Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2016 – 01:28 PM EDT

PDB ID	:	5DJW
Title	:	Crystal structure of Family 31 alpha-glucosidase (BT_3299) from Bacteroides thetaiotaomicron
Authors	:	Chaudet, M.M.; Rose, D.R.
Deposited on	:	2015-09-02
Resolution	:	2.70 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

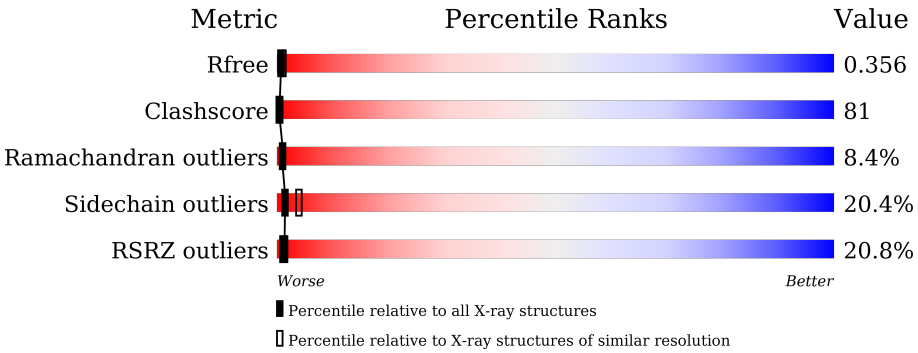
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 <=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	697	18% 22% 45% 15% • 16%
1	B	697	17% 22% 45% 14% • 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9139 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 Alpha-glucosidase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4569	2924	782	843	20			
1	B	587	Total	C	N	O	S	0	0	0
			4547	2913	783	831	20			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8A2K6
A	685	HIS	-	expression tag	UNP Q8A2K6
A	686	HIS	-	expression tag	UNP Q8A2K6
A	687	HIS	-	expression tag	UNP Q8A2K6
A	688	HIS	-	expression tag	UNP Q8A2K6
A	689	HIS	-	expression tag	UNP Q8A2K6
A	690	HIS	-	expression tag	UNP Q8A2K6
A	691	LEU	-	expression tag	UNP Q8A2K6
A	692	ARG	-	expression tag	UNP Q8A2K6
A	693	VAL	-	expression tag	UNP Q8A2K6
A	694	PRO	-	expression tag	UNP Q8A2K6
A	695	ARG	-	expression tag	UNP Q8A2K6
A	696	GLY	-	expression tag	UNP Q8A2K6
A	697	SER	-	expression tag	UNP Q8A2K6
B	1	MET	-	initiating methionine	UNP Q8A2K6
B	685	HIS	-	expression tag	UNP Q8A2K6
B	686	HIS	-	expression tag	UNP Q8A2K6
B	687	HIS	-	expression tag	UNP Q8A2K6
B	688	HIS	-	expression tag	UNP Q8A2K6
B	689	HIS	-	expression tag	UNP Q8A2K6
B	690	HIS	-	expression tag	UNP Q8A2K6
B	691	LEU	-	expression tag	UNP Q8A2K6
B	692	ARG	-	expression tag	UNP Q8A2K6
B	693	VAL	-	expression tag	UNP Q8A2K6
B	694	PRO	-	expression tag	UNP Q8A2K6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	695	ARG	-	expression tag	UNP Q8A2K6
B	696	GLY	-	expression tag	UNP Q8A2K6
B	697	SER	-	expression tag	UNP Q8A2K6

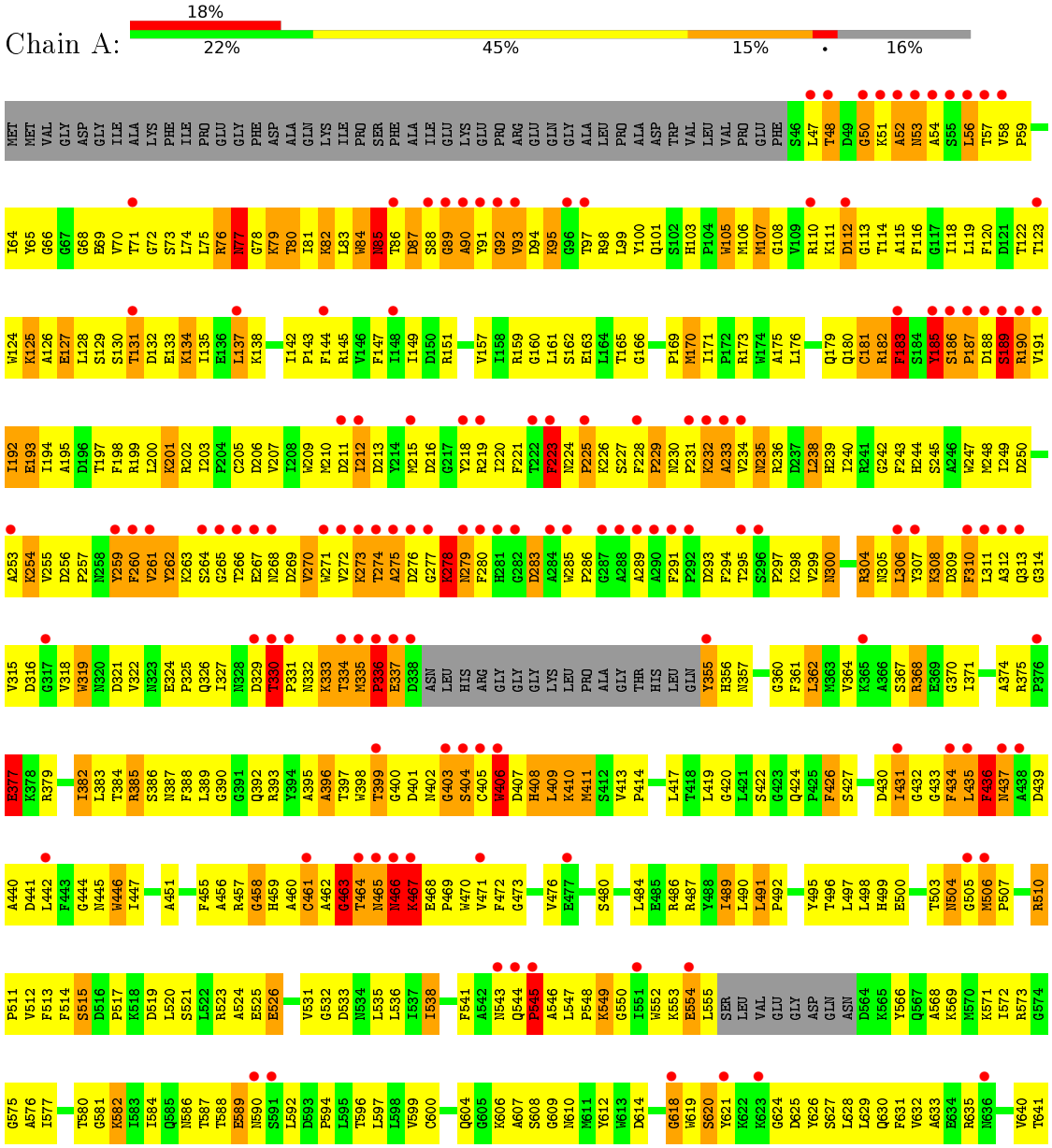
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	15	Total O 15 15	0	0
2	B	8	Total O 8 8	0	0

3 Residue-property plots (i)

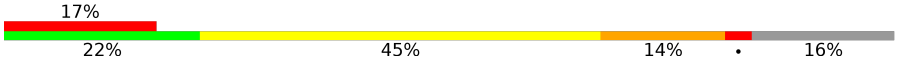
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

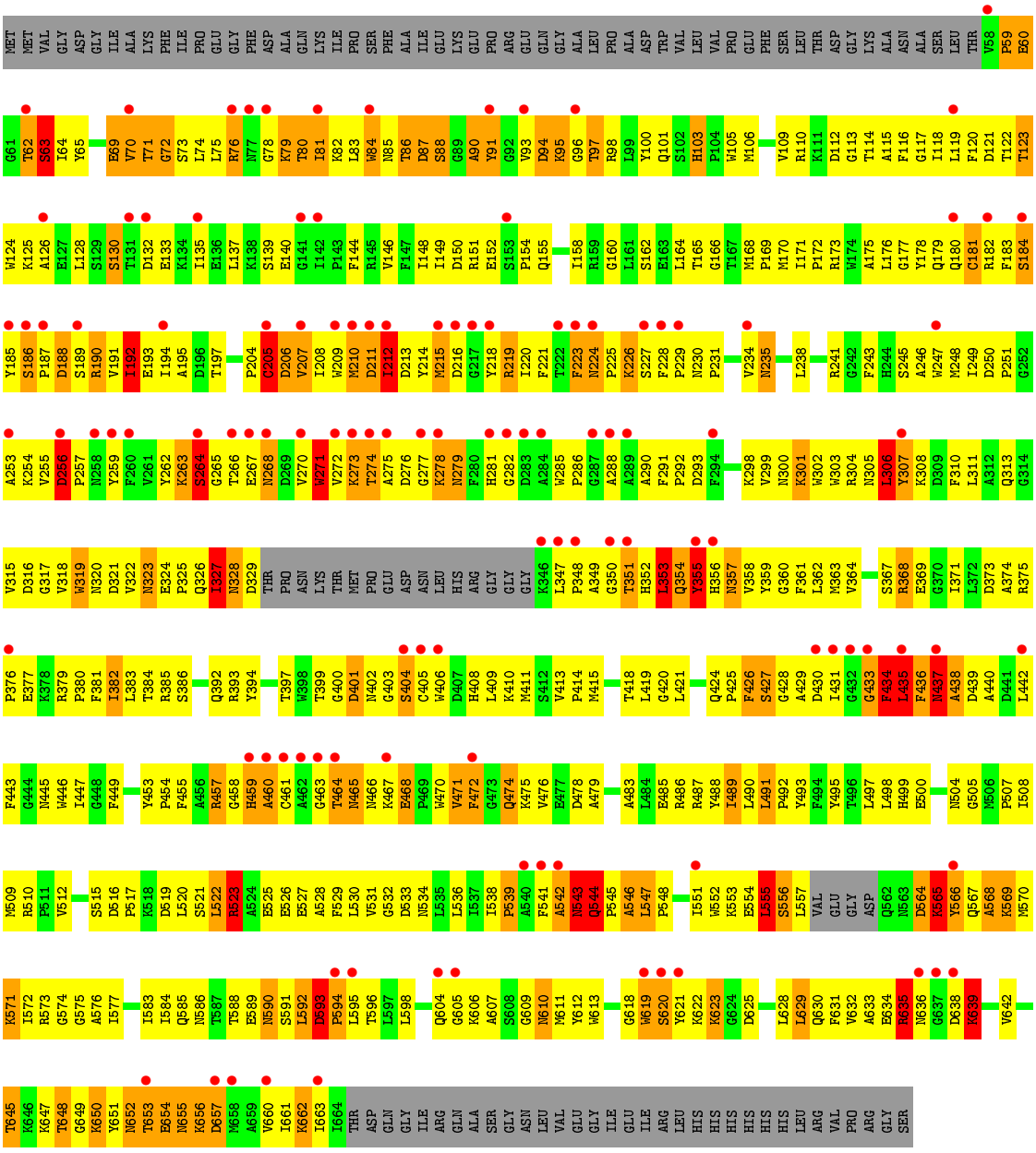
- Molecule 1: Alpha-glucosidase II



- Molecule 1: Alpha-glucosidase II

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.26Å 74.86Å 94.43Å 90.00° 95.70° 90.00°	Depositor
Resolution (Å)	47.55 – 2.70 47.55 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.55-2.70) 100.0 (47.55-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.330 , 0.390 0.304 , 0.356	Depositor DCC
R_{free} test set	1714 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 89.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	9139	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.84	3/4694 (0.1%)	0.98	16/6370 (0.3%)
1	B	1.10	2/4672 (0.0%)	1.00	16/6342 (0.3%)
All	All	0.98	5/9366 (0.1%)	0.99	32/12712 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	18
1	B	0	20
All	All	0	38

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	434	PHE	C-N	-49.64	0.19	1.34
1	B	594	PRO	C-N	13.36	1.64	1.34
1	A	50	GLY	C-N	9.53	1.55	1.34
1	A	143	PRO	N-CD	5.13	1.55	1.47
1	A	545	PRO	N-CD	5.13	1.55	1.47

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	50	GLY	O-C-N	-18.38	93.30	122.70
1	B	326	GLN	C-N-CA	14.11	156.97	121.70
1	A	309	ASP	CB-CA-C	-13.73	82.94	110.40
1	B	434	PHE	CA-C-N	-11.30	92.34	117.20
1	B	327	ILE	CA-C-N	-10.55	93.98	117.20
1	B	434	PHE	O-C-N	10.44	139.41	122.70
1	A	463	GLY	N-CA-C	-10.37	87.19	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	50	GLY	C-N-CA	-9.11	98.92	121.70
1	A	330	THR	C-N-CD	-8.15	102.67	120.60
1	B	434	PHE	C-N-CA	-8.06	101.54	121.70
1	A	225	PRO	CB-CA-C	-7.59	93.02	112.00
1	B	206	ASP	N-CA-C	7.50	131.24	111.00
1	B	326	GLN	O-C-N	-7.24	111.12	122.70
1	B	544	GLN	N-CA-C	-7.05	91.97	111.00
1	A	89	GLY	N-CA-C	-6.81	96.08	113.10
1	A	620	SER	N-CA-C	-6.75	92.77	111.00
1	B	208	ILE	N-CA-C	-6.48	93.51	111.00
1	A	265	GLY	N-CA-C	-6.40	97.11	113.10
1	B	327	ILE	O-C-N	6.38	132.91	122.70
1	B	62	THR	N-CA-C	6.28	127.96	111.00
1	B	91	TYR	N-CA-CB	6.19	121.74	110.60
1	B	433	GLY	N-CA-C	5.78	127.56	113.10
1	A	142	ILE	C-N-CD	5.68	140.33	128.40
1	A	618	GLY	N-CA-C	-5.63	99.03	113.10
1	A	545	PRO	CA-N-CD	-5.60	103.66	111.50
1	A	377	GLU	N-CA-C	5.58	126.06	111.00
1	B	401	ASP	N-CA-C	-5.46	96.25	111.00
1	A	403	GLY	N-CA-C	-5.43	99.52	113.10
1	A	186	SER	C-N-CD	-5.34	108.85	120.60
1	A	310	PHE	CB-CA-C	-5.12	100.16	110.40
1	B	205	CYS	C-N-CA	5.12	134.49	121.70
1	B	327	ILE	N-CA-C	5.07	124.67	111.00

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	TYR	Peptide
1	A	235	ASN	Peptide
1	A	259	TYR	Peptide
1	A	330	THR	Peptide
1	A	336	PRO	Peptide
1	A	377	GLU	Peptide
1	A	396	ALA	Peptide
1	A	399	THR	Peptide
1	A	436	PHE	Peptide
1	A	458	GLY	Peptide
1	A	463	GLY	Peptide
1	A	464	THR	Peptide

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Mol	Chain	Res	Type	Group
1	A	50	GLY	Mainchain
1	A	504	ASN	Peptide
1	A	541	PHE	Peptide
1	A	620	SER	Peptide
1	A	652	ASN	Peptide
1	A	77	ASN	Peptide
1	B	188	ASP	Peptide
1	B	192	ILE	Peptide
1	B	205	CYS	Peptide
1	B	223	PHE	Peptide
1	B	256	ASP	Peptide
1	B	264	SER	Peptide
1	B	276	ASP	Peptide
1	B	306	LEU	Peptide
1	B	327	ILE	Mainchain
1	B	353	LEU	Mainchain
1	B	355	TYR	Peptide
1	B	434	PHE	Mainchain
1	B	544	GLN	Peptide
1	B	551	ILE	Peptide
1	B	593	ASP	Peptide
1	B	619	TRP	Peptide
1	B	622	LYS	Peptide
1	B	635	ARG	Peptide
1	B	648	THR	Peptide
1	B	90	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4569	0	4348	730	5
1	B	4547	0	4343	709	1
2	A	15	0	0	8	1
2	B	8	0	0	3	0
All	All	9139	0	8691	1435	6

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 81.

All (1435) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:VAL:CG1	1:A:336:PRO:HG2	1.40	1.51
1:B:553:LYS:CB	1:B:572:ILE:HG22	1.36	1.50
1:B:256:ASP:O	1:B:259:TYR:CD2	1.73	1.40
1:B:552:TRP:CB	1:B:571:LYS:HE2	1.49	1.39
1:A:256:ASP:O	1:A:259:TYR:CD2	1.73	1.39
1:B:181:CYS:SG	1:B:211:ASP:CB	2.12	1.37
1:A:324:GLU:OE2	1:A:385:ARG:NH1	1.57	1.37
1:A:84:TRP:CD1	1:A:85:ASN:N	1.89	1.36
1:A:101:GLN:NE2	1:A:387:ASN:HB3	1.41	1.35
1:A:280:PHE:CE1	1:A:336:PRO:HD2	1.67	1.30
1:B:379:ARG:NE	1:B:618:GLY:O	1.62	1.30
1:B:406:TRP:CZ2	1:B:541:PHE:HD2	1.48	1.29
1:B:328:ASN:CB	1:B:348:PRO:HB3	1.59	1.29
1:A:224:ASN:HB3	1:A:227:SER:CB	1.63	1.28
1:A:330:THR:HG21	2:A:712:HOH:O	1.14	1.28
1:B:347:LEU:O	1:B:350:GLY:N	1.67	1.27
1:B:406:TRP:NE1	1:B:541:PHE:CE2	2.02	1.26
1:A:436:PHE:CZ	1:A:459:HIS:HE1	1.51	1.26
1:A:272:VAL:CG1	1:A:336:PRO:CG	2.14	1.25
1:A:379:ARG:NH2	1:A:618:GLY:O	1.69	1.25
1:B:188:ASP:OD1	1:B:191:VAL:HG22	1.33	1.24
1:A:436:PHE:HZ	1:A:459:HIS:CE1	1.56	1.24
1:B:219:ARG:NH1	1:B:254:LYS:HG2	1.50	1.23
1:A:436:PHE:CZ	1:A:459:HIS:CE1	2.25	1.22
1:B:214:TYR:OH	1:B:248:MET:O	1.52	1.22
1:A:193:GLU:O	1:A:197:THR:OG1	1.54	1.21
1:B:166:GLY:O	1:B:392:GLN:NE2	1.74	1.20
1:A:57:THR:HG23	1:A:134:LYS:CD	1.71	1.20
1:B:245:SER:OG	1:B:247:TRP:NE1	1.73	1.20
1:A:627:SER:HA	1:A:647:LYS:NZ	1.58	1.19
1:A:192:ILE:HG21	1:A:195:ALA:HB3	1.26	1.18
1:A:80:THR:HB	1:A:129:SER:CB	1.72	1.18
1:A:86:THR:O	1:A:88:SER:N	1.77	1.17
1:A:272:VAL:CG2	1:A:280:PHE:HB2	1.74	1.17
1:A:272:VAL:HG13	1:A:336:PRO:CG	1.71	1.17
1:A:233:ALA:CB	1:A:312:ALA:HA	1.72	1.17
1:B:306:LEU:HD13	1:B:307:TYR:HA	1.17	1.17
1:A:225:PRO:O	1:A:229:PRO:HG3	1.43	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:TRP:CZ2	1:B:541:PHE:CD2	2.32	1.16
1:B:211:ASP:O	1:B:212:ILE:CG2	1.94	1.15
1:B:189:SER:O	1:B:191:VAL:N	1.76	1.15
1:B:178:TYR:HB3	1:B:205:CYS:HB3	1.15	1.15
1:B:406:TRP:NE1	1:B:541:PHE:CD2	2.16	1.14
1:A:224:ASN:HB3	1:A:227:SER:HB3	1.14	1.12
1:A:223:PHE:CZ	1:A:311:LEU:CB	2.32	1.12
1:A:57:THR:CG2	1:A:134:LYS:HD2	1.78	1.12
1:A:225:PRO:O	1:A:229:PRO:CG	1.96	1.12
1:A:80:THR:HB	1:A:129:SER:CA	1.79	1.12
1:B:263:LYS:HA	1:B:265:GLY:H	1.10	1.11
1:B:307:TYR:CD2	1:B:374:ALA:HB2	1.85	1.11
1:B:586:ASN:HB2	1:B:589:GLU:HG3	1.19	1.11
1:A:182:ARG:NH2	1:A:190:ARG:CB	2.13	1.10
1:A:256:ASP:O	1:A:259:TYR:HD2	1.15	1.10
1:B:553:LYS:CB	1:B:572:ILE:CG2	2.30	1.10
1:B:256:ASP:O	1:B:259:TYR:CE2	2.05	1.09
1:A:101:GLN:NE2	1:A:387:ASN:CB	2.15	1.09
1:A:53:ASN:O	1:A:144:PHE:HZ	1.33	1.09
1:A:266:THR:O	1:A:267:GLU:HB2	1.46	1.09
1:A:627:SER:HA	1:A:647:LYS:HZ1	0.95	1.09
1:A:647:LYS:NZ	1:A:648:THR:O	1.85	1.09
1:B:186:SER:HB3	1:B:187:PRO:CD	1.82	1.08
1:A:87:ASP:HA	1:A:100:TYR:HE1	1.15	1.08
1:B:404:SER:O	1:B:442:LEU:CD2	2.02	1.08
1:B:552:TRP:CB	1:B:571:LYS:CE	2.32	1.08
1:A:272:VAL:HG22	1:A:280:PHE:HB2	1.09	1.07
1:B:219:ARG:NH1	1:B:254:LYS:CG	2.16	1.07
1:B:211:ASP:O	1:B:212:ILE:HG23	1.50	1.07
1:B:406:TRP:CE2	1:B:541:PHE:CD2	2.42	1.07
1:B:219:ARG:HH11	1:B:254:LYS:CG	1.67	1.07
1:A:294:PHE:HB3	1:A:362:LEU:HD22	1.36	1.07
1:A:84:TRP:CE2	1:A:356:HIS:CD2	2.43	1.07
1:A:84:TRP:HD1	1:A:85:ASN:N	1.38	1.07
1:A:80:THR:HB	1:A:129:SER:HA	1.34	1.07
1:B:186:SER:HB3	1:B:187:PRO:HD3	1.30	1.06
1:A:179:GLN:HB3	1:A:209:TRP:HE1	1.20	1.06
1:A:238:LEU:O	1:A:243:PHE:HB2	1.52	1.06
1:A:625:ASP:HA	1:A:651:TYR:CB	1.85	1.06
1:B:178:TYR:HB3	1:B:205:CYS:CB	1.85	1.05
1:B:328:ASN:HB2	1:B:348:PRO:HB3	1.11	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ASP:CA	1:A:651:TYR:CB	2.34	1.05
1:A:460:ALA:HB3	1:A:467:LYS:HD3	1.39	1.05
1:B:566:TYR:HA	1:B:567:GLN:HG2	1.36	1.04
1:A:192:ILE:O	1:A:194:ILE:N	1.90	1.04
1:A:86:THR:HG21	1:A:333:LYS:CB	1.88	1.04
1:B:194:ILE:CG2	1:B:470:TRP:HZ2	1.70	1.04
1:B:323:ASN:OD1	1:B:386:SER:HB3	1.58	1.04
1:A:280:PHE:CD1	1:A:336:PRO:HD2	1.91	1.04
1:B:194:ILE:HG22	1:B:470:TRP:CZ2	1.92	1.04
1:A:280:PHE:CE1	1:A:336:PRO:CD	2.42	1.03
1:A:506:MET:HB3	1:A:507:PRO:HD2	1.39	1.03
1:B:454:PRO:CD	1:B:509:MET:HE3	1.88	1.03
1:A:263:LYS:O	1:A:266:THR:CB	2.05	1.03
1:B:72:GLY:HA2	1:B:73:SER:HB2	1.39	1.03
1:B:210:MET:HB2	1:B:211:ASP:CB	1.88	1.03
1:B:328:ASN:HB2	1:B:348:PRO:CB	1.90	1.02
1:B:402:ASN:ND2	1:B:446:TRP:CH2	2.26	1.02
1:B:139:SER:HB3	1:B:144:PHE:HE2	1.19	1.02
1:B:70:VAL:HG22	1:B:71:THR:H	1.25	1.02
1:A:233:ALA:HB2	1:A:312:ALA:HA	1.03	1.02
1:A:87:ASP:HA	1:A:100:TYR:CE1	1.95	1.02
1:A:53:ASN:O	1:A:144:PHE:CZ	2.13	1.02
1:A:433:GLY:O	1:A:460:ALA:HA	1.55	1.02
1:A:119:LEU:HD13	1:A:389:LEU:HD21	1.41	1.01
1:B:270:VAL:CG2	1:B:292:PRO:HA	1.90	1.01
1:B:590:ASN:O	1:B:591:SER:OG	1.77	1.01
1:A:192:ILE:CG2	1:A:195:ALA:HB3	1.91	1.01
1:A:182:ARG:NH2	1:A:190:ARG:HB2	1.75	1.00
1:A:512:VAL:O	1:A:515:SER:OG	1.75	1.00
1:B:189:SER:O	1:B:191:VAL:HG13	1.60	1.00
1:A:506:MET:HB3	1:A:507:PRO:CD	1.90	1.00
1:B:256:ASP:O	1:B:259:TYR:HD2	1.16	1.00
1:B:221:PHE:CE1	1:B:306:LEU:HG	1.97	1.00
1:A:229:PRO:C	1:A:231:PRO:CD	2.29	1.00
1:B:545:PRO:HG2	1:B:547:LEU:HD13	1.42	1.00
1:A:580:THR:OG1	1:A:596:THR:O	1.80	1.00
1:B:307:TYR:O	2:B:701:HOH:O	1.80	0.99
1:A:131:THR:HG22	1:A:132:ASP:H	1.24	0.99
1:A:512:VAL:HG13	1:A:548:PRO:HD3	1.42	0.99
1:A:101:GLN:HE21	1:A:387:ASN:HB3	0.83	0.99
1:A:248:MET:HB2	1:A:319:TRP:CZ2	1.98	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:LEU:O	1:B:523:ARG:HB2	1.61	0.99
1:A:78:GLY:HA2	1:A:131:THR:HA	1.42	0.98
1:A:219:ARG:HH22	1:A:256:ASP:CB	1.77	0.98
1:B:306:LEU:HD13	1:B:307:TYR:CA	1.93	0.98
1:A:229:PRO:C	1:A:231:PRO:HD3	1.81	0.98
1:B:188:ASP:OD1	1:B:191:VAL:CG2	2.12	0.98
1:A:182:ARG:HH22	1:A:190:ARG:CB	1.73	0.98
1:B:74:LEU:HD23	1:B:75:LEU:H	1.27	0.98
1:A:627:SER:CA	1:A:647:LYS:NZ	2.27	0.98
1:B:554:GLU:O	1:B:555:LEU:HB2	1.60	0.98
1:B:328:ASN:CG	1:B:348:PRO:HB3	1.83	0.97
1:B:368:ARG:HG3	1:B:382:ILE:HG21	1.46	0.97
1:A:331:PRO:O	1:A:332:ASN:OD1	1.80	0.97
1:A:74:LEU:HD12	1:A:76:ARG:O	1.64	0.97
1:A:517:PRO:O	1:A:523:ARG:NH2	1.95	0.97
1:B:306:LEU:CD1	1:B:307:TYR:HA	1.94	0.97
1:A:228:PHE:C	1:A:230:ASN:H	1.66	0.96
1:B:248:MET:HB2	1:B:319:TRP:CZ2	2.00	0.96
1:A:101:GLN:HG2	1:A:387:ASN:N	1.79	0.96
1:B:194:ILE:CG2	1:B:470:TRP:CZ2	2.48	0.96
1:B:117:GLY:N	1:B:149:ILE:O	1.97	0.96
1:B:434:PHE:O	1:B:436:PHE:N	1.89	0.95
1:B:594:PRO:O	1:B:596:THR:N	1.97	0.95
1:A:192:ILE:C	1:A:194:ILE:H	1.65	0.95
1:B:406:TRP:HZ2	1:B:541:PHE:HD2	1.07	0.95
1:B:263:LYS:HA	1:B:265:GLY:N	1.79	0.95
1:B:573:ARG:HH11	1:B:573:ARG:HG2	1.30	0.95
1:A:525:GLU:OE1	1:A:545:PRO:HG2	1.65	0.95
1:A:119:LEU:CD1	1:A:389:LEU:HD21	1.97	0.95
1:A:228:PHE:O	1:A:231:PRO:HD3	1.64	0.95
1:A:641:THR:HB	1:A:643:LYS:HE3	1.49	0.95
1:A:86:THR:HG22	1:A:87:ASP:OD1	1.66	0.95
1:A:224:ASN:HB3	1:A:227:SER:HB2	1.49	0.94
1:A:233:ALA:HB2	1:A:312:ALA:CA	1.96	0.94
1:B:118:ILE:HD11	1:B:120:PHE:CE1	2.01	0.94
1:B:328:ASN:CB	1:B:348:PRO:CB	2.42	0.94
1:B:555:LEU:HD23	1:B:570:MET:HE3	1.49	0.94
1:A:272:VAL:HG11	1:A:336:PRO:CG	1.96	0.94
1:B:307:TYR:HD2	1:B:374:ALA:HB2	1.28	0.94
1:B:593:ASP:CB	1:B:594:PRO:HD3	1.97	0.94
1:B:512:VAL:HG23	1:B:528:ALA:O	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLN:HG2	1:A:387:ASN:H	1.33	0.94
1:A:223:PHE:CE2	1:A:311:LEU:CB	2.51	0.93
1:B:219:ARG:HH12	1:B:254:LYS:HG2	1.33	0.93
1:B:402:ASN:HB2	1:B:430:ASP:HB2	1.47	0.93
1:A:272:VAL:HG11	1:A:336:PRO:HG2	1.49	0.93
1:B:454:PRO:HD3	1:B:509:MET:HE3	1.50	0.93
1:A:256:ASP:O	1:A:259:TYR:CE2	2.21	0.93
1:A:275:ALA:O	1:A:277:GLY:N	2.00	0.93
1:A:179:GLN:OE1	1:A:455:PHE:HE1	1.52	0.93
1:A:277:GLY:O	1:A:278:LYS:HB2	1.66	0.93
1:A:179:GLN:HG2	1:A:207:VAL:HB	1.49	0.92
1:A:84:TRP:CZ3	1:A:356:HIS:HB2	2.04	0.92
1:A:225:PRO:C	1:A:229:PRO:HG3	1.88	0.92
1:B:434:PHE:HD2	1:B:435:LEU:HA	1.35	0.92
1:B:545:PRO:HG2	1:B:547:LEU:CD1	2.00	0.92
1:A:101:GLN:HE21	1:A:387:ASN:CB	1.77	0.91
1:B:593:ASP:HB2	1:B:594:PRO:HD3	1.51	0.91
1:A:182:ARG:HH21	1:A:190:ARG:HB2	1.34	0.91
1:B:415:MET:O	1:B:418:THR:HG22	1.70	0.91
1:A:84:TRP:CE3	1:A:125:LYS:HG2	2.06	0.91
1:B:479:ALA:HB2	1:B:566:TYR:CD2	2.06	0.91
1:B:82:LYS:HG2	1:B:83:LEU:N	1.86	0.91
1:B:209:TRP:CB	1:B:246:ALA:HB3	2.00	0.91
1:B:306:LEU:HD21	1:B:310:PHE:HB3	1.51	0.90
1:A:224:ASN:CB	1:A:227:SER:HB3	2.00	0.90
1:A:269:ASP:HB2	1:A:279:ASN:HD22	1.34	0.90
1:A:329:ASP:OD1	1:A:330:THR:N	2.04	0.90
1:A:434:PHE:CD2	1:A:461:CYS:HB3	2.06	0.90
1:B:188:ASP:O	1:B:227:SER:OG	1.88	0.90
1:B:510:ARG:HB2	1:B:530:LEU:HB2	1.50	0.90
1:B:555:LEU:HD23	1:B:570:MET:CE	2.01	0.90
1:B:170:MET:HE1	1:B:499:HIS:HA	1.54	0.90
1:B:439:ASP:OD1	1:B:440:ALA:N	2.05	0.90
1:B:328:ASN:ND2	1:B:328:ASN:O	2.05	0.89
1:A:229:PRO:O	1:A:231:PRO:HD2	1.72	0.89
1:B:219:ARG:NH1	1:B:254:LYS:CD	2.34	0.89
1:A:101:GLN:CG	1:A:387:ASN:H	1.85	0.89
1:A:101:GLN:CG	1:A:387:ASN:N	2.35	0.89
1:A:610:ASN:O	2:A:701:HOH:O	1.91	0.89
1:B:194:ILE:O	1:B:197:THR:HB	1.72	0.89
1:A:230:ASN:N	1:A:231:PRO:HD3	1.87	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ASP:O	1:B:212:ILE:HG22	1.72	0.88
1:B:211:ASP:C	1:B:212:ILE:HG22	1.92	0.88
1:A:627:SER:CA	1:A:647:LYS:HZ1	1.82	0.88
1:A:549:LYS:HG3	1:A:550:GLY:N	1.88	0.88
1:A:119:LEU:HD11	1:A:389:LEU:CD2	2.04	0.88
1:B:245:SER:O	1:B:316:ASP:O	1.91	0.88
1:A:653:THR:O	1:A:654:GLU:HB2	1.70	0.88
1:A:272:VAL:CG2	1:A:280:PHE:CB	2.51	0.88
1:B:347:LEU:O	1:B:350:GLY:CA	2.20	0.88
1:A:230:ASN:N	1:A:231:PRO:CD	2.36	0.87
1:A:76:ARG:NH2	1:A:524:ALA:HB2	1.89	0.87
1:A:82:LYS:NZ	1:A:97:THR:HA	1.88	0.87
1:B:433:GLY:HA3	1:B:460:ALA:HB3	1.57	0.87
1:B:406:TRP:HZ2	1:B:541:PHE:CD2	1.81	0.87
1:B:525:GLU:OE1	1:B:545:PRO:O	1.93	0.87
1:B:86:THR:CG2	1:B:98:ARG:O	2.23	0.87
1:A:119:LEU:CD1	1:A:389:LEU:CD2	2.52	0.87
1:A:549:LYS:HG3	1:A:550:GLY:H	1.40	0.87
1:B:454:PRO:HD2	1:B:509:MET:HE3	1.57	0.87
1:B:81:ILE:HG12	1:B:82:LYS:N	1.89	0.87
1:B:454:PRO:CD	1:B:509:MET:CE	2.52	0.86
1:B:546:ALA:O	1:B:547:LEU:HB2	1.74	0.86
1:A:86:THR:HG21	1:A:333:LYS:HB3	1.55	0.86
1:B:406:TRP:CE2	1:B:541:PHE:HD2	1.87	0.86
1:A:80:THR:CB	1:A:129:SER:HA	2.04	0.86
1:B:406:TRP:HE3	1:B:442:LEU:CD1	1.88	0.86
1:A:236:ARG:HG2	1:A:240:ILE:HG13	1.58	0.86
1:A:324:GLU:HG3	1:A:386:SER:OG	1.75	0.86
1:B:474:GLN:O	1:B:474:GLN:NE2	2.08	0.86
1:A:436:PHE:HE2	1:A:467:LYS:CB	1.88	0.86
1:A:500:GLU:O	1:A:505:GLY:N	2.08	0.86
1:A:286:PRO:HG2	1:A:289:ALA:HB2	1.57	0.86
1:A:413:VAL:HB	1:A:414:PRO:HD3	1.55	0.85
1:A:464:THR:HG22	1:A:465:ASN:H	1.41	0.85
1:B:194:ILE:HG21	1:B:470:TRP:HZ2	1.40	0.85
1:A:71:THR:CB	1:A:93:VAL:O	2.23	0.85
1:A:94:ASP:C	1:A:95:LYS:HG3	1.97	0.85
1:B:436:PHE:O	1:B:438:ALA:N	2.09	0.85
1:A:186:SER:CB	1:A:187:PRO:HD3	2.07	0.84
1:B:64:ILE:H	1:B:76:ARG:HH21	1.25	0.84
1:B:454:PRO:HD3	1:B:509:MET:CE	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PHE:O	1:A:230:ASN:N	2.10	0.84
1:A:577:ILE:O	2:A:702:HOH:O	1.95	0.84
1:B:353:LEU:C	1:B:354:GLN:HG2	1.98	0.84
1:A:330:THR:HB	1:A:331:PRO:HD2	1.58	0.84
1:A:182:ARG:NH2	1:A:190:ARG:CG	2.39	0.84
1:A:81:ILE:N	1:A:128:LEU:O	2.11	0.84
1:A:641:THR:HB	1:A:643:LYS:CE	2.08	0.84
1:A:625:ASP:C	1:A:651:TYR:CB	2.47	0.84
1:B:210:MET:CB	1:B:211:ASP:CB	2.56	0.83
1:A:434:PHE:O	1:A:435:LEU:HB2	1.77	0.83
1:B:479:ALA:HA	1:B:566:TYR:CE2	2.14	0.83
1:B:479:ALA:HB2	1:B:566:TYR:HD2	1.43	0.83
1:B:101:GLN:O	2:B:702:HOH:O	1.94	0.83
1:A:182:ARG:HH22	1:A:190:ARG:HB3	1.40	0.83
1:A:273:LYS:O	1:A:275:ALA:N	2.11	0.83
1:A:406:TRP:CE3	1:A:442:LEU:HD13	2.13	0.83
1:B:139:SER:HB3	1:B:144:PHE:CE2	2.09	0.83
1:A:76:ARG:CZ	1:A:524:ALA:HB2	2.09	0.83
1:A:232:LYS:HA	1:A:311:LEU:HA	1.57	0.83
1:A:268:ASN:HB3	1:A:299:VAL:HG22	1.58	0.83
1:B:165:THR:O	1:B:393:ARG:HD2	1.80	0.82
1:B:256:ASP:HB3	1:B:257:PRO:CD	2.09	0.82
1:A:466:ASN:HB3	1:A:471:VAL:HG11	1.62	0.82
1:A:192:ILE:CG2	1:A:195:ALA:CB	2.57	0.82
1:B:437:ASN:HA	1:B:465:ASN:OD1	1.78	0.82
1:A:272:VAL:HG13	1:A:336:PRO:HG2	0.83	0.82
1:B:270:VAL:HG22	1:B:292:PRO:HA	1.61	0.82
1:A:238:LEU:O	1:A:243:PHE:CB	2.28	0.82
1:A:269:ASP:HA	1:A:291:PHE:O	1.80	0.81
1:B:404:SER:O	1:B:442:LEU:HD22	1.80	0.81
1:B:209:TRP:HB2	1:B:246:ALA:HB3	1.61	0.81
1:B:62:THR:O	1:B:63:SER:HB2	1.79	0.81
1:A:272:VAL:HG13	1:A:336:PRO:O	1.81	0.81
1:B:270:VAL:HG22	1:B:271:TRP:N	1.93	0.81
1:B:479:ALA:CA	1:B:566:TYR:HE2	1.93	0.81
1:A:318:VAL:HG23	1:A:382:ILE:HD12	1.62	0.81
1:A:229:PRO:C	1:A:231:PRO:HD2	2.00	0.80
1:A:440:ALA:HB1	1:A:476:VAL:HG21	1.63	0.80
1:B:86:THR:HG21	1:B:98:ARG:O	1.81	0.80
1:B:189:SER:C	1:B:191:VAL:H	1.85	0.80
1:B:406:TRP:HE3	1:B:442:LEU:HD13	1.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:TYR:O	1:A:260:PHE:HD1	1.64	0.80
1:B:132:ASP:O	1:B:133:GLU:HB2	1.80	0.80
1:B:414:PRO:HG3	1:B:526:GLU:HB3	1.64	0.80
1:B:404:SER:O	1:B:442:LEU:HD21	1.81	0.80
1:A:462:ALA:C	1:A:463:GLY:O	2.01	0.80
1:B:219:ARG:HH11	1:B:254:LYS:CD	1.93	0.79
1:B:322:VAL:O	1:B:324:GLU:N	2.15	0.79
1:B:74:LEU:CD2	1:B:75:LEU:H	1.94	0.79
1:A:280:PHE:CE2	1:A:335:MET:HB3	2.18	0.79
1:A:486:ARG:O	1:A:489:ILE:HG22	1.82	0.79
1:A:587:THR:O	1:A:590:ASN:HB2	1.82	0.79
1:B:132:ASP:O	1:B:133:GLU:CB	2.30	0.79
1:A:402:ASN:HB3	1:A:433:GLY:HA3	1.63	0.79
1:A:436:PHE:CE2	1:A:467:LYS:HB2	2.18	0.79
1:B:63:SER:HA	1:B:76:ARG:NH2	1.99	0.79
1:A:268:ASN:CB	1:A:299:VAL:HG22	2.13	0.78
1:A:84:TRP:HD1	1:A:85:ASN:CA	1.96	0.78
1:A:162:SER:O	1:A:166:GLY:N	2.16	0.78
1:A:192:ILE:HG21	1:A:195:ALA:CB	2.10	0.78
1:A:219:ARG:NH2	1:A:256:ASP:CB	2.46	0.78
1:A:324:GLU:N	1:A:325:PRO:HA	1.97	0.78
1:B:256:ASP:CB	1:B:257:PRO:CD	2.61	0.78
1:A:283:ASP:H	1:A:327:ILE:HG23	1.48	0.78
1:B:507:PRO:O	1:B:510:ARG:NE	2.16	0.78
1:B:541:PHE:O	1:B:542:ALA:HB2	1.84	0.78
1:A:112:ASP:CG	1:A:113:GLY:H	1.86	0.78
1:A:192:ILE:CG2	1:A:195:ALA:H	1.97	0.78
1:A:101:GLN:HG2	1:A:387:ASN:CA	2.14	0.78
1:A:436:PHE:HE2	1:A:467:LYS:HB2	1.48	0.78
1:B:277:GLY:C	1:B:278:LYS:HD3	2.04	0.77
1:A:308:LYS:HD2	1:A:371:ILE:HG12	1.66	0.77
1:B:212:ILE:HG13	1:B:213:ASP:N	1.98	0.77
1:B:479:ALA:CA	1:B:566:TYR:CE2	2.68	0.77
1:A:223:PHE:HZ	1:A:311:LEU:CB	1.97	0.77
1:B:454:PRO:HD2	1:B:509:MET:CE	2.14	0.77
1:A:436:PHE:CE2	1:A:460:ALA:HB2	2.20	0.77
1:B:256:ASP:HB3	1:B:257:PRO:HD2	1.66	0.77
1:A:274:THR:O	1:A:275:ALA:CB	2.33	0.77
1:A:285:TRP:HE1	1:A:322:VAL:HG21	1.49	0.77
1:A:305:ASN:OD1	1:A:307:TYR:HB3	1.84	0.77
1:B:402:ASN:CB	1:B:430:ASP:HB2	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ASN:ND2	1:B:446:TRP:CZ2	2.47	0.77
1:A:225:PRO:CA	1:A:229:PRO:HG3	2.14	0.77
1:A:404:SER:HB2	1:A:436:PHE:HA	1.67	0.77
1:A:618:GLY:HA3	1:A:621:TYR:CE2	2.20	0.77
1:B:245:SER:HG	1:B:247:TRP:HE1	1.23	0.77
1:A:133:GLU:HA	1:A:134:LYS:HE3	1.66	0.76
1:A:207:VAL:HG13	1:A:244:HIS:O	1.84	0.76
1:A:262:TYR:CE1	1:A:264:SER:OG	2.38	0.76
1:A:430:ASP:HB3	1:A:459:HIS:HB3	1.68	0.76
1:B:525:GLU:OE2	1:B:527:GLU:CB	2.34	0.76
1:A:74:LEU:HD13	1:A:79:LYS:CE	2.16	0.76
1:A:272:VAL:HG22	1:A:280:PHE:CB	2.03	0.76
1:A:92:GLY:O	1:A:93:VAL:CB	2.33	0.76
1:A:436:PHE:CZ	1:A:460:ALA:HB2	2.19	0.76
1:A:431:ILE:CG2	1:A:446:TRP:HB3	2.16	0.76
1:A:618:GLY:HA3	1:A:621:TYR:CZ	2.21	0.75
1:B:406:TRP:CE3	1:B:442:LEU:CD1	2.69	0.75
1:B:126:ALA:HB1	1:B:137:LEU:HD21	1.67	0.75
1:B:90:ALA:O	1:B:91:TYR:O	2.05	0.75
1:B:210:MET:CA	1:B:211:ASP:CB	2.64	0.75
1:B:453:TYR:HA	1:B:509:MET:CE	2.15	0.75
1:A:182:ARG:NH2	1:A:190:ARG:HG3	2.02	0.75
1:A:74:LEU:HD13	1:A:79:LYS:HE3	1.68	0.75
1:A:329:ASP:O	1:A:330:THR:OG1	2.05	0.75
1:B:464:THR:O	1:B:465:ASN:HB3	1.85	0.75
1:B:586:ASN:HB2	1:B:589:GLU:CG	2.10	0.75
1:B:81:ILE:HG21	1:B:128:LEU:HB3	1.66	0.75
1:A:84:TRP:HA	1:A:357:ASN:OD1	1.87	0.75
1:B:211:ASP:C	1:B:212:ILE:CG2	2.45	0.75
1:B:91:TYR:CD2	1:B:415:MET:HE1	2.21	0.74
1:B:358:VAL:O	1:B:362:LEU:HG	1.87	0.74
1:A:581:GLY:O	1:A:582:LYS:HB3	1.86	0.74
1:A:274:THR:O	1:A:275:ALA:HB3	1.87	0.74
1:A:504:ASN:OD1	1:A:505:GLY:HA2	1.87	0.74
1:B:459:HIS:CG	1:B:460:ALA:N	2.56	0.74
1:B:652:ASN:ND2	1:B:657:ASP:OD1	2.20	0.74
1:A:57:THR:HG23	1:A:134:LYS:HD2	0.85	0.74
1:A:84:TRP:CZ3	1:A:356:HIS:CB	2.71	0.74
1:B:78:GLY:O	1:B:79:LYS:HB2	1.86	0.74
1:B:428:GLY:HA3	1:B:455:PHE:O	1.87	0.74
1:B:575:GLY:HA2	1:B:606:LYS:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:MET:CE	1:B:128:LEU:HD22	2.17	0.74
1:B:379:ARG:CD	1:B:618:GLY:O	2.35	0.74
1:A:179:GLN:OE1	1:A:455:PHE:CE1	2.40	0.73
1:B:256:ASP:CG	1:B:257:PRO:HD3	2.09	0.73
1:B:379:ARG:CG	1:B:618:GLY:O	2.36	0.73
1:B:566:TYR:CA	1:B:567:GLN:HG2	2.15	0.73
1:A:171:ILE:HD12	1:A:175:ALA:HB3	1.69	0.73
1:A:627:SER:CA	1:A:647:LYS:HZ3	1.98	0.73
1:B:307:TYR:HD2	1:B:374:ALA:CB	2.01	0.73
1:B:538:ILE:CD1	1:B:545:PRO:HG3	2.19	0.73
1:A:587:THR:HB	1:A:590:ASN:HD22	1.52	0.73
1:B:151:ARG:HH12	1:B:160:GLY:HA3	1.52	0.73
1:B:186:SER:CB	1:B:187:PRO:CD	2.60	0.73
1:B:224:ASN:H	1:B:225:PRO:HD2	1.52	0.73
1:B:87:ASP:HB3	1:B:324:GLU:OE1	1.88	0.73
1:A:538:ILE:HD12	1:A:569:LYS:HB3	1.69	0.73
1:B:402:ASN:HB2	1:B:430:ASP:CB	2.19	0.73
1:B:635:ARG:HE	1:B:636:ASN:HD22	1.35	0.73
1:B:83:LEU:N	1:B:83:LEU:HD12	2.02	0.73
1:A:436:PHE:CE1	1:A:459:HIS:CE1	2.77	0.73
1:B:180:GLN:O	1:B:181:CYS:HB2	1.88	0.73
1:B:93:VAL:O	1:B:97:THR:N	2.22	0.73
1:A:84:TRP:CZ3	1:A:125:LYS:HG2	2.23	0.72
1:B:204:PRO:CB	1:B:585:GLN:HA	2.18	0.72
1:B:166:GLY:HA3	1:B:393:ARG:HD2	1.71	0.72
1:A:179:GLN:HB3	1:A:209:TRP:NE1	2.02	0.72
1:A:436:PHE:CE2	1:A:460:ALA:CB	2.71	0.72
1:A:84:TRP:O	1:A:85:ASN:HB2	1.89	0.72
1:A:272:VAL:HG11	1:A:336:PRO:HG3	1.69	0.72
1:A:434:PHE:O	1:A:435:LEU:CB	2.36	0.72
1:A:236:ARG:NH1	1:B:661:ILE:HG23	2.04	0.72
1:A:266:THR:O	1:A:267:GLU:CB	2.32	0.72
1:A:506:MET:CB	1:A:507:PRO:CD	2.66	0.72
1:B:552:TRP:HA	1:B:571:LYS:HD3	1.72	0.72
1:A:80:THR:HA	1:A:129:SER:HA	1.70	0.72
1:B:545:PRO:O	1:B:546:ALA:CB	2.37	0.72
1:A:84:TRP:CH2	1:A:356:HIS:HB2	2.24	0.72
1:A:74:LEU:CD1	1:A:76:ARG:O	2.37	0.72
1:A:80:THR:CB	1:A:129:SER:CB	2.61	0.72
1:A:223:PHE:CD2	1:A:231:PRO:HB2	2.24	0.72
1:B:527:GLU:CB	1:B:543:ASN:ND2	2.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:THR:HB	1:B:64:ILE:HD11	1.72	0.71
1:A:236:ARG:HG2	1:A:240:ILE:CG1	2.21	0.71
1:B:118:ILE:HD11	1:B:120:PHE:HE1	1.54	0.71
1:B:493:TYR:OH	1:B:531:VAL:O	2.04	0.71
1:B:431:ILE:HA	1:B:446:TRP:CE2	2.26	0.71
1:B:178:TYR:HB3	1:B:205:CYS:SG	2.30	0.71
1:A:84:TRP:HZ2	1:A:334:THR:CG2	2.03	0.71
1:A:397:THR:HG21	1:A:424:GLN:HG2	1.73	0.71
1:B:413:VAL:HB	1:B:414:PRO:HD3	1.73	0.71
1:B:100:TYR:HE2	1:B:400:GLY:HA2	1.55	0.71
1:B:270:VAL:CG2	1:B:292:PRO:CA	2.67	0.71
1:A:324:GLU:CD	1:A:385:ARG:NH1	2.45	0.70
1:B:206:ASP:HB2	1:B:488:TYR:HH	1.55	0.70
1:B:82:LYS:C	1:B:83:LEU:HD12	2.10	0.70
1:A:84:TRP:HE3	1:A:125:LYS:HG2	1.52	0.70
1:A:225:PRO:O	1:A:229:PRO:HG2	1.91	0.70
1:B:209:TRP:HH2	1:B:459:HIS:CD2	2.10	0.70
1:B:453:TYR:HA	1:B:509:MET:HE2	1.72	0.70
1:A:625:ASP:CB	1:A:651:TYR:CB	2.69	0.70
1:A:73:SER:H	1:A:95:LYS:HE3	1.56	0.70
1:B:231:PRO:O	1:B:235:ASN:OD1	2.09	0.70
1:B:270:VAL:HG21	1:B:292:PRO:HB3	1.73	0.70
1:A:209:TRP:HE3	1:A:319:TRP:CE3	2.09	0.70
1:A:440:ALA:HB1	1:A:476:VAL:CG2	2.22	0.70
1:A:486:ARG:O	1:A:489:ILE:CG2	2.40	0.70
1:A:641:THR:HB	1:A:643:LYS:NZ	2.06	0.70
1:A:627:SER:CB	1:A:647:LYS:NZ	2.54	0.70
1:B:306:LEU:HD22	1:B:306:LEU:C	2.12	0.70
1:A:192:ILE:HG22	1:A:195:ALA:H	1.57	0.69
1:B:183:PHE:HA	1:B:212:ILE:H	1.54	0.69
1:B:459:HIS:CG	1:B:460:ALA:H	2.10	0.69
1:A:224:ASN:CB	1:A:227:SER:CB	2.57	0.69
1:B:270:VAL:HG22	1:B:271:TRP:H	1.57	0.69
1:B:270:VAL:HG13	1:B:271:TRP:CE3	2.27	0.69
1:B:545:PRO:CG	1:B:547:LEU:CD1	2.70	0.69
1:B:70:VAL:HG22	1:B:71:THR:N	2.03	0.69
1:B:184:SER:OG	1:B:185:TYR:N	2.24	0.69
1:B:328:ASN:CG	1:B:348:PRO:CB	2.58	0.69
1:B:81:ILE:HG12	1:B:82:LYS:H	1.55	0.69
1:A:330:THR:CB	1:A:331:PRO:HD2	2.22	0.69
1:A:84:TRP:CZ2	1:A:356:HIS:CD2	2.79	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LYS:N	1:B:278:LYS:HD3	2.07	0.69
1:B:171:ILE:HD12	1:B:175:ALA:HB3	1.73	0.69
1:A:131:THR:HG22	1:A:132:ASP:N	2.04	0.69
1:B:306:LEU:HD21	1:B:310:PHE:CB	2.23	0.69
1:A:409:LEU:HD23	1:A:410:LYS:N	2.08	0.69
1:A:434:PHE:CD2	1:A:461:CYS:CB	2.75	0.69
1:B:485:GLU:O	1:B:489:ILE:HG23	1.93	0.69
1:B:552:TRP:CB	1:B:571:LYS:CD	2.71	0.69
1:A:191:VAL:O	1:A:192:ILE:HB	1.92	0.69
1:B:298:LYS:O	1:B:301:LYS:HE3	1.94	0.69
1:A:192:ILE:C	1:A:194:ILE:N	2.37	0.68
1:A:232:LYS:O	1:A:233:ALA:HB3	1.92	0.68
1:A:266:THR:CB	1:A:268:ASN:OD1	2.41	0.68
1:A:232:LYS:HA	1:A:311:LEU:CA	2.18	0.68
1:B:64:ILE:O	1:B:74:LEU:CD2	2.41	0.68
1:A:466:ASN:O	1:A:467:LYS:HB3	1.92	0.68
1:B:520:LEU:HD12	1:B:520:LEU:N	2.09	0.68
1:B:552:TRP:CB	1:B:571:LYS:HD3	2.23	0.68
1:A:332:ASN:C	1:A:333:LYS:HG2	2.14	0.68
1:B:470:TRP:C	1:B:472:PHE:H	1.94	0.68
1:A:538:ILE:CG2	1:A:544:GLN:O	2.41	0.68
1:B:256:ASP:C	1:B:259:TYR:CE2	2.66	0.68
1:B:406:TRP:CE3	1:B:442:LEU:HD12	2.28	0.68
1:A:307:TYR:O	1:A:310:PHE:HD2	1.76	0.68
1:A:84:TRP:HZ2	1:A:334:THR:HG21	1.59	0.68
1:B:215:MET:HB2	1:B:218:TYR:HA	1.76	0.68
1:B:248:MET:HB2	1:B:319:TRP:CE2	2.29	0.68
1:B:300:ASN:O	1:B:304:ARG:N	2.25	0.68
1:B:64:ILE:N	1:B:76:ARG:HH21	1.91	0.68
1:A:228:PHE:C	1:A:230:ASN:N	2.34	0.68
1:A:538:ILE:HG21	1:A:544:GLN:O	1.94	0.68
1:A:577:ILE:HB	1:A:609:GLY:HA3	1.75	0.68
1:B:210:MET:HA	1:B:211:ASP:CB	2.24	0.68
1:A:86:THR:HG21	1:A:333:LYS:HB2	1.74	0.67
1:A:628:LEU:HB3	1:A:648:THR:HB	1.75	0.67
1:B:474:GLN:O	1:B:478:ASP:OD2	2.12	0.67
1:A:202:ARG:HD3	1:B:583:ILE:HD12	1.75	0.67
1:A:84:TRP:CD2	1:A:356:HIS:CD2	2.81	0.67
1:A:68:GLY:HA2	1:A:422:SER:CB	2.25	0.67
1:A:649:GLY:O	1:A:650:LYS:HB2	1.93	0.67
1:B:63:SER:HA	1:B:76:ARG:HH21	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:PHE:CE2	1:A:455:PHE:HB2	2.30	0.67
1:A:586:ASN:OD1	1:A:588:THR:HB	1.93	0.67
1:B:534:ASN:CG	1:B:576:ALA:HB1	2.14	0.67
1:B:63:SER:H	1:B:76:ARG:HH22	1.43	0.67
1:B:81:ILE:CG2	1:B:128:LEU:CB	2.73	0.67
1:B:516:ASP:HB3	1:B:519:ASP:HB2	1.77	0.67
1:A:307:TYR:HA	1:A:310:PHE:CE2	2.29	0.67
1:B:178:TYR:CB	1:B:205:CYS:HB3	2.08	0.67
1:B:347:LEU:O	1:B:350:GLY:HA2	1.95	0.67
1:A:171:ILE:HD12	1:A:175:ALA:CB	2.24	0.67
1:A:379:ARG:CZ	1:A:618:GLY:O	2.42	0.67
1:B:256:ASP:CB	1:B:257:PRO:HD3	2.24	0.67
1:A:106:MET:O	1:A:107:MET:HB3	1.92	0.66
1:A:308:LYS:HD2	1:A:371:ILE:CG1	2.25	0.66
1:A:128:LEU:HD23	1:A:137:LEU:HB2	1.77	0.66
1:A:239:HIS:HE1	1:A:316:ASP:OD2	1.76	0.66
1:A:460:ALA:CB	1:A:467:LYS:HD3	2.22	0.66
1:B:193:GLU:HB3	1:B:195:ALA:HB3	1.78	0.66
1:B:209:TRP:HB3	1:B:246:ALA:HB3	1.73	0.66
1:B:434:PHE:CD2	1:B:435:LEU:HA	2.25	0.66
1:B:204:PRO:HB2	1:B:584:ILE:O	1.95	0.66
1:A:491:LEU:HD21	1:A:590:ASN:OD1	1.95	0.66
1:A:126:ALA:O	1:A:127:GLU:HB2	1.95	0.66
1:B:307:TYR:H	1:B:307:TYR:HD1	1.44	0.66
1:B:605:GLY:O	1:B:606:LYS:HG3	1.96	0.66
1:A:165:THR:CG2	1:A:390:GLY:HA2	2.26	0.66
1:A:128:LEU:CD2	1:A:137:LEU:HB2	2.26	0.66
1:A:575:GLY:HA2	1:A:606:LYS:O	1.95	0.66
1:B:81:ILE:CG2	1:B:128:LEU:HB3	2.25	0.66
1:A:589:GLU:OE1	2:A:703:HOH:O	2.12	0.66
1:B:367:SER:O	1:B:371:ILE:HD12	1.96	0.66
1:B:479:ALA:HB2	1:B:566:TYR:CE2	2.31	0.66
1:B:573:ARG:NH1	1:B:574:GLY:O	2.29	0.66
1:B:78:GLY:O	1:B:79:LYS:CB	2.44	0.66
1:A:552:TRP:O	1:A:572:ILE:O	2.14	0.66
1:B:459:HIS:ND1	1:B:460:ALA:N	2.43	0.66
1:B:545:PRO:O	1:B:546:ALA:HB2	1.95	0.66
1:A:272:VAL:CG2	1:A:280:PHE:CA	2.74	0.66
1:A:500:GLU:O	1:A:505:GLY:CA	2.44	0.66
1:A:512:VAL:CG1	1:A:548:PRO:HD3	2.22	0.66
1:B:612:TYR:OH	1:B:621:TYR:HB3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:CYS:O	1:A:406:TRP:HB2	1.94	0.65
1:A:500:GLU:O	1:A:505:GLY:HA3	1.96	0.65
1:B:538:ILE:HD12	1:B:545:PRO:HG3	1.77	0.65
1:B:606:LYS:NZ	1:B:634:GLU:HG3	2.10	0.65
1:A:464:THR:CG2	1:A:465:ASN:H	2.10	0.65
1:B:483:ALA:O	1:B:486:ARG:HB2	1.97	0.65
1:B:81:ILE:HG21	1:B:128:LEU:CB	2.26	0.65
1:B:228:PHE:N	1:B:229:PRO:HD3	2.12	0.65
1:B:557:LEU:HD12	1:B:557:LEU:H	1.61	0.65
1:A:215:MET:HE3	1:A:218:TYR:HA	1.79	0.65
1:B:124:TRP:O	1:B:140:GLU:CB	2.44	0.65
1:B:106:MET:HE1	1:B:128:LEU:HD22	1.76	0.65
1:B:270:VAL:CG2	1:B:271:TRP:N	2.59	0.65
1:B:512:VAL:CG2	1:B:528:ALA:O	2.43	0.65
1:B:100:TYR:CE2	1:B:400:GLY:HA2	2.31	0.65
1:A:248:MET:HB2	1:A:319:TRP:CH2	2.32	0.65
1:B:479:ALA:CB	1:B:566:TYR:CD2	2.79	0.65
1:B:594:PRO:C	1:B:596:THR:H	1.98	0.65
1:B:522:LEU:HD23	1:B:522:LEU:N	2.12	0.65
1:B:64:ILE:H	1:B:76:ARG:NH2	1.94	0.65
1:A:84:TRP:CE2	1:A:356:HIS:HD2	2.14	0.65
1:B:82:LYS:HE2	1:B:84:TRP:HB3	1.78	0.65
1:A:538:ILE:CD1	1:A:569:LYS:HB3	2.27	0.65
1:B:554:GLU:O	1:B:555:LEU:CB	2.41	0.65
1:B:63:SER:CA	1:B:76:ARG:NH2	2.60	0.64
1:A:74:LEU:HD22	1:A:79:LYS:HD2	1.79	0.64
1:A:84:TRP:CD1	1:A:85:ASN:CA	2.75	0.64
1:A:84:TRP:HD1	1:A:85:ASN:HA	1.62	0.64
1:B:118:ILE:CD1	1:B:120:PHE:CE1	2.79	0.64
1:B:91:TYR:CD2	1:B:415:MET:CE	2.81	0.64
1:B:593:ASP:CB	1:B:594:PRO:CD	2.70	0.64
1:A:84:TRP:O	1:A:85:ASN:CB	2.45	0.64
1:B:520:LEU:HD12	1:B:520:LEU:H	1.61	0.64
1:A:306:LEU:HA	1:A:374:ALA:HB2	1.77	0.64
1:A:626:TYR:O	1:A:650:LYS:N	2.31	0.64
1:B:436:PHE:C	1:B:438:ALA:H	2.00	0.64
1:B:609:GLY:O	1:B:631:PHE:N	2.16	0.64
1:B:115:ALA:HB3	1:B:154:PRO:HA	1.79	0.64
1:B:277:GLY:C	1:B:278:LYS:CD	2.66	0.64
1:A:80:THR:CA	1:A:129:SER:HA	2.27	0.64
1:B:165:THR:O	1:B:393:ARG:CD	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:VAL:CG1	1:A:262:TYR:N	2.59	0.64
1:A:618:GLY:CA	1:A:621:TYR:CZ	2.79	0.64
1:B:406:TRP:HZ2	1:B:541:PHE:HB2	1.63	0.64
1:B:517:PRO:O	1:B:523:ARG:NH2	2.31	0.64
1:A:84:TRP:CD2	1:A:356:HIS:HD2	2.16	0.63
1:A:90:ALA:C	1:A:92:GLY:H	2.01	0.63
1:A:111:LYS:O	1:A:112:ASP:O	2.16	0.63
1:A:165:THR:O	1:A:393:ARG:NH1	2.29	0.63
1:A:105:TRP:CE2	1:A:161:LEU:HD22	2.34	0.63
1:B:81:ILE:HG22	1:B:128:LEU:O	1.98	0.63
1:A:420:GLY:HA3	1:A:507:PRO:HG3	1.80	0.63
1:A:52:ALA:O	1:A:53:ASN:ND2	2.32	0.63
1:B:181:CYS:O	1:B:459:HIS:CD2	2.51	0.63
1:A:211:ASP:O	1:A:212:ILE:HG22	1.98	0.63
1:A:461:CYS:SG	1:A:462:ALA:N	2.72	0.63
1:B:566:TYR:N	1:B:567:GLN:HA	2.12	0.63
1:A:72:GLY:H	1:A:411:MET:HE1	1.62	0.63
1:A:101:GLN:HG3	1:A:387:ASN:N	2.14	0.63
1:A:552:TRP:CH2	1:A:573:ARG:HG3	2.34	0.63
1:B:117:GLY:O	1:B:148:ILE:HA	1.98	0.63
1:B:188:ASP:OD2	1:B:192:ILE:CD1	2.46	0.63
1:B:255:VAL:HG23	1:B:255:VAL:O	1.99	0.63
1:B:245:SER:O	1:B:316:ASP:C	2.36	0.62
1:B:590:ASN:C	1:B:591:SER:OG	2.37	0.62
1:B:434:PHE:HD2	1:B:435:LEU:CA	2.08	0.62
1:B:435:LEU:O	1:B:436:PHE:CB	2.48	0.62
1:B:206:ASP:HB2	1:B:488:TYR:OH	1.98	0.62
1:A:133:GLU:CA	1:A:134:LYS:HE3	2.29	0.62
1:B:305:ASN:ND2	1:B:307:TYR:CE1	2.67	0.62
1:B:590:ASN:ND2	1:B:590:ASN:O	2.29	0.62
1:A:99:LEU:N	1:A:99:LEU:HD12	2.13	0.62
1:B:557:LEU:HD12	1:B:557:LEU:N	2.15	0.62
1:A:462:ALA:O	1:A:463:GLY:O	2.17	0.62
1:B:132:ASP:O	1:B:133:GLU:HG2	1.99	0.62
1:B:109:VAL:O	1:B:110:ARG:HB3	1.99	0.62
1:B:279:ASN:OD1	1:B:279:ASN:N	2.33	0.62
1:A:462:ALA:O	1:A:463:GLY:C	2.36	0.62
1:B:509:MET:HG3	1:B:529:PHE:CD2	2.35	0.62
1:B:82:LYS:HG2	1:B:83:LEU:H	1.64	0.62
1:A:182:ARG:O	1:A:183:PHE:HB2	2.00	0.62
1:A:272:VAL:HG21	1:A:280:PHE:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:TYR:O	1:A:310:PHE:CD2	2.53	0.62
1:A:322:VAL:HG13	1:A:326:GLN:OE1	2.00	0.62
1:B:194:ILE:HG22	1:B:470:TRP:CH2	2.33	0.62
1:B:263:LYS:CA	1:B:265:GLY:H	2.00	0.62
1:B:431:ILE:HA	1:B:446:TRP:NE1	2.15	0.62
1:A:151:ARG:HH12	1:A:160:GLY:HA3	1.65	0.62
1:B:86:THR:HG22	1:B:98:ARG:O	1.99	0.62
1:B:512:VAL:HG13	1:B:548:PRO:HG3	1.82	0.61
1:A:397:THR:HG23	1:A:424:GLN:NE2	2.15	0.61
1:A:65:TYR:O	1:A:106:MET:HG2	2.00	0.61
1:A:74:LEU:HD13	1:A:79:LYS:CD	2.30	0.61
1:B:223:PHE:CB	1:B:224:ASN:HA	2.29	0.61
1:B:369:GLU:O	1:B:373:ASP:HB2	2.00	0.61
1:B:185:TYR:O	1:B:212:ILE:HD13	2.00	0.61
1:B:188:ASP:HB3	1:B:189:SER:HA	1.81	0.61
1:B:256:ASP:C	1:B:259:TYR:HE2	2.01	0.61
1:B:270:VAL:CG2	1:B:271:TRP:H	2.13	0.61
1:B:305:ASN:ND2	1:B:307:TYR:HE1	1.97	0.61
1:A:431:ILE:HG22	1:A:446:TRP:HB3	1.80	0.61
1:A:286:PRO:CG	1:A:289:ALA:HB2	2.31	0.61
1:B:171:ILE:HB	1:B:172:PRO:HD2	1.82	0.61
1:B:151:ARG:HH12	1:B:160:GLY:CA	2.12	0.61
1:B:247:TRP:CD1	1:B:315:VAL:HG13	2.36	0.61
1:B:651:TYR:CG	1:B:652:ASN:N	2.68	0.61
1:A:101:GLN:NE2	1:A:387:ASN:HB2	2.14	0.61
1:B:264:SER:OG	1:B:302:TRP:NE1	2.25	0.61
1:A:431:ILE:HG22	1:A:431:ILE:O	2.01	0.61
1:B:479:ALA:N	1:B:566:TYR:HE2	1.98	0.61
1:B:519:ASP:OD1	1:B:521:SER:N	2.32	0.61
1:B:590:ASN:C	1:B:591:SER:HG	2.01	0.61
1:A:230:ASN:HD21	1:A:234:VAL:CB	2.14	0.60
1:A:430:ASP:HB3	1:A:459:HIS:CB	2.30	0.60
1:A:625:ASP:HB3	1:A:651:TYR:CB	2.31	0.60
1:B:173:ARG:NH1	1:B:495:TYR:CE2	2.68	0.60
1:B:285:TRP:HB2	1:B:286:PRO:HD3	1.83	0.60
1:B:162:SER:HB2	1:B:504:ASN:O	2.00	0.60
1:B:101:GLN:HB3	1:B:103:HIS:CE1	2.37	0.60
1:B:64:ILE:HG12	1:B:76:ARG:NH2	2.16	0.60
1:A:627:SER:CB	1:A:647:LYS:HE2	2.30	0.60
1:A:269:ASP:HB2	1:A:279:ASN:ND2	2.14	0.60
1:A:654:GLU:C	1:A:655:ASN:HD22	2.03	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:GLU:O	1:B:268:ASN:CB	2.49	0.60
1:B:593:ASP:HB3	1:B:594:PRO:HD3	1.83	0.60
1:A:330:THR:HB	1:A:331:PRO:CD	2.31	0.60
1:A:228:PHE:O	1:A:231:PRO:CD	2.46	0.60
1:A:257:PRO:HA	1:A:259:TYR:CE2	2.37	0.60
1:A:231:PRO:O	1:A:311:LEU:CB	2.50	0.60
1:A:94:ASP:O	1:A:95:LYS:CB	2.49	0.60
1:A:185:TYR:O	1:A:187:PRO:O	2.19	0.60
1:A:582:LYS:HE2	1:A:594:PRO:HD2	1.82	0.60
1:A:89:GLY:O	1:A:90:ALA:HB2	2.01	0.60
1:B:552:TRP:CA	1:B:571:LYS:HD3	2.32	0.60
1:B:573:ARG:NH1	1:B:573:ARG:HG2	2.05	0.60
1:A:629:LEU:HD22	1:A:644:LEU:HD11	1.83	0.59
1:B:545:PRO:CG	1:B:547:LEU:HD11	2.31	0.59
1:B:257:PRO:HA	1:B:259:TYR:CE2	2.38	0.59
1:B:638:ASP:CG	1:B:639:LYS:HG2	2.22	0.59
1:A:280:PHE:CZ	1:A:335:MET:HA	2.38	0.59
1:A:90:ALA:C	1:A:92:GLY:N	2.55	0.59
1:B:74:LEU:HD23	1:B:75:LEU:N	2.08	0.59
1:B:352:HIS:O	1:B:353:LEU:CB	2.50	0.59
1:B:90:ALA:O	1:B:91:TYR:C	2.41	0.59
1:A:233:ALA:C	1:A:235:ASN:N	2.56	0.59
1:A:431:ILE:HG23	1:A:446:TRP:HB3	1.83	0.59
1:A:432:GLY:HA3	1:A:459:HIS:NE2	2.18	0.59
1:B:402:ASN:HB2	1:B:430:ASP:OD2	2.02	0.59
1:A:209:TRP:HH2	1:A:383:LEU:CD1	2.15	0.58
1:A:64:ILE:O	1:A:77:ASN:ND2	2.28	0.58
1:B:177:GLY:H	1:B:487:ARG:HH21	1.50	0.58
1:A:410:LYS:NZ	1:A:413:VAL:HG21	2.18	0.58
1:A:465:ASN:C	1:A:466:ASN:OD1	2.42	0.58
1:B:285:TRP:N	1:B:286:PRO:HD2	2.17	0.58
1:A:126:ALA:HB3	1:A:137:LEU:HD11	1.85	0.58
1:A:280:PHE:CD1	1:A:336:PRO:CD	2.77	0.58
1:A:362:LEU:HD23	1:A:362:LEU:O	2.02	0.58
1:A:51:LYS:O	1:A:52:ALA:O	2.21	0.58
1:A:652:ASN:O	1:A:653:THR:OG1	2.20	0.58
1:B:128:LEU:HG	1:B:137:LEU:HD12	1.84	0.58
1:B:266:THR:O	1:B:267:GLU:HB3	2.02	0.58
1:B:64:ILE:O	1:B:74:LEU:HD21	2.03	0.58
1:B:180:GLN:OE1	1:B:181:CYS:HA	2.02	0.58
1:A:464:THR:HG22	1:A:465:ASN:N	2.14	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ALA:CB	1:B:137:LEU:HD21	2.34	0.58
1:B:219:ARG:NH1	1:B:254:LYS:HD2	2.19	0.58
1:B:381:PHE:CE1	1:B:383:LEU:HD21	2.38	0.58
1:B:364:VAL:HG21	1:B:384:THR:HB	1.84	0.58
1:A:262:TYR:HD1	1:A:262:TYR:O	1.85	0.58
1:B:270:VAL:O	1:B:271:TRP:CB	2.51	0.58
1:A:88:SER:CB	1:A:98:ARG:O	2.52	0.58
1:B:204:PRO:HB2	1:B:585:GLN:HA	1.86	0.58
1:B:307:TYR:CD2	1:B:374:ALA:CB	2.73	0.58
1:B:479:ALA:CB	1:B:566:TYR:CE2	2.86	0.58
1:B:507:PRO:O	1:B:510:ARG:CD	2.52	0.58
1:A:624:GLY:O	1:A:650:LYS:O	2.21	0.58
1:B:220:ILE:HG21	1:B:250:ASP:O	2.04	0.58
1:B:264:SER:HG	1:B:302:TRP:HE1	1.40	0.58
1:A:635:ARG:HB2	1:A:640:VAL:HG22	1.86	0.58
1:B:223:PHE:HB2	1:B:224:ASN:HA	1.84	0.58
1:A:165:THR:O	1:A:165:THR:HG22	2.03	0.57
1:A:399:THR:HG22	1:A:399:THR:O	2.03	0.57
1:A:451:ALA:O	1:A:487:ARG:HD2	2.04	0.57
1:A:84:TRP:CG	1:A:85:ASN:N	2.48	0.57
1:B:178:TYR:CB	1:B:205:CYS:SG	2.92	0.57
1:B:270:VAL:HG21	1:B:292:PRO:CB	2.34	0.57
1:A:170:MET:HE2	1:A:498:LEU:HG	1.86	0.57
1:B:257:PRO:CA	1:B:259:TYR:CE2	2.87	0.57
1:B:566:TYR:N	1:B:566:TYR:CD1	2.72	0.57
1:B:59:PRO:HB2	1:B:62:THR:OG1	2.03	0.57
1:A:112:ASP:CG	1:A:113:GLY:N	2.57	0.57
1:A:210:MET:HG3	1:A:247:TRP:CH2	2.39	0.57
1:A:259:TYR:O	1:A:260:PHE:CD1	2.53	0.57
1:A:398:TRP:HH2	1:A:401:ASP:OD1	1.86	0.57
1:B:577:ILE:HG13	1:B:607:ALA:HB1	1.85	0.57
1:A:538:ILE:HD12	1:A:569:LYS:CB	2.33	0.57
1:B:328:ASN:HB2	1:B:348:PRO:CA	2.35	0.57
1:B:507:PRO:O	1:B:510:ARG:HD3	2.05	0.57
1:B:106:MET:HE2	1:B:128:LEU:HD22	1.86	0.57
1:B:379:ARG:HG3	1:B:618:GLY:O	2.04	0.57
1:B:81:ILE:CG2	1:B:128:LEU:O	2.52	0.57
1:A:233:ALA:C	1:A:235:ASN:H	2.08	0.57
1:A:406:TRP:CD1	1:A:409:LEU:HD22	2.39	0.57
1:B:274:THR:HA	1:B:352:HIS:NE2	2.16	0.57
1:A:209:TRP:HH2	1:A:383:LEU:HD12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ALA:CB	1:A:476:VAL:HG21	2.34	0.57
1:A:573:ARG:O	1:A:576:ALA:HB3	2.04	0.57
1:B:183:PHE:HA	1:B:212:ILE:N	2.18	0.57
1:B:629:LEU:CD2	1:B:647:LYS:HD2	2.35	0.57
1:B:629:LEU:HD22	1:B:647:LYS:HD2	1.86	0.57
1:A:66:GLY:HA3	1:A:106:MET:HA	1.87	0.57
1:A:120:PHE:HB3	1:A:144:PHE:CE1	2.40	0.57
1:B:298:LYS:HA	1:B:301:LYS:CE	2.34	0.57
1:B:298:LYS:HA	1:B:301:LYS:HE3	1.85	0.57
1:B:474:GLN:HA	1:B:474:GLN:HE21	1.70	0.57
1:B:94:ASP:O	1:B:96:GLY:N	2.32	0.57
1:A:118:ILE:CG1	1:A:120:PHE:CE1	2.87	0.56
1:A:78:GLY:CA	1:A:131:THR:HA	2.28	0.56
1:B:542:ALA:O	1:B:543:ASN:O	2.23	0.56
1:B:488:TYR:HD2	1:B:584:ILE:CG2	2.17	0.56
1:A:330:THR:CB	1:A:331:PRO:CD	2.77	0.56
1:A:597:LEU:HD21	1:A:631:PHE:CD1	2.40	0.56
1:B:72:GLY:HA2	1:B:73:SER:CB	2.16	0.56
1:A:259:TYR:CE2	1:A:262:TYR:CD1	2.92	0.56
1:A:432:GLY:HA3	1:A:436:PHE:HE1	1.69	0.56
1:A:53:ASN:O	1:A:54:ALA:HB2	2.05	0.56
1:A:82:LYS:NZ	1:A:97:THR:CA	2.66	0.56
1:A:94:ASP:O	1:A:95:LYS:HB2	2.05	0.56
1:B:472:PHE:O	1:B:476:VAL:HG21	2.05	0.56
1:A:456:ALA:HA	2:A:704:HOH:O	2.05	0.56
1:A:85:ASN:HB3	1:A:99:LEU:O	2.05	0.56
1:B:213:ASP:HB3	1:B:218:TYR:CE1	2.41	0.56
1:B:467:LYS:O	1:B:468:GLU:CB	2.53	0.56
1:A:236:ARG:NE	1:A:240:ILE:HD11	2.20	0.56
1:A:360:GLY:O	1:A:364:VAL:HG12	2.06	0.56
1:A:525:GLU:OE1	1:A:545:PRO:CG	2.47	0.56
1:B:541:PHE:O	1:B:542:ALA:CB	2.50	0.56
1:A:388:PHE:CD1	1:A:389:LEU:N	2.73	0.56
1:A:633:ALA:HB2	1:A:642:VAL:HG22	1.87	0.56
1:B:402:ASN:ND2	1:B:446:TRP:HH2	1.99	0.56
1:B:534:ASN:ND2	1:B:576:ALA:HB1	2.21	0.56
1:A:444:GLY:O	1:A:566:TYR:HB3	2.05	0.56
1:B:132:ASP:O	1:B:133:GLU:CG	2.54	0.56
1:B:536:LEU:HD21	1:B:548:PRO:HD2	1.87	0.56
1:B:555:LEU:O	1:B:557:LEU:N	2.36	0.56
1:B:606:LYS:HZ3	1:B:634:GLU:HG3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:TRP:CZ2	1:A:573:ARG:HG3	2.41	0.56
1:A:304:ARG:HB2	1:A:370:GLY:HA2	1.88	0.56
1:B:375:ARG:HG2	1:B:376:PRO:HD2	1.87	0.56
1:B:553:LYS:CB	1:B:572:ILE:H	2.19	0.56
1:A:125:LYS:CE	1:A:355:TYR:HA	2.36	0.56
1:A:231:PRO:C	1:A:233:ALA:H	2.09	0.56
1:A:618:GLY:N	1:A:621:TYR:OH	2.39	0.56
1:B:190:ARG:HG2	1:B:194:ILE:HG12	1.88	0.56
1:B:212:ILE:HG13	1:B:213:ASP:H	1.71	0.56
1:B:306:LEU:HD13	1:B:307:TYR:N	2.21	0.56
1:B:430:ASP:O	1:B:431:ILE:HB	2.06	0.56
1:B:135:ILE:HG23	1:B:135:ILE:O	2.06	0.55
1:B:117:GLY:O	1:B:149:ILE:N	2.38	0.55
1:A:403:GLY:HA2	1:A:435:LEU:HB3	1.89	0.55
1:A:86:THR:HG21	1:A:333:LYS:CG	2.36	0.55
1:B:70:VAL:O	1:B:415:MET:HG3	2.06	0.55
1:A:123:THR:HG23	1:A:355:TYR:HD2	1.72	0.55
1:A:532:GLY:O	1:A:533:ASP:HB2	2.05	0.55
1:A:627:SER:CB	1:A:647:LYS:CE	2.84	0.55
1:B:403:GLY:HA3	1:B:408:HIS:ND1	2.21	0.55
1:B:101:GLN:HB3	1:B:103:HIS:HE1	1.70	0.55
1:B:262:TYR:O	1:B:263:LYS:CB	2.53	0.55
1:B:270:VAL:HG23	1:B:292:PRO:HA	1.85	0.55
1:B:635:ARG:HG3	1:B:635:ARG:O	2.07	0.55
1:A:224:ASN:CB	1:A:227:SER:HB2	2.29	0.55
1:A:436:PHE:CE2	1:A:467:LYS:CB	2.76	0.55
1:B:654:GLU:N	1:B:655:ASN:HA	2.21	0.55
1:A:149:ILE:CG2	1:A:151:ARG:HG3	2.37	0.55
1:A:355:TYR:CD1	1:A:355:TYR:N	2.72	0.55
1:A:572:ILE:HD13	1:A:600:CYS:HB2	1.89	0.55
1:A:496:THR:HA	1:A:612:TYR:HB3	1.88	0.55
1:B:500:GLU:O	1:B:504:ASN:HB2	2.06	0.55
1:A:432:GLY:HA3	1:A:459:HIS:CE1	2.42	0.55
1:B:248:MET:HG3	1:B:319:TRP:NE1	2.22	0.55
1:B:182:ARG:HB2	1:B:461:CYS:HB2	1.87	0.55
1:A:272:VAL:HG21	1:A:280:PHE:CA	2.35	0.55
1:B:181:CYS:O	1:B:459:HIS:HD2	1.90	0.55
1:A:125:LYS:HE3	1:A:355:TYR:HA	1.89	0.55
1:A:433:GLY:O	1:A:460:ALA:CA	2.43	0.55
1:A:233:ALA:HB3	1:A:312:ALA:HA	1.82	0.54
1:A:308:LYS:HB3	1:A:315:VAL:CG1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:VAL:HB	1:A:535:LEU:HD23	1.89	0.54
1:B:188:ASP:OD2	1:B:192:ILE:HD12	2.07	0.54
1:B:285:TRP:HB2	1:B:286:PRO:CD	2.36	0.54
1:B:584:ILE:HG13	1:B:589:GLU:HB2	1.89	0.54
1:A:507:PRO:O	1:A:510:ARG:NE	2.26	0.54
1:B:406:TRP:CZ2	1:B:541:PHE:HB2	2.42	0.54
1:A:151:ARG:HH12	1:A:160:GLY:CA	2.21	0.54
1:A:84:TRP:CD1	1:A:85:ASN:HA	2.40	0.54
1:B:118:ILE:HD11	1:B:146:VAL:HG13	1.90	0.54
1:B:69:GLU:HB3	1:B:101:GLN:HB2	1.88	0.54
1:A:441:ASP:O	1:A:445:ASN:ND2	2.35	0.54
1:B:453:TYR:HA	1:B:509:MET:HE1	1.88	0.54
1:A:212:ILE:CG2	1:A:213:ASP:N	2.70	0.54
1:A:245:SER:O	1:A:316:ASP:HB2	2.08	0.54
1:A:431:ILE:C	1:A:459:HIS:CD2	2.80	0.54
1:B:158:ILE:HG21	1:B:507:PRO:CD	2.37	0.54
1:B:270:VAL:O	1:B:271:TRP:HB2	2.07	0.54
1:A:410:LYS:HZ3	1:A:413:VAL:HG21	1.72	0.54
1:B:255:VAL:HG21	1:B:281:HIS:CD2	2.43	0.54
1:B:459:HIS:O	1:B:460:ALA:CB	2.56	0.54
1:A:330:THR:CG2	2:A:712:HOH:O	1.97	0.54
1:A:457:ARG:HG2	1:A:458:GLY:O	2.07	0.54
1:B:458:GLY:O	1:B:459:HIS:HB2	2.07	0.54
1:B:633:ALA:HB2	1:B:642:VAL:HG22	1.90	0.54
1:A:264:SER:C	1:A:266:THR:N	2.60	0.54
1:A:100:TYR:CG	1:A:385:ARG:HD3	2.43	0.54
1:A:406:TRP:CD2	1:A:442:LEU:HD13	2.42	0.54
1:A:618:GLY:N	1:A:621:TYR:CZ	2.76	0.54
1:B:590:ASN:HD22	1:B:590:ASN:C	2.08	0.54
1:A:383:LEU:CD2	1:A:396:ALA:HB3	2.37	0.54
1:A:440:ALA:HB2	1:A:472:PHE:HB3	1.91	0.54
1:A:85:ASN:OD1	1:A:88:SER:CB	2.56	0.54
1:B:118:ILE:CG1	1:B:120:PHE:CE1	2.91	0.54
1:B:612:TYR:HB2	1:B:628:LEU:HD12	1.90	0.54
1:B:446:TRP:O	1:B:446:TRP:HD1	1.91	0.53
1:A:504:ASN:OD1	1:A:505:GLY:CA	2.56	0.53
1:A:192:ILE:HG23	1:A:195:ALA:H	1.71	0.53
1:A:210:MET:HG3	1:A:247:TRP:CZ3	2.43	0.53
1:B:106:MET:HE3	1:B:135:ILE:HG13	1.89	0.53
1:B:638:ASP:C	1:B:639:LYS:HG2	2.28	0.53
1:A:236:ARG:HD3	1:B:661:ILE:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ARG:HH11	1:B:254:LYS:HD2	1.69	0.53
1:B:291:PHE:CD1	1:B:291:PHE:N	2.76	0.53
1:A:402:ASN:OD1	1:A:408:HIS:HB3	2.08	0.53
1:A:464:THR:CG2	1:A:465:ASN:N	2.72	0.53
1:A:84:TRP:CZ2	1:A:356:HIS:CG	2.97	0.53
1:A:72:GLY:HA3	1:A:95:LYS:HG2	1.89	0.53
1:B:299:VAL:O	1:B:303:TRP:N	2.29	0.53
1:A:74:LEU:O	1:A:75:LEU:C	2.46	0.53
1:B:555:LEU:HB3	1:B:570:MET:HE2	1.89	0.53
1:A:119:LEU:HD11	1:A:389:LEU:HD23	1.88	0.53
1:A:133:GLU:C	1:A:134:LYS:HE3	2.28	0.53
1:A:436:PHE:HE2	1:A:467:LYS:HB3	1.72	0.53
1:B:594:PRO:C	1:B:596:THR:N	2.59	0.53
1:B:651:TYR:CD2	1:B:652:ASN:N	2.68	0.53
1:B:74:LEU:CD2	1:B:75:LEU:N	2.68	0.53
1:A:272:VAL:HG21	1:A:280:PHE:CB	2.39	0.53
1:B:254:LYS:HE2	1:B:286:PRO:O	2.09	0.53
1:B:273:LYS:O	1:B:352:HIS:HE1	1.92	0.53
1:A:186:SER:CB	1:A:187:PRO:CD	2.85	0.53
1:A:229:PRO:CA	1:A:231:PRO:HD3	2.38	0.53
1:B:512:VAL:HG12	1:B:522:LEU:HD13	1.90	0.53
1:A:79:LYS:HZ2	1:A:95:LYS:HD3	1.74	0.52
1:B:633:ALA:CB	1:B:642:VAL:HG22	2.40	0.52
1:A:630:GLN:HB3	1:A:645:THR:OG1	2.09	0.52
1:B:59:PRO:O	1:B:60:GLU:HB2	2.09	0.52
1:A:236:ARG:O	1:A:240:ILE:HG13	2.09	0.52
1:A:306:LEU:CD1	1:A:374:ALA:HA	2.39	0.52
1:A:468:GLU:HB2	1:A:471:VAL:HG23	1.91	0.52
1:A:627:SER:HB3	1:A:647:LYS:HE2	1.91	0.52
1:A:238:LEU:O	1:A:243:PHE:CA	2.57	0.52
1:A:101:GLN:HG3	1:A:387:ASN:H	1.68	0.52
1:A:519:ASP:OD1	1:A:521:SER:N	2.42	0.52
1:A:587:THR:HB	1:A:590:ASN:ND2	2.21	0.52
1:B:189:SER:O	1:B:191:VAL:CG1	2.44	0.52
1:A:111:LYS:HG2	1:A:520:LEU:HD11	1.92	0.52
1:A:226:LYS:C	1:A:228:PHE:H	2.11	0.52
1:B:181:CYS:O	1:B:459:HIS:HB2	2.10	0.52
1:B:459:HIS:CE1	1:B:460:ALA:HA	2.44	0.52
1:B:555:LEU:HD23	1:B:570:MET:HE2	1.88	0.52
1:B:470:TRP:C	1:B:472:PHE:N	2.58	0.52
1:A:379:ARG:NH2	1:A:614:ASP:OD2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:PHE:CD2	1:B:434:PHE:C	2.83	0.52
1:A:268:ASN:O	1:A:293:ASP:CB	2.58	0.52
1:A:466:ASN:N	1:A:466:ASN:OD1	2.43	0.52
1:B:225:PRO:O	1:B:226:LYS:O	2.28	0.52
1:B:65:TYR:OH	1:B:523:ARG:HG2	2.09	0.52
1:A:587:THR:CB	1:A:590:ASN:HD22	2.22	0.52
1:B:285:TRP:CB	1:B:286:PRO:CD	2.88	0.52
1:A:407:ASP:O	1:A:411:MET:HB2	2.10	0.51
1:A:627:SER:HB2	1:A:647:LYS:CE	2.40	0.51
1:A:72:GLY:C	1:A:74:LEU:H	2.14	0.51
1:B:182:ARG:HE	1:B:466:ASN:HA	1.73	0.51
1:B:91:TYR:CE2	1:B:415:MET:CE	2.93	0.51
1:A:232:LYS:O	1:A:233:ALA:CB	2.57	0.51
1:A:630:GLN:HB3	1:A:645:THR:HG1	1.75	0.51
1:A:108:GLY:O	1:A:115:ALA:HA	2.11	0.51
1:B:323:ASN:OD1	1:B:360:GLY:HA3	2.10	0.51
1:A:293:ASP:O	1:A:299:VAL:HB	2.11	0.51
1:A:209:TRP:CH2	1:A:383:LEU:HD12	2.44	0.51
1:B:123:THR:CG2	1:B:124:TRP:HE3	2.23	0.51
1:B:307:TYR:CD1	1:B:307:TYR:N	2.78	0.51
1:B:158:ILE:HG21	1:B:507:PRO:HD2	1.91	0.51
1:B:510:ARG:NH1	1:B:533:ASP:OD1	2.43	0.51
1:B:632:VAL:O	1:B:642:VAL:HG13	2.11	0.51
1:A:145:ARG:HE	1:A:147:PHE:HE2	1.58	0.51
1:A:165:THR:HG21	1:A:390:GLY:HA2	1.91	0.51
1:A:497:LEU:HD11	1:A:532:GLY:HA3	1.92	0.51
1:A:621:TYR:HB2	1:A:625:ASP:H	1.74	0.51
1:B:227:SER:O	1:B:228:PHE:HB2	2.09	0.51
1:B:270:VAL:O	1:B:271:TRP:CG	2.64	0.51
1:A:230:ASN:ND2	1:A:234:VAL:CB	2.74	0.51
1:A:245:SER:CB	1:A:314:GLY:O	2.58	0.51
1:A:511:PRO:HG2	1:A:514:PHE:CG	2.46	0.51
1:A:627:SER:HB2	1:A:647:LYS:HE2	1.92	0.51
1:B:251:PRO:HG3	1:B:363:MET:SD	2.51	0.51
1:B:350:GLY:O	1:B:352:HIS:N	2.39	0.51
1:B:584:ILE:CG1	1:B:589:GLU:HB2	2.41	0.51
1:A:105:TRP:HH2	1:A:157:VAL:CG1	2.24	0.51
1:A:225:PRO:HA	1:A:229:PRO:HG3	1.88	0.51
1:B:543:ASN:O	1:B:545:PRO:HD3	2.11	0.51
1:A:101:GLN:HG3	1:A:386:SER:HA	1.93	0.51
1:A:304:ARG:HB3	1:A:370:GLY:CA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:TRP:CE3	1:A:319:TRP:CE3	2.96	0.51
1:A:405:CYS:SG	1:A:408:HIS:ND1	2.84	0.51
1:B:353:LEU:O	1:B:354:GLN:HG2	2.11	0.51
1:B:487:ARG:O	1:B:490:LEU:HB2	2.11	0.51
1:A:126:ALA:CB	1:A:137:LEU:HD11	2.41	0.51
1:B:509:MET:HG3	1:B:529:PHE:HD2	1.73	0.51
1:A:48:THR:CB	1:A:53:ASN:HB2	2.41	0.50
1:A:607:ALA:HB3	1:A:633:ALA:HB3	1.92	0.50
1:B:86:THR:O	1:B:100:TYR:CD1	2.63	0.50
1:B:403:GLY:C	1:B:405:CYS:H	2.15	0.50
1:B:534:ASN:OD1	1:B:573:ARG:NE	2.44	0.50
1:B:638:ASP:C	1:B:639:LYS:CG	2.79	0.50
1:A:472:PHE:HB2	1:A:476:VAL:HG21	1.92	0.50
1:B:321:ASP:O	1:B:322:VAL:HB	2.11	0.50
1:A:94:ASP:C	1:A:95:LYS:CG	2.67	0.50
1:A:86:THR:O	1:A:87:ASP:C	2.45	0.50
1:B:557:LEU:CD1	1:B:557:LEU:N	2.73	0.50
1:A:262:TYR:CD1	1:A:262:TYR:C	2.85	0.50
1:A:457:ARG:N	2:A:704:HOH:O	2.36	0.50
1:A:641:THR:CB	1:A:643:LYS:NZ	2.67	0.50
1:B:406:TRP:CZ3	1:B:442:LEU:HD12	2.46	0.50
1:B:516:ASP:HB3	1:B:519:ASP:CB	2.39	0.50
1:A:179:GLN:CB	1:A:209:TRP:HE1	2.08	0.50
1:A:324:GLU:N	1:A:325:PRO:CA	2.72	0.50
1:A:384:THR:HG22	1:A:395:ALA:HB1	1.93	0.50
1:A:552:TRP:HB3	1:A:571:LYS:HB3	1.92	0.50
1:B:348:PRO:HG2	1:B:348:PRO:O	2.12	0.50
1:B:567:GLN:O	1:B:568:ALA:HB3	2.12	0.50
1:A:120:PHE:HB2	1:A:137:LEU:HD22	1.92	0.50
1:B:248:MET:HG2	1:B:249:ILE:N	2.26	0.50
1:B:485:GLU:HG2	1:B:583:ILE:CG2	2.41	0.50
1:B:649:GLY:O	1:B:650:LYS:CB	2.59	0.50
1:B:63:SER:CA	1:B:76:ARG:HH21	2.22	0.50
1:B:72:GLY:CA	1:B:73:SER:HB2	2.24	0.50
1:B:62:THR:O	1:B:63:SER:CB	2.54	0.49
1:A:180:GLN:HG3	1:A:181:CYS:N	2.27	0.49
1:A:236:ARG:HG2	1:A:240:ILE:CD1	2.42	0.49
1:B:361:PHE:CZ	1:B:394:TYR:HE2	2.30	0.49
1:B:364:VAL:CG2	1:B:384:THR:HB	2.42	0.49
1:B:437:ASN:O	1:B:438:ALA:HB3	2.11	0.49
1:A:181:CYS:HB3	1:A:209:TRP:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:PRO:HG3	1:A:526:GLU:HB2	1.94	0.49
1:B:182:ARG:NE	1:B:466:ASN:HA	2.27	0.49
1:B:83:LEU:N	1:B:83:LEU:CD1	2.73	0.49
1:A:182:ARG:HD3	1:A:194:ILE:HG13	1.95	0.49
1:A:77:ASN:N	1:A:77:ASN:ND2	2.60	0.49
1:B:270:VAL:HG13	1:B:271:TRP:CD2	2.48	0.49
1:A:84:TRP:NE1	1:A:356:HIS:CD2	2.80	0.49
1:B:228:PHE:N	1:B:229:PRO:CD	2.75	0.49
1:B:257:PRO:HA	1:B:259:TYR:HE2	1.76	0.49
1:B:64:ILE:N	1:B:76:ARG:NH2	2.56	0.49
1:A:280:PHE:CE1	1:A:336:PRO:HD3	2.41	0.49
1:A:420:GLY:CA	1:A:507:PRO:HG3	2.43	0.49
1:B:179:GLN:OE1	1:B:455:PHE:HE1	1.95	0.49
1:B:311:LEU:HD23	1:B:315:VAL:HB	1.93	0.49
1:A:192:ILE:CG2	1:A:195:ALA:N	2.73	0.49
1:B:212:ILE:CG1	1:B:213:ASP:N	2.73	0.49
1:B:379:ARG:CG	1:B:619:TRP:HA	2.43	0.49
1:B:592:LEU:HG	1:B:592:LEU:O	2.13	0.49
1:B:593:ASP:HB3	1:B:594:PRO:CD	2.41	0.49
1:B:604:GLN:HA	1:B:604:GLN:NE2	2.28	0.49
1:A:125:LYS:HE2	1:A:356:HIS:H	1.78	0.49
1:B:109:VAL:HB	1:B:523:ARG:NH1	2.28	0.49
1:B:379:ARG:HG3	1:B:619:TRP:HA	1.95	0.49
1:B:70:VAL:HG13	1:B:71:THR:N	2.28	0.49
1:A:105:TRP:CZ2	1:A:161:LEU:HD22	2.47	0.49
1:A:170:MET:CE	1:A:498:LEU:HG	2.42	0.49
1:A:84:TRP:CH2	1:A:356:HIS:CB	2.96	0.49
1:A:619:TRP:O	1:A:621:TYR:CD1	2.66	0.49
1:B:204:PRO:HB3	1:B:585:GLN:HA	1.92	0.49
1:B:219:ARG:HH11	1:B:254:LYS:CB	2.23	0.49
1:A:100:TYR:CD1	1:A:385:ARG:HD3	2.47	0.49
1:A:459:HIS:ND1	1:A:460:ALA:HB2	2.28	0.49
1:A:503:THR:HG23	1:A:504:ASN:N	2.27	0.49
1:A:336:PRO:O	1:A:336:PRO:HG2	2.12	0.48
1:A:173:ARG:HH21	1:A:590:ASN:HB3	1.78	0.48
1:A:261:VAL:HG13	1:A:262:TYR:N	2.28	0.48
1:A:466:ASN:O	1:A:467:LYS:NZ	2.34	0.48
1:B:187:PRO:HA	1:B:188:ASP:C	2.33	0.48
1:B:443:PHE:CD2	1:B:472:PHE:CE2	3.01	0.48
1:A:379:ARG:HE	1:A:618:GLY:C	2.16	0.48
1:B:356:HIS:O	1:B:357:ASN:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:HIS:ND1	1:B:460:ALA:HA	2.28	0.48
1:A:383:LEU:HD23	1:A:396:ALA:HB3	1.95	0.48
1:B:181:CYS:O	1:B:459:HIS:CB	2.62	0.48
1:B:471:VAL:O	1:B:471:VAL:HG12	2.13	0.48
1:A:304:ARG:CB	1:A:370:GLY:CA	2.91	0.48
1:A:434:PHE:N	1:A:434:PHE:CD1	2.82	0.48
1:A:572:ILE:HG23	1:A:572:ILE:O	2.14	0.48
1:B:115:ALA:CB	1:B:154:PRO:HA	2.41	0.48
1:B:118:ILE:CG1	1:B:120:PHE:CZ	2.97	0.48
1:B:171:ILE:HD12	1:B:175:ALA:CB	2.42	0.48
1:B:434:PHE:C	1:B:434:PHE:HD2	2.17	0.48
1:B:634:GLU:O	1:B:635:ARG:CG	2.62	0.48
1:A:264:SER:C	1:A:266:THR:H	2.15	0.48
1:A:101:GLN:CD	1:A:387:ASN:CB	2.80	0.48
1:A:82:LYS:HD2	1:A:98:ARG:H	1.78	0.48
1:B:257:PRO:C	1:B:259:TYR:CE2	2.87	0.48
1:B:536:LEU:CD2	1:B:548:PRO:HD2	2.44	0.48
1:A:307:TYR:HA	1:A:310:PHE:CD2	2.49	0.48
1:A:308:LYS:H	1:A:308:LYS:HG3	1.52	0.48
1:A:86:THR:CG2	1:A:333:LYS:HB3	2.37	0.48
1:A:456:ALA:CA	2:A:704:HOH:O	2.60	0.48
1:A:173:ARG:HD3	1:A:495:TYR:CE2	2.49	0.48
1:A:69:GLU:C	1:A:70:VAL:CG1	2.82	0.48
1:B:472:PHE:O	1:B:476:VAL:CG2	2.61	0.48
1:A:192:ILE:HG22	1:A:195:ALA:N	2.26	0.48
1:A:262:TYR:HD1	1:A:262:TYR:C	2.17	0.48
1:B:188:ASP:HB3	1:B:189:SER:CA	2.43	0.48
1:B:351:THR:OG1	1:B:351:THR:O	2.32	0.48
1:B:610:ASN:HA	1:B:629:LEU:O	2.13	0.48
1:B:63:SER:N	1:B:76:ARG:HH22	2.10	0.48
1:B:118:ILE:HD13	1:B:148:ILE:CG1	2.43	0.48
1:A:382:ILE:HG13	1:A:383:LEU:N	2.29	0.47
1:A:413:VAL:HB	1:A:414:PRO:CD	2.36	0.47
1:A:72:GLY:HA3	1:A:95:LYS:CG	2.43	0.47
1:B:118:ILE:CD1	1:B:146:VAL:HG13	2.44	0.47
1:B:173:ARG:O	1:B:176:LEU:HB2	2.14	0.47
1:B:285:TRP:CB	1:B:286:PRO:HD3	2.44	0.47
1:B:449:PHE:CB	1:B:539:PRO:HG3	2.43	0.47
1:A:259:TYR:CE1	1:A:262:TYR:O	2.67	0.47
1:A:312:ALA:HB2	1:A:315:VAL:H	1.79	0.47
1:A:68:GLY:N	1:A:422:SER:OG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:THR:CB	1:A:590:ASN:ND2	2.77	0.47
1:B:171:ILE:O	1:B:379:ARG:NH1	2.43	0.47
1:B:224:ASN:H	1:B:225:PRO:CD	2.26	0.47
1:B:247:TRP:HD1	1:B:315:VAL:HG13	1.79	0.47
1:A:361:PHE:C	1:A:361:PHE:CD1	2.87	0.47
1:A:91:TYR:O	1:A:92:GLY:C	2.53	0.47
1:B:248:MET:HB2	1:B:319:TRP:CH2	2.45	0.47
1:B:158:ILE:HD11	1:B:421:LEU:CD2	2.43	0.47
1:A:278:LYS:HD3	1:A:279:ASN:OD1	2.15	0.47
1:A:285:TRP:N	1:A:286:PRO:CD	2.77	0.47
1:A:367:SER:CB	1:A:382:ILE:HD13	2.45	0.47
1:A:436:PHE:CE2	1:A:460:ALA:HB1	2.49	0.47
1:A:489:ILE:O	1:A:489:ILE:HG13	2.13	0.47
1:A:379:ARG:NE	1:A:618:GLY:O	2.47	0.47
1:B:216:ASP:C	1:B:218:TYR:H	2.17	0.47
1:B:443:PHE:CD2	1:B:472:PHE:HE2	2.32	0.47
1:B:75:LEU:N	1:B:75:LEU:HD22	2.30	0.47
1:A:465:ASN:O	1:A:466:ASN:CB	2.63	0.47
1:B:420:GLY:HA3	1:B:507:PRO:HB3	1.96	0.47
1:B:527:GLU:CB	1:B:543:ASN:HD22	2.28	0.47
1:B:538:ILE:O	1:B:538:ILE:HG23	2.15	0.47
1:B:324:GLU:N	1:B:325:PRO:HA	2.30	0.47
1:A:160:GLY:HA2	1:A:163:GLU:CD	2.35	0.47
1:B:259:TYR:CE1	1:B:262:TYR:O	2.68	0.47
1:B:259:TYR:HE1	1:B:263:LYS:CB	2.28	0.47
1:B:270:VAL:CG2	1:B:292:PRO:HB3	2.44	0.47
1:B:415:MET:O	1:B:418:THR:CG2	2.53	0.47
1:B:449:PHE:HB3	1:B:539:PRO:HG3	1.97	0.47
1:B:534:ASN:CG	1:B:576:ALA:CB	2.83	0.47
1:A:398:TRP:HE3	1:A:398:TRP:O	1.98	0.47
1:A:171:ILE:HG13	1:A:498:LEU:HD21	1.96	0.47
1:B:246:ALA:HA	1:B:317:GLY:O	2.15	0.47
1:A:120:PHE:CB	1:A:137:LEU:HD22	2.45	0.47
1:A:402:ASN:HB3	1:A:433:GLY:CA	2.38	0.47
1:A:457:ARG:HG2	1:A:458:GLY:N	2.30	0.47
1:A:519:ASP:OD1	1:A:521:SER:HB2	2.15	0.47
1:B:272:VAL:O	1:B:274:THR:N	2.47	0.47
1:B:430:ASP:O	1:B:457:ARG:O	2.32	0.47
1:B:498:LEU:HA	1:B:508:ILE:HD11	1.97	0.47
1:B:488:TYR:HB3	1:B:584:ILE:HG22	1.97	0.47
1:A:124:TRP:CZ2	1:A:355:TYR:CE1	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:TRP:N	1:A:209:TRP:CD1	2.83	0.46
1:A:76:ARG:HH11	1:A:523:ARG:HB3	1.80	0.46
1:A:86:THR:CG2	1:A:87:ASP:N	2.77	0.46
1:B:304:ARG:O	1:B:307:TYR:HB3	2.15	0.46
1:A:131:THR:CG2	1:A:132:ASP:H	2.05	0.46
1:A:262:TYR:HE1	1:A:264:SER:HG	1.59	0.46
1:A:272:VAL:CG1	1:A:336:PRO:CB	2.87	0.46
1:A:405:CYS:O	1:A:406:TRP:CB	2.63	0.46
1:A:432:GLY:CA	1:A:436:PHE:HE1	2.28	0.46
1:A:627:SER:HB2	1:A:647:LYS:NZ	2.29	0.46
1:B:411:MET:C	1:B:414:PRO:HD2	2.34	0.46
1:A:312:ALA:HB2	1:A:315:VAL:N	2.30	0.46
1:A:460:ALA:HB3	1:A:467:LYS:CD	2.28	0.46
1:B:257:PRO:CA	1:B:259:TYR:HE2	2.26	0.46
1:A:392:GLN:HA	1:A:395:ALA:O	2.16	0.46
1:A:506:MET:CB	1:A:507:PRO:HD2	2.26	0.46
1:A:69:GLU:C	1:A:70:VAL:HG13	2.35	0.46
1:A:76:ARG:NH1	1:A:523:ARG:HB3	2.30	0.46
1:A:86:THR:HG22	1:A:87:ASP:N	2.31	0.46
1:B:409:LEU:HB2	1:B:446:TRP:CE3	2.50	0.46
1:B:542:ALA:C	1:B:543:ASN:OD1	2.54	0.46
1:A:447:ILE:HA	1:A:447:ILE:HD12	1.71	0.46
1:A:544:GLN:CB	1:A:545:PRO:HA	2.45	0.46
1:B:204:PRO:HB3	1:B:585:GLN:CD	2.36	0.46
1:B:630:GLN:HG2	1:B:645:THR:OG1	2.16	0.46
1:A:101:GLN:HG2	1:A:387:ASN:C	2.35	0.46
1:A:81:ILE:O	1:A:128:LEU:N	2.48	0.46
1:A:431:ILE:HG13	1:A:447:ILE:HD13	1.97	0.46
1:A:506:MET:HE2	1:A:506:MET:HB2	1.94	0.46
1:A:118:ILE:HG12	1:A:120:PHE:CE1	2.50	0.46
1:A:253:ALA:O	1:A:289:ALA:HA	2.15	0.46
1:A:436:PHE:CD2	1:A:460:ALA:HB1	2.51	0.46
1:B:285:TRP:N	1:B:286:PRO:CD	2.78	0.46
1:B:162:SER:OG	1:B:505:GLY:HA3	2.14	0.46
1:B:612:TYR:OH	1:B:621:TYR:CB	2.64	0.46
1:B:86:THR:HG23	1:B:88:SER:OG	2.15	0.46
1:B:87:ASP:N	1:B:87:ASP:OD1	2.38	0.46
1:A:89:GLY:HA3	1:A:100:TYR:CE2	2.51	0.46
1:A:245:SER:CB	1:A:247:TRP:HE1	2.29	0.46
1:A:170:MET:HE3	1:A:499:HIS:HA	1.98	0.46
1:A:627:SER:CB	1:A:647:LYS:HZ3	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:HD2	1:A:193:GLU:OE1	2.15	0.46
1:A:233:ALA:O	1:A:235:ASN:N	2.49	0.46
1:A:176:LEU:HD11	1:A:495:TYR:HD1	1.81	0.46
1:B:565:LYS:C	1:B:566:TYR:CD1	2.90	0.46
1:A:431:ILE:O	1:A:459:HIS:NE2	2.49	0.45
1:A:465:ASN:HB3	1:A:466:ASN:OD1	2.16	0.45
1:A:491:LEU:CB	1:A:492:PRO:HD3	2.46	0.45
1:A:536:LEU:HD23	1:A:571:LYS:HD3	1.98	0.45
1:A:581:GLY:O	1:A:582:LYS:CB	2.58	0.45
1:A:628:LEU:N	1:A:647:LYS:HZ3	2.13	0.45
1:B:112:ASP:HB2	1:B:114:THR:H	1.80	0.45
1:B:356:HIS:O	1:B:357:ASN:CB	2.65	0.45
1:B:634:GLU:O	1:B:635:ARG:HG3	2.15	0.45
1:A:306:LEU:HD12	1:A:374:ALA:HA	1.99	0.45
1:B:424:GLN:HG3	1:B:424:GLN:O	2.14	0.45
1:B:486:ARG:O	1:B:489:ILE:HG13	2.16	0.45
1:A:194:ILE:HD12	1:A:470:TRP:HZ2	1.81	0.45
1:A:278:LYS:CD	1:A:279:ASN:H	2.30	0.45
1:B:653:THR:C	1:B:654:GLU:HG2	2.36	0.45
1:B:126:ALA:HB1	1:B:137:LEU:CD2	2.41	0.45
1:B:304:ARG:HG2	1:B:369:GLU:HB2	1.97	0.45
1:B:162:SER:CB	1:B:504:ASN:O	2.63	0.45
1:B:530:LEU:HB3	1:B:532:GLY:O	2.15	0.45
1:B:173:ARG:HD2	1:B:613:TRP:CH2	2.50	0.45
1:B:635:ARG:HE	1:B:636:ASN:ND2	2.09	0.45
1:A:179:GLN:CG	1:A:207:VAL:HB	2.33	0.45
1:A:77:ASN:N	1:A:77:ASN:HD22	2.14	0.45
1:B:620:SER:HB3	1:B:621:TYR:H	1.59	0.45
1:A:236:ARG:HE	1:A:240:ILE:HD11	1.82	0.45
1:A:272:VAL:CG1	1:A:336:PRO:HG3	2.24	0.45
1:A:203:ILE:CG2	1:A:484:LEU:HD12	2.47	0.45
1:A:545:PRO:O	1:A:546:ALA:C	2.51	0.45
1:B:350:GLY:C	1:B:352:HIS:N	2.69	0.45
1:B:91:TYR:CE2	1:B:415:MET:HE1	2.51	0.45
1:A:431:ILE:HG23	1:A:446:TRP:CB	2.46	0.45
1:A:467:LYS:NZ	1:A:467:LYS:HB3	2.32	0.45
1:B:168:MET:HA	1:B:392:GLN:O	2.17	0.45
1:A:130:SER:HB3	1:A:135:ILE:HA	1.99	0.45
1:A:270:VAL:HG12	1:A:293:ASP:HA	1.98	0.45
1:A:73:SER:N	1:A:95:LYS:HE3	2.29	0.45
1:B:116:PHE:HA	1:B:150:ASP:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:PHE:HA	1:B:212:ILE:CA	2.46	0.45
1:B:262:TYR:O	1:B:262:TYR:CD2	2.70	0.45
1:B:565:LYS:C	1:B:566:TYR:HD1	2.20	0.45
1:A:293:ASP:O	1:A:299:VAL:CB	2.64	0.45
1:A:84:TRP:CH2	1:A:356:HIS:CG	3.05	0.45
1:A:410:LYS:HZ3	1:A:413:VAL:CG2	2.30	0.45
1:A:75:LEU:HD12	1:A:75:LEU:HA	1.78	0.45
1:B:223:PHE:HB2	1:B:224:ASN:CA	2.47	0.45
1:B:91:TYR:CE2	1:B:415:MET:HE3	2.51	0.45
1:A:271:TRP:O	1:A:337:GLU:OE2	2.34	0.45
1:A:361:PHE:CD2	1:A:388:PHE:HB3	2.52	0.45
1:A:434:PHE:CE2	1:A:461:CYS:CB	3.00	0.45
1:B:106:MET:CE	1:B:135:ILE:HG13	2.47	0.45
1:B:273:LYS:O	1:B:352:HIS:CE1	2.70	0.45
1:B:382:ILE:O	1:B:383:LEU:HD23	2.17	0.45
1:B:402:ASN:HB2	1:B:430:ASP:CG	2.38	0.45
1:B:437:ASN:CA	1:B:465:ASN:OD1	2.57	0.45
1:A:324:GLU:OE2	1:A:385:ARG:HD2	2.17	0.44
1:A:410:LYS:O	1:A:414:PRO:HD2	2.18	0.44
1:A:409:LEU:HA	1:A:446:TRP:CZ2	2.52	0.44
1:A:426:PHE:CD2	1:A:455:PHE:HB2	2.50	0.44
1:B:245:SER:OG	1:B:247:TRP:CD1	2.52	0.44
1:B:323:ASN:OD1	1:B:360:GLY:CA	2.65	0.44
1:A:248:MET:HB2	1:A:319:TRP:CE2	2.47	0.44
1:A:402:ASN:O	1:A:434:PHE:O	2.34	0.44
1:A:627:SER:HB2	1:A:647:LYS:HZ3	1.83	0.44
1:B:458:GLY:O	1:B:459:HIS:CB	2.66	0.44
1:B:499:HIS:CE1	1:B:612:TYR:CE2	3.05	0.44
1:B:474:GLN:CA	1:B:474:GLN:NE2	2.80	0.44
1:A:86:THR:CG2	1:A:87:ASP:OD1	2.53	0.44
1:A:89:GLY:O	1:A:90:ALA:CB	2.65	0.44
1:B:270:VAL:CG2	1:B:292:PRO:CB	2.96	0.44
1:B:270:VAL:HG23	1:B:293:ASP:H	1.83	0.44
1:B:652:ASN:ND2	1:B:656:LYS:O	2.51	0.44
1:A:236:ARG:HH11	1:B:661:ILE:HG23	1.78	0.44
1:A:398:TRP:CE3	1:A:398:TRP:O	2.70	0.44
1:A:520:LEU:HA	1:A:520:LEU:HD23	1.80	0.44
1:A:72:GLY:C	1:A:74:LEU:N	2.70	0.44
1:B:257:PRO:O	1:B:259:TYR:CE2	2.70	0.44
1:B:311:LEU:HD23	1:B:311:LEU:HA	1.83	0.44
1:A:297:PRO:HA	1:A:300:ASN:ND2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:GLN:HA	1:B:425:PRO:HD3	1.88	0.44
1:A:256:ASP:HA	1:A:257:PRO:HD3	1.86	0.44
1:B:180:GLN:O	1:B:181:CYS:CB	2.60	0.44
1:B:419:LEU:HD13	1:B:427:SER:HB3	2.00	0.44
1:B:520:LEU:CD1	1:B:520:LEU:N	2.79	0.44
1:B:577:ILE:HA	1:B:598:LEU:O	2.18	0.44
1:B:62:THR:HB	1:B:64:ILE:CD1	2.46	0.44
1:B:93:VAL:O	1:B:97:THR:CA	2.65	0.44
1:A:538:ILE:O	1:A:568:ALA:HB1	2.17	0.44
1:A:577:ILE:HB	1:A:609:GLY:CA	2.47	0.44
1:B:229:PRO:HD2	1:B:230:ASN:H	1.83	0.44
1:A:111:LYS:C	1:A:112:ASP:O	2.55	0.44
1:A:182:ARG:O	1:A:183:PHE:CB	2.66	0.44
1:A:211:ASP:OD1	1:A:212:ILE:HB	2.18	0.44
1:B:224:ASN:O	1:B:228:PHE:O	2.36	0.44
1:B:433:GLY:HA3	1:B:460:ALA:CB	2.40	0.44
1:B:446:TRP:O	1:B:446:TRP:CD1	2.70	0.44
1:B:541:PHE:O	1:B:541:PHE:CD1	2.70	0.44
1:A:173:ARG:HG2	1:A:491:LEU:HD11	1.99	0.43
1:A:525:GLU:HB2	1:A:546:ALA:HB3	1.99	0.43
1:B:493:TYR:O	1:B:497:LEU:HG	2.18	0.43
1:A:466:ASN:CB	1:A:471:VAL:HG11	2.39	0.43
1:A:83:LEU:O	1:A:84:TRP:HB2	2.17	0.43
1:B:224:ASN:HB3	1:B:225:PRO:HD3	2.00	0.43
1:B:459:HIS:O	1:B:460:ALA:HB3	2.19	0.43
1:B:661:ILE:H	1:B:661:ILE:HG13	1.56	0.43
1:A:107:MET:HA	1:A:116:PHE:O	2.18	0.43
1:A:212:ILE:O	1:A:215:MET:HE2	2.18	0.43
1:B:274:THR:CG2	1:B:275:ALA:N	2.80	0.43
1:B:306:LEU:HD22	1:B:306:LEU:O	2.17	0.43
1:B:320:ASN:O	1:B:385:ARG:N	2.38	0.43
1:A:413:VAL:O	1:A:417:LEU:HG	2.19	0.43
1:A:525:GLU:OE2	1:A:545:PRO:CD	2.66	0.43
1:A:629:LEU:HD22	1:A:644:LEU:HD21	1.99	0.43
1:A:84:TRP:HA	1:A:357:ASN:CG	2.38	0.43
1:B:227:SER:O	1:B:228:PHE:CB	2.63	0.43
1:A:126:ALA:O	1:A:127:GLU:CB	2.66	0.43
1:A:305:ASN:O	1:A:306:LEU:CB	2.66	0.43
1:B:446:TRP:C	1:B:446:TRP:CD1	2.92	0.43
1:B:491:LEU:N	1:B:492:PRO:CD	2.81	0.43
1:B:538:ILE:CG2	1:B:569:LYS:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:PRO:O	1:B:60:GLU:CB	2.65	0.43
1:A:197:THR:O	1:A:201:LYS:HG3	2.18	0.43
1:A:249:ILE:HG22	1:A:250:ASP:N	2.34	0.43
1:A:84:TRP:HA	1:A:357:ASN:HD21	1.83	0.43
1:A:84:TRP:HA	1:A:357:ASN:ND2	2.33	0.43
1:A:577:ILE:HG12	1:A:599:VAL:HG22	2.00	0.43
1:B:179:GLN:HA	1:B:207:VAL:O	2.17	0.43
1:B:282:GLY:O	1:B:288:ALA:HA	2.18	0.43
1:B:305:ASN:HD21	1:B:307:TYR:HE1	1.67	0.43
1:B:606:LYS:HZ1	1:B:634:GLU:HG3	1.81	0.43
1:B:635:ARG:HE	1:B:636:ASN:HB2	1.83	0.43
1:A:466:ASN:O	1:A:467:LYS:CB	2.64	0.43
1:B:121:ASP:O	1:B:144:PHE:HB2	2.18	0.43
1:B:118:ILE:HG13	1:B:120:PHE:CZ	2.54	0.43
1:B:169:PRO:HD2	2:B:704:HOH:O	2.19	0.43
1:B:623:LYS:HB2	1:B:625:ASP:H	1.84	0.43
1:A:397:THR:O	1:A:398:TRP:CD1	2.71	0.43
1:B:180:GLN:O	1:B:209:TRP:O	2.36	0.43
1:B:180:GLN:OE1	1:B:181:CYS:N	2.51	0.43
1:B:461:CYS:HB3	1:B:463:GLY:H	1.83	0.43
1:A:304:ARG:HB3	1:A:370:GLY:HA3	2.01	0.43
1:A:313:GLN:O	1:A:313:GLN:HG3	2.19	0.43
1:B:426:PHE:CE2	1:B:455:PHE:HB2	2.54	0.43
1:B:443:PHE:CG	1:B:472:PHE:CE2	3.07	0.43
1:B:479:ALA:CB	1:B:566:TYR:HD2	2.19	0.43
1:A:238:LEU:O	1:A:243:PHE:N	2.52	0.42
1:A:434:PHE:CE2	1:A:461:CYS:HB2	2.54	0.42
1:A:459:HIS:C	1:A:459:HIS:ND1	2.73	0.42
1:B:91:TYR:CG	1:B:415:MET:HE1	2.53	0.42
1:B:586:ASN:HB3	1:B:588:THR:H	1.84	0.42
1:B:85:ASN:HB2	1:B:356:HIS:HD2	1.84	0.42
1:A:105:TRP:CH2	1:A:157:VAL:CG1	3.01	0.42
1:A:587:THR:HG22	1:A:590:ASN:HD21	1.84	0.42
1:A:649:GLY:O	1:A:650:LYS:CB	2.65	0.42
1:B:307:TYR:HD2	1:B:374:ALA:CA	2.31	0.42
1:A:271:TRP:CD1	1:A:271:TRP:N	2.84	0.42
1:A:319:TRP:CD1	1:A:321:ASP:HB2	2.54	0.42
1:A:367:SER:HB3	1:A:382:ILE:HD13	2.01	0.42
1:A:503:THR:CG2	1:A:504:ASN:N	2.82	0.42
1:B:253:ALA:HB3	1:B:290:ALA:HB3	2.00	0.42
1:B:255:VAL:HG12	1:B:262:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:GLY:CA	1:B:278:LYS:HD3	2.49	0.42
1:A:199:ARG:NH2	1:A:242:GLY:O	2.51	0.42
1:A:300:ASN:O	1:A:304:ARG:HG2	2.20	0.42
1:A:84:TRP:CZ2	1:A:334:THR:HG21	2.46	0.42
1:A:402:ASN:CB	1:A:433:GLY:HA3	2.42	0.42
1:A:159:ARG:HG2	1:A:504:ASN:HB2	2.01	0.42
1:A:58:VAL:CG2	1:A:116:PHE:HZ	2.32	0.42
1:B:59:PRO:HD3	1:B:133:GLU:O	2.19	0.42
1:B:209:TRP:HE1	1:B:457:ARG:HD2	1.85	0.42
1:B:223:PHE:CB	1:B:224:ASN:CA	2.96	0.42
1:B:474:GLN:C	1:B:474:GLN:NE2	2.73	0.42
1:B:635:ARG:CD	1:B:639:LYS:O	2.68	0.42
1:B:81:ILE:CG2	1:B:128:LEU:HB2	2.49	0.42
1:B:85:ASN:OD1	1:B:100:TYR:O	2.37	0.42
1:A:254:LYS:HA	1:A:289:ALA:HA	2.01	0.42
1:A:58:VAL:H	1:A:134:LYS:HD3	1.85	0.42
1:A:645:THR:O	1:A:646:LYS:HD2	2.19	0.42
1:B:158:ILE:HD11	1:B:421:LEU:HD22	2.01	0.42
1:B:193:GLU:OE1	1:B:241:ARG:NH1	2.53	0.42
1:B:183:PHE:HA	1:B:212:ILE:HA	2.01	0.42
1:B:493:TYR:HE2	1:B:531:VAL:HG12	1.85	0.42
1:A:431:ILE:C	1:A:459:HIS:NE2	2.73	0.42
1:A:439:ASP:N	1:A:439:ASP:OD1	2.47	0.42
1:A:238:LEU:HA	1:A:238:LEU:HD12	1.84	0.42
1:A:82:LYS:HB2	1:A:98:ARG:CB	2.50	0.42
1:B:122:THR:HB	1:B:144:PHE:CD2	2.54	0.42
1:B:224:ASN:HB3	1:B:225:PRO:CD	2.49	0.42
1:B:431:ILE:HD13	1:B:447:ILE:HD12	2.01	0.42
1:A:181:CYS:O	1:A:182:ARG:HB2	2.19	0.42
1:A:262:TYR:CD1	1:A:262:TYR:O	2.70	0.42
1:B:112:ASP:CB	1:B:114:THR:H	2.32	0.42
1:B:231:PRO:HB2	1:B:313:GLN:HB3	2.02	0.42
1:B:371:ILE:HG21	1:B:380:PRO:HB3	2.01	0.42
1:A:272:VAL:HG13	1:A:336:PRO:CB	2.39	0.42
1:A:536:LEU:HB3	1:A:571:LYS:HB2	2.02	0.42
1:B:368:ARG:HD2	1:B:394:TYR:O	2.19	0.42
1:A:162:SER:O	1:A:166:GLY:CA	2.68	0.42
1:A:198:PHE:CD1	1:A:205:CYS:HB2	2.55	0.42
1:A:254:LYS:HB2	1:A:286:PRO:HB2	2.02	0.42
1:A:293:ASP:C	1:A:295:THR:H	2.23	0.42
1:A:307:TYR:HA	1:A:310:PHE:HE2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LYS:HE2	1:A:308:LYS:HB2	1.77	0.42
1:A:103:HIS:HB3	1:A:389:LEU:HD13	2.01	0.42
1:A:397:THR:CG2	1:A:424:GLN:HG2	2.45	0.42
1:A:490:LEU:HA	1:A:490:LEU:HD23	1.80	0.42
1:A:525:GLU:OE2	1:A:545:PRO:HD2	2.20	0.42
1:A:58:VAL:HG13	1:A:59:PRO:O	2.19	0.42
1:B:81:ILE:HG23	1:B:128:LEU:CB	2.48	0.42
1:B:80:THR:OG1	1:B:130:SER:OG	2.07	0.42
1:A:133:GLU:HA	1:A:134:LYS:CE	2.44	0.41
1:A:220:ILE:O	1:A:221:PHE:HB2	2.19	0.41
1:A:587:THR:HG22	1:A:590:ASN:ND2	2.34	0.41
1:A:94:ASP:O	1:A:95:LYS:CG	2.68	0.41
1:B:406:TRP:HZ2	1:B:541:PHE:CB	2.30	0.41
1:A:242:GLY:HA3	1:A:586:ASN:ND2	2.35	0.41
1:A:68:GLY:HA2	1:A:422:SER:OG	2.20	0.41
1:B:238:LEU:O	1:B:243:PHE:HB2	2.19	0.41
1:B:404:SER:C	1:B:442:LEU:HD21	2.41	0.41
1:B:485:GLU:HG2	1:B:583:ILE:HG23	2.02	0.41
1:B:538:ILE:HD11	1:B:545:PRO:HG3	2.00	0.41
1:B:566:TYR:C	1:B:567:GLN:HG2	2.41	0.41
1:B:611:MET:HE2	1:B:611:MET:HB2	1.80	0.41
1:B:621:TYR:N	1:B:621:TYR:CD1	2.88	0.41
1:B:94:ASP:C	1:B:96:GLY:N	2.74	0.41
1:A:471:VAL:C	1:A:473:GLY:H	2.24	0.41
1:B:158:ILE:HG21	1:B:507:PRO:HD3	2.02	0.41
1:B:189:SER:OG	1:B:190:ARG:N	2.53	0.41
1:B:348:PRO:HA	1:B:349:ALA:HA	1.57	0.41
1:B:249:ILE:HG22	1:B:250:ASP:N	2.35	0.41
1:B:406:TRP:NE1	1:B:541:PHE:HE2	1.95	0.41
1:B:649:GLY:O	1:B:650:LYS:HB2	2.20	0.41
1:B:323:ASN:O	1:B:359:TYR:HD2	2.04	0.41
1:B:109:VAL:HB	1:B:523:ARG:HH11	1.85	0.41
1:A:278:LYS:HD3	1:A:279:ASN:H	1.85	0.41
1:B:109:VAL:HG12	1:B:113:GLY:HA2	2.03	0.41
1:B:187:PRO:HA	1:B:188:ASP:O	2.21	0.41
1:A:182:ARG:HH21	1:A:190:ARG:CB	2.00	0.41
1:A:332:ASN:C	1:A:333:LYS:CG	2.81	0.41
1:A:361:PHE:HD2	1:A:388:PHE:HB3	1.85	0.41
1:A:468:GLU:OE1	1:A:470:TRP:NE1	2.54	0.41
1:A:486:ARG:C	1:A:489:ILE:HG22	2.39	0.41
1:A:586:ASN:OD1	1:A:588:THR:CB	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:LYS:CA	1:B:301:LYS:HE3	2.50	0.41
1:B:464:THR:O	1:B:465:ASN:CB	2.60	0.41
1:B:653:THR:HB	1:B:654:GLU:HG2	2.02	0.41
1:A:469:PRO:HD2	1:A:470:TRP:CZ3	2.56	0.41
1:B:474:GLN:CA	1:B:474:GLN:HE21	2.33	0.41
1:B:612:TYR:C	1:B:612:TYR:CD1	2.93	0.41
1:A:189:SER:HB2	1:A:190:ARG:H	1.69	0.41
1:A:375:ARG:HD2	1:A:375:ARG:C	2.41	0.41
1:A:491:LEU:HB3	1:A:492:PRO:HD3	2.02	0.41
1:B:375:ARG:HA	1:B:376:PRO:HD2	1.77	0.41
1:A:134:LYS:CE	1:A:134:LYS:N	2.83	0.41
1:A:191:VAL:O	1:A:192:ILE:CB	2.61	0.41
1:B:270:VAL:HB	1:B:299:VAL:HG22	2.02	0.41
1:A:268:ASN:O	1:A:293:ASP:HB2	2.21	0.41
1:A:304:ARG:HG2	1:A:304:ARG:H	1.58	0.41
1:A:368:ARG:HB2	1:A:382:ILE:HG21	2.03	0.41
1:B:253:ALA:H	1:B:290:ALA:H	1.68	0.41
1:B:318:VAL:O	1:B:382:ILE:HA	2.21	0.41
1:B:328:ASN:O	1:B:329:ASP:CB	2.69	0.41
1:B:429:ALA:HB3	1:B:453:TYR:CZ	2.56	0.41
1:B:547:LEU:HA	1:B:548:PRO:HD3	1.96	0.41
1:B:95:LYS:HG2	1:B:96:GLY:N	2.35	0.41
1:A:434:PHE:N	1:A:434:PHE:HD1	2.19	0.40
1:A:53:ASN:OD1	1:A:138:LYS:HG2	2.21	0.40
1:B:421:LEU:HA	1:B:421:LEU:HD23	1.82	0.40
1:B:590:ASN:ND2	1:B:590:ASN:C	2.72	0.40
1:B:94:ASP:O	1:B:95:LYS:HB3	2.21	0.40
1:A:249:ILE:CG2	1:A:250:ASP:N	2.83	0.40
1:B:179:GLN:HA	1:B:207:VAL:HG23	1.44	0.40
1:B:328:ASN:ND2	1:B:328:ASN:C	2.73	0.40
1:A:180:GLN:O	1:A:209:TRP:HD1	2.04	0.40
1:A:123:THR:CG2	1:A:355:TYR:HD2	2.33	0.40
1:B:176:LEU:HD11	1:B:498:LEU:HD22	2.03	0.40
1:B:70:VAL:CG2	1:B:71:THR:H	2.02	0.40
1:A:312:ALA:HB3	1:A:313:GLN:HA	1.32	0.40
1:A:308:LYS:HB3	1:A:315:VAL:HG11	2.02	0.40
1:B:454:PRO:HD3	1:B:509:MET:HE2	1.94	0.40
1:B:605:GLY:C	1:B:606:LYS:HG3	2.41	0.40
1:A:169:PRO:HG2	1:A:393:ARG:O	2.22	0.40
1:A:254:LYS:HG2	1:A:255:VAL:H	1.86	0.40
1:A:262:TYR:HE1	1:A:264:SER:OG	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:THR:HG23	1:B:419:LEU:N	2.36	0.40
1:B:470:TRP:O	1:B:472:PHE:N	2.55	0.40
1:B:75:LEU:N	1:B:75:LEU:CD2	2.84	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:GLU:OE1	1:A:653:THR:OG1[2_557]	0.80	1.40
1:A:521:SER:OG	1:B:377:GLU:CB[2_557]	1.36	0.84
1:A:554:GLU:CD	1:A:653:THR:OG1[2_557]	1.72	0.48
1:A:554:GLU:OE2	1:A:652:ASN:O[2_557]	1.90	0.30
1:A:554:GLU:OE1	1:A:653:THR:CB[2_557]	1.98	0.22
2:A:714:HOH:O	2:A:715:HOH:O[2_547]	2.14	0.06

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	582/697 (84%)	471 (81%)	66 (11%)	45 (8%)	1 1
1	B	581/697 (83%)	464 (80%)	64 (11%)	53 (9%)	1 1
All	All	1163/1394 (83%)	935 (80%)	130 (11%)	98 (8%)	1 1

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	TRP
1	A	87	ASP
1	A	90	ALA
1	A	93	VAL
1	A	112	ASP

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Mol	Chain	Res	Type
1	A	127	GLU
1	A	193	GLU
1	A	229	PRO
1	A	274	THR
1	A	275	ALA
1	A	276	ASP
1	A	278	LYS
1	A	437	ASN
1	A	467	LYS
1	A	506	MET
1	A	545	PRO
1	A	650	LYS
1	A	654	GLU
1	B	59	PRO
1	B	72	GLY
1	B	181	CYS
1	B	190	ARG
1	B	211	ASP
1	B	212	ILE
1	B	215	MET
1	B	226	LYS
1	B	263	LYS
1	B	268	ASN
1	B	271	TRP
1	B	323	ASN
1	B	327	ILE
1	B	353	LEU
1	B	355	TYR
1	B	434	PHE
1	B	435	LEU
1	B	437	ASN
1	B	542	ALA
1	B	546	ALA
1	B	564	ASP
1	B	565	LYS
1	B	593	ASP
1	B	595	LEU
1	B	663	ILE
1	A	52	ALA
1	A	53	ASN
1	A	56	LEU
1	A	85	ASN

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Mol	Chain	Res	Type
1	A	92	GLY
1	A	182	ARG
1	A	400	GLY
1	A	406	TRP
1	A	435	LEU
1	B	60	GLU
1	B	63	SER
1	B	79	LYS
1	B	460	ALA
1	B	468	GLU
1	B	523	ARG
1	B	555	LEU
1	B	568	ALA
1	B	639	LYS
1	B	657	ASP
1	A	48	THR
1	A	95	LYS
1	A	131	THR
1	A	187	PRO
1	A	189	SER
1	A	233	ALA
1	A	466	ASN
1	A	554	GLU
1	A	582	LYS
1	B	84	TRP
1	B	97	THR
1	B	184	SER
1	B	224	ASN
1	B	438	ALA
1	B	459	HIS
1	B	543	ASN
1	B	635	ARG
1	B	650	LYS
1	B	662	LYS
1	A	183	PHE
1	A	223	PHE
1	A	232	LYS
1	A	273	LYS
1	B	125	LYS
1	A	107	MET
1	A	192	ILE
1	A	336	PRO

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Mol	Chain	Res	Type
1	B	186	SER
1	B	471	VAL
1	B	544	GLN
1	B	547	LEU
1	B	556	SER
1	A	330	THR
1	B	436	PHE
1	A	431	ILE
1	B	539	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	464/579 (80%)	369 (80%)	95 (20%)	1 4
1	B	462/579 (80%)	368 (80%)	94 (20%)	1 4
All	All	926/1158 (80%)	737 (80%)	189 (20%)	1 4

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	56	LEU
1	A	76	ARG
1	A	77	ASN
1	A	79	LYS
1	A	80	THR
1	A	82	LYS
1	A	85	ASN
1	A	105	TRP
1	A	110	ARG
1	A	114	THR
1	A	122	THR
1	A	125	LYS
1	A	134	LYS

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Mol	Chain	Res	Type
1	A	137	LEU
1	A	170	MET
1	A	181	CYS
1	A	183	PHE
1	A	185	TYR
1	A	188	ASP
1	A	189	SER
1	A	190	ARG
1	A	200	LEU
1	A	201	LYS
1	A	206	ASP
1	A	212	ILE
1	A	216	ASP
1	A	223	PHE
1	A	238	LEU
1	A	254	LYS
1	A	260	PHE
1	A	261	VAL
1	A	262	TYR
1	A	270	VAL
1	A	278	LYS
1	A	279	ASN
1	A	283	ASP
1	A	298	LYS
1	A	300	ASN
1	A	304	ARG
1	A	306	LEU
1	A	308	LYS
1	A	319	TRP
1	A	333	LYS
1	A	334	THR
1	A	335	MET
1	A	337	GLU
1	A	355	TYR
1	A	362	LEU
1	A	368	ARG
1	A	377	GLU
1	A	382	ILE
1	A	385	ARG
1	A	404	SER
1	A	406	TRP
1	A	408	HIS

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Mol	Chain	Res	Type
1	A	409	LEU
1	A	410	LYS
1	A	411	MET
1	A	419	LEU
1	A	426	PHE
1	A	427	SER
1	A	434	PHE
1	A	436	PHE
1	A	437	ASN
1	A	446	TRP
1	A	461	CYS
1	A	465	ASN
1	A	466	ASN
1	A	467	LYS
1	A	480	SER
1	A	489	ILE
1	A	491	LEU
1	A	510	ARG
1	A	513	PHE
1	A	515	SER
1	A	526	GLU
1	A	538	ILE
1	A	543	ASN
1	A	547	LEU
1	A	549	LYS
1	A	553	LYS
1	A	555	LEU
1	A	584	ILE
1	A	589	GLU
1	A	592	LEU
1	A	604	GLN
1	A	608	SER
1	A	632	VAL
1	A	643	LYS
1	A	646	LYS
1	A	647	LYS
1	A	650	LYS
1	A	652	ASN
1	A	653	THR
1	B	63	SER
1	B	69	GLU
1	B	70	VAL

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Mol	Chain	Res	Type
1	B	71	THR
1	B	76	ARG
1	B	80	THR
1	B	81	ILE
1	B	86	THR
1	B	87	ASP
1	B	88	SER
1	B	94	ASP
1	B	95	LYS
1	B	103	HIS
1	B	105	TRP
1	B	119	LEU
1	B	123	THR
1	B	130	SER
1	B	152	GLU
1	B	155	GLN
1	B	164	LEU
1	B	192	ILE
1	B	207	VAL
1	B	210	MET
1	B	212	ILE
1	B	219	ARG
1	B	234	VAL
1	B	235	ASN
1	B	256	ASP
1	B	264	SER
1	B	271	TRP
1	B	273	LYS
1	B	274	THR
1	B	278	LYS
1	B	279	ASN
1	B	301	LYS
1	B	306	LEU
1	B	307	TYR
1	B	308	LYS
1	B	319	TRP
1	B	328	ASN
1	B	351	THR
1	B	354	GLN
1	B	355	TYR
1	B	357	ASN
1	B	368	ARG

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Mol	Chain	Res	Type
1	B	382	ILE
1	B	397	THR
1	B	399	THR
1	B	401	ASP
1	B	404	SER
1	B	410	LYS
1	B	426	PHE
1	B	427	SER
1	B	434	PHE
1	B	435	LEU
1	B	437	ASN
1	B	445	ASN
1	B	457	ARG
1	B	464	THR
1	B	465	ASN
1	B	472	PHE
1	B	474	GLN
1	B	475	LYS
1	B	489	ILE
1	B	491	LEU
1	B	515	SER
1	B	522	LEU
1	B	523	ARG
1	B	543	ASN
1	B	544	GLN
1	B	555	LEU
1	B	556	SER
1	B	564	ASP
1	B	565	LYS
1	B	566	TYR
1	B	569	LYS
1	B	571	LYS
1	B	590	ASN
1	B	592	LEU
1	B	610	ASN
1	B	620	SER
1	B	623	LYS
1	B	629	LEU
1	B	635	ARG
1	B	639	LYS
1	B	645	THR
1	B	648	THR

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Mol	Chain	Res	Type
1	B	652	ASN
1	B	653	THR
1	B	654	GLU
1	B	655	ASN
1	B	656	LYS
1	B	660	VAL
1	B	662	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	230	ASN
1	A	235	ASN
1	A	239	HIS
1	A	258	ASN
1	A	328	ASN
1	A	356	HIS
1	A	424	GLN
1	A	655	ASN
1	B	281	HIS
1	B	305	ASN
1	B	352	HIS
1	B	357	ASN
1	B	474	GLN
1	B	604	GLN
1	B	636	ASN
1	B	655	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	594:PRO	C	595:LEU	N	1.64
1	B	434:PHE	C	435:LEU	N	0.19

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, 95^{th} 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	588/697 (84%)	1.22	128 (21%)	1	1	10, 42, 120, 162	0
1	B	587/697 (84%)	1.18	116 (19%)	1	1	11, 43, 110, 166	0
All	All	1175/1394 (84%)	1.20	244 (20%)	1	1	10, 42, 117, 166	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	THR	11.0
1	A	260	PHE	8.6
1	B	637	GLY	8.3
1	B	58	VAL	8.0
1	B	211	ASP	7.2
1	A	93	VAL	6.9
1	A	271	TRP	6.7
1	B	274	THR	6.7
1	A	186	SER	6.5
1	B	259	TYR	6.5
1	A	273	LYS	6.3
1	A	544	GLN	6.1
1	A	312	ALA	5.8
1	A	48	THR	5.7
1	A	91	TYR	5.6
1	B	281	HIS	5.6
1	B	437	ASN	5.6
1	A	54	ALA	5.5
1	A	435	LEU	5.5
1	B	461	CYS	5.4
1	A	183	PHE	5.4
1	A	222	THR	5.3
1	B	222	THR	5.1
1	A	50	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	228	PHE	5.1
1	B	277	GLY	5.1
1	A	47	LEU	5.0
1	A	275	ALA	5.0
1	B	619	TRP	5.0
1	A	233	ALA	4.9
1	B	288	ALA	4.9
1	B	376	PRO	4.9
1	B	132	ASP	4.8
1	B	348	PRO	4.7
1	A	461	CYS	4.7
1	A	290	ALA	4.7
1	B	268	ASN	4.6
1	B	76	ARG	4.6
1	A	313	GLN	4.5
1	A	277	GLY	4.5
1	B	464	THR	4.5
1	B	462	ALA	4.4
1	B	270	VAL	4.4
1	B	658	MET	4.4
1	A	187	PRO	4.3
1	A	276	ASP	4.3
1	A	284	ALA	4.3
1	B	215	MET	4.3
1	A	272	VAL	4.3
1	A	231	PRO	4.2
1	B	621	TYR	4.2
1	B	135	ILE	4.2
1	A	331	PRO	4.1
1	A	89	GLY	4.1
1	A	131	THR	4.0
1	B	210	MET	4.0
1	A	465	ASN	4.0
1	A	291	PHE	4.0
1	B	260	PHE	4.0
1	A	92	GLY	3.9
1	B	212	ILE	3.9
1	B	432	GLY	3.8
1	A	56	LEU	3.7
1	A	434	PHE	3.7
1	A	86	THR	3.7
1	B	131	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	335	MET	3.7
1	B	638	ASP	3.7
1	B	636	ASN	3.7
1	A	261	VAL	3.7
1	B	566	TYR	3.7
1	A	336	PRO	3.7
1	B	228	PHE	3.6
1	B	77	ASN	3.6
1	A	188	ASP	3.6
1	B	186	SER	3.6
1	A	464	THR	3.6
1	A	281	HIS	3.6
1	A	292	PRO	3.6
1	B	267	GLU	3.5
1	A	185	TYR	3.5
1	A	232	LYS	3.5
1	B	141	GLY	3.5
1	B	620	SER	3.4
1	B	266	THR	3.4
1	A	471	VAL	3.3
1	A	52	ALA	3.3
1	B	258	ASN	3.3
1	B	653	THR	3.3
1	A	55	SER	3.3
1	A	110	ARG	3.3
1	B	234	VAL	3.2
1	A	191	VAL	3.2
1	B	283	ASP	3.2
1	B	93	VAL	3.1
1	A	311	LEU	3.1
1	A	264	SER	3.1
1	A	404	SER	3.1
1	A	148	ILE	3.1
1	B	278	LYS	3.1
1	A	112	ASP	3.1
1	B	209	TRP	3.0
1	B	216	ASP	3.0
1	A	190	ARG	3.0
1	A	296	SER	3.0
1	A	58	VAL	3.0
1	B	406	TRP	3.0
1	B	70	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	604	GLN	3.0
1	A	90	ALA	3.0
1	B	289	ALA	3.0
1	A	618	GLY	3.0
1	B	355	TYR	2.9
1	B	404	SER	2.9
1	B	78	GLY	2.9
1	B	541	PHE	2.9
1	A	376	PRO	2.9
1	A	554	GLU	2.9
1	B	182	ARG	2.9
1	A	189	SER	2.9
1	B	126	ALA	2.9
1	A	265	GLY	2.8
1	B	272	VAL	2.8
1	A	97	THR	2.8
1	A	438	ALA	2.8
1	A	591	SER	2.8
1	B	595	LEU	2.8
1	A	399	THR	2.8
1	A	96	GLY	2.8
1	B	350	GLY	2.8
1	A	545	PRO	2.8
1	B	460	ALA	2.8
1	B	256	ASP	2.7
1	A	405	CYS	2.7
1	A	467	LYS	2.7
1	A	287	GLY	2.7
1	B	224	ASN	2.7
1	B	287	GLY	2.7
1	A	53	ASN	2.7
1	B	307	TYR	2.7
1	A	289	ALA	2.7
1	B	119	LEU	2.7
1	B	542	ALA	2.7
1	A	234	VAL	2.7
1	A	280	PHE	2.7
1	A	259	TYR	2.7
1	A	51	LYS	2.7
1	B	431	ILE	2.7
1	B	467	LYS	2.7
1	B	142	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	185	TYR	2.6
1	B	663	ILE	2.6
1	A	365	LYS	2.6
1	B	282	GLY	2.6
1	B	351	THR	2.6
1	B	472	PHE	2.6
1	A	279	ASN	2.6
1	A	310	PHE	2.6
1	A	406	TRP	2.5
1	A	338	ASP	2.5
1	A	223	PHE	2.5
1	B	81	ILE	2.5
1	A	267	GLU	2.5
1	A	253	ALA	2.5
1	B	433	GLY	2.5
1	A	219	ARG	2.5
1	B	91	TYR	2.5
1	A	285	TRP	2.5
1	A	268	ASN	2.5
1	A	621	TYR	2.4
1	B	347	LEU	2.4
1	B	84	TRP	2.4
1	B	227	SER	2.4
1	A	437	ASN	2.4
1	B	194	ILE	2.4
1	A	590	ASN	2.4
1	B	217	GLY	2.4
1	A	295	THR	2.4
1	A	215	MET	2.4
1	A	218	TYR	2.4
1	A	334	THR	2.4
1	A	88	SER	2.4
1	B	180	GLN	2.4
1	A	212	ILE	2.4
1	B	657	ASP	2.4
1	A	282	GLY	2.4
1	A	506	MET	2.4
1	A	137	LEU	2.4
1	A	288	ALA	2.4
1	B	153	SER	2.4
1	A	144	PHE	2.3
1	A	477	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	284	ALA	2.3
1	B	540	ALA	2.3
1	B	463	GLY	2.3
1	B	187	PRO	2.3
1	A	57	THR	2.2
1	B	62	THR	2.2
1	B	551	ILE	2.2
1	B	184	SER	2.2
1	A	442	LEU	2.2
1	A	623	LYS	2.2
1	A	355	TYR	2.2
1	B	96	GLY	2.2
1	A	543	ASN	2.2
1	B	435	LEU	2.2
1	B	229	PRO	2.2
1	A	636	ASN	2.2
1	B	207	VAL	2.2
1	B	442	LEU	2.2
1	B	459	HIS	2.2
1	A	307	TYR	2.2
1	B	660	VAL	2.2
1	A	403	GLY	2.2
1	B	247	TRP	2.2
1	B	223	PHE	2.2
1	A	505	GLY	2.1
1	B	346	LYS	2.1
1	A	71	THR	2.1
1	A	551	ILE	2.1
1	B	218	TYR	2.1
1	A	317	GLY	2.1
1	A	337	GLU	2.1
1	A	123	THR	2.1
1	A	466	ASN	2.1
1	A	266	THR	2.1
1	B	430	ASP	2.1
1	B	356	HIS	2.1
1	B	264	SER	2.1
1	B	405	CYS	2.1
1	B	253	ALA	2.1
1	B	275	ALA	2.1
1	A	329	ASP	2.1
1	A	306	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	431	ILE	2.1
1	A	330	THR	2.1
1	B	189	SER	2.0
1	A	225	PRO	2.0
1	B	594	PRO	2.0
1	B	205	CYS	2.0
1	B	605	GLY	2.0
1	B	273	LYS	2.0
1	A	211	ASP	2.0
1	B	294	PHE	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.