



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:50 AM UTC

PDB ID : 2ZIX / pdb_00002zix
Title : Crystal structure of the Mus81-Eme1 complex
Authors : Chang, J.H.; Kim, J.J.; Choi, J.M.; Lee, J.H.; Cho, Y.
Deposited on : 2008-02-25
Resolution : 3.50 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

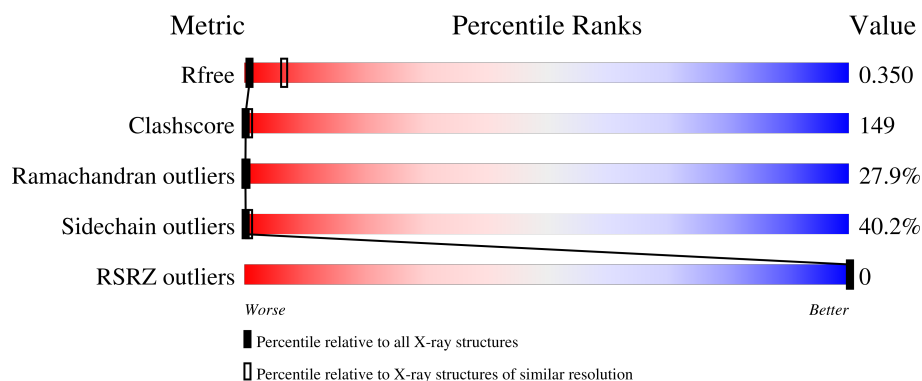
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	307	
2	B	341	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4154 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 Crossover junction endonuclease MUS81.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2136	1340	397	391	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	245	MET	-	initiating methionine	UNP Q96NY9

- Molecule 2 is a protein called Crossover junction endonuclease EME1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	0	0	0
			2018	1269	354	383	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	230	MET	-	expression tag	UNP Q96AY2
B	231	GLY	-	expression tag	UNP Q96AY2
B	232	SER	-	expression tag	UNP Q96AY2
B	233	SER	-	expression tag	UNP Q96AY2
B	234	HIS	-	expression tag	UNP Q96AY2
B	235	HIS	-	expression tag	UNP Q96AY2
B	236	HIS	-	expression tag	UNP Q96AY2
B	237	HIS	-	expression tag	UNP Q96AY2
B	238	HIS	-	expression tag	UNP Q96AY2
B	239	HIS	-	expression tag	UNP Q96AY2
B	240	SER	-	expression tag	UNP Q96AY2
B	241	GLN	-	expression tag	UNP Q96AY2
B	242	ASP	-	expression tag	UNP Q96AY2
B	243	PRO	-	expression tag	UNP Q96AY2
B	244	ASN	-	expression tag	UNP Q96AY2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	245	SER	-	expression tag	UNP Q96AY2

R533	R534	G535	E536	GLY	VAL	THR	SER	T541	S542	R543	R544	I545	G546	P547	E548	L549	S550	R551	R552	I553	Y554	L555	Q556	M557	T558	T559	L560	Q561	P562	H563	L564	S565	L566	D567	S568	ALA	ASP
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	85.81Å 85.81Å 176.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.50 20.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	92.7 (20.00-3.50) 92.7 (20.00-3.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.69 (at 3.52Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.285 , 0.346 0.283 , 0.350	Depositor DCC
R_{free} test set	441 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.06 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.188 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4154	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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, 0.333 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	0.74	1/2168 (0.0%)	1.36	20/2923 (0.7%)
2	B	0.74	2/2043 (0.1%)	1.31	27/2765 (1.0%)
All	All	0.74	3/4211 (0.1%)	1.34	47/5688 (0.8%)

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	1	6
2	B	0	9
All	All	1	15

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	484	ARG	CG-CD	7.76	1.75	1.52
2	B	474	ALA	C-O	6.63	1.32	1.24
1	A	380	PRO	CG-CD	5.07	1.68	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	ASP	N-CA-C	-20.72	87.44	113.55
1	A	548	GLY	CA-C-N	13.66	136.91	119.84
1	A	548	GLY	C-N-CA	13.66	136.91	119.84
1	A	543	LEU	N-CA-C	-9.92	103.31	114.62
2	B	504	TYR	CA-C-N	8.98	129.56	119.32
2	B	504	TYR	C-N-CA	8.98	129.56	119.32
1	A	380	PRO	CB-CA-C	8.13	124.98	111.56
2	B	257	ASP	CA-C-N	8.12	129.99	119.84
2	B	257	ASP	C-N-CA	8.12	129.99	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	PRO	N-CA-C	7.99	128.94	112.47
1	A	424	GLN	N-CA-C	6.68	125.03	110.80
2	B	290	SER	N-CA-C	6.50	114.99	108.75
2	B	282	ILE	N-CA-C	6.40	115.56	106.53
2	B	255	VAL	N-CA-C	6.31	117.92	108.96
2	B	307	VAL	N-CA-C	6.26	117.04	107.77
2	B	492	VAL	N-CA-C	6.23	116.99	107.77
2	B	463	SER	N-CA-C	6.23	118.32	108.79
2	B	409	GLU	N-CA-C	-6.22	105.47	114.12
2	B	313	LEU	N-CA-C	6.09	118.55	108.99
1	A	276	GLY	N-CA-C	-6.01	107.73	114.40
2	B	451	LEU	N-CA-C	5.98	119.41	110.14
1	A	271	LEU	N-CA-C	5.95	117.31	107.20
1	A	491	ALA	N-CA-C	5.87	123.31	110.80
1	A	328	LEU	N-CA-C	5.82	119.01	109.76
2	B	534	ARG	N-CA-C	5.66	117.62	108.34
2	B	292	THR	N-CA-C	5.65	117.77	109.24
1	A	377	LEU	N-CA-C	5.63	117.61	108.26
2	B	436	THR	N-CA-C	-5.57	107.73	114.75
2	B	522	GLU	N-CA-C	-5.57	98.94	110.80
2	B	350	ILE	N-CA-C	-5.55	107.38	113.43
2	B	476	ARG	N-CA-C	5.54	117.53	108.55
1	A	301	ARG	N-CA-C	5.49	117.61	108.99
1	A	453	LEU	N-CA-C	5.45	122.42	110.80
1	A	482	VAL	CB-CA-C	-5.43	102.38	111.29
2	B	438	ALA	N-CA-C	-5.37	105.32	111.07
1	A	530	ARG	N-CA-C	5.33	117.18	108.76
1	A	330	HIS	N-CA-C	5.27	118.17	109.85
2	B	513	ALA	N-CA-C	-5.24	106.15	112.54
2	B	561	GLN	CA-C-N	5.15	126.28	119.84
2	B	561	GLN	C-N-CA	5.15	126.28	119.84
2	B	309	GLU	CA-C-N	5.08	126.18	119.84
2	B	309	GLU	C-N-CA	5.08	126.18	119.84
2	B	551	ARG	N-CA-C	-5.07	105.45	111.69
1	A	505	ALA	N-CA-C	-5.06	105.84	111.36
2	B	530	ILE	CB-CA-C	-5.03	103.04	111.29
1	A	491	ALA	CA-C-N	5.01	130.72	121.70
1	A	491	ALA	C-N-CA	5.01	130.72	121.70

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
1	A	380	PRO	CA

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	ARG	Peptide
1	A	338	ASP	Peptide
1	A	378	SER	Peptide
1	A	379	LEU	Peptide
1	A	431	ARG	Peptide
1	A	453	LEU	Peptide
2	B	272	ALA	Peptide
2	B	276	MET	Peptide
2	B	278	CYS	Peptide
2	B	351	THR	Peptide
2	B	430	LYS	Peptide
2	B	450	LYS	Peptide
2	B	461	LEU	Peptide
2	B	463	SER	Peptide
2	B	560	LEU	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	2136	0	2188	694	1
2	B	2018	0	2033	648	1
All	All	4154	0	4221	1249	2

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 149.

All (1249) 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)
2:B:484:ARG:CG	2:B:484:ARG:CD	1.75	1.64
1:A:491:ALA:CB	1:A:492:ALA:HB2	1.30	1.59
1:A:414:LEU:HD21	2:B:413:VAL:CG2	1.41	1.47
1:A:414:LEU:CD2	2:B:413:VAL:HG21	1.43	1.45
1:A:491:ALA:HB3	1:A:492:ALA:CB	1.44	1.44
1:A:272:CYS:HB2	1:A:311:VAL:CG2	1.51	1.37
2:B:253:ILE:HG13	2:B:279:ARG:O	1.21	1.28
1:A:272:CYS:CB	1:A:311:VAL:HG21	1.66	1.25
1:A:497:TYR:CD1	1:A:503:LEU:HD13	1.74	1.23
1:A:308:PHE:O	1:A:309:VAL:HG23	1.39	1.23
1:A:536:LEU:O	1:A:540:LEU:HB2	1.35	1.22
1:A:312:ALA:N	1:A:325:GLU:OE1	1.69	1.21
2:B:290:SER:O	2:B:291:VAL:HG13	1.38	1.19
1:A:296:VAL:CG1	1:A:416:THR:HG21	1.73	1.18
1:A:336:ARG:CB	1:A:339:ASP:HB2	1.75	1.17
1:A:532:LEU:HD13	1:A:533:GLY:H	1.00	1.15
1:A:536:LEU:O	1:A:540:LEU:CB	1.95	1.13
1:A:499:THR:HG21	2:B:560:LEU:HG	1.23	1.12
2:B:268:GLN:HG3	2:B:432:LEU:HB3	1.29	1.12
1:A:507:TYR:HE1	1:A:541:SER:OG	1.31	1.11
2:B:544:ARG:HA	2:B:544:ARG:NE	1.59	1.11
1:A:332:VAL:HA	1:A:365:VAL:O	1.51	1.11
1:A:305:VAL:HG22	1:A:356:LEU:HB2	1.32	1.10
1:A:291:LEU:HD13	1:A:412:LEU:HD13	1.21	1.10
2:B:263:MET:HE1	2:B:429:TRP:CZ2	1.86	1.10
2:B:483:ARG:HA	2:B:486:ILE:HG13	1.32	1.10
2:B:506:SER:HB3	2:B:509:LEU:HG	1.31	1.10
1:A:291:LEU:HD22	1:A:412:LEU:CD2	1.82	1.09
1:A:359:CYS:HB2	1:A:361:LEU:HD22	1.30	1.09
2:B:492:VAL:HG13	2:B:497:ALA:CB	1.79	1.09
1:A:493:LEU:HD21	1:A:523:ILE:HG21	1.34	1.08
1:A:532:LEU:CD1	1:A:536:LEU:HD13	1.84	1.08
2:B:249:LEU:HA	2:B:445:GLU:OE1	1.53	1.08
1:A:369:GLU:O	1:A:371:HIS:CE1	2.06	1.08
1:A:492:ALA:HB3	1:A:493:LEU:HD12	1.29	1.08
1:A:336:ARG:HD2	1:A:338:ASP:HB3	1.35	1.08
1:A:369:GLU:HG3	1:A:370:GLU:N	1.51	1.08
1:A:402:THR:CB	1:A:408:SER:HA	1.83	1.08
2:B:253:ILE:CG1	2:B:279:ARG:O	2.02	1.08
1:A:291:LEU:CD2	1:A:412:LEU:HD22	1.83	1.07
1:A:334:ARG:HE	1:A:367:LEU:HD22	1.02	1.07
1:A:296:VAL:HG13	1:A:416:THR:HG21	1.25	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:VAL:CG2	1:A:365:VAL:HB	1.84	1.06
1:A:369:GLU:CG	1:A:370:GLU:H	1.66	1.06
1:A:477:ARG:HG2	1:A:477:ARG:HH11	0.99	1.06
1:A:402:THR:HB	1:A:408:SER:CA	1.84	1.06
1:A:530:ARG:HG2	1:A:530:ARG:HH21	0.95	1.05
1:A:332:VAL:HG22	1:A:365:VAL:HB	1.06	1.05
1:A:540:LEU:O	1:A:543:LEU:HD21	1.56	1.05
1:A:418:GLY:O	1:A:421:ARG:NH2	1.89	1.05
1:A:329:ASP:HB2	1:A:362:GLU:OE1	1.57	1.04
1:A:404:ASP:O	1:A:408:SER:HB3	1.57	1.04
1:A:310:TRP:O	1:A:327:VAL:HB	1.55	1.04
2:B:511:VAL:HA	2:B:514:TYR:HB2	1.37	1.03
1:A:263:ARG:NH1	1:A:264:PRO:HD2	1.73	1.03
2:B:257:ASP:CB	2:B:288:PRO:HB3	1.87	1.03
2:B:551:ARG:HH12	2:B:566:LEU:HB3	1.22	1.03
1:A:334:ARG:HG3	1:A:367:LEU:HB2	1.40	1.03
1:A:364:ARG:O	1:A:397:PHE:HA	1.57	1.03
1:A:331:ILE:HG22	1:A:361:LEU:HB3	1.38	1.03
1:A:458:ASP:O	1:A:462:GLY:CA	2.07	1.02
1:A:532:LEU:HD11	1:A:536:LEU:CD1	1.87	1.02
1:A:419:LEU:HD12	1:A:422:LEU:CD2	1.90	1.02
1:A:305:VAL:HG13	1:A:356:LEU:HD22	1.39	1.02
2:B:316:LEU:CB	2:B:363:ILE:HG22	1.90	1.02
2:B:435:PHE:CD2	2:B:435:PHE:O	2.13	1.02
2:B:531:GLN:NE2	2:B:534:ARG:HG3	1.74	1.02
1:A:332:VAL:HG22	1:A:365:VAL:CB	1.89	1.01
1:A:264:PRO:HA	1:A:427:THR:HA	1.43	1.01
1:A:383:THR:HG22	1:A:386:GLN:NE2	1.75	1.00
2:B:257:ASP:HB2	2:B:288:PRO:HB3	1.38	1.00
2:B:305:ASP:O	2:B:306:TRP:CE3	2.13	1.00
1:A:523:ILE:HG23	1:A:525:CYS:SG	2.00	1.00
1:A:532:LEU:HD13	1:A:533:GLY:N	1.73	1.00
2:B:290:SER:HA	2:B:313:LEU:O	1.60	1.00
1:A:326:LEU:CD2	1:A:428:LEU:HD11	1.90	1.00
1:A:480:MET:HA	1:A:485:VAL:CG1	1.92	1.00
2:B:316:LEU:HB2	2:B:363:ILE:HG22	1.43	0.99
2:B:271:GLY:N	2:B:274:GLN:HB3	1.75	0.99
1:A:497:TYR:CB	1:A:503:LEU:HD22	1.93	0.99
2:B:265:GLY:O	2:B:269:LEU:N	1.96	0.99
2:B:260:LEU:HD13	2:B:289:CYS:HA	1.44	0.99
1:A:336:ARG:HB3	1:A:339:ASP:CB	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:SER:O	1:A:499:THR:HB	1.58	0.98
2:B:493:SER:O	2:B:496:MET:N	1.95	0.98
1:A:336:ARG:HB3	1:A:339:ASP:HB2	1.00	0.98
1:A:308:PHE:O	1:A:309:VAL:CG2	2.12	0.98
1:A:480:MET:HE1	2:B:460:CYS:O	1.63	0.97
2:B:524:GLN:HG2	2:B:551:ARG:HB2	1.44	0.97
1:A:287:LEU:HD13	1:A:405:ILE:HG22	1.47	0.97
2:B:280:CYS:O	2:B:281:VAL:HG23	1.65	0.97
2:B:273:LEU:HD13	2:B:437:CYS:SG	2.05	0.96
1:A:329:ASP:CB	1:A:362:GLU:OE1	2.11	0.96
1:A:541:SER:HA	1:A:544:TYR:HB2	1.46	0.96
1:A:369:GLU:HG3	1:A:370:GLU:H	0.81	0.96
2:B:247:GLU:OE1	2:B:250:LYS:NZ	1.97	0.96
2:B:287:VAL:HG21	2:B:350:ILE:HG12	1.47	0.95
1:A:341:CYS:O	1:A:343:SER:N	1.99	0.95
2:B:542:SER:O	2:B:543:ARG:HG3	1.66	0.95
2:B:492:VAL:HG13	2:B:497:ALA:HB2	1.48	0.95
1:A:262:LEU:O	1:A:263:ARG:HB3	1.65	0.94
1:A:419:LEU:HD12	1:A:422:LEU:HD22	1.48	0.94
1:A:369:GLU:HA	1:A:402:THR:O	1.67	0.94
1:A:326:LEU:HD23	1:A:428:LEU:HD11	1.49	0.94
1:A:423:TYR:HB2	1:A:449:PRO:HB3	1.47	0.94
2:B:365:ASP:OD1	2:B:366:GLN:N	2.01	0.94
1:A:369:GLU:CG	1:A:370:GLU:N	2.25	0.94
1:A:530:ARG:HG2	1:A:530:ARG:NH2	1.73	0.94
2:B:544:ARG:HA	2:B:544:ARG:CZ	1.98	0.94
1:A:463:ALA:O	1:A:465:LYS:N	1.99	0.93
2:B:416:GLN:HE21	2:B:416:GLN:N	1.67	0.93
1:A:402:THR:HB	1:A:408:SER:HA	0.94	0.93
1:A:495:ASP:O	1:A:498:SER:OG	1.85	0.93
1:A:383:THR:HG22	1:A:386:GLN:HE22	1.27	0.93
2:B:354:THR:HG23	2:B:357:LYS:HB2	1.51	0.93
2:B:416:GLN:C	2:B:418:HIS:H	1.76	0.93
1:A:421:ARG:H	1:A:421:ARG:HE	0.98	0.93
1:A:399:VAL:O	1:A:400:LYS:HG2	1.69	0.93
1:A:328:LEU:O	1:A:330:HIS:N	2.02	0.93
1:A:480:MET:HA	1:A:485:VAL:HG11	1.50	0.92
2:B:273:LEU:CD1	2:B:437:CYS:SG	2.58	0.92
2:B:314:VAL:HG22	2:B:361:LEU:HD13	1.51	0.92
2:B:435:PHE:O	2:B:435:PHE:HD2	1.51	0.92
2:B:316:LEU:O	2:B:363:ILE:HA	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:TYR:HD1	1:A:503:LEU:HD13	1.22	0.92
1:A:538:ARG:HH22	2:B:473:LEU:C	1.78	0.91
1:A:421:ARG:HE	1:A:421:ARG:N	1.67	0.91
1:A:293:ARG:HG2	1:A:293:ARG:HH11	1.36	0.91
1:A:307:ASP:OD2	1:A:334:ARG:N	2.04	0.91
1:A:477:ARG:HG2	1:A:477:ARG:NH1	1.77	0.91
2:B:555:LEU:C	2:B:557:MET:H	1.79	0.91
1:A:307:ASP:OD2	1:A:333:GLU:HA	1.71	0.91
1:A:395:ASP:HB2	1:A:397:PHE:CD1	2.06	0.91
2:B:255:VAL:HG13	2:B:281:VAL:O	1.71	0.91
1:A:312:ALA:O	1:A:313:GLN:HG2	1.71	0.91
2:B:433:ALA:C	2:B:435:PHE:H	1.79	0.90
1:A:331:ILE:CG2	1:A:361:LEU:HB3	2.01	0.90
1:A:551:THR:OG1	2:B:476:ARG:HG3	1.72	0.90
2:B:268:GLN:HG3	2:B:432:LEU:CB	2.02	0.90
1:A:391:THR:HA	1:A:395:ASP:OD2	1.71	0.89
1:A:395:ASP:CB	1:A:397:PHE:CE1	2.55	0.89
2:B:255:VAL:HG13	2:B:281:VAL:C	1.98	0.89
2:B:263:MET:HE1	2:B:429:TRP:CH2	2.06	0.89
2:B:518:PHE:O	2:B:523:ARG:HG3	1.72	0.89
1:A:268:ARG:NH1	1:A:314:GLU:O	2.06	0.89
1:A:285:PRO:HB2	1:A:288:LEU:HB2	1.53	0.88
2:B:312:VAL:O	2:B:360:SER:N	2.05	0.88
1:A:543:LEU:HG	1:A:544:TYR:N	1.89	0.88
2:B:482:TRP:NE1	2:B:504:TYR:O	2.07	0.88
1:A:422:LEU:HD11	2:B:418:HIS:CE1	2.09	0.88
2:B:264:GLU:O	2:B:429:TRP:CZ2	2.27	0.88
2:B:433:ALA:HA	2:B:436:THR:HB	1.55	0.87
2:B:492:VAL:HG13	2:B:497:ALA:HB3	1.53	0.87
1:A:334:ARG:NE	1:A:367:LEU:HD22	1.88	0.87
1:A:420:GLN:H	1:A:421:ARG:HH21	1.21	0.87
1:A:491:ALA:CB	1:A:492:ALA:CB	2.21	0.87
2:B:491:ARG:H	2:B:491:ARG:HD2	1.38	0.87
1:A:532:LEU:HD11	1:A:536:LEU:HD13	0.92	0.87
2:B:264:GLU:O	2:B:429:TRP:HZ2	1.57	0.87
2:B:511:VAL:HA	2:B:514:TYR:CB	2.04	0.87
1:A:270:LEU:HD12	1:A:271:LEU:H	1.37	0.86
1:A:477:ARG:HG3	2:B:460:CYS:SG	2.15	0.86
2:B:509:LEU:O	2:B:512:GLN:N	2.08	0.86
1:A:413:ALA:HA	1:A:417:ARG:NH1	1.90	0.86
1:A:518:THR:OG1	1:A:521:SER:OG	1.92	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ARG:O	1:A:420:GLN:HB2	1.76	0.86
1:A:341:CYS:C	1:A:343:SER:H	1.79	0.86
1:A:353:LYS:NZ	1:A:357:LYS:NZ	2.24	0.85
1:A:456:PHE:HD1	1:A:457:SER:N	1.75	0.85
1:A:543:LEU:HG	1:A:544:TYR:H	1.40	0.85
2:B:493:SER:O	2:B:496:MET:HG3	1.75	0.85
1:A:326:LEU:HD22	1:A:428:LEU:HD21	1.59	0.85
2:B:313:LEU:HB2	2:B:360:SER:HB2	1.59	0.85
2:B:483:ARG:O	2:B:486:ILE:N	2.08	0.85
2:B:257:ASP:OD2	2:B:285:GLN:HG2	1.76	0.84
2:B:555:LEU:O	2:B:557:MET:N	2.10	0.84
1:A:413:ALA:C	1:A:415:LEU:H	1.83	0.84
2:B:405:ARG:C	2:B:407:ASP:H	1.86	0.84
1:A:336:ARG:HG3	1:A:369:GLU:HG2	1.59	0.84
2:B:461:LEU:O	2:B:462:GLU:HG2	1.77	0.84
2:B:483:ARG:HD2	2:B:483:ARG:C	2.03	0.84
2:B:305:ASP:O	2:B:306:TRP:HE3	1.59	0.84
2:B:365:ASP:O	2:B:366:GLN:HB2	1.76	0.84
2:B:250:LYS:O	2:B:251:HIS:HB2	1.78	0.84
1:A:261:GLU:OE1	1:A:428:LEU:O	1.95	0.83
1:A:360:GLY:H	1:A:459:PHE:HE2	1.23	0.83
1:A:336:ARG:HD2	1:A:338:ASP:CB	2.08	0.83
1:A:476:ALA:HA	1:A:479:LEU:HB2	1.59	0.83
2:B:324:MET:SD	2:B:342:THR:HA	2.18	0.82
1:A:413:ALA:HA	1:A:417:ARG:HH12	1.42	0.82
2:B:287:VAL:HB	2:B:350:ILE:HD11	1.61	0.82
2:B:289:CYS:O	2:B:314:VAL:HA	1.79	0.82
1:A:530:ARG:HH21	1:A:530:ARG:CG	1.87	0.82
1:A:540:LEU:O	1:A:543:LEU:CD2	2.28	0.82
1:A:296:VAL:HG13	1:A:416:THR:CG2	2.08	0.82
1:A:270:LEU:CD1	1:A:271:LEU:H	1.93	0.81
1:A:337:LEU:HD22	1:A:376:ASN:ND2	1.95	0.81
1:A:514:LYS:H	1:A:514:LYS:CD	1.93	0.81
2:B:287:VAL:HG21	2:B:350:ILE:CG1	2.09	0.81
2:B:514:TYR:OH	2:B:553:ILE:HG22	1.80	0.81
1:A:284:ARG:N	1:A:286:GLU:HG2	1.94	0.81
1:A:272:CYS:CB	1:A:311:VAL:CG2	2.41	0.81
2:B:416:GLN:NE2	2:B:416:GLN:H	1.77	0.81
1:A:263:ARG:HH11	1:A:264:PRO:HD2	1.45	0.81
1:A:264:PRO:CA	1:A:427:THR:HA	2.11	0.81
1:A:419:LEU:HD12	1:A:422:LEU:HD23	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:LEU:HD12	2:B:507:PRO:HG2	1.60	0.81
2:B:420:GLU:O	2:B:421:ALA:HB3	1.81	0.81
2:B:290:SER:O	2:B:291:VAL:CG1	2.27	0.80
1:A:390:ASN:O	1:A:392:GLN:N	2.14	0.80
2:B:544:ARG:NE	2:B:544:ARG:CA	2.38	0.80
2:B:531:GLN:NE2	2:B:534:ARG:CG	2.45	0.80
2:B:413:VAL:HG23	2:B:413:VAL:O	1.81	0.80
1:A:491:ALA:HB1	1:A:492:ALA:HB2	1.57	0.80
1:A:344:ILE:O	1:A:344:ILE:HG13	1.80	0.80
1:A:478:GLN:HA	1:A:481:GLN:OE1	1.82	0.80
1:A:458:ASP:O	1:A:462:GLY:N	2.15	0.80
1:A:290:GLU:OE2	1:A:291:LEU:HD23	1.82	0.80
1:A:371:HIS:HE1	1:A:403:ALA:HA	1.46	0.80
1:A:497:TYR:HB3	1:A:503:LEU:HB2	1.64	0.79
1:A:499:THR:CG2	2:B:560:LEU:HG	2.09	0.79
1:A:508:ASP:OD2	1:A:509:ALA:N	2.14	0.79
1:A:404:ASP:HB2	1:A:406:LYS:H	1.47	0.79
1:A:455:THR:OG1	1:A:456:PHE:N	2.13	0.79
2:B:312:VAL:H	2:B:359:LEU:HA	1.44	0.79
1:A:353:LYS:HZ1	1:A:357:LYS:NZ	1.80	0.79
1:A:507:TYR:CE1	1:A:544:TYR:HB3	2.17	0.79
1:A:456:PHE:HD1	1:A:457:SER:H	1.30	0.79
1:A:523:ILE:CG2	1:A:525:CYS:SG	2.70	0.79
2:B:432:LEU:HD23	2:B:436:THR:HG21	1.65	0.79
1:A:270:LEU:HD23	1:A:311:VAL:O	1.83	0.79
2:B:467:GLY:HA2	2:B:484:ARG:NH2	1.97	0.79
1:A:366:TYR:CD1	1:A:391:THR:HG21	2.18	0.79
1:A:460:ASN:CG	1:A:461:ALA:H	1.91	0.79
2:B:351:THR:HA	2:B:354:THR:O	1.83	0.78
1:A:393:VAL:HG11	2:B:443:VAL:HG22	1.63	0.78
1:A:414:LEU:HD21	2:B:413:VAL:CB	2.11	0.78
1:A:512:THR:O	1:A:515:GLU:HG2	1.83	0.78
2:B:314:VAL:CG2	2:B:361:LEU:CD1	2.61	0.78
1:A:480:MET:HA	1:A:485:VAL:HG12	1.65	0.78
2:B:316:LEU:HB3	2:B:363:ILE:HG22	1.64	0.78
2:B:451:LEU:CD2	2:B:454:GLU:OE2	2.31	0.78
2:B:492:VAL:CG1	2:B:497:ALA:CB	2.61	0.78
2:B:255:VAL:HG12	2:B:256:LEU:H	1.49	0.78
2:B:317:ARG:HG3	2:B:364:VAL:HG23	1.65	0.78
1:A:523:ILE:HG23	1:A:524:LYS:H	1.49	0.77
1:A:326:LEU:HD22	1:A:428:LEU:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:272:ALA:O	2:B:437:CYS:SG	2.43	0.77
1:A:535:ALA:O	1:A:538:ARG:N	2.18	0.77
2:B:256:LEU:CD1	2:B:282:ILE:HG23	2.15	0.77
2:B:486:ILE:HG22	2:B:489:LEU:HD22	1.64	0.77
1:A:307:ASP:OD2	1:A:333:GLU:CA	2.33	0.77
1:A:477:ARG:HB3	2:B:488:GLN:HG3	1.64	0.77
2:B:324:MET:HE1	2:B:346:PHE:HB2	1.67	0.77
2:B:416:GLN:HE21	2:B:416:GLN:H	1.29	0.77
1:A:260:LEU:HD22	1:A:455:THR:HG21	1.65	0.76
1:A:458:ASP:O	1:A:462:GLY:HA3	1.85	0.76
2:B:289:CYS:O	2:B:314:VAL:HB	1.84	0.76
2:B:359:LEU:CD2	2:B:421:ALA:HB2	2.16	0.76
1:A:419:LEU:CD1	1:A:422:LEU:HD23	2.15	0.76
1:A:366:TYR:HD1	1:A:391:THR:HG21	1.51	0.76
2:B:555:LEU:HD23	2:B:559:THR:HG22	1.67	0.76
1:A:336:ARG:HG3	1:A:369:GLU:CG	2.14	0.76
2:B:492:VAL:CG1	2:B:497:ALA:HB3	2.15	0.76
1:A:411:TYR:O	1:A:415:LEU:HG	1.85	0.76
2:B:256:LEU:HD12	2:B:282:ILE:HG23	1.68	0.76
1:A:395:ASP:HB2	1:A:397:PHE:CE1	2.20	0.76
2:B:480:LEU:O	2:B:483:ARG:HB3	1.84	0.76
1:A:266:GLU:HG2	1:A:268:ARG:HG2	1.67	0.76
1:A:395:ASP:HB3	1:A:397:PHE:CE1	2.20	0.76
1:A:404:ASP:HB2	1:A:406:LYS:HB3	1.68	0.76
1:A:502:SER:O	1:A:506:ALA:CB	2.34	0.76
2:B:416:GLN:C	2:B:418:HIS:N	2.41	0.76
1:A:536:LEU:O	1:A:540:LEU:HB3	1.84	0.75
2:B:316:LEU:C	2:B:363:ILE:HA	2.10	0.75
2:B:267:GLY:O	2:B:268:GLN:HB2	1.84	0.75
2:B:290:SER:CA	2:B:313:LEU:O	2.35	0.75
1:A:266:GLU:HG2	1:A:268:ARG:HE	1.51	0.75
1:A:419:LEU:CG	1:A:422:LEU:HD23	2.16	0.75
2:B:326:ASP:OD1	2:B:326:ASP:N	2.19	0.75
2:B:314:VAL:CG2	2:B:361:LEU:HD13	2.16	0.75
2:B:433:ALA:CA	2:B:436:THR:HB	2.16	0.75
1:A:419:LEU:CD1	1:A:422:LEU:CD2	2.65	0.75
1:A:538:ARG:NH2	2:B:473:LEU:CA	2.50	0.75
2:B:314:VAL:HG22	2:B:361:LEU:CD1	2.16	0.75
2:B:451:LEU:HD21	2:B:454:GLU:OE2	1.85	0.75
2:B:490:ASN:O	2:B:492:VAL:N	2.20	0.75
1:A:417:ARG:H	1:A:417:ARG:HD2	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:489:LEU:HB2	2:B:492:VAL:HG21	1.69	0.75
1:A:507:TYR:OH	1:A:541:SER:HB2	1.87	0.74
2:B:289:CYS:O	2:B:314:VAL:CB	2.35	0.74
2:B:316:LEU:HB2	2:B:363:ILE:CG2	2.15	0.74
2:B:327:ASN:N	2:B:327:ASN:HD22	1.85	0.74
1:A:419:LEU:HD11	2:B:414:ASP:OD1	1.86	0.74
2:B:481:VAL:O	2:B:483:ARG:N	2.20	0.74
1:A:289:ARG:O	1:A:293:ARG:HB2	1.87	0.74
2:B:483:ARG:HB2	2:B:501:VAL:HG21	1.68	0.74
1:A:369:GLU:C	1:A:371:HIS:CE1	2.65	0.74
2:B:271:GLY:H	2:B:274:GLN:HB3	1.52	0.74
2:B:287:VAL:HG11	2:B:350:ILE:HG13	1.69	0.74
2:B:459:PHE:O	2:B:461:LEU:HD23	1.87	0.74
2:B:555:LEU:CD2	2:B:559:THR:HG22	2.17	0.74
2:B:427:GLN:O	2:B:428:SER:HB2	1.87	0.74
1:A:272:CYS:N	1:A:311:VAL:HG22	2.03	0.73
1:A:432:PRO:O	1:A:452:SER:HA	1.88	0.73
2:B:283:GLU:HG2	2:B:284:ALA:H	1.51	0.73
1:A:497:TYR:HB2	1:A:503:LEU:HD22	1.70	0.73
1:A:502:SER:O	1:A:506:ALA:HB3	1.88	0.73
1:A:308:PHE:O	1:A:309:VAL:CB	2.35	0.73
1:A:399:VAL:HG21	2:B:435:PHE:CE1	2.24	0.73
1:A:485:VAL:HG12	1:A:485:VAL:O	1.85	0.73
2:B:526:LEU:O	2:B:527:LEU:HD23	1.89	0.73
2:B:550:SER:HA	2:B:553:ILE:HD13	1.70	0.73
1:A:296:VAL:HG11	1:A:416:THR:HG21	1.68	0.73
1:A:371:HIS:CE1	1:A:403:ALA:HA	2.23	0.73
2:B:471:VAL:HB	2:B:476:ARG:O	1.89	0.73
2:B:496:MET:O	2:B:499:ALA:N	2.18	0.73
2:B:509:LEU:O	2:B:510:LEU:C	2.30	0.73
1:A:262:LEU:O	1:A:263:ARG:CB	2.36	0.73
1:A:422:LEU:HD11	2:B:418:HIS:HE1	1.52	0.73
2:B:257:ASP:HB3	2:B:285:GLN:HB2	1.68	0.73
1:A:399:VAL:HG21	2:B:435:PHE:HE1	1.54	0.72
1:A:274:ASP:OD2	1:A:277:GLU:OE1	2.07	0.72
1:A:420:GLN:H	1:A:421:ARG:NH2	1.86	0.72
2:B:550:SER:HA	2:B:553:ILE:CD1	2.19	0.72
1:A:492:ALA:HB3	1:A:493:LEU:CD1	2.16	0.72
2:B:511:VAL:CA	2:B:514:TYR:HB2	2.17	0.72
1:A:305:VAL:HG22	1:A:356:LEU:CB	2.16	0.72
2:B:309:GLU:HB3	2:B:310:PRO:HD2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:CYS:H	1:A:311:VAL:HG22	1.55	0.72
1:A:413:ALA:C	1:A:415:LEU:N	2.45	0.72
2:B:364:VAL:HG12	2:B:426:VAL:HG11	1.71	0.72
2:B:471:VAL:HG12	2:B:477:GLY:HA3	1.72	0.72
2:B:551:ARG:NH1	2:B:566:LEU:HB3	1.99	0.72
2:B:519:SER:O	2:B:523:ARG:HG3	1.88	0.72
1:A:284:ARG:HA	1:A:286:GLU:H	1.54	0.72
2:B:260:LEU:HD22	2:B:289:CYS:C	2.14	0.72
2:B:289:CYS:O	2:B:314:VAL:CA	2.37	0.72
2:B:315:LEU:HD22	2:B:316:LEU:N	2.05	0.72
1:A:422:LEU:HD12	1:A:422:LEU:O	1.89	0.72
2:B:483:ARG:CA	2:B:486:ILE:HG13	2.16	0.72
2:B:551:ARG:C	2:B:553:ILE:H	1.96	0.72
1:A:329:ASP:O	1:A:362:GLU:HB3	1.89	0.71
2:B:491:ARG:H	2:B:491:ARG:CD	2.03	0.71
1:A:264:PRO:HA	1:A:427:THR:CA	2.19	0.71
1:A:381:GLU:HA	1:A:384:LEU:HD23	1.72	0.71
1:A:538:ARG:NH2	2:B:473:LEU:C	2.48	0.71
2:B:260:LEU:HD22	2:B:289:CYS:O	1.88	0.71
2:B:555:LEU:C	2:B:557:MET:N	2.43	0.71
1:A:541:SER:C	1:A:543:LEU:H	1.98	0.71
1:A:546:SER:HB2	2:B:506:SER:OG	1.90	0.71
2:B:273:LEU:HD12	2:B:437:CYS:SG	2.30	0.71
1:A:263:ARG:HG2	1:A:266:GLU:OE1	1.90	0.71
1:A:340:LEU:O	1:A:343:SER:HB3	1.91	0.70
2:B:488:GLN:O	2:B:489:LEU:HD12	1.91	0.70
2:B:261:LEU:HD23	2:B:262:GLN:HG3	1.73	0.70
1:A:316:ASN:HD21	1:A:321:ALA:N	1.90	0.70
1:A:362:GLU:O	1:A:363:ARG:HD2	1.90	0.70
1:A:391:THR:HA	1:A:395:ASP:CG	2.15	0.70
2:B:495:GLU:O	2:B:532:VAL:HG13	1.92	0.70
1:A:270:LEU:HG	1:A:271:LEU:N	2.07	0.70
1:A:520:LEU:O	1:A:521:SER:C	2.33	0.70
1:A:497:TYR:CG	1:A:503:LEU:HD22	2.26	0.70
2:B:284:ALA:O	2:B:285:GLN:OE1	2.10	0.70
2:B:450:LYS:CB	2:B:451:LEU:HD12	2.20	0.70
2:B:551:ARG:O	2:B:554:TYR:N	2.25	0.70
1:A:369:GLU:O	1:A:371:HIS:ND1	2.24	0.70
1:A:524:LYS:O	1:A:530:ARG:O	2.09	0.70
2:B:354:THR:HG21	2:B:359:LEU:HD22	1.73	0.70
2:B:529:ASP:O	2:B:530:ILE:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLU:OE2	1:A:291:LEU:CD2	2.39	0.69
1:A:457:SER:O	1:A:458:ASP:C	2.35	0.69
2:B:281:VAL:C	2:B:282:ILE:HD13	2.16	0.69
2:B:420:GLU:O	2:B:421:ALA:CB	2.39	0.69
1:A:419:LEU:HG	1:A:422:LEU:HD23	1.73	0.69
1:A:273:VAL:HA	1:A:308:PHE:HB3	1.73	0.69
1:A:293:ARG:HH11	1:A:293:ARG:CG	2.04	0.69
1:A:323:PRO:O	1:A:324:GLY:O	2.09	0.69
2:B:317:ARG:CG	2:B:364:VAL:HG23	2.22	0.69
1:A:499:THR:CB	2:B:560:LEU:O	2.40	0.69
1:A:260:LEU:HD22	1:A:455:THR:CG2	2.22	0.69
1:A:536:LEU:HD23	1:A:536:LEU:C	2.18	0.69
2:B:467:GLY:HA2	2:B:484:ARG:HH22	1.56	0.69
1:A:404:ASP:O	1:A:408:SER:CB	2.39	0.69
1:A:422:LEU:O	1:A:422:LEU:CD1	2.40	0.69
2:B:482:TRP:CD1	2:B:505:PRO:O	2.46	0.69
1:A:417:ARG:HD2	1:A:417:ARG:N	2.07	0.69
2:B:309:GLU:HB3	2:B:310:PRO:CD	2.21	0.68
2:B:416:GLN:HE21	2:B:416:GLN:CA	2.05	0.68
1:A:458:ASP:O	1:A:462:GLY:C	2.36	0.68
1:A:492:ALA:CB	1:A:493:LEU:HD12	2.15	0.68
1:A:480:MET:O	1:A:482:VAL:N	2.26	0.68
1:A:356:LEU:HD11	1:A:459:PHE:HB3	1.76	0.68
1:A:420:GLN:N	1:A:421:ARG:HH21	1.91	0.68
1:A:499:THR:HB	2:B:560:LEU:O	1.92	0.68
2:B:480:LEU:HD12	2:B:481:VAL:H	1.57	0.68
2:B:514:TYR:OH	2:B:553:ILE:C	2.37	0.68
1:A:305:VAL:O	1:A:356:LEU:HB3	1.94	0.68
2:B:504:TYR:HD2	2:B:510:LEU:HD22	1.58	0.68
1:A:394:ILE:O	1:A:395:ASP:C	2.37	0.68
2:B:288:PRO:C	2:B:290:SER:H	2.02	0.68
2:B:317:ARG:HA	2:B:364:VAL:N	2.09	0.68
1:A:497:TYR:HA	1:A:502:SER:HB2	1.75	0.68
1:A:366:TYR:C	1:A:367:LEU:HD12	2.18	0.68
2:B:488:GLN:H	2:B:488:GLN:NE2	1.92	0.68
1:A:304:HIS:O	1:A:305:VAL:HB	1.93	0.67
1:A:541:SER:O	1:A:543:LEU:N	2.27	0.67
2:B:317:ARG:HA	2:B:364:VAL:H	1.58	0.67
2:B:253:ILE:O	2:B:294:ARG:HG3	1.94	0.67
1:A:382:SER:O	1:A:385:LEU:N	2.23	0.67
2:B:481:VAL:HG12	2:B:485:GLN:HG3	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LEU:HB3	1:A:376:ASN:ND2	2.10	0.67
2:B:551:ARG:C	2:B:553:ILE:N	2.51	0.67
1:A:523:ILE:HG23	1:A:524:LYS:N	2.10	0.67
1:A:538:ARG:NH2	2:B:473:LEU:HB3	2.10	0.67
1:A:310:TRP:O	1:A:327:VAL:CB	2.39	0.67
2:B:548:GLU:HG3	2:B:549:LEU:HD22	1.76	0.67
1:A:456:PHE:CD1	1:A:457:SER:N	2.61	0.67
2:B:506:SER:CB	2:B:509:LEU:HG	2.17	0.67
1:A:285:PRO:C	1:A:287:LEU:H	2.03	0.67
2:B:255:VAL:HG12	2:B:256:LEU:N	2.10	0.66
1:A:481:GLN:NE2	2:B:485:GLN:HG2	2.10	0.66
2:B:491:ARG:O	2:B:496:MET:SD	2.53	0.66
1:A:336:ARG:CD	1:A:338:ASP:HB3	2.20	0.66
1:A:270:LEU:CG	1:A:271:LEU:H	2.08	0.66
1:A:272:CYS:SG	1:A:301:ARG:HG2	2.35	0.66
2:B:327:ASN:HD22	2:B:327:ASN:H	1.43	0.66
2:B:542:SER:O	2:B:543:ARG:CG	2.41	0.66
1:A:371:HIS:CD2	1:A:401:ARG:HG2	2.30	0.66
2:B:457:PHE:O	2:B:458:SER:HB3	1.95	0.66
1:A:285:PRO:O	1:A:287:LEU:N	2.28	0.66
1:A:296:VAL:CG1	1:A:416:THR:CG2	2.65	0.66
1:A:351:GLU:HG3	1:A:352:GLN:N	2.11	0.66
2:B:484:ARG:CG	2:B:484:ARG:NE	2.59	0.66
1:A:329:ASP:HB3	1:A:362:GLU:OE1	1.95	0.66
1:A:337:LEU:HB3	1:A:376:ASN:HD21	1.59	0.66
2:B:260:LEU:HD21	2:B:315:LEU:HB3	1.77	0.66
2:B:361:LEU:HB3	2:B:422:GLN:O	1.96	0.66
2:B:469:VAL:CG2	2:B:484:ARG:HD3	2.25	0.66
2:B:524:GLN:O	2:B:550:SER:O	2.14	0.66
1:A:404:ASP:HB2	1:A:406:LYS:N	2.11	0.66
1:A:289:ARG:CG	1:A:289:ARG:HH21	2.08	0.66
1:A:360:GLY:N	1:A:459:PHE:HE2	1.94	0.66
2:B:359:LEU:O	2:B:421:ALA:HA	1.94	0.66
2:B:483:ARG:HD2	2:B:484:ARG:N	2.11	0.66
1:A:460:ASN:CG	1:A:461:ALA:N	2.52	0.65
2:B:492:VAL:HA	2:B:496:MET:SD	2.35	0.65
2:B:551:ARG:NH1	2:B:568:SER:O	2.29	0.65
1:A:486:SER:HB3	1:A:489:LYS:H	1.60	0.65
2:B:528:ALA:HA	2:B:546:GLY:HA2	1.79	0.65
1:A:382:SER:O	1:A:385:LEU:HB2	1.97	0.65
1:A:353:LYS:HZ2	1:A:353:LYS:HB3	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:LEU:HG	2:B:250:LYS:H	1.62	0.65
1:A:550:LEU:HD12	2:B:505:PRO:O	1.96	0.65
2:B:551:ARG:HH12	2:B:566:LEU:CB	2.04	0.65
2:B:359:LEU:HG	2:B:421:ALA:HB2	1.79	0.65
2:B:430:LYS:O	2:B:431:GLU:HG2	1.95	0.65
1:A:497:TYR:HB3	1:A:503:LEU:HD22	1.76	0.65
2:B:314:VAL:HG23	2:B:361:LEU:CD1	2.26	0.65
2:B:496:MET:C	2:B:498:SER:H	2.05	0.65
2:B:503:ALA:C	2:B:504:TYR:HD1	2.05	0.65
1:A:312:ALA:C	1:A:313:GLN:HG2	2.20	0.64
1:A:521:SER:O	1:A:532:LEU:HB3	1.96	0.64
1:A:457:SER:HA	1:A:460:ASN:OD1	1.96	0.64
1:A:532:LEU:CD1	1:A:533:GLY:N	2.57	0.64
2:B:491:ARG:O	2:B:496:MET:HE1	1.97	0.64
1:A:333:GLU:O	1:A:334:ARG:HB2	1.97	0.64
2:B:315:LEU:HD13	2:B:315:LEU:O	1.97	0.64
2:B:315:LEU:HA	2:B:362:VAL:HG13	1.79	0.64
2:B:494:LEU:HD23	2:B:494:LEU:H	1.62	0.64
1:A:328:LEU:C	1:A:330:HIS:H	2.04	0.64
2:B:255:VAL:O	2:B:292:THR:O	2.16	0.64
2:B:252:ILE:CG2	2:B:253:ILE:N	2.60	0.64
2:B:473:LEU:O	2:B:474:ALA:O	2.15	0.64
1:A:337:LEU:HD22	1:A:376:ASN:HD22	1.61	0.64
1:A:471:VAL:HB	2:B:562:PRO:HA	1.80	0.64
1:A:476:ALA:O	1:A:479:LEU:N	2.31	0.64
1:A:356:LEU:O	1:A:356:LEU:HG	1.96	0.64
2:B:542:SER:C	2:B:543:ARG:HG3	2.22	0.64
1:A:353:LYS:HZ3	1:A:357:LYS:NZ	1.96	0.63
1:A:272:CYS:HB2	1:A:311:VAL:HG21	0.69	0.63
2:B:433:ALA:C	2:B:435:PHE:N	2.50	0.63
1:A:272:CYS:O	1:A:308:PHE:HB3	1.98	0.63
1:A:326:LEU:HG	1:A:455:THR:CG2	2.28	0.63
1:A:357:LYS:HD2	1:A:358:ARG:N	2.14	0.63
1:A:498:SER:O	1:A:499:THR:CB	2.39	0.63
2:B:257:ASP:CG	2:B:288:PRO:HB3	2.23	0.63
1:A:353:LYS:NZ	1:A:357:LYS:HZ2	1.94	0.63
1:A:270:LEU:CG	1:A:271:LEU:N	2.62	0.63
1:A:414:LEU:HD11	2:B:413:VAL:HB	1.81	0.63
1:A:534:PRO:O	1:A:537:SER:OG	2.16	0.63
2:B:252:ILE:HG23	2:B:294:ARG:O	1.98	0.63
2:B:531:GLN:NE2	2:B:533:ARG:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:GLN:NE2	2:B:484:ARG:HG2	2.13	0.62
2:B:409:GLU:O	2:B:413:VAL:HG13	1.99	0.62
2:B:433:ALA:HB1	2:B:437:CYS:HB2	1.80	0.62
2:B:503:ALA:C	2:B:505:PRO:HD3	2.24	0.62
2:B:271:GLY:C	2:B:273:LEU:H	2.07	0.62
1:A:260:LEU:HD13	1:A:455:THR:HG23	1.80	0.62
1:A:291:LEU:HD22	1:A:412:LEU:HD22	0.87	0.62
1:A:322:ASN:N	1:A:323:PRO:HD3	2.14	0.62
2:B:495:GLU:O	2:B:532:VAL:CG1	2.48	0.62
2:B:354:THR:HG21	2:B:359:LEU:HD13	1.80	0.62
1:A:366:TYR:HB2	1:A:397:PHE:HD2	1.63	0.62
1:A:478:GLN:HB2	2:B:485:GLN:HB3	1.82	0.62
2:B:313:LEU:HD12	2:B:361:LEU:H	1.64	0.62
2:B:317:ARG:HB2	2:B:319:GLU:HG2	1.82	0.62
1:A:311:VAL:C	1:A:325:GLU:OE1	2.40	0.62
2:B:511:VAL:O	2:B:515:GLN:HG2	1.99	0.61
2:B:481:VAL:CG1	2:B:485:GLN:HE21	2.13	0.61
2:B:551:ARG:O	2:B:553:ILE:N	2.33	0.61
1:A:514:LYS:H	1:A:514:LYS:HD2	1.64	0.61
2:B:487:GLN:O	2:B:489:LEU:N	2.33	0.61
2:B:316:LEU:N	2:B:362:VAL:O	2.31	0.61
1:A:266:GLU:HG2	1:A:268:ARG:NE	2.15	0.61
2:B:365:ASP:CG	2:B:367:GLU:H	2.08	0.61
1:A:333:GLU:HB3	1:A:366:TYR:CD2	2.36	0.61
1:A:353:LYS:HZ1	1:A:357:LYS:HZ1	1.46	0.61
1:A:493:LEU:HD21	1:A:523:ILE:CG2	2.23	0.61
1:A:550:LEU:CD1	2:B:505:PRO:O	2.49	0.61
2:B:257:ASP:OD2	2:B:285:GLN:CG	2.48	0.61
1:A:266:GLU:OE2	1:A:268:ARG:NH2	2.32	0.61
1:A:330:HIS:HB3	1:A:363:ARG:O	2.01	0.61
1:A:520:LEU:CD1	1:A:536:LEU:HD22	2.31	0.61
2:B:501:VAL:HG12	2:B:501:VAL:O	2.01	0.60
2:B:543:ARG:C	2:B:544:ARG:HE	2.08	0.60
1:A:275:ILE:C	1:A:277:GLU:H	2.08	0.60
1:A:337:LEU:CD2	1:A:376:ASN:ND2	2.64	0.60
1:A:465:LYS:H	1:A:465:LYS:HD2	1.65	0.60
2:B:254:VAL:HG22	2:B:293:TRP:CD1	2.36	0.60
1:A:382:SER:OG	1:A:383:THR:N	2.30	0.60
1:A:499:THR:HG21	2:B:560:LEU:HA	1.83	0.60
1:A:545:CYS:C	2:B:508:GLN:HG3	2.26	0.60
1:A:332:VAL:CA	1:A:365:VAL:O	2.38	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:CYS:C	1:A:343:SER:N	2.47	0.60
2:B:291:VAL:O	2:B:312:VAL:HG12	2.02	0.60
2:B:471:VAL:CG1	2:B:477:GLY:O	2.49	0.60
1:A:522:THR:HA	1:A:532:LEU:CB	2.31	0.60
2:B:284:ALA:O	2:B:285:GLN:CD	2.44	0.60
2:B:507:PRO:O	2:B:508:GLN:C	2.43	0.60
1:A:354:PHE:HA	1:A:357:LYS:HB2	1.83	0.60
1:A:359:CYS:HB2	1:A:361:LEU:CD2	2.21	0.60
1:A:538:ARG:HH22	2:B:473:LEU:CA	2.14	0.60
2:B:504:TYR:N	2:B:505:PRO:HD3	2.16	0.60
2:B:405:ARG:C	2:B:407:ASP:N	2.56	0.60
2:B:551:ARG:CZ	2:B:568:SER:O	2.49	0.60
2:B:256:LEU:HD12	2:B:282:ILE:CG2	2.32	0.60
1:A:347:GLY:HA3	2:B:464:ASP:CG	2.27	0.59
1:A:456:PHE:O	1:A:458:ASP:N	2.25	0.59
2:B:347:VAL:HG22	2:B:351:THR:OG1	2.02	0.59
2:B:451:LEU:HD23	2:B:454:GLU:OE2	2.02	0.59
1:A:307:ASP:OD2	1:A:333:GLU:C	2.44	0.59
1:A:471:VAL:O	1:A:471:VAL:HG12	2.01	0.59
1:A:551:THR:OG1	2:B:476:ARG:CG	2.47	0.59
2:B:271:GLY:C	2:B:273:LEU:N	2.59	0.59
2:B:293:TRP:HZ2	2:B:439:PHE:HZ	1.50	0.59
1:A:550:LEU:HD12	2:B:506:SER:HA	1.84	0.59
1:A:336:ARG:CG	1:A:370:GLU:HB3	2.32	0.59
1:A:476:ALA:C	1:A:479:LEU:H	2.11	0.59
1:A:499:THR:HG23	1:A:501:ALA:N	2.18	0.59
2:B:269:LEU:C	2:B:269:LEU:HD13	2.26	0.59
2:B:459:PHE:O	2:B:461:LEU:CD2	2.51	0.59
1:A:354:PHE:HD1	1:A:357:LYS:HE2	1.67	0.59
1:A:406:LYS:HG2	1:A:407:GLU:N	2.17	0.59
1:A:423:TYR:HD2	1:A:426:HIS:HD2	1.51	0.59
1:A:474:VAL:HB	2:B:556:GLN:OE1	2.01	0.59
1:A:404:ASP:CB	1:A:406:LYS:HB3	2.32	0.59
2:B:255:VAL:O	2:B:292:THR:HG22	2.03	0.59
2:B:255:VAL:CG1	2:B:256:LEU:H	2.15	0.59
2:B:254:VAL:HG12	2:B:254:VAL:O	2.03	0.59
2:B:315:LEU:HD22	2:B:315:LEU:C	2.28	0.59
2:B:429:TRP:HA	2:B:429:TRP:CE3	2.36	0.59
1:A:405:ILE:HA	1:A:408:SER:OG	2.03	0.59
2:B:432:LEU:CD2	2:B:436:THR:HG21	2.33	0.59
1:A:399:VAL:O	1:A:400:LYS:CG	2.47	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ILE:O	1:A:524:LYS:HB2	2.03	0.58
2:B:507:PRO:O	2:B:509:LEU:N	2.36	0.58
2:B:544:ARG:HA	2:B:544:ARG:HE	1.61	0.58
1:A:390:ASN:C	1:A:392:GLN:H	2.11	0.58
2:B:252:ILE:HG22	2:B:253:ILE:N	2.17	0.58
1:A:275:ILE:HG22	1:A:275:ILE:O	2.02	0.58
2:B:531:GLN:HE21	2:B:534:ARG:HG3	1.63	0.58
1:A:331:ILE:CG2	1:A:361:LEU:HG	2.33	0.58
1:A:395:ASP:N	1:A:395:ASP:OD1	2.35	0.58
1:A:398:PHE:HB2	2:B:422:GLN:HE21	1.67	0.58
1:A:543:LEU:HA	1:A:546:SER:OG	2.03	0.58
2:B:324:MET:SD	2:B:342:THR:CA	2.91	0.58
2:B:293:TRP:HZ2	2:B:439:PHE:CZ	2.21	0.58
1:A:491:ALA:HB3	1:A:492:ALA:HB2	0.60	0.58
1:A:538:ARG:HH21	2:B:473:LEU:HA	1.68	0.58
2:B:324:MET:SD	2:B:342:THR:HB	2.44	0.58
1:A:316:ASN:ND2	1:A:321:ALA:N	2.51	0.58
1:A:423:TYR:CD2	1:A:426:HIS:HD2	2.22	0.58
1:A:502:SER:O	1:A:506:ALA:HB2	2.03	0.58
2:B:249:LEU:HA	2:B:445:GLU:CD	2.27	0.58
2:B:258:PRO:HB3	2:B:282:ILE:HB	1.84	0.58
2:B:506:SER:HB3	2:B:509:LEU:CG	2.22	0.58
1:A:266:GLU:CG	1:A:268:ARG:HG2	2.34	0.58
1:A:289:ARG:HG2	1:A:289:ARG:NH2	2.19	0.58
1:A:503:LEU:HD12	1:A:507:TYR:HD2	1.69	0.58
2:B:480:LEU:CD1	2:B:481:VAL:H	2.17	0.58
1:A:470:SER:C	1:A:472:ARG:H	2.12	0.58
1:A:542:GLN:O	1:A:546:SER:OG	2.22	0.58
2:B:354:THR:CG2	2:B:357:LYS:HB2	2.31	0.58
2:B:421:ALA:O	2:B:422:GLN:OE1	2.21	0.57
2:B:433:ALA:HA	2:B:437:CYS:N	2.19	0.57
2:B:527:LEU:HD12	2:B:553:ILE:HD13	1.86	0.57
2:B:257:ASP:HB2	2:B:288:PRO:CB	2.23	0.57
2:B:481:VAL:HA	2:B:484:ARG:HB3	1.86	0.57
1:A:349:PHE:O	1:A:353:LYS:N	2.28	0.57
2:B:416:GLN:O	2:B:418:HIS:N	2.38	0.57
1:A:337:LEU:CD2	1:A:376:ASN:HD21	2.18	0.57
1:A:396:GLY:N	1:A:397:PHE:HD1	2.03	0.57
1:A:520:LEU:HD11	1:A:536:LEU:CD2	2.35	0.57
2:B:268:GLN:CD	2:B:430:LYS:HA	2.30	0.57
2:B:281:VAL:CG1	2:B:282:ILE:N	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:VAL:CG1	2:B:426:VAL:HG21	2.35	0.57
2:B:412:LEU:HA	2:B:415:LEU:HD21	1.87	0.57
2:B:547:PRO:C	2:B:549:LEU:H	2.13	0.57
1:A:334:ARG:HG3	1:A:367:LEU:CB	2.25	0.57
1:A:464:ILE:HA	1:A:467:LYS:HB3	1.87	0.57
2:B:254:VAL:HG22	2:B:293:TRP:HD1	1.69	0.57
2:B:526:LEU:N	2:B:550:SER:OG	2.38	0.57
2:B:271:GLY:C	2:B:274:GLN:H	2.12	0.57
1:A:305:VAL:CG2	1:A:356:LEU:HB2	2.20	0.57
2:B:316:LEU:O	2:B:364:VAL:N	2.36	0.57
2:B:442:ALA:C	2:B:444:ALA:H	2.13	0.57
1:A:497:TYR:CD1	1:A:503:LEU:CD1	2.68	0.57
1:A:514:LYS:H	1:A:514:LYS:HD3	1.67	0.57
1:A:539:THR:HA	1:A:542:GLN:NE2	2.20	0.57
1:A:541:SER:C	1:A:543:LEU:N	2.63	0.57
1:A:477:ARG:CB	2:B:488:GLN:HG3	2.34	0.56
2:B:254:VAL:O	2:B:280:CYS:HA	2.05	0.56
2:B:359:LEU:CG	2:B:421:ALA:HB2	2.35	0.56
2:B:426:VAL:HG12	2:B:428:SER:H	1.70	0.56
2:B:483:ARG:C	2:B:485:GLN:N	2.61	0.56
2:B:484:ARG:CD	2:B:484:ARG:CB	2.75	0.56
1:A:331:ILE:HG13	1:A:332:VAL:N	2.20	0.56
2:B:429:TRP:O	2:B:431:GLU:N	2.37	0.56
2:B:553:ILE:O	2:B:554:TYR:C	2.47	0.56
1:A:356:LEU:C	1:A:359:CYS:SG	2.88	0.56
1:A:486:SER:HB3	1:A:489:LYS:HB2	1.88	0.56
1:A:512:THR:HG23	1:A:515:GLU:OE2	2.05	0.56
1:A:538:ARG:NH2	2:B:473:LEU:CB	2.69	0.56
1:A:336:ARG:CG	1:A:369:GLU:HG2	2.34	0.56
1:A:361:LEU:O	1:A:364:ARG:HG3	2.05	0.56
1:A:400:LYS:HA	2:B:424:GLN:NE2	2.21	0.56
1:A:470:SER:HB2	2:B:563:HIS:HA	1.88	0.56
1:A:481:GLN:HE22	2:B:485:GLN:HG2	1.70	0.56
2:B:433:ALA:N	2:B:436:THR:HB	2.20	0.56
2:B:483:ARG:NH1	2:B:484:ARG:HA	2.20	0.56
2:B:493:SER:O	2:B:495:GLU:N	2.39	0.56
1:A:264:PRO:HG3	1:A:427:THR:OG1	2.05	0.56
1:A:347:GLY:HA3	2:B:464:ASP:OD2	2.05	0.56
1:A:366:TYR:HB2	1:A:397:PHE:CD2	2.40	0.56
1:A:423:TYR:O	1:A:424:GLN:O	2.23	0.56
1:A:469:GLN:O	2:B:565:SER:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:THR:CG2	1:A:502:SER:H	2.18	0.56
2:B:283:GLU:O	2:B:284:ALA:O	2.23	0.56
2:B:357:LYS:O	2:B:358:ALA:HB3	2.06	0.56
1:A:336:ARG:CD	1:A:338:ASP:CB	2.82	0.56
2:B:251:HIS:ND1	2:B:295:ARG:NH2	2.53	0.56
1:A:331:ILE:HG21	1:A:361:LEU:HG	1.87	0.56
2:B:261:LEU:HD23	2:B:261:LEU:N	2.21	0.56
2:B:283:GLU:HG2	2:B:284:ALA:N	2.17	0.56
2:B:444:ALA:HB3	2:B:445:GLU:OE2	2.06	0.56
2:B:494:LEU:HD23	2:B:494:LEU:N	2.18	0.56
1:A:491:ALA:CA	1:A:492:ALA:CB	2.83	0.55
1:A:538:ARG:NH2	2:B:473:LEU:HA	2.21	0.55
2:B:313:LEU:HD12	2:B:361:LEU:N	2.21	0.55
2:B:261:LEU:N	2:B:261:LEU:CD2	2.69	0.55
1:A:359:CYS:CB	1:A:361:LEU:HD22	2.20	0.55
1:A:381:GLU:O	1:A:382:SER:C	2.49	0.55
2:B:416:GLN:HE21	2:B:417:LEU:H	1.55	0.55
1:A:398:PHE:CG	2:B:422:GLN:NE2	2.75	0.55
1:A:407:GLU:HA	1:A:410:ALA:HB2	1.88	0.55
1:A:550:LEU:CD2	2:B:478:LEU:HB2	2.36	0.55
2:B:271:GLY:O	2:B:275:THR:N	2.30	0.55
1:A:409:ALA:O	1:A:412:LEU:HB3	2.06	0.55
1:A:463:ALA:O	1:A:464:ILE:C	2.49	0.55
1:A:522:THR:OG1	1:A:523:ILE:N	2.40	0.55
1:A:401:ARG:O	1:A:403:ALA:N	2.39	0.55
1:A:467:LYS:HG3	1:A:468:ALA:N	2.22	0.55
2:B:482:TRP:O	2:B:483:ARG:HB2	2.07	0.55
1:A:307:ASP:C	1:A:308:PHE:CD1	2.85	0.55
1:A:362:GLU:C	1:A:363:ARG:HD2	2.32	0.55
1:A:367:LEU:CD2	1:A:400:LYS:HB2	2.37	0.55
1:A:453:LEU:HD12	1:A:454:LEU:HB2	1.89	0.55
1:A:496:ARG:HB3	1:A:497:TYR:CD2	2.41	0.55
2:B:305:ASP:C	2:B:306:TRP:CE3	2.85	0.55
2:B:507:PRO:HB2	2:B:508:GLN:HE21	1.70	0.55
1:A:523:ILE:CG2	1:A:524:LYS:H	2.18	0.55
2:B:527:LEU:HD12	2:B:553:ILE:CD1	2.37	0.55
1:A:336:ARG:HA	1:A:369:GLU:HG2	1.89	0.55
1:A:413:ALA:CA	1:A:417:ARG:NH1	2.68	0.55
2:B:518:PHE:CD2	2:B:519:SER:N	2.75	0.54
1:A:284:ARG:CA	1:A:286:GLU:HG2	2.37	0.54
1:A:298:HIS:ND1	1:A:298:HIS:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LEU:C	1:A:330:HIS:N	2.64	0.54
1:A:499:THR:OG1	2:B:560:LEU:O	2.24	0.54
1:A:548:GLY:N	2:B:509:LEU:HD21	2.22	0.54
1:A:518:THR:OG1	1:A:518:THR:O	2.20	0.54
2:B:261:LEU:HD23	2:B:261:LEU:H	1.71	0.54
2:B:269:LEU:C	2:B:269:LEU:CD1	2.80	0.54
2:B:351:THR:HG22	2:B:351:THR:O	2.07	0.54
2:B:488:GLN:C	2:B:489:LEU:HD12	2.32	0.54
1:A:421:ARG:N	1:A:421:ARG:NE	2.49	0.54
2:B:264:GLU:HB3	2:B:429:TRP:CE2	2.42	0.54
2:B:276:MET:SD	2:B:437:CYS:HB3	2.48	0.54
2:B:342:THR:O	2:B:342:THR:OG1	2.23	0.54
2:B:517:CYS:O	2:B:518:PHE:O	2.26	0.54
1:A:270:LEU:HG	1:A:271:LEU:H	1.69	0.54
1:A:338:ASP:C	1:A:341:CYS:H	2.16	0.54
2:B:248:CYS:O	2:B:249:LEU:O	2.26	0.54
2:B:265:GLY:C	2:B:267:GLY:N	2.63	0.54
1:A:261:GLU:HA	1:A:428:LEU:HG	1.89	0.54
2:B:271:GLY:O	2:B:274:GLN:N	2.40	0.54
2:B:435:PHE:CD2	2:B:435:PHE:C	2.85	0.54
2:B:508:GLN:HE21	2:B:508:GLN:H	1.53	0.54
1:A:463:ALA:C	1:A:465:LYS:N	2.63	0.54
1:A:530:ARG:NH2	1:A:530:ARG:CG	2.54	0.54
1:A:546:SER:C	1:A:548:GLY:H	2.15	0.54
2:B:405:ARG:O	2:B:407:ASP:N	2.41	0.54
2:B:496:MET:C	2:B:498:SER:N	2.65	0.54
2:B:514:TYR:CZ	2:B:553:ILE:HG22	2.41	0.54
2:B:518:PHE:O	2:B:519:SER:O	2.25	0.54
2:B:543:ARG:HB3	2:B:543:ARG:CZ	2.36	0.54
2:B:314:VAL:O	2:B:362:VAL:N	2.33	0.54
1:A:354:PHE:O	1:A:354:PHE:CG	2.61	0.54
2:B:364:VAL:HG12	2:B:426:VAL:HG21	1.90	0.54
2:B:416:GLN:HE21	2:B:417:LEU:N	2.05	0.54
2:B:471:VAL:HG12	2:B:477:GLY:O	2.08	0.54
2:B:472:ASP:O	2:B:473:LEU:C	2.50	0.54
1:A:289:ARG:HH21	1:A:289:ARG:HG2	1.71	0.54
2:B:427:GLN:O	2:B:428:SER:CB	2.56	0.54
2:B:436:THR:O	2:B:436:THR:HG22	2.07	0.54
2:B:527:LEU:HD12	2:B:553:ILE:HG12	1.90	0.54
2:B:531:GLN:HE22	2:B:534:ARG:CG	2.20	0.54
2:B:548:GLU:OE2	2:B:549:LEU:HD21	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLU:O	1:A:371:HIS:NE2	2.41	0.53
2:B:314:VAL:HG23	2:B:361:LEU:HD12	1.90	0.53
1:A:514:LYS:CD	1:A:514:LYS:N	2.67	0.53
1:A:550:LEU:HD21	2:B:478:LEU:HB2	1.89	0.53
1:A:371:HIS:ND1	1:A:371:HIS:N	2.56	0.53
1:A:395:ASP:C	1:A:397:PHE:CE1	2.86	0.53
2:B:313:LEU:HG	2:B:314:VAL:N	2.22	0.53
2:B:527:LEU:HD12	2:B:553:ILE:CG1	2.39	0.53
1:A:551:THR:OG1	2:B:475:GLY:O	2.25	0.53
2:B:314:VAL:CG2	2:B:361:LEU:HD12	2.38	0.53
2:B:312:VAL:O	2:B:359:LEU:HB2	2.08	0.53
1:A:306:GLY:O	1:A:307:ASP:C	2.50	0.53
2:B:271:GLY:HA2	2:B:275:THR:HG23	1.89	0.53
2:B:316:LEU:O	2:B:363:ILE:CA	2.51	0.53
1:A:278:THR:O	1:A:280:GLY:N	2.41	0.53
1:A:347:GLY:O	1:A:349:PHE:N	2.42	0.53
1:A:394:ILE:HG23	1:A:395:ASP:N	2.23	0.53
1:A:513:PRO:HD2	1:A:514:LYS:NZ	2.24	0.53
2:B:318:ALA:HA	2:B:321:PHE:HB3	1.91	0.53
1:A:476:ALA:HA	1:A:479:LEU:CB	2.35	0.53
1:A:538:ARG:NH2	1:A:539:THR:HG22	2.23	0.53
1:A:534:PRO:O	1:A:535:ALA:C	2.51	0.53
2:B:287:VAL:CB	2:B:350:ILE:HD11	2.35	0.53
2:B:293:TRP:HE1	2:B:440:THR:HG22	1.74	0.53
2:B:413:VAL:CG2	2:B:413:VAL:O	2.54	0.53
1:A:497:TYR:HA	1:A:502:SER:CB	2.39	0.53
1:A:341:CYS:O	1:A:344:ILE:N	2.35	0.52
1:A:381:GLU:O	1:A:382:SER:O	2.27	0.52
1:A:389:THR:O	1:A:390:ASN:C	2.50	0.52
1:A:390:ASN:C	1:A:392:GLN:N	2.66	0.52
1:A:480:MET:HG2	1:A:486:SER:O	2.08	0.52
1:A:518:THR:O	1:A:519:LEU:C	2.52	0.52
2:B:254:VAL:CG2	2:B:293:TRP:HD1	2.22	0.52
2:B:270:LEU:HD11	2:B:274:GLN:NE2	2.24	0.52
2:B:551:ARG:NH1	2:B:566:LEU:HD23	2.24	0.52
2:B:321:PHE:CD1	2:B:321:PHE:C	2.87	0.52
2:B:325:ILE:HD13	2:B:411:ALA:HB1	1.91	0.52
2:B:468:GLY:H	2:B:484:ARG:NH2	2.06	0.52
2:B:524:GLN:CG	2:B:551:ARG:HB2	2.29	0.52
2:B:566:LEU:C	2:B:568:SER:N	2.64	0.52
1:A:337:LEU:HB2	1:A:368:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:ARG:HH11	1:A:477:ARG:CG	1.91	0.52
2:B:514:TYR:OH	2:B:554:TYR:N	2.42	0.52
2:B:533:ARG:HD3	2:B:541:THR:N	2.25	0.52
1:A:338:ASP:O	1:A:341:CYS:N	2.37	0.52
1:A:398:PHE:CB	2:B:422:GLN:HE21	2.20	0.52
2:B:351:THR:HG23	2:B:354:THR:O	2.10	0.52
2:B:483:ARG:C	2:B:486:ILE:H	2.16	0.52
1:A:332:VAL:HG22	1:A:365:VAL:CA	2.38	0.52
2:B:327:ASN:N	2:B:327:ASN:ND2	2.51	0.52
2:B:416:GLN:N	2:B:416:GLN:NE2	2.39	0.52
1:A:356:LEU:O	1:A:356:LEU:CG	2.57	0.52
2:B:313:LEU:HD12	2:B:361:LEU:C	2.34	0.52
1:A:395:ASP:CB	1:A:397:PHE:HE1	2.22	0.52
1:A:478:GLN:O	2:B:485:GLN:CD	2.52	0.52
1:A:507:TYR:CE1	1:A:541:SER:OG	2.22	0.52
2:B:254:VAL:HA	2:B:293:TRP:HA	1.91	0.52
2:B:422:GLN:OE1	2:B:422:GLN:HA	2.10	0.52
2:B:426:VAL:HG12	2:B:427:GLN:N	2.24	0.52
1:A:291:LEU:HD13	1:A:412:LEU:CD1	2.15	0.52
1:A:393:VAL:HG11	2:B:443:VAL:CG2	2.37	0.52
1:A:548:GLY:HA2	2:B:509:LEU:HD11	1.92	0.52
2:B:457:PHE:O	2:B:458:SER:CB	2.57	0.52
2:B:554:TYR:O	2:B:558:THR:N	2.43	0.52
2:B:252:ILE:CG2	2:B:253:ILE:H	2.22	0.52
2:B:548:GLU:O	2:B:552:ARG:HD2	2.10	0.52
2:B:519:SER:O	2:B:523:ARG:CG	2.58	0.52
1:A:325:GLU:OE2	1:A:327:VAL:HG12	2.10	0.51
2:B:445:GLU:HG3	2:B:447:PRO:HD2	1.91	0.51
1:A:331:ILE:HG13	1:A:332:VAL:H	1.74	0.51
1:A:367:LEU:HD23	1:A:402:THR:HG23	1.91	0.51
1:A:457:SER:O	1:A:460:ASN:OD1	2.28	0.51
2:B:311:THR:O	2:B:312:VAL:HG13	2.09	0.51
2:B:351:THR:HG23	2:B:355:ALA:HA	1.92	0.51
1:A:353:LYS:NZ	1:A:353:LYS:C	2.68	0.51
1:A:367:LEU:HG	1:A:400:LYS:HB2	1.91	0.51
1:A:485:VAL:CG1	1:A:485:VAL:O	2.57	0.51
1:A:536:LEU:HD23	1:A:537:SER:N	2.24	0.51
1:A:544:TYR:HA	2:B:508:GLN:NE2	2.26	0.51
2:B:482:TRP:HA	2:B:482:TRP:CE3	2.45	0.51
1:A:334:ARG:CG	1:A:367:LEU:HB2	2.29	0.51
2:B:322:VAL:HA	2:B:325:ILE:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:GLN:O	2:B:432:LEU:O	2.28	0.51
2:B:310:PRO:O	2:B:357:LYS:CG	2.59	0.51
2:B:446:ALA:H	2:B:447:PRO:CD	2.23	0.51
2:B:491:ARG:O	2:B:496:MET:CE	2.59	0.51
1:A:366:TYR:O	1:A:367:LEU:HD12	2.11	0.51
2:B:260:LEU:HD13	2:B:289:CYS:CA	2.28	0.51
2:B:433:ALA:O	2:B:435:PHE:N	2.44	0.51
1:A:385:LEU:O	1:A:389:THR:HG23	2.10	0.51
2:B:347:VAL:HG23	2:B:350:ILE:HG22	1.93	0.51
2:B:493:SER:C	2:B:495:GLU:N	2.69	0.51
1:A:538:ARG:HH22	2:B:473:LEU:HB3	1.76	0.51
2:B:270:LEU:HG	2:B:274:GLN:OE1	2.11	0.51
2:B:509:LEU:N	2:B:509:LEU:HD23	2.26	0.51
1:A:461:ALA:O	1:A:464:ILE:HB	2.11	0.50
2:B:288:PRO:C	2:B:290:SER:N	2.68	0.50
2:B:504:TYR:HD2	2:B:510:LEU:CD2	2.23	0.50
1:A:342:SER:O	1:A:346:ASP:OD2	2.29	0.50
1:A:347:GLY:CA	2:B:464:ASP:OD2	2.59	0.50
1:A:470:SER:O	1:A:474:VAL:HG23	2.11	0.50
2:B:414:ASP:C	2:B:415:LEU:HD23	2.37	0.50
1:A:503:LEU:O	1:A:504:LEU:HD23	2.12	0.50
1:A:546:SER:HB2	2:B:506:SER:CB	2.40	0.50
2:B:260:LEU:CD2	2:B:289:CYS:O	2.59	0.50
1:A:348:ARG:O	1:A:349:PHE:C	2.53	0.50
1:A:414:LEU:O	1:A:418:GLY:HA3	2.12	0.50
1:A:293:ARG:CG	1:A:293:ARG:NH1	2.69	0.50
1:A:414:LEU:CD2	2:B:413:VAL:HG11	2.42	0.50
1:A:333:GLU:O	1:A:366:TYR:HA	2.12	0.50
1:A:336:ARG:HG3	1:A:370:GLU:HB3	1.94	0.50
1:A:482:VAL:HA	2:B:469:VAL:O	2.12	0.50
2:B:347:VAL:O	2:B:349:ASP:N	2.44	0.50
1:A:520:LEU:O	1:A:522:THR:O	2.30	0.50
2:B:526:LEU:C	2:B:527:LEU:HG	2.35	0.50
1:A:414:LEU:HD21	2:B:413:VAL:HG21	0.58	0.50
2:B:282:ILE:HD13	2:B:282:ILE:N	2.27	0.50
2:B:293:TRP:CH2	2:B:311:THR:OG1	2.65	0.49
2:B:486:ILE:HG22	2:B:489:LEU:CD2	2.39	0.49
1:A:263:ARG:C	1:A:265:GLY:H	2.19	0.49
1:A:405:ILE:O	1:A:408:SER:OG	2.27	0.49
1:A:418:GLY:O	1:A:420:GLN:N	2.43	0.49
1:A:431:ARG:HB2	1:A:432:PRO:C	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:VAL:CG1	2:B:556:GLN:OE1	2.59	0.49
1:A:517:GLU:HB3	1:A:538:ARG:HG3	1.94	0.49
2:B:455:THR:OG1	2:B:456:THR:N	2.46	0.49
1:A:326:LEU:HG	1:A:455:THR:HG22	1.93	0.49
1:A:370:GLU:C	1:A:371:HIS:ND1	2.70	0.49
1:A:514:LYS:HD2	1:A:514:LYS:N	2.27	0.49
1:A:348:ARG:O	1:A:349:PHE:O	2.29	0.49
1:A:422:LEU:CD1	2:B:418:HIS:HE1	2.23	0.49
2:B:365:ASP:OD1	2:B:367:GLU:N	2.43	0.49
2:B:525:ASN:O	2:B:525:ASN:OD1	2.30	0.49
1:A:497:TYR:CD2	1:A:497:TYR:N	2.80	0.49
2:B:293:TRP:NE1	2:B:440:THR:HG22	2.28	0.49
2:B:364:VAL:HG21	2:B:429:TRP:HZ3	1.77	0.49
2:B:486:ILE:HB	2:B:497:ALA:HB1	1.94	0.49
1:A:285:PRO:CB	1:A:288:LEU:HB2	2.36	0.49
1:A:430:SER:O	1:A:453:LEU:O	2.31	0.49
1:A:543:LEU:HB2	2:B:507:PRO:HD2	1.95	0.49
2:B:315:LEU:HA	2:B:362:VAL:CG1	2.41	0.49
1:A:520:LEU:O	1:A:522:THR:N	2.46	0.49
2:B:354:THR:HG21	2:B:359:LEU:CD2	2.42	0.49
1:A:275:ILE:C	1:A:277:GLU:N	2.69	0.49
1:A:365:VAL:HG12	1:A:367:LEU:CD1	2.43	0.49
2:B:248:CYS:SG	2:B:249:LEU:N	2.86	0.49
2:B:259:VAL:O	2:B:288:PRO:O	2.31	0.49
2:B:295:ARG:HB3	2:B:307:VAL:HB	1.95	0.49
2:B:506:SER:H	2:B:509:LEU:HD12	1.78	0.49
1:A:273:VAL:HA	1:A:308:PHE:CD1	2.48	0.48
1:A:411:TYR:O	1:A:412:LEU:C	2.56	0.48
2:B:471:VAL:HG11	2:B:478:LEU:HD23	1.95	0.48
1:A:304:HIS:ND1	1:A:304:HIS:N	2.61	0.48
1:A:309:VAL:HG13	1:A:310:TRP:H	1.79	0.48
1:A:413:ALA:HB1	1:A:417:ARG:NH2	2.28	0.48
1:A:543:LEU:C	1:A:545:CYS:H	2.21	0.48
1:A:539:THR:OG1	1:A:540:LEU:N	2.46	0.48
2:B:313:LEU:HG	2:B:361:LEU:HA	1.96	0.48
2:B:542:SER:C	2:B:543:ARG:CG	2.83	0.48
1:A:272:CYS:N	1:A:311:VAL:CG2	2.76	0.48
1:A:333:GLU:C	1:A:366:TYR:HD2	2.21	0.48
1:A:393:VAL:CG1	2:B:443:VAL:CG2	2.91	0.48
2:B:433:ALA:HB1	2:B:437:CYS:SG	2.53	0.48
2:B:443:VAL:HG23	2:B:443:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:472:ASP:O	2:B:474:ALA:O	2.31	0.48
1:A:338:ASP:O	1:A:341:CYS:HB2	2.14	0.48
2:B:486:ILE:CG2	2:B:489:LEU:HD22	2.41	0.48
1:A:270:LEU:HD12	1:A:271:LEU:N	2.18	0.48
2:B:259:VAL:O	2:B:260:LEU:HB2	2.12	0.48
2:B:483:ARG:CB	2:B:501:VAL:HG21	2.40	0.48
1:A:284:ARG:HA	1:A:286:GLU:N	2.24	0.48
1:A:393:VAL:CG1	2:B:443:VAL:HG22	2.40	0.48
1:A:508:ASP:OD2	1:A:508:ASP:C	2.57	0.48
1:A:534:PRO:HG2	1:A:535:ALA:H	1.79	0.48
1:A:391:THR:O	1:A:395:ASP:HB2	2.14	0.48
2:B:411:ALA:O	2:B:415:LEU:HD21	2.14	0.48
1:A:453:LEU:HB2	1:A:454:LEU:HD23	1.95	0.48
2:B:362:VAL:HG22	2:B:363:ILE:N	2.29	0.48
1:A:453:LEU:HG	1:A:454:LEU:N	2.29	0.47
1:A:524:LYS:C	1:A:525:CYS:SG	2.97	0.47
2:B:482:TRP:O	2:B:501:VAL:HG21	2.14	0.47
1:A:364:ARG:O	1:A:397:PHE:CA	2.46	0.47
1:A:274:ASP:OD2	1:A:277:GLU:CD	2.57	0.47
2:B:310:PRO:O	2:B:357:LYS:HG2	2.15	0.47
2:B:495:GLU:O	2:B:499:ALA:HB2	2.14	0.47
1:A:354:PHE:C	1:A:357:LYS:HB2	2.40	0.47
2:B:525:ASN:HA	2:B:550:SER:HB3	1.94	0.47
2:B:550:SER:HA	2:B:553:ILE:HD12	1.96	0.47
2:B:482:TRP:CH2	2:B:510:LEU:HG	2.50	0.47
1:A:300:VAL:HG13	1:A:300:VAL:O	2.13	0.47
2:B:259:VAL:O	2:B:260:LEU:CB	2.62	0.47
2:B:471:VAL:HG12	2:B:477:GLY:CA	2.43	0.47
2:B:482:TRP:O	2:B:501:VAL:HG11	2.14	0.47
1:A:275:ILE:HA	1:A:278:THR:OG1	2.14	0.47
1:A:331:ILE:HB	1:A:361:LEU:HG	1.95	0.47
1:A:365:VAL:HG13	1:A:398:PHE:HB3	1.97	0.47
1:A:494:VAL:O	1:A:498:SER:CA	2.63	0.47
1:A:548:GLY:HA2	2:B:509:LEU:HD21	1.94	0.47
2:B:310:PRO:C	2:B:357:LYS:HE2	2.39	0.47
2:B:473:LEU:C	2:B:474:ALA:O	2.57	0.47
2:B:507:PRO:O	2:B:510:LEU:N	2.47	0.47
2:B:556:GLN:O	2:B:556:GLN:HG3	2.15	0.47
1:A:284:ARG:HA	1:A:286:GLU:HG2	1.97	0.47
1:A:404:ASP:HB2	1:A:406:LYS:CB	2.40	0.47
2:B:261:LEU:HD23	2:B:262:GLN:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:GLU:O	2:B:429:TRP:CE2	2.67	0.47
2:B:295:ARG:C	2:B:307:VAL:HG23	2.39	0.47
2:B:483:ARG:C	2:B:485:GLN:H	2.21	0.47
2:B:542:SER:O	2:B:543:ARG:CB	2.61	0.47
1:A:351:GLU:HA	2:B:459:PHE:HE2	1.79	0.47
1:A:476:ALA:O	1:A:477:ARG:C	2.58	0.47
1:A:486:SER:CB	1:A:489:LYS:HB2	2.45	0.47
2:B:289:CYS:C	2:B:314:VAL:HG12	2.40	0.47
2:B:415:LEU:O	2:B:418:HIS:HB2	2.14	0.47
1:A:307:ASP:HB2	1:A:333:GLU:HA	1.97	0.47
1:A:349:PHE:CE1	1:A:353:LYS:HG3	2.50	0.47
1:A:471:VAL:O	1:A:471:VAL:CG1	2.63	0.47
1:A:546:SER:O	2:B:508:GLN:HB2	2.15	0.47
1:A:331:ILE:CG2	1:A:361:LEU:CB	2.83	0.46
1:A:432:PRO:HA	1:A:453:LEU:HA	1.97	0.46
1:A:522:THR:HA	1:A:532:LEU:HB3	1.97	0.46
2:B:281:VAL:HG12	2:B:282:ILE:N	2.30	0.46
2:B:471:VAL:CG1	2:B:477:GLY:HA3	2.43	0.46
2:B:559:THR:CG2	2:B:561:GLN:NE2	2.78	0.46
1:A:457:SER:CA	1:A:460:ASN:OD1	2.64	0.46
1:A:326:LEU:HD22	1:A:428:LEU:CD1	2.41	0.46
1:A:354:PHE:HA	1:A:357:LYS:HZ3	1.79	0.46
1:A:369:GLU:CA	1:A:402:THR:O	2.54	0.46
1:A:477:ARG:NH1	1:A:477:ARG:CG	2.59	0.46
1:A:497:TYR:C	1:A:502:SER:OG	2.58	0.46
2:B:255:VAL:CG1	2:B:256:LEU:N	2.75	0.46
2:B:280:CYS:O	2:B:281:VAL:CG2	2.51	0.46
2:B:287:VAL:O	2:B:289:CYS:N	2.48	0.46
2:B:508:GLN:H	2:B:508:GLN:NE2	2.13	0.46
1:A:369:GLU:O	1:A:371:HIS:CG	2.68	0.46
1:A:522:THR:C	1:A:523:ILE:HG22	2.41	0.46
2:B:409:GLU:O	2:B:412:LEU:HG	2.15	0.46
2:B:471:VAL:HG11	2:B:477:GLY:O	2.15	0.46
2:B:483:ARG:HG2	2:B:497:ALA:O	2.16	0.46
2:B:543:ARG:O	2:B:544:ARG:NE	2.42	0.46
2:B:554:TYR:CD1	2:B:558:THR:HB	2.50	0.46
1:A:477:ARG:HG3	2:B:460:CYS:CB	2.45	0.46
2:B:347:VAL:HG13	2:B:348:THR:N	2.30	0.46
1:A:264:PRO:HB3	1:A:427:THR:CB	2.46	0.46
1:A:270:LEU:HD11	1:A:299:THR:OG1	2.14	0.46
1:A:337:LEU:N	1:A:368:VAL:HG13	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLN:O	1:A:519:LEU:HB2	2.15	0.46
1:A:523:ILE:C	1:A:524:LYS:HD2	2.40	0.46
1:A:326:LEU:HD22	1:A:428:LEU:CD2	2.37	0.46
2:B:482:TRP:HA	2:B:482:TRP:HE3	1.81	0.46
2:B:555:LEU:HD21	2:B:559:THR:HG22	1.94	0.46
2:B:433:ALA:HB1	2:B:437:CYS:CB	2.44	0.46
2:B:439:PHE:CG	2:B:440:THR:N	2.82	0.46
1:A:285:PRO:HG3	1:A:288:LEU:HD12	1.98	0.46
1:A:362:GLU:HG2	1:A:363:ARG:HG2	1.97	0.46
1:A:458:ASP:O	1:A:463:ALA:N	2.48	0.46
1:A:474:VAL:HG12	1:A:478:GLN:OE1	2.15	0.46
1:A:539:THR:HA	1:A:542:GLN:CD	2.41	0.46
2:B:305:ASP:C	2:B:306:TRP:CD2	2.94	0.46
2:B:410:GLU:HA	2:B:413:VAL:HG22	1.97	0.46
1:A:266:GLU:HG2	1:A:268:ARG:CG	2.43	0.46
1:A:369:GLU:O	1:A:370:GLU:C	2.59	0.46
1:A:394:ILE:HG23	1:A:395:ASP:H	1.81	0.46
1:A:497:TYR:HB3	1:A:503:LEU:CB	2.40	0.46
2:B:527:LEU:HB2	2:B:550:SER:HB2	1.98	0.46
2:B:547:PRO:O	2:B:549:LEU:N	2.49	0.46
1:A:326:LEU:HG	1:A:455:THR:HG21	1.97	0.45
1:A:328:LEU:HD21	1:A:330:HIS:ND1	2.31	0.45
1:A:471:VAL:HA	1:A:474:VAL:HG23	1.97	0.45
1:A:475:PHE:HD1	1:A:475:PHE:O	1.98	0.45
1:A:261:GLU:O	1:A:262:LEU:HB2	2.17	0.45
1:A:353:LYS:HZ3	1:A:357:LYS:HZ2	1.60	0.45
1:A:457:SER:O	1:A:459:PHE:N	2.48	0.45
2:B:263:MET:HE1	2:B:429:TRP:HZ2	1.65	0.45
2:B:268:GLN:CG	2:B:432:LEU:HB3	2.22	0.45
2:B:317:ARG:CB	2:B:319:GLU:HG2	2.45	0.45
2:B:433:ALA:HA	2:B:436:THR:CB	2.36	0.45
2:B:478:LEU:O	2:B:479:ALA:C	2.59	0.45
1:A:299:THR:HG21	1:A:301:ARG:NH2	2.31	0.45
2:B:263:MET:CE	2:B:429:TRP:CZ2	2.80	0.45
2:B:269:LEU:CD1	2:B:270:LEU:N	2.79	0.45
2:B:491:ARG:HD2	2:B:491:ARG:N	2.20	0.45
2:B:496:MET:C	2:B:499:ALA:H	2.17	0.45
1:A:287:LEU:HD21	1:A:409:ALA:HB2	1.98	0.45
1:A:389:THR:HG21	2:B:438:ALA:CB	2.46	0.45
1:A:395:ASP:C	1:A:397:PHE:CD1	2.95	0.45
1:A:499:THR:HG1	2:B:560:LEU:C	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:ILE:HG23	2:B:253:ILE:H	1.81	0.45
2:B:264:GLU:HB3	2:B:429:TRP:CZ2	2.52	0.45
2:B:316:LEU:O	2:B:364:VAL:HG22	2.15	0.45
2:B:321:PHE:CE1	2:B:325:ILE:HD11	2.51	0.45
1:A:347:GLY:CA	2:B:464:ASP:CG	2.90	0.45
2:B:293:TRP:HZ3	2:B:311:THR:O	2.00	0.45
2:B:527:LEU:HD23	2:B:527:LEU:HA	1.73	0.45
1:A:268:ARG:NH1	1:A:314:GLU:HA	2.31	0.45
1:A:423:TYR:HD2	1:A:426:HIS:CD2	2.34	0.45
1:A:550:LEU:HD23	1:A:551:THR:N	2.32	0.45
2:B:309:GLU:HA	2:B:309:GLU:OE2	2.17	0.45
2:B:314:VAL:O	2:B:361:LEU:HD12	2.17	0.45
1:A:469:GLN:HE21	1:A:469:GLN:HB3	1.50	0.45
1:A:493:LEU:CD2	1:A:523:ILE:HD13	2.46	0.45
2:B:359:LEU:HD23	2:B:359:LEU:N	2.32	0.45
2:B:507:PRO:C	2:B:509:LEU:N	2.74	0.45
2:B:527:LEU:CD1	2:B:553:ILE:HG12	2.47	0.45
2:B:559:THR:HG23	2:B:561:GLN:H	1.82	0.45
1:A:285:PRO:C	1:A:287:LEU:N	2.66	0.45
1:A:294:LEU:CD2	1:A:413:ALA:HB2	2.46	0.45
1:A:535:ALA:O	1:A:536:LEU:C	2.60	0.45
2:B:257:ASP:HA	2:B:258:PRO:HD2	1.64	0.45
2:B:359:LEU:HD23	2:B:421:ALA:HB2	1.93	0.45
1:A:288:LEU:C	1:A:290:GLU:N	2.73	0.45
1:A:349:PHE:CE2	1:A:350:ARG:HG2	2.52	0.45
1:A:524:LYS:O	1:A:525:CYS:O	2.35	0.45
2:B:270:LEU:C	2:B:274:GLN:HB3	2.39	0.45
2:B:516:GLN:OE1	2:B:516:GLN:N	2.50	0.45
1:A:288:LEU:HB3	1:A:289:ARG:H	1.65	0.44
1:A:340:LEU:O	1:A:341:CYS:C	2.58	0.44
1:A:371:HIS:NE2	1:A:401:ARG:HG2	2.31	0.44
1:A:476:ALA:C	1:A:478:GLN:N	2.73	0.44
1:A:522:THR:O	1:A:523:ILE:HB	2.17	0.44
1:A:536:LEU:C	1:A:536:LEU:CD2	2.90	0.44
2:B:290:SER:HB2	2:B:291:VAL:H	1.59	0.44
2:B:348:THR:C	2:B:349:ASP:OD1	2.61	0.44
1:A:294:LEU:HD23	1:A:417:ARG:HH22	1.83	0.44
1:A:353:LYS:HD3	1:A:395:ASP:OD2	2.18	0.44
1:A:354:PHE:CE2	1:A:466:ASN:ND2	2.85	0.44
1:A:390:ASN:O	1:A:391:THR:C	2.61	0.44
2:B:261:LEU:HD11	2:B:282:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:GLN:OE1	2:B:430:LYS:HA	2.16	0.44
1:A:354:PHE:HE2	1:A:466:ASN:HD21	1.63	0.44
1:A:385:LEU:HD13	2:B:434:ASP:O	2.16	0.44
1:A:542:GLN:HA	1:A:545:CYS:HG	1.82	0.44
1:A:548:GLY:HA3	1:A:549:PRO:HD2	1.64	0.44
2:B:482:TRP:O	2:B:483:ARG:CB	2.65	0.44
2:B:543:ARG:O	2:B:544:ARG:NH2	2.50	0.44
1:A:331:ILE:CB	1:A:361:LEU:HG	2.47	0.44
1:A:395:ASP:C	1:A:397:PHE:HE1	2.25	0.44
1:A:414:LEU:HD21	2:B:413:VAL:CG1	2.47	0.44
1:A:494:VAL:O	1:A:497:TYR:C	2.61	0.44
2:B:270:LEU:HD12	2:B:274:GLN:HB2	2.00	0.44
2:B:453:ASP:O	2:B:454:GLU:HG2	2.18	0.44
2:B:480:LEU:CD1	2:B:481:VAL:N	2.81	0.44
2:B:488:GLN:H	2:B:488:GLN:CD	2.24	0.44
1:A:394:ILE:O	1:A:396:GLY:N	2.50	0.44
1:A:423:TYR:CD2	1:A:423:TYR:C	2.95	0.44
1:A:464:ILE:C	1:A:466:ASN:H	2.25	0.44
1:A:481:GLN:C	1:A:482:VAL:CG2	2.90	0.44
2:B:263:MET:HB2	2:B:263:MET:HE2	1.55	0.44
1:A:288:LEU:C	1:A:290:GLU:H	2.25	0.44
1:A:383:THR:HG22	1:A:386:GLN:CD	2.38	0.44
1:A:422:LEU:O	1:A:422:LEU:HD13	2.17	0.44
2:B:441:LYS:O	2:B:442:ALA:HB3	2.17	0.44
1:A:260:LEU:CB	1:A:430:SER:HB2	2.48	0.44
1:A:267:TYR:CD1	1:A:267:TYR:N	2.86	0.44
1:A:456:PHE:C	1:A:458:ASP:H	2.21	0.44
2:B:305:ASP:O	2:B:306:TRP:CD2	2.65	0.44
2:B:253:ILE:O	2:B:294:ARG:N	2.51	0.43
2:B:256:LEU:CD1	2:B:282:ILE:CG2	2.90	0.43
2:B:257:ASP:N	2:B:285:GLN:OE1	2.49	0.43
2:B:365:ASP:CG	2:B:366:GLN:N	2.74	0.43
2:B:431:GLU:O	2:B:433:ALA:N	2.42	0.43
1:A:337:LEU:CB	1:A:368:VAL:HG11	2.48	0.43
1:A:342:SER:HA	1:A:345:ILE:HG22	1.99	0.43
1:A:367:LEU:CG	1:A:400:LYS:HB2	2.48	0.43
1:A:528:LEU:HD23	1:A:528:LEU:O	2.18	0.43
2:B:285:GLN:CB	2:B:288:PRO:HG3	2.48	0.43
1:A:351:GLU:O	1:A:354:PHE:N	2.51	0.43
1:A:352:GLN:HA	1:A:355:ARG:HB3	1.99	0.43
1:A:513:PRO:HD2	1:A:514:LYS:HZ3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:VAL:HA	2:B:325:ILE:CD1	2.47	0.43
1:A:477:ARG:HB3	2:B:488:GLN:CG	2.42	0.43
1:A:486:SER:OG	1:A:488:GLU:HG3	2.19	0.43
2:B:350:ILE:O	2:B:350:ILE:HG23	2.18	0.43
2:B:503:ALA:C	2:B:504:TYR:CD1	2.92	0.43
1:A:270:LEU:CD2	1:A:311:VAL:O	2.62	0.43
1:A:532:LEU:HA	1:A:532:LEU:HD22	1.61	0.43
2:B:260:LEU:HD21	2:B:315:LEU:H	1.83	0.43
2:B:565:SER:O	2:B:566:LEU:C	2.61	0.43
1:A:338:ASP:O	1:A:341:CYS:CB	2.66	0.43
1:A:499:THR:HG22	1:A:502:SER:H	1.83	0.43
1:A:548:GLY:CA	2:B:509:LEU:HD21	2.48	0.43
1:A:260:LEU:HB2	1:A:430:SER:HB2	2.00	0.43
1:A:331:ILE:HG21	1:A:361:LEU:HB3	1.95	0.43
1:A:481:GLN:O	1:A:482:VAL:HG22	2.19	0.43
2:B:433:ALA:C	2:B:436:THR:H	2.27	0.43
1:A:269:VAL:CG1	1:A:270:LEU:N	2.82	0.43
1:A:414:LEU:CD2	2:B:413:VAL:CG2	2.35	0.43
1:A:414:LEU:HB3	1:A:415:LEU:HD23	2.01	0.43
2:B:260:LEU:CD1	2:B:315:LEU:HD12	2.48	0.43
2:B:309:GLU:CB	2:B:310:PRO:CD	2.92	0.43
2:B:432:LEU:O	2:B:433:ALA:CB	2.67	0.43
2:B:455:THR:OG1	2:B:457:PHE:N	2.42	0.43
2:B:482:TRP:CD1	2:B:505:PRO:C	2.97	0.43
2:B:517:CYS:HB2	2:B:523:ARG:HG2	1.99	0.43
2:B:526:LEU:O	2:B:527:LEU:CD2	2.64	0.43
1:A:260:LEU:HA	1:A:260:LEU:HD23	1.74	0.43
1:A:267:TYR:CE2	1:A:423:TYR:CZ	3.07	0.43
1:A:337:LEU:N	1:A:368:VAL:CG1	2.82	0.43
1:A:358:ARG:O	1:A:359:CYS:C	2.61	0.43
2:B:261:LEU:CD2	2:B:262:GLN:HG3	2.46	0.43
2:B:293:TRP:CZ3	2:B:311:THR:O	2.72	0.43
2:B:483:ARG:HH11	2:B:484:ARG:HA	1.83	0.43
1:A:498:SER:N	1:A:502:SER:OG	2.52	0.42
2:B:357:LYS:O	2:B:358:ALA:CB	2.67	0.42
1:A:300:VAL:O	1:A:300:VAL:CG1	2.67	0.42
1:A:347:GLY:O	1:A:348:ARG:C	2.62	0.42
2:B:317:ARG:HG3	2:B:364:VAL:CG2	2.45	0.42
2:B:482:TRP:HH2	2:B:510:LEU:HG	1.84	0.42
1:A:309:VAL:HG13	1:A:310:TRP:N	2.34	0.42
1:A:365:VAL:HG12	1:A:367:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:MET:CA	1:A:485:VAL:HG12	2.44	0.42
2:B:253:ILE:HD12	2:B:279:ARG:HB2	2.01	0.42
2:B:254:VAL:O	2:B:280:CYS:HB3	2.19	0.42
2:B:416:GLN:NE2	2:B:416:GLN:CA	2.76	0.42
2:B:453:ASP:C	2:B:454:GLU:HG2	2.45	0.42
2:B:547:PRO:C	2:B:549:LEU:N	2.76	0.42
1:A:309:VAL:CG1	1:A:310:TRP:N	2.83	0.42
1:A:354:PHE:HB3	2:B:459:PHE:HZ	1.84	0.42
2:B:412:LEU:O	2:B:415:LEU:HG	2.20	0.42
2:B:471:VAL:HG11	2:B:478:LEU:CD2	2.49	0.42
1:A:350:ARG:HA	1:A:353:LYS:HB2	2.02	0.42
1:A:385:LEU:HA	1:A:388:VAL:HG23	2.01	0.42
1:A:453:LEU:HG	1:A:454:LEU:H	1.84	0.42
1:A:260:LEU:HD12	1:A:430:SER:O	2.19	0.42
1:A:354:PHE:HB3	2:B:459:PHE:CZ	2.54	0.42
1:A:404:ASP:C	1:A:406:LYS:N	2.77	0.42
1:A:405:ILE:CA	1:A:408:SER:OG	2.68	0.42
1:A:501:ALA:HB3	2:B:560:LEU:HD12	2.01	0.42
2:B:490:ASN:HB2	2:B:552:ARG:HH22	1.84	0.42
2:B:252:ILE:HA	2:B:295:ARG:HA	2.01	0.42
2:B:464:ASP:HB2	2:B:467:GLY:N	2.35	0.42
2:B:566:LEU:O	2:B:567:ASP:C	2.63	0.42
1:A:426:HIS:HB2	1:A:427:THR:H	1.53	0.42
1:A:501:ALA:CB	2:B:560:LEU:HD12	2.50	0.42
1:A:345:ILE:HD12	1:A:345:ILE:HA	1.88	0.42
1:A:472:ARG:HG2	2:B:457:PHE:HE1	1.85	0.42
1:A:551:THR:OG1	2:B:476:ARG:HA	2.20	0.42
2:B:343:LEU:CD1	2:B:348:THR:O	2.68	0.42
2:B:354:THR:HG21	2:B:359:LEU:CD1	2.46	0.42
1:A:413:ALA:O	1:A:415:LEU:N	2.53	0.42
1:A:522:THR:HA	1:A:532:LEU:HB2	2.01	0.42
2:B:416:GLN:NE2	2:B:417:LEU:H	2.15	0.42
2:B:480:LEU:O	2:B:481:VAL:C	2.61	0.42
2:B:511:VAL:C	2:B:514:TYR:HB2	2.44	0.42
1:A:308:PHE:O	1:A:309:VAL:HB	2.17	0.41
1:A:474:VAL:CB	2:B:556:GLN:OE1	2.66	0.41
1:A:497:TYR:HB3	1:A:503:LEU:CD2	2.49	0.41
1:A:424:GLN:HE21	1:A:424:GLN:HB3	1.61	0.41
1:A:463:ALA:C	1:A:465:LYS:H	2.28	0.41
1:A:543:LEU:HB2	2:B:507:PRO:CD	2.50	0.41
2:B:252:ILE:HD11	2:B:295:ARG:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:GLY:O	2:B:269:LEU:HB3	2.19	0.41
2:B:359:LEU:CD2	2:B:359:LEU:N	2.83	0.41
1:A:275:ILE:O	1:A:275:ILE:CG2	2.67	0.41
1:A:480:MET:HE3	1:A:480:MET:HB2	1.90	0.41
1:A:522:THR:O	1:A:523:ILE:CB	2.67	0.41
2:B:255:VAL:HG22	2:B:281:VAL:N	2.35	0.41
2:B:270:LEU:HG	2:B:274:GLN:CD	2.45	0.41
1:A:470:SER:C	1:A:472:ARG:N	2.77	0.41
2:B:268:GLN:NE2	2:B:430:LYS:HA	2.36	0.41
1:A:290:GLU:OE2	1:A:291:LEU:HD21	2.19	0.41
2:B:271:GLY:O	2:B:273:LEU:N	2.54	0.41
2:B:309:GLU:OE2	2:B:310:PRO:HD3	2.20	0.41
2:B:313:LEU:HD12	2:B:361:LEU:CA	2.50	0.41
2:B:319:GLU:HB2	2:B:320:ALA:H	1.77	0.41
1:A:299:THR:HG21	1:A:301:ARG:CZ	2.51	0.41
1:A:396:GLY:N	1:A:397:PHE:CD1	2.87	0.41
1:A:486:SER:HB3	1:A:489:LYS:N	2.30	0.41
2:B:494:LEU:H	2:B:494:LEU:CD2	2.21	0.41
2:B:501:VAL:O	2:B:501:VAL:CG1	2.67	0.41
2:B:555:LEU:HD23	2:B:555:LEU:HA	1.83	0.41
1:A:398:PHE:CG	1:A:399:VAL:N	2.88	0.41
1:A:465:LYS:O	1:A:466:ASN:HB2	2.21	0.41
2:B:493:SER:N	2:B:496:MET:SD	2.94	0.41
2:B:496:MET:O	2:B:500:VAL:HG22	2.21	0.41
1:A:274:ASP:OD1	1:A:276:GLY:N	2.54	0.41
1:A:333:GLU:HB3	1:A:366:TYR:CE2	2.55	0.41
1:A:499:THR:OG1	2:B:560:LEU:C	2.63	0.41
1:A:538:ARG:CZ	1:A:542:GLN:HE22	2.33	0.41
2:B:258:PRO:CA	2:B:282:ILE:HG22	2.51	0.41
2:B:264:GLU:HB3	2:B:429:TRP:NE1	2.36	0.41
2:B:269:LEU:HD12	2:B:270:LEU:N	2.36	0.41
2:B:290:SER:CA	2:B:314:VAL:HG12	2.51	0.41
2:B:413:VAL:O	2:B:414:ASP:HB2	2.20	0.41
2:B:496:MET:O	2:B:498:SER:N	2.53	0.41
1:A:478:GLN:HB2	2:B:485:GLN:OE1	2.21	0.41
2:B:264:GLU:C	2:B:429:TRP:HE1	2.29	0.41
2:B:315:LEU:HD22	2:B:316:LEU:CA	2.50	0.41
2:B:458:SER:O	2:B:461:LEU:HG	2.21	0.41
1:A:353:LYS:HZ3	1:A:353:LYS:C	2.29	0.40
2:B:255:VAL:O	2:B:292:THR:C	2.65	0.40
1:A:268:ARG:NH1	1:A:314:GLU:C	2.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:468:GLY:H	2:B:484:ARG:HH22	1.68	0.40
2:B:487:GLN:HA	2:B:492:VAL:HG11	2.03	0.40
1:A:357:LYS:N	1:A:359:CYS:SG	2.95	0.40
1:A:388:VAL:O	1:A:391:THR:N	2.53	0.40
1:A:389:THR:HG21	2:B:438:ALA:HB3	2.03	0.40
1:A:478:GLN:O	2:B:485:GLN:NE2	2.54	0.40
1:A:524:LYS:HA	1:A:530:ARG:O	2.21	0.40
1:A:272:CYS:O	1:A:308:PHE:CB	2.67	0.40
1:A:296:VAL:HG11	1:A:416:THR:CG2	2.44	0.40
2:B:517:CYS:C	2:B:518:PHE:O	2.63	0.40
1:A:328:LEU:HD21	1:A:330:HIS:CE1	2.56	0.40
1:A:328:LEU:HD12	1:A:329:ASP:N	2.37	0.40
1:A:337:LEU:CB	1:A:376:ASN:HD21	2.31	0.40
1:A:389:THR:OG1	1:A:390:ASN:N	2.54	0.40
1:A:479:LEU:O	1:A:481:GLN:N	2.53	0.40
1:A:491:ALA:CB	1:A:492:ALA:CA	2.96	0.40
1:A:546:SER:C	1:A:548:GLY:N	2.80	0.40
2:B:318:ALA:HB1	2:B:321:PHE:HD2	1.87	0.40

All (2) 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)
2:B:266:GLY:O	2:B:266:GLY:O[6_555]	1.90	0.30
1:A:380:PRO:CD	1:A:538:ARG:NH1[4_555]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	262/307 (85%)	127 (48%)	59 (22%)	76 (29%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	247/341 (72%)	100 (40%)	81 (33%)	66 (27%)	0	0
All	All	509/648 (78%)	227 (45%)	140 (28%)	142 (28%)	0	0

All (142) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	LEU
1	A	263	ARG
1	A	279	ARG
1	A	285	PRO
1	A	305	VAL
1	A	324	GLY
1	A	329	ASP
1	A	334	ARG
1	A	349	PHE
1	A	359	CYS
1	A	362	GLU
1	A	370	GLU
1	A	373	SER
1	A	380	PRO
1	A	382	SER
1	A	388	VAL
1	A	418	GLY
1	A	424	GLN
1	A	464	ILE
1	A	481	GLN
1	A	499	THR
1	A	510	CYS
1	A	523	ILE
1	A	531	ASN
1	A	535	ALA
1	A	536	LEU
1	A	542	GLN
2	B	249	LEU
2	B	260	LEU
2	B	268	GLN
2	B	284	ALA
2	B	291	VAL
2	B	306	TRP
2	B	349	ASP
2	B	406	VAL
2	B	414	ASP

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Mol	Chain	Res	Type
2	B	417	LEU
2	B	426	VAL
2	B	428	SER
2	B	430	LYS
2	B	432	LEU
2	B	440	THR
2	B	442	ALA
2	B	445	GLU
2	B	474	ALA
2	B	482	TRP
2	B	483	ARG
2	B	491	ARG
2	B	494	LEU
2	B	518	PHE
2	B	519	SER
2	B	532	VAL
2	B	543	ARG
2	B	552	ARG
2	B	556	GLN
2	B	563	HIS
1	A	286	GLU
1	A	295	HIS
1	A	307	ASP
1	A	309	VAL
1	A	310	TRP
1	A	327	VAL
1	A	342	SER
1	A	348	ARG
1	A	378	SER
1	A	381	GLU
1	A	391	THR
1	A	402	THR
1	A	406	LYS
1	A	428	LEU
1	A	457	SER
1	A	466	ASN
1	A	491	ALA
1	A	492	ALA
1	A	524	LYS
1	A	525	CYS
1	A	526	GLY
1	A	529	GLN

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Mol	Chain	Res	Type
1	A	549	PRO
2	B	285	GLN
2	B	308	GLU
2	B	310	PRO
2	B	312	VAL
2	B	361	LEU
2	B	433	ALA
2	B	435	PHE
2	B	473	LEU
2	B	488	GLN
2	B	497	ALA
2	B	503	ALA
2	B	548	GLU
2	B	566	LEU
1	A	265	GLY
1	A	273	VAL
1	A	288	LEU
1	A	414	LEU
1	A	416	THR
1	A	458	ASP
1	A	475	PHE
1	A	476	ALA
1	A	519	LEU
1	A	534	PRO
1	A	538	ARG
2	B	272	ALA
2	B	421	ALA
2	B	423	ALA
2	B	446	ALA
2	B	458	SER
2	B	479	ALA
2	B	487	GLN
2	B	547	PRO
1	A	264	PRO
1	A	325	GLU
1	A	427	THR
1	A	453	LEU
1	A	521	SER
1	A	546	SER
2	B	250	LYS
2	B	258	PRO
2	B	348	THR

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Mol	Chain	Res	Type
2	B	462	GLU
2	B	507	PRO
2	B	508	GLN
2	B	522	GLU
1	A	347	GLY
1	A	390	ASN
1	A	419	LEU
1	A	460	ASN
1	A	471	VAL
1	A	547	TYR
2	B	265	GLY
2	B	343	LEU
2	B	434	ASP
2	B	468	GLY
2	B	248	CYS
2	B	281	VAL
2	B	444	ALA
2	B	530	ILE
2	B	535	GLY
1	A	431	ARG
1	A	379	LEU
1	A	500	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/260 (90%)	141 (60%)	92 (40%)	0	1
2	B	220/290 (76%)	130 (59%)	90 (41%)	0	0
All	All	453/550 (82%)	271 (60%)	182 (40%)	0	1

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	GLU

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Mol	Chain	Res	Type
1	A	263	ARG
1	A	266	GLU
1	A	267	TYR
1	A	268	ARG
1	A	269	VAL
1	A	271	LEU
1	A	286	GLU
1	A	289	ARG
1	A	293	ARG
1	A	294	LEU
1	A	297	THR
1	A	298	HIS
1	A	299	THR
1	A	303	LEU
1	A	304	HIS
1	A	305	VAL
1	A	308	PHE
1	A	309	VAL
1	A	313	GLN
1	A	314	GLU
1	A	327	VAL
1	A	331	ILE
1	A	337	LEU
1	A	339	ASP
1	A	340	LEU
1	A	342	SER
1	A	343	SER
1	A	344	ILE
1	A	346	ASP
1	A	351	GLU
1	A	353	LYS
1	A	357	LYS
1	A	358	ARG
1	A	361	LEU
1	A	364	ARG
1	A	369	GLU
1	A	371	HIS
1	A	373	SER
1	A	374	VAL
1	A	375	HIS
1	A	376	ASN
1	A	377	LEU

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Mol	Chain	Res	Type
1	A	379	LEU
1	A	380	PRO
1	A	385	LEU
1	A	391	THR
1	A	392	GLN
1	A	395	ASP
1	A	399	VAL
1	A	400	LYS
1	A	404	ASP
1	A	405	ILE
1	A	412	LEU
1	A	414	LEU
1	A	416	THR
1	A	417	ARG
1	A	421	ARG
1	A	422	LEU
1	A	423	TYR
1	A	428	LEU
1	A	429	ARG
1	A	430	SER
1	A	431	ARG
1	A	450	LEU
1	A	454	LEU
1	A	464	ILE
1	A	469	GLN
1	A	477	ARG
1	A	478	GLN
1	A	482	VAL
1	A	483	ARG
1	A	485	VAL
1	A	488	GLU
1	A	498	SER
1	A	503	LEU
1	A	504	LEU
1	A	512	THR
1	A	516	GLN
1	A	517	GLU
1	A	520	LEU
1	A	523	ILE
1	A	524	LYS
1	A	525	CYS
1	A	529	GLN

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Mol	Chain	Res	Type
1	A	530	ARG
1	A	532	LEU
1	A	539	THR
1	A	540	LEU
1	A	543	LEU
1	A	550	LEU
1	A	551	THR
2	B	247	GLU
2	B	254	VAL
2	B	257	ASP
2	B	260	LEU
2	B	261	LEU
2	B	262	GLN
2	B	263	MET
2	B	269	LEU
2	B	274	GLN
2	B	278	CYS
2	B	282	ILE
2	B	285	GLN
2	B	287	VAL
2	B	289	CYS
2	B	290	SER
2	B	292	THR
2	B	293	TRP
2	B	305	ASP
2	B	312	VAL
2	B	313	LEU
2	B	315	LEU
2	B	316	LEU
2	B	319	GLU
2	B	322	VAL
2	B	326	ASP
2	B	327	ASN
2	B	342	THR
2	B	343	LEU
2	B	348	THR
2	B	353	LYS
2	B	359	LEU
2	B	364	VAL
2	B	365	ASP
2	B	367	GLU
2	B	409	GLU

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Mol	Chain	Res	Type
2	B	410	GLU
2	B	416	GLN
2	B	417	LEU
2	B	419	THR
2	B	424	GLN
2	B	425	ILE
2	B	427	GLN
2	B	429	TRP
2	B	432	LEU
2	B	434	ASP
2	B	439	PHE
2	B	443	VAL
2	B	445	GLU
2	B	451	LEU
2	B	452	ARG
2	B	455	THR
2	B	457	PHE
2	B	459	PHE
2	B	461	LEU
2	B	463	SER
2	B	472	ASP
2	B	473	LEU
2	B	476	ARG
2	B	478	LEU
2	B	480	LEU
2	B	483	ARG
2	B	486	ILE
2	B	487	GLN
2	B	488	GLN
2	B	491	ARG
2	B	494	LEU
2	B	496	MET
2	B	500	VAL
2	B	510	LEU
2	B	514	TYR
2	B	522	GLU
2	B	526	LEU
2	B	529	ASP
2	B	530	ILE
2	B	531	GLN
2	B	534	ARG
2	B	536	GLU

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Mol	Chain	Res	Type
2	B	542	SER
2	B	543	ARG
2	B	544	ARG
2	B	545	ILE
2	B	548	GLU
2	B	552	ARG
2	B	555	LEU
2	B	558	THR
2	B	559	THR
2	B	560	LEU
2	B	565	SER
2	B	566	LEU
2	B	568	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	GLN
1	A	313	GLN
1	A	371	HIS
1	A	376	ASN
1	A	386	GLN
1	A	424	GLN
1	A	426	HIS
1	A	466	ASN
1	A	469	GLN
1	A	481	GLN
1	A	542	GLN
2	B	327	ASN
2	B	416	GLN
2	B	422	GLN
2	B	485	GLN
2	B	487	GLN
2	B	490	ASN
2	B	508	GLN
2	B	515	GLN
2	B	525	ASN
2	B	531	GLN

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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	270/307 (87%)	-1.22	0 100 100	8, 34, 44, 53	0
2	B	259/341 (75%)	-1.23	0 100 100	15, 35, 45, 52	0
All	All	529/648 (81%)	-1.23	0 100 100	8, 34, 44, 53	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.