	769	LYS	3.3
1	C	448	VAL	3.3
1	A	207	ILE	3.3
1	A	250	LEU	3.3
1	B	852	PRO	3.3
1	F	443	VAL	3.3
1	B	621	GLY	3.3
1	A	404	LEU	3.3
1	F	82	SER	3.3
1	A	244	GLU	3.3
1	D	60	THR	3.3
1	F	563	PHE	3.2
1	A	678	THR	3.2
1	C	498	LYS	3.2
1	D	248	LYS	3.2
1	D	801	PHE	3.2
1	F	746	ILE	3.2
1	F	449	LEU	3.2
1	F	945	ILE	3.2
1	A	246	PHE	3.2
1	C	831	ALA	3.2
1	F	868	LEU	3.2
1	D	334	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	995	ALA	3.2
1	C	867	ARG	3.2
1	C	166	ILE	3.2
1	C	839	GLU	3.2
1	D	854	GLY	3.2
1	D	770	LYS	3.1
1	A	316	PHE	3.1
1	B	806	SER	3.1
1	C	80	SER	3.1
1	C	303	ALA	3.1
1	F	806	SER	3.1
1	D	960	LEU	3.1
1	C	83	ASP	3.1
1	D	463	THR	3.1
1	D	858	ASP	3.1
1	F	398	MET	3.1
1	D	247	GLY	3.1
1	D	615	PHE	3.1
1	F	733	GLN	3.1
1	B	768	VAL	3.1
1	B	690	LEU	3.1
1	F	921	LEU	3.1
1	B	412	VAL	3.1
1	E	773	VAL	3.1
1	A	763	ILE	3.1
1	D	977	MET	3.1
1	E	145	THR	3.1
1	C	400	LEU	3.1
1	D	838	GLY	3.1
1	D	721	LEU	3.1
1	E	240	LEU	3.1
1	F	409	ALA	3.0
1	A	343	THR	3.0
1	E	369	THR	3.0
1	F	768	VAL	3.0
1	D	321	LEU	3.0
1	D	857	TYR	3.0
1	F	246	PHE	3.0
1	D	713	LEU	3.0
1	D	401	ALA	3.0
1	A	408	ASP	3.0
1	D	462	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	392	THR	3.0
1	F	315	PRO	3.0
1	B	758	TYR	3.0
1	D	310	LEU	3.0
1	F	193	LEU	3.0
1	F	789	TRP	3.0
1	F	474	ILE	3.0
1	E	137	LEU	3.0
1	D	30	LEU	3.0
1	C	941	ASN	3.0
1	B	851	LEU	3.0
1	F	473	THR	3.0
1	D	383	LEU	2.9
1	F	407	ASP	2.9
1	A	29	LYS	2.9
1	F	829	GLY	2.9
1	F	400	LEU	2.9
1	E	317	PHE	2.9
1	E	617	PHE	2.9
1	E	806	SER	2.9
1	F	888	LEU	2.9
1	B	307	ARG	2.9
1	B	410	ILE	2.9
1	E	184	MET	2.9
1	F	892	TYR	2.9
1	F	166	ILE	2.9
1	A	31	PRO	2.9
1	F	242	SER	2.9
1	B	105	VAL	2.9
1	C	768	VAL	2.9
1	E	982	PHE	2.9
1	E	892	TYR	2.9
1	F	356	TYR	2.9
1	B	876	LEU	2.9
1	E	934	THR	2.9
1	F	55	LYS	2.9
1	C	390	ILE	2.9
1	B	240	LEU	2.9
1	F	69	MET	2.9
1	B	400	LEU	2.8
1	E	92	LEU	2.8
1	E	193	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	729	ILE	2.8
1	B	615	PHE	2.8
1	D	749	THR	2.8
1	A	976	LEU	2.8
1	E	821	GLY	2.8
1	E	204	ILE	2.8
1	D	246	PHE	2.8
1	E	763	ILE	2.8
1	F	396	PHE	2.8
1	B	121	GLU	2.8
1	B	842	GLU	2.8
1	B	836	SER	2.8
1	D	325	TYR	2.8
1	C	832	ALA	2.8
1	A	179	GLY	2.8
1	A	996	GLY	2.8
1	B	488	LEU	2.8
1	D	493	CYS	2.8
1	F	679	GLY	2.8
1	C	763	ILE	2.8
1	D	1037	ASN	2.8
1	E	618	ALA	2.8
1	A	617	PHE	2.8
1	F	839	GLU	2.8
1	C	822	LEU	2.8
1	F	814	PRO	2.8
1	F	759	VAL	2.8
1	F	773	VAL	2.8
1	B	461	GLY	2.8
1	C	840	ALA	2.8
1	E	86	GLY	2.8
1	A	315	PRO	2.8
1	B	396	PHE	2.8
1	E	207	ILE	2.7
1	E	786	ILE	2.7
1	B	312	LYS	2.7
1	D	759	VAL	2.7
1	A	62	THR	2.7
1	C	618	ALA	2.7
1	F	107	VAL	2.7
1	E	743	ILE	2.7
1	D	624	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	59	ASP	2.7
1	F	405	LEU	2.7
1	F	444	GLY	2.7
1	C	855	VAL	2.7
1	C	620	ARG	2.7
1	E	270	LEU	2.7
1	A	899	PHE	2.7
1	A	368	PRO	2.7
1	E	859	TRP	2.7
1	E	714	THR	2.7
1	D	708	LYS	2.7
1	D	771	VAL	2.7
1	D	102	ILE	2.7
1	D	324	VAL	2.7
1	D	85	THR	2.7
1	D	681	ASP	2.7
1	D	714	THR	2.7
1	D	182	TYR	2.7
1	C	888	LEU	2.7
1	C	398	MET	2.7
1	D	715	SER	2.7
1	C	789	TRP	2.7
1	C	871	ASN	2.7
1	D	982	PHE	2.7
1	F	470	PHE	2.7
1	B	531	VAL	2.7
1	C	300	LEU	2.6
1	E	888	LEU	2.6
1	D	243	THR	2.6
1	E	837	THR	2.6
1	B	534	ILE	2.6
1	D	403	GLY	2.6
1	C	207	ILE	2.6
1	C	499	PRO	2.6
1	E	198	LEU	2.6
1	A	411	VAL	2.6
1	D	761	ASP	2.6
1	F	91	THR	2.6
1	E	249	ILE	2.6
1	C	502	LYS	2.6
1	F	764	ASP	2.6
1	A	853	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	207	ILE	2.6
1	C	406	VAL	2.6
1	D	677	ALA	2.6
1	C	263	ARG	2.6
1	C	762	PHE	2.6
1	E	309	GLU	2.6
1	F	920	GLY	2.6
1	A	712	MET	2.6
1	D	48	SER	2.6
1	C	851	LEU	2.6
1	C	760	ASN	2.6
1	B	815	ARG	2.6
1	D	11	PHE	2.6
1	F	56	THR	2.6
1	A	791	VAL	2.6
1	E	406	VAL	2.6
1	F	715	SER	2.6
1	B	623	ASN	2.6
1	A	91	THR	2.6
1	A	874	PRO	2.6
1	B	355	MET	2.6
1	B	80	SER	2.6
1	D	701	GLN	2.6
1	E	26	ALA	2.6
1	F	325	TYR	2.6
1	A	852	PRO	2.6
1	C	442	LEU	2.6
1	B	104	GLN	2.5
1	C	829	GLY	2.5
1	F	245	GLU	2.5
1	B	184	MET	2.5
1	F	784	ASP	2.5
1	E	1020	PHE	2.5
1	B	926	TYR	2.5
1	E	383	LEU	2.5
1	C	410	ILE	2.5
1	D	762	PHE	2.5
1	D	605	ASN	2.5
1	D	789	TRP	2.5
1	C	306	ILE	2.5
1	B	784	ASP	2.5
1	E	784	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	773	VAL	2.5
1	E	925	VAL	2.5
1	F	502	LYS	2.5
1	A	300	LEU	2.5
1	A	449	LEU	2.5
1	C	445	ILE	2.5
1	B	460	GLY	2.5
1	E	272	GLY	2.5
1	C	828	LEU	2.5
1	F	293	LEU	2.5
1	D	671	ILE	2.5
1	F	641	GLU	2.5
1	E	239	ARG	2.5
1	E	1007	VAL	2.5
1	B	859	TRP	2.5
1	C	362	PHE	2.5
1	F	93	THR	2.5
1	A	771	VAL	2.5
1	A	864	TYR	2.5
1	C	54	ALA	2.5
1	C	322	LYS	2.5
1	A	278	ILE	2.5
1	F	314	GLU	2.5
1	A	87	THR	2.5
1	C	321	LEU	2.5
1	C	473	THR	2.5
1	D	486	LEU	2.4
1	F	605	ASN	2.4
1	B	244	GLU	2.4
1	B	439	GLN	2.4
1	D	687	GLN	2.4
1	E	798	MET	2.4
1	D	621	GLY	2.4
1	F	766	GLY	2.4
1	B	694	LYS	2.4
1	C	210	GLN	2.4
1	E	63	GLN	2.4
1	A	953	MET	2.4
1	E	816	LEU	2.4
1	B	807	SER	2.4
1	D	617	PHE	2.4
1	C	315	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	773	VAL	2.4
1	D	712	MET	2.4
1	E	246	PHE	2.4
1	F	178	PHE	2.4
1	F	65	ILE	2.4
1	B	642	ASN	2.4
1	E	348	ILE	2.4
1	B	697	GLN	2.4
1	E	717	ARG	2.4
1	F	241	THR	2.4
1	A	323	ILE	2.4
1	D	270	LEU	2.4
1	F	944	LEU	2.4
1	D	678	THR	2.4
1	E	388	PHE	2.4
1	D	125	GLN	2.4
1	E	395	MET	2.4
1	A	837	THR	2.4
1	D	809	TRP	2.4
1	C	1011	MET	2.4
1	D	82	SER	2.4
1	F	372	VAL	2.4
1	D	200	PRO	2.4
1	F	47	ALA	2.4
1	A	249	ILE	2.4
1	A	713	LEU	2.4
1	C	615	PHE	2.4
1	D	733	GLN	2.4
1	F	453	PHE	2.4
1	C	493	CYS	2.4
1	A	786	ILE	2.4
1	D	763	ILE	2.4
1	A	790	TYR	2.3
1	B	323	ILE	2.3
1	C	308	ALA	2.3
1	A	43	VAL	2.3
1	E	330	THR	2.3
1	B	616	GLY	2.3
1	A	162	MET	2.3
1	A	839	GLU	2.3
1	F	383	LEU	2.3
1	F	404	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	62	THR	2.3
1	D	358	PHE	2.3
1	E	295	THR	2.3
1	A	48	SER	2.3
1	C	449	LEU	2.3
1	A	355	MET	2.3
1	B	183	ALA	2.3
1	B	921	LEU	2.3
1	E	706	ALA	2.3
1	E	129	VAL	2.3
1	E	208	LYS	2.3
1	E	621	GLY	2.3
1	C	772	TYR	2.3
1	D	706	ALA	2.3
1	D	976	LEU	2.3
1	E	278	ILE	2.3
1	A	399	VAL	2.3
1	F	482	VAL	2.3
1	E	496	MET	2.3
1	E	815	ARG	2.3
1	A	1037	ASN	2.3
1	E	733	GLN	2.3
1	D	385	ALA	2.3
1	D	926	TYR	2.3
1	A	838	GLY	2.3
1	A	241	THR	2.3
1	C	605	ASN	2.3
1	D	618	ALA	2.3
1	A	398	MET	2.3
1	B	434	SER	2.3
1	A	182	TYR	2.3
1	E	804	PHE	2.3
1	E	993	THR	2.3
1	E	1022	VAL	2.3
1	E	462	SER	2.3
1	D	773	VAL	2.3
1	E	384	ALA	2.3
1	E	767	ARG	2.3
1	C	783	PRO	2.3
1	A	680	PHE	2.3
1	C	389	SER	2.3
1	A	706	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	173	GLY	2.3
1	A	764	ASP	2.3
1	A	72	ILE	2.3
1	A	445	ILE	2.3
1	D	67	GLN	2.3
1	B	844	MET	2.2
1	F	463	THR	2.2
1	C	9	PRO	2.2
1	E	898	PRO	2.2
1	A	982	PHE	2.2
1	B	771	VAL	2.2
1	B	805	SER	2.2
1	B	207	ILE	2.2
1	A	482	VAL	2.2
1	F	32	VAL	2.2
1	F	877	TYR	2.2
1	C	481	SER	2.2
1	F	869	SER	2.2
1	C	270	LEU	2.2
1	B	841	MET	2.2
1	D	830	GLN	2.2
1	F	790	TYR	2.2
1	B	250	LEU	2.2
1	B	94	PHE	2.2
1	A	85	THR	2.2
1	A	645	GLU	2.2
1	E	901	VAL	2.2
1	F	817	GLU	2.2
1	B	837	THR	2.2
1	E	391	ASN	2.2
1	B	762	PHE	2.2
1	B	689	GLY	2.2
1	E	839	GLU	2.2
1	E	36	PRO	2.2
1	B	310	LEU	2.2
1	B	695	LEU	2.2
1	E	83	ASP	2.2
1	E	495	THR	2.2
1	C	619	GLY	2.2
1	E	766	GLY	2.2
1	E	304	ALA	2.2
1	F	874	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	81	ASN	2.2
1	A	27	ILE	2.2
1	B	1003	VAL	2.2
1	D	64	VAL	2.2
1	D	207	ILE	2.2
1	F	462	SER	2.2
1	C	761	ASP	2.2
1	A	410	ILE	2.2
1	C	93	THR	2.2
1	C	417	GLU	2.2
1	E	85	THR	2.2
1	F	85	THR	2.2
1	A	833	PRO	2.2
1	A	689	GLY	2.2
1	C	248	LYS	2.2
1	B	739	LEU	2.1
1	E	300	LEU	2.1
1	F	250	LEU	2.1
1	D	336	SER	2.1
1	D	65	ILE	2.1
1	B	816	LEU	2.1
1	E	719	ASN	2.1
1	B	982	PHE	2.1
1	C	458	PHE	2.1
1	E	316	PHE	2.1
1	A	946	VAL	2.1
1	B	50	PRO	2.1
1	C	759	VAL	2.1
1	F	102	ILE	2.1
1	B	465	ALA	2.1
1	C	325	TYR	2.1
1	F	248	LYS	2.1
1	F	500	ILE	2.1
1	B	435	MET	2.1
1	E	299	ALA	2.1
1	E	727	PHE	2.1
1	A	716	VAL	2.1
1	B	63	GLN	2.1
1	E	65	ILE	2.1
1	F	10	ILE	2.1
1	A	690	LEU	2.1
1	D	822	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	636	ASP	2.1
1	A	385	ALA	2.1
1	A	842	GLU	2.1
1	C	38	ILE	2.1
1	F	964	THR	2.1
1	D	865	GLN	2.1
1	E	48	SER	2.1
1	A	178	PHE	2.1
1	F	307	ARG	2.1
1	C	1038	GLU	2.1
1	B	369	THR	2.1
1	E	624	THR	2.1
1	A	270	LEU	2.1
1	F	440	GLY	2.1
1	C	617	PHE	2.1
1	D	727	PHE	2.1
1	F	866	GLU	2.1
1	C	399	VAL	2.1
1	E	106	GLN	2.1
1	B	49	TYR	2.1
1	C	57	VAL	2.1
1	E	708	LYS	2.1
1	F	925	VAL	2.1
1	A	619	GLY	2.1
1	B	960	LEU	2.1
1	B	413	VAL	2.1
1	E	385	ALA	2.1
1	F	183	ALA	2.1
1	D	233	SER	2.1
1	D	81	ASN	2.1
1	D	61	VAL	2.1
1	A	310	LEU	2.1
1	C	240	LEU	2.1
1	C	675	GLY	2.1
1	D	79	SER	2.1
1	D	691	GLY	2.1
1	F	408	ASP	2.1
1	D	758	TYR	2.0
1	B	472	ILE	2.0
1	D	90	ILE	2.0
1	F	739	LEU	2.0
1	A	386	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	439	GLN	2.0
1	D	140	VAL	2.0
1	F	933	THR	2.0
1	B	67	GLN	2.0
1	E	641	GLU	2.0
1	E	325	TYR	2.0
1	B	487	ILE	2.0
1	E	262	LEU	2.0
1	F	100	ALA	2.0
1	B	922	THR	2.0
1	D	179	GLY	2.0
1	E	994	GLY	2.0
1	D	78	MET	2.0
1	F	95	GLU	2.0
1	D	1039	ASP	2.0
1	B	769	LYS	2.0
1	E	843	LEU	2.0
1	F	118	LEU	2.0
1	A	136	PHE	2.0
1	A	184	MET	2.0
1	C	317	PHE	2.0
1	E	833	PRO	2.0
1	B	817	GLU	2.0
1	E	125	GLN	2.0
1	B	289	LEU	2.0
1	C	674	LEU	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	LMT	F	1101	35/35	0.88	0.58	2.80	35,82,93,99	0
2	LMT	B	1101	35/35	0.81	0.52	2.26	58,82,95,98	0
2	LMT	D	1101	35/35	0.83	0.38	1.71	38,77,87,92	0
2	LMT	E	1101	35/35	0.76	0.51	1.54	54,94,105,108	0
2	LMT	A	1101	35/35	0.85	0.40	1.34	62,71,84,86	0
2	LMT	C	1101	35/35	0.83	0.35	0.74	30,75,84,93	0
3	NI	C	1102	1/1	0.96	0.22	-	80,80,80,80	0
3	NI	E	1102	1/1	0.96	0.13	-	96,96,96,96	0
3	NI	A	1102	1/1	0.99	0.12	-	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.