



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:05 PM GMT

PDB ID : 4QSL
Title : Crystal Structure of Listeria Monocytogenes Pyruvate Carboxylase
Authors : Choi, P.H.; Tong, L.
Deposited on : 2014-07-04
Resolution : 3.28 Å(reported)

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

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

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

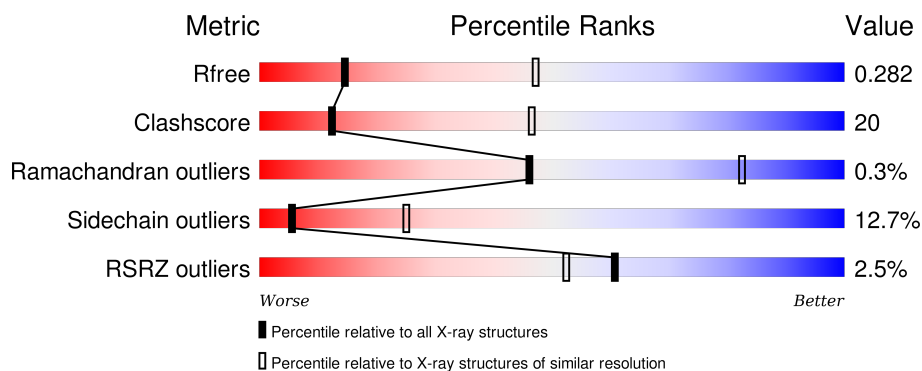
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1756 (3.36-3.20)
Clashscore	102246	1941 (3.36-3.20)
Ramachandran outliers	100387	1905 (3.36-3.20)
Sidechain outliers	100360	1903 (3.36-3.20)
RSRZ outliers	91569	1764 (3.36-3.20)

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	1146	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>28%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	1146	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>26%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	1146	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>25%</div> <div>•</div> <div>18%</div> </div> </div>
1	D	1146	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>27%</div> <div>5%</div> <div>10%</div> </div> </div>
1	E	1146	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>26%</div> <div>•</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	1146	<div><div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>59%28%8%</div></div></div>
1	G	1146	<div><div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>53%25%18%</div></div></div>
1	H	1146	<div><div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>57%28%5%10%</div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 60495 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.

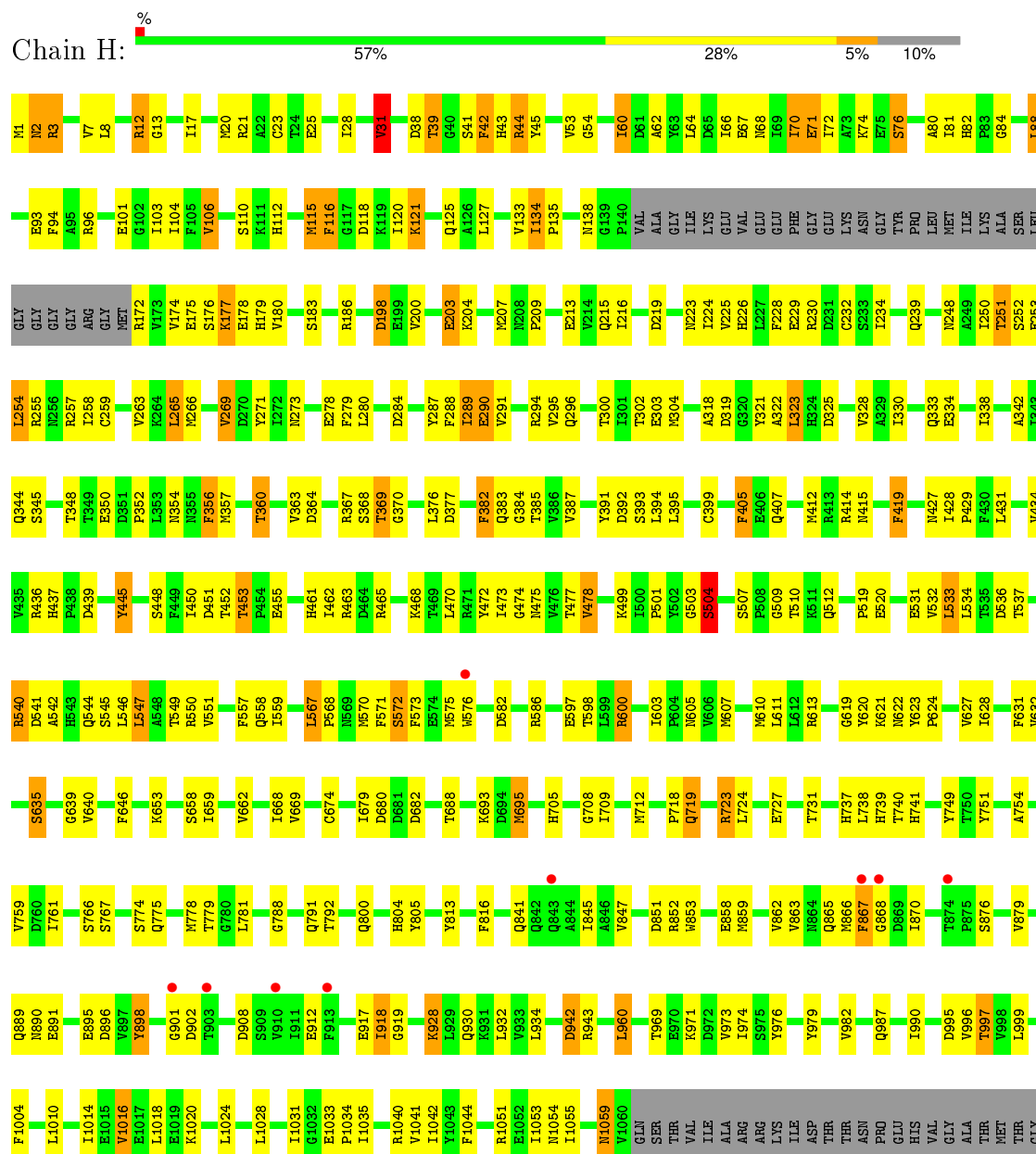
- Molecule 1 is a protein called Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	1029	Total	C	N	O	S	0	0	0
			7881	4992	1351	1504	34			
1	F	1052	Total	C	N	O	S	0	0	0
			7969	5063	1353	1518	35			
1	E	1031	Total	C	N	O	S	0	0	0
			7492	4716	1292	1459	25			
1	G	942	Total	C	N	O	S	0	0	0
			6909	4338	1202	1341	28			
1	D	1029	Total	C	N	O	S	0	0	0
			7881	4992	1351	1504	34			
1	A	1052	Total	C	N	O	S	0	0	0
			7969	5063	1353	1518	35			
1	B	1031	Total	C	N	O	S	0	0	0
			7492	4716	1292	1459	25			
1	C	941	Total	C	N	O	S	0	0	0
			6902	4333	1201	1340	28			

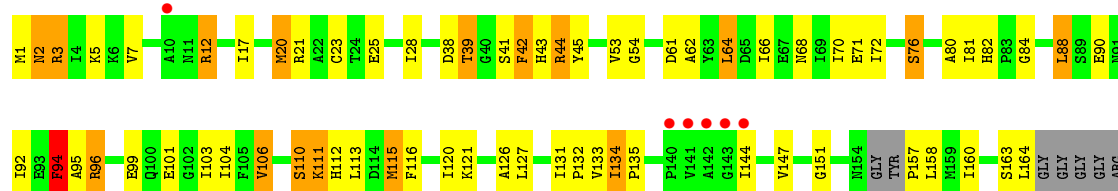
3 Residue-property plots

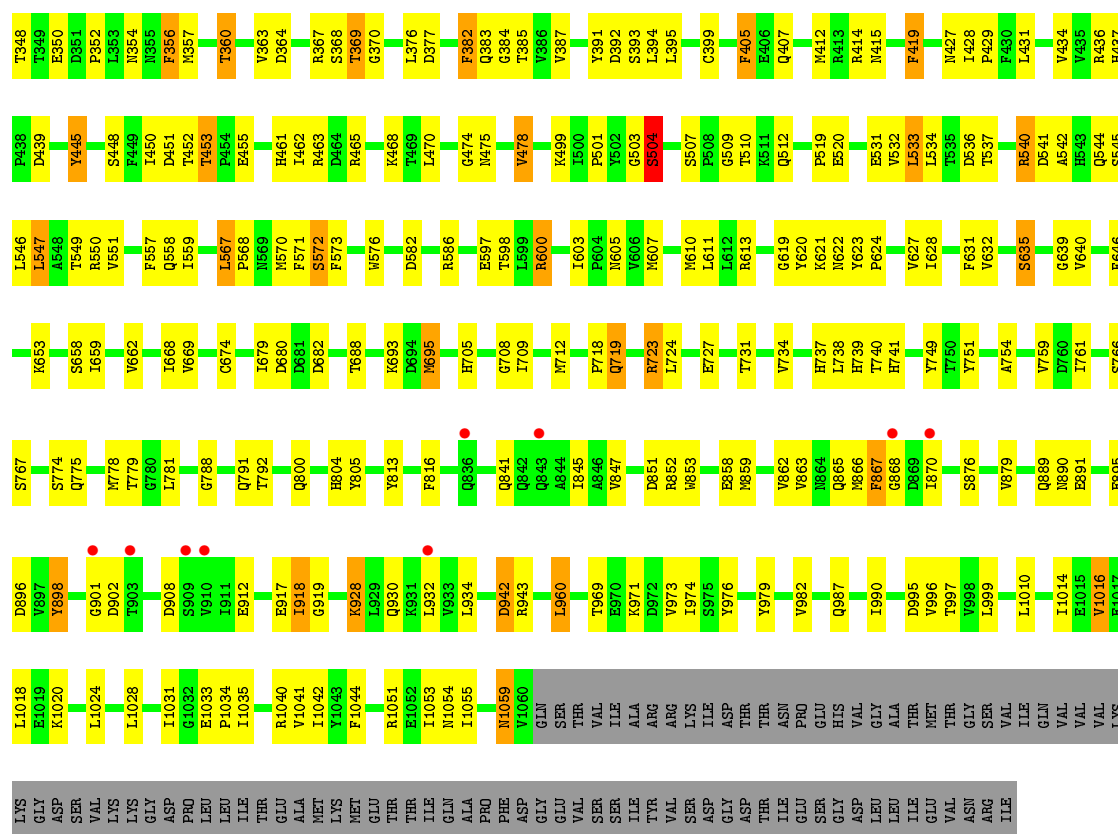
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Pyruvate carboxylase

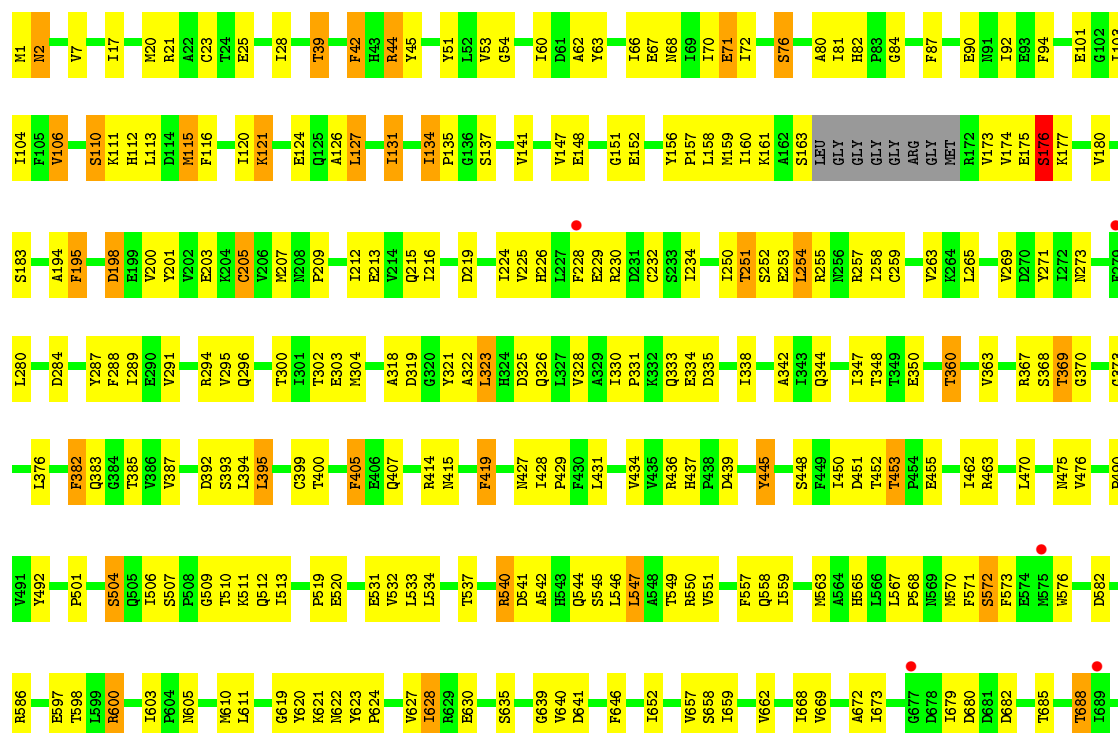


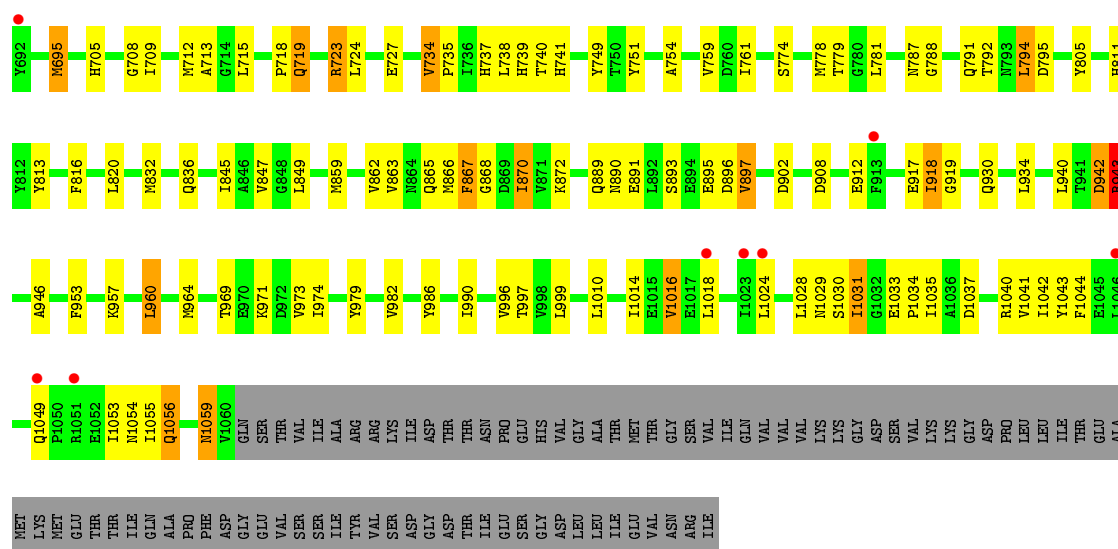




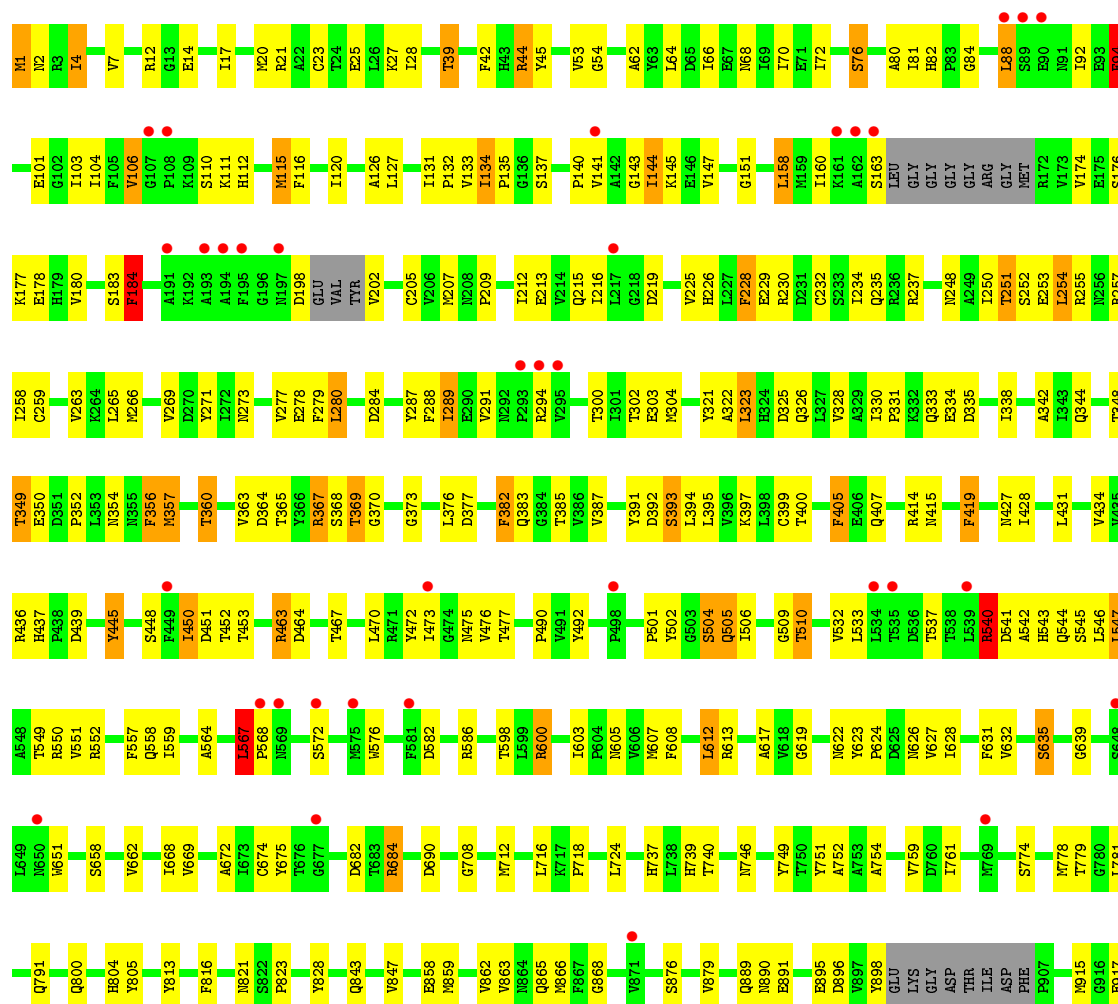


• Molecule 1: Pyruvate carboxylase

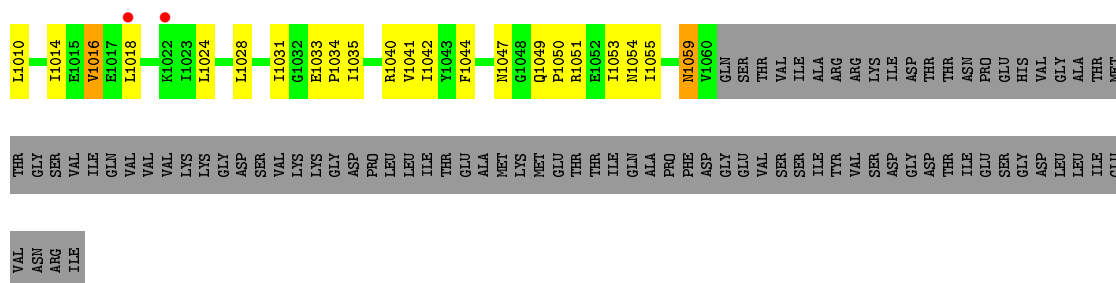




• Molecule 1: Pyruvate carboxylase







4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.36Å 132.62Å 257.54Å 86.65° 79.84° 70.07°	Depositor
Resolution (Å)	47.16 – 3.28 47.11 – 3.28	Depositor EDS
% Data completeness (in resolution range)	88.9 (47.16-3.28) 88.4 (47.11-3.28)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.238 , 0.284 0.235 , 0.282	Depositor DCC
R_{free} test set	7628 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	116.2	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 86.7	EDS
Estimated twinning fraction	0.398 for h,h-k,h-l 0.007 for -h,-h+k,-l 0.007 for -h,-k,-h+l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 151833 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	60495	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.46	0/8136	0.74	5/11083 (0.0%)
1	B	0.45	0/7639	0.72	7/10443 (0.1%)
1	C	0.46	0/7031	0.73	6/9586 (0.1%)
1	D	0.47	0/8042	0.74	9/10933 (0.1%)
1	E	0.45	0/7639	0.72	9/10443 (0.1%)
1	F	0.46	0/8136	0.74	6/11083 (0.1%)
1	G	0.47	0/7039	0.73	6/9597 (0.1%)
1	H	0.48	0/8042	0.74	9/10933 (0.1%)
All	All	0.46	0/61704	0.73	57/84101 (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	D	0	1
1	F	0	1
1	H	0	1
All	All	0	3

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	115	MET	CA-CB-CG	8.11	127.09	113.30
1	H	115	MET	CA-CB-CG	8.08	127.04	113.30
1	G	690	ASP	CB-CG-OD1	7.87	125.38	118.30
1	C	690	ASP	CB-CG-OD1	7.80	125.32	118.30
1	H	478	VAL	CB-CA-C	-7.79	96.61	111.40
1	D	478	VAL	CB-CA-C	-7.27	97.59	111.40
1	A	943	ARG	NE-CZ-NH2	-7.19	116.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	943	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	B	184	PHE	N-CA-CB	6.50	122.31	110.60
1	E	184	PHE	N-CA-CB	6.50	122.29	110.60
1	E	4	ILE	CG1-CB-CG2	-6.41	97.30	111.40
1	F	943	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	H	478	VAL	CA-CB-CG2	6.38	120.46	110.90
1	A	628	ILE	CG1-CB-CG2	-6.34	97.45	111.40
1	B	4	ILE	CG1-CB-CG2	-6.32	97.49	111.40
1	F	628	ILE	CG1-CB-CG2	-6.32	97.50	111.40
1	D	478	VAL	CA-CB-CG2	6.24	120.26	110.90
1	A	943	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	H	367	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	D	367	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	C	96	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	G	94	PHE	CB-CG-CD1	6.13	125.09	120.80
1	H	31	VAL	CB-CA-C	-6.11	99.79	111.40
1	C	94	PHE	CB-CG-CD1	6.04	125.03	120.80
1	D	31	VAL	CB-CA-C	-5.95	100.09	111.40
1	E	94	PHE	CB-CG-CD1	5.91	124.94	120.80
1	B	450	ILE	CA-CB-CG1	5.89	122.19	111.00
1	A	1029	ASN	N-CA-CB	5.87	121.16	110.60
1	E	540	ARG	CG-CD-NE	5.86	124.10	111.80
1	B	94	PHE	CB-CG-CD1	5.85	124.90	120.80
1	F	1029	ASN	N-CA-CB	5.85	121.13	110.60
1	C	588	LEU	CB-CG-CD1	-5.85	101.06	111.00
1	D	695	MET	CG-SD-CE	5.74	109.38	100.20
1	G	588	LEU	CB-CG-CD1	-5.72	101.28	111.00
1	G	96	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	H	695	MET	CG-SD-CE	5.67	109.27	100.20
1	H	115	MET	N-CA-CB	-5.55	100.61	110.60
1	H	960	LEU	CB-CG-CD2	5.53	120.40	111.00
1	D	115	MET	N-CA-CB	-5.51	100.68	110.60
1	B	463	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	960	LEU	CB-CG-CD2	5.36	120.11	111.00
1	C	690	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	H	567	LEU	CB-CG-CD2	5.35	120.09	111.00
1	E	144	ILE	CB-CA-C	-5.33	100.95	111.60
1	G	690	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	B	540	ARG	CG-CD-NE	5.29	122.91	111.80
1	D	567	LEU	CB-CG-CD2	5.27	119.95	111.00
1	F	1056	GLN	N-CA-CB	5.21	119.97	110.60
1	A	1056	GLN	N-CA-CB	5.19	119.94	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	94	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	E	463	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	G	94	PHE	CB-CG-CD2	-5.09	117.24	120.80
1	E	567	LEU	CA-CB-CG	5.08	126.99	115.30
1	B	567	LEU	CA-CB-CG	5.07	126.96	115.30
1	E	143	GLY	N-CA-C	5.07	125.77	113.10
1	F	159	MET	CG-SD-CE	5.05	108.28	100.20
1	C	832	MET	CG-SD-CE	5.01	108.22	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	504	SER	Peptide
1	F	504	SER	Peptide
1	H	504	SER	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	7969	0	7573	289	0
1	B	7492	0	6807	324	0
1	C	6902	0	6371	288	0
1	D	7881	0	7579	288	0
1	E	7492	0	6807	311	0
1	F	7969	0	7573	299	0
1	G	6909	0	6379	282	0
1	H	7881	0	7579	298	0
All	All	60495	0	56668	2299	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (2299) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:SER:OG	1:D:412:MET:CE	1.67	1.40
1:H:345:SER:OG	1:H:412:MET:CE	1.68	1.39
1:E:280:LEU:HD12	1:E:289:ILE:CG2	1.54	1.37
1:B:280:LEU:HD12	1:B:289:ILE:CG2	1.55	1.37
1:B:279:PHE:N	1:B:289:ILE:HD11	1.37	1.36
1:E:279:PHE:N	1:E:289:ILE:HD11	1.39	1.35
1:H:345:SER:OG	1:H:412:MET:HE1	1.21	1.25
1:D:345:SER:OG	1:D:412:MET:HE1	1.21	1.24
1:E:180:VAL:HG12	1:E:184:PHE:CZ	1.72	1.23
1:E:144:ILE:HG22	1:E:184:PHE:CE2	1.78	1.19
1:B:279:PHE:CA	1:B:289:ILE:HD11	1.71	1.18
1:E:14:GLU:OE2	1:E:397:LYS:CE	1.91	1.17
1:E:279:PHE:CA	1:E:289:ILE:HD11	1.72	1.17
1:B:180:VAL:HG12	1:B:184:PHE:CZ	1.78	1.17
1:B:14:GLU:OE2	1:B:397:LYS:CE	1.91	1.17
1:B:279:PHE:CA	1:B:289:ILE:CD1	2.22	1.15
1:B:612:LEU:HD11	1:B:617:ALA:HA	1.20	1.15
1:E:612:LEU:HD11	1:E:617:ALA:HA	1.20	1.15
1:E:279:PHE:CA	1:E:289:ILE:CD1	2.23	1.14
1:G:960:LEU:HD12	1:G:968:PRO:HG3	1.25	1.13
1:C:960:LEU:HD12	1:C:968:PRO:HG3	1.25	1.13
1:D:254:LEU:HD22	1:D:258:ILE:HD11	1.32	1.11
1:H:254:LEU:HD22	1:H:258:ILE:HD11	1.32	1.11
1:E:280:LEU:HD12	1:E:289:ILE:HG21	1.13	1.10
1:B:280:LEU:HD12	1:B:289:ILE:HG21	1.13	1.10
1:G:61:ASP:HA	1:G:64:LEU:HD12	1.29	1.09
1:C:61:ASP:HA	1:C:64:LEU:HD12	1.29	1.09
1:D:8:LEU:HA	1:D:31:VAL:HG23	1.24	1.09
1:H:8:LEU:HA	1:H:31:VAL:HG23	1.23	1.09
1:B:144:ILE:HG22	1:B:184:PHE:CE2	1.87	1.08
1:B:158:LEU:HD13	1:B:174:VAL:HB	1.30	1.07
1:B:612:LEU:CD1	1:B:617:ALA:HA	1.86	1.03
1:E:612:LEU:CD1	1:E:617:ALA:HA	1.87	1.03
1:D:345:SER:OG	1:D:412:MET:HE3	1.53	1.02
1:C:164:LEU:HA	1:C:195:PHE:HE1	1.22	1.02
1:H:345:SER:OG	1:H:412:MET:HE3	1.54	1.01
1:E:279:PHE:C	1:E:289:ILE:CD1	2.29	1.01
1:B:279:PHE:C	1:B:289:ILE:CD1	2.29	1.01
1:A:219:ASP:HB3	1:A:323:LEU:HD23	1.42	1.01
1:E:219:ASP:HB3	1:E:323:LEU:HD23	1.43	1.01
1:B:219:ASP:HB3	1:B:323:LEU:HD23	1.43	1.01
1:E:144:ILE:HG22	1:E:184:PHE:CZ	1.96	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:369:THR:OG1	1:F:415:ASN:ND2	1.94	1.00
1:A:369:THR:OG1	1:A:415:ASN:ND2	1.94	1.00
1:F:219:ASP:HB3	1:F:323:LEU:HD23	1.44	1.00
1:G:219:ASP:HB3	1:G:323:LEU:HD23	1.42	0.99
1:G:576:TRP:HE1	1:G:596:LEU:HB2	1.27	0.99
1:A:156:TYR:O	1:A:176:SER:HB2	1.61	0.99
1:E:144:ILE:CG2	1:E:184:PHE:CE2	2.44	0.99
1:F:126:ALA:O	1:F:131:ILE:CD1	2.10	0.99
1:C:219:ASP:HB3	1:C:323:LEU:HD23	1.43	0.99
1:C:576:TRP:HE1	1:C:596:LEU:HB2	1.28	0.99
1:G:960:LEU:CD1	1:G:968:PRO:HG3	1.91	0.98
1:C:960:LEU:CD1	1:C:968:PRO:HG3	1.91	0.98
1:H:503:GLY:O	1:C:5:LYS:NZ	1.96	0.98
1:E:915:MET:O	1:E:940:LEU:CB	2.11	0.98
1:A:126:ALA:O	1:A:131:ILE:CD1	2.10	0.98
1:E:280:LEU:CD1	1:E:289:ILE:CG2	2.41	0.98
1:B:280:LEU:CD1	1:B:289:ILE:CG2	2.41	0.98
1:G:367:ARG:HH12	1:G:1049:GLN:CB	1.77	0.97
1:H:219:ASP:HB3	1:H:323:LEU:HD23	1.43	0.97
1:D:369:THR:OG1	1:D:415:ASN:ND2	1.96	0.97
1:C:369:THR:OG1	1:C:415:ASN:ND2	1.98	0.97
1:G:369:THR:OG1	1:G:415:ASN:ND2	1.98	0.97
1:B:158:LEU:HD12	1:B:174:VAL:O	1.64	0.97
1:D:219:ASP:HB3	1:D:323:LEU:HD23	1.44	0.96
1:B:369:THR:OG1	1:B:415:ASN:ND2	1.99	0.96
1:E:369:THR:OG1	1:E:415:ASN:ND2	1.99	0.96
1:F:126:ALA:O	1:F:131:ILE:HD13	1.65	0.96
1:H:369:THR:OG1	1:H:415:ASN:ND2	1.98	0.96
1:A:126:ALA:O	1:A:131:ILE:HD13	1.66	0.96
1:C:367:ARG:HH12	1:C:1049:GLN:CB	1.80	0.95
1:B:14:GLU:OE2	1:B:397:LYS:HE3	1.66	0.95
1:C:164:LEU:HA	1:C:195:PHE:CE1	2.02	0.95
1:C:960:LEU:HD11	1:C:968:PRO:HB3	1.48	0.95
1:G:960:LEU:HD11	1:G:968:PRO:HB3	1.48	0.94
1:E:14:GLU:OE2	1:E:397:LYS:HE3	1.66	0.94
1:E:280:LEU:CD1	1:E:289:ILE:HG21	1.97	0.93
1:E:14:GLU:OE2	1:E:397:LYS:NZ	2.02	0.93
1:E:564:ALA:HB2	1:E:603:ILE:HG22	1.49	0.93
1:B:280:LEU:CD1	1:B:289:ILE:HG21	1.98	0.93
1:B:564:ALA:HB2	1:B:603:ILE:HG22	1.49	0.93
1:B:14:GLU:OE2	1:B:397:LYS:NZ	2.02	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ARG:HD2	1:C:104:ILE:HD11	1.51	0.92
1:G:3:ARG:HD2	1:G:104:ILE:HD11	1.53	0.90
1:D:3:ARG:HD2	1:D:104:ILE:HD11	1.52	0.90
1:B:279:PHE:HA	1:B:289:ILE:HD13	1.50	0.90
1:H:3:ARG:HD2	1:H:104:ILE:HD11	1.52	0.90
1:G:576:TRP:NE1	1:G:596:LEU:HB2	1.86	0.89
1:F:943:ARG:HD3	1:F:946:ALA:HB2	1.55	0.89
1:E:279:PHE:HA	1:E:289:ILE:HD13	1.51	0.89
1:A:943:ARG:HD3	1:A:946:ALA:HB2	1.55	0.89
1:B:279:PHE:CA	1:B:289:ILE:HD13	2.00	0.89
1:B:970:GLU:O	1:B:973:VAL:HG22	1.72	0.89
1:C:576:TRP:NE1	1:C:596:LEU:HB2	1.86	0.89
1:B:279:PHE:HA	1:B:289:ILE:CD1	2.01	0.88
1:E:970:GLU:O	1:E:973:VAL:HG22	1.73	0.88
1:E:279:PHE:CA	1:E:289:ILE:HD13	2.01	0.88
1:B:278:GLU:C	1:B:289:ILE:HD11	1.92	0.88
1:E:279:PHE:HA	1:E:289:ILE:CD1	2.01	0.88
1:C:227:LEU:HD23	1:C:306:THR:HG21	1.55	0.88
1:E:278:GLU:C	1:E:289:ILE:HD11	1.94	0.87
1:A:347:ILE:O	1:A:395:LEU:HD12	1.74	0.86
1:F:347:ILE:O	1:F:395:LEU:HD12	1.74	0.86
1:D:45:TYR:CE1	1:C:1047:ASN:HB3	2.09	0.86
1:G:61:ASP:HA	1:G:64:LEU:CD1	2.05	0.85
1:C:61:ASP:HA	1:C:64:LEU:CD1	2.06	0.85
1:B:279:PHE:N	1:B:289:ILE:CD1	2.32	0.85
1:H:45:TYR:CE1	1:G:1047:ASN:HB3	2.11	0.84
1:E:147:VAL:O	1:E:151:GLY:N	2.09	0.84
1:E:279:PHE:N	1:E:289:ILE:CD1	2.33	0.83
1:E:180:VAL:HG12	1:E:184:PHE:HZ	1.35	0.83
1:B:915:MET:O	1:B:940:LEU:CB	2.26	0.83
1:D:172:ARG:HH12	1:D:186:ARG:CB	1.92	0.83
1:B:101:GLU:HB2	1:B:103:ILE:HD13	1.60	0.82
1:E:101:GLU:HB2	1:E:103:ILE:HD13	1.60	0.82
1:B:180:VAL:HG12	1:B:184:PHE:HZ	1.37	0.82
1:B:144:ILE:HG22	1:B:184:PHE:CZ	2.14	0.82
1:C:227:LEU:CD2	1:C:306:THR:HG21	2.10	0.82
1:E:349:THR:HG22	1:E:393:SER:O	1.80	0.82
1:C:147:VAL:O	1:C:151:GLY:N	2.11	0.81
1:F:51:TYR:CE1	1:E:1021:GLY:HA3	2.15	0.81
1:G:250:ILE:HD11	1:G:255:ARG:HB3	1.62	0.81
1:G:147:VAL:O	1:G:151:GLY:N	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:5:LYS:NZ	1:D:503:GLY:O	2.12	0.81
1:H:172:ARG:HH12	1:H:186:ARG:CB	1.94	0.81
1:H:8:LEU:HA	1:H:31:VAL:CG2	2.08	0.81
1:B:349:THR:HG22	1:B:393:SER:O	1.81	0.81
1:F:673:ILE:HG22	1:F:695:MET:CE	2.11	0.81
1:F:147:VAL:O	1:F:151:GLY:N	2.12	0.80
1:A:147:VAL:O	1:A:151:GLY:N	2.12	0.80
1:C:250:ILE:HD11	1:C:255:ARG:HB3	1.63	0.80
1:A:673:ILE:HG22	1:A:695:MET:CE	2.12	0.80
1:D:8:LEU:HA	1:D:31:VAL:CG2	2.09	0.80
1:D:254:LEU:CD2	1:D:258:ILE:HD11	2.11	0.80
1:H:254:LEU:CD2	1:H:258:ILE:HD11	2.11	0.80
1:G:61:ASP:CA	1:G:64:LEU:HD12	2.12	0.80
1:B:144:ILE:CG2	1:B:184:PHE:CE2	2.64	0.80
1:G:3:ARG:HG3	1:G:319:ASP:OD1	1.82	0.80
1:A:344:GLN:HG3	1:A:399:CYS:SG	2.22	0.80
1:C:61:ASP:CA	1:C:64:LEU:HD12	2.12	0.80
1:G:219:ASP:HB3	1:G:323:LEU:CD2	2.12	0.80
1:C:3:ARG:HG3	1:C:319:ASP:OD1	1.82	0.80
1:E:843:GLN:O	1:E:847:VAL:HG23	1.81	0.80
1:C:344:GLN:HG3	1:C:399:CYS:SG	2.23	0.79
1:E:979:TYR:HB3	1:E:982:VAL:HG22	1.63	0.79
1:H:3:ARG:HG3	1:H:319:ASP:OD1	1.82	0.79
1:B:876:SER:O	1:B:879:VAL:HG12	1.81	0.79
1:B:843:GLN:O	1:B:847:VAL:HG23	1.81	0.79
1:D:3:ARG:HG3	1:D:319:ASP:OD1	1.82	0.79
1:C:66:ILE:O	1:C:70:ILE:HD12	1.83	0.79
1:A:979:TYR:HB3	1:A:982:VAL:HG22	1.65	0.79
1:E:876:SER:O	1:E:879:VAL:HG12	1.82	0.79
1:G:66:ILE:O	1:G:70:ILE:HD12	1.83	0.79
1:C:219:ASP:HB3	1:C:323:LEU:CD2	2.13	0.79
1:B:979:TYR:HB3	1:B:982:VAL:HG22	1.64	0.79
1:F:943:ARG:O	1:F:943:ARG:HG2	1.81	0.79
1:D:344:GLN:HG3	1:D:399:CYS:SG	2.23	0.79
1:A:943:ARG:O	1:A:943:ARG:HG2	1.81	0.78
1:B:72:ILE:O	1:B:76:SER:OG	2.01	0.78
1:C:501:PRO:O	1:C:504:SER:OG	2.01	0.78
1:E:72:ILE:O	1:E:76:SER:OG	2.01	0.78
1:G:344:GLN:HG3	1:G:399:CYS:SG	2.23	0.78
1:F:979:TYR:HB3	1:F:982:VAL:HG22	1.65	0.78
1:A:219:ASP:HB3	1:A:323:LEU:CD2	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:344:GLN:HG3	1:H:399:CYS:SG	2.23	0.78
1:H:876:SER:O	1:H:879:VAL:HG12	1.83	0.78
1:E:344:GLN:HG3	1:E:399:CYS:SG	2.24	0.78
1:F:344:GLN:HG3	1:F:399:CYS:SG	2.24	0.78
1:B:66:ILE:O	1:B:70:ILE:HD12	1.82	0.78
1:E:66:ILE:O	1:E:70:ILE:HD12	1.82	0.78
1:H:510:THR:HG22	1:H:607:MET:SD	2.22	0.78
1:A:66:ILE:O	1:A:70:ILE:HD12	1.82	0.78
1:A:72:ILE:O	1:A:76:SER:OG	2.02	0.78
1:B:219:ASP:HB3	1:B:323:LEU:CD2	2.13	0.78
1:F:986:TYR:CE1	1:F:990:ILE:HD12	2.19	0.78
1:B:344:GLN:HG3	1:B:399:CYS:SG	2.24	0.78
1:F:72:ILE:O	1:F:76:SER:OG	2.02	0.78
1:E:219:ASP:HB3	1:E:323:LEU:CD2	2.13	0.78
1:D:876:SER:O	1:D:879:VAL:HG12	1.83	0.78
1:F:66:ILE:O	1:F:70:ILE:HD12	1.82	0.78
1:H:72:ILE:O	1:H:76:SER:OG	2.01	0.78
1:F:504:SER:HB2	1:F:505:GLN:CG	2.13	0.78
1:D:72:ILE:O	1:D:76:SER:OG	2.01	0.77
1:G:501:PRO:O	1:G:504:SER:OG	2.02	0.77
1:D:219:ASP:HB3	1:D:323:LEU:CD2	2.14	0.77
1:A:986:TYR:CE1	1:A:990:ILE:HD12	2.20	0.77
1:C:540:ARG:NH2	1:C:541:ASP:OD1	2.18	0.77
1:B:160:ILE:HD11	1:B:174:VAL:CG2	2.14	0.77
1:H:219:ASP:HB3	1:H:323:LEU:CD2	2.15	0.77
1:D:510:THR:HG22	1:D:607:MET:SD	2.23	0.77
1:G:72:ILE:O	1:G:76:SER:OG	2.01	0.77
1:E:280:LEU:HD12	1:E:289:ILE:HG23	1.64	0.77
1:F:219:ASP:HB3	1:F:323:LEU:CD2	2.14	0.77
1:B:280:LEU:HD12	1:B:289:ILE:HG23	1.65	0.77
1:C:72:ILE:O	1:C:76:SER:OG	2.02	0.77
1:G:540:ARG:NH2	1:G:541:ASP:OD1	2.18	0.77
1:C:88:LEU:HB3	1:C:94:PHE:HD2	1.50	0.77
1:E:501:PRO:O	1:E:504:SER:OG	2.03	0.77
1:B:160:ILE:HD11	1:B:174:VAL:HG21	1.67	0.76
1:G:526:VAL:O	1:G:529:GLN:N	2.18	0.76
1:C:526:VAL:O	1:C:529:GLN:N	2.18	0.76
1:D:979:TYR:HB3	1:D:982:VAL:HG22	1.64	0.76
1:G:519:PRO:HB2	1:G:705:HIS:NE2	2.00	0.76
1:B:144:ILE:HG22	1:B:184:PHE:CD2	2.21	0.76
1:G:960:LEU:HD11	1:G:968:PRO:CB	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:960:LEU:HD11	1:C:968:PRO:CB	2.15	0.76
1:C:691:TYR:O	1:C:695:MET:HG2	1.85	0.76
1:B:228:PHE:HD2	1:B:338:ILE:HD11	1.50	0.76
1:C:519:PRO:HB2	1:C:705:HIS:NE2	2.00	0.76
1:G:691:TYR:O	1:G:695:MET:HG2	1.85	0.76
1:B:88:LEU:HB3	1:B:94:PHE:HD2	1.50	0.76
1:F:51:TYR:CE1	1:E:1021:GLY:CA	2.69	0.76
1:B:82:HIS:HD2	1:B:84:GLY:H	1.33	0.76
1:G:88:LEU:HB3	1:G:94:PHE:HD2	1.52	0.75
1:E:228:PHE:HD2	1:E:338:ILE:HD11	1.50	0.75
1:A:501:PRO:O	1:A:504:SER:OG	2.04	0.75
1:F:124:GLU:O	1:F:127:LEU:HG	1.86	0.75
1:E:88:LEU:HB3	1:E:94:PHE:HD2	1.51	0.75
1:B:501:PRO:O	1:B:504:SER:OG	2.04	0.75
1:H:979:TYR:HB3	1:H:982:VAL:HG22	1.65	0.75
1:E:82:HIS:HD2	1:E:84:GLY:H	1.34	0.75
1:F:501:PRO:O	1:F:504:SER:OG	2.05	0.75
1:A:51:TYR:CE1	1:B:1021:GLY:HA3	2.21	0.75
1:H:82:HIS:HD2	1:H:84:GLY:H	1.34	0.75
1:G:685:THR:O	1:G:688:THR:HG23	1.87	0.75
1:C:685:THR:O	1:C:688:THR:HG23	1.87	0.74
1:A:124:GLU:O	1:A:127:LEU:HG	1.86	0.74
1:D:82:HIS:HD2	1:D:84:GLY:H	1.35	0.74
1:E:88:LEU:HD12	1:E:94:PHE:CD2	2.23	0.74
1:H:960:LEU:CD1	1:H:976:TYR:CG	2.71	0.74
1:D:45:TYR:CD1	1:C:1047:ASN:HB3	2.22	0.74
1:D:501:PRO:O	1:D:504:SER:OG	2.05	0.74
1:E:800:GLN:O	1:E:804:HIS:ND1	2.20	0.74
1:B:800:GLN:O	1:B:804:HIS:ND1	2.20	0.74
1:B:88:LEU:HD12	1:B:94:PHE:CD2	2.23	0.73
1:D:960:LEU:CD1	1:D:976:TYR:CG	2.71	0.73
1:D:384:GLY:HA3	1:C:1050:PRO:HD3	1.69	0.73
1:D:13:GLY:O	1:D:17:ILE:HD12	1.87	0.73
1:H:13:GLY:O	1:H:17:ILE:HD12	1.87	0.73
1:H:501:PRO:O	1:H:504:SER:OG	2.05	0.73
1:D:800:GLN:O	1:D:804:HIS:ND1	2.20	0.73
1:G:960:LEU:CD1	1:G:968:PRO:CG	2.65	0.73
1:C:960:LEU:CD1	1:C:968:PRO:CG	2.65	0.73
1:D:45:TYR:CE1	1:C:1047:ASN:CB	2.71	0.73
1:F:82:HIS:HD2	1:F:84:GLY:H	1.36	0.73
1:B:141:VAL:HG11	1:B:147:VAL:HG22	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:ALA:O	1:F:131:ILE:HD11	1.87	0.72
1:H:960:LEU:HD13	1:H:976:TYR:CG	2.23	0.72
1:D:960:LEU:HD13	1:D:976:TYR:CG	2.24	0.72
1:A:82:HIS:HD2	1:A:84:GLY:H	1.36	0.72
1:G:227:LEU:HD22	1:G:306:THR:HG21	1.71	0.72
1:F:627:VAL:HG23	1:F:628:ILE:HD12	1.68	0.72
1:B:160:ILE:CD1	1:B:174:VAL:CG2	2.67	0.72
1:B:81:ILE:O	1:B:106:VAL:HG23	1.90	0.72
1:A:627:VAL:HG23	1:A:628:ILE:HD12	1.68	0.72
1:G:175:GLU:HG2	1:G:179:HIS:CD2	2.24	0.72
1:A:156:TYR:O	1:A:176:SER:CB	2.36	0.72
1:H:45:TYR:CD1	1:G:1047:ASN:HB3	2.24	0.72
1:A:126:ALA:O	1:A:131:ILE:HD11	1.88	0.72
1:E:234:ILE:HD11	1:E:445:TYR:CZ	2.25	0.72
1:A:519:PRO:HB2	1:A:705:HIS:NE2	2.05	0.72
1:C:500:ILE:HG21	1:C:565:HIS:CD2	2.24	0.72
1:C:510:THR:OG1	1:C:607:MET:HG3	1.90	0.72
1:E:81:ILE:O	1:E:106:VAL:HG23	1.90	0.72
1:C:228:PHE:CE2	1:C:338:ILE:HG13	2.24	0.72
1:F:519:PRO:HB2	1:F:705:HIS:NE2	2.06	0.71
1:H:519:PRO:HB2	1:H:705:HIS:NE2	2.05	0.71
1:A:234:ILE:HD11	1:A:445:TYR:CZ	2.25	0.71
1:B:990:ILE:HD11	1:B:995:ASP:HA	1.72	0.71
1:G:82:HIS:HD2	1:G:84:GLY:H	1.35	0.71
1:G:127:LEU:HD22	1:G:133:VAL:HG21	1.71	0.71
1:C:82:HIS:HD2	1:C:84:GLY:H	1.35	0.71
1:E:990:ILE:HD11	1:E:995:ASP:HA	1.72	0.71
1:E:279:PHE:C	1:E:289:ILE:HD13	2.08	0.71
1:D:279:PHE:CA	1:D:289:ILE:HD11	2.20	0.71
1:B:158:LEU:CD1	1:B:174:VAL:O	2.38	0.71
1:B:234:ILE:HD11	1:B:445:TYR:CZ	2.25	0.71
1:F:234:ILE:HD11	1:F:445:TYR:CZ	2.26	0.71
1:G:88:LEU:HD12	1:G:94:PHE:CD2	2.25	0.71
1:A:51:TYR:CE1	1:B:1021:GLY:CA	2.74	0.71
1:G:510:THR:OG1	1:G:607:MET:HG3	1.91	0.71
1:H:279:PHE:CA	1:H:289:ILE:HD11	2.21	0.71
1:B:279:PHE:C	1:B:289:ILE:HD13	2.09	0.71
1:H:45:TYR:CE1	1:G:1047:ASN:CB	2.73	0.71
1:F:504:SER:HB2	1:F:505:GLN:HG3	1.73	0.71
1:H:21:ARG:NH2	1:G:418:GLU:OE2	2.23	0.71
1:B:437:HIS:CD2	1:B:439:ASP:H	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:HIS:ND1	1:C:259:CYS:HB3	2.06	0.71
1:F:414:ARG:HD3	1:E:25:GLU:HG3	1.72	0.71
1:D:175:GLU:OE2	1:D:175:GLU:N	2.23	0.71
1:F:511:LYS:HZ3	1:F:641:ASP:CG	1.94	0.71
1:C:88:LEU:HD12	1:C:94:PHE:CD2	2.26	0.70
1:H:234:ILE:HD11	1:H:445:TYR:CZ	2.25	0.70
1:C:127:LEU:HD22	1:C:133:VAL:HG21	1.72	0.70
1:E:437:HIS:CD2	1:E:439:ASP:H	2.08	0.70
1:D:60:ILE:H	1:D:60:ILE:HD13	1.53	0.70
1:E:64:LEU:HD23	1:E:88:LEU:HD23	1.73	0.70
1:H:134:ILE:HD12	1:H:287:TYR:HB3	1.74	0.70
1:H:60:ILE:H	1:H:60:ILE:HD13	1.54	0.70
1:E:14:GLU:OE2	1:E:397:LYS:HE2	1.90	0.70
1:E:157:PRO:O	1:E:158:LEU:HD23	1.92	0.70
1:B:510:THR:OG1	1:B:607:MET:HG3	1.90	0.70
1:B:64:LEU:HD23	1:B:88:LEU:HD23	1.74	0.70
1:F:1010:LEU:HD21	1:F:1031:ILE:HD11	1.74	0.70
1:B:14:GLU:OE2	1:B:397:LYS:HE2	1.90	0.70
1:F:657:VAL:HG22	1:F:943:ARG:NH2	2.06	0.70
1:A:363:VAL:O	1:A:383:GLN:O	2.10	0.70
1:D:519:PRO:HB2	1:D:705:HIS:NE2	2.07	0.70
1:H:64:LEU:HD23	1:H:88:LEU:HD23	1.74	0.70
1:D:234:ILE:HD11	1:D:445:TYR:CZ	2.26	0.70
1:D:370:GLY:O	1:C:21:ARG:NH1	2.25	0.70
1:F:363:VAL:O	1:F:383:GLN:O	2.10	0.69
1:A:657:VAL:HG22	1:A:943:ARG:NH2	2.07	0.69
1:E:82:HIS:HA	1:E:106:VAL:HG23	1.74	0.69
1:B:82:HIS:HA	1:B:106:VAL:HG23	1.74	0.69
1:C:363:VAL:O	1:C:383:GLN:O	2.09	0.69
1:C:234:ILE:HD11	1:C:445:TYR:CZ	2.28	0.69
1:D:64:LEU:HD23	1:D:88:LEU:HD23	1.75	0.69
1:F:657:VAL:HG22	1:F:943:ARG:HH22	1.58	0.69
1:F:134:ILE:HD12	1:F:287:TYR:HB3	1.74	0.69
1:D:363:VAL:O	1:D:383:GLN:O	2.10	0.69
1:A:657:VAL:HG22	1:A:943:ARG:HH22	1.58	0.69
1:A:370:GLY:O	1:B:21:ARG:NH1	2.26	0.69
1:G:363:VAL:O	1:G:383:GLN:O	2.10	0.69
1:E:180:VAL:HG12	1:E:184:PHE:CE1	2.28	0.68
1:D:134:ILE:HD12	1:D:287:TYR:HB3	1.75	0.68
1:H:800:GLN:O	1:H:804:HIS:ND1	2.20	0.68
1:A:863:VAL:HA	1:A:866:MET:HG3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:PRO:O	1:F:158:LEU:HD23	1.93	0.68
1:G:234:ILE:HD11	1:G:445:TYR:CZ	2.28	0.68
1:C:279:PHE:N	1:C:289:ILE:HD11	2.09	0.68
1:H:363:VAL:O	1:H:383:GLN:O	2.10	0.68
1:H:279:PHE:N	1:H:289:ILE:HD11	2.09	0.68
1:D:21:ARG:NH1	1:C:370:GLY:O	2.27	0.68
1:D:70:ILE:O	1:D:74:LYS:HG2	1.94	0.68
1:F:673:ILE:CG2	1:F:695:MET:CE	2.71	0.68
1:H:863:VAL:HA	1:H:866:MET:HG3	1.74	0.68
1:E:363:VAL:O	1:E:383:GLN:O	2.10	0.68
1:G:582:ASP:OD2	1:G:586:ARG:NH1	2.26	0.68
1:D:279:PHE:N	1:D:289:ILE:HD11	2.09	0.68
1:A:1010:LEU:HD21	1:A:1031:ILE:HD11	1.75	0.68
1:A:157:PRO:O	1:A:158:LEU:HD23	1.94	0.68
1:C:582:ASP:OD2	1:C:586:ARG:NH1	2.26	0.68
1:F:679:ILE:HD13	1:F:724:LEU:HD13	1.74	0.68
1:G:279:PHE:N	1:G:289:ILE:HD11	2.09	0.68
1:A:134:ILE:HD12	1:A:287:TYR:HB3	1.75	0.68
1:B:363:VAL:O	1:B:383:GLN:O	2.10	0.68
1:A:673:ILE:CG2	1:A:695:MET:CE	2.71	0.68
1:H:70:ILE:O	1:H:74:LYS:HG2	1.94	0.68
1:F:863:VAL:HA	1:F:866:MET:HG3	1.75	0.68
1:B:143:GLY:O	1:B:147:VAL:HG23	1.94	0.68
1:H:582:ASP:OD2	1:H:586:ARG:NH1	2.27	0.68
1:D:990:ILE:HD11	1:D:995:ASP:HA	1.76	0.67
1:D:582:ASP:OD2	1:D:586:ARG:NH1	2.28	0.67
1:B:158:LEU:N	1:B:158:LEU:HD12	2.09	0.67
1:D:863:VAL:HA	1:D:866:MET:HG3	1.75	0.67
1:E:160:ILE:HD11	1:E:174:VAL:HG21	1.75	0.67
1:H:384:GLY:HA3	1:G:1050:PRO:HD3	1.75	0.67
1:B:582:ASP:OD2	1:B:586:ARG:NH1	2.27	0.67
1:D:21:ARG:NH1	1:C:370:GLY:C	2.47	0.67
1:A:679:ILE:HD13	1:A:724:LEU:HD13	1.75	0.67
1:E:603:ILE:HG13	1:E:608:PHE:CZ	2.30	0.67
1:B:603:ILE:HG13	1:B:608:PHE:CZ	2.30	0.67
1:C:66:ILE:HG13	1:C:88:LEU:HD11	1.77	0.67
1:C:198:ASP:O	1:C:200:VAL:HG23	1.95	0.67
1:H:990:ILE:HD11	1:H:995:ASP:HA	1.77	0.67
1:H:8:LEU:CA	1:H:31:VAL:HG23	2.16	0.67
1:B:603:ILE:HG13	1:B:608:PHE:HZ	1.60	0.67
1:F:198:ASP:O	1:F:200:VAL:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:673:ILE:CG2	1:F:695:MET:HE3	2.25	0.66
1:B:437:HIS:HD2	1:B:439:ASP:N	1.91	0.66
1:F:550:ARG:HG3	1:F:816:PHE:CD1	2.30	0.66
1:A:582:ASP:OD2	1:A:586:ARG:NH1	2.28	0.66
1:E:437:HIS:HD2	1:E:439:ASP:N	1.92	0.66
1:G:198:ASP:O	1:G:200:VAL:HG23	1.96	0.66
1:E:582:ASP:OD2	1:E:586:ARG:NH1	2.27	0.66
1:G:365:THR:HG21	1:G:1051:ARG:HD3	1.77	0.66
1:A:21:ARG:NH1	1:B:370:GLY:O	2.28	0.66
1:E:603:ILE:HG13	1:E:608:PHE:HZ	1.60	0.66
1:A:550:ARG:HG3	1:A:816:PHE:CD1	2.31	0.66
1:C:365:THR:HG21	1:C:1051:ARG:HD3	1.78	0.66
1:D:1:MET:HE1	1:D:319:ASP:HB2	1.78	0.66
1:G:250:ILE:HD11	1:G:255:ARG:CB	2.25	0.66
1:A:673:ILE:CG2	1:A:695:MET:HE3	2.26	0.66
1:G:66:ILE:HG13	1:G:88:LEU:HD11	1.78	0.66
1:A:414:ARG:HD3	1:B:25:GLU:HG3	1.77	0.66
1:D:679:ILE:HD13	1:D:724:LEU:HD13	1.76	0.66
1:C:1:MET:HE1	1:C:319:ASP:HB2	1.78	0.66
1:G:227:LEU:CD2	1:G:306:THR:HG21	2.26	0.66
1:F:250:ILE:HD11	1:F:255:ARG:HB2	1.77	0.66
1:A:198:ASP:O	1:A:200:VAL:HG23	1.95	0.66
1:F:582:ASP:OD2	1:F:586:ARG:NH1	2.29	0.66
1:E:250:ILE:HD11	1:E:255:ARG:HB2	1.76	0.66
1:F:504:SER:HB2	1:F:505:GLN:HG2	1.76	0.66
1:B:147:VAL:O	1:B:151:GLY:N	2.28	0.66
1:G:278:GLU:C	1:G:289:ILE:HD11	2.16	0.66
1:H:250:ILE:HD11	1:H:255:ARG:HB2	1.78	0.66
1:F:120:ILE:HD12	1:F:121:LYS:N	2.11	0.66
1:B:250:ILE:HD11	1:B:255:ARG:HB2	1.77	0.66
1:D:370:GLY:C	1:C:21:ARG:NH1	2.50	0.65
1:A:250:ILE:HD11	1:A:255:ARG:HB2	1.78	0.65
1:D:120:ILE:HD12	1:D:121:LYS:N	2.11	0.65
1:D:250:ILE:HD11	1:D:255:ARG:HB2	1.78	0.65
1:H:176:SER:O	1:H:179:HIS:ND1	2.26	0.65
1:B:158:LEU:HD13	1:B:174:VAL:CB	2.18	0.65
1:G:1:MET:HE1	1:G:319:ASP:HB2	1.78	0.65
1:H:1:MET:HE1	1:H:319:ASP:HB2	1.78	0.65
1:C:278:GLU:C	1:C:289:ILE:HD11	2.17	0.65
1:H:120:ILE:HD12	1:H:121:LYS:N	2.11	0.65
1:H:679:ILE:HD13	1:H:724:LEU:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:659:ILE:HG23	1:H:669:VAL:HG11	1.79	0.65
1:A:151:GLY:HA2	1:A:158:LEU:HD11	1.78	0.65
1:C:250:ILE:HD11	1:C:255:ARG:CB	2.26	0.65
1:F:370:GLY:O	1:E:21:ARG:NH1	2.30	0.65
1:C:120:ILE:HD12	1:C:121:LYS:N	2.11	0.65
1:F:21:ARG:NH1	1:E:370:GLY:O	2.29	0.65
1:G:127:LEU:CD2	1:G:133:VAL:HG21	2.26	0.65
1:H:66:ILE:HG13	1:H:88:LEU:HD11	1.79	0.65
1:D:66:ILE:HG13	1:D:88:LEU:HD11	1.79	0.65
1:A:120:ILE:HD12	1:A:121:LYS:N	2.12	0.65
1:H:352:PRO:HA	1:H:356:PHE:CD1	2.32	0.65
1:B:603:ILE:HD12	1:B:608:PHE:CE1	2.32	0.65
1:B:141:VAL:CG1	1:B:147:VAL:HG22	2.27	0.65
1:D:659:ILE:HG23	1:D:669:VAL:HG11	1.79	0.65
1:A:1:MET:HE1	1:A:319:ASP:HB2	1.77	0.64
1:A:470:LEU:HD22	1:A:1044:PHE:CD2	2.32	0.64
1:G:960:LEU:HD13	1:G:961:LYS:N	2.12	0.64
1:C:127:LEU:CD2	1:C:133:VAL:HG21	2.27	0.64
1:D:550:ARG:HG3	1:D:816:PHE:CD1	2.33	0.64
1:B:464:ASP:OD2	1:B:467:THR:OG1	2.15	0.64
1:E:603:ILE:HD12	1:E:608:PHE:CE1	2.33	0.64
1:F:943:ARG:HD3	1:F:946:ALA:CB	2.27	0.64
1:E:464:ASP:OD2	1:E:467:THR:OG1	2.15	0.64
1:H:901:GLY:HA3	1:H:932:LEU:HD22	1.79	0.64
1:F:1:MET:HE1	1:F:319:ASP:HB2	1.78	0.64
1:E:952:ASN:OD1	1:E:955:GLU:N	2.19	0.64
1:C:960:LEU:HD13	1:C:961:LYS:N	2.12	0.64
1:E:66:ILE:HG13	1:E:88:LEU:HD11	1.78	0.64
1:B:952:ASN:OD1	1:B:955:GLU:N	2.19	0.64
1:A:25:GLU:HG3	1:B:414:ARG:HD3	1.80	0.64
1:B:66:ILE:HG13	1:B:88:LEU:HD11	1.78	0.64
1:H:550:ARG:HG3	1:H:816:PHE:CD1	2.33	0.64
1:B:144:ILE:CG2	1:B:184:PHE:CD2	2.81	0.64
1:A:943:ARG:HD3	1:A:946:ALA:CB	2.27	0.64
1:F:504:SER:CB	1:F:505:GLN:HG2	2.28	0.64
1:D:901:GLY:HA3	1:D:932:LEU:HD22	1.79	0.64
1:H:546:LEU:HB3	1:H:547:LEU:HD13	1.80	0.64
1:H:328:VAL:HG12	1:H:330:ILE:HG13	1.80	0.64
1:D:328:VAL:HG12	1:D:330:ILE:HG13	1.80	0.64
1:G:174:VAL:HG12	1:G:176:SER:H	1.63	0.64
1:D:198:ASP:O	1:D:200:VAL:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:500:ILE:HG21	1:G:565:HIS:CD2	2.33	0.64
1:H:198:ASP:O	1:H:200:VAL:HG23	1.97	0.64
1:C:540:ARG:HH21	1:C:541:ASP:CG	2.01	0.64
1:B:228:PHE:CE2	1:B:338:ILE:HG13	2.33	0.63
1:G:120:ILE:HD12	1:G:121:LYS:N	2.12	0.63
1:E:550:ARG:HG3	1:E:816:PHE:CD1	2.34	0.63
1:B:740:THR:HG22	1:B:751:TYR:CE1	2.33	0.63
1:A:659:ILE:HG23	1:A:669:VAL:HG11	1.80	0.63
1:D:546:LEU:HB3	1:D:547:LEU:HD13	1.81	0.63
1:E:740:THR:HG22	1:E:751:TYR:CE1	2.33	0.63
1:B:254:LEU:HD22	1:B:258:ILE:HD11	1.80	0.63
1:F:659:ILE:HG23	1:F:669:VAL:HG11	1.80	0.63
1:A:370:GLY:C	1:B:21:ARG:NH1	2.51	0.63
1:C:227:LEU:HD23	1:C:306:THR:CG2	2.29	0.63
1:E:228:PHE:CE2	1:E:338:ILE:HG13	2.34	0.63
1:H:541:ASP:OD2	1:H:739:HIS:CE1	2.52	0.63
1:B:550:ARG:HG3	1:B:816:PHE:CD1	2.34	0.63
1:C:254:LEU:HD22	1:C:258:ILE:HD11	1.81	0.63
1:G:659:ILE:HG23	1:G:669:VAL:HG11	1.79	0.63
1:E:254:LEU:HD22	1:E:258:ILE:HD11	1.81	0.63
1:B:328:VAL:HG12	1:B:330:ILE:HG13	1.81	0.63
1:D:680:ASP:OD1	1:D:723:ARG:NH1	2.31	0.63
1:F:328:VAL:HG12	1:F:330:ILE:HG13	1.81	0.63
1:G:550:ARG:HG3	1:G:816:PHE:CD1	2.33	0.63
1:E:352:PRO:HA	1:E:356:PHE:CD1	2.33	0.63
1:C:328:VAL:HG12	1:C:330:ILE:HG13	1.81	0.63
1:C:174:VAL:HG12	1:C:176:SER:H	1.64	0.63
1:H:290:GLU:OE2	1:H:291:VAL:N	2.31	0.63
1:A:597:GLU:OE1	1:A:971:LYS:NZ	2.26	0.63
1:F:470:LEU:HD22	1:F:1044:PHE:CD2	2.34	0.63
1:D:740:THR:HG22	1:D:751:TYR:CE1	2.34	0.62
1:G:254:LEU:HD22	1:G:258:ILE:HD11	1.81	0.62
1:A:740:THR:HG22	1:A:751:TYR:CE1	2.35	0.62
1:E:328:VAL:HG12	1:E:330:ILE:HG13	1.81	0.62
1:H:942:ASP:OD1	1:H:942:ASP:N	2.32	0.62
1:B:141:VAL:HG21	1:B:202:VAL:CB	2.28	0.62
1:H:740:THR:HG22	1:H:751:TYR:CE1	2.34	0.62
1:D:352:PRO:HA	1:D:356:PHE:CD1	2.34	0.62
1:C:659:ILE:HG23	1:C:669:VAL:HG11	1.80	0.62
1:H:680:ASP:OD1	1:H:723:ARG:NH1	2.32	0.62
1:D:541:ASP:OD2	1:D:739:HIS:CE1	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:940:LEU:O	1:B:941:THR:HG22	1.99	0.62
1:G:540:ARG:HH21	1:G:541:ASP:CG	2.03	0.62
1:C:526:VAL:O	1:C:529:GLN:CB	2.47	0.62
1:B:437:HIS:HD2	1:B:439:ASP:H	1.46	0.62
1:A:254:LEU:HD22	1:A:258:ILE:HD11	1.80	0.62
1:G:546:LEU:HB3	1:G:547:LEU:HD13	1.81	0.62
1:C:832:MET:HG3	1:C:833:PRO:CD	2.30	0.62
1:F:740:THR:HG22	1:F:751:TYR:CE1	2.35	0.62
1:D:624:PRO:O	1:D:627:VAL:HG22	1.99	0.62
1:D:942:ASP:OD1	1:D:942:ASP:N	2.33	0.62
1:F:624:PRO:O	1:F:627:VAL:HG22	2.00	0.62
1:A:541:ASP:OD2	1:A:739:HIS:CE1	2.52	0.62
1:G:624:PRO:O	1:G:627:VAL:HG22	2.00	0.62
1:C:624:PRO:O	1:C:627:VAL:HG22	2.00	0.62
1:A:624:PRO:O	1:A:627:VAL:HG22	2.00	0.62
1:G:328:VAL:HG12	1:G:330:ILE:HG13	1.82	0.62
1:B:352:PRO:HA	1:B:356:PHE:CD1	2.34	0.62
1:C:546:LEU:HB3	1:C:547:LEU:HD13	1.82	0.62
1:A:219:ASP:CB	1:A:323:LEU:HD23	2.27	0.61
1:H:17:ILE:HD11	1:H:43:HIS:HB3	1.82	0.61
1:F:370:GLY:C	1:E:21:ARG:NH1	2.53	0.61
1:F:254:LEU:HD22	1:F:258:ILE:HD11	1.81	0.61
1:G:526:VAL:O	1:G:529:GLN:CB	2.48	0.61
1:C:550:ARG:HG3	1:C:816:PHE:CD1	2.35	0.61
1:F:25:GLU:HG3	1:E:414:ARG:HD3	1.83	0.61
1:F:546:LEU:HB3	1:F:547:LEU:HD13	1.82	0.61
1:H:624:PRO:O	1:H:627:VAL:HG22	2.00	0.61
1:D:177:LYS:HG3	1:D:178:GLU:H	1.64	0.61
1:G:352:PRO:HA	1:G:356:PHE:CD1	2.35	0.61
1:E:180:VAL:CG1	1:E:184:PHE:CZ	2.66	0.61
1:C:537:THR:O	1:C:540:ARG:O	2.18	0.61
1:B:624:PRO:O	1:B:627:VAL:HG22	2.00	0.61
1:H:537:THR:O	1:H:540:ARG:O	2.19	0.61
1:G:832:MET:HG3	1:G:833:PRO:CD	2.31	0.61
1:F:151:GLY:HA2	1:F:158:LEU:HD11	1.81	0.61
1:G:537:THR:O	1:G:540:ARG:O	2.18	0.61
1:E:624:PRO:O	1:E:627:VAL:HG22	2.00	0.61
1:A:328:VAL:HG12	1:A:330:ILE:HG13	1.82	0.61
1:F:174:VAL:HG12	1:F:176:SER:H	1.64	0.61
1:F:541:ASP:OD2	1:F:739:HIS:CE1	2.53	0.61
1:H:360:THR:HA	1:H:387:VAL:CG2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:LEU:HB3	1:B:547:LEU:HD13	1.83	0.61
1:C:352:PRO:HA	1:C:356:PHE:CD1	2.35	0.61
1:D:537:THR:O	1:D:540:ARG:O	2.19	0.61
1:E:749:TYR:CZ	1:G:752:ALA:HB1	2.36	0.61
1:E:219:ASP:CB	1:E:323:LEU:HD23	2.27	0.61
1:E:234:ILE:HD11	1:E:445:TYR:CE1	2.36	0.61
1:G:360:THR:HA	1:G:387:VAL:CG2	2.31	0.61
1:A:832:MET:HG2	1:A:836:GLN:HG2	1.81	0.61
1:F:175:GLU:OE2	1:F:175:GLU:N	2.33	0.61
1:C:360:THR:HA	1:C:387:VAL:CG2	2.31	0.61
1:H:360:THR:HA	1:H:387:VAL:HG23	1.83	0.61
1:A:942:ASP:N	1:A:942:ASP:OD1	2.33	0.61
1:H:254:LEU:O	1:H:258:ILE:HD12	2.01	0.60
1:B:219:ASP:CB	1:B:323:LEU:HD23	2.27	0.60
1:A:21:ARG:NH1	1:B:370:GLY:C	2.53	0.60
1:B:234:ILE:HD11	1:B:445:TYR:CE1	2.36	0.60
1:E:213:GLU:OE2	1:E:232:CYS:SG	2.54	0.60
1:A:175:GLU:OE2	1:A:175:GLU:N	2.34	0.60
1:F:942:ASP:OD1	1:F:942:ASP:N	2.33	0.60
1:D:254:LEU:O	1:D:258:ILE:HD12	2.01	0.60
1:B:537:THR:O	1:B:540:ARG:O	2.19	0.60
1:A:546:LEU:HB3	1:A:547:LEU:HD13	1.83	0.60
1:G:110:SER:HA	1:G:113:LEU:HD12	1.82	0.60
1:G:576:TRP:CD1	1:G:596:LEU:HB2	2.37	0.60
1:F:126:ALA:C	1:F:131:ILE:HD11	2.21	0.60
1:E:537:THR:O	1:E:540:ARG:O	2.19	0.60
1:C:576:TRP:CD1	1:C:596:LEU:HB2	2.37	0.60
1:D:17:ILE:HD11	1:D:43:HIS:HB3	1.84	0.60
1:F:1031:ILE:HG22	1:F:1042:ILE:HG13	1.84	0.60
1:C:110:SER:HA	1:C:113:LEU:HD12	1.82	0.60
1:D:360:THR:HA	1:D:387:VAL:CG2	2.31	0.60
1:A:174:VAL:HG12	1:A:176:SER:H	1.66	0.60
1:C:541:ASP:OD2	1:C:739:HIS:CE1	2.55	0.60
1:F:680:ASP:OD1	1:F:723:ARG:NH1	2.33	0.60
1:F:537:THR:O	1:F:540:ARG:O	2.19	0.60
1:A:537:THR:O	1:A:540:ARG:O	2.19	0.60
1:E:546:LEU:HB3	1:E:547:LEU:HD13	1.84	0.60
1:E:979:TYR:HB3	1:E:982:VAL:CG2	2.31	0.60
1:A:1031:ILE:HG22	1:A:1042:ILE:HG13	1.84	0.60
1:F:611:LEU:HD11	1:F:646:PHE:CE1	2.37	0.60
1:B:213:GLU:OE2	1:B:232:CYS:SG	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:GLU:HG3	1:C:414:ARG:HD3	1.83	0.60
1:F:832:MET:HG2	1:F:836:GLN:HG2	1.81	0.60
1:H:611:LEU:HD11	1:H:646:PHE:CE1	2.37	0.60
1:B:160:ILE:HD12	1:B:174:VAL:HG23	1.84	0.60
1:H:219:ASP:CB	1:H:323:LEU:HD23	2.27	0.60
1:E:382:PHE:CE1	1:E:385:THR:HB	2.36	0.60
1:H:12:ARG:NH2	1:H:38:ASP:OD1	2.34	0.60
1:G:552:ARG:HA	1:G:588:LEU:HD11	1.83	0.60
1:F:126:ALA:CA	1:F:131:ILE:HD11	2.31	0.60
1:G:541:ASP:OD2	1:G:739:HIS:CE1	2.55	0.60
1:C:589:ASN:OD1	1:C:989:MET:HE1	2.02	0.60
1:D:12:ARG:NH2	1:D:38:ASP:OD1	2.34	0.60
1:E:940:LEU:O	1:E:941:THR:HG22	2.02	0.60
1:A:979:TYR:HB3	1:A:982:VAL:CG2	2.32	0.60
1:A:234:ILE:HD11	1:A:445:TYR:CE1	2.36	0.60
1:H:134:ILE:HD12	1:H:287:TYR:CB	2.32	0.60
1:D:360:THR:HA	1:D:387:VAL:HG23	1.84	0.60
1:E:360:THR:HA	1:E:387:VAL:CG2	2.31	0.60
1:A:680:ASP:OD1	1:A:723:ARG:NH1	2.33	0.60
1:D:219:ASP:CB	1:D:323:LEU:HD23	2.28	0.59
1:E:437:HIS:HD2	1:E:439:ASP:H	1.47	0.59
1:D:290:GLU:OE2	1:D:291:VAL:N	2.32	0.59
1:G:589:ASN:OD1	1:G:989:MET:HE1	2.02	0.59
1:C:470:LEU:HD22	1:C:1044:PHE:CD2	2.37	0.59
1:B:360:THR:HA	1:B:387:VAL:CG2	2.32	0.59
1:A:563:MET:HE1	1:A:573:PHE:CD2	2.36	0.59
1:F:979:TYR:HB3	1:F:982:VAL:CG2	2.32	0.59
1:E:541:ASP:OD2	1:E:739:HIS:CE1	2.55	0.59
1:H:370:GLY:O	1:G:21:ARG:NH1	2.36	0.59
1:H:414:ARG:HD3	1:G:25:GLU:HG3	1.82	0.59
1:F:21:ARG:NH1	1:E:370:GLY:C	2.55	0.59
1:E:280:LEU:N	1:E:289:ILE:HD13	2.18	0.59
1:D:45:TYR:CE2	1:C:1047:ASN:O	2.55	0.59
1:D:979:TYR:HB3	1:D:982:VAL:CG2	2.33	0.59
1:F:234:ILE:HD11	1:F:445:TYR:CE1	2.37	0.59
1:G:470:LEU:HD22	1:G:1044:PHE:CD2	2.38	0.59
1:D:611:LEU:HD11	1:D:646:PHE:CE1	2.37	0.59
1:A:110:SER:HA	1:A:113:LEU:HD12	1.83	0.59
1:F:134:ILE:HD12	1:F:287:TYR:CB	2.32	0.59
1:C:552:ARG:HA	1:C:588:LEU:HD11	1.84	0.59
1:E:470:LEU:HD22	1:E:1044:PHE:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:SER:HA	1:F:113:LEU:HD12	1.83	0.59
1:E:266:MET:HE2	1:E:277:VAL:HG22	1.84	0.59
1:B:979:TYR:HB3	1:B:982:VAL:CG2	2.32	0.59
1:G:360:THR:HA	1:G:387:VAL:HG23	1.83	0.59
1:B:541:ASP:OD2	1:B:739:HIS:CE1	2.56	0.59
1:A:126:ALA:C	1:A:131:ILE:HD11	2.22	0.59
1:H:234:ILE:HD11	1:H:445:TYR:CE1	2.37	0.59
1:E:14:GLU:CD	1:E:397:LYS:HE3	2.22	0.59
1:A:134:ILE:HD12	1:A:287:TYR:CB	2.32	0.59
1:C:360:THR:HA	1:C:387:VAL:HG23	1.83	0.59
1:A:865:GLN:HA	1:A:868:GLY:O	2.03	0.59
1:A:126:ALA:CA	1:A:131:ILE:HD11	2.32	0.59
1:D:45:TYR:CZ	1:C:1047:ASN:HB3	2.38	0.59
1:F:511:LYS:NZ	1:F:641:ASP:OD1	2.35	0.59
1:H:134:ILE:CD1	1:H:287:TYR:CB	2.81	0.59
1:H:64:LEU:CD2	1:H:88:LEU:HD23	2.33	0.59
1:A:611:LEU:HD11	1:A:646:PHE:CE1	2.38	0.59
1:B:382:PHE:CE1	1:B:385:THR:HB	2.38	0.59
1:B:280:LEU:N	1:B:289:ILE:HD13	2.18	0.58
1:D:322:ALA:N	1:D:325:ASP:OD2	2.36	0.58
1:A:511:LYS:NZ	1:A:641:ASP:OD1	2.35	0.58
1:B:64:LEU:CD2	1:B:88:LEU:HD23	2.32	0.58
1:H:979:TYR:HB3	1:H:982:VAL:CG2	2.34	0.58
1:D:134:ILE:HD12	1:D:287:TYR:CB	2.33	0.58
1:H:470:LEU:HD22	1:H:1044:PHE:CD2	2.38	0.58
1:E:141:VAL:HG21	1:E:202:VAL:CB	2.33	0.58
1:E:64:LEU:CD2	1:E:88:LEU:HD23	2.32	0.58
1:F:134:ILE:CD1	1:F:287:TYR:CB	2.81	0.58
1:E:360:THR:HA	1:E:387:VAL:HG23	1.84	0.58
1:F:563:MET:HE1	1:F:573:PHE:CD2	2.37	0.58
1:B:14:GLU:CD	1:B:397:LYS:HE3	2.23	0.58
1:E:228:PHE:CD2	1:E:338:ILE:HD11	2.37	0.58
1:D:64:LEU:CD2	1:D:88:LEU:HD23	2.34	0.58
1:B:360:THR:HA	1:B:387:VAL:HG23	1.84	0.58
1:C:653:LYS:O	1:C:943:ARG:HD3	2.03	0.58
1:D:470:LEU:HD22	1:D:1044:PHE:CD2	2.38	0.58
1:G:653:LYS:O	1:G:943:ARG:HD3	2.03	0.58
1:H:322:ALA:N	1:H:325:ASP:OD2	2.36	0.58
1:H:45:TYR:CE2	1:G:1047:ASN:O	2.57	0.58
1:D:234:ILE:HD11	1:D:445:TYR:CE1	2.38	0.58
1:B:348:THR:OG1	1:B:350:GLU:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:898:TYR:HD1	1:D:928:LYS:CE	2.16	0.58
1:B:470:LEU:HD22	1:B:1044:PHE:CD2	2.39	0.58
1:A:134:ILE:CD1	1:A:287:TYR:CB	2.81	0.58
1:H:550:ARG:HG3	1:H:816:PHE:CE1	2.39	0.58
1:F:92:ILE:HD13	1:F:113:LEU:HB2	1.86	0.58
1:E:823:PRO:O	1:G:767:SER:HB3	2.04	0.58
1:F:322:ALA:N	1:F:325:ASP:OD2	2.36	0.58
1:E:322:ALA:N	1:E:325:ASP:OD2	2.36	0.58
1:E:278:GLU:HB2	1:E:289:ILE:HG13	1.84	0.58
1:B:266:MET:HE2	1:B:277:VAL:HG22	1.85	0.58
1:B:603:ILE:CD1	1:B:608:PHE:CE1	2.86	0.58
1:D:134:ILE:CD1	1:D:287:TYR:CB	2.82	0.58
1:H:898:TYR:HD1	1:H:928:LYS:CE	2.16	0.58
1:A:511:LYS:HZ3	1:A:641:ASP:CG	2.07	0.58
1:A:360:THR:HA	1:A:387:VAL:CG2	2.33	0.58
1:E:603:ILE:CD1	1:E:608:PHE:CE1	2.86	0.58
1:B:101:GLU:CB	1:B:103:ILE:HD13	2.32	0.58
1:H:177:LYS:HG3	1:H:178:GLU:H	1.68	0.58
1:A:322:ALA:N	1:A:325:ASP:OD2	2.37	0.58
1:F:382:PHE:CE1	1:F:385:THR:HB	2.38	0.58
1:G:53:VAL:HG13	1:G:54:GLY:N	2.18	0.58
1:D:174:VAL:C	1:D:175:GLU:OE2	2.42	0.57
1:C:234:ILE:HD11	1:C:445:TYR:CE1	2.38	0.57
1:H:175:GLU:HB2	1:H:179:HIS:CG	2.39	0.57
1:B:952:ASN:C	1:B:952:ASN:OD1	2.42	0.57
1:B:823:PRO:O	1:C:767:SER:HB3	2.04	0.57
1:F:360:THR:HA	1:F:387:VAL:CG2	2.34	0.57
1:F:865:GLN:HA	1:F:868:GLY:O	2.04	0.57
1:B:749:TYR:CZ	1:C:752:ALA:HB1	2.39	0.57
1:F:213:GLU:OE2	1:F:232:CYS:SG	2.54	0.57
1:B:278:GLU:C	1:B:289:ILE:CD1	2.69	0.57
1:B:278:GLU:HB2	1:B:289:ILE:HG13	1.85	0.57
1:E:101:GLU:CB	1:E:103:ILE:HD13	2.32	0.57
1:C:228:PHE:HE2	1:C:338:ILE:HG13	1.70	0.57
1:E:952:ASN:OD1	1:E:952:ASN:C	2.42	0.57
1:C:53:VAL:HG13	1:C:54:GLY:H	1.70	0.57
1:A:213:GLU:OE2	1:A:232:CYS:SG	2.54	0.57
1:G:164:LEU:HA	1:G:195:PHE:HE1	1.68	0.57
1:G:367:ARG:NH1	1:G:1049:GLN:CB	2.60	0.57
1:G:520:GLU:OE1	1:G:705:HIS:CD2	2.57	0.57
1:G:53:VAL:HG13	1:G:54:GLY:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:VAL:HG13	1:C:54:GLY:N	2.18	0.57
1:A:92:ILE:HD13	1:A:113:LEU:HB2	1.87	0.57
1:F:360:THR:HA	1:F:387:VAL:HG23	1.86	0.57
1:B:322:ALA:N	1:B:325:ASP:OD2	2.37	0.57
1:D:550:ARG:HG3	1:D:816:PHE:CE1	2.40	0.57
1:A:360:THR:HA	1:A:387:VAL:HG23	1.86	0.57
1:D:865:GLN:HA	1:D:868:GLY:O	2.04	0.57
1:F:80:ALA:HB2	1:F:104:ILE:HB	1.87	0.57
1:D:551:VAL:HA	1:D:813:TYR:CE2	2.40	0.57
1:C:520:GLU:OE1	1:C:705:HIS:CD2	2.57	0.57
1:C:160:ILE:HG22	1:C:200:VAL:CG1	2.34	0.57
1:E:926:PRO:O	1:E:927:GLU:HB2	2.03	0.57
1:E:348:THR:OG1	1:E:350:GLU:HG3	2.05	0.57
1:B:603:ILE:HD12	1:B:608:PHE:HE1	1.69	0.57
1:F:986:TYR:CZ	1:F:990:ILE:HD12	2.38	0.57
1:G:160:ILE:HG22	1:G:200:VAL:CG1	2.34	0.57
1:A:550:ARG:HG3	1:A:816:PHE:CE1	2.40	0.57
1:E:349:THR:HG23	1:E:393:SER:CB	2.35	0.57
1:G:234:ILE:HD11	1:G:445:TYR:CE1	2.39	0.57
1:E:651:TRP:CZ2	1:E:920:GLN:HG3	2.40	0.57
1:A:673:ILE:HG22	1:A:695:MET:HE1	1.87	0.57
1:A:986:TYR:CZ	1:A:990:ILE:HD12	2.39	0.57
1:C:540:ARG:HH21	1:C:541:ASP:CB	2.18	0.57
1:B:504:SER:O	1:B:506:ILE:HG12	2.05	0.57
1:G:550:ARG:HG3	1:G:816:PHE:CE1	2.40	0.57
1:B:394:LEU:HD12	1:B:395:LEU:N	2.20	0.57
1:A:557:PHE:CE1	1:A:598:THR:HB	2.40	0.57
1:A:382:PHE:CE1	1:A:385:THR:HB	2.39	0.57
1:F:304:MET:HE3	1:F:342:ALA:HB1	1.87	0.57
1:H:623:TYR:HB3	1:H:627:VAL:HG21	1.87	0.57
1:G:126:ALA:HB1	1:G:131:ILE:HD11	1.87	0.57
1:H:557:PHE:CE1	1:H:598:THR:HB	2.40	0.57
1:F:713:ALA:HB3	1:F:715:LEU:CD1	2.34	0.57
1:B:926:PRO:O	1:B:927:GLU:HB2	2.04	0.57
1:B:651:TRP:CZ2	1:B:920:GLN:HG3	2.40	0.57
1:F:673:ILE:HG22	1:F:695:MET:HE1	1.87	0.56
1:G:540:ARG:HH21	1:G:541:ASP:HA	1.69	0.56
1:F:859:MET:O	1:F:863:VAL:HG23	2.05	0.56
1:B:859:MET:O	1:B:863:VAL:HG23	2.05	0.56
1:G:322:ALA:N	1:G:325:ASP:OD2	2.38	0.56
1:A:304:MET:HE3	1:A:342:ALA:HB1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:623:TYR:HB3	1:D:627:VAL:HG21	1.88	0.56
1:E:394:LEU:HD12	1:E:395:LEU:N	2.20	0.56
1:B:865:GLN:HA	1:B:868:GLY:O	2.05	0.56
1:E:859:MET:O	1:E:863:VAL:HG23	2.05	0.56
1:E:865:GLN:HA	1:E:868:GLY:O	2.05	0.56
1:B:53:VAL:HG13	1:B:54:GLY:N	2.20	0.56
1:H:382:PHE:CE1	1:H:385:THR:HB	2.40	0.56
1:E:14:GLU:CD	1:E:397:LYS:CE	2.70	0.56
1:D:8:LEU:CA	1:D:31:VAL:HG23	2.16	0.56
1:G:576:TRP:CZ2	1:G:592:PRO:HB2	2.40	0.56
1:E:603:ILE:HD12	1:E:608:PHE:HE1	1.70	0.56
1:H:45:TYR:CZ	1:G:1047:ASN:HB3	2.41	0.56
1:F:673:ILE:HG22	1:F:695:MET:HE3	1.85	0.56
1:B:304:MET:HE3	1:B:342:ALA:HB1	1.87	0.56
1:G:540:ARG:HH21	1:G:541:ASP:CB	2.19	0.56
1:H:859:MET:O	1:H:863:VAL:HG23	2.05	0.56
1:G:92:ILE:HD13	1:G:113:LEU:HB2	1.87	0.56
1:C:92:ILE:HD13	1:C:113:LEU:HB2	1.87	0.56
1:F:348:THR:OG1	1:F:350:GLU:HG3	2.05	0.56
1:A:348:THR:OG1	1:A:350:GLU:HG3	2.05	0.56
1:H:551:VAL:HA	1:H:813:TYR:CE2	2.40	0.56
1:D:382:PHE:CE1	1:D:385:THR:HB	2.40	0.56
1:C:126:ALA:HB1	1:C:131:ILE:HD11	1.88	0.56
1:C:576:TRP:CZ2	1:C:592:PRO:HB2	2.40	0.56
1:A:859:MET:O	1:A:863:VAL:HG23	2.06	0.56
1:D:859:MET:O	1:D:863:VAL:HG23	2.05	0.56
1:E:550:ARG:HG3	1:E:816:PHE:CE1	2.41	0.56
1:C:322:ALA:N	1:C:325:ASP:OD2	2.38	0.56
1:E:278:GLU:C	1:E:289:ILE:CD1	2.70	0.56
1:B:158:LEU:H	1:B:158:LEU:HD12	1.67	0.56
1:A:321:TYR:HB3	1:A:325:ASP:OD2	2.05	0.56
1:F:321:TYR:HB3	1:F:325:ASP:OD2	2.05	0.56
1:A:80:ALA:HB2	1:A:104:ILE:HB	1.88	0.56
1:E:80:ALA:HB2	1:E:104:ILE:HB	1.88	0.56
1:E:209:PRO:HB2	1:E:280:LEU:HD23	1.87	0.56
1:B:88:LEU:HB3	1:B:94:PHE:CD2	2.37	0.56
1:B:987:GLN:O	1:B:990:ILE:HG22	2.05	0.56
1:E:987:GLN:O	1:E:990:ILE:HG22	2.05	0.56
1:H:1031:ILE:HG23	1:H:1042:ILE:HG13	1.88	0.56
1:D:1031:ILE:HG23	1:D:1042:ILE:HG13	1.88	0.56
1:B:450:ILE:HG22	1:B:451:ASP:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1041:VAL:HG12	1:F:1043:TYR:CE1	2.40	0.56
1:B:209:PRO:HB2	1:B:280:LEU:HD23	1.87	0.56
1:D:321:TYR:HB3	1:D:325:ASP:OD2	2.06	0.56
1:H:134:ILE:HD11	1:H:287:TYR:HB2	1.87	0.56
1:D:134:ILE:HD11	1:D:287:TYR:HB2	1.87	0.56
1:C:278:GLU:C	1:C:289:ILE:CD1	2.74	0.56
1:G:278:GLU:C	1:G:289:ILE:CD1	2.74	0.56
1:F:160:ILE:HG22	1:F:200:VAL:CG1	2.35	0.56
1:G:164:LEU:HA	1:G:195:PHE:CE1	2.40	0.56
1:B:367:ARG:HH12	1:B:1049:GLN:HB2	1.70	0.56
1:A:506:ILE:HD11	1:A:565:HIS:CE1	2.41	0.56
1:B:14:GLU:CD	1:B:397:LYS:CE	2.71	0.56
1:G:304:MET:HE3	1:G:342:ALA:HB1	1.87	0.56
1:D:898:TYR:CD1	1:D:928:LYS:HE2	2.40	0.56
1:D:557:PHE:CE1	1:D:598:THR:HB	2.41	0.56
1:H:321:TYR:HB3	1:H:325:ASP:OD2	2.06	0.56
1:F:550:ARG:HG3	1:F:816:PHE:CE1	2.41	0.56
1:D:908:ASP:O	1:D:912:GLU:HG3	2.06	0.56
1:E:53:VAL:HG13	1:E:54:GLY:N	2.20	0.56
1:A:630:GLU:HG2	1:A:953:PHE:HE1	1.70	0.56
1:H:908:ASP:O	1:H:912:GLU:HG3	2.06	0.56
1:F:557:PHE:CE1	1:F:598:THR:HB	2.41	0.56
1:H:898:TYR:CD1	1:H:928:LYS:HE2	2.40	0.56
1:H:865:GLN:HA	1:H:868:GLY:O	2.06	0.56
1:H:600:ARG:NH1	1:H:603:ILE:O	2.39	0.56
1:E:505:GLN:HA	1:E:505:GLN:OE1	2.05	0.56
1:B:349:THR:HG23	1:B:393:SER:CB	2.36	0.55
1:A:160:ILE:HG22	1:A:200:VAL:CG1	2.36	0.55
1:H:175:GLU:N	1:H:175:GLU:OE2	2.39	0.55
1:H:541:ASP:OD2	1:H:741:HIS:HE1	1.89	0.55
1:G:348:THR:OG1	1:G:350:GLU:HG3	2.05	0.55
1:E:147:VAL:HG21	1:E:184:PHE:CE1	2.40	0.55
1:D:80:ALA:HB2	1:D:104:ILE:HB	1.88	0.55
1:H:80:ALA:HB2	1:H:104:ILE:HB	1.88	0.55
1:A:673:ILE:HG22	1:A:695:MET:HE3	1.86	0.55
1:H:510:THR:CG2	1:H:607:MET:SD	2.92	0.55
1:F:986:TYR:CE1	1:F:990:ILE:CD1	2.89	0.55
1:F:1031:ILE:CG2	1:F:1042:ILE:HG13	2.36	0.55
1:C:832:MET:HG3	1:C:833:PRO:HD2	1.88	0.55
1:B:80:ALA:HB2	1:B:104:ILE:HB	1.88	0.55
1:E:367:ARG:HH12	1:E:1049:GLN:HB2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:557:PHE:CE1	1:G:598:THR:HB	2.41	0.55
1:C:348:THR:OG1	1:C:350:GLU:HG3	2.05	0.55
1:E:88:LEU:HB3	1:E:94:PHE:CD2	2.38	0.55
1:B:126:ALA:HB1	1:B:131:ILE:HD11	1.88	0.55
1:H:394:LEU:HD12	1:H:395:LEU:N	2.21	0.55
1:H:348:THR:OG1	1:H:350:GLU:HG3	2.06	0.55
1:F:53:VAL:HG13	1:F:54:GLY:N	2.21	0.55
1:B:82:HIS:HA	1:B:106:VAL:CG2	2.37	0.55
1:E:82:HIS:HA	1:E:106:VAL:CG2	2.37	0.55
1:H:960:LEU:CD1	1:H:976:TYR:CD1	2.89	0.55
1:D:960:LEU:CD1	1:D:976:TYR:CD1	2.89	0.55
1:B:623:TYR:HB3	1:B:627:VAL:HG21	1.89	0.55
1:C:557:PHE:CE1	1:C:598:THR:HB	2.42	0.55
1:G:620:TYR:CD2	1:G:621:LYS:N	2.74	0.55
1:A:713:ALA:HB3	1:A:715:LEU:CD1	2.35	0.55
1:D:345:SER:CB	1:D:412:MET:CE	2.81	0.55
1:A:394:LEU:HD12	1:A:395:LEU:N	2.22	0.55
1:A:986:TYR:CE1	1:A:990:ILE:CD1	2.90	0.55
1:F:134:ILE:HD11	1:F:287:TYR:HB2	1.87	0.55
1:A:1031:ILE:CG2	1:A:1042:ILE:HG13	2.37	0.55
1:H:987:GLN:O	1:H:990:ILE:HG22	2.07	0.55
1:C:550:ARG:HG3	1:C:816:PHE:CE1	2.42	0.55
1:A:1041:VAL:HG12	1:A:1043:TYR:CE1	2.41	0.55
1:H:53:VAL:HG13	1:H:54:GLY:N	2.20	0.55
1:A:134:ILE:HD11	1:A:287:TYR:HB2	1.87	0.55
1:A:740:THR:HG22	1:A:751:TYR:CZ	2.42	0.55
1:G:1031:ILE:HG23	1:G:1042:ILE:HG13	1.89	0.55
1:C:1031:ILE:HG23	1:C:1042:ILE:HG13	1.89	0.55
1:F:630:GLU:HG2	1:F:953:PHE:HE1	1.71	0.55
1:D:348:THR:OG1	1:D:350:GLU:HG3	2.06	0.55
1:D:177:LYS:O	1:D:180:VAL:HG23	2.07	0.55
1:A:53:VAL:HG13	1:A:54:GLY:N	2.21	0.55
1:D:465:ARG:HG2	1:D:465:ARG:O	2.07	0.55
1:D:987:GLN:O	1:D:990:ILE:HG22	2.07	0.55
1:E:160:ILE:CD1	1:E:174:VAL:CG2	2.85	0.55
1:B:550:ARG:HG3	1:B:816:PHE:CE1	2.42	0.55
1:H:465:ARG:O	1:H:465:ARG:HG2	2.07	0.55
1:C:540:ARG:HH21	1:C:541:ASP:HA	1.71	0.55
1:D:928:LYS:O	1:D:932:LEU:HD12	2.07	0.55
1:B:551:VAL:HA	1:B:813:TYR:CE2	2.42	0.55
1:C:394:LEU:HD12	1:C:395:LEU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:259:CYS:O	1:H:263:VAL:HG23	2.07	0.55
1:E:1031:ILE:HG23	1:E:1042:ILE:HG13	1.89	0.55
1:E:126:ALA:HB1	1:E:131:ILE:HD11	1.89	0.55
1:H:622:ASN:ND2	1:H:917:GLU:O	2.40	0.55
1:A:63:TYR:HB2	1:A:87:PHE:CD2	2.42	0.55
1:H:345:SER:CB	1:H:412:MET:CE	2.81	0.54
1:D:44:ARG:HD3	1:D:45:TYR:CD1	2.42	0.54
1:B:235:GLN:O	1:B:450:ILE:HG13	2.07	0.54
1:D:259:CYS:O	1:D:263:VAL:HG23	2.08	0.54
1:H:228:PHE:CE2	1:H:338:ILE:HG13	2.42	0.54
1:B:1031:ILE:HG23	1:B:1042:ILE:HG13	1.89	0.54
1:G:80:ALA:HB2	1:G:104:ILE:HB	1.88	0.54
1:F:394:LEU:HD12	1:F:395:LEU:N	2.23	0.54
1:D:510:THR:CG2	1:D:607:MET:SD	2.93	0.54
1:H:928:LYS:O	1:H:932:LEU:HD12	2.07	0.54
1:D:53:VAL:HG13	1:D:54:GLY:N	2.21	0.54
1:D:394:LEU:HD12	1:D:395:LEU:N	2.22	0.54
1:B:472:TYR:OH	1:B:1004:PHE:CD2	2.59	0.54
1:E:259:CYS:O	1:E:263:VAL:HG23	2.07	0.54
1:E:304:MET:HE3	1:E:342:ALA:HB1	1.88	0.54
1:B:740:THR:HG22	1:B:751:TYR:CZ	2.41	0.54
1:F:600:ARG:NH1	1:F:603:ILE:O	2.40	0.54
1:A:600:ARG:NH1	1:A:603:ILE:O	2.40	0.54
1:A:908:ASP:O	1:A:912:GLU:HG3	2.06	0.54
1:C:620:TYR:CD2	1:C:621:LYS:N	2.75	0.54
1:H:44:ARG:HD3	1:H:45:TYR:CD1	2.42	0.54
1:F:134:ILE:CD1	1:F:287:TYR:HB3	2.36	0.54
1:F:160:ILE:CG2	1:F:200:VAL:HG11	2.37	0.54
1:G:160:ILE:CG2	1:G:200:VAL:HG11	2.37	0.54
1:G:832:MET:HG3	1:G:833:PRO:HD2	1.89	0.54
1:G:20:MET:CE	1:G:43:HIS:O	2.55	0.54
1:G:394:LEU:HD12	1:G:395:LEU:N	2.22	0.54
1:G:620:TYR:HD2	1:G:621:LYS:N	2.05	0.54
1:C:195:PHE:N	1:C:195:PHE:CD2	2.75	0.54
1:F:623:TYR:HB3	1:F:627:VAL:HG21	1.88	0.54
1:B:120:ILE:HD12	1:B:140:PRO:HG3	1.88	0.54
1:C:177:LYS:O	1:C:180:VAL:HG23	2.08	0.54
1:D:600:ARG:NH1	1:D:603:ILE:O	2.41	0.54
1:E:209:PRO:CB	1:E:280:LEU:HD23	2.38	0.54
1:D:21:ARG:HH12	1:C:370:GLY:C	2.11	0.54
1:C:259:CYS:O	1:C:263:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:740:THR:HG22	1:F:751:TYR:CZ	2.43	0.54
1:E:551:VAL:HA	1:E:813:TYR:CE2	2.43	0.54
1:B:259:CYS:O	1:B:263:VAL:HG23	2.07	0.54
1:F:567:LEU:N	1:F:568:PRO:CD	2.70	0.54
1:C:80:ALA:HB2	1:C:104:ILE:HB	1.88	0.54
1:F:395:LEU:HD12	1:F:395:LEU:H	1.71	0.54
1:B:228:PHE:HD2	1:B:338:ILE:CD1	2.21	0.54
1:E:740:THR:HG22	1:E:751:TYR:CZ	2.42	0.54
1:D:541:ASP:OD2	1:D:741:HIS:HE1	1.91	0.54
1:C:600:ARG:NH1	1:C:603:ILE:O	2.41	0.54
1:F:259:CYS:O	1:F:263:VAL:HG23	2.07	0.54
1:C:20:MET:CE	1:C:43:HIS:O	2.56	0.54
1:A:160:ILE:CG2	1:A:200:VAL:HG11	2.38	0.54
1:F:120:ILE:HD12	1:F:121:LYS:HG2	1.90	0.54
1:E:623:TYR:HB3	1:E:627:VAL:HG21	1.90	0.54
1:G:177:LYS:O	1:G:180:VAL:HG23	2.08	0.54
1:D:597:GLU:OE1	1:D:971:LYS:NZ	2.26	0.54
1:H:25:GLU:HG3	1:G:414:ARG:HD3	1.89	0.54
1:A:126:ALA:HB1	1:A:131:ILE:HD11	1.90	0.54
1:B:600:ARG:NH1	1:B:603:ILE:O	2.41	0.54
1:H:862:VAL:O	1:H:866:MET:HG2	2.08	0.54
1:C:160:ILE:CG2	1:C:200:VAL:HG11	2.38	0.54
1:H:597:GLU:OE1	1:H:971:LYS:NZ	2.26	0.54
1:E:472:TYR:OH	1:E:1004:PHE:CD2	2.60	0.54
1:F:502:TYR:CD1	1:F:503:GLY:N	2.76	0.54
1:H:509:GLY:N	1:H:512:GLN:OE1	2.39	0.54
1:G:259:CYS:O	1:G:263:VAL:HG23	2.08	0.54
1:F:870:ILE:O	1:F:872:LYS:NZ	2.39	0.54
1:E:278:GLU:CB	1:E:289:ILE:HG13	2.38	0.54
1:B:209:PRO:CB	1:B:280:LEU:HD23	2.38	0.54
1:F:63:TYR:HB2	1:F:87:PHE:CD2	2.43	0.54
1:A:571:PHE:CD2	1:A:572:SER:HB3	2.44	0.54
1:B:278:GLU:CB	1:B:289:ILE:HG13	2.38	0.53
1:E:147:VAL:HG11	1:E:180:VAL:CG1	2.38	0.53
1:E:228:PHE:HD2	1:E:338:ILE:CD1	2.21	0.53
1:D:862:VAL:O	1:D:866:MET:HG2	2.08	0.53
1:E:160:ILE:HD11	1:E:174:VAL:CG2	2.38	0.53
1:E:321:TYR:HB3	1:E:325:ASP:OD2	2.08	0.53
1:A:259:CYS:O	1:A:263:VAL:HG23	2.08	0.53
1:B:160:ILE:HD12	1:B:174:VAL:CG2	2.37	0.53
1:F:66:ILE:HG23	1:F:94:PHE:CD1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:TYR:HB3	1:A:627:VAL:HG21	1.88	0.53
1:A:134:ILE:CD1	1:A:287:TYR:HB3	2.37	0.53
1:B:53:VAL:HG13	1:B:54:GLY:H	1.72	0.53
1:F:908:ASP:O	1:F:912:GLU:HG3	2.07	0.53
1:G:609:GLN:HE22	1:G:737:HIS:HE1	1.54	0.53
1:E:266:MET:HE2	1:E:277:VAL:CG2	2.37	0.53
1:E:600:ARG:NH1	1:E:603:ILE:O	2.41	0.53
1:B:321:TYR:HB3	1:B:325:ASP:OD2	2.09	0.53
1:H:53:VAL:HG13	1:H:54:GLY:H	1.73	0.53
1:A:870:ILE:O	1:A:872:LYS:NZ	2.40	0.53
1:A:849:LEU:HD12	1:A:849:LEU:N	2.22	0.53
1:G:600:ARG:NH1	1:G:603:ILE:O	2.41	0.53
1:F:849:LEU:HD12	1:F:849:LEU:N	2.22	0.53
1:E:120:ILE:HD12	1:E:140:PRO:HG3	1.89	0.53
1:B:81:ILE:O	1:B:106:VAL:CG2	2.57	0.53
1:A:225:VAL:HG13	1:A:333:GLN:NE2	2.23	0.53
1:D:622:ASN:ND2	1:D:917:GLU:O	2.41	0.53
1:F:571:PHE:CD2	1:F:572:SER:HB3	2.44	0.53
1:D:414:ARG:HD3	1:C:25:GLU:HG3	1.89	0.53
1:D:304:MET:HE3	1:D:342:ALA:HB1	1.90	0.53
1:C:228:PHE:CD2	1:C:338:ILE:CG1	2.92	0.53
1:A:134:ILE:HG22	1:A:203:GLU:HB3	1.89	0.53
1:A:120:ILE:HD12	1:A:121:LYS:HG2	1.91	0.53
1:G:195:PHE:CD2	1:G:195:PHE:N	2.76	0.53
1:D:225:VAL:HG13	1:D:333:GLN:NE2	2.23	0.53
1:C:620:TYR:HD2	1:C:621:LYS:N	2.06	0.53
1:D:571:PHE:CD2	1:D:572:SER:HB3	2.44	0.53
1:D:509:GLY:N	1:D:512:GLN:OE1	2.40	0.53
1:F:597:GLU:OE1	1:F:971:LYS:NZ	2.26	0.53
1:G:219:ASP:CB	1:G:323:LEU:HD23	2.26	0.53
1:F:126:ALA:HB1	1:F:131:ILE:HD11	1.90	0.53
1:F:54:GLY:HA3	1:F:62:ALA:HB1	1.91	0.53
1:E:81:ILE:O	1:E:106:VAL:CG2	2.57	0.53
1:F:134:ILE:CD1	1:F:287:TYR:HB2	2.39	0.53
1:A:134:ILE:CD1	1:A:287:TYR:HB2	2.38	0.53
1:D:53:VAL:HG13	1:D:54:GLY:H	1.73	0.53
1:F:177:LYS:O	1:F:180:VAL:HG23	2.09	0.53
1:D:788:GLY:N	1:A:719:GLN:HG2	2.24	0.53
1:G:1059:ASN:N	1:G:1059:ASN:OD1	2.41	0.53
1:A:395:LEU:HD12	1:A:395:LEU:H	1.73	0.53
1:H:304:MET:HE3	1:H:342:ALA:HB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:740:THR:HG22	1:D:751:TYR:CZ	2.44	0.53
1:A:567:LEU:N	1:A:568:PRO:CD	2.71	0.53
1:D:251:THR:HG23	1:D:254:LEU:HB2	1.91	0.53
1:F:134:ILE:HG22	1:F:203:GLU:HB3	1.90	0.53
1:H:120:ILE:HD12	1:H:121:LYS:HG2	1.90	0.53
1:H:740:THR:HG22	1:H:751:TYR:CZ	2.44	0.53
1:F:541:ASP:OD2	1:F:741:HIS:HE1	1.92	0.53
1:F:225:VAL:HG13	1:F:333:GLN:NE2	2.24	0.53
1:D:213:GLU:OE2	1:D:232:CYS:SG	2.55	0.53
1:E:752:ALA:HB1	1:G:749:TYR:CZ	2.43	0.53
1:H:1059:ASN:N	1:H:1059:ASN:OD1	2.42	0.53
1:D:1059:ASN:OD1	1:D:1059:ASN:N	2.42	0.53
1:E:280:LEU:CD1	1:E:289:ILE:HG22	2.37	0.53
1:H:251:THR:HG23	1:H:254:LEU:HB2	1.91	0.53
1:F:251:THR:HG23	1:F:254:LEU:HB2	1.90	0.53
1:G:509:GLY:N	1:G:512:GLN:OE1	2.39	0.53
1:A:66:ILE:HG23	1:A:94:PHE:CD1	2.44	0.52
1:G:540:ARG:NH2	1:G:541:ASP:HA	2.25	0.52
1:E:53:VAL:HG13	1:E:54:GLY:H	1.73	0.52
1:F:195:PHE:N	1:F:195:PHE:CD2	2.77	0.52
1:D:228:PHE:CE2	1:D:338:ILE:HG13	2.44	0.52
1:G:227:LEU:HD21	1:G:308:ILE:HD12	1.91	0.52
1:A:1010:LEU:HA	1:A:1028:LEU:HD23	1.91	0.52
1:C:609:GLN:HE22	1:C:737:HIS:HE1	1.55	0.52
1:F:551:VAL:HA	1:F:813:TYR:CE2	2.44	0.52
1:F:475:ASN:HA	1:F:1055:ILE:HG21	1.92	0.52
1:F:2:ASN:HB2	1:F:321:TYR:OH	2.10	0.52
1:A:251:THR:HG23	1:A:254:LEU:HB2	1.90	0.52
1:A:54:GLY:HA3	1:A:62:ALA:HB1	1.91	0.52
1:D:1010:LEU:HA	1:D:1028:LEU:HD23	1.91	0.52
1:A:551:VAL:HA	1:A:813:TYR:CE2	2.44	0.52
1:B:266:MET:HE2	1:B:277:VAL:CG2	2.38	0.52
1:E:251:THR:HG23	1:E:254:LEU:HB2	1.90	0.52
1:A:541:ASP:OD2	1:A:741:HIS:HE1	1.92	0.52
1:A:53:VAL:HG13	1:A:54:GLY:H	1.74	0.52
1:F:509:GLY:N	1:F:512:GLN:OE1	2.40	0.52
1:B:280:LEU:CD1	1:B:289:ILE:HG22	2.38	0.52
1:E:143:GLY:O	1:E:147:VAL:HG23	2.10	0.52
1:H:134:ILE:CD1	1:H:287:TYR:HB2	2.39	0.52
1:H:134:ILE:CD1	1:H:287:TYR:HB3	2.36	0.52
1:G:160:ILE:CG2	1:G:200:VAL:CG1	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:HIS:ND1	1:B:259:CYS:HB3	2.24	0.52
1:E:472:TYR:OH	1:E:1004:PHE:O	2.27	0.52
1:F:230:ARG:NH2	1:F:296:GLN:OE1	2.43	0.52
1:A:195:PHE:N	1:A:195:PHE:CD2	2.78	0.52
1:D:996:VAL:O	1:D:999:LEU:HD12	2.09	0.52
1:C:304:MET:HE3	1:C:342:ALA:HB1	1.91	0.52
1:F:53:VAL:HG13	1:F:54:GLY:H	1.74	0.52
1:A:230:ARG:NH2	1:A:296:GLN:OE1	2.43	0.52
1:A:177:LYS:O	1:A:180:VAL:HG23	2.09	0.52
1:D:230:ARG:NH2	1:D:296:GLN:OE1	2.42	0.52
1:C:1059:ASN:OD1	1:C:1059:ASN:N	2.42	0.52
1:C:219:ASP:CB	1:C:323:LEU:HD23	2.28	0.52
1:D:134:ILE:CD1	1:D:287:TYR:HB2	2.39	0.52
1:D:120:ILE:HD12	1:D:121:LYS:HG2	1.91	0.52
1:C:251:THR:HG23	1:C:254:LEU:HB2	1.90	0.52
1:F:1041:VAL:CG1	1:F:1043:TYR:CE1	2.92	0.52
1:E:54:GLY:HA3	1:E:62:ALA:HB1	1.90	0.52
1:D:54:GLY:HA3	1:D:62:ALA:HB1	1.91	0.52
1:C:213:GLU:OE2	1:C:232:CYS:SG	2.54	0.52
1:B:160:ILE:CD1	1:B:174:VAL:HG23	2.39	0.52
1:G:251:THR:HG23	1:G:254:LEU:HB2	1.90	0.52
1:H:996:VAL:O	1:H:999:LEU:HD12	2.10	0.52
1:C:996:VAL:O	1:C:999:LEU:HD12	2.09	0.52
1:C:160:ILE:CG2	1:C:200:VAL:CG1	2.88	0.52
1:A:2:ASN:HB2	1:A:321:TYR:OH	2.10	0.52
1:G:164:LEU:HD22	1:G:195:PHE:CZ	2.44	0.52
1:H:225:VAL:HG13	1:H:333:GLN:NE2	2.25	0.52
1:B:472:TYR:OH	1:B:1004:PHE:O	2.28	0.52
1:A:996:VAL:O	1:A:999:LEU:HD12	2.09	0.52
1:E:180:VAL:CG1	1:E:184:PHE:HZ	2.14	0.52
1:D:2:ASN:HB2	1:D:321:TYR:OH	2.10	0.52
1:G:250:ILE:CD1	1:G:255:ARG:HB3	2.37	0.52
1:H:177:LYS:O	1:H:180:VAL:HG23	2.10	0.52
1:C:54:GLY:HA3	1:C:62:ALA:HB1	1.92	0.52
1:D:226:HIS:H	1:D:333:GLN:HE22	1.58	0.52
1:C:23:CYS:HB3	1:C:28:ILE:HB	1.92	0.52
1:A:475:ASN:HA	1:A:1055:ILE:HG21	1.92	0.52
1:E:557:PHE:CE1	1:E:598:THR:HB	2.45	0.52
1:E:266:MET:CE	1:E:277:VAL:HG22	2.39	0.51
1:C:367:ARG:NH1	1:C:1049:GLN:CB	2.63	0.51
1:H:541:ASP:OD2	1:H:741:HIS:CE1	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:LYS:CG	1:D:178:GLU:H	2.22	0.51
1:G:54:GLY:HA3	1:G:62:ALA:HB1	1.93	0.51
1:B:54:GLY:HA3	1:B:62:ALA:HB1	1.91	0.51
1:D:465:ARG:CG	1:D:465:ARG:O	2.58	0.51
1:H:115:MET:HG2	1:H:125:GLN:HG3	1.92	0.51
1:F:996:VAL:O	1:F:999:LEU:HD12	2.09	0.51
1:D:475:ASN:HA	1:D:1055:ILE:HG21	1.92	0.51
1:C:509:GLY:N	1:C:512:GLN:OE1	2.40	0.51
1:E:147:VAL:HG21	1:E:184:PHE:HE1	1.74	0.51
1:F:1010:LEU:HA	1:F:1028:LEU:HD23	1.92	0.51
1:G:17:ILE:HA	1:G:20:MET:HG3	1.91	0.51
1:H:54:GLY:HA3	1:H:62:ALA:HB1	1.92	0.51
1:H:226:HIS:H	1:H:333:GLN:HE22	1.58	0.51
1:A:734:VAL:HG12	1:A:735:PRO:HD2	1.92	0.51
1:G:23:CYS:HB3	1:G:28:ILE:HB	1.92	0.51
1:B:557:PHE:CE1	1:B:598:THR:HB	2.45	0.51
1:C:88:LEU:HB3	1:C:94:PHE:CD2	2.38	0.51
1:H:66:ILE:HG23	1:H:94:PHE:HD1	1.75	0.51
1:D:120:ILE:HD12	1:D:121:LYS:H	1.76	0.51
1:B:356:PHE:CD1	1:B:356:PHE:N	2.79	0.51
1:E:540:ARG:NH2	1:E:541:ASP:OD1	2.44	0.51
1:G:225:VAL:HG13	1:G:333:GLN:NE2	2.26	0.51
1:G:228:PHE:CE2	1:G:338:ILE:HG13	2.45	0.51
1:G:996:VAL:O	1:G:999:LEU:HD12	2.09	0.51
1:B:996:VAL:O	1:B:999:LEU:HD12	2.10	0.51
1:H:475:ASN:HA	1:H:1055:ILE:HG21	1.93	0.51
1:E:996:VAL:O	1:E:999:LEU:HD12	2.10	0.51
1:B:158:LEU:CD1	1:B:174:VAL:HB	2.22	0.51
1:G:540:ARG:HH21	1:G:541:ASP:CA	2.23	0.51
1:F:2:ASN:HB3	1:F:319:ASP:OD2	2.11	0.51
1:B:131:ILE:HD12	1:B:132:PRO:O	2.10	0.51
1:H:465:ARG:O	1:H:465:ARG:CG	2.58	0.51
1:E:131:ILE:HD12	1:E:132:PRO:O	2.10	0.51
1:H:1010:LEU:HA	1:H:1028:LEU:HD23	1.92	0.51
1:H:571:PHE:CD2	1:H:572:SER:HB3	2.45	0.51
1:H:93:GLU:O	1:H:96:ARG:HG2	2.11	0.51
1:F:734:VAL:HG12	1:F:735:PRO:HD2	1.93	0.51
1:B:266:MET:CE	1:B:277:VAL:HG22	2.40	0.51
1:B:288:PHE:CD1	1:B:288:PHE:C	2.84	0.51
1:C:194:ALA:C	1:C:195:PHE:HD2	2.14	0.51
1:H:2:ASN:HB2	1:H:321:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:VAL:HG13	1:C:333:GLN:NE2	2.26	0.51
1:F:862:VAL:O	1:F:866:MET:HG2	2.09	0.51
1:F:160:ILE:CG2	1:F:200:VAL:CG1	2.88	0.51
1:B:251:THR:HG23	1:B:254:LEU:HB2	1.91	0.51
1:B:475:ASN:HA	1:B:1055:ILE:HG21	1.92	0.51
1:H:278:GLU:C	1:H:289:ILE:CD1	2.79	0.51
1:C:228:PHE:CD2	1:C:338:ILE:HG13	2.46	0.51
1:A:2:ASN:HB3	1:A:319:ASP:OD2	2.11	0.51
1:E:749:TYR:CZ	1:G:752:ALA:CB	2.94	0.51
1:A:1041:VAL:CG1	1:A:1043:TYR:CE1	2.93	0.51
1:D:754:ALA:HB1	1:D:759:VAL:HG11	1.92	0.51
1:G:183:SER:HA	1:G:186:ARG:HD2	1.92	0.51
1:E:475:ASN:HA	1:E:1055:ILE:HG21	1.92	0.51
1:C:183:SER:HA	1:C:186:ARG:HD2	1.92	0.51
1:E:279:PHE:C	1:E:289:ILE:HD12	2.26	0.51
1:H:120:ILE:HD12	1:H:121:LYS:H	1.76	0.51
1:A:506:ILE:CD1	1:A:565:HIS:CE1	2.93	0.51
1:E:675:TYR:CE2	1:E:716:LEU:CD1	2.93	0.51
1:A:509:GLY:N	1:A:512:GLN:OE1	2.41	0.51
1:D:93:GLU:O	1:D:96:ARG:HG2	2.11	0.51
1:B:279:PHE:C	1:B:289:ILE:HD12	2.26	0.51
1:E:180:VAL:O	1:E:184:PHE:CE2	2.64	0.51
1:C:250:ILE:CD1	1:C:255:ARG:HB3	2.37	0.51
1:B:552:ARG:HD2	1:B:1004:PHE:CD1	2.46	0.51
1:E:626:ASN:CG	1:E:950:PRO:HB3	2.31	0.51
1:B:626:ASN:CG	1:B:950:PRO:HB3	2.31	0.51
1:H:230:ARG:NH2	1:H:296:GLN:OE1	2.43	0.51
1:D:112:HIS:CE1	1:D:271:TYR:HA	2.46	0.51
1:F:44:ARG:HD3	1:F:45:TYR:CD1	2.46	0.51
1:E:12:ARG:CZ	1:E:391:TYR:CD1	2.94	0.51
1:C:2:ASN:HB3	1:C:319:ASP:OD2	2.11	0.51
1:D:134:ILE:CD1	1:D:287:TYR:HB3	2.38	0.51
1:G:131:ILE:HD12	1:G:132:PRO:O	2.11	0.51
1:C:131:ILE:HD12	1:C:132:PRO:O	2.11	0.51
1:G:134:ILE:HG22	1:G:203:GLU:HB3	1.93	0.51
1:H:754:ALA:HB1	1:H:759:VAL:HG11	1.93	0.51
1:H:354:ASN:HD22	1:H:357:MET:CB	2.23	0.51
1:A:754:ALA:HB1	1:A:759:VAL:HG11	1.93	0.51
1:G:2:ASN:HB3	1:G:319:ASP:OD2	2.12	0.51
1:A:862:VAL:O	1:A:866:MET:HG2	2.10	0.51
1:C:832:MET:HG3	1:C:833:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:LYS:NZ	1:A:641:ASP:CG	2.64	0.51
1:E:226:HIS:H	1:E:333:GLN:HE22	1.58	0.51
1:H:737:HIS:HA	1:H:761:ILE:O	2.11	0.51
1:H:788:GLY:N	1:F:719:GLN:HG2	2.25	0.51
1:B:12:ARG:CZ	1:B:391:TYR:CD1	2.94	0.51
1:A:44:ARG:HD3	1:A:45:TYR:CD1	2.46	0.51
1:A:1059:ASN:N	1:A:1059:ASN:OD1	2.42	0.51
1:H:960:LEU:HD13	1:H:976:TYR:CD2	2.46	0.50
1:A:160:ILE:CG2	1:A:200:VAL:CG1	2.89	0.50
1:D:662:VAL:HB	1:D:669:VAL:HG22	1.93	0.50
1:A:1:MET:HE1	1:A:319:ASP:CB	2.40	0.50
1:F:1:MET:HE1	1:F:319:ASP:CB	2.41	0.50
1:D:541:ASP:OD2	1:D:741:HIS:CE1	2.64	0.50
1:E:752:ALA:CB	1:G:749:TYR:CZ	2.94	0.50
1:C:475:ASN:HA	1:C:1055:ILE:HG21	1.92	0.50
1:D:719:GLN:HG2	1:A:788:GLY:N	2.26	0.50
1:D:115:MET:HG2	1:D:125:GLN:HG3	1.93	0.50
1:F:737:HIS:HA	1:F:761:ILE:O	2.12	0.50
1:E:502:TYR:HD1	1:E:503:GLY:N	2.08	0.50
1:H:112:HIS:CE1	1:H:271:TYR:HA	2.46	0.50
1:D:278:GLU:C	1:D:289:ILE:CD1	2.79	0.50
1:B:228:PHE:CD2	1:B:338:ILE:HD11	2.37	0.50
1:C:510:THR:OG1	1:C:607:MET:CG	2.58	0.50
1:C:651:TRP:NE1	1:C:653:LYS:CB	2.75	0.50
1:B:226:HIS:H	1:B:333:GLN:HE22	1.58	0.50
1:A:215:GLN:C	1:A:216:ILE:HD12	2.32	0.50
1:C:44:ARG:HD3	1:C:45:TYR:CD1	2.46	0.50
1:B:675:TYR:CE2	1:B:716:LEU:CD1	2.94	0.50
1:H:453:THR:HG22	1:H:455:GLU:OE1	2.11	0.50
1:G:475:ASN:HA	1:G:1055:ILE:HG21	1.92	0.50
1:D:44:ARG:HD3	1:D:45:TYR:CE1	2.46	0.50
1:G:127:LEU:HD22	1:G:133:VAL:CG2	2.41	0.50
1:C:120:ILE:HD12	1:C:121:LYS:H	1.76	0.50
1:H:356:PHE:N	1:H:356:PHE:HD1	2.10	0.50
1:E:540:ARG:HH21	1:E:541:ASP:CG	2.15	0.50
1:E:541:ASP:HA	1:E:544:GLN:HB3	1.94	0.50
1:D:453:THR:HG22	1:D:455:GLU:OE1	2.12	0.50
1:E:23:CYS:HB3	1:E:28:ILE:HB	1.92	0.50
1:A:737:HIS:HA	1:A:761:ILE:O	2.12	0.50
1:G:1010:LEU:HA	1:G:1028:LEU:HD23	1.93	0.50
1:F:1059:ASN:OD1	1:F:1059:ASN:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:116:PHE:CD1	1:H:116:PHE:N	2.77	0.50
1:B:180:VAL:CG1	1:B:184:PHE:CZ	2.72	0.50
1:H:42:PHE:HA	1:H:45:TYR:CD2	2.46	0.50
1:H:662:VAL:HB	1:H:669:VAL:HG22	1.94	0.50
1:F:570:MET:HG3	1:F:573:PHE:HE1	1.76	0.50
1:H:428:ILE:HA	1:H:431:LEU:HD12	1.93	0.50
1:G:662:VAL:HB	1:G:669:VAL:HG22	1.93	0.50
1:G:194:ALA:C	1:G:195:PHE:HD2	2.15	0.50
1:G:737:HIS:HA	1:G:761:ILE:O	2.11	0.50
1:C:610:MET:HG2	1:C:640:VAL:HG11	1.94	0.50
1:D:7:VAL:HG11	1:D:23:CYS:SG	2.52	0.50
1:G:112:HIS:O	1:G:116:PHE:HD2	1.95	0.50
1:C:453:THR:HG22	1:C:455:GLU:OE1	2.12	0.50
1:F:219:ASP:CB	1:F:323:LEU:HD23	2.28	0.50
1:H:2:ASN:HB3	1:H:319:ASP:OD2	2.11	0.50
1:C:540:ARG:HH21	1:C:541:ASP:CA	2.24	0.50
1:D:66:ILE:HG23	1:D:94:PHE:HD1	1.76	0.50
1:E:552:ARG:HD2	1:E:1004:PHE:CD1	2.46	0.50
1:C:134:ILE:HG22	1:C:203:GLU:HB3	1.94	0.50
1:E:112:HIS:CE1	1:E:271:TYR:HA	2.47	0.50
1:G:610:MET:HG2	1:G:640:VAL:HG11	1.94	0.50
1:F:754:ALA:HB1	1:F:759:VAL:HG11	1.94	0.50
1:H:44:ARG:HD3	1:H:45:TYR:CE1	2.47	0.50
1:C:304:MET:HE2	1:C:399:CYS:CB	2.41	0.50
1:H:356:PHE:CD1	1:H:356:PHE:N	2.79	0.50
1:G:832:MET:HG3	1:G:833:PRO:HD3	1.94	0.50
1:C:589:ASN:OD1	1:C:989:MET:CE	2.60	0.50
1:G:7:VAL:HG11	1:G:23:CYS:SG	2.52	0.50
1:C:551:VAL:HA	1:C:813:TYR:CE2	2.46	0.50
1:C:1010:LEU:HA	1:C:1028:LEU:HD23	1.93	0.50
1:C:215:GLN:C	1:C:216:ILE:HD12	2.32	0.50
1:F:112:HIS:CE1	1:F:271:TYR:HA	2.47	0.50
1:G:453:THR:HG22	1:G:455:GLU:OE1	2.12	0.50
1:B:23:CYS:HB3	1:B:28:ILE:HB	1.93	0.50
1:H:567:LEU:N	1:H:568:PRO:CD	2.73	0.50
1:D:42:PHE:HA	1:D:45:TYR:CD2	2.46	0.50
1:D:12:ARG:NH1	1:D:391:TYR:CB	2.74	0.50
1:G:589:ASN:OD1	1:G:989:MET:CE	2.60	0.50
1:C:230:ARG:NH2	1:C:296:GLN:OE1	2.45	0.50
1:D:532:VAL:HG12	1:D:791:GLN:O	2.12	0.50
1:B:180:VAL:HG12	1:B:184:PHE:CE1	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ASN:HB3	1:D:319:ASP:OD2	2.11	0.50
1:B:228:PHE:CD2	1:B:338:ILE:CG1	2.95	0.50
1:E:228:PHE:CD2	1:E:338:ILE:CG1	2.95	0.50
1:H:17:ILE:HA	1:H:20:MET:HG3	1.93	0.50
1:H:21:ARG:NH1	1:G:370:GLY:O	2.44	0.50
1:G:510:THR:OG1	1:G:607:MET:CG	2.58	0.50
1:A:134:ILE:CG2	1:A:203:GLU:HB3	2.42	0.50
1:D:176:SER:OG	1:D:177:LYS:HE2	2.12	0.50
1:C:737:HIS:HA	1:C:761:ILE:O	2.12	0.50
1:H:532:VAL:HG12	1:H:791:GLN:O	2.12	0.50
1:D:737:HIS:HA	1:D:761:ILE:O	2.12	0.50
1:F:622:ASN:ND2	1:F:917:GLU:O	2.45	0.50
1:H:719:GLN:HG2	1:F:788:GLY:N	2.27	0.50
1:G:44:ARG:HD3	1:G:45:TYR:CD1	2.47	0.50
1:A:112:HIS:CE1	1:A:271:TYR:HA	2.47	0.50
1:F:541:ASP:OD2	1:F:741:HIS:CE1	2.65	0.49
1:A:226:HIS:H	1:A:333:GLN:HE22	1.58	0.49
1:C:7:VAL:HG11	1:C:23:CYS:SG	2.52	0.49
1:B:134:ILE:HD12	1:B:287:TYR:CB	2.42	0.49
1:E:428:ILE:HA	1:E:431:LEU:HD12	1.94	0.49
1:D:116:PHE:CD1	1:D:116:PHE:N	2.77	0.49
1:D:546:LEU:CD1	1:D:774:SER:HB2	2.42	0.49
1:E:356:PHE:N	1:E:356:PHE:CD1	2.81	0.49
1:B:540:ARG:HA	1:B:543:HIS:HE2	1.77	0.49
1:A:570:MET:HG3	1:A:573:PHE:HE1	1.77	0.49
1:G:213:GLU:O	1:G:229:GLU:HA	2.12	0.49
1:G:428:ILE:HA	1:G:431:LEU:HD12	1.93	0.49
1:H:265:LEU:HG	1:H:266:MET:HE2	1.94	0.49
1:B:177:LYS:O	1:B:178:GLU:CB	2.60	0.49
1:F:532:VAL:HG12	1:F:791:GLN:O	2.12	0.49
1:G:111:LYS:O	1:G:115:MET:HG2	2.12	0.49
1:F:134:ILE:CG2	1:F:203:GLU:HB3	2.43	0.49
1:D:356:PHE:N	1:D:356:PHE:CD1	2.80	0.49
1:C:662:VAL:HB	1:C:669:VAL:HG22	1.94	0.49
1:C:546:LEU:CD1	1:C:774:SER:HB2	2.43	0.49
1:F:712:MET:O	1:F:741:HIS:HD2	1.95	0.49
1:C:356:PHE:N	1:C:356:PHE:CD1	2.81	0.49
1:E:546:LEU:CD1	1:E:774:SER:HB2	2.43	0.49
1:F:42:PHE:HA	1:F:45:TYR:CD2	2.47	0.49
1:F:428:ILE:HA	1:F:431:LEU:HD12	1.94	0.49
1:B:754:ALA:HB1	1:B:759:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:754:ALA:HB1	1:E:759:VAL:HG11	1.94	0.49
1:E:1010:LEU:HA	1:E:1028:LEU:HD23	1.94	0.49
1:H:7:VAL:HG11	1:H:23:CYS:SG	2.52	0.49
1:D:17:ILE:HA	1:D:20:MET:HG3	1.94	0.49
1:C:226:HIS:H	1:C:333:GLN:HE22	1.58	0.49
1:D:370:GLY:C	1:C:21:ARG:HH12	2.14	0.49
1:B:356:PHE:N	1:B:356:PHE:HD1	2.09	0.49
1:F:226:HIS:H	1:F:333:GLN:HE22	1.59	0.49
1:D:213:GLU:O	1:D:229:GLU:HA	2.12	0.49
1:H:708:GLY:HA2	1:H:737:HIS:O	2.12	0.49
1:H:851:ASP:OD2	1:H:852:ARG:N	2.45	0.49
1:B:1010:LEU:HA	1:B:1028:LEU:HD23	1.94	0.49
1:C:112:HIS:O	1:C:116:PHE:HD2	1.96	0.49
1:D:428:ILE:HA	1:D:431:LEU:HD12	1.94	0.49
1:G:754:ALA:HB1	1:G:759:VAL:HG11	1.94	0.49
1:H:474:GLY:O	1:H:478:VAL:HG23	2.12	0.49
1:G:88:LEU:HB3	1:G:94:PHE:CD2	2.39	0.49
1:C:540:ARG:NH2	1:C:541:ASP:HA	2.26	0.49
1:G:520:GLU:OE1	1:G:705:HIS:NE2	2.45	0.49
1:C:127:LEU:HD22	1:C:133:VAL:CG2	2.42	0.49
1:C:17:ILE:HA	1:C:20:MET:HG3	1.94	0.49
1:H:546:LEU:CD1	1:H:774:SER:HB2	2.42	0.49
1:A:541:ASP:OD2	1:A:741:HIS:CE1	2.66	0.49
1:H:12:ARG:NH1	1:H:391:TYR:CB	2.75	0.49
1:A:563:MET:HB3	1:A:573:PHE:HE2	1.75	0.49
1:A:42:PHE:HA	1:A:45:TYR:CD2	2.47	0.49
1:G:230:ARG:NH2	1:G:296:GLN:OE1	2.46	0.49
1:A:622:ASN:ND2	1:A:917:GLU:O	2.46	0.49
1:F:111:LYS:O	1:F:115:MET:HG2	2.12	0.49
1:B:112:HIS:CE1	1:B:271:TYR:HA	2.47	0.49
1:B:567:LEU:N	1:B:568:PRO:CD	2.75	0.49
1:B:603:ILE:CD1	1:B:608:PHE:CZ	2.95	0.49
1:G:176:SER:O	1:G:179:HIS:CD2	2.65	0.49
1:A:370:GLY:C	1:B:21:ARG:HH12	2.16	0.49
1:H:176:SER:OG	1:H:177:LYS:HE2	2.12	0.49
1:D:356:PHE:N	1:D:356:PHE:HD1	2.11	0.49
1:G:546:LEU:CD1	1:G:774:SER:HB2	2.43	0.49
1:G:356:PHE:CD1	1:G:356:PHE:N	2.81	0.49
1:B:541:ASP:HA	1:B:544:GLN:HB3	1.95	0.49
1:E:226:HIS:ND1	1:E:259:CYS:HB3	2.27	0.49
1:G:215:GLN:C	1:G:216:ILE:HD12	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:551:VAL:HA	1:G:813:TYR:CE2	2.47	0.49
1:A:453:THR:HG22	1:A:455:GLU:OE1	2.12	0.49
1:B:368:SER:HA	1:B:419:PHE:CE1	2.48	0.49
1:G:519:PRO:HB2	1:G:705:HIS:HE2	1.76	0.49
1:C:520:GLU:OE1	1:C:705:HIS:NE2	2.46	0.49
1:E:228:PHE:CD2	1:E:338:ILE:HG13	2.48	0.49
1:H:540:ARG:O	1:H:542:ALA:N	2.43	0.49
1:B:546:LEU:CD1	1:B:774:SER:HB2	2.43	0.49
1:A:226:HIS:ND1	1:A:259:CYS:HB3	2.28	0.49
1:G:182:GLU:O	1:G:186:ARG:HD2	2.13	0.49
1:F:708:GLY:HA2	1:F:737:HIS:O	2.13	0.49
1:H:23:CYS:HB3	1:H:28:ILE:HB	1.95	0.49
1:B:112:HIS:O	1:B:116:PHE:HD2	1.95	0.49
1:C:754:ALA:HB1	1:C:759:VAL:HG11	1.94	0.49
1:G:532:VAL:HG12	1:G:791:GLN:O	2.13	0.49
1:G:437:HIS:CE1	1:G:439:ASP:HB2	2.48	0.49
1:D:851:ASP:OD2	1:D:852:ARG:N	2.45	0.49
1:E:567:LEU:N	1:E:568:PRO:CD	2.75	0.49
1:B:428:ILE:HA	1:B:431:LEU:HD12	1.95	0.49
1:E:215:GLN:C	1:E:216:ILE:HD12	2.33	0.49
1:B:510:THR:OG1	1:B:607:MET:CG	2.59	0.49
1:A:511:LYS:NZ	1:A:641:ASP:OD2	2.46	0.49
1:E:7:VAL:HG11	1:E:23:CYS:SG	2.53	0.49
1:G:112:HIS:CE1	1:G:271:TYR:HA	2.47	0.49
1:E:112:HIS:O	1:E:116:PHE:HD2	1.95	0.49
1:A:532:VAL:HG12	1:A:791:GLN:O	2.12	0.49
1:D:567:LEU:N	1:D:568:PRO:CD	2.74	0.49
1:F:453:THR:HG22	1:F:455:GLU:OE1	2.12	0.49
1:A:111:LYS:O	1:A:115:MET:HG2	2.13	0.49
1:C:519:PRO:HB2	1:C:705:HIS:HE2	1.75	0.49
1:D:960:LEU:HD13	1:D:976:TYR:CD2	2.47	0.49
1:D:540:ARG:O	1:D:542:ALA:N	2.43	0.49
1:E:225:VAL:HG13	1:E:333:GLN:NE2	2.28	0.49
1:A:708:GLY:HA2	1:A:737:HIS:O	2.13	0.49
1:D:23:CYS:HB3	1:D:28:ILE:HB	1.95	0.49
1:E:708:GLY:HA2	1:E:737:HIS:O	2.13	0.49
1:C:532:VAL:HG12	1:C:791:GLN:O	2.13	0.49
1:E:64:LEU:CD2	1:E:88:LEU:CD2	2.91	0.49
1:A:712:MET:O	1:A:741:HIS:HD2	1.96	0.49
1:F:534:LEU:O	1:F:570:MET:HE3	2.12	0.49
1:F:213:GLU:O	1:F:229:GLU:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:226:HIS:H	1:G:333:GLN:HE22	1.58	0.49
1:C:182:GLU:O	1:C:186:ARG:HD2	2.13	0.49
1:D:708:GLY:HA2	1:D:737:HIS:O	2.13	0.49
1:C:112:HIS:CE1	1:C:271:TYR:HA	2.47	0.49
1:C:111:LYS:O	1:C:115:MET:HG2	2.13	0.49
1:F:23:CYS:HB3	1:F:28:ILE:HB	1.94	0.49
1:F:918:ILE:HD12	1:F:919:GLY:H	1.78	0.49
1:B:708:GLY:HA2	1:B:737:HIS:O	2.13	0.49
1:H:918:ILE:HD12	1:H:919:GLY:H	1.77	0.49
1:A:7:VAL:HG11	1:A:23:CYS:SG	2.53	0.49
1:H:42:PHE:HA	1:H:45:TYR:HD2	1.78	0.48
1:D:620:TYR:CE2	1:D:621:LYS:HE3	2.47	0.48
1:F:563:MET:HB3	1:F:573:PHE:HE2	1.76	0.48
1:C:213:GLU:O	1:C:229:GLU:HA	2.13	0.48
1:A:709:ILE:HB	1:A:738:LEU:CD1	2.43	0.48
1:F:215:GLN:C	1:F:216:ILE:HD12	2.34	0.48
1:B:44:ARG:HD3	1:B:45:TYR:CD1	2.47	0.48
1:E:288:PHE:C	1:E:288:PHE:CD1	2.87	0.48
1:D:42:PHE:HA	1:D:45:TYR:HD2	1.78	0.48
1:F:662:VAL:HB	1:F:669:VAL:HG22	1.95	0.48
1:D:541:ASP:HA	1:D:544:GLN:HB3	1.94	0.48
1:C:356:PHE:HD1	1:C:356:PHE:N	2.12	0.48
1:A:546:LEU:CD1	1:A:774:SER:HB2	2.42	0.48
1:H:226:HIS:ND1	1:H:259:CYS:HB3	2.28	0.48
1:F:226:HIS:ND1	1:F:259:CYS:HB3	2.28	0.48
1:B:7:VAL:HG11	1:B:23:CYS:SG	2.53	0.48
1:F:709:ILE:HB	1:F:738:LEU:CD1	2.43	0.48
1:A:918:ILE:HD12	1:A:919:GLY:H	1.78	0.48
1:C:12:ARG:NH1	1:C:38:ASP:OD2	2.46	0.48
1:C:960:LEU:HD11	1:C:968:PRO:CG	2.36	0.48
1:H:712:MET:O	1:H:741:HIS:HD2	1.96	0.48
1:H:611:LEU:HD11	1:H:646:PHE:CD1	2.48	0.48
1:A:213:GLU:O	1:A:229:GLU:HA	2.12	0.48
1:B:12:ARG:CZ	1:B:391:TYR:HD1	2.25	0.48
1:G:42:PHE:HA	1:G:45:TYR:CD2	2.47	0.48
1:A:228:PHE:CE2	1:A:338:ILE:HG13	2.48	0.48
1:B:532:VAL:HG12	1:B:791:GLN:O	2.12	0.48
1:D:215:GLN:C	1:D:216:ILE:HD12	2.34	0.48
1:E:532:VAL:HG12	1:E:791:GLN:O	2.12	0.48
1:D:534:LEU:O	1:D:570:MET:HE3	2.12	0.48
1:G:960:LEU:HD11	1:G:968:PRO:CG	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:TYR:CB	1:A:157:PRO:HD3	2.43	0.48
1:A:21:ARG:HH12	1:B:370:GLY:C	2.17	0.48
1:F:546:LEU:CD1	1:F:774:SER:HB2	2.42	0.48
1:G:356:PHE:HD1	1:G:356:PHE:N	2.12	0.48
1:D:611:LEU:HD11	1:D:646:PHE:CD1	2.48	0.48
1:A:23:CYS:HB3	1:A:28:ILE:HB	1.95	0.48
1:F:228:PHE:CE2	1:F:338:ILE:HG13	2.48	0.48
1:E:44:ARG:HD3	1:E:45:TYR:CD1	2.48	0.48
1:F:611:LEU:HD11	1:F:646:PHE:CD1	2.48	0.48
1:A:534:LEU:O	1:A:570:MET:HE3	2.13	0.48
1:G:182:GLU:O	1:G:186:ARG:NE	2.45	0.48
1:E:12:ARG:CZ	1:E:391:TYR:HD1	2.25	0.48
1:A:533:LEU:O	1:A:761:ILE:HA	2.14	0.48
1:H:213:GLU:OE2	1:H:232:CYS:SG	2.55	0.48
1:D:474:GLY:O	1:D:478:VAL:HG23	2.13	0.48
1:G:992:LYS:HE3	1:G:993:TYR:CZ	2.47	0.48
1:G:12:ARG:NH1	1:G:38:ASP:OD2	2.47	0.48
1:B:662:VAL:HB	1:B:669:VAL:HG22	1.94	0.48
1:G:473:ILE:O	1:G:477:THR:OG1	2.26	0.48
1:G:567:LEU:N	1:G:568:PRO:CD	2.76	0.48
1:G:960:LEU:C	1:G:960:LEU:HD13	2.33	0.48
1:C:960:LEU:C	1:C:960:LEU:HD13	2.33	0.48
1:E:603:ILE:CD1	1:E:608:PHE:CZ	2.96	0.48
1:C:1:MET:HE1	1:C:319:ASP:CB	2.42	0.48
1:B:64:LEU:CD2	1:B:88:LEU:CD2	2.91	0.48
1:B:82:HIS:CD2	1:B:84:GLY:H	2.23	0.48
1:B:228:PHE:CD2	1:B:338:ILE:HG13	2.48	0.48
1:A:611:LEU:HD11	1:A:646:PHE:CD1	2.48	0.48
1:B:626:ASN:ND2	1:B:950:PRO:HB3	2.28	0.48
1:F:7:VAL:HG11	1:F:23:CYS:SG	2.54	0.48
1:H:213:GLU:O	1:H:229:GLU:HA	2.14	0.48
1:C:473:ILE:O	1:C:477:THR:OG1	2.26	0.48
1:H:534:LEU:O	1:H:570:MET:HE3	2.13	0.48
1:F:473:ILE:O	1:F:477:THR:OG1	2.26	0.48
1:C:992:LYS:HE3	1:C:993:TYR:CZ	2.48	0.48
1:B:180:VAL:O	1:B:184:PHE:CE2	2.67	0.48
1:D:712:MET:O	1:D:741:HIS:HD2	1.96	0.48
1:E:626:ASN:ND2	1:E:950:PRO:HB3	2.28	0.48
1:E:737:HIS:HA	1:E:761:ILE:O	2.13	0.48
1:B:737:HIS:HA	1:B:761:ILE:O	2.13	0.48
1:G:144:ILE:HG23	1:G:184:PHE:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:HIS:CE1	1:D:439:ASP:HB2	2.49	0.48
1:G:1:MET:HE1	1:G:319:ASP:CB	2.43	0.48
1:C:176:SER:O	1:C:179:HIS:CD2	2.66	0.48
1:F:42:PHE:HA	1:F:45:TYR:HD2	1.78	0.48
1:F:533:LEU:O	1:F:761:ILE:HA	2.14	0.48
1:D:265:LEU:HG	1:D:266:MET:HE2	1.95	0.48
1:D:918:ILE:HD12	1:D:919:GLY:H	1.78	0.48
1:C:963:LYS:HA	1:C:963:LYS:HE3	1.96	0.48
1:B:144:ILE:HD12	1:B:145:LYS:H	1.79	0.48
1:F:120:ILE:HD12	1:F:121:LYS:H	1.76	0.48
1:C:175:GLU:HG3	1:C:179:HIS:CD2	2.48	0.48
1:F:541:ASP:HA	1:F:544:GLN:HB3	1.95	0.48
1:B:749:TYR:CZ	1:C:752:ALA:CB	2.97	0.48
1:E:662:VAL:HB	1:E:669:VAL:HG22	1.94	0.48
1:C:428:ILE:HA	1:C:431:LEU:HD12	1.94	0.48
1:C:437:HIS:CE1	1:C:439:ASP:HB2	2.49	0.48
1:D:354:ASN:HD22	1:D:357:MET:CB	2.26	0.48
1:E:280:LEU:N	1:E:289:ILE:CD1	2.74	0.48
1:A:541:ASP:HA	1:A:544:GLN:HB3	1.95	0.48
1:H:370:GLY:C	1:G:21:ARG:NH1	2.68	0.48
1:F:1041:VAL:HG11	1:F:1043:TYR:HE1	1.77	0.48
1:C:42:PHE:HA	1:C:45:TYR:CD2	2.48	0.48
1:A:112:HIS:O	1:A:116:PHE:HD2	1.95	0.48
1:A:428:ILE:HA	1:A:431:LEU:HD12	1.96	0.48
1:H:437:HIS:CE1	1:H:439:ASP:HB2	2.49	0.48
1:H:709:ILE:HB	1:H:738:LEU:CD1	2.44	0.48
1:H:1:MET:HE1	1:H:319:ASP:CB	2.43	0.47
1:F:347:ILE:O	1:F:395:LEU:CD1	2.55	0.47
1:C:510:THR:OG1	1:C:607:MET:SD	2.71	0.47
1:F:511:LYS:NZ	1:F:641:ASP:CG	2.64	0.47
1:F:370:GLY:C	1:E:21:ARG:HH12	2.18	0.47
1:G:120:ILE:HD12	1:G:121:LYS:H	1.79	0.47
1:G:651:TRP:NE1	1:G:653:LYS:CB	2.77	0.47
1:D:226:HIS:ND1	1:D:259:CYS:HB3	2.29	0.47
1:G:533:LEU:O	1:G:761:ILE:HA	2.14	0.47
1:H:559:ILE:HD13	1:H:805:TYR:CG	2.49	0.47
1:B:180:VAL:CG1	1:B:184:PHE:HZ	2.17	0.47
1:A:662:VAL:HB	1:A:669:VAL:HG22	1.95	0.47
1:C:533:LEU:O	1:C:761:ILE:HA	2.15	0.47
1:E:675:TYR:CE2	1:E:716:LEU:HD12	2.49	0.47
1:G:42:PHE:HA	1:G:45:TYR:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HE1	1:D:319:ASP:CB	2.43	0.47
1:E:64:LEU:HD23	1:E:88:LEU:CD2	2.44	0.47
1:H:82:HIS:CD2	1:H:84:GLY:H	2.24	0.47
1:A:194:ALA:HB1	1:A:195:PHE:CE2	2.49	0.47
1:C:182:GLU:O	1:C:186:ARG:NE	2.46	0.47
1:G:144:ILE:HA	1:G:184:PHE:CE2	2.50	0.47
1:B:752:ALA:HB1	1:C:749:TYR:CZ	2.48	0.47
1:E:368:SER:HA	1:E:419:PHE:CE1	2.49	0.47
1:H:610:MET:HG2	1:H:640:VAL:HG11	1.95	0.47
1:E:509:GLY:HA3	1:E:605:ASN:O	2.14	0.47
1:B:280:LEU:N	1:B:289:ILE:CD1	2.75	0.47
1:G:510:THR:OG1	1:G:607:MET:SD	2.71	0.47
1:H:64:LEU:CD2	1:H:88:LEU:CD2	2.92	0.47
1:H:898:TYR:HD1	1:H:928:LYS:HE2	1.77	0.47
1:D:176:SER:O	1:D:179:HIS:ND1	2.26	0.47
1:F:112:HIS:O	1:F:116:PHE:HD2	1.96	0.47
1:F:437:HIS:CE1	1:F:439:ASP:HB2	2.49	0.47
1:B:1:MET:HE2	1:B:4:ILE:O	2.13	0.47
1:E:356:PHE:N	1:E:356:PHE:HD1	2.11	0.47
1:F:509:GLY:HA3	1:F:605:ASN:O	2.14	0.47
1:C:509:GLY:HA3	1:C:605:ASN:O	2.14	0.47
1:C:567:LEU:N	1:C:568:PRO:CD	2.77	0.47
1:E:354:ASN:ND2	1:E:357:MET:HB3	2.29	0.47
1:B:215:GLN:C	1:B:216:ILE:HD12	2.35	0.47
1:E:1:MET:HE2	1:E:4:ILE:O	2.14	0.47
1:E:134:ILE:HD12	1:E:287:TYR:CB	2.44	0.47
1:D:709:ILE:HB	1:D:738:LEU:CD1	2.45	0.47
1:H:304:MET:HE2	1:H:399:CYS:CB	2.44	0.47
1:H:620:TYR:CE2	1:H:621:LYS:HE3	2.48	0.47
1:H:352:PRO:HA	1:H:356:PHE:CE1	2.49	0.47
1:B:540:ARG:O	1:B:542:ALA:N	2.46	0.47
1:E:540:ARG:O	1:E:542:ALA:N	2.45	0.47
1:B:225:VAL:HG13	1:B:333:GLN:NE2	2.30	0.47
1:F:996:VAL:O	1:F:997:THR:C	2.53	0.47
1:A:509:GLY:HA3	1:A:605:ASN:O	2.14	0.47
1:A:42:PHE:HA	1:A:45:TYR:HD2	1.79	0.47
1:H:631:PHE:CD2	1:H:631:PHE:C	2.88	0.47
1:D:405:PHE:CD2	1:D:405:PHE:C	2.88	0.47
1:D:369:THR:O	1:D:376:LEU:HD11	2.15	0.47
1:C:3:ARG:CD	1:C:104:ILE:HD11	2.35	0.47
1:C:227:LEU:HD22	1:C:306:THR:HG21	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ILE:O	1:A:395:LEU:CD1	2.55	0.47
1:B:64:LEU:HD23	1:B:88:LEU:CD2	2.44	0.47
1:C:226:HIS:CE1	1:C:259:CYS:HB3	2.49	0.47
1:A:120:ILE:HD12	1:A:121:LYS:H	1.78	0.47
1:H:546:LEU:HD11	1:H:774:SER:HB2	1.97	0.47
1:C:90:GLU:HA	1:C:113:LEU:HD22	1.97	0.47
1:G:509:GLY:HA3	1:G:605:ASN:O	2.14	0.47
1:C:708:GLY:HA2	1:C:737:HIS:O	2.14	0.47
1:B:675:TYR:CE2	1:B:716:LEU:HD12	2.50	0.47
1:E:533:LEU:O	1:E:761:ILE:HA	2.15	0.47
1:B:533:LEU:O	1:B:761:ILE:HA	2.15	0.47
1:E:450:ILE:HG22	1:E:451:ASP:N	2.29	0.47
1:C:778:MET:HG3	1:C:779:THR:N	2.29	0.47
1:G:963:LYS:HA	1:G:963:LYS:HE3	1.96	0.47
1:A:437:HIS:CE1	1:A:439:ASP:HB2	2.50	0.47
1:A:559:ILE:HD13	1:A:805:TYR:CG	2.50	0.47
1:E:1018:LEU:HD11	1:E:1024:LEU:HD11	1.95	0.47
1:H:450:ILE:HG22	1:H:451:ASP:N	2.29	0.47
1:B:559:ILE:HD13	1:B:805:TYR:CG	2.50	0.47
1:E:111:LYS:O	1:E:115:MET:HG2	2.14	0.47
1:G:157:PRO:O	1:G:205:CYS:HB2	2.15	0.47
1:D:559:ILE:HD13	1:D:805:TYR:CG	2.49	0.47
1:D:64:LEU:CD2	1:D:88:LEU:CD2	2.93	0.47
1:B:17:ILE:HA	1:B:20:MET:HG3	1.96	0.47
1:H:541:ASP:HA	1:H:544:GLN:HB3	1.96	0.47
1:E:213:GLU:O	1:E:229:GLU:HA	2.14	0.47
1:F:540:ARG:O	1:F:542:ALA:N	2.45	0.47
1:B:651:TRP:CE2	1:B:920:GLN:HG3	2.50	0.47
1:B:111:LYS:O	1:B:115:MET:HG2	2.14	0.47
1:D:70:ILE:HG21	1:D:101:GLU:HG3	1.96	0.47
1:E:17:ILE:HA	1:E:20:MET:HG3	1.97	0.47
1:H:619:GLY:HA3	1:H:623:TYR:HE2	1.80	0.47
1:A:1041:VAL:HG11	1:A:1043:TYR:HE1	1.78	0.47
1:G:708:GLY:HA2	1:G:737:HIS:O	2.14	0.47
1:F:194:ALA:HB1	1:F:195:PHE:CE2	2.50	0.47
1:E:4:ILE:HD12	1:E:319:ASP:OD1	2.14	0.47
1:E:559:ILE:HD13	1:E:805:TYR:CG	2.50	0.47
1:G:300:THR:O	1:G:303:GLU:HB2	2.14	0.47
1:G:778:MET:HG3	1:G:779:THR:N	2.29	0.47
1:D:610:MET:HG2	1:D:640:VAL:HG11	1.96	0.47
1:H:473:ILE:O	1:H:477:THR:OG1	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:546:LEU:HD11	1:D:774:SER:HB2	1.97	0.47
1:D:116:PHE:HD1	1:D:116:PHE:N	2.13	0.47
1:B:1018:LEU:HD11	1:B:1024:LEU:HD11	1.96	0.47
1:B:1041:VAL:HG22	1:B:1054:ASN:OD1	2.15	0.47
1:E:1041:VAL:HG22	1:E:1054:ASN:OD1	2.15	0.47
1:B:622:ASN:ND2	1:B:917:GLU:O	2.47	0.47
1:H:369:THR:O	1:H:376:LEU:HD11	2.15	0.46
1:G:90:GLU:HA	1:G:113:LEU:HD22	1.97	0.46
1:B:213:GLU:O	1:B:229:GLU:HA	2.14	0.46
1:B:718:PRO:HG2	1:B:749:TYR:CD2	2.50	0.46
1:E:651:TRP:CE2	1:E:920:GLN:HG3	2.50	0.46
1:H:116:PHE:HD1	1:H:116:PHE:N	2.13	0.46
1:G:1041:VAL:HG22	1:G:1054:ASN:OD1	2.15	0.46
1:G:81:ILE:HG13	1:G:103:ILE:HG21	1.97	0.46
1:F:106:VAL:HG13	1:F:318:ALA:HB2	1.97	0.46
1:D:369:THR:HG1	1:D:415:ASN:ND2	2.07	0.46
1:G:134:ILE:HD12	1:G:287:TYR:CB	2.45	0.46
1:C:134:ILE:HD12	1:C:287:TYR:CB	2.45	0.46
1:C:81:ILE:HG13	1:C:103:ILE:HG21	1.97	0.46
1:C:106:VAL:HG13	1:C:318:ALA:HB2	1.97	0.46
1:A:148:GLU:O	1:A:152:GLU:N	2.46	0.46
1:C:300:THR:O	1:C:303:GLU:HB2	2.14	0.46
1:D:300:THR:O	1:D:303:GLU:HB2	2.15	0.46
1:F:369:THR:O	1:F:376:LEU:HD11	2.14	0.46
1:D:82:HIS:CD2	1:D:84:GLY:H	2.25	0.46
1:H:21:ARG:NH1	1:G:370:GLY:C	2.68	0.46
1:A:563:MET:CE	1:A:573:PHE:CE2	2.98	0.46
1:G:20:MET:HE3	1:G:43:HIS:O	2.15	0.46
1:H:509:GLY:HA3	1:H:605:ASN:O	2.16	0.46
1:A:847:VAL:HG11	1:A:889:GLN:OE1	2.15	0.46
1:C:42:PHE:HA	1:C:45:TYR:HD2	1.80	0.46
1:C:1041:VAL:HG22	1:C:1054:ASN:OD1	2.15	0.46
1:A:513:ILE:HD12	1:A:513:ILE:N	2.30	0.46
1:F:21:ARG:HH12	1:E:370:GLY:C	2.19	0.46
1:G:3:ARG:CD	1:G:104:ILE:HD11	2.35	0.46
1:B:70:ILE:HG21	1:B:101:GLU:HG3	1.98	0.46
1:E:70:ILE:HG21	1:E:101:GLU:HG3	1.98	0.46
1:C:20:MET:HE3	1:C:43:HIS:O	2.15	0.46
1:F:1041:VAL:CG1	1:F:1043:TYR:HE1	2.29	0.46
1:G:106:VAL:HG13	1:G:318:ALA:HB2	1.97	0.46
1:B:300:THR:O	1:B:303:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:PRO:HB2	1:A:335:ASP:HB2	1.97	0.46
1:B:509:GLY:HA3	1:B:605:ASN:O	2.15	0.46
1:D:631:PHE:CD2	1:D:631:PHE:C	2.89	0.46
1:H:405:PHE:C	1:H:405:PHE:CD2	2.89	0.46
1:H:319:ASP:OD2	1:H:321:TYR:HE2	1.99	0.46
1:F:620:TYR:CD2	1:F:621:LYS:HB3	2.51	0.46
1:F:1010:LEU:HD21	1:F:1031:ILE:CD1	2.42	0.46
1:B:540:ARG:HA	1:B:543:HIS:NE2	2.31	0.46
1:F:847:VAL:HG11	1:F:889:GLN:OE1	2.16	0.46
1:H:106:VAL:HG13	1:H:318:ALA:HB2	1.97	0.46
1:F:559:ILE:HD13	1:F:805:TYR:CG	2.51	0.46
1:F:513:ILE:N	1:F:513:ILE:HD12	2.30	0.46
1:E:369:THR:O	1:E:376:LEU:HD11	2.16	0.46
1:B:81:ILE:HG13	1:B:103:ILE:HG21	1.96	0.46
1:H:70:ILE:HG21	1:H:101:GLU:HG3	1.97	0.46
1:E:718:PRO:HG2	1:E:749:TYR:CD2	2.50	0.46
1:D:847:VAL:HG11	1:D:889:GLN:OE1	2.15	0.46
1:D:319:ASP:OD2	1:D:321:TYR:HE2	1.99	0.46
1:E:82:HIS:CD2	1:E:84:GLY:H	2.24	0.46
1:C:546:LEU:HD11	1:C:774:SER:HB2	1.97	0.46
1:A:540:ARG:O	1:A:542:ALA:N	2.45	0.46
1:D:509:GLY:HA3	1:D:605:ASN:O	2.16	0.46
1:F:331:PRO:HB2	1:F:335:ASP:HB2	1.98	0.46
1:E:177:LYS:O	1:E:178:GLU:CB	2.62	0.46
1:B:778:MET:HG3	1:B:779:THR:N	2.30	0.46
1:E:300:THR:O	1:E:303:GLU:HB2	2.15	0.46
1:A:369:THR:O	1:A:376:LEU:HD11	2.15	0.46
1:D:304:MET:HE2	1:D:399:CYS:CB	2.46	0.46
1:A:68:ASN:O	1:A:72:ILE:HG13	2.16	0.46
1:F:68:ASN:O	1:F:72:ILE:HG13	2.16	0.46
1:F:546:LEU:HD11	1:F:774:SER:HB2	1.98	0.46
1:A:546:LEU:HD11	1:A:774:SER:HB2	1.98	0.46
1:H:215:GLN:C	1:H:216:ILE:HD12	2.36	0.46
1:D:81:ILE:HG13	1:D:103:ILE:HG21	1.98	0.46
1:A:106:VAL:HG13	1:A:318:ALA:HB2	1.98	0.46
1:E:266:MET:CE	1:E:277:VAL:CG2	2.94	0.46
1:G:576:TRP:CD1	1:G:596:LEU:HD22	2.51	0.46
1:B:369:THR:O	1:B:376:LEU:HD11	2.16	0.46
1:H:541:ASP:OD2	1:H:739:HIS:HE1	1.99	0.46
1:D:619:GLY:HA3	1:D:623:TYR:HE2	1.81	0.46
1:E:546:LEU:HD11	1:E:774:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:996:VAL:O	1:A:997:THR:C	2.54	0.46
1:H:81:ILE:HG13	1:H:103:ILE:HG21	1.98	0.46
1:A:794:LEU:HD12	1:A:795:ASP:O	2.16	0.46
1:E:622:ASN:ND2	1:E:917:GLU:O	2.48	0.46
1:A:893:SER:O	1:A:897:VAL:HG13	2.16	0.46
1:F:794:LEU:HD12	1:F:795:ASP:O	2.16	0.46
1:A:1018:LEU:HD11	1:A:1024:LEU:HD11	1.97	0.46
1:H:280:LEU:HG	1:H:289:ILE:HG12	1.98	0.46
1:C:304:MET:HE2	1:C:399:CYS:HB2	1.98	0.46
1:A:620:TYR:CD2	1:A:621:LYS:HB3	2.51	0.46
1:H:177:LYS:CG	1:H:178:GLU:H	2.25	0.46
1:D:898:TYR:HD1	1:D:928:LYS:HE2	1.77	0.46
1:D:541:ASP:OD2	1:D:739:HIS:HE1	1.99	0.46
1:D:533:LEU:O	1:D:761:ILE:HA	2.15	0.46
1:F:1018:LEU:HD11	1:F:1024:LEU:HD11	1.97	0.46
1:D:257:ARG:NH2	1:D:284:ASP:O	2.49	0.46
1:B:288:PHE:CD1	1:B:289:ILE:N	2.84	0.45
1:C:369:THR:O	1:C:376:LEU:HD11	2.16	0.45
1:F:156:TYR:CB	1:F:157:PRO:HD3	2.46	0.45
1:G:546:LEU:HD11	1:G:774:SER:HB2	1.97	0.45
1:A:541:ASP:OD2	1:A:739:HIS:HE1	1.98	0.45
1:D:12:ARG:HH12	1:D:391:TYR:HB2	1.81	0.45
1:G:226:HIS:ND1	1:G:259:CYS:HB3	2.31	0.45
1:D:106:VAL:HG13	1:D:318:ALA:HB2	1.97	0.45
1:E:778:MET:HG3	1:E:779:THR:N	2.31	0.45
1:E:209:PRO:CG	1:E:280:LEU:HD23	2.47	0.45
1:B:266:MET:CE	1:B:277:VAL:CG2	2.94	0.45
1:B:278:GLU:O	1:B:289:ILE:HG12	2.16	0.45
1:G:369:THR:O	1:G:376:LEU:HD11	2.16	0.45
1:H:3:ARG:CD	1:H:104:ILE:HD11	2.35	0.45
1:B:68:ASN:O	1:B:72:ILE:HG13	2.16	0.45
1:E:155:GLY:O	1:E:158:LEU:HD21	2.15	0.45
1:G:160:ILE:HG22	1:G:200:VAL:HG11	1.97	0.45
1:H:12:ARG:HH12	1:H:391:TYR:HB2	1.82	0.45
1:B:134:ILE:CD1	1:B:287:TYR:CB	2.95	0.45
1:H:847:VAL:HG11	1:H:889:GLN:OE1	2.15	0.45
1:A:610:MET:HG2	1:A:640:VAL:HG11	1.97	0.45
1:F:148:GLU:O	1:F:152:GLU:N	2.47	0.45
1:C:559:ILE:HD13	1:C:805:TYR:CG	2.51	0.45
1:F:17:ILE:HA	1:F:20:MET:HG3	1.98	0.45
1:E:437:HIS:CD2	1:E:439:ASP:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:LEU:HD23	1:H:88:LEU:CD2	2.45	0.45
1:G:365:THR:HG21	1:G:1051:ARG:CD	2.43	0.45
1:H:766:SER:O	1:H:767:SER:C	2.55	0.45
1:C:1018:LEU:HD11	1:C:1024:LEU:HD11	1.97	0.45
1:E:257:ARG:NH2	1:E:284:ASP:O	2.49	0.45
1:G:559:ILE:HD13	1:G:805:TYR:CG	2.51	0.45
1:F:610:MET:HG2	1:F:640:VAL:HG11	1.97	0.45
1:B:448:SER:O	1:B:452:THR:HG23	2.16	0.45
1:A:778:MET:HG3	1:A:779:THR:N	2.31	0.45
1:D:450:ILE:HG22	1:D:451:ASP:N	2.31	0.45
1:E:278:GLU:O	1:E:289:ILE:HG12	2.16	0.45
1:A:673:ILE:HG21	1:A:695:MET:HE3	1.98	0.45
1:F:70:ILE:HG21	1:F:101:GLU:HG3	1.99	0.45
1:G:68:ASN:O	1:G:72:ILE:HG13	2.16	0.45
1:C:160:ILE:HG22	1:C:200:VAL:HG11	1.98	0.45
1:F:563:MET:CE	1:F:573:PHE:CE2	2.99	0.45
1:G:164:LEU:HD22	1:G:195:PHE:CE1	2.50	0.45
1:H:847:VAL:HG12	1:H:847:VAL:O	2.17	0.45
1:E:253:GLU:OE2	1:E:257:ARG:NH1	2.50	0.45
1:F:893:SER:O	1:F:897:VAL:HG13	2.17	0.45
1:G:331:PRO:HB2	1:G:335:ASP:HB2	1.98	0.45
1:H:257:ARG:NH2	1:H:284:ASP:O	2.49	0.45
1:A:448:SER:O	1:A:452:THR:HG23	2.16	0.45
1:C:331:PRO:HB2	1:C:335:ASP:HB2	1.98	0.45
1:B:354:ASN:ND2	1:B:357:MET:HB3	2.31	0.45
1:D:280:LEU:HG	1:D:289:ILE:HG12	1.99	0.45
1:E:81:ILE:HG13	1:E:103:ILE:HG21	1.97	0.45
1:E:68:ASN:O	1:E:72:ILE:HG13	2.16	0.45
1:D:68:ASN:O	1:D:72:ILE:HG13	2.16	0.45
1:D:996:VAL:O	1:D:997:THR:C	2.54	0.45
1:B:752:ALA:CB	1:C:749:TYR:CZ	3.00	0.45
1:H:1018:LEU:HD11	1:H:1024:LEU:HD11	1.97	0.45
1:H:778:MET:HG3	1:H:779:THR:N	2.32	0.45
1:B:257:ARG:NH2	1:B:284:ASP:O	2.49	0.45
1:H:930:GLN:O	1:H:934:LEU:HG	2.16	0.45
1:H:472:TYR:OH	1:H:1004:PHE:O	2.27	0.45
1:E:684:ARG:HH11	1:E:684:ARG:HA	1.82	0.45
1:D:3:ARG:CD	1:D:104:ILE:HD11	2.35	0.45
1:A:657:VAL:HG22	1:A:943:ARG:CZ	2.47	0.45
1:H:68:ASN:O	1:H:72:ILE:HG13	2.16	0.45
1:B:228:PHE:CD1	1:B:228:PHE:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:ILE:O	1:H:21:ARG:HG3	2.17	0.45
1:F:541:ASP:OD2	1:F:739:HIS:HE1	1.99	0.45
1:A:1041:VAL:CG1	1:A:1043:TYR:HE1	2.30	0.45
1:G:996:VAL:O	1:G:997:THR:C	2.54	0.45
1:G:134:ILE:CG2	1:G:203:GLU:HB3	2.47	0.45
1:H:533:LEU:O	1:H:761:ILE:HA	2.15	0.45
1:G:144:ILE:HG23	1:G:184:PHE:HD2	1.80	0.45
1:H:653:LYS:O	1:H:943:ARG:HD3	2.15	0.45
1:F:288:PHE:C	1:F:288:PHE:CD1	2.90	0.45
1:C:448:SER:O	1:C:452:THR:HG23	2.17	0.45
1:F:405:PHE:C	1:F:405:PHE:CD2	2.89	0.45
1:F:160:ILE:HG22	1:F:200:VAL:HG11	1.98	0.45
1:G:352:PRO:HA	1:G:356:PHE:CE1	2.52	0.45
1:B:546:LEU:HD11	1:B:774:SER:HB2	1.98	0.45
1:B:253:GLU:OE2	1:B:257:ARG:NH1	2.50	0.45
1:A:960:LEU:CD2	1:A:964:MET:HB2	2.46	0.45
1:E:448:SER:O	1:E:452:THR:HG23	2.17	0.45
1:D:930:GLN:O	1:D:934:LEU:HG	2.17	0.45
1:F:450:ILE:HG22	1:F:451:ASP:N	2.29	0.45
1:D:653:LYS:O	1:D:943:ARG:HD3	2.15	0.45
1:D:1018:LEU:HD11	1:D:1024:LEU:HD11	1.98	0.45
1:G:1018:LEU:HD11	1:G:1024:LEU:HD11	1.98	0.45
1:F:673:ILE:HG21	1:F:695:MET:HE3	1.98	0.45
1:A:304:MET:HE2	1:A:399:CYS:CB	2.47	0.45
1:B:437:HIS:CD2	1:B:439:ASP:N	2.73	0.45
1:A:1010:LEU:HD21	1:A:1031:ILE:CD1	2.44	0.45
1:B:543:HIS:ND1	1:B:551:VAL:HB	2.31	0.45
1:F:502:TYR:HD1	1:F:503:GLY:N	2.14	0.45
1:F:44:ARG:HD3	1:F:45:TYR:CE1	2.51	0.45
1:D:847:VAL:HG12	1:D:847:VAL:O	2.17	0.45
1:A:300:THR:O	1:A:303:GLU:HB2	2.16	0.45
1:C:794:LEU:HD12	1:C:795:ASP:O	2.17	0.45
1:C:368:SER:HA	1:C:419:PHE:CE1	2.52	0.45
1:C:576:TRP:CD1	1:C:596:LEU:HD22	2.52	0.45
1:F:657:VAL:HG22	1:F:943:ARG:CZ	2.47	0.45
1:D:64:LEU:HD23	1:D:88:LEU:CD2	2.45	0.45
1:E:352:PRO:HA	1:E:356:PHE:CE1	2.51	0.45
1:B:619:GLY:HA3	1:B:623:TYR:HE2	1.80	0.45
1:A:257:ARG:NH2	1:A:284:ASP:O	2.50	0.45
1:F:960:LEU:CD2	1:F:964:MET:HB2	2.46	0.45
1:F:131:ILE:O	1:F:131:ILE:HG12	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ILE:O	1:A:131:ILE:HG12	2.14	0.45
1:H:369:THR:HG1	1:H:415:ASN:ND2	2.10	0.45
1:H:234:ILE:CD1	1:H:445:TYR:CZ	2.98	0.45
1:B:510:THR:OG1	1:B:607:MET:SD	2.73	0.45
1:D:118:ASP:OD2	1:D:120:ILE:HG13	2.17	0.45
1:D:352:PRO:HA	1:D:356:PHE:CE1	2.51	0.45
1:G:20:MET:HE1	1:G:43:HIS:O	2.15	0.45
1:B:367:ARG:NH1	1:B:1049:GLN:HB2	2.31	0.45
1:E:54:GLY:HA3	1:E:62:ALA:CB	2.47	0.45
1:H:996:VAL:O	1:H:997:THR:C	2.54	0.45
1:A:44:ARG:HD3	1:A:45:TYR:CE1	2.52	0.45
1:F:253:GLU:OE2	1:F:257:ARG:NH1	2.50	0.45
1:G:368:SER:HA	1:G:419:PHE:CE1	2.52	0.45
1:A:450:ILE:HG22	1:A:451:ASP:N	2.30	0.45
1:D:1041:VAL:HG22	1:D:1054:ASN:OD1	2.17	0.45
1:C:257:ARG:NH2	1:C:284:ASP:O	2.49	0.45
1:H:693:LYS:HG2	1:H:731:THR:OG1	2.16	0.45
1:F:778:MET:HG3	1:F:779:THR:N	2.32	0.45
1:G:70:ILE:HG21	1:G:101:GLU:HG3	1.98	0.44
1:A:70:ILE:HG21	1:A:101:GLU:HG3	1.99	0.44
1:A:160:ILE:HG22	1:A:200:VAL:HG11	1.98	0.44
1:H:414:ARG:NH1	1:G:21:ARG:HD3	2.32	0.44
1:B:996:VAL:O	1:B:997:THR:C	2.56	0.44
1:C:134:ILE:CG2	1:C:203:GLU:HB3	2.47	0.44
1:E:42:PHE:HA	1:E:45:TYR:CD2	2.52	0.44
1:F:257:ARG:NH2	1:F:284:ASP:O	2.50	0.44
1:D:448:SER:O	1:D:452:THR:HG23	2.16	0.44
1:B:209:PRO:CG	1:B:280:LEU:HD23	2.48	0.44
1:A:17:ILE:HA	1:A:20:MET:HG3	1.99	0.44
1:C:70:ILE:HG21	1:C:101:GLU:HG3	1.98	0.44
1:C:17:ILE:O	1:C:21:ARG:HG3	2.17	0.44
1:H:118:ASP:OD2	1:H:120:ILE:HG13	2.17	0.44
1:E:952:ASN:OD1	1:E:952:ASN:O	2.35	0.44
1:C:352:PRO:HA	1:C:356:PHE:CE1	2.53	0.44
1:C:651:TRP:HE1	1:C:653:LYS:CB	2.31	0.44
1:B:54:GLY:HA3	1:B:62:ALA:CB	2.48	0.44
1:E:367:ARG:NH1	1:E:1049:GLN:HB2	2.31	0.44
1:A:253:GLU:OE2	1:A:257:ARG:NH1	2.50	0.44
1:G:257:ARG:NH2	1:G:284:ASP:O	2.49	0.44
1:F:448:SER:O	1:F:452:THR:HG23	2.17	0.44
1:H:718:PRO:HG2	1:H:749:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:930:GLN:O	1:F:934:LEU:HG	2.17	0.44
1:E:331:PRO:HB2	1:E:335:ASP:HB2	1.97	0.44
1:C:365:THR:HG21	1:C:1051:ARG:CD	2.45	0.44
1:F:319:ASP:OD2	1:F:321:TYR:HE2	2.00	0.44
1:D:253:GLU:OE2	1:D:257:ARG:NH1	2.50	0.44
1:G:794:LEU:HD12	1:G:795:ASP:O	2.17	0.44
1:F:368:SER:HA	1:F:419:PHE:CE1	2.51	0.44
1:H:448:SER:O	1:H:452:THR:HG23	2.16	0.44
1:G:741:HIS:CD2	1:G:775:GLN:HE21	2.36	0.44
1:F:51:TYR:CE1	1:E:1021:GLY:HA2	2.50	0.44
1:C:68:ASN:O	1:C:72:ILE:HG13	2.17	0.44
1:E:234:ILE:CD1	1:E:445:TYR:CZ	2.98	0.44
1:D:712:MET:N	1:D:712:MET:SD	2.89	0.44
1:A:90:GLU:HA	1:A:113:LEU:HD22	2.00	0.44
1:C:996:VAL:O	1:C:997:THR:C	2.55	0.44
1:E:626:ASN:OD1	1:E:950:PRO:HB3	2.17	0.44
1:B:626:ASN:OD1	1:B:950:PRO:HB3	2.17	0.44
1:H:427:ASN:ND2	1:H:431:LEU:HD11	2.31	0.44
1:H:1041:VAL:HG22	1:H:1054:ASN:OD1	2.17	0.44
1:H:368:SER:HA	1:H:419:PHE:CE1	2.53	0.44
1:G:405:PHE:CD2	1:G:405:PHE:C	2.90	0.44
1:B:952:ASN:O	1:B:952:ASN:OD1	2.35	0.44
1:E:619:GLY:HA3	1:E:623:TYR:HE2	1.81	0.44
1:A:570:MET:HG3	1:A:573:PHE:CE1	2.52	0.44
1:A:509:GLY:N	1:A:605:ASN:HB2	2.33	0.44
1:E:427:ASN:ND2	1:E:431:LEU:HD11	2.32	0.44
1:B:44:ARG:HD3	1:B:45:TYR:CE1	2.52	0.44
1:C:718:PRO:HG2	1:C:749:TYR:CD2	2.52	0.44
1:E:134:ILE:CD1	1:E:287:TYR:CB	2.96	0.44
1:H:300:THR:O	1:H:303:GLU:HB2	2.17	0.44
1:E:746:ASN:HD22	1:G:748:ILE:HG21	1.82	0.44
1:A:1014:ILE:HD12	1:A:1016:VAL:HG12	2.00	0.44
1:B:821:ASN:N	1:B:821:ASN:OD1	2.49	0.44
1:G:519:PRO:CB	1:G:705:HIS:NE2	2.78	0.44
1:D:17:ILE:O	1:D:21:ARG:HG3	2.18	0.44
1:C:20:MET:HE1	1:C:43:HIS:O	2.16	0.44
1:G:718:PRO:HG2	1:G:749:TYR:CD2	2.52	0.44
1:F:709:ILE:HB	1:F:738:LEU:HD12	1.99	0.44
1:C:12:ARG:NH2	1:C:391:TYR:CD2	2.85	0.44
1:D:693:LYS:HG2	1:D:731:THR:OG1	2.17	0.44
1:G:448:SER:O	1:G:452:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1014:ILE:HD12	1:F:1016:VAL:HG12	2.00	0.44
1:F:619:GLY:HA3	1:F:623:TYR:HE2	1.81	0.44
1:E:156:TYR:N	1:E:157:PRO:CD	2.80	0.44
1:F:679:ILE:CD1	1:F:724:LEU:HD13	2.44	0.44
1:B:540:ARG:NH2	1:B:541:ASP:OD1	2.51	0.44
1:F:90:GLU:HA	1:F:113:LEU:HD22	2.00	0.44
1:A:54:GLY:HA3	1:A:62:ALA:CB	2.48	0.44
1:C:186:ARG:CZ	1:C:186:ARG:HB3	2.47	0.44
1:B:42:PHE:HA	1:B:45:TYR:CD2	2.53	0.44
1:E:1:MET:HE1	1:E:4:ILE:HB	2.00	0.44
1:H:253:GLU:OE2	1:H:257:ARG:NH1	2.51	0.44
1:B:631:PHE:CD2	1:B:631:PHE:C	2.91	0.44
1:A:930:GLN:O	1:A:934:LEU:HG	2.17	0.44
1:F:17:ILE:O	1:F:21:ARG:HG3	2.17	0.44
1:C:519:PRO:CB	1:C:705:HIS:NE2	2.78	0.44
1:A:234:ILE:CD1	1:A:445:TYR:CZ	2.99	0.44
1:D:234:ILE:CD1	1:D:445:TYR:CZ	2.99	0.44
1:A:319:ASP:OD2	1:A:321:TYR:HE2	2.01	0.44
1:E:996:VAL:O	1:E:997:THR:C	2.56	0.44
1:E:44:ARG:HD3	1:E:45:TYR:CE1	2.53	0.44
1:C:992:LYS:HE3	1:C:993:TYR:CE2	2.53	0.44
1:D:81:ILE:O	1:D:106:VAL:HG23	2.18	0.44
1:C:741:HIS:CD2	1:C:775:GLN:HE21	2.36	0.44
1:E:147:VAL:HG11	1:E:180:VAL:HG11	2.00	0.44
1:D:279:PHE:C	1:D:289:ILE:HD11	2.38	0.44
1:E:369:THR:OG1	1:E:370:GLY:N	2.50	0.44
1:D:45:TYR:CD1	1:C:1047:ASN:CB	2.97	0.44
1:B:228:PHE:HD1	1:B:228:PHE:N	2.16	0.44
1:G:278:GLU:CB	1:G:289:ILE:CD1	2.96	0.44
1:E:160:ILE:HD12	1:E:174:VAL:CG2	2.47	0.44
1:F:847:VAL:HG12	1:F:847:VAL:O	2.17	0.44
1:H:81:ILE:O	1:H:106:VAL:HG23	2.18	0.44
1:B:684:ARG:HA	1:B:684:ARG:HH11	1.83	0.44
1:F:673:ILE:HG21	1:F:695:MET:CE	2.48	0.43
1:G:278:GLU:HB2	1:G:289:ILE:CD1	2.48	0.43
1:F:570:MET:HG3	1:F:573:PHE:CE1	2.52	0.43
1:G:230:ARG:HD3	1:G:302:THR:OG1	2.18	0.43
1:D:766:SER:O	1:D:767:SER:C	2.57	0.43
1:D:1033:GLU:HG3	1:D:1034:PRO:HD2	2.00	0.43
1:D:969:THR:O	1:D:973:VAL:HG23	2.18	0.43
1:B:746:ASN:HD22	1:C:748:ILE:HG21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:PHE:CD1	1:E:228:PHE:N	2.87	0.43
1:C:278:GLU:HB2	1:C:289:ILE:CD1	2.48	0.43
1:C:288:PHE:C	1:C:288:PHE:CD1	2.91	0.43
1:D:898:TYR:HD1	1:D:928:LYS:HE3	1.81	0.43
1:F:54:GLY:HA3	1:F:62:ALA:CB	2.48	0.43
1:A:847:VAL:HG12	1:A:847:VAL:O	2.17	0.43
1:A:754:ALA:HB1	1:A:759:VAL:CG1	2.49	0.43
1:B:331:PRO:HB2	1:B:335:ASP:HB2	1.98	0.43
1:G:288:PHE:CD1	1:G:288:PHE:C	2.91	0.43
1:F:300:THR:O	1:F:303:GLU:HB2	2.17	0.43
1:H:279:PHE:C	1:H:289:ILE:HD11	2.38	0.43
1:E:349:THR:HG23	1:E:393:SER:HB2	2.00	0.43
1:C:279:PHE:CA	1:C:289:ILE:HD11	2.48	0.43
1:H:898:TYR:H	1:H:898:TYR:HD2	1.65	0.43
1:H:712:MET:SD	1:H:712:MET:N	2.90	0.43
1:C:600:ARG:HG3	1:C:639:GLY:HA3	1.99	0.43
1:B:134:ILE:HG23	1:B:135:PRO:HD2	2.00	0.43
1:G:712:MET:SD	1:G:712:MET:N	2.88	0.43
1:E:821:ASN:N	1:E:821:ASN:OD1	2.49	0.43
1:A:17:ILE:O	1:A:21:ARG:HG3	2.18	0.43
1:F:234:ILE:CD1	1:F:445:TYR:CZ	2.99	0.43
1:C:278:GLU:CB	1:C:289:ILE:CD1	2.96	0.43
1:H:741:HIS:CE1	1:H:775:GLN:NE2	2.86	0.43
1:D:427:ASN:ND2	1:D:431:LEU:HD11	2.32	0.43
1:G:81:ILE:O	1:G:106:VAL:HG23	2.18	0.43
1:H:969:THR:O	1:H:973:VAL:HG23	2.18	0.43
1:B:174:VAL:HG12	1:B:176:SER:H	1.83	0.43
1:A:673:ILE:HG21	1:A:695:MET:CE	2.49	0.43
1:E:847:VAL:HG12	1:E:847:VAL:O	2.18	0.43
1:G:620:TYR:CE1	1:G:978:LEU:O	2.72	0.43
1:G:12:ARG:NH2	1:G:391:TYR:CD2	2.85	0.43
1:H:709:ILE:HB	1:H:738:LEU:HD12	2.00	0.43
1:D:709:ILE:HB	1:D:738:LEU:HD12	2.00	0.43
1:D:368:SER:HA	1:D:419:PHE:CE1	2.54	0.43
1:C:158:LEU:C	1:C:205:CYS:SG	2.97	0.43
1:F:173:VAL:HG13	1:F:205:CYS:SG	2.58	0.43
1:E:847:VAL:CG1	1:E:889:GLN:OE1	2.67	0.43
1:C:540:ARG:O	1:C:542:ALA:N	2.46	0.43
1:A:619:GLY:HA3	1:A:623:TYR:HE2	1.82	0.43
1:H:898:TYR:HD1	1:H:928:LYS:HE3	1.82	0.43
1:B:352:PRO:HA	1:B:356:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:GLY:HA3	1:C:62:ALA:CB	2.48	0.43
1:G:600:ARG:HG3	1:G:639:GLY:HA3	1.99	0.43
1:C:230:ARG:HD3	1:C:302:THR:OG1	2.19	0.43
1:G:288:PHE:CE2	1:G:291:VAL:HG23	2.54	0.43
1:A:1033:GLU:HG3	1:A:1034:PRO:HD2	2.00	0.43
1:E:288:PHE:CE2	1:E:291:VAL:HG23	2.53	0.43
1:E:288:PHE:CD1	1:E:289:ILE:N	2.86	0.43
1:B:603:ILE:CG1	1:B:608:PHE:CZ	3.00	0.43
1:C:541:ASP:OD2	1:C:739:HIS:HE1	2.01	0.43
1:H:519:PRO:HB2	1:H:705:HIS:CD2	2.53	0.43
1:B:234:ILE:CD1	1:B:445:TYR:CZ	2.99	0.43
1:C:288:PHE:CE2	1:C:291:VAL:HG23	2.54	0.43
1:G:279:PHE:CA	1:G:289:ILE:HD11	2.48	0.43
1:H:174:VAL:HG12	1:H:176:SER:H	1.84	0.43
1:E:17:ILE:O	1:E:21:ARG:HG3	2.18	0.43
1:G:54:GLY:HA3	1:G:62:ALA:CB	2.49	0.43
1:B:427:ASN:ND2	1:B:431:LEU:HD11	2.33	0.43
1:A:81:ILE:HG13	1:A:103:ILE:HG21	2.00	0.43
1:E:631:PHE:CD2	1:E:631:PHE:C	2.92	0.43
1:A:368:SER:HA	1:A:419:PHE:CE1	2.53	0.43
1:H:8:LEU:CA	1:H:31:VAL:CG2	2.89	0.43
1:A:126:ALA:CB	1:A:131:ILE:HD11	2.48	0.43
1:E:603:ILE:CG1	1:E:608:PHE:CZ	3.00	0.43
1:F:51:TYR:CD1	1:E:1021:GLY:HA2	2.54	0.43
1:B:847:VAL:CG1	1:B:889:GLN:OE1	2.67	0.43
1:F:66:ILE:HG23	1:F:94:PHE:HD1	1.81	0.43
1:G:540:ARG:O	1:G:542:ALA:N	2.46	0.43
1:H:600:ARG:HG3	1:H:639:GLY:HA3	2.00	0.43
1:C:44:ARG:HD3	1:C:45:TYR:CE1	2.53	0.43
1:B:39:THR:HG22	1:B:44:ARG:HH21	1.82	0.43
1:E:134:ILE:HG23	1:E:135:PRO:HD2	2.00	0.43
1:G:959:GLU:O	1:G:963:LYS:HG2	2.18	0.43
1:F:126:ALA:CB	1:F:131:ILE:HD11	2.48	0.43
1:B:82:HIS:HB2	1:B:106:VAL:HG21	2.00	0.43
1:D:54:GLY:HA3	1:D:62:ALA:CB	2.48	0.43
1:C:620:TYR:CE1	1:C:978:LEU:O	2.72	0.43
1:E:675:TYR:CE2	1:E:716:LEU:HD13	2.54	0.43
1:E:39:THR:HG22	1:E:44:ARG:HH21	1.82	0.43
1:F:81:ILE:HG13	1:F:103:ILE:HG21	2.00	0.43
1:B:448:SER:O	1:B:452:THR:CG2	2.67	0.43
1:D:841:GLN:HG2	1:D:853:TRP:CZ2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:778:MET:HG3	1:D:779:THR:N	2.34	0.43
1:A:718:PRO:HG2	1:A:749:TYR:CD2	2.53	0.43
1:C:674:CYS:HB3	1:C:712:MET:HE1	2.01	0.43
1:D:718:PRO:HG2	1:D:749:TYR:CD2	2.53	0.43
1:F:867:PHE:CD1	1:F:867:PHE:N	2.85	0.43
1:D:39:THR:HG22	1:D:44:ARG:HH21	1.84	0.43
1:H:45:TYR:CD1	1:G:1047:ASN:CB	2.99	0.43
1:F:50:ALA:O	1:E:1021:GLY:O	2.37	0.43
1:B:847:VAL:O	1:B:847:VAL:HG12	2.19	0.43
1:G:541:ASP:OD2	1:G:739:HIS:HE1	2.02	0.43
1:A:679:ILE:CD1	1:A:724:LEU:HD13	2.44	0.43
1:D:898:TYR:H	1:D:898:TYR:HD2	1.65	0.43
1:H:674:CYS:HB3	1:H:712:MET:HE1	2.01	0.43
1:A:563:MET:HB3	1:A:573:PHE:CE2	2.53	0.43
1:C:39:THR:HG22	1:C:44:ARG:HH21	1.83	0.43
1:G:992:LYS:HE3	1:G:993:TYR:CE2	2.54	0.43
1:F:209:PRO:HB2	1:F:280:LEU:HD22	2.01	0.43
1:H:39:THR:HG22	1:H:44:ARG:HH21	1.84	0.42
1:E:82:HIS:HB2	1:E:106:VAL:HG21	2.00	0.42
1:F:304:MET:HE2	1:F:399:CYS:CB	2.49	0.42
1:A:519:PRO:HB2	1:A:705:HIS:CD2	2.54	0.42
1:F:519:PRO:HB2	1:F:705:HIS:CD2	2.54	0.42
1:B:464:ASP:CG	1:B:467:THR:OG1	2.58	0.42
1:A:563:MET:HE1	1:A:573:PHE:CE2	2.52	0.42
1:B:718:PRO:CG	1:B:749:TYR:CD2	3.02	0.42
1:C:348:THR:HG22	1:C:394:LEU:HA	2.01	0.42
1:H:54:GLY:HA3	1:H:62:ALA:CB	2.49	0.42
1:F:754:ALA:HB1	1:F:759:VAL:CG1	2.49	0.42
1:C:959:GLU:O	1:C:963:LYS:HG2	2.19	0.42
1:C:427:ASN:ND2	1:C:431:LEU:HD11	2.34	0.42
1:H:631:PHE:O	1:H:635:SER:OG	2.37	0.42
1:E:448:SER:O	1:E:452:THR:CG2	2.67	0.42
1:C:712:MET:N	1:C:712:MET:SD	2.89	0.42
1:H:1033:GLU:HG3	1:H:1034:PRO:HD2	2.01	0.42
1:A:288:PHE:CD1	1:A:288:PHE:C	2.92	0.42
1:A:867:PHE:N	1:A:867:PHE:CD1	2.86	0.42
1:A:405:PHE:CD2	1:A:405:PHE:C	2.91	0.42
1:H:867:PHE:CD1	1:H:867:PHE:N	2.85	0.42
1:B:405:PHE:C	1:B:405:PHE:CD2	2.92	0.42
1:B:288:PHE:CE2	1:B:291:VAL:HG23	2.54	0.42
1:H:278:GLU:C	1:H:289:ILE:HD11	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:THR:HG23	1:B:393:SER:HB2	2.01	0.42
1:A:620:TYR:HD1	1:A:979:TYR:CE1	2.38	0.42
1:F:500:ILE:HG22	1:F:501:PRO:O	2.19	0.42
1:E:464:ASP:CG	1:E:467:THR:OG1	2.58	0.42
1:B:540:ARG:HH21	1:B:541:ASP:CG	2.23	0.42
1:F:39:THR:HG22	1:F:44:ARG:HH21	1.84	0.42
1:A:672:ALA:HA	1:A:708:GLY:O	2.20	0.42
1:C:134:ILE:HG23	1:C:135:PRO:HD2	1.99	0.42
1:A:709:ILE:HB	1:A:738:LEU:HD12	1.99	0.42
1:E:712:MET:SD	1:E:712:MET:N	2.89	0.42
1:A:969:THR:O	1:A:973:VAL:HG23	2.19	0.42
1:C:1014:ILE:HD12	1:C:1016:VAL:HG12	2.01	0.42
1:A:209:PRO:HB2	1:A:280:LEU:HD22	2.01	0.42
1:F:1033:GLU:HG3	1:F:1034:PRO:HD2	2.01	0.42
1:D:278:GLU:C	1:D:289:ILE:HD11	2.40	0.42
1:E:600:ARG:HG3	1:E:639:GLY:HA3	2.01	0.42
1:H:21:ARG:CZ	1:G:418:GLU:OE2	2.68	0.42
1:F:134:ILE:HG23	1:F:135:PRO:HD2	2.01	0.42
1:D:600:ARG:HG3	1:D:639:GLY:HA3	2.01	0.42
1:A:39:THR:HG22	1:A:44:ARG:HH21	1.84	0.42
1:A:81:ILE:O	1:A:106:VAL:HG23	2.19	0.42
1:G:674:CYS:HB3	1:G:712:MET:HE1	2.01	0.42
1:B:712:MET:SD	1:B:712:MET:N	2.89	0.42
1:F:969:THR:O	1:F:973:VAL:HG23	2.19	0.42
1:G:1014:ILE:HD12	1:G:1016:VAL:HG12	2.01	0.42
1:G:304:MET:CE	1:G:399:CYS:CB	2.98	0.42
1:E:228:PHE:N	1:E:228:PHE:HD1	2.18	0.42
1:H:134:ILE:HG21	1:H:203:GLU:HB2	2.01	0.42
1:D:519:PRO:HB2	1:D:705:HIS:CD2	2.54	0.42
1:A:134:ILE:HG23	1:A:135:PRO:HD2	2.01	0.42
1:F:563:MET:HB3	1:F:573:PHE:CE2	2.54	0.42
1:G:44:ARG:HD3	1:G:45:TYR:CE1	2.54	0.42
1:F:428:ILE:HB	1:F:429:PRO:HD3	2.01	0.42
1:C:81:ILE:O	1:C:106:VAL:HG23	2.19	0.42
1:D:463:ARG:HG3	1:D:468:LYS:HE3	2.02	0.42
1:E:490:PRO:HD2	1:E:492:TYR:CE2	2.54	0.42
1:C:144:ILE:HA	1:C:184:PHE:CE2	2.54	0.42
1:D:8:LEU:CA	1:D:31:VAL:CG2	2.89	0.42
1:B:600:ARG:HG3	1:B:639:GLY:HA3	2.01	0.42
1:F:620:TYR:HD1	1:F:979:TYR:CE1	2.38	0.42
1:D:680:ASP:HB3	1:A:787:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:741:HIS:CE1	1:D:775:GLN:NE2	2.87	0.42
1:G:17:ILE:O	1:G:21:ARG:HG3	2.20	0.42
1:F:713:ALA:HB3	1:F:715:LEU:HD12	1.99	0.42
1:C:509:GLY:N	1:C:605:ASN:HB2	2.34	0.42
1:B:675:TYR:CE2	1:B:716:LEU:HD13	2.54	0.42
1:B:754:ALA:HB1	1:B:759:VAL:CG1	2.49	0.42
1:F:81:ILE:O	1:F:106:VAL:HG23	2.19	0.42
1:B:674:CYS:HB3	1:B:712:MET:HE1	2.00	0.42
1:E:373:GLY:O	1:E:400:THR:HA	2.19	0.42
1:G:1033:GLU:HG3	1:G:1034:PRO:HD2	2.00	0.42
1:E:304:MET:HE2	1:E:399:CYS:CB	2.49	0.42
1:A:519:PRO:CB	1:A:705:HIS:NE2	2.80	0.42
1:D:898:TYR:CD1	1:D:928:LYS:CE	2.99	0.42
1:H:680:ASP:HB3	1:F:787:ASN:ND2	2.35	0.42
1:E:718:PRO:CG	1:E:749:TYR:CD2	3.02	0.42
1:E:348:THR:HG22	1:E:394:LEU:HA	2.01	0.42
1:H:115:MET:CG	1:H:125:GLN:HG3	2.48	0.42
1:D:754:ALA:HB1	1:D:759:VAL:CG1	2.49	0.42
1:A:288:PHE:CE2	1:A:291:VAL:HG23	2.55	0.42
1:B:862:VAL:O	1:B:866:MET:N	2.52	0.42
1:B:365:THR:CG2	1:B:1050:PRO:O	2.67	0.42
1:F:718:PRO:HG2	1:F:749:TYR:CD2	2.54	0.42
1:E:144:ILE:HD12	1:E:145:LYS:H	1.83	0.42
1:E:304:MET:CE	1:E:399:CYS:HB2	2.49	0.42
1:H:41:SER:OG	1:H:43:HIS:HD2	2.02	0.42
1:C:586:ARG:NH1	1:C:586:ARG:HB2	2.34	0.42
1:G:348:THR:HG22	1:G:394:LEU:HA	2.02	0.42
1:H:224:ILE:HG22	1:H:263:VAL:HG13	2.02	0.42
1:G:134:ILE:HG23	1:G:135:PRO:HD2	1.99	0.42
1:D:631:PHE:O	1:D:635:SER:OG	2.38	0.42
1:F:288:PHE:CE2	1:F:291:VAL:HG23	2.55	0.42
1:C:448:SER:O	1:C:452:THR:CG2	2.67	0.42
1:E:828:TYR:CE2	1:G:783:TYR:HB3	2.54	0.42
1:E:862:VAL:O	1:E:866:MET:N	2.52	0.42
1:D:867:PHE:N	1:D:867:PHE:CD1	2.86	0.42
1:H:209:PRO:HB2	1:H:280:LEU:HD22	2.01	0.42
1:C:217:LEU:HD12	1:C:227:LEU:HD11	2.01	0.42
1:G:304:MET:CE	1:G:399:CYS:HB2	2.49	0.42
1:H:519:PRO:CB	1:H:705:HIS:NE2	2.80	0.42
1:H:754:ALA:HB1	1:H:759:VAL:CG1	2.49	0.42
1:G:39:THR:HG22	1:G:44:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ASN:ND2	1:A:431:LEU:HD11	2.35	0.42
1:H:1014:ILE:HD12	1:H:1016:VAL:HG12	2.01	0.42
1:B:828:TYR:CE2	1:C:783:TYR:HB3	2.54	0.42
1:A:161:LYS:HB2	1:A:201:TYR:CE2	2.54	0.42
1:D:209:PRO:HB2	1:D:280:LEU:HD22	2.01	0.42
1:A:157:PRO:C	1:A:205:CYS:HB2	2.40	0.42
1:C:304:MET:CE	1:C:399:CYS:HB2	2.49	0.42
1:B:17:ILE:O	1:B:21:ARG:HG3	2.19	0.42
1:D:134:ILE:HG21	1:D:203:GLU:HB2	2.02	0.42
1:H:898:TYR:CD1	1:H:928:LYS:CE	2.99	0.42
1:G:427:ASN:ND2	1:G:431:LEU:HD11	2.35	0.42
1:E:754:ALA:HB1	1:E:759:VAL:CG1	2.49	0.42
1:A:428:ILE:HB	1:A:429:PRO:HD3	2.02	0.42
1:A:448:SER:O	1:A:452:THR:CG2	2.68	0.42
1:B:490:PRO:HD2	1:B:492:TYR:CE2	2.55	0.42
1:B:278:GLU:C	1:B:289:ILE:CG1	2.89	0.42
1:A:66:ILE:HG23	1:A:94:PHE:HD1	1.83	0.42
1:F:82:HIS:CD2	1:F:84:GLY:H	2.26	0.42
1:H:198:ASP:N	1:H:198:ASP:OD1	2.53	0.42
1:F:563:MET:HE1	1:F:573:PHE:CE2	2.53	0.42
1:B:348:THR:HG22	1:B:394:LEU:HA	2.02	0.42
1:D:224:ILE:HG22	1:D:263:VAL:HG13	2.02	0.42
1:E:42:PHE:HA	1:E:45:TYR:HD2	1.83	0.42
1:F:161:LYS:HB2	1:F:201:TYR:CE2	2.54	0.42
1:B:473:ILE:O	1:B:477:THR:OG1	2.26	0.42
1:H:288:PHE:C	1:H:288:PHE:CD1	2.92	0.41
1:B:304:MET:CE	1:B:399:CYS:HB2	2.50	0.41
1:C:519:PRO:HB2	1:C:705:HIS:CD2	2.54	0.41
1:D:174:VAL:CA	1:D:175:GLU:OE2	2.68	0.41
1:G:586:ARG:HB2	1:G:586:ARG:NH1	2.35	0.41
1:C:198:ASP:N	1:C:198:ASP:OD1	2.53	0.41
1:D:198:ASP:N	1:D:198:ASP:OD1	2.53	0.41
1:A:63:TYR:HB2	1:A:87:PHE:CE2	2.54	0.41
1:A:847:VAL:HB	1:A:849:LEU:CD1	2.50	0.41
1:F:509:GLY:N	1:F:605:ASN:HB2	2.35	0.41
1:B:675:TYR:HE2	1:B:716:LEU:HA	1.84	0.41
1:B:133:VAL:HG12	1:B:134:ILE:N	2.35	0.41
1:G:754:ALA:HB1	1:G:759:VAL:CG1	2.50	0.41
1:D:448:SER:O	1:D:452:THR:CG2	2.67	0.41
1:H:448:SER:O	1:H:452:THR:CG2	2.67	0.41
1:D:1014:ILE:HD12	1:D:1016:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1014:ILE:HD12	1:E:1016:VAL:HG12	2.01	0.41
1:B:266:MET:HE1	1:B:291:VAL:CG1	2.50	0.41
1:G:519:PRO:HB2	1:G:705:HIS:CD2	2.54	0.41
1:A:600:ARG:HG3	1:A:639:GLY:HA3	2.02	0.41
1:F:194:ALA:C	1:F:195:PHE:CD2	2.94	0.41
1:F:230:ARG:HD3	1:F:302:THR:OG1	2.20	0.41
1:A:230:ARG:HD3	1:A:302:THR:OG1	2.20	0.41
1:E:672:ALA:HA	1:E:708:GLY:O	2.19	0.41
1:G:448:SER:O	1:G:452:THR:CG2	2.68	0.41
1:E:473:ILE:O	1:E:477:THR:OG1	2.26	0.41
1:H:463:ARG:HG3	1:H:468:LYS:HE3	2.03	0.41
1:H:280:LEU:HD23	1:H:280:LEU:HA	1.92	0.41
1:B:158:LEU:HA	1:B:205:CYS:H	1.85	0.41
1:D:45:TYR:CE1	1:C:1047:ASN:CG	2.94	0.41
1:H:304:MET:CE	1:H:399:CYS:HB2	2.50	0.41
1:H:134:ILE:HG23	1:H:135:PRO:HD2	2.02	0.41
1:C:41:SER:OG	1:C:43:HIS:HD2	2.03	0.41
1:E:212:ILE:HG23	1:E:229:GLU:HB2	2.02	0.41
1:A:194:ALA:C	1:A:195:PHE:CD2	2.94	0.41
1:F:672:ALA:HA	1:F:708:GLY:O	2.21	0.41
1:C:754:ALA:HB1	1:C:759:VAL:CG1	2.50	0.41
1:G:144:ILE:HA	1:G:184:PHE:HE2	1.84	0.41
1:F:448:SER:O	1:F:452:THR:CG2	2.68	0.41
1:H:718:PRO:CG	1:H:749:TYR:CD2	3.04	0.41
1:B:1033:GLU:HG3	1:B:1034:PRO:HD2	2.01	0.41
1:C:1033:GLU:HG3	1:C:1034:PRO:HD2	2.01	0.41
1:B:1014:ILE:HD12	1:B:1016:VAL:HG12	2.02	0.41
1:C:85:TYR:CZ	1:C:297:VAL:HG22	2.55	0.41
1:H:841:GLN:HG2	1:H:853:TRP:CZ2	2.55	0.41
1:A:685:THR:O	1:A:688:THR:HG23	2.21	0.41
1:B:369:THR:OG1	1:B:370:GLY:N	2.53	0.41
1:F:519:PRO:CB	1:F:705:HIS:NE2	2.81	0.41
1:D:679:ILE:CD1	1:D:724:LEU:HD13	2.45	0.41
1:E:7:VAL:HG12	1:E:28:ILE:CG2	2.50	0.41
1:D:428:ILE:HB	1:D:429:PRO:HD3	2.02	0.41
1:A:137:SER:CB	1:A:141:VAL:HG22	2.50	0.41
1:D:628:ILE:O	1:D:632:VAL:HG23	2.21	0.41
1:D:280:LEU:HD23	1:D:280:LEU:HA	1.92	0.41
1:H:17:ILE:HD11	1:H:43:HIS:CB	2.49	0.41
1:A:82:HIS:CD2	1:A:84:GLY:H	2.26	0.41
1:H:134:ILE:CG2	1:H:203:GLU:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:SER:OG	1:G:43:HIS:HD2	2.03	0.41
1:F:600:ARG:HG3	1:F:639:GLY:HA3	2.02	0.41
1:F:63:TYR:HB2	1:F:87:PHE:CE2	2.55	0.41
1:E:675:TYR:HE2	1:E:716:LEU:HA	1.84	0.41
1:E:674:CYS:HB3	1:E:712:MET:HE1	2.01	0.41
1:H:628:ILE:O	1:H:632:VAL:HG23	2.21	0.41
1:C:405:PHE:CD2	1:C:405:PHE:C	2.93	0.41
1:G:672:ALA:HA	1:G:708:GLY:O	2.20	0.41
1:D:115:MET:CG	1:D:125:GLN:HG3	2.49	0.41
1:B:7:VAL:HG12	1:B:28:ILE:CG2	2.50	0.41
1:B:672:ALA:HA	1:B:708:GLY:O	2.20	0.41
1:G:158:LEU:C	1:G:205:CYS:SG	2.99	0.41
1:G:95:ALA:O	1:G:99:GLU:HG3	2.21	0.41
1:E:266:MET:HE1	1:E:291:VAL:CG1	2.51	0.41
1:F:157:PRO:O	1:F:205:CYS:HB2	2.20	0.41
1:E:304:MET:CE	1:E:399:CYS:CB	2.98	0.41
1:A:198:ASP:N	1:A:198:ASP:OD1	2.54	0.41
1:A:470:LEU:HB3	1:A:1044:PHE:CE2	2.55	0.41
1:F:1044:PHE:HE2	1:F:1053:ILE:HD11	1.86	0.41
1:B:450:ILE:CG2	1:B:451:ASP:N	2.84	0.41
1:G:134:ILE:CD1	1:G:287:TYR:CB	2.98	0.41
1:H:428:ILE:HB	1:H:429:PRO:HD3	2.03	0.41
1:F:288:PHE:CD1	1:F:289:ILE:N	2.89	0.41
1:B:631:PHE:O	1:B:635:SER:OG	2.38	0.41
1:E:1033:GLU:HG3	1:E:1034:PRO:HD2	2.02	0.41
1:F:490:PRO:HD2	1:F:492:TYR:CE2	2.56	0.41
1:D:138:ASN:N	1:D:138:ASN:OD1	2.52	0.41
1:G:589:ASN:CG	1:G:989:MET:HE2	2.40	0.41
1:G:766:SER:O	1:G:767:SER:C	2.59	0.41
1:A:224:ILE:HG22	1:A:263:VAL:HG13	2.03	0.41
1:F:847:VAL:HB	1:F:849:LEU:CD1	2.51	0.41
1:C:672:ALA:HA	1:C:708:GLY:O	2.20	0.41
1:F:427:ASN:ND2	1:F:431:LEU:HD11	2.36	0.41
1:B:42:PHE:HA	1:B:45:TYR:HD2	1.84	0.41
1:E:631:PHE:O	1:E:635:SER:OG	2.38	0.41
1:F:67:GLU:O	1:F:71:GLU:HG2	2.21	0.41
1:B:373:GLY:O	1:B:400:THR:HA	2.20	0.41
1:A:304:MET:CE	1:A:399:CYS:HB2	2.50	0.41
1:B:304:MET:CE	1:B:399:CYS:CB	2.99	0.41
1:D:41:SER:OG	1:D:43:HIS:HD2	2.03	0.41
1:D:134:ILE:HG23	1:D:135:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ILE:HG23	1:B:229:GLU:HB2	2.03	0.41
1:C:589:ASN:CG	1:C:989:MET:HE2	2.40	0.41
1:G:1044:PHE:HE2	1:G:1053:ILE:HD11	1.85	0.41
1:D:1044:PHE:HE2	1:D:1053:ILE:HD11	1.85	0.41
1:F:224:ILE:HG22	1:F:263:VAL:HG13	2.03	0.41
1:G:509:GLY:N	1:G:605:ASN:HB2	2.35	0.41
1:C:718:PRO:CG	1:C:749:TYR:CD2	3.04	0.41
1:E:133:VAL:HG12	1:E:134:ILE:N	2.36	0.41
1:H:536:ASP:HB3	1:H:573:PHE:HD1	1.86	0.41
1:C:95:ALA:O	1:C:99:GLU:HG3	2.21	0.41
1:H:138:ASN:OD1	1:H:138:ASN:N	2.53	0.41
1:A:67:GLU:O	1:A:71:GLU:HG2	2.21	0.41
1:A:490:PRO:HD2	1:A:492:TYR:CE2	2.56	0.41
1:H:288:PHE:CD1	1:H:289:ILE:N	2.89	0.41
1:C:304:MET:CE	1:C:399:CYS:CB	2.99	0.41
1:F:88:LEU:HB3	1:F:94:PHE:CD2	2.56	0.41
1:A:51:TYR:CE1	1:B:1021:GLY:HA2	2.54	0.41
1:D:134:ILE:CG2	1:D:203:GLU:HB2	2.51	0.41
1:H:382:PHE:CD1	1:H:385:THR:HB	2.56	0.41
1:B:12:ARG:NE	1:B:391:TYR:CD1	2.89	0.41
1:H:67:GLU:O	1:H:71:GLU:HG2	2.21	0.41
1:F:685:THR:O	1:F:688:THR:HG23	2.21	0.41
1:D:258:ILE:CG2	1:D:279:PHE:CD2	3.04	0.40
1:H:45:TYR:CE1	1:G:1047:ASN:CG	2.95	0.40
1:H:620:TYR:HD1	1:H:979:TYR:CE1	2.39	0.40
1:F:862:VAL:O	1:F:866:MET:N	2.53	0.40
1:D:862:VAL:O	1:D:866:MET:N	2.54	0.40
1:G:198:ASP:O	1:G:200:VAL:CG2	2.68	0.40
1:H:679:ILE:CD1	1:H:724:LEU:HD13	2.46	0.40
1:G:651:TRP:HE1	1:G:653:LYS:CB	2.35	0.40
1:E:12:ARG:NE	1:E:391:TYR:CD1	2.90	0.40
1:C:134:ILE:CD1	1:C:287:TYR:CB	2.98	0.40
1:H:265:LEU:O	1:H:269:VAL:HG22	2.20	0.40
1:G:373:GLY:O	1:G:400:THR:HA	2.20	0.40
1:E:365:THR:CG2	1:E:1050:PRO:O	2.68	0.40
1:F:911:ILE:O	1:F:915:MET:N	2.50	0.40
1:C:536:ASP:HB3	1:C:573:PHE:HD1	1.86	0.40
1:H:258:ILE:CG2	1:H:279:PHE:CD2	3.04	0.40
1:D:620:TYR:HD1	1:D:979:TYR:CE1	2.39	0.40
1:B:505:GLN:C	1:B:506:ILE:HG12	2.41	0.40
1:D:13:GLY:C	1:D:17:ILE:HD12	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:SER:CB	1:B:141:VAL:HG22	2.50	0.40
1:H:133:VAL:HG12	1:H:134:ILE:N	2.36	0.40
1:C:234:ILE:CD1	1:C:445:TYR:CZ	3.01	0.40
1:A:862:VAL:O	1:A:866:MET:N	2.53	0.40
1:G:198:ASP:OD1	1:G:198:ASP:N	2.52	0.40
1:H:177:LYS:HG2	1:H:179:HIS:CE1	2.56	0.40
1:A:1044:PHE:HE2	1:A:1053:ILE:HD11	1.86	0.40
1:E:540:ARG:NH1	1:E:578:GLY:HA3	2.37	0.40
1:F:540:ARG:HD2	1:F:540:ARG:HH11	1.69	0.40
1:A:212:ILE:HG23	1:A:229:GLU:HB2	2.04	0.40
1:A:713:ALA:HB3	1:A:715:LEU:HD12	2.01	0.40
1:G:718:PRO:CG	1:G:749:TYR:CD2	3.05	0.40
1:E:278:GLU:C	1:E:289:ILE:CG1	2.90	0.40
1:A:173:VAL:HG13	1:A:205:CYS:SG	2.61	0.40
1:F:304:MET:CE	1:F:399:CYS:HB2	2.50	0.40
1:F:198:ASP:N	1:F:198:ASP:OD1	2.55	0.40
1:E:541:ASP:OD2	1:E:739:HIS:HE1	2.01	0.40
1:C:1044:PHE:HE2	1:C:1053:ILE:HD11	1.86	0.40
1:D:67:GLU:O	1:D:71:GLU:HG2	2.21	0.40
1:C:979:TYR:CB	1:C:982:VAL:HG22	2.51	0.40
1:C:631:PHE:O	1:C:635:SER:OG	2.37	0.40
1:H:862:VAL:O	1:H:866:MET:N	2.54	0.40
1:B:541:ASP:OD2	1:B:739:HIS:HE1	2.02	0.40
1:H:1044:PHE:HE2	1:H:1053:ILE:HD11	1.86	0.40
1:D:265:LEU:O	1:D:269:VAL:HG22	2.20	0.40
1:F:331:PRO:HG2	1:F:336:ILE:HG12	2.03	0.40
1:C:472:TYR:OH	1:C:1004:PHE:O	2.28	0.40
1:B:230:ARG:HD3	1:B:302:THR:OG1	2.21	0.40
1:G:472:TYR:OH	1:G:1004:PHE:O	2.28	0.40
1:F:131:ILE:N	1:F:131:ILE:HD13	2.36	0.40
1:D:45:TYR:CZ	1:C:1047:ASN:O	2.74	0.40
1:D:304:MET:CE	1:D:399:CYS:HB2	2.51	0.40
1:C:288:PHE:CD1	1:C:289:ILE:N	2.90	0.40
1:F:470:LEU:HB3	1:F:1044:PHE:CE2	2.56	0.40
1:D:674:CYS:HB3	1:D:712:MET:HE1	2.04	0.40
1:H:230:ARG:HD3	1:H:302:THR:OG1	2.21	0.40
1:F:266:MET:HE1	1:F:271:TYR:CE1	2.56	0.40
1:G:212:ILE:HG23	1:G:229:GLU:HB2	2.04	0.40
1:A:373:GLY:O	1:A:400:THR:HA	2.22	0.40
1:D:536:ASP:HB3	1:D:573:PHE:HD1	1.87	0.40
1:B:628:ILE:O	1:B:632:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:137:SER:CB	1:F:141:VAL:HG22	2.51	0.40
1:E:405:PHE:CD2	1:E:405:PHE:C	2.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1048/1146 (91%)	988 (94%)	57 (5%)	3 (0%)	46	82
1	B	1021/1146 (89%)	966 (95%)	53 (5%)	2 (0%)	52	86
1	C	933/1146 (81%)	882 (94%)	47 (5%)	4 (0%)	39	78
1	D	1025/1146 (89%)	967 (94%)	55 (5%)	3 (0%)	46	82
1	E	1021/1146 (89%)	962 (94%)	56 (6%)	3 (0%)	46	82
1	F	1048/1146 (91%)	992 (95%)	54 (5%)	2 (0%)	52	86
1	G	934/1146 (82%)	881 (94%)	49 (5%)	4 (0%)	39	78
1	H	1025/1146 (89%)	966 (94%)	56 (6%)	3 (0%)	46	82
All	All	8055/9168 (88%)	7604 (94%)	427 (5%)	24 (0%)	46	82

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	273	ASN
1	F	273	ASN
1	E	273	ASN
1	G	176	SER
1	G	273	ASN
1	D	273	ASN
1	A	273	ASN
1	B	273	ASN

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Mol	Chain	Res	Type
1	C	176	SER
1	C	273	ASN
1	A	176	SER
1	F	176	SER
1	D	176	SER
1	H	997	THR
1	E	506	ILE
1	G	506	ILE
1	C	506	ILE
1	H	1035	ILE
1	E	1035	ILE
1	G	1035	ILE
1	D	1035	ILE
1	B	1035	ILE
1	C	1035	ILE
1	A	1035	ILE

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	814/981 (83%)	710 (87%)	104 (13%)	5	24
1	B	719/981 (73%)	626 (87%)	93 (13%)	5	24
1	C	676/981 (69%)	587 (87%)	89 (13%)	5	23
1	D	819/981 (84%)	719 (88%)	100 (12%)	6	27
1	E	719/981 (73%)	625 (87%)	94 (13%)	5	23
1	F	814/981 (83%)	710 (87%)	104 (13%)	5	24
1	G	677/981 (69%)	591 (87%)	86 (13%)	5	25
1	H	819/981 (84%)	718 (88%)	101 (12%)	6	26
All	All	6057/7848 (77%)	5286 (87%)	771 (13%)	5	25

All (771) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	2	ASN
1	H	3	ARG
1	H	12	ARG
1	H	31	VAL
1	H	39	THR
1	H	42	PHE
1	H	44	ARG
1	H	60	ILE
1	H	70	ILE
1	H	71	GLU
1	H	76	SER
1	H	88	LEU
1	H	106	VAL
1	H	110	SER
1	H	116	PHE
1	H	121	LYS
1	H	127	LEU
1	H	134	ILE
1	H	177	LYS
1	H	183	SER
1	H	198	ASP
1	H	203	GLU
1	H	204	LYS
1	H	207	MET
1	H	223	ASN
1	H	239	GLN
1	H	248	ASN
1	H	251	THR
1	H	252	SER
1	H	254	LEU
1	H	265	LEU
1	H	269	VAL
1	H	289	ILE
1	H	290	GLU
1	H	294	ARG
1	H	295	VAL
1	H	323	LEU
1	H	334	GLU
1	H	356	PHE
1	H	360	THR
1	H	364	ASP
1	H	369	THR
1	H	377	ASP

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Mol	Chain	Res	Type
1	H	382	PHE
1	H	392	ASP
1	H	393	SER
1	H	405	PHE
1	H	407	GLN
1	H	419	PHE
1	H	434	VAL
1	H	436	ARG
1	H	445	TYR
1	H	453	THR
1	H	461	HIS
1	H	462	ILE
1	H	499	LYS
1	H	504	SER
1	H	507	SER
1	H	520	GLU
1	H	531	GLU
1	H	533	LEU
1	H	540	ARG
1	H	545	SER
1	H	547	LEU
1	H	549	THR
1	H	558	GLN
1	H	572	SER
1	H	575	MET
1	H	576	TRP
1	H	600	ARG
1	H	613	ARG
1	H	635	SER
1	H	658	SER
1	H	668	ILE
1	H	682	ASP
1	H	688	THR
1	H	695	MET
1	H	719	GLN
1	H	723	ARG
1	H	727	GLU
1	H	781	LEU
1	H	792	THR
1	H	845	ILE
1	H	858	GLU
1	H	867	PHE

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Mol	Chain	Res	Type
1	H	870	ILE
1	H	890	ASN
1	H	891	GLU
1	H	895	GLU
1	H	896	ASP
1	H	898	TYR
1	H	902	ASP
1	H	918	ILE
1	H	928	LYS
1	H	942	ASP
1	H	974	ILE
1	H	1016	VAL
1	H	1020	LYS
1	H	1040	ARG
1	H	1051	ARG
1	H	1059	ASN
1	F	2	ASN
1	F	39	THR
1	F	42	PHE
1	F	44	ARG
1	F	60	ILE
1	F	71	GLU
1	F	76	SER
1	F	106	VAL
1	F	110	SER
1	F	115	MET
1	F	121	LYS
1	F	127	LEU
1	F	131	ILE
1	F	134	ILE
1	F	159	MET
1	F	163	SER
1	F	183	SER
1	F	195	PHE
1	F	198	ASP
1	F	205	CYS
1	F	207	MET
1	F	239	GLN
1	F	251	THR
1	F	252	SER
1	F	254	LEU
1	F	265	LEU

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Mol	Chain	Res	Type
1	F	269	VAL
1	F	289	ILE
1	F	294	ARG
1	F	295	VAL
1	F	323	LEU
1	F	326	GLN
1	F	334	GLU
1	F	360	THR
1	F	367	ARG
1	F	369	THR
1	F	382	PHE
1	F	392	ASP
1	F	393	SER
1	F	395	LEU
1	F	405	PHE
1	F	407	GLN
1	F	419	PHE
1	F	434	VAL
1	F	436	ARG
1	F	445	TYR
1	F	453	THR
1	F	462	ILE
1	F	463	ARG
1	F	476	VAL
1	F	504	SER
1	F	505	GLN
1	F	507	SER
1	F	510	THR
1	F	520	GLU
1	F	531	GLU
1	F	540	ARG
1	F	545	SER
1	F	547	LEU
1	F	549	THR
1	F	558	GLN
1	F	572	SER
1	F	576	TRP
1	F	600	ARG
1	F	635	SER
1	F	652	ILE
1	F	658	SER
1	F	668	ILE

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Mol	Chain	Res	Type
1	F	682	ASP
1	F	695	MET
1	F	719	GLN
1	F	723	ARG
1	F	727	GLU
1	F	734	VAL
1	F	781	LEU
1	F	792	THR
1	F	794	LEU
1	F	811	HIS
1	F	820	LEU
1	F	845	ILE
1	F	867	PHE
1	F	870	ILE
1	F	890	ASN
1	F	891	GLU
1	F	895	GLU
1	F	896	ASP
1	F	897	VAL
1	F	902	ASP
1	F	918	ILE
1	F	940	LEU
1	F	942	ASP
1	F	943	ARG
1	F	957	LYS
1	F	960	LEU
1	F	974	ILE
1	F	1016	VAL
1	F	1030	SER
1	F	1031	ILE
1	F	1037	ASP
1	F	1040	ARG
1	F	1049	GLN
1	F	1054	ASN
1	F	1056	GLN
1	F	1059	ASN
1	E	1	MET
1	E	2	ASN
1	E	27	LYS
1	E	39	THR
1	E	44	ARG
1	E	76	SER

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Mol	Chain	Res	Type
1	E	88	LEU
1	E	92	ILE
1	E	94	PHE
1	E	106	VAL
1	E	110	SER
1	E	115	MET
1	E	127	LEU
1	E	134	ILE
1	E	144	ILE
1	E	163	SER
1	E	183	SER
1	E	184	PHE
1	E	198	ASP
1	E	207	MET
1	E	228	PHE
1	E	237	ARG
1	E	248	ASN
1	E	251	THR
1	E	252	SER
1	E	254	LEU
1	E	265	LEU
1	E	269	VAL
1	E	280	LEU
1	E	289	ILE
1	E	294	ARG
1	E	323	LEU
1	E	326	GLN
1	E	334	GLU
1	E	349	THR
1	E	356	PHE
1	E	357	MET
1	E	360	THR
1	E	364	ASP
1	E	367	ARG
1	E	369	THR
1	E	377	ASP
1	E	382	PHE
1	E	392	ASP
1	E	393	SER
1	E	405	PHE
1	E	407	GLN
1	E	419	PHE

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Mol	Chain	Res	Type
1	E	434	VAL
1	E	436	ARG
1	E	445	TYR
1	E	453	THR
1	E	463	ARG
1	E	476	VAL
1	E	502	TYR
1	E	504	SER
1	E	505	GLN
1	E	507	SER
1	E	510	THR
1	E	531	GLU
1	E	540	ARG
1	E	545	SER
1	E	547	LEU
1	E	549	THR
1	E	558	GLN
1	E	567	LEU
1	E	572	SER
1	E	576	TRP
1	E	600	ARG
1	E	612	LEU
1	E	613	ARG
1	E	635	SER
1	E	658	SER
1	E	668	ILE
1	E	682	ASP
1	E	684	ARG
1	E	690	ASP
1	E	724	LEU
1	E	781	LEU
1	E	858	GLU
1	E	890	ASN
1	E	891	GLU
1	E	895	GLU
1	E	896	ASP
1	E	898	TYR
1	E	920	GLN
1	E	927	GLU
1	E	949	GLU
1	E	952	ASN
1	E	960	LEU

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Mol	Chain	Res	Type
1	E	974	ILE
1	E	1016	VAL
1	E	1040	ARG
1	E	1059	ASN
1	G	2	ASN
1	G	3	ARG
1	G	12	ARG
1	G	20	MET
1	G	39	THR
1	G	42	PHE
1	G	44	ARG
1	G	64	LEU
1	G	71	GLU
1	G	76	SER
1	G	88	LEU
1	G	94	PHE
1	G	96	ARG
1	G	106	VAL
1	G	110	SER
1	G	111	LYS
1	G	115	MET
1	G	134	ILE
1	G	163	SER
1	G	179	HIS
1	G	183	SER
1	G	186	ARG
1	G	195	PHE
1	G	198	ASP
1	G	205	CYS
1	G	207	MET
1	G	248	ASN
1	G	251	THR
1	G	252	SER
1	G	254	LEU
1	G	265	LEU
1	G	269	VAL
1	G	289	ILE
1	G	294	ARG
1	G	295	VAL
1	G	323	LEU
1	G	326	GLN
1	G	334	GLU

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Mol	Chain	Res	Type
1	G	356	PHE
1	G	360	THR
1	G	364	ASP
1	G	367	ARG
1	G	369	THR
1	G	377	ASP
1	G	392	ASP
1	G	393	SER
1	G	405	PHE
1	G	407	GLN
1	G	419	PHE
1	G	434	VAL
1	G	436	ARG
1	G	445	TYR
1	G	453	THR
1	G	458	LYS
1	G	462	ILE
1	G	476	VAL
1	G	494	GLU
1	G	502	TYR
1	G	504	SER
1	G	507	SER
1	G	510	THR
1	G	540	ARG
1	G	545	SER
1	G	547	LEU
1	G	549	THR
1	G	558	GLN
1	G	572	SER
1	G	576	TRP
1	G	588	LEU
1	G	600	ARG
1	G	635	SER
1	G	651	TRP
1	G	658	SER
1	G	668	ILE
1	G	682	ASP
1	G	698	GLU
1	G	717	LYS
1	G	737	HIS
1	G	781	LEU
1	G	792	THR

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Mol	Chain	Res	Type
1	G	794	LEU
1	G	960	LEU
1	G	962	GLU
1	G	1016	VAL
1	G	1040	ARG
1	G	1059	ASN
1	D	2	ASN
1	D	3	ARG
1	D	12	ARG
1	D	31	VAL
1	D	39	THR
1	D	42	PHE
1	D	44	ARG
1	D	60	ILE
1	D	70	ILE
1	D	71	GLU
1	D	76	SER
1	D	88	LEU
1	D	106	VAL
1	D	110	SER
1	D	116	PHE
1	D	121	LYS
1	D	127	LEU
1	D	134	ILE
1	D	177	LYS
1	D	183	SER
1	D	198	ASP
1	D	203	GLU
1	D	204	LYS
1	D	207	MET
1	D	223	ASN
1	D	248	ASN
1	D	251	THR
1	D	252	SER
1	D	254	LEU
1	D	265	LEU
1	D	269	VAL
1	D	289	ILE
1	D	290	GLU
1	D	294	ARG
1	D	295	VAL
1	D	323	LEU

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Mol	Chain	Res	Type
1	D	334	GLU
1	D	356	PHE
1	D	360	THR
1	D	364	ASP
1	D	369	THR
1	D	377	ASP
1	D	382	PHE
1	D	392	ASP
1	D	393	SER
1	D	405	PHE
1	D	407	GLN
1	D	419	PHE
1	D	434	VAL
1	D	436	ARG
1	D	445	TYR
1	D	453	THR
1	D	461	HIS
1	D	462	ILE
1	D	499	LYS
1	D	504	SER
1	D	507	SER
1	D	520	GLU
1	D	531	GLU
1	D	533	LEU
1	D	540	ARG
1	D	545	SER
1	D	547	LEU
1	D	549	THR
1	D	558	GLN
1	D	572	SER
1	D	576	TRP
1	D	600	ARG
1	D	613	ARG
1	D	635	SER
1	D	658	SER
1	D	668	ILE
1	D	682	ASP
1	D	688	THR
1	D	695	MET
1	D	719	GLN
1	D	723	ARG
1	D	727	GLU

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Mol	Chain	Res	Type
1	D	734	VAL
1	D	781	LEU
1	D	792	THR
1	D	845	ILE
1	D	858	GLU
1	D	867	PHE
1	D	870	ILE
1	D	890	ASN
1	D	891	GLU
1	D	895	GLU
1	D	896	ASP
1	D	898	TYR
1	D	902	ASP
1	D	918	ILE
1	D	928	LYS
1	D	942	ASP
1	D	974	ILE
1	D	1016	VAL
1	D	1020	LYS
1	D	1040	ARG
1	D	1051	ARG
1	D	1059	ASN
1	A	2	ASN
1	A	39	THR
1	A	42	PHE
1	A	44	ARG
1	A	60	ILE
1	A	71	GLU
1	A	76	SER
1	A	106	VAL
1	A	110	SER
1	A	115	MET
1	A	121	LYS
1	A	127	LEU
1	A	131	ILE
1	A	134	ILE
1	A	159	MET
1	A	163	SER
1	A	176	SER
1	A	183	SER
1	A	195	PHE
1	A	198	ASP

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Mol	Chain	Res	Type
1	A	205	CYS
1	A	207	MET
1	A	251	THR
1	A	252	SER
1	A	254	LEU
1	A	265	LEU
1	A	269	VAL
1	A	289	ILE
1	A	294	ARG
1	A	295	VAL
1	A	323	LEU
1	A	326	GLN
1	A	334	GLU
1	A	360	THR
1	A	367	ARG
1	A	369	THR
1	A	382	PHE
1	A	392	ASP
1	A	393	SER
1	A	395	LEU
1	A	405	PHE
1	A	407	GLN
1	A	419	PHE
1	A	434	VAL
1	A	436	ARG
1	A	445	TYR
1	A	453	THR
1	A	462	ILE
1	A	463	ARG
1	A	476	VAL
1	A	504	SER
1	A	507	SER
1	A	510	THR
1	A	520	GLU
1	A	531	GLU
1	A	540	ARG
1	A	545	SER
1	A	547	LEU
1	A	549	THR
1	A	558	GLN
1	A	572	SER
1	A	576	TRP

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Mol	Chain	Res	Type
1	A	600	ARG
1	A	635	SER
1	A	652	ILE
1	A	658	SER
1	A	668	ILE
1	A	682	ASP
1	A	688	THR
1	A	695	MET
1	A	719	GLN
1	A	723	ARG
1	A	727	GLU
1	A	734	VAL
1	A	781	LEU
1	A	792	THR
1	A	794	LEU
1	A	811	HIS
1	A	820	LEU
1	A	845	ILE
1	A	867	PHE
1	A	870	ILE
1	A	890	ASN
1	A	891	GLU
1	A	895	GLU
1	A	896	ASP
1	A	897	VAL
1	A	902	ASP
1	A	918	ILE
1	A	940	LEU
1	A	942	ASP
1	A	943	ARG
1	A	957	LYS
1	A	960	LEU
1	A	974	ILE
1	A	1016	VAL
1	A	1030	SER
1	A	1031	ILE
1	A	1037	ASP
1	A	1040	ARG
1	A	1049	GLN
1	A	1054	ASN
1	A	1056	GLN
1	A	1059	ASN

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Mol	Chain	Res	Type
1	B	1	MET
1	B	2	ASN
1	B	27	LYS
1	B	39	THR
1	B	44	ARG
1	B	76	SER
1	B	88	LEU
1	B	92	ILE
1	B	94	PHE
1	B	106	VAL
1	B	110	SER
1	B	115	MET
1	B	127	LEU
1	B	134	ILE
1	B	144	ILE
1	B	158	LEU
1	B	163	SER
1	B	183	SER
1	B	184	PHE
1	B	198	ASP
1	B	207	MET
1	B	228	PHE
1	B	237	ARG
1	B	248	ASN
1	B	251	THR
1	B	252	SER
1	B	254	LEU
1	B	265	LEU
1	B	269	VAL
1	B	280	LEU
1	B	289	ILE
1	B	294	ARG
1	B	323	LEU
1	B	326	GLN
1	B	334	GLU
1	B	349	THR
1	B	356	PHE
1	B	357	MET
1	B	360	THR
1	B	364	ASP
1	B	367	ARG
1	B	369	THR

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Mol	Chain	Res	Type
1	B	377	ASP
1	B	382	PHE
1	B	392	ASP
1	B	393	SER
1	B	405	PHE
1	B	407	GLN
1	B	419	PHE
1	B	434	VAL
1	B	436	ARG
1	B	445	TYR
1	B	453	THR
1	B	463	ARG
1	B	476	VAL
1	B	502	TYR
1	B	504	SER
1	B	505	GLN
1	B	510	THR
1	B	540	ARG
1	B	545	SER
1	B	547	LEU
1	B	549	THR
1	B	558	GLN
1	B	567	LEU
1	B	572	SER
1	B	576	TRP
1	B	600	ARG
1	B	612	LEU
1	B	613	ARG
1	B	635	SER
1	B	658	SER
1	B	668	ILE
1	B	682	ASP
1	B	684	ARG
1	B	690	ASP
1	B	724	LEU
1	B	781	LEU
1	B	858	GLU
1	B	890	ASN
1	B	891	GLU
1	B	895	GLU
1	B	896	ASP
1	B	898	TYR

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Mol	Chain	Res	Type
1	B	920	GLN
1	B	927	GLU
1	B	949	GLU
1	B	952	ASN
1	B	960	LEU
1	B	974	ILE
1	B	1016	VAL
1	B	1040	ARG
1	B	1059	ASN
1	C	2	ASN
1	C	3	ARG
1	C	12	ARG
1	C	20	MET
1	C	39	THR
1	C	42	PHE
1	C	44	ARG
1	C	64	LEU
1	C	71	GLU
1	C	76	SER
1	C	88	LEU
1	C	94	PHE
1	C	96	ARG
1	C	106	VAL
1	C	110	SER
1	C	111	LYS
1	C	115	MET
1	C	134	ILE
1	C	172	ARG
1	C	175	GLU
1	C	179	HIS
1	C	183	SER
1	C	186	ARG
1	C	195	PHE
1	C	198	ASP
1	C	203	GLU
1	C	205	CYS
1	C	207	MET
1	C	248	ASN
1	C	251	THR
1	C	252	SER
1	C	254	LEU
1	C	265	LEU

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Mol	Chain	Res	Type
1	C	269	VAL
1	C	289	ILE
1	C	294	ARG
1	C	295	VAL
1	C	323	LEU
1	C	326	GLN
1	C	334	GLU
1	C	356	PHE
1	C	360	THR
1	C	364	ASP
1	C	367	ARG
1	C	369	THR
1	C	377	ASP
1	C	392	ASP
1	C	393	SER
1	C	405	PHE
1	C	407	GLN
1	C	419	PHE
1	C	434	VAL
1	C	436	ARG
1	C	445	TYR
1	C	453	THR
1	C	458	LYS
1	C	462	ILE
1	C	476	VAL
1	C	494	GLU
1	C	502	TYR
1	C	504	SER
1	C	507	SER
1	C	510	THR
1	C	531	GLU
1	C	540	ARG
1	C	545	SER
1	C	547	LEU
1	C	549	THR
1	C	558	GLN
1	C	572	SER
1	C	576	TRP
1	C	588	LEU
1	C	600	ARG
1	C	635	SER
1	C	651	TRP

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Mol	Chain	Res	Type
1	C	658	SER
1	C	668	ILE
1	C	682	ASP
1	C	698	GLU
1	C	717	LYS
1	C	737	HIS
1	C	781	LEU
1	C	792	THR
1	C	794	LEU
1	C	960	LEU
1	C	962	GLU
1	C	1016	VAL
1	C	1040	ARG
1	C	1059	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	2	ASN
1	H	43	HIS
1	H	82	HIS
1	H	112	HIS
1	H	221	HIS
1	H	226	HIS
1	H	333	GLN
1	H	337	HIS
1	H	354	ASN
1	H	415	ASN
1	H	479	ASN
1	H	558	GLN
1	H	741	HIS
1	H	787	ASN
1	H	842	GLN
1	H	890	ASN
1	F	2	ASN
1	F	43	HIS
1	F	82	HIS
1	F	112	HIS
1	F	179	HIS
1	F	221	HIS
1	F	226	HIS
1	F	333	GLN

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Mol	Chain	Res	Type
1	F	337	HIS
1	F	383	GLN
1	F	415	ASN
1	F	461	HIS
1	F	479	ASN
1	F	505	GLN
1	F	558	GLN
1	F	565	HIS
1	F	741	HIS
1	F	787	ASN
1	F	830	HIS
1	F	865	GLN
1	F	890	ASN
1	F	1029	ASN
1	E	2	ASN
1	E	43	HIS
1	E	82	HIS
1	E	112	HIS
1	E	221	HIS
1	E	226	HIS
1	E	333	GLN
1	E	337	HIS
1	E	354	ASN
1	E	383	GLN
1	E	415	ASN
1	E	437	HIS
1	E	479	ASN
1	E	558	GLN
1	E	637	GLN
1	E	746	ASN
1	E	787	ASN
1	E	842	GLN
1	E	865	GLN
1	G	2	ASN
1	G	43	HIS
1	G	82	HIS
1	G	112	HIS
1	G	221	HIS
1	G	226	HIS
1	G	333	GLN
1	G	337	HIS
1	G	383	GLN

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Mol	Chain	Res	Type
1	G	415	ASN
1	G	461	HIS
1	G	479	ASN
1	G	558	GLN
1	G	737	HIS
1	G	746	ASN
1	G	787	ASN
1	G	830	HIS
1	D	2	ASN
1	D	43	HIS
1	D	82	HIS
1	D	112	HIS
1	D	221	HIS
1	D	226	HIS
1	D	333	GLN
1	D	337	HIS
1	D	354	ASN
1	D	383	GLN
1	D	415	ASN
1	D	479	ASN
1	D	486	HIS
1	D	558	GLN
1	D	741	HIS
1	D	787	ASN
1	D	842	GLN
1	D	890	ASN
1	A	2	ASN
1	A	43	HIS
1	A	82	HIS
1	A	112	HIS
1	A	179	HIS
1	A	221	HIS
1	A	226	HIS
1	A	333	GLN
1	A	337	HIS
1	A	383	GLN
1	A	415	ASN
1	A	461	HIS
1	A	479	ASN
1	A	558	GLN
1	A	565	HIS
1	A	741	HIS

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Mol	Chain	Res	Type
1	A	787	ASN
1	A	830	HIS
1	A	865	GLN
1	A	890	ASN
1	A	1029	ASN
1	B	43	HIS
1	B	82	HIS
1	B	112	HIS
1	B	221	HIS
1	B	226	HIS
1	B	333	GLN
1	B	337	HIS
1	B	354	ASN
1	B	383	GLN
1	B	415	ASN
1	B	437	HIS
1	B	479	ASN
1	B	505	GLN
1	B	558	GLN
1	B	637	GLN
1	B	746	ASN
1	B	787	ASN
1	B	842	GLN
1	B	865	GLN
1	C	2	ASN
1	C	43	HIS
1	C	82	HIS
1	C	112	HIS
1	C	221	HIS
1	C	226	HIS
1	C	333	GLN
1	C	337	HIS
1	C	415	ASN
1	C	479	ASN
1	C	558	GLN
1	C	565	HIS
1	C	737	HIS
1	C	746	ASN
1	C	787	ASN
1	C	830	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	1052/1146 (91%)	-0.20	13 (1%) 81 74	74, 124, 168, 201	0
1	B	1031/1146 (89%)	-0.10	36 (3%) 48 39	72, 153, 205, 246	0
1	C	941/1146 (82%)	0.02	51 (5%) 29 22	72, 147, 212, 265	0
1	D	1029/1146 (89%)	-0.18	12 (1%) 81 74	58, 118, 188, 231	0
1	E	1031/1146 (89%)	-0.13	39 (3%) 44 34	68, 149, 205, 248	0
1	F	1052/1146 (91%)	-0.23	9 (0%) 85 81	72, 123, 168, 204	0
1	G	942/1146 (82%)	-0.05	33 (3%) 48 39	70, 141, 208, 267	0
1	H	1029/1146 (89%)	-0.19	9 (0%) 85 81	59, 114, 185, 232	0
All	All	8107/9168 (88%)	-0.14	202 (2%) 61 52	58, 132, 199, 267	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	675	TYR	8.0
1	C	726	GLY	6.6
1	C	675	TYR	6.2
1	E	194	ALA	5.9
1	B	194	ALA	5.7
1	B	535	THR	5.6
1	H	901	GLY	5.5
1	C	718	PRO	5.1
1	G	719	GLN	5.0
1	E	108	PRO	5.0
1	E	535	THR	5.0
1	B	572	SER	5.0
1	E	293	PRO	4.8
1	E	572	SER	4.8
1	H	903	THR	4.7
1	G	674	CYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	G	718	PRO	4.4
1	B	581	PHE	4.4
1	E	575	MET	4.4
1	C	719	GLN	4.4
1	B	294	ARG	4.3
1	A	1018	LEU	4.3
1	G	734	VAL	4.2
1	C	206	VAL	4.2
1	F	692	TYR	4.1
1	C	721	ALA	4.1
1	G	650	ASN	4.0
1	E	193	ALA	4.0
1	G	730	ASP	4.0
1	B	293	PRO	4.0
1	B	108	PRO	3.9
1	E	294	ARG	3.9
1	C	734	VAL	3.8
1	D	909	SER	3.8
1	C	707	LEU	3.7
1	E	534	LEU	3.7
1	G	696	ALA	3.6
1	C	674	CYS	3.6
1	G	141	VAL	3.6
1	B	871	VAL	3.5
1	C	202	VAL	3.5
1	C	1022	LYS	3.5
1	F	1018	LEU	3.5
1	H	868	GLY	3.5
1	D	843	GLN	3.5
1	E	107	GLY	3.4
1	H	913	PHE	3.4
1	B	569	ASN	3.4
1	A	692	TYR	3.3
1	G	726	GLY	3.3
1	B	89	SER	3.3
1	C	291	VAL	3.3
1	D	903	THR	3.2
1	C	292	ASN	3.2
1	B	648	SER	3.2
1	C	281	VAL	3.2
1	B	568	PRO	3.2
1	C	143	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	201	TYR	3.2
1	E	163	SER	3.1
1	E	568	PRO	3.1
1	C	216	ILE	3.1
1	F	1023	ILE	3.1
1	C	575	MET	3.1
1	F	1046	LEU	3.0
1	G	806	TRP	3.0
1	B	193	ALA	3.0
1	A	1046	LEU	3.0
1	C	141	VAL	3.0
1	C	160	ILE	3.0
1	E	90	GLU	3.0
1	C	276	THR	2.9
1	C	724	LEU	2.9
1	G	967	GLU	2.9
1	G	678	ASP	2.9
1	G	805	TYR	2.9
1	C	595	ARG	2.9
1	D	932	LEU	2.9
1	H	843	GLN	2.8
1	G	144	ILE	2.8
1	E	676	THR	2.8
1	C	142	ALA	2.8
1	E	197	ASN	2.8
1	B	575	MET	2.8
1	B	534	LEU	2.8
1	G	676	THR	2.8
1	E	998	VAL	2.8
1	E	709	ILE	2.7
1	C	498	PRO	2.7
1	E	677	GLY	2.7
1	B	90	GLU	2.7
1	E	292	ASN	2.7
1	A	1023	ILE	2.7
1	G	143	GLY	2.7
1	C	1018	LEU	2.7
1	G	751	TYR	2.7
1	G	207	MET	2.7
1	E	569	ASN	2.7
1	D	868	GLY	2.7
1	B	88	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	133	VAL	2.7
1	B	163	SER	2.6
1	C	293	PRO	2.6
1	C	706	ILE	2.6
1	H	910	VAL	2.6
1	C	551	VAL	2.6
1	D	870	ILE	2.6
1	B	107	GLY	2.6
1	G	813	TYR	2.6
1	G	142	ALA	2.5
1	A	689	ILE	2.5
1	B	162	ALA	2.5
1	A	677	GLY	2.5
1	F	1024	LEU	2.5
1	B	1028	LEU	2.5
1	E	567	LEU	2.5
1	F	675	TYR	2.5
1	C	669	VAL	2.5
1	B	677	GLY	2.5
1	C	725	ILE	2.5
1	C	650	ASN	2.4
1	E	195	PHE	2.4
1	E	642	VAL	2.4
1	E	716	LEU	2.4
1	B	539	LEU	2.4
1	D	836	GLN	2.4
1	G	786	VAL	2.4
1	G	710	LYS	2.4
1	G	679	ILE	2.4
1	C	277	VAL	2.4
1	C	89	SER	2.4
1	D	87	PHE	2.4
1	E	648	SER	2.4
1	G	740	THR	2.4
1	G	575	MET	2.3
1	E	735	PRO	2.3
1	B	195	PHE	2.3
1	G	140	PRO	2.3
1	G	202	VAL	2.3
1	C	722	TYR	2.3
1	B	769	MET	2.3
1	C	278	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	277	VAL	2.3
1	G	551	VAL	2.3
1	C	538	THR	2.3
1	E	539	LEU	2.3
1	A	228	PHE	2.3
1	E	198	ASP	2.3
1	E	871	VAL	2.3
1	G	293	PRO	2.3
1	E	749	TYR	2.3
1	D	227	LEU	2.3
1	B	650	ASN	2.2
1	C	805	TYR	2.2
1	E	941	THR	2.2
1	H	867	PHE	2.2
1	D	901	GLY	2.2
1	B	295	VAL	2.2
1	F	575	MET	2.2
1	A	575	MET	2.2
1	C	118	ASP	2.2
1	E	581	PHE	2.2
1	C	559	ILE	2.2
1	C	975	SER	2.2
1	G	10	ALA	2.2
1	B	197	ASN	2.2
1	D	910	VAL	2.2
1	A	913	PHE	2.2
1	C	740	THR	2.1
1	E	643	PHE	2.1
1	B	217	LEU	2.1
1	B	161	LYS	2.1
1	C	266	MET	2.1
1	E	162	ALA	2.1
1	G	677	GLY	2.1
1	A	1049	GLN	2.1
1	B	498	PRO	2.1
1	E	191	ALA	2.1
1	C	806	TRP	2.1
1	C	703	GLY	2.1
1	B	1008	MET	2.1
1	D	216	ILE	2.1
1	B	191	ALA	2.1
1	A	1024	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	473	ILE	2.1
1	C	749	TYR	2.1
1	A	279	PHE	2.1
1	A	1051	ARG	2.1
1	C	735	PRO	2.1
1	E	89	SER	2.0
1	E	939	PRO	2.0
1	B	449	PHE	2.0
1	H	576	TRP	2.0
1	C	147	VAL	2.0
1	E	995	ASP	2.0
1	C	203	GLU	2.0
1	F	1017	GLU	2.0
1	E	669	VAL	2.0
1	B	141	VAL	2.0
1	H	874	THR	2.0
1	C	207	MET	2.0
1	G	724	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.