



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:10 AM UTC

PDB ID : 1KTV / pdb_00001ktv
Title : Crystal Structure of Elongation Factor G Dimer Without Nucleotide
Authors : Laurberg, M.; Kristensen, O.; Su, X.D.; Liljas, A.
Deposited on : 2002-01-17
Resolution : 3.80 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

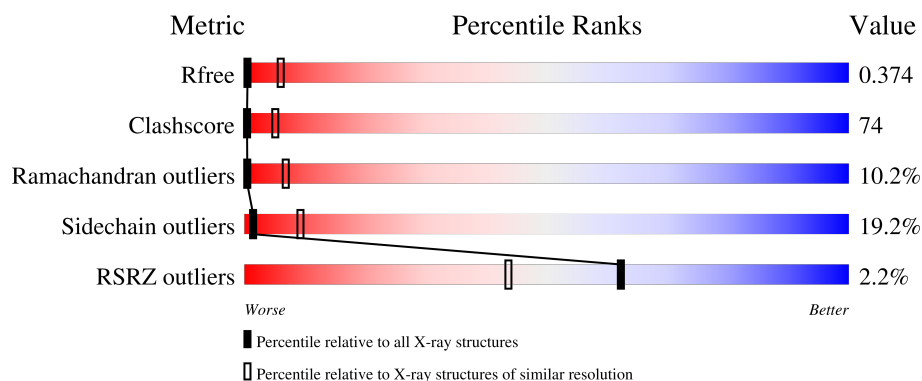
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	691	
1	B	691	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9914 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.

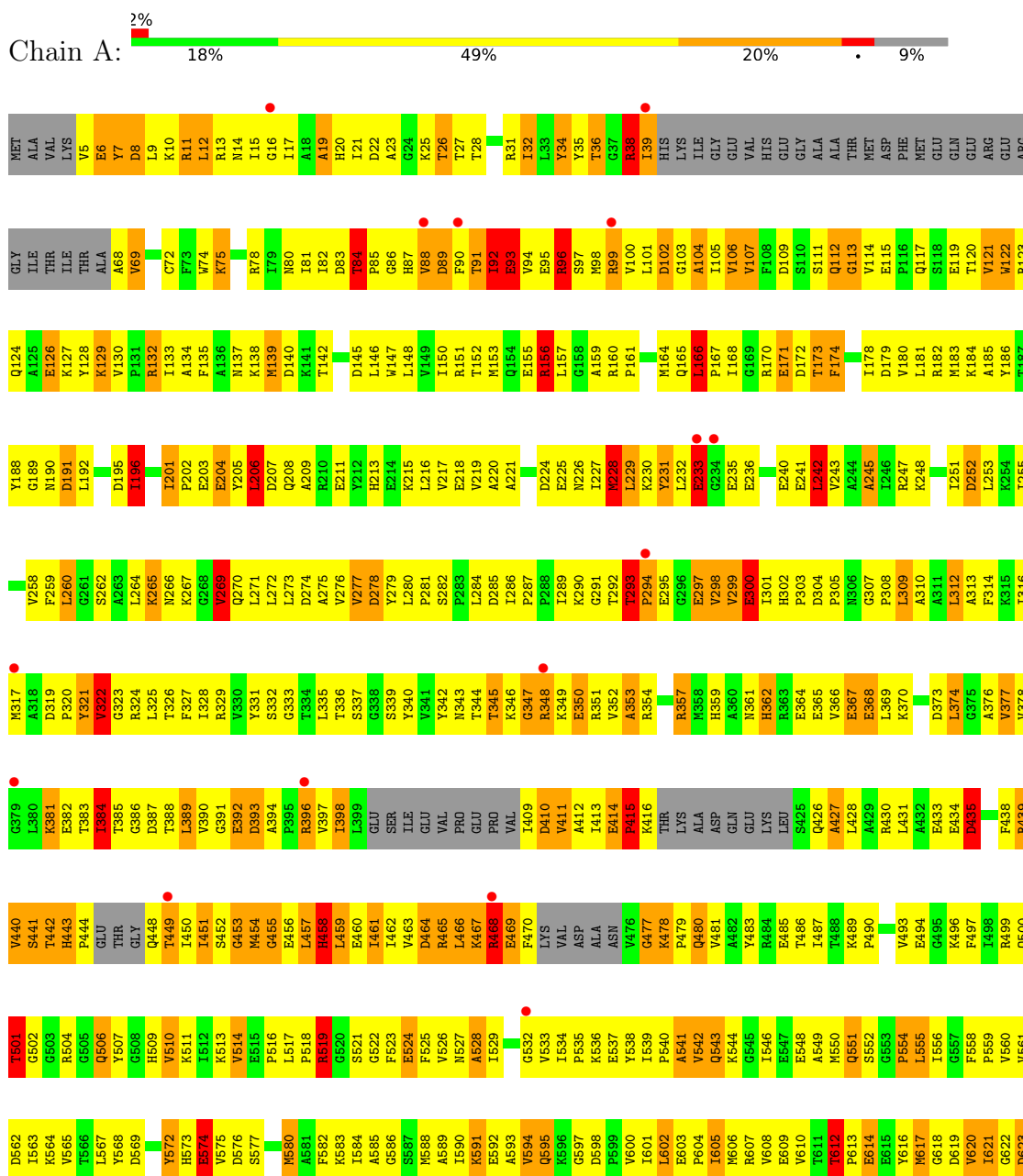
- Molecule 1 is a protein called ELONGATION FACTOR G.

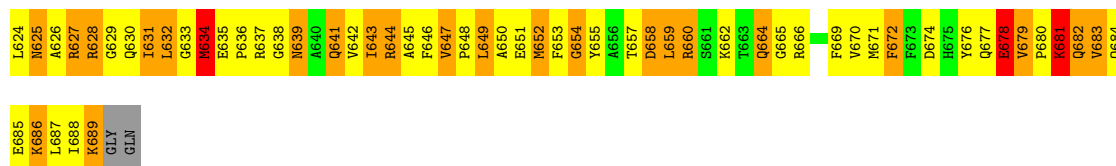
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	632	Total	C	N	O	S	0	0	0
			4957	3157	849	933	18			
1	B	632	Total	C	N	O	S	0	0	0
			4957	3157	849	933	18			

3 Residue-property plots

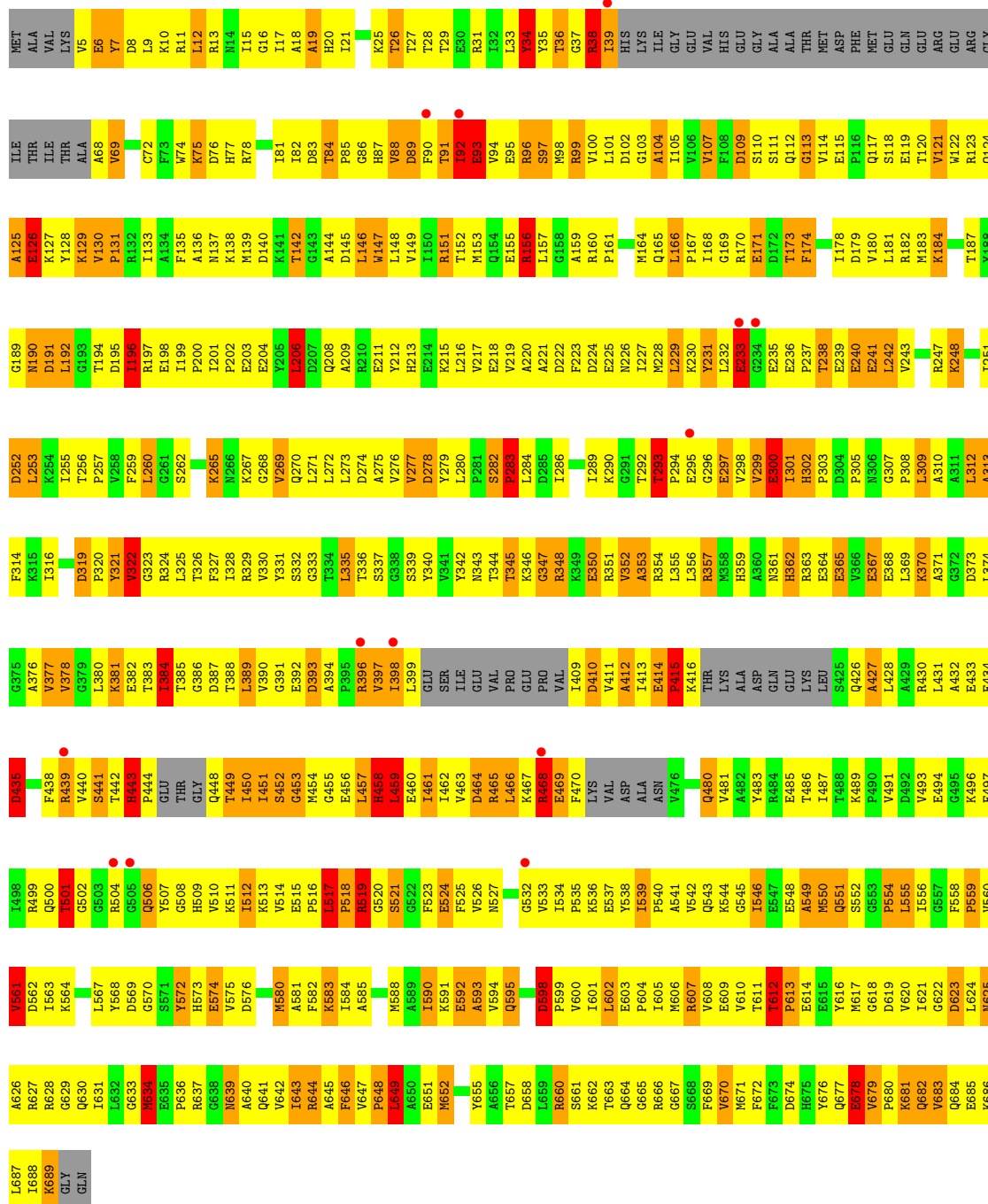
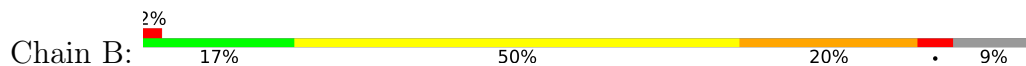
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: ELONGATION FACTOR G





• Molecule 1: ELONGATION FACTOR G



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.99Å 103.55Å 176.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.73 – 3.80 39.73 – 3.80	Depositor EDS
% Data completeness (in resolution range)	82.4 (39.73-3.80) 82.3 (39.73-3.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.287 , 0.374 0.278 , 0.374	Depositor DCC
R_{free} test set	727 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9914	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2024e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.79	5/5048 (0.1%)	1.33	64/6829 (0.9%)
1	B	0.83	3/5048 (0.1%)	1.36	69/6829 (1.0%)
All	All	0.81	8/10096 (0.1%)	1.34	133/13658 (1.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	TRP	NE1-CE2	-10.20	1.26	1.37
1	A	106	VAL	CA-CB	-6.11	1.46	1.53
1	B	302	HIS	CA-C	-5.92	1.46	1.52
1	A	122	TRP	NE1-CE2	5.79	1.43	1.37
1	A	542	VAL	CA-CB	-5.23	1.48	1.54
1	B	598	ASP	CA-C	-5.23	1.50	1.53
1	A	634	MET	SD-CE	5.19	1.92	1.79
1	A	228	MET	SD-CE	-5.09	1.66	1.79

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	533	VAL	N-CA-C	-16.01	96.95	112.96
1	B	533	VAL	N-CA-C	-15.94	97.03	112.96
1	A	458	HIS	N-CA-C	-13.12	96.54	112.54
1	B	458	HIS	N-CA-C	-11.18	99.09	111.28
1	B	236	GLU	CA-C-N	10.86	130.62	119.76
1	B	236	GLU	C-N-CA	10.86	130.62	119.76
1	A	465	ARG	N-CA-C	-10.28	100.28	112.92
1	B	521	SER	N-CA-C	-10.03	96.71	110.35
1	A	451	ILE	N-CA-C	-8.85	98.03	109.80
1	B	465	ARG	N-CA-C	-8.77	102.13	112.92
1	A	173	THR	N-CA-C	-8.72	102.44	113.43
1	B	480	GLN	N-CA-C	8.67	122.89	110.14
1	B	450	ILE	N-CA-C	8.60	119.41	106.42
1	B	147	TRP	CD2-CE2-CZ2	-8.27	114.13	122.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	SER	N-CA-C	-8.11	99.49	110.36
1	A	121	VAL	N-CA-C	-8.06	102.48	110.30
1	A	453	GLY	N-CA-C	7.90	131.90	113.18
1	B	256	THR	CA-C-N	7.85	127.87	119.78
1	B	256	THR	C-N-CA	7.85	127.87	119.78
1	A	477	GLY	N-CA-C	7.69	122.69	111.24
1	A	299	VAL	N-CA-C	7.66	119.76	108.65
1	B	551	GLN	N-CA-C	7.35	119.93	111.11
1	A	594	VAL	CB-CA-C	-7.26	102.51	112.02
1	B	450	ILE	CB-CA-C	-7.10	104.06	111.23
1	B	453	GLY	N-CA-C	7.05	129.88	113.18
1	B	441	SER	N-CA-C	7.02	120.94	109.85
1	B	459	LEU	N-CA-C	-7.01	103.68	111.82
1	A	294	PRO	N-CA-C	-6.97	100.95	111.41
1	B	439	ARG	N-CA-C	6.93	120.05	108.13
1	B	121	VAL	N-CA-C	-6.92	103.59	110.30
1	B	300	GLU	N-CA-C	6.83	119.98	108.23
1	A	255	ILE	N-CA-C	6.80	117.95	108.23
1	B	255	ILE	N-CA-C	6.80	120.19	108.90
1	A	285	ASP	N-CA-C	-6.78	103.81	111.14
1	A	414	GLU	CA-C-N	6.78	128.31	119.84
1	A	414	GLU	C-N-CA	6.78	128.31	119.84
1	A	441	SER	N-CA-C	6.76	120.18	109.50
1	B	173	THR	N-CA-C	-6.72	104.12	112.72
1	A	459	LEU	N-CA-C	-6.68	104.07	111.82
1	B	546	ILE	N-CA-C	-6.68	104.00	110.42
1	A	156	ARG	N-CA-C	6.65	118.19	111.07
1	A	521	SER	N-CA-C	-6.65	101.31	110.35
1	A	132	ARG	N-CA-C	6.64	119.41	108.99
1	B	461	ILE	N-CA-C	-6.62	103.01	112.35
1	A	583	LYS	N-CA-C	-6.61	104.69	112.89
1	B	309	LEU	N-CA-C	6.61	120.26	110.48
1	A	231	TYR	N-CA-C	-6.60	103.78	110.97
1	A	93	GLU	N-CA-C	-6.58	96.78	110.80
1	B	517	LEU	N-CA-C	-6.46	102.00	110.39
1	A	480	GLN	N-CA-C	6.32	119.83	109.72
1	A	461	ILE	N-CA-C	-6.28	103.49	112.35
1	A	612	THR	CA-C-N	-6.28	113.82	120.03
1	A	612	THR	C-N-CA	-6.28	113.82	120.03
1	A	245	ALA	N-CA-C	-6.20	104.06	111.69
1	A	412	ALA	N-CA-C	6.18	121.90	113.37
1	B	299	VAL	N-CA-C	6.14	119.08	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	THR	CA-C-N	-6.12	113.97	120.03
1	A	293	THR	C-N-CA	-6.12	113.97	120.03
1	B	469	GLU	N-CA-C	-6.11	104.70	111.36
1	A	8	ASP	N-CA-C	-6.10	97.89	108.69
1	B	452	SER	N-CA-C	6.07	119.41	108.48
1	B	293	THR	CA-C-N	-6.03	113.36	120.11
1	B	293	THR	C-N-CA	-6.03	113.36	120.11
1	B	397	VAL	N-CA-C	6.02	118.67	108.86
1	A	233	GLU	N-CA-C	-5.99	98.05	110.80
1	A	659	LEU	N-CA-C	-5.98	104.09	111.33
1	B	278	ASP	N-CA-C	5.97	117.46	111.07
1	B	156	ARG	N-CA-C	5.93	118.70	111.82
1	A	293	THR	N-CA-C	-5.92	102.69	110.39
1	B	451	ILE	N-CA-C	-5.91	100.44	109.78
1	B	319	ASP	CA-C-N	5.90	125.60	119.05
1	B	319	ASP	C-N-CA	5.90	125.60	119.05
1	B	147	TRP	CE2-CD2-CE3	5.89	124.69	118.80
1	B	412	ALA	N-CA-C	5.89	123.35	110.80
1	B	607	ARG	N-CA-C	-5.88	99.59	109.07
1	B	519	ARG	N-CA-C	-5.87	101.62	110.24
1	A	278	ASP	N-CA-C	5.85	118.16	111.02
1	A	168	ILE	N-CA-C	-5.76	100.14	108.89
1	B	612	THR	CB-CA-C	-5.72	101.69	109.42
1	B	125	ALA	N-CA-C	-5.70	104.27	111.11
1	A	81	ILE	N-CA-C	5.68	115.52	106.88
1	B	414	GLU	CA-C-N	5.67	126.93	119.84
1	B	414	GLU	C-N-CA	5.67	126.93	119.84
1	A	605	ILE	N-CA-C	-5.66	102.28	109.58
1	A	439	ARG	N-CA-C	5.64	117.84	108.13
1	A	469	GLU	N-CA-C	-5.63	105.29	111.82
1	B	613	PRO	N-CA-C	-5.62	102.62	111.34
1	B	233	GLU	N-CA-C	-5.61	98.85	110.80
1	A	433	GLU	N-CA-C	-5.56	104.91	110.97
1	B	109	ASP	N-CA-C	-5.52	99.52	108.41
1	A	528	ALA	N-CA-C	-5.51	106.91	113.97
1	B	282	SER	N-CA-C	-5.50	102.53	110.40
1	A	658	ASP	N-CA-C	-5.50	104.92	111.03
1	B	93	GLU	N-CA-C	-5.49	99.10	110.80
1	A	281	PRO	N-CA-C	5.46	120.66	111.32
1	B	231	TYR	N-CA-C	-5.45	105.24	111.07
1	B	313	ALA	N-CA-C	-5.44	100.82	109.96
1	B	443	HIS	N-CA-C	5.41	121.76	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	ALA	N-CA-C	-5.39	105.30	111.07
1	B	130	VAL	CA-C-N	5.36	125.62	119.83
1	B	130	VAL	C-N-CA	5.36	125.62	119.83
1	A	628	ARG	N-CA-C	-5.34	106.72	113.23
1	A	594	VAL	N-CA-C	5.32	115.53	110.53
1	B	370	LYS	N-CA-C	5.32	117.55	110.53
1	A	166	LEU	CA-C-N	-5.28	113.24	119.84
1	A	166	LEU	C-N-CA	-5.28	113.24	119.84
1	A	533	VAL	CA-C-O	5.25	123.70	119.29
1	A	150	ILE	CB-CA-C	-5.24	104.03	112.16
1	A	519	ARG	N-CA-C	-5.23	102.30	110.10
1	A	551	GLN	N-CA-C	5.20	117.35	111.11
1	A	620	VAL	N-CA-C	-5.20	106.62	111.45
1	B	512	ILE	N-CA-C	5.19	115.15	108.82
1	A	309	LEU	N-CA-C	5.19	117.41	110.35
1	A	84	THR	CA-C-N	5.18	126.32	119.84
1	A	84	THR	C-N-CA	5.18	126.32	119.84
1	A	621	ILE	N-CA-C	-5.18	106.18	112.76
1	A	96	ARG	N-CA-C	-5.17	105.53	111.07
1	A	300	GLU	N-CA-C	5.15	117.09	108.23
1	B	142	THR	N-CA-C	5.15	121.77	110.80
1	B	190	ASN	N-CA-C	5.14	115.95	108.14
1	A	236	GLU	CA-C-N	5.12	125.03	119.85
1	A	236	GLU	C-N-CA	5.12	125.03	119.85
1	B	433	GLU	N-CA-C	-5.12	105.38	110.97
1	B	8	ASP	N-CA-C	-5.12	99.26	108.48
1	B	34	TYR	N-CA-C	-5.09	105.62	111.07
1	B	198	GLU	N-CA-C	-5.06	102.79	110.28
1	B	674	ASP	N-CA-C	5.04	119.42	113.12
1	B	115	GLU	CA-C-N	5.03	126.13	119.84
1	B	115	GLU	C-N-CA	5.03	126.13	119.84
1	B	598	ASP	CA-C-N	5.03	124.94	119.76
1	B	598	ASP	C-N-CA	5.03	124.94	119.76
1	B	549	ALA	N-CA-C	-5.02	104.89	111.02
1	B	583	LYS	N-CA-C	-5.01	107.02	113.23

There are no chirality outliers.

There are no planarity outliers.

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	4957	0	5021	738	0
1	B	4957	0	5021	753	0
All	All	9914	0	10042	1479	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 74.

All (1479) 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:B:411:VAL:HB	1:B:453:GLY:CA	1.63	1.28
1:A:411:VAL:HB	1:A:453:GLY:CA	1.69	1.19
1:A:411:VAL:HB	1:A:453:GLY:HA2	1.26	1.09
1:B:276:VAL:HG13	1:B:280:LEU:HD12	1.29	1.08
1:B:321:TYR:O	1:B:322:VAL:HG22	1.51	1.08
1:A:276:VAL:HG13	1:A:280:LEU:HD12	1.35	1.05
1:B:5:VAL:HG13	1:B:6:GLU:H	1.16	1.05
1:B:87:HIS:NE2	1:B:90:PHE:HB2	1.72	1.05
1:A:87:HIS:NE2	1:A:90:PHE:HB2	1.73	1.03
1:B:6:GLU:HG2	1:B:7:TYR:H	1.19	1.03
1:B:411:VAL:CB	1:B:453:GLY:HA3	1.89	1.02
1:A:221:ALA:HB1	1:A:228:MET:HE3	1.41	1.00
1:B:329:ARG:HA	1:B:374:LEU:HB3	1.43	0.99
1:A:5:VAL:HG13	1:A:6:GLU:H	1.26	0.99
1:A:434:GLU:O	1:A:435:ASP:HB2	1.63	0.97
1:A:459:LEU:HD12	1:A:459:LEU:H	1.28	0.97
1:A:612:THR:HG21	1:A:620:VAL:HG21	1.44	0.96
1:B:434:GLU:O	1:B:435:ASP:HB2	1.62	0.96
1:B:411:VAL:HB	1:B:453:GLY:HA3	0.98	0.96
1:A:411:VAL:HB	1:A:453:GLY:HA3	1.48	0.95
1:A:329:ARG:HG3	1:A:374:LEU:HD23	1.48	0.95
1:B:457:LEU:HG	1:B:460:GLU:HB2	1.48	0.94
1:B:413:ILE:HD11	1:B:454:MET:O	1.67	0.94
1:A:224:ASP:HB3	1:A:227:ILE:HG13	1.49	0.94
1:B:346:LYS:HE3	1:B:382:GLU:O	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:ILE:HG13	1:B:689:LYS:NZ	1.83	0.94
1:A:6:GLU:HG2	1:A:7:TYR:H	1.31	0.93
1:A:213:HIS:O	1:A:217:VAL:HG23	1.69	0.92
1:A:203:GLU:HA	1:A:206:LEU:HD23	1.49	0.92
1:B:561:VAL:O	1:B:563:ILE:HG23	1.70	0.92
1:B:203:GLU:HA	1:B:206:LEU:HD23	1.51	0.92
1:A:633:GLY:O	1:A:634:MET:HB3	1.68	0.91
1:A:181:LEU:HD21	1:A:243:VAL:HG22	1.52	0.91
1:B:6:GLU:CG	1:B:7:TYR:H	1.83	0.90
1:A:99:ARG:HD3	1:A:99:ARG:O	1.72	0.90
1:B:181:LEU:HD21	1:B:243:VAL:HG22	1.52	0.90
1:A:183:MET:HE1	1:A:209:ALA:HB1	1.51	0.90
1:A:427:ALA:HA	1:A:470:PHE:CE2	2.05	0.90
1:B:354:ARG:HG3	1:B:378:VAL:CG1	2.02	0.89
1:A:522:GLY:HA3	1:B:194:THR:O	1.73	0.89
1:A:11:ARG:HG3	1:A:11:ARG:HH11	1.37	0.88
1:B:99:ARG:O	1:B:99:ARG:HD3	1.73	0.88
1:A:426:GLN:HE21	1:A:430:ARG:NH2	1.70	0.88
1:A:657:THR:HA	1:A:660:ARG:HB2	1.56	0.87
1:A:346:LYS:HZ1	1:A:383:THR:HA	1.39	0.87
1:B:123:ARG:NH2	1:B:639:ASN:HB3	1.89	0.87
1:B:5:VAL:HG13	1:B:6:GLU:N	1.90	0.87
1:A:550:MET:SD	1:A:563:ILE:HD11	2.15	0.86
1:B:11:ARG:HG3	1:B:11:ARG:HH11	1.40	0.86
1:A:454:MET:HG2	1:A:455:GLY:H	1.39	0.86
1:B:290:LYS:HB3	1:B:298:VAL:HG12	1.54	0.86
1:B:213:HIS:O	1:B:217:VAL:HG23	1.75	0.86
1:B:224:ASP:HB3	1:B:227:ILE:HG13	1.58	0.86
1:B:329:ARG:HG3	1:B:374:LEU:HD23	1.57	0.86
1:A:321:TYR:O	1:A:322:VAL:HG22	1.74	0.86
1:B:164:MET:O	1:B:180:VAL:HG22	1.76	0.86
1:B:6:GLU:HG2	1:B:7:TYR:N	1.90	0.86
1:B:426:GLN:HE21	1:B:430:ARG:NH2	1.73	0.86
1:A:84:THR:HG22	1:A:85:PRO:HD2	1.58	0.85
1:A:329:ARG:HA	1:A:374:LEU:HB3	1.59	0.85
1:A:346:LYS:HE3	1:A:382:GLU:O	1.75	0.85
1:B:87:HIS:HE2	1:B:90:PHE:HB2	1.34	0.85
1:A:348:ARG:HH11	1:A:348:ARG:HB3	1.38	0.84
1:A:536:LYS:HA	1:A:539:ILE:HD12	1.58	0.84
1:A:500:GLN:C	1:A:502:GLY:H	1.82	0.84
1:B:339:SER:O	1:B:352:VAL:HG12	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ILE:HG23	1:A:133:ILE:HG13	1.60	0.84
1:B:481:VAL:HB	1:B:483:TYR:CE2	2.13	0.84
1:A:354:ARG:HG3	1:A:378:VAL:CG1	2.08	0.83
1:A:427:ALA:HA	1:A:470:PHE:CD2	2.12	0.83
1:A:309:LEU:HA	1:A:332:SER:O	1.79	0.83
1:A:680:PRO:HB2	1:A:682:GLN:HE21	1.44	0.83
1:B:612:THR:HG21	1:B:620:VAL:HG21	1.61	0.83
1:A:6:GLU:CG	1:A:7:TYR:H	1.91	0.82
1:B:289:ILE:HG23	1:B:301:ILE:HB	1.60	0.82
1:B:388:THR:HG21	1:B:397:VAL:O	1.78	0.82
1:A:411:VAL:CB	1:A:453:GLY:HA2	2.08	0.82
1:B:312:LEU:HD22	1:B:313:ALA:O	1.80	0.82
1:B:457:LEU:HG	1:B:460:GLU:CB	2.09	0.82
1:B:300:GLU:HB3	1:B:302:HIS:CE1	2.15	0.81
1:B:348:ARG:HH11	1:B:348:ARG:HB3	1.41	0.81
1:A:102:ASP:HB3	1:A:286:ILE:HD11	1.63	0.81
1:A:518:PRO:HG2	1:B:39:ILE:CG2	2.11	0.81
1:B:294:PRO:O	1:B:295:GLU:HB3	1.80	0.81
1:A:327:PHE:CE1	1:A:376:ALA:HB2	2.16	0.81
1:A:129:LYS:O	1:A:129:LYS:HG2	1.80	0.81
1:A:343:ASN:HD21	1:A:387:ASP:HB3	1.44	0.81
1:B:681:LYS:H	1:B:681:LYS:HD3	1.44	0.81
1:A:157:LEU:O	1:A:639:ASN:HB2	1.81	0.80
1:A:221:ALA:HB1	1:A:228:MET:HG3	1.63	0.80
1:B:221:ALA:HB1	1:B:228:MET:HE3	1.64	0.80
1:A:290:LYS:HA	1:A:299:VAL:O	1.81	0.80
1:A:481:VAL:HG13	1:A:649:LEU:HD12	1.61	0.80
1:B:680:PRO:HB2	1:B:682:GLN:HE21	1.45	0.80
1:B:519:ARG:HA	1:B:562:ASP:OD2	1.81	0.80
1:A:201:ILE:HD12	1:A:201:ILE:H	1.45	0.79
1:B:354:ARG:HG3	1:B:378:VAL:HG12	1.64	0.79
1:A:457:LEU:HG	1:A:460:GLU:HB2	1.65	0.79
1:B:427:ALA:HA	1:B:470:PHE:CE2	2.18	0.79
1:B:683:VAL:O	1:B:687:LEU:HG	1.83	0.79
1:A:221:ALA:CB	1:A:228:MET:HE3	2.12	0.79
1:B:688:ILE:HG13	1:B:689:LYS:HZ2	1.45	0.79
1:B:91:THR:O	1:B:93:GLU:N	2.16	0.79
1:B:119:GLU:O	1:B:122:TRP:HB3	1.83	0.79
1:B:357:ARG:HG3	1:B:357:ARG:HH11	1.47	0.79
1:A:165:GLN:HB2	1:A:178:ILE:O	1.82	0.79
1:B:97:SER:O	1:B:101:LEU:HD22	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HD21	1:A:208:GLN:HG2	1.63	0.79
1:B:165:GLN:HG3	1:B:260:LEU:CD1	2.12	0.78
1:B:411:VAL:HB	1:B:453:GLY:HA2	1.65	0.78
1:A:119:GLU:O	1:A:122:TRP:HB3	1.84	0.78
1:A:127:LYS:HB2	1:A:637:ARG:NH1	1.97	0.78
1:A:601:ILE:HD12	1:A:684:GLN:HG3	1.65	0.78
1:B:165:GLN:HB2	1:B:178:ILE:O	1.82	0.78
1:A:6:GLU:HG2	1:A:7:TYR:N	1.98	0.78
1:A:518:PRO:HG2	1:B:39:ILE:HG23	1.66	0.78
1:A:191:ASP:HA	1:A:265:LYS:O	1.83	0.78
1:A:5:VAL:HG13	1:A:6:GLU:N	1.98	0.78
1:A:290:LYS:HB3	1:A:298:VAL:HG12	1.65	0.78
1:A:573:HIS:ND1	1:A:576:ASP:HB2	1.98	0.78
1:A:190:ASN:HD21	1:A:195:ASP:HB2	1.48	0.77
1:A:388:THR:HG21	1:A:397:VAL:O	1.84	0.77
1:A:506:GLN:HA	1:A:576:ASP:O	1.83	0.77
1:A:606:MET:HB2	1:A:647:VAL:O	1.84	0.77
1:A:132:ARG:NH1	1:A:132:ARG:HG2	1.99	0.77
1:B:500:GLN:C	1:B:502:GLY:H	1.92	0.77
1:B:634:MET:HE3	1:B:634:MET:O	1.84	0.77
1:A:634:MET:HE3	1:A:634:MET:O	1.85	0.77
1:A:459:LEU:HD12	1:A:459:LEU:N	1.99	0.77
1:B:38:ARG:CG	1:B:39:ILE:H	1.97	0.77
1:B:276:VAL:CG1	1:B:280:LEU:HD12	2.12	0.77
1:A:25:LYS:NZ	1:A:84:THR:OG1	2.18	0.76
1:B:290:LYS:HA	1:B:299:VAL:O	1.86	0.76
1:A:221:ALA:HB1	1:A:228:MET:CE	2.15	0.76
1:A:688:ILE:HG13	1:A:689:LYS:NZ	2.01	0.76
1:A:548:GLU:O	1:A:551:GLN:HB2	1.85	0.76
1:B:634:MET:SD	1:B:634:MET:C	2.69	0.76
1:B:541:ALA:O	1:B:544:LYS:HB3	1.86	0.76
1:B:113:GLY:HA2	1:B:149:VAL:HG22	1.67	0.75
1:B:357:ARG:HB3	1:B:364:GLU:HB3	1.66	0.75
1:A:340:TYR:HB2	1:A:392:GLU:OE2	1.86	0.75
1:B:454:MET:HG2	1:B:455:GLY:H	1.51	0.75
1:A:157:LEU:C	1:A:639:ASN:HD22	1.94	0.75
1:B:517:LEU:HD22	1:B:521:SER:CB	2.15	0.75
1:B:345:THR:HG23	1:B:388:THR:H	1.51	0.75
1:B:455:GLY:O	1:B:458:HIS:HB3	1.86	0.75
1:A:346:LYS:NZ	1:A:383:THR:HA	2.01	0.75
1:A:294:PRO:O	1:A:295:GLU:HB3	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLU:OE1	1:B:666:ARG:NH1	2.19	0.75
1:A:357:ARG:HH22	1:A:373:ASP:CG	1.95	0.75
1:B:454:MET:HB3	1:B:458:HIS:CD2	2.22	0.75
1:A:34:TYR:CD1	1:A:34:TYR:C	2.64	0.74
1:A:535:PRO:HG2	1:A:538:TYR:CD2	2.22	0.74
1:A:681:LYS:HE3	1:A:682:GLN:HE22	1.52	0.74
1:A:91:THR:O	1:A:93:GLU:N	2.20	0.74
1:A:90:PHE:O	1:A:94:VAL:HG23	1.86	0.74
1:B:91:THR:O	1:B:94:VAL:N	2.18	0.74
1:B:652:MET:HE3	1:B:655:TYR:CD2	2.23	0.74
1:A:361:ASN:O	1:A:362:HIS:ND1	2.21	0.74
1:B:608:VAL:HG12	1:B:609:GLU:N	2.03	0.74
1:B:633:GLY:O	1:B:634:MET:HB3	1.87	0.74
1:B:319:ASP:HB2	1:B:325:LEU:HD12	1.67	0.74
1:A:605:ILE:HD11	1:A:677:GLN:HB3	1.69	0.74
1:A:91:THR:O	1:A:94:VAL:N	2.16	0.73
1:B:276:VAL:HG13	1:B:280:LEU:CD1	2.14	0.73
1:A:631:ILE:HD12	1:A:631:ILE:N	2.04	0.73
1:B:350:GLU:OE1	1:B:380:LEU:HD22	1.89	0.73
1:B:590:ILE:O	1:B:594:VAL:HG23	1.88	0.73
1:A:348:ARG:NH2	1:A:382:GLU:HG3	2.04	0.73
1:A:500:GLN:O	1:A:502:GLY:N	2.21	0.73
1:A:680:PRO:HG2	1:A:683:VAL:HG23	1.71	0.73
1:B:602:LEU:HD12	1:B:678:GLU:HA	1.69	0.73
1:B:11:ARG:HG3	1:B:11:ARG:NH1	2.03	0.73
1:A:293:THR:HG23	1:A:297:GLU:O	1.88	0.73
1:A:303:PRO:HA	1:A:331:TYR:O	1.87	0.73
1:B:468:ARG:NE	1:B:468:ARG:HA	2.04	0.73
1:B:443:HIS:ND1	1:B:450:ILE:HD11	2.04	0.73
1:B:229:LEU:H	1:B:229:LEU:CD1	2.02	0.73
1:B:201:ILE:HD12	1:B:201:ILE:H	1.54	0.73
1:A:190:ASN:ND2	1:A:195:ASP:HB2	2.02	0.72
1:B:459:LEU:H	1:B:459:LEU:HD12	1.53	0.72
1:B:605:ILE:CD1	1:B:677:GLN:HB3	2.19	0.72
1:A:680:PRO:HG2	1:A:683:VAL:CG2	2.20	0.72
1:B:606:MET:HB2	1:B:647:VAL:O	1.88	0.72
1:B:5:VAL:CG1	1:B:6:GLU:H	1.93	0.72
1:B:346:LYS:HZ1	1:B:383:THR:HA	1.55	0.72
1:A:165:GLN:HG3	1:A:260:LEU:HD13	1.71	0.72
1:A:357:ARG:HG3	1:A:357:ARG:HH11	1.54	0.71
1:A:166:LEU:CD2	1:A:208:GLN:HG2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ASN:O	1:B:362:HIS:ND1	2.23	0.71
1:A:114:VAL:HG11	1:A:157:LEU:HD11	1.72	0.71
1:A:413:ILE:HD11	1:A:454:MET:O	1.91	0.71
1:B:359:HIS:ND1	1:B:362:HIS:NE2	2.38	0.71
1:B:38:ARG:HG3	1:B:39:ILE:H	1.56	0.71
1:B:517:LEU:HD22	1:B:521:SER:HB3	1.71	0.71
1:A:605:ILE:CD1	1:A:677:GLN:HB3	2.20	0.70
1:A:500:GLN:O	1:A:501:THR:HG22	1.91	0.70
1:A:631:ILE:HD12	1:A:631:ILE:H	1.56	0.70
1:B:480:GLN:HE22	1:B:558:PHE:HZ	1.38	0.70
1:A:276:VAL:CG1	1:A:280:LEU:HD12	2.18	0.70
1:B:127:LYS:HB2	1:B:637:ARG:NH1	2.07	0.70
1:B:427:ALA:O	1:B:431:LEU:HG	1.92	0.70
1:B:554:PRO:HG2	1:B:594:VAL:HB	1.72	0.70
1:B:409:ILE:O	1:B:411:VAL:N	2.24	0.70
1:B:688:ILE:HG13	1:B:689:LYS:HZ1	1.57	0.70
1:A:524:GLU:OE1	1:A:564:LYS:HE3	1.91	0.70
1:B:191:ASP:HA	1:B:265:LYS:O	1.92	0.70
1:B:300:GLU:HB3	1:B:302:HIS:HE1	1.55	0.70
1:B:109:ASP:OD1	1:B:111:SER:HB2	1.92	0.70
1:A:295:GLU:HA	1:B:26:THR:OG1	1.91	0.69
1:A:459:LEU:H	1:A:459:LEU:CD1	2.03	0.69
1:A:289:ILE:HG23	1:A:301:ILE:HB	1.74	0.69
1:A:426:GLN:HE21	1:A:430:ARG:HH21	1.38	0.69
1:B:129:LYS:HG2	1:B:253:LEU:HD11	1.74	0.69
1:B:416:LYS:HA	1:B:449:THR:O	1.91	0.69
1:B:414:GLU:HB3	1:B:452:SER:HB2	1.74	0.69
1:B:120:THR:HA	1:B:123:ARG:HG3	1.74	0.69
1:B:354:ARG:HG3	1:B:378:VAL:HG11	1.74	0.69
1:A:11:ARG:HG3	1:A:11:ARG:NH1	2.04	0.69
1:A:132:ARG:HG2	1:A:132:ARG:HH11	1.57	0.69
1:A:427:ALA:HA	1:A:470:PHE:HE2	1.57	0.69
1:B:152:THR:O	1:B:155:GLU:N	2.25	0.69
1:B:84:THR:HG22	1:B:85:PRO:HD2	1.73	0.69
1:B:414:GLU:HB3	1:B:452:SER:CB	2.22	0.69
1:A:8:ASP:HB3	1:A:11:ARG:CG	2.23	0.69
1:A:191:ASP:O	1:A:192:LEU:HD23	1.93	0.69
1:A:359:HIS:ND1	1:A:362:HIS:NE2	2.40	0.69
1:A:170:ARG:H	1:A:173:THR:HB	1.56	0.68
1:A:416:LYS:HA	1:A:449:THR:O	1.92	0.68
1:A:486:THR:O	1:A:600:VAL:HG22	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:PRO:HG2	1:B:538:TYR:CD2	2.28	0.68
1:A:628:ARG:HD2	1:A:648:PRO:HG2	1.75	0.68
1:B:293:THR:HG23	1:B:297:GLU:O	1.93	0.68
1:B:329:ARG:HA	1:B:374:LEU:CB	2.23	0.68
1:B:681:LYS:HD3	1:B:681:LYS:N	2.08	0.68
1:A:184:LYS:HE2	1:A:186:TYR:OH	1.94	0.68
1:B:96:ARG:NH2	1:B:386:GLY:HA3	2.09	0.68
1:B:427:ALA:HA	1:B:470:PHE:CD2	2.29	0.68
1:B:552:SER:O	1:B:591:LYS:HE3	1.94	0.68
1:A:467:LYS:HG2	1:A:467:LYS:O	1.94	0.68
1:A:357:ARG:NH2	1:A:373:ASP:OD2	2.26	0.68
1:A:554:PRO:HG2	1:A:594:VAL:HB	1.75	0.68
1:A:384:ILE:C	1:A:387:ASP:OD2	2.37	0.68
1:B:26:THR:HG22	1:B:27:THR:N	2.07	0.68
1:B:95:GLU:HB2	1:B:128:TYR:OH	1.93	0.68
1:B:328:ILE:O	1:B:374:LEU:HB2	1.94	0.67
1:B:114:VAL:HG11	1:B:157:LEU:HD11	1.74	0.67
1:B:367:GLU:O	1:B:368:GLU:HB3	1.95	0.67
1:A:339:SER:O	1:A:352:VAL:HG12	1.94	0.67
1:B:573:HIS:ND1	1:B:576:ASP:HB2	2.08	0.67
1:A:683:VAL:O	1:A:687:LEU:HG	1.94	0.67
1:B:348:ARG:CZ	1:B:382:GLU:HG3	2.25	0.67
1:A:270:GLN:O	1:A:273:LEU:HB2	1.94	0.67
1:A:415:PRO:HD2	1:A:451:ILE:O	1.94	0.67
1:A:631:ILE:H	1:A:631:ILE:CD1	2.07	0.67
1:B:324:ARG:NH2	1:B:383:THR:O	2.28	0.67
1:A:229:LEU:HD12	1:A:229:LEU:H	1.60	0.67
1:A:322:VAL:HB	1:A:378:VAL:HG21	1.77	0.67
1:B:321:TYR:O	1:B:322:VAL:CG2	2.36	0.67
1:B:345:THR:CG2	1:B:388:THR:H	2.08	0.67
1:A:606:MET:HE3	1:A:671:MET:SD	2.34	0.67
1:B:78:ARG:NH2	1:B:357:ARG:HE	1.93	0.67
1:B:549:ALA:HA	1:B:591:LYS:NZ	2.09	0.67
1:B:549:ALA:HA	1:B:591:LYS:HZ3	1.60	0.67
1:A:326:THR:O	1:A:377:VAL:HG12	1.95	0.66
1:B:327:PHE:CE1	1:B:376:ALA:HB2	2.29	0.66
1:A:608:VAL:HG22	1:A:671:MET:HB3	1.77	0.66
1:B:348:ARG:NH2	1:B:382:GLU:HG3	2.09	0.66
1:B:500:GLN:O	1:B:502:GLY:N	2.29	0.66
1:B:85:PRO:HG3	1:B:94:VAL:HA	1.76	0.66
1:A:8:ASP:HB3	1:A:11:ARG:HG2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:VAL:O	1:A:563:ILE:HG23	1.95	0.66
1:A:609:GLU:O	1:A:669:PHE:HA	1.95	0.66
1:B:102:ASP:HB3	1:B:286:ILE:HD11	1.76	0.66
1:B:165:GLN:HG3	1:B:260:LEU:HD13	1.75	0.66
1:B:680:PRO:O	1:B:683:VAL:HG23	1.94	0.66
1:A:98:MET:O	1:A:101:LEU:HD23	1.96	0.66
1:B:680:PRO:HG2	1:B:683:VAL:CG2	2.25	0.66
1:A:220:ALA:O	1:A:221:ALA:C	2.35	0.66
1:B:628:ARG:HD2	1:B:648:PRO:HG2	1.77	0.66
1:A:348:ARG:HB3	1:A:348:ARG:NH1	2.09	0.66
1:A:468:ARG:HA	1:A:468:ARG:NE	2.11	0.66
1:A:671:MET:C	1:A:672:PHE:HD1	2.04	0.66
1:B:146:LEU:HD23	1:B:146:LEU:O	1.96	0.66
1:B:616:TYR:O	1:B:618:GLY:N	2.28	0.66
1:B:657:THR:HA	1:B:660:ARG:HB2	1.77	0.66
1:A:669:PHE:O	1:A:670:VAL:CG2	2.43	0.66
1:B:457:LEU:HG	1:B:460:GLU:CG	2.26	0.65
1:B:292:THR:O	1:B:398:ILE:HD12	1.96	0.65
1:B:485:GLU:HA	1:B:600:VAL:O	1.96	0.65
1:B:259:PHE:CE2	1:B:275:ALA:HB1	2.31	0.65
1:B:558:PHE:O	1:B:559:PRO:C	2.39	0.65
1:A:78:ARG:NH2	1:A:357:ARG:HE	1.94	0.65
1:A:219:VAL:O	1:A:220:ALA:C	2.39	0.65
1:A:469:GLU:C	1:A:470:PHE:HD1	2.04	0.65
1:A:500:GLN:C	1:A:502:GLY:N	2.52	0.65
1:B:38:ARG:O	1:B:39:ILE:HG22	1.97	0.65
1:B:546:ILE:HG23	1:B:590:ILE:HG13	1.79	0.65
1:B:247:ARG:HD2	1:B:278:ASP:O	1.97	0.65
1:B:309:LEU:HG	1:B:310:ALA:N	2.10	0.65
1:A:606:MET:HE3	1:A:671:MET:HG3	1.78	0.65
1:B:69:VAL:HG12	1:B:69:VAL:O	1.97	0.65
1:B:230:LYS:O	1:B:235:GLU:N	2.30	0.65
1:A:342:TYR:O	1:A:390:VAL:HG22	1.96	0.65
1:B:221:ALA:HB1	1:B:228:MET:CE	2.27	0.65
1:A:290:LYS:HB3	1:A:298:VAL:CG1	2.27	0.65
1:B:15:ILE:HG22	1:B:103:GLY:HA3	1.79	0.65
1:B:548:GLU:O	1:B:551:GLN:HB2	1.96	0.65
1:B:456:GLU:C	1:B:458:HIS:H	2.05	0.64
1:B:605:ILE:HD13	1:B:677:GLN:HB3	1.78	0.64
1:B:519:ARG:HG2	1:B:676:TYR:O	1.96	0.64
1:B:137:ASN:OD1	1:B:138:LYS:N	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:SER:OG	1:B:354:ARG:HA	1.97	0.64
1:A:201:ILE:HD12	1:A:201:ILE:N	2.13	0.64
1:A:354:ARG:HG3	1:A:378:VAL:HG11	1.78	0.64
1:A:410:ASP:O	1:A:411:VAL:HG22	1.97	0.64
1:A:573:HIS:O	1:A:575:VAL:N	2.31	0.64
1:B:603:GLU:OE2	1:B:679:VAL:HG23	1.97	0.64
1:A:16:GLY:N	1:A:101:LEU:HD12	2.12	0.64
1:A:499:ARG:HG3	1:A:500:GLN:H	1.61	0.64
1:B:426:GLN:O	1:B:427:ALA:CB	2.44	0.64
1:A:602:LEU:HB3	1:A:676:TYR:HD2	1.63	0.64
1:B:309:LEU:C	1:B:309:LEU:HD23	2.23	0.64
1:B:585:ALA:HA	1:B:588:MET:SD	2.37	0.64
1:B:105:ILE:HG12	1:B:133:ILE:HD11	1.80	0.64
1:B:260:LEU:C	1:B:260:LEU:HD22	2.23	0.64
1:A:19:ALA:HB3	1:A:25:LYS:HB2	1.80	0.64
1:A:157:LEU:N	1:A:157:LEU:HD12	2.12	0.64
1:A:31:ARG:O	1:A:32:ILE:C	2.38	0.64
1:B:523:PHE:CD1	1:B:524:GLU:N	2.66	0.64
1:B:103:GLY:O	1:B:104:ALA:HB2	1.96	0.64
1:A:367:GLU:O	1:A:368:GLU:HB3	1.98	0.63
1:B:348:ARG:HB3	1:B:348:ARG:NH1	2.12	0.63
1:A:189:GLY:HA3	1:A:195:ASP:CG	2.23	0.63
1:A:606:MET:O	1:A:646:PHE:HA	1.97	0.63
1:B:148:LEU:HD12	1:B:148:LEU:O	1.99	0.63
1:B:580:MET:O	1:B:584:ILE:HD13	1.97	0.63
1:A:165:GLN:HG3	1:A:260:LEU:CD1	2.27	0.63
1:A:309:LEU:CD1	1:A:335:LEU:HB2	2.29	0.63
1:B:218:GLU:O	1:B:221:ALA:HB3	1.99	0.63
1:B:309:LEU:HA	1:B:332:SER:O	1.98	0.63
1:A:549:ALA:HA	1:A:591:LYS:NZ	2.14	0.63
1:B:218:GLU:O	1:B:221:ALA:N	2.31	0.63
1:B:415:PRO:HD2	1:B:451:ILE:O	1.99	0.63
1:A:164:MET:HB2	1:A:258:VAL:O	1.97	0.63
1:A:604:PRO:HG2	1:A:649:LEU:HB3	1.78	0.63
1:B:342:TYR:O	1:B:390:VAL:HG22	1.98	0.63
1:A:461:ILE:O	1:A:465:ARG:HG3	1.99	0.63
1:B:92:ILE:HD13	1:B:92:ILE:N	2.13	0.63
1:A:230:LYS:O	1:A:235:GLU:N	2.31	0.63
1:B:78:ARG:CZ	1:B:357:ARG:HH21	2.12	0.63
1:B:426:GLN:HE21	1:B:430:ARG:HH21	1.44	0.63
1:A:17:ILE:HD13	1:A:28:THR:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:CE1	1:A:269:VAL:HG21	2.34	0.62
1:A:68:ALA:HB3	1:A:327:PHE:CE2	2.34	0.62
1:A:426:GLN:O	1:A:427:ALA:CB	2.47	0.62
1:A:426:GLN:O	1:A:427:ALA:HB3	1.99	0.62
1:A:526:VAL:CG1	1:A:527:ASN:N	2.62	0.62
1:A:606:MET:HE3	1:A:671:MET:CG	2.29	0.62
1:A:681:LYS:N	1:A:681:LYS:HD3	2.14	0.62
1:A:688:ILE:HG13	1:A:689:LYS:HZ2	1.63	0.62
1:B:110:SER:OG	1:B:136:ALA:HB1	1.99	0.62
1:B:221:ALA:HB1	1:B:228:MET:HG3	1.82	0.62
1:B:229:LEU:H	1:B:229:LEU:HD12	1.63	0.62
1:B:681:LYS:HE3	1:B:682:GLN:HE22	1.63	0.62
1:A:74:TRP:CE3	1:A:273:LEU:HD13	2.35	0.62
1:B:616:TYR:O	1:B:620:VAL:HG23	1.98	0.62
1:A:19:ALA:HB2	1:A:107:VAL:HG13	1.81	0.62
1:A:326:THR:HB	1:A:377:VAL:HG13	1.81	0.62
1:A:542:VAL:HG22	1:A:582:PHE:HB3	1.80	0.62
1:B:458:HIS:O	1:B:461:ILE:HB	1.98	0.62
1:A:96:ARG:O	1:A:100:VAL:HG22	1.99	0.62
1:A:139:MET:HE2	1:A:260:LEU:HB2	1.80	0.62
1:A:339:SER:H	1:A:352:VAL:HG13	1.65	0.62
1:A:526:VAL:HG12	1:A:527:ASN:N	2.14	0.62
1:B:610:VAL:HG22	1:B:669:PHE:CB	2.30	0.62
1:B:416:LYS:HD3	1:B:416:LYS:C	2.25	0.62
1:B:550:MET:SD	1:B:563:ILE:HD11	2.40	0.62
1:A:99:ARG:NE	1:A:289:ILE:HD12	2.14	0.62
1:B:157:LEU:O	1:B:639:ASN:HB2	1.99	0.62
1:B:506:GLN:HA	1:B:576:ASP:O	2.00	0.62
1:B:689:LYS:NZ	1:B:689:LYS:HB2	2.15	0.62
1:B:218:GLU:O	1:B:221:ALA:CB	2.48	0.62
1:A:240:GLU:CD	1:A:240:GLU:H	2.08	0.61
1:A:590:ILE:O	1:A:592:GLU:N	2.33	0.61
1:B:457:LEU:CG	1:B:460:GLU:HB2	2.25	0.61
1:B:681:LYS:H	1:B:681:LYS:CD	2.13	0.61
1:A:229:LEU:H	1:A:229:LEU:CD1	2.13	0.61
1:B:319:ASP:HB2	1:B:325:LEU:CD1	2.29	0.61
1:B:441:SER:HB3	1:B:450:ILE:HG13	1.82	0.61
1:B:685:GLU:O	1:B:688:ILE:HG12	2.00	0.61
1:B:689:LYS:HB2	1:B:689:LYS:HZ3	1.65	0.61
1:A:120:THR:HA	1:A:123:ARG:HG3	1.83	0.61
1:A:215:LYS:O	1:A:219:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:SER:OG	1:B:265:LYS:HB2	2.01	0.61
1:A:247:ARG:HG2	1:A:251:ILE:HD11	1.82	0.61
1:A:416:LYS:HD3	1:A:416:LYS:C	2.25	0.61
1:B:427:ALA:HA	1:B:470:PHE:HE2	1.64	0.61
1:B:439:ARG:HB2	1:B:439:ARG:HH11	1.65	0.61
1:B:521:SER:O	1:B:562:ASP:OD1	2.18	0.61
1:A:123:ARG:NH2	1:A:639:ASN:HB3	2.15	0.61
1:A:140:ASP:HA	1:A:171:GLU:O	2.01	0.61
1:A:634:MET:SD	1:A:634:MET:C	2.84	0.61
1:B:98:MET:O	1:B:101:LEU:HD23	2.00	0.61
1:B:481:VAL:HG13	1:B:649:LEU:HD12	1.81	0.61
1:A:159:ALA:O	1:A:161:PRO:HD3	2.00	0.61
1:A:409:ILE:O	1:A:411:VAL:N	2.32	0.61
1:A:552:SER:O	1:A:591:LYS:HE3	2.00	0.61
1:B:129:LYS:HG2	1:B:129:LYS:O	2.00	0.61
1:B:303:PRO:HA	1:B:331:TYR:O	1.99	0.61
1:B:538:TYR:O	1:B:541:ALA:N	2.30	0.61
1:A:68:ALA:HB2	1:A:317:MET:SD	2.40	0.61
1:A:653:PHE:O	1:A:655:TYR:N	2.33	0.61
1:B:457:LEU:HA	1:B:460:GLU:HB2	1.82	0.61
1:A:247:ARG:HD2	1:A:278:ASP:O	2.01	0.61
1:A:309:LEU:C	1:A:309:LEU:HD23	2.26	0.61
1:A:517:LEU:HB2	1:A:562:ASP:C	2.26	0.61
1:A:632:LEU:HG	1:A:644:ARG:O	2.00	0.61
1:A:129:LYS:HG2	1:A:253:LEU:HD11	1.83	0.61
1:A:354:ARG:HG3	1:A:378:VAL:HG12	1.83	0.61
1:A:457:LEU:HG	1:A:460:GLU:CB	2.30	0.61
1:A:572:TYR:N	1:A:572:TYR:HD1	1.97	0.61
1:B:411:VAL:CB	1:B:453:GLY:CA	2.57	0.61
1:A:103:GLY:O	1:A:104:ALA:HB2	1.99	0.61
1:A:218:GLU:O	1:A:221:ALA:HB3	2.01	0.61
1:A:411:VAL:O	1:A:411:VAL:HG23	1.99	0.61
1:A:669:PHE:O	1:A:670:VAL:HG22	1.99	0.61
1:A:122:TRP:CD2	1:A:157:LEU:HD23	2.35	0.60
1:A:343:ASN:ND2	1:A:387:ASP:HB3	2.15	0.60
1:B:156:ARG:HB3	1:B:666:ARG:HH12	1.66	0.60
1:A:457:LEU:C	1:A:460:GLU:H	2.09	0.60
1:B:35:TYR:CZ	1:B:269:VAL:HG21	2.36	0.60
1:B:220:ALA:O	1:B:221:ALA:C	2.43	0.60
1:B:467:LYS:O	1:B:467:LYS:HG2	2.00	0.60
1:A:262:SER:OG	1:A:265:LYS:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:LYS:CG	1:B:509:HIS:ND1	2.64	0.60
1:A:17:ILE:HD13	1:A:28:THR:CG2	2.31	0.60
1:A:443:HIS:ND1	1:A:450:ILE:HD11	2.17	0.60
1:B:501:THR:HG22	1:B:504:ARG:O	2.02	0.60
1:B:608:VAL:CG1	1:B:609:GLU:N	2.65	0.60
1:A:85:PRO:HG3	1:A:94:VAL:HA	1.83	0.60
1:A:348:ARG:CZ	1:A:382:GLU:HG3	2.30	0.60
1:A:601:ILE:CD1	1:A:684:GLN:HG3	2.32	0.60
1:B:69:VAL:HG21	1:B:314:PHE:HZ	1.66	0.60
1:B:87:HIS:CE1	1:B:90:PHE:HB2	2.36	0.60
1:A:38:ARG:CG	1:A:39:ILE:H	2.15	0.60
1:A:132:ARG:HH11	1:A:132:ARG:CG	2.11	0.60
1:A:215:LYS:O	1:A:218:GLU:HB3	2.01	0.60
1:A:340:TYR:CE1	1:A:351:ARG:HB2	2.37	0.60
1:A:454:MET:HG2	1:A:455:GLY:N	2.11	0.60
1:B:121:VAL:O	1:B:124:GLN:HB2	2.02	0.60
1:A:286:ILE:HD12	1:A:286:ILE:H	1.65	0.60
1:A:602:LEU:HD12	1:A:678:GLU:HA	1.84	0.60
1:A:89:ASP:OD1	1:A:89:ASP:N	2.31	0.60
1:A:295:GLU:HA	1:B:26:THR:CB	2.31	0.60
1:A:603:GLU:OE2	1:A:648:PRO:HB3	2.01	0.60
1:B:549:ALA:O	1:B:550:MET:C	2.43	0.60
1:B:679:VAL:O	1:B:679:VAL:CG1	2.49	0.60
1:B:604:PRO:HG2	1:B:649:LEU:HB3	1.83	0.60
1:A:518:PRO:HG2	1:B:39:ILE:HG21	1.84	0.59
1:A:631:ILE:HA	1:A:645:ALA:HB2	1.84	0.59
1:B:92:ILE:HG12	1:B:92:ILE:O	2.01	0.59
1:A:538:TYR:O	1:A:541:ALA:N	2.35	0.59
1:B:90:PHE:O	1:B:94:VAL:HG23	2.01	0.59
1:B:183:MET:HE1	1:B:209:ALA:CB	2.32	0.59
1:B:325:LEU:HD23	1:B:378:VAL:HG23	1.84	0.59
1:A:204:GLU:OE1	1:A:204:GLU:N	2.35	0.59
1:B:13:ARG:HG2	1:B:13:ARG:HH11	1.67	0.59
1:A:121:VAL:O	1:A:124:GLN:HB2	2.02	0.59
1:A:171:GLU:HG3	1:A:172:ASP:H	1.66	0.59
1:A:572:TYR:N	1:A:572:TYR:CD1	2.69	0.59
1:A:634:MET:HB2	1:A:642:VAL:O	2.02	0.59
1:B:247:ARG:HG2	1:B:251:ILE:HD11	1.85	0.59
1:B:616:TYR:C	1:B:618:GLY:H	2.09	0.59
1:B:613:PRO:HG3	1:B:666:ARG:HE	1.67	0.59
1:A:101:LEU:HD23	1:A:101:LEU:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:MET:HE2	1:B:257:PRO:HB3	1.85	0.59
1:A:165:GLN:CB	1:A:178:ILE:O	2.50	0.59
1:A:327:PHE:CD1	1:A:376:ALA:HB2	2.37	0.59
1:A:497:PHE:CG	1:A:584:ILE:HG21	2.37	0.59
1:B:78:ARG:CZ	1:B:357:ARG:HE	2.16	0.59
1:A:357:ARG:HB3	1:A:364:GLU:HB3	1.83	0.59
1:B:122:TRP:CD2	1:B:157:LEU:HD23	2.38	0.59
1:B:340:TYR:HB2	1:B:392:GLU:OE2	2.03	0.59
1:B:340:TYR:CE1	1:B:351:ARG:HB2	2.37	0.59
1:B:499:ARG:HG3	1:B:500:GLN:H	1.66	0.59
1:A:122:TRP:CE2	1:A:157:LEU:HD23	2.38	0.59
1:B:229:LEU:HD12	1:B:229:LEU:N	2.17	0.59
1:B:160:ARG:HG3	1:B:160:ARG:HH11	1.67	0.58
1:B:290:LYS:HB3	1:B:298:VAL:CG1	2.30	0.58
1:B:443:HIS:O	1:B:448:GLN:N	2.35	0.58
1:B:627:ARG:NH2	1:B:658:ASP:OD2	2.36	0.58
1:A:487:ILE:HD12	1:A:489:LYS:O	2.02	0.58
1:B:350:GLU:OE1	1:B:380:LEU:CD2	2.51	0.58
1:B:439:ARG:HB2	1:B:439:ARG:NH1	2.17	0.58
1:B:563:ILE:O	1:B:563:ILE:HG13	2.04	0.58
1:A:90:PHE:O	1:A:91:THR:O	2.21	0.58
1:A:266:ASN:C	1:A:267:LYS:HG2	2.28	0.58
1:A:455:GLY:O	1:A:459:LEU:CD1	2.51	0.58
1:A:181:LEU:HD21	1:A:243:VAL:CG2	2.29	0.58
1:A:345:THR:HG22	1:A:398:ILE:HG22	1.85	0.58
1:B:457:LEU:HG	1:B:460:GLU:HG2	1.85	0.58
1:B:534:ILE:HD12	1:B:582:PHE:HE2	1.67	0.58
1:A:157:LEU:N	1:A:157:LEU:CD1	2.66	0.58
1:B:183:MET:HE1	1:B:209:ALA:HB1	1.84	0.58
1:B:500:GLN:C	1:B:502:GLY:N	2.61	0.58
1:B:99:ARG:HD3	1:B:99:ARG:C	2.27	0.58
1:B:322:VAL:HB	1:B:378:VAL:HG21	1.84	0.58
1:B:468:ARG:HG2	1:B:468:ARG:HH11	1.68	0.58
1:B:494:GLU:HG3	1:B:509:HIS:CE1	2.39	0.58
1:B:681:LYS:HA	1:B:684:GLN:HB3	1.86	0.58
1:A:305:PRO:O	1:A:333:GLY:HA2	2.02	0.58
1:A:573:HIS:ND1	1:A:576:ASP:OD2	2.37	0.58
1:A:69:VAL:HG21	1:A:314:PHE:HZ	1.68	0.58
1:A:549:ALA:HA	1:A:591:LYS:HZ3	1.69	0.58
1:B:6:GLU:CG	1:B:7:TYR:N	2.53	0.58
1:B:259:PHE:CE2	1:B:275:ALA:CB	2.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ILE:C	1:B:387:ASP:OD2	2.48	0.57
1:A:26:THR:HG22	1:A:27:THR:N	2.18	0.57
1:A:443:HIS:O	1:A:448:GLN:N	2.36	0.57
1:A:580:MET:O	1:A:584:ILE:HD13	2.03	0.57
1:A:616:TYR:O	1:A:618:GLY:N	2.38	0.57
1:A:481:VAL:HB	1:A:483:TYR:CE2	2.39	0.57
1:B:34:TYR:CD1	1:B:34:TYR:C	2.77	0.57
1:B:339:SER:H	1:B:352:VAL:HG13	1.68	0.57
1:A:201:ILE:H	1:A:201:ILE:CD1	2.16	0.57
1:A:519:ARG:HA	1:A:562:ASP:OD2	2.05	0.57
1:A:631:ILE:HA	1:A:645:ALA:CB	2.33	0.57
1:A:681:LYS:CE	1:A:682:GLN:HE22	2.18	0.57
1:B:331:TYR:O	1:B:371:ALA:HB1	2.04	0.57
1:B:434:GLU:O	1:B:434:GLU:HG2	2.05	0.57
1:A:324:ARG:NH2	1:A:383:THR:O	2.35	0.57
1:B:182:ARG:HH11	1:B:239:GLU:CD	2.11	0.57
1:B:235:GLU:O	1:B:237:PRO:HD3	2.04	0.57
1:B:560:VAL:O	1:B:561:VAL:HG13	2.04	0.57
1:B:658:ASP:O	1:B:662:LYS:HG2	2.05	0.57
1:A:99:ARG:HD3	1:A:99:ARG:C	2.28	0.57
1:A:228:MET:O	1:A:231:TYR:HB3	2.04	0.57
1:A:273:LEU:O	1:A:276:VAL:N	2.38	0.57
1:A:523:PHE:HE1	1:A:565:VAL:HG23	1.69	0.57
1:A:681:LYS:HD3	1:A:681:LYS:H	1.68	0.57
1:B:432:ALA:HA	1:B:438:PHE:HZ	1.69	0.57
1:A:152:THR:O	1:A:155:GLU:N	2.38	0.57
1:A:542:VAL:CG2	1:A:582:PHE:HB3	2.35	0.57
1:B:469:GLU:C	1:B:470:PHE:HD1	2.13	0.57
1:B:636:PRO:HB3	1:B:641:GLN:OE1	2.05	0.57
1:A:443:HIS:HB2	1:A:450:ILE:CD1	2.35	0.57
1:A:658:ASP:O	1:A:662:LYS:HG2	2.05	0.57
1:B:426:GLN:O	1:B:427:ALA:HB3	2.04	0.57
1:B:606:MET:O	1:B:646:PHE:HA	2.03	0.57
1:A:277:VAL:HG22	1:A:278:ASP:N	2.19	0.57
1:A:416:LYS:O	1:A:449:THR:HG22	2.05	0.57
1:A:439:ARG:HB2	1:A:439:ARG:HH11	1.70	0.57
1:A:613:PRO:HG3	1:A:666:ARG:HE	1.69	0.57
1:B:319:ASP:CG	1:B:320:PRO:HD2	2.30	0.57
1:A:95:GLU:HB2	1:A:128:TYR:OH	2.04	0.56
1:A:139:MET:CE	1:A:260:LEU:HB2	2.35	0.56
1:A:631:ILE:N	1:A:631:ILE:CD1	2.67	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:MET:HE1	1:A:641:GLN:OE1	2.05	0.56
1:B:409:ILE:C	1:B:411:VAL:H	2.13	0.56
1:B:549:ALA:O	1:B:551:GLN:N	2.38	0.56
1:B:85:PRO:HG3	1:B:94:VAL:HG22	1.87	0.56
1:B:289:ILE:CG2	1:B:301:ILE:HB	2.33	0.56
1:A:373:ASP:C	1:A:374:LEU:HG	2.30	0.56
1:A:456:GLU:O	1:A:458:HIS:N	2.38	0.56
1:A:458:HIS:CE1	1:A:462:ILE:HD11	2.40	0.56
1:A:458:HIS:HA	1:A:461:ILE:CD1	2.35	0.56
1:A:597:GLY:O	1:A:598:ASP:C	2.48	0.56
1:B:123:ARG:HH22	1:B:639:ASN:HB3	1.67	0.56
1:B:321:TYR:C	1:B:322:VAL:HG13	2.29	0.56
1:B:500:GLN:O	1:B:501:THR:HG22	2.05	0.56
1:B:523:PHE:CZ	1:B:525:PHE:HB2	2.40	0.56
1:B:592:GLU:O	1:B:595:GLN:HG2	2.05	0.56
1:B:602:LEU:HB3	1:B:676:TYR:HD2	1.70	0.56
1:B:608:VAL:HG21	1:B:647:VAL:CG1	2.35	0.56
1:B:118:SER:O	1:B:121:VAL:HB	2.04	0.56
1:B:496:LYS:O	1:B:588:MET:HE1	2.05	0.56
1:B:526:VAL:CG1	1:B:527:ASN:N	2.68	0.56
1:A:410:ASP:C	1:A:411:VAL:HG22	2.31	0.56
1:B:17:ILE:HG22	1:B:17:ILE:O	2.05	0.56
1:A:448:GLN:O	1:A:449:THR:CB	2.53	0.56
1:A:590:ILE:O	1:A:591:LYS:C	2.49	0.56
1:A:672:PHE:CD1	1:A:672:PHE:N	2.74	0.56
1:B:524:GLU:OE1	1:B:564:LYS:HE3	2.05	0.56
1:A:344:THR:C	1:A:346:LYS:H	2.13	0.56
1:A:439:ARG:HB2	1:A:439:ARG:NH1	2.20	0.56
1:A:626:ALA:C	1:A:628:ARG:H	2.13	0.56
1:B:457:LEU:CA	1:B:460:GLU:HB2	2.35	0.56
1:B:468:ARG:HG2	1:B:468:ARG:NH1	2.21	0.56
1:A:300:GLU:HB3	1:A:302:HIS:CE1	2.41	0.56
1:B:7:TYR:C	1:B:7:TYR:CD1	2.83	0.56
1:B:411:VAL:HG23	1:B:411:VAL:O	2.06	0.56
1:B:517:LEU:HD23	1:B:518:PRO:HD2	1.87	0.56
1:B:601:ILE:HD12	1:B:684:GLN:HG3	1.88	0.56
1:B:652:MET:HE3	1:B:655:TYR:CG	2.39	0.56
1:A:91:THR:O	1:A:92:ILE:C	2.49	0.56
1:A:292:THR:HB	1:A:398:ILE:HD12	1.87	0.56
1:A:220:ALA:HB1	1:A:227:ILE:HD12	1.87	0.56
1:A:377:VAL:HG22	1:A:377:VAL:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LEU:CD1	1:A:466:LEU:HD12	2.36	0.56
1:A:669:PHE:C	1:A:670:VAL:HG23	2.31	0.56
1:A:114:VAL:HG11	1:A:157:LEU:CD1	2.36	0.55
1:A:558:PHE:O	1:A:559:PRO:C	2.47	0.55
1:B:101:LEU:HD23	1:B:101:LEU:H	1.71	0.55
1:B:228:MET:O	1:B:231:TYR:N	2.39	0.55
1:B:457:LEU:C	1:B:460:GLU:H	2.13	0.55
1:B:526:VAL:HG12	1:B:527:ASN:N	2.20	0.55
1:A:38:ARG:O	1:A:39:ILE:HG22	2.06	0.55
1:A:129:LYS:O	1:A:129:LYS:CG	2.53	0.55
1:A:247:ARG:NH1	1:A:251:ILE:HD11	2.22	0.55
1:A:157:LEU:C	1:A:639:ASN:ND2	2.65	0.55
1:B:98:MET:HA	1:B:101:LEU:CD2	2.36	0.55
1:B:189:GLY:HA3	1:B:195:ASP:CG	2.32	0.55
1:A:5:VAL:HG22	1:A:6:GLU:N	2.22	0.55
1:A:114:VAL:CG1	1:A:157:LEU:HD11	2.36	0.55
1:A:688:ILE:HG13	1:A:689:LYS:HZ1	1.70	0.55
1:A:164:MET:O	1:A:180:VAL:HG22	2.06	0.55
1:B:36:THR:HG22	1:B:74:TRP:HB2	1.89	0.55
1:B:431:LEU:HD11	1:B:466:LEU:HD12	1.89	0.55
1:A:15:ILE:HG22	1:A:103:GLY:HA3	1.89	0.55
1:B:432:ALA:HA	1:B:438:PHE:CZ	2.41	0.55
1:A:9:LEU:HD12	1:A:12:LEU:HD13	1.88	0.55
1:A:590:ILE:C	1:A:592:GLU:N	2.64	0.55
1:B:486:THR:OG1	1:B:561:VAL:O	2.23	0.55
1:B:496:LYS:HG2	1:B:509:HIS:ND1	2.21	0.55
1:B:636:PRO:HA	1:B:641:GLN:HG2	1.89	0.55
1:A:160:ARG:HG3	1:A:160:ARG:HH11	1.72	0.55
1:A:343:ASN:HD22	1:A:389:LEU:HD11	1.71	0.55
1:A:634:MET:HB2	1:A:643:ILE:HA	1.89	0.55
1:A:677:GLN:O	1:A:678:GLU:O	2.24	0.55
1:B:85:PRO:CG	1:B:94:VAL:HG22	2.37	0.54
1:B:295:GLU:HG3	1:B:295:GLU:O	2.07	0.54
1:B:410:ASP:O	1:B:411:VAL:HG22	2.07	0.54
1:A:84:THR:CG2	1:A:85:PRO:HD2	2.34	0.54
1:B:112:GLN:O	1:B:113:GLY:C	2.51	0.54
1:B:605:ILE:HD11	1:B:677:GLN:HB3	1.89	0.54
1:B:608:VAL:HG21	1:B:647:VAL:HG11	1.89	0.54
1:B:610:VAL:HG22	1:B:669:PHE:HB3	1.89	0.54
1:A:133:ILE:HG23	1:A:280:LEU:HD21	1.90	0.54
1:A:309:LEU:HG	1:A:310:ALA:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG21	1:A:325:LEU:HD21	1.89	0.54
1:A:431:LEU:HD11	1:A:466:LEU:HD12	1.90	0.54
1:B:38:ARG:CG	1:B:39:ILE:N	2.69	0.54
1:B:357:ARG:CB	1:B:364:GLU:HB3	2.36	0.54
1:A:276:VAL:HG13	1:A:280:LEU:CD1	2.25	0.54
1:A:608:VAL:HG22	1:A:671:MET:CB	2.37	0.54
1:B:204:GLU:N	1:B:204:GLU:OE1	2.41	0.54
1:B:277:VAL:HG22	1:B:278:ASP:N	2.22	0.54
1:B:637:ARG:O	1:B:637:ARG:HG3	2.06	0.54
1:A:92:ILE:HG12	1:A:92:ILE:O	2.07	0.54
1:A:35:TYR:CZ	1:A:269:VAL:HG21	2.43	0.54
1:B:486:THR:O	1:B:600:VAL:HG22	2.08	0.54
1:B:606:MET:HE3	1:B:671:MET:HG3	1.90	0.54
1:A:343:ASN:HB2	1:A:389:LEU:HD12	1.90	0.54
1:A:434:GLU:O	1:A:435:ASP:CB	2.48	0.54
1:B:169:GLY:C	1:B:174:PHE:HA	2.33	0.54
1:B:356:LEU:HD23	1:B:365:GLU:HA	1.90	0.54
1:B:585:ALA:O	1:B:588:MET:HB2	2.08	0.54
1:A:156:ARG:HB3	1:A:666:ARG:HH12	1.73	0.54
1:A:224:ASP:HB3	1:A:227:ILE:CG1	2.32	0.54
1:A:312:LEU:HD22	1:A:313:ALA:O	2.07	0.54
1:A:523:PHE:HE1	1:A:565:VAL:CG2	2.21	0.54
1:B:17:ILE:HD13	1:B:28:THR:HG22	1.87	0.54
1:B:159:ALA:O	1:B:161:PRO:HD3	2.08	0.54
1:B:534:ILE:HG23	1:B:582:PHE:CE2	2.43	0.54
1:B:535:PRO:HB2	1:B:537:GLU:OE1	2.08	0.54
1:B:536:LYS:HA	1:B:539:ILE:HD12	1.90	0.54
1:B:631:ILE:HD12	1:B:631:ILE:H	1.73	0.54
1:A:272:LEU:O	1:A:276:VAL:HG23	2.08	0.54
1:A:357:ARG:CB	1:A:364:GLU:HB3	2.38	0.54
1:A:679:VAL:CG1	1:A:679:VAL:O	2.54	0.54
1:B:342:TYR:OH	1:B:347:GLY:HA2	2.07	0.54
1:B:538:TYR:O	1:B:539:ILE:C	2.51	0.54
1:B:680:PRO:CB	1:B:682:GLN:HE21	2.16	0.54
1:B:11:ARG:HA	1:B:77:HIS:HD2	1.73	0.53
1:B:19:ALA:HB2	1:B:107:VAL:CG1	2.38	0.53
1:B:247:ARG:HD2	1:B:279:TYR:HA	1.90	0.53
1:B:634:MET:HB2	1:B:642:VAL:O	2.08	0.53
1:A:78:ARG:CZ	1:A:357:ARG:HE	2.21	0.53
1:A:504:ARG:HG2	1:A:504:ARG:HH11	1.72	0.53
1:A:507:TYR:N	1:A:576:ASP:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:ILE:HG22	1:A:585:ALA:N	2.23	0.53
1:B:443:HIS:ND1	1:B:450:ILE:CD1	2.71	0.53
1:A:127:LYS:HE2	1:A:637:ARG:NH2	2.22	0.53
1:A:361:ASN:O	1:A:362:HIS:CB	2.56	0.53
1:A:494:GLU:HB2	1:A:511:LYS:HG2	1.90	0.53
1:A:610:VAL:HA	1:A:669:PHE:HA	1.90	0.53
1:A:636:PRO:HB3	1:A:641:GLN:OE1	2.08	0.53
1:B:147:TRP:O	1:B:151:ARG:HB2	2.08	0.53
1:A:391:GLY:O	1:A:393:ASP:N	2.40	0.53
1:B:5:VAL:HG22	1:B:6:GLU:N	2.23	0.53
1:B:173:THR:O	1:B:174:PHE:C	2.51	0.53
1:B:220:ALA:HB1	1:B:227:ILE:HD12	1.90	0.53
1:A:229:LEU:HD12	1:A:229:LEU:N	2.21	0.53
1:A:381:LYS:O	1:A:382:GLU:HB2	2.08	0.53
1:A:652:MET:HG3	1:A:652:MET:O	2.09	0.53
1:B:138:LYS:C	1:B:140:ASP:H	2.15	0.53
1:B:542:VAL:HG22	1:B:582:PHE:HB3	1.91	0.53
1:B:652:MET:HG2	1:B:671:MET:HE1	1.91	0.53
1:B:679:VAL:HG13	1:B:683:VAL:HB	1.90	0.53
1:A:119:GLU:OE1	1:A:666:ARG:NH1	2.41	0.53
1:A:170:ARG:N	1:A:173:THR:HB	2.23	0.53
1:B:38:ARG:HG3	1:B:39:ILE:N	2.23	0.53
1:B:114:VAL:HG12	1:B:114:VAL:O	2.08	0.53
1:B:271:LEU:O	1:B:274:ASP:N	2.40	0.53
1:B:610:VAL:HG22	1:B:669:PHE:HB2	1.90	0.53
1:A:343:ASN:OD1	1:A:346:LYS:HB2	2.08	0.53
1:A:525:PHE:CE1	1:A:543:GLN:NE2	2.76	0.53
1:A:669:PHE:C	1:A:670:VAL:CG2	2.81	0.53
1:A:679:VAL:HG22	1:A:683:VAL:HG21	1.91	0.53
1:B:168:ILE:HD11	1:B:178:ILE:HD11	1.90	0.53
1:B:392:GLU:O	1:B:392:GLU:HG3	2.08	0.53
1:A:525:PHE:HB3	1:B:197:ARG:HB3	1.90	0.53
1:B:504:ARG:HG2	1:B:504:ARG:HH11	1.73	0.53
1:A:608:VAL:HG12	1:A:609:GLU:N	2.23	0.53
1:B:357:ARG:HG3	1:B:357:ARG:NH1	2.19	0.53
1:B:684:GLN:O	1:B:688:ILE:HG23	2.09	0.53
1:A:106:VAL:O	1:A:134:ALA:HA	2.09	0.53
1:A:410:ASP:O	1:A:411:VAL:CG2	2.57	0.53
1:A:657:THR:CA	1:A:660:ARG:HB2	2.33	0.53
1:A:13:ARG:HG2	1:A:13:ARG:HH11	1.73	0.52
1:A:301:ILE:O	1:A:301:ILE:HG22	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:TYR:C	1:A:618:GLY:H	2.17	0.52
1:A:636:PRO:HA	1:A:641:GLN:HG2	1.91	0.52
1:B:182:ARG:NH1	1:B:239:GLU:OE2	2.43	0.52
1:B:240:GLU:O	1:B:241:GLU:C	2.50	0.52
1:A:252:ASP:O	1:A:253:LEU:HB2	2.09	0.52
1:A:653:PHE:C	1:A:655:TYR:N	2.66	0.52
1:B:181:LEU:HD12	1:B:242:LEU:HD23	1.92	0.52
1:B:374:LEU:HD12	1:B:374:LEU:O	2.08	0.52
1:B:35:TYR:C	1:B:37:GLY:N	2.66	0.52
1:B:343:ASN:C	1:B:343:ASN:OD1	2.52	0.52
1:B:355:LEU:HD23	1:B:377:VAL:HA	1.89	0.52
1:B:434:GLU:O	1:B:435:ASP:CB	2.46	0.52
1:B:454:MET:HG2	1:B:455:GLY:N	2.23	0.52
1:A:450:ILE:O	1:A:450:ILE:HG13	2.09	0.52
1:A:458:HIS:HA	1:A:461:ILE:HG13	1.92	0.52
1:A:486:THR:HG22	1:A:487:ILE:O	2.10	0.52
1:B:38:ARG:C	1:B:39:ILE:HG22	2.34	0.52
1:B:519:ARG:CA	1:B:562:ASP:OD2	2.56	0.52
1:B:590:ILE:O	1:B:591:LYS:C	2.50	0.52
1:B:681:LYS:O	1:B:685:GLU:HB2	2.10	0.52
1:A:17:ILE:CD1	1:A:28:THR:HG22	2.40	0.52
1:A:178:ILE:HD13	1:A:185:ALA:HB2	1.91	0.52
1:B:431:LEU:CD1	1:B:466:LEU:HD12	2.40	0.52
1:B:517:LEU:CD2	1:B:518:PRO:HD2	2.39	0.52
1:A:7:TYR:CD1	1:A:7:TYR:C	2.87	0.52
1:A:203:GLU:HA	1:A:206:LEU:CD2	2.31	0.52
1:B:629:GLY:HA2	1:B:646:PHE:O	2.09	0.52
1:A:221:ALA:CB	1:A:228:MET:HG3	2.37	0.52
1:A:326:THR:O	1:A:377:VAL:CG1	2.58	0.52
1:B:221:ALA:CB	1:B:228:MET:HE3	2.39	0.52
1:A:82:ILE:HD12	1:A:101:LEU:HB3	1.91	0.52
1:A:646:PHE:CZ	1:A:674:ASP:OD2	2.63	0.52
1:A:148:LEU:HD12	1:A:148:LEU:O	2.10	0.52
1:B:78:ARG:NH2	1:B:357:ARG:HH21	2.08	0.52
1:B:346:LYS:NZ	1:B:383:THR:HA	2.23	0.52
1:B:361:ASN:O	1:B:362:HIS:CB	2.57	0.52
1:B:96:ARG:O	1:B:100:VAL:HG22	2.10	0.51
1:B:114:VAL:HG11	1:B:157:LEU:CD1	2.40	0.51
1:B:219:VAL:HG12	1:B:223:PHE:HE2	1.75	0.51
1:B:312:LEU:CD2	1:B:313:ALA:O	2.54	0.51
1:B:672:PHE:CD1	1:B:672:PHE:N	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ILE:HD11	1:B:384:ILE:C	2.35	0.51
1:B:319:ASP:CG	1:B:363:ARG:HH12	2.18	0.51
1:B:391:GLY:O	1:B:393:ASP:N	2.43	0.51
1:A:69:VAL:HG12	1:A:69:VAL:O	2.10	0.51
1:A:114:VAL:HG12	1:A:114:VAL:O	2.09	0.51
1:A:325:LEU:HD23	1:A:378:VAL:HG23	1.92	0.51
1:B:91:THR:O	1:B:92:ILE:C	2.52	0.51
1:B:129:LYS:O	1:B:129:LYS:CG	2.59	0.51
1:B:218:GLU:O	1:B:219:VAL:C	2.52	0.51
1:B:428:LEU:O	1:B:432:ALA:HB2	2.11	0.51
1:A:97:SER:O	1:A:101:LEU:HD22	2.10	0.51
1:A:411:VAL:CB	1:A:453:GLY:HA3	2.33	0.51
1:B:20:HIS:CG	1:B:21:ILE:H	2.28	0.51
1:B:211:GLU:OE2	1:B:215:LYS:HE3	2.10	0.51
1:B:274:ASP:O	1:B:278:ASP:HB2	2.11	0.51
1:B:481:VAL:HB	1:B:483:TYR:CZ	2.45	0.51
1:A:409:ILE:C	1:A:411:VAL:H	2.19	0.51
1:B:648:PRO:O	1:B:649:LEU:C	2.53	0.51
1:A:272:LEU:O	1:A:275:ALA:HB3	2.11	0.51
1:A:291:GLY:H	1:A:299:VAL:H	1.57	0.51
1:A:411:VAL:CB	1:A:453:GLY:CA	2.63	0.51
1:B:13:ARG:HG2	1:B:13:ARG:NH1	2.25	0.51
1:B:138:LYS:O	1:B:140:ASP:N	2.43	0.51
1:B:352:VAL:HG23	1:B:377:VAL:HG23	1.93	0.51
1:B:608:VAL:O	1:B:644:ARG:HA	2.10	0.51
1:A:182:ARG:HB2	1:A:184:LYS:HD3	1.93	0.51
1:B:26:THR:O	1:B:27:THR:C	2.54	0.51
1:B:170:ARG:H	1:B:173:THR:HB	1.75	0.51
1:B:322:VAL:HG21	1:B:325:LEU:HD21	1.92	0.51
1:A:427:ALA:O	1:A:431:LEU:HG	2.11	0.51
1:A:501:THR:HG22	1:A:504:ARG:O	2.11	0.51
1:B:485:GLU:OE2	1:B:556:ILE:CG1	2.59	0.51
1:A:541:ALA:O	1:A:544:LYS:HB3	2.11	0.51
1:B:19:ALA:HB3	1:B:25:LYS:HB2	1.93	0.51
1:B:534:ILE:HD12	1:B:582:PHE:CE2	2.45	0.51
1:A:260:LEU:HD22	1:A:260:LEU:C	2.36	0.50
1:A:539:ILE:HB	1:A:540:PRO:HD3	1.93	0.50
1:B:649:LEU:O	1:B:652:MET:HB3	2.11	0.50
1:A:493:VAL:HG21	1:A:593:ALA:HB2	1.92	0.50
1:B:286:ILE:N	1:B:286:ILE:HD12	2.26	0.50
1:B:410:ASP:C	1:B:411:VAL:HG22	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:LEU:HA	1:B:431:LEU:HB2	1.93	0.50
1:A:295:GLU:HA	1:B:26:THR:HB	1.93	0.50
1:B:190:ASN:ND2	1:B:195:ASP:HB2	2.26	0.50
1:A:216:LEU:O	1:A:217:VAL:C	2.54	0.50
1:B:74:TRP:O	1:B:75:LYS:C	2.55	0.50
1:B:94:VAL:HG11	1:B:124:GLN:OE1	2.11	0.50
1:B:381:LYS:C	1:B:383:THR:H	2.19	0.50
1:B:416:LYS:HG2	1:B:449:THR:HB	1.94	0.50
1:B:680:PRO:HG2	1:B:683:VAL:HG21	1.93	0.50
1:A:135:PHE:HE2	1:A:137:ASN:ND2	2.10	0.50
1:B:330:VAL:CG1	1:B:371:ALA:HA	2.41	0.50
1:B:590:ILE:HG22	1:B:591:LYS:N	2.26	0.50
1:A:157:LEU:O	1:A:639:ASN:CB	2.55	0.50
1:A:336:THR:HG22	1:A:368:GLU:HB3	1.94	0.50
1:B:621:ILE:O	1:B:625:ASN:HB2	2.12	0.50
1:B:630:GLN:HB2	1:B:646:PHE:HB2	1.93	0.50
1:A:137:ASN:OD1	1:A:138:LYS:N	2.42	0.50
1:B:608:VAL:CG2	1:B:647:VAL:CG1	2.89	0.50
1:A:109:ASP:OD1	1:A:111:SER:HB2	2.10	0.50
1:A:312:LEU:CD2	1:A:313:ALA:N	2.75	0.50
1:A:653:PHE:O	1:A:654:GLY:C	2.55	0.50
1:B:82:ILE:HD12	1:B:101:LEU:HB3	1.93	0.50
1:B:485:GLU:OE2	1:B:556:ILE:HG13	2.12	0.50
1:A:274:ASP:O	1:A:278:ASP:HB2	2.12	0.50
1:A:316:ILE:HD11	1:A:384:ILE:C	2.36	0.50
1:A:543:GLN:HE22	1:B:199:ILE:HG22	1.76	0.50
1:B:508:GLY:O	1:B:585:ALA:HB2	2.12	0.50
1:A:85:PRO:HG3	1:A:94:VAL:HG22	1.93	0.49
1:A:123:ARG:O	1:A:126:GLU:HB3	2.12	0.49
1:A:145:ASP:O	1:A:148:LEU:HB3	2.12	0.49
1:A:468:ARG:HH11	1:A:468:ARG:HG2	1.77	0.49
1:B:573:HIS:ND1	1:B:576:ASP:OD2	2.45	0.49
1:A:10:LYS:HG2	1:A:284:LEU:HD21	1.93	0.49
1:A:34:TYR:CD1	1:A:34:TYR:O	2.65	0.49
1:A:38:ARG:C	1:A:39:ILE:HG22	2.37	0.49
1:A:295:GLU:O	1:A:295:GLU:HG3	2.11	0.49
1:A:312:LEU:HD23	1:A:387:ASP:O	2.12	0.49
1:A:361:ASN:O	1:A:362:HIS:HB3	2.12	0.49
1:A:458:HIS:O	1:A:461:ILE:HB	2.12	0.49
1:A:616:TYR:OH	1:A:664:GLN:NE2	2.45	0.49
1:B:34:TYR:OH	1:B:38:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:GLN:O	1:B:273:LEU:N	2.41	0.49
1:B:613:PRO:HA	1:B:640:ALA:CB	2.42	0.49
1:B:631:ILE:HA	1:B:645:ALA:CB	2.41	0.49
1:A:349:LYS:C	1:A:350:GLU:HG2	2.36	0.49
1:A:506:GLN:CA	1:A:576:ASP:O	2.58	0.49
1:A:680:PRO:O	1:A:682:GLN:N	2.45	0.49
1:B:182:ARG:HB2	1:B:184:LYS:HD3	1.94	0.49
1:B:270:GLN:O	1:B:273:LEU:HB2	2.12	0.49
1:B:312:LEU:O	1:B:328:ILE:HA	2.12	0.49
1:B:388:THR:C	1:B:389:LEU:HD13	2.38	0.49
1:B:448:GLN:O	1:B:449:THR:CB	2.60	0.49
1:B:491:VAL:CG2	1:B:593:ALA:HB1	2.41	0.49
1:A:19:ALA:HB2	1:A:107:VAL:CG1	2.43	0.49
1:A:443:HIS:HB2	1:A:450:ILE:HD13	1.93	0.49
1:A:514:VAL:HA	1:A:564:LYS:O	2.12	0.49
1:B:196:ILE:HG23	1:B:196:ILE:O	2.13	0.49
1:A:87:HIS:CE1	1:A:90:PHE:HB2	2.45	0.49
1:A:190:ASN:ND2	1:A:195:ASP:CB	2.74	0.49
1:B:16:GLY:N	1:B:101:LEU:HD12	2.27	0.49
1:B:572:TYR:CD1	1:B:572:TYR:N	2.80	0.49
1:A:20:HIS:CE1	1:A:117:GLN:HE22	2.31	0.49
1:A:102:ASP:HB3	1:A:286:ILE:CD1	2.40	0.49
1:A:138:LYS:C	1:A:140:ASP:H	2.21	0.49
1:A:147:TRP:H	1:A:147:TRP:CD1	2.23	0.49
1:A:352:VAL:O	1:A:353:ALA:O	2.31	0.49
1:A:507:TYR:CD1	1:A:507:TYR:C	2.91	0.49
1:A:608:VAL:HG13	1:A:670:VAL:O	2.12	0.49
1:B:26:THR:O	1:B:29:THR:N	2.45	0.49
1:B:247:ARG:O	1:B:248:LYS:C	2.56	0.49
1:B:330:VAL:HG12	1:B:371:ALA:HA	1.95	0.49
1:A:292:THR:O	1:A:398:ILE:HD12	2.12	0.49
1:A:385:THR:HG22	1:A:386:GLY:N	2.28	0.49
1:A:468:ARG:HG2	1:A:468:ARG:NH1	2.28	0.49
1:B:539:ILE:O	1:B:542:VAL:HB	2.12	0.49
1:B:628:ARG:HH12	1:B:651:GLU:HB2	1.76	0.49
1:B:679:VAL:O	1:B:679:VAL:HG12	2.12	0.49
1:A:8:ASP:HB3	1:A:11:ARG:HG3	1.92	0.49
1:A:414:GLU:HB3	1:A:452:SER:CB	2.43	0.49
1:B:68:ALA:HB3	1:B:327:PHE:CE2	2.48	0.49
1:B:88:VAL:HG12	1:B:89:ASP:N	2.27	0.49
1:B:211:GLU:O	1:B:215:LYS:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:PRO:CG	1:A:538:TYR:CD2	2.94	0.49
1:A:680:PRO:O	1:A:683:VAL:HG23	2.12	0.49
1:B:89:ASP:N	1:B:89:ASP:OD1	2.39	0.49
1:A:82:ILE:HD12	1:A:101:LEU:CB	2.43	0.49
1:B:572:TYR:N	1:B:572:TYR:HD1	2.10	0.49
1:B:634:MET:HB2	1:B:643:ILE:HA	1.94	0.49
1:A:183:MET:HE1	1:A:209:ALA:CB	2.35	0.48
1:A:92:ILE:N	1:A:92:ILE:HD13	2.28	0.48
1:A:181:LEU:CD2	1:A:243:VAL:HG22	2.33	0.48
1:A:499:ARG:HG3	1:A:500:GLN:N	2.27	0.48
1:B:122:TRP:CE3	1:B:157:LEU:HD23	2.48	0.48
1:B:152:THR:O	1:B:153:MET:C	2.55	0.48
1:B:342:TYR:HE1	1:B:347:GLY:C	2.20	0.48
1:B:343:ASN:OD1	1:B:343:ASN:O	2.30	0.48
1:B:461:ILE:O	1:B:465:ARG:HG3	2.14	0.48
1:B:590:ILE:C	1:B:592:GLU:N	2.70	0.48
1:A:462:ILE:O	1:A:466:LEU:HB2	2.14	0.48
1:A:608:VAL:HG13	1:A:669:PHE:HD2	1.78	0.48
1:A:657:THR:HA	1:A:660:ARG:CB	2.36	0.48
1:B:96:ARG:C	1:B:98:MET:H	2.20	0.48
1:B:325:LEU:CD2	1:B:378:VAL:HG23	2.42	0.48
1:B:385:THR:HG22	1:B:386:GLY:N	2.28	0.48
1:B:584:ILE:HG22	1:B:585:ALA:N	2.29	0.48
1:A:146:LEU:HD12	1:A:167:PRO:HD3	1.96	0.48
1:A:535:PRO:HB2	1:A:537:GLU:OE1	2.13	0.48
1:A:573:HIS:C	1:A:575:VAL:N	2.72	0.48
1:A:669:PHE:CD2	1:A:670:VAL:N	2.81	0.48
1:B:631:ILE:HA	1:B:645:ALA:HB2	1.95	0.48
1:A:38:ARG:CD	1:A:39:ILE:H	2.26	0.48
1:A:456:GLU:C	1:A:458:HIS:H	2.21	0.48
1:A:607:ARG:NH1	1:A:672:PHE:CG	2.81	0.48
1:B:20:HIS:CE1	1:B:117:GLN:HE22	2.30	0.48
1:B:68:ALA:O	1:B:69:VAL:HG23	2.14	0.48
1:B:456:GLU:C	1:B:458:HIS:N	2.69	0.48
1:B:652:MET:CE	1:B:655:TYR:CD2	2.95	0.48
1:A:485:GLU:OE1	1:A:555:LEU:HB2	2.12	0.48
1:A:628:ARG:HH12	1:A:651:GLU:HB2	1.79	0.48
1:B:166:LEU:CD2	1:B:208:GLN:HG2	2.43	0.48
1:B:191:ASP:O	1:B:192:LEU:HD23	2.12	0.48
1:B:212:TYR:CD1	1:B:215:LYS:HD2	2.48	0.48
1:B:456:GLU:O	1:B:458:HIS:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:THR:O	1:A:174:PHE:C	2.56	0.48
1:A:203:GLU:CA	1:A:206:LEU:HD23	2.32	0.48
1:A:312:LEU:HD23	1:A:313:ALA:H	1.77	0.48
1:A:457:LEU:HA	1:A:460:GLU:HB2	1.95	0.48
1:B:74:TRP:CE3	1:B:273:LEU:HD13	2.47	0.48
1:B:170:ARG:N	1:B:173:THR:HB	2.28	0.48
1:B:271:LEU:O	1:B:272:LEU:C	2.56	0.48
1:B:626:ALA:C	1:B:628:ARG:H	2.20	0.48
1:A:218:GLU:O	1:A:219:VAL:C	2.57	0.48
1:A:241:GLU:O	1:A:245:ALA:HB2	2.14	0.48
1:A:466:LEU:O	1:A:470:PHE:N	2.35	0.48
1:A:510:VAL:HB	1:A:567:LEU:HD11	1.95	0.48
1:B:344:THR:O	1:B:346:LYS:N	2.47	0.48
1:B:491:VAL:HG21	1:B:593:ALA:HB1	1.96	0.48
1:B:494:GLU:CD	1:B:509:HIS:HE1	2.22	0.48
1:B:517:LEU:HD23	1:B:518:PRO:CD	2.43	0.48
1:B:520:GLY:N	1:B:562:ASP:OD2	2.46	0.48
1:A:96:ARG:C	1:A:98:MET:H	2.20	0.48
1:A:105:ILE:HG23	1:A:133:ILE:CG1	2.37	0.48
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.78	0.48
1:B:151:ARG:HG2	1:B:151:ARG:HH11	1.79	0.48
1:B:270:GLN:O	1:B:271:LEU:C	2.55	0.48
1:B:388:THR:CG2	1:B:397:VAL:O	2.57	0.48
1:A:192:LEU:HA	1:A:266:ASN:HD22	1.78	0.48
1:A:273:LEU:O	1:A:274:ASP:C	2.56	0.48
1:A:345:THR:CG2	1:A:388:THR:H	2.27	0.48
1:A:361:ASN:O	1:A:362:HIS:CG	2.67	0.48
1:A:455:GLY:O	1:A:459:LEU:HD11	2.14	0.48
1:B:305:PRO:C	1:B:307:GLY:H	2.21	0.48
1:B:509:HIS:CD2	1:B:570:GLY:HA2	2.49	0.48
1:A:428:LEU:HD12	1:A:428:LEU:H	1.79	0.47
1:A:457:LEU:CG	1:A:460:GLU:HB2	2.42	0.47
1:A:523:PHE:N	1:B:194:THR:O	2.42	0.47
1:B:464:ASP:O	1:B:468:ARG:HB2	2.14	0.47
1:A:620:VAL:C	1:A:622:GLY:N	2.69	0.47
1:B:19:ALA:HB2	1:B:107:VAL:HG13	1.96	0.47
1:A:672:PHE:HD1	1:A:672:PHE:N	2.11	0.47
1:B:329:ARG:CG	1:B:374:LEU:HD23	2.36	0.47
1:B:335:LEU:O	1:B:335:LEU:HG	2.05	0.47
1:A:19:ALA:CB	1:A:107:VAL:HG13	2.43	0.47
1:A:466:LEU:O	1:A:468:ARG:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:C	1:B:39:ILE:CG2	2.86	0.47
1:B:361:ASN:O	1:B:362:HIS:CG	2.67	0.47
1:B:647:VAL:HG21	1:B:652:MET:SD	2.55	0.47
1:A:573:HIS:HB3	1:A:576:ASP:HB2	1.96	0.47
1:B:260:LEU:C	1:B:260:LEU:CD2	2.87	0.47
1:B:343:ASN:HD21	1:B:387:ASP:HB3	1.80	0.47
1:B:494:GLU:HG3	1:B:509:HIS:HE1	1.80	0.47
1:B:624:LEU:HD13	1:B:655:TYR:OH	2.15	0.47
1:B:165:GLN:CB	1:B:178:ILE:O	2.58	0.47
1:B:181:LEU:CD1	1:B:242:LEU:HD23	2.44	0.47
1:B:342:TYR:HE1	1:B:347:GLY:O	1.97	0.47
1:B:680:PRO:HG2	1:B:683:VAL:HG23	1.95	0.47
1:A:88:VAL:HG12	1:A:89:ASP:N	2.29	0.47
1:A:312:LEU:HD23	1:A:313:ALA:N	2.30	0.47
1:B:25:LYS:HZ1	1:B:84:THR:H	1.63	0.47
1:B:35:TYR:CE1	1:B:269:VAL:HG21	2.50	0.47
1:B:123:ARG:HH21	1:B:639:ASN:HB3	1.78	0.47
1:B:164:MET:HG3	1:B:259:PHE:CE1	2.49	0.47
1:B:228:MET:O	1:B:229:LEU:C	2.56	0.47
1:B:308:PRO:HB2	1:B:394:ALA:HB1	1.95	0.47
1:B:309:LEU:CD1	1:B:335:LEU:HB2	2.45	0.47
1:B:544:LYS:HD3	1:B:583:LYS:HD3	1.95	0.47
1:B:584:ILE:O	1:B:588:MET:HG3	2.15	0.47
1:A:477:GLY:C	1:A:479:PRO:HD3	2.40	0.47
1:A:689:LYS:NZ	1:A:689:LYS:HB2	2.30	0.47
1:B:131:PRO:HG3	1:B:253:LEU:HD21	1.96	0.47
1:B:336:THR:HG22	1:B:368:GLU:HB3	1.97	0.47
1:B:396:ARG:HG2	1:B:396:ARG:O	2.15	0.47
1:B:538:TYR:O	1:B:540:PRO:N	2.48	0.47
1:A:38:ARG:HD2	1:A:39:ILE:H	1.78	0.47
1:A:321:TYR:C	1:A:323:GLY:H	2.22	0.47
1:A:546:ILE:HG23	1:A:590:ILE:HG13	1.96	0.47
1:B:518:PRO:O	1:B:519:ARG:C	2.57	0.47
1:A:438:PHE:O	1:A:439:ARG:HG3	2.15	0.47
1:B:82:ILE:HD12	1:B:101:LEU:CB	2.46	0.47
1:B:187:THR:HG23	1:B:187:THR:O	2.15	0.47
1:B:231:TYR:CD1	1:B:231:TYR:C	2.93	0.47
1:A:105:ILE:HG12	1:A:133:ILE:HD11	1.96	0.46
1:A:322:VAL:HG12	1:A:354:ARG:NH2	2.31	0.46
1:A:329:ARG:HG2	1:A:329:ARG:HH11	1.80	0.46
1:A:629:GLY:HA2	1:A:646:PHE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:ILE:HD13	1:A:643:ILE:N	2.30	0.46
1:B:114:VAL:CG1	1:B:157:LEU:HD11	2.42	0.46
1:B:240:GLU:H	1:B:240:GLU:CD	2.23	0.46
1:B:286:ILE:HD12	1:B:286:ILE:H	1.78	0.46
1:B:443:HIS:HB2	1:B:450:ILE:CD1	2.45	0.46
1:B:462:ILE:O	1:B:466:LEU:HB2	2.15	0.46
1:B:549:ALA:HB3	1:B:590:ILE:HG21	1.97	0.46
1:B:688:ILE:O	1:B:689:LYS:HD3	2.14	0.46
1:A:36:THR:HG22	1:A:74:TRP:HB2	1.97	0.46
1:B:78:ARG:CZ	1:B:357:ARG:NH2	2.78	0.46
1:B:485:GLU:OE1	1:B:555:LEU:HB2	2.15	0.46
1:B:677:GLN:NE2	1:B:678:GLU:H	2.14	0.46
1:A:96:ARG:C	1:A:98:MET:N	2.70	0.46
1:A:312:LEU:HD21	1:A:386:GLY:HA2	1.96	0.46
1:A:573:HIS:CE1	1:A:576:ASP:OD2	2.68	0.46
1:A:610:VAL:HG22	1:A:669:PHE:HB2	1.97	0.46
1:A:660:ARG:O	1:A:665:GLY:N	2.48	0.46
1:B:361:ASN:O	1:B:362:HIS:HB3	2.15	0.46
1:A:38:ARG:HD2	1:A:39:ILE:O	2.16	0.46
1:A:85:PRO:HD3	1:A:97:SER:OG	2.16	0.46
1:A:513:LYS:HG3	1:A:568:TYR:CE1	2.51	0.46
1:B:313:ALA:HA	1:B:327:PHE:O	2.16	0.46
1:B:620:VAL:C	1:B:622:GLY:N	2.72	0.46
1:A:103:GLY:O	1:A:104:ALA:CB	2.64	0.46
1:A:343:ASN:HD22	1:A:389:LEU:CD1	2.28	0.46
1:A:359:HIS:HD1	1:A:362:HIS:CE1	2.33	0.46
1:A:232:LEU:O	1:A:233:GLU:HB2	2.15	0.46
1:A:328:ILE:O	1:A:374:LEU:HB2	2.14	0.46
1:B:229:LEU:CD1	1:B:229:LEU:N	2.69	0.46
1:B:346:LYS:C	1:B:348:ARG:H	2.24	0.46
1:B:353:ALA:HB3	1:B:378:VAL:O	2.16	0.46
1:B:535:PRO:HD3	1:B:572:TYR:CD2	2.50	0.46
1:B:590:ILE:O	1:B:592:GLU:N	2.49	0.46
1:B:621:ILE:HG23	1:B:631:ILE:HG12	1.97	0.46
1:B:38:ARG:CD	1:B:39:ILE:H	2.28	0.46
1:B:517:LEU:HB2	1:B:562:ASP:C	2.41	0.46
1:B:616:TYR:C	1:B:618:GLY:N	2.71	0.46
1:B:623:ASP:O	1:B:626:ALA:HB3	2.16	0.46
1:A:434:GLU:O	1:A:434:GLU:HG2	2.14	0.46
1:A:443:HIS:HA	1:A:444:PRO:HD3	1.78	0.46
1:A:572:TYR:HD1	1:A:572:TYR:H	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ASP:O	1:B:148:LEU:HB3	2.16	0.46
1:B:344:THR:C	1:B:346:LYS:H	2.23	0.46
1:B:443:HIS:HA	1:B:444:PRO:HD3	1.78	0.46
1:A:112:GLN:O	1:A:113:GLY:C	2.59	0.46
1:A:305:PRO:C	1:A:307:GLY:H	2.24	0.46
1:A:312:LEU:O	1:A:328:ILE:HA	2.15	0.46
1:A:344:THR:O	1:A:346:LYS:N	2.48	0.46
1:A:610:VAL:HG22	1:A:669:PHE:CB	2.46	0.46
1:A:626:ALA:C	1:A:628:ARG:N	2.73	0.46
1:B:352:VAL:HG13	1:B:352:VAL:O	2.16	0.46
1:B:685:GLU:O	1:B:688:ILE:CG1	2.62	0.46
1:A:339:SER:H	1:A:352:VAL:CG1	2.28	0.46
1:A:416:LYS:C	1:A:416:LYS:CD	2.88	0.46
1:A:538:TYR:O	1:A:539:ILE:C	2.58	0.46
1:A:680:PRO:C	1:A:682:GLN:N	2.74	0.46
1:B:178:ILE:HG22	1:B:179:ASP:N	2.31	0.46
1:B:232:LEU:O	1:B:233:GLU:HB2	2.15	0.46
1:B:309:LEU:CG	1:B:310:ALA:N	2.77	0.46
1:B:546:ILE:O	1:B:550:MET:HG2	2.15	0.46
1:A:264:LEU:O	1:A:265:LYS:HD3	2.15	0.45
1:A:275:ALA:O	1:A:276:VAL:C	2.56	0.45
1:B:10:LYS:HG2	1:B:284:LEU:HD21	1.97	0.45
1:B:157:LEU:N	1:B:157:LEU:HD12	2.30	0.45
1:B:170:ARG:O	1:B:173:THR:N	2.42	0.45
1:B:439:ARG:NH1	1:B:439:ARG:CB	2.79	0.45
1:B:466:LEU:HB3	1:B:467:LYS:H	1.60	0.45
1:B:602:LEU:CD1	1:B:678:GLU:HA	2.42	0.45
1:A:192:LEU:HA	1:A:266:ASN:ND2	2.31	0.45
1:A:523:PHE:CD1	1:A:524:GLU:N	2.84	0.45
1:B:103:GLY:O	1:B:104:ALA:CB	2.61	0.45
1:A:68:ALA:O	1:A:69:VAL:HG23	2.17	0.45
1:A:455:GLY:O	1:A:459:LEU:HD12	2.16	0.45
1:A:621:ILE:O	1:A:625:ASN:HB2	2.16	0.45
1:A:630:GLN:O	1:A:631:ILE:C	2.60	0.45
1:B:27:THR:O	1:B:28:THR:C	2.60	0.45
1:B:539:ILE:HB	1:B:540:PRO:HD3	1.97	0.45
1:B:611:THR:O	1:B:667:GLY:HA2	2.17	0.45
1:A:345:THR:HG23	1:A:388:THR:H	1.82	0.45
1:A:481:VAL:HG21	1:A:650:ALA:HB2	1.98	0.45
1:A:669:PHE:HE2	1:A:671:MET:HE2	1.81	0.45
1:B:199:ILE:HB	1:B:200:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:LEU:O	1:B:432:ALA:CB	2.65	0.45
1:B:554:PRO:O	1:B:555:LEU:O	2.35	0.45
1:A:99:ARG:HD2	1:A:289:ILE:HD12	1.99	0.45
1:A:188:TYR:CB	1:A:267:LYS:HD3	2.47	0.45
1:A:340:TYR:CB	1:A:392:GLU:OE2	2.61	0.45
1:A:344:THR:CG2	1:A:396:ARG:HB2	2.46	0.45
1:A:364:GLU:HG2	1:A:366:VAL:HG13	1.99	0.45
1:A:688:ILE:O	1:A:689:LYS:HD3	2.17	0.45
1:B:201:ILE:H	1:B:201:ILE:CD1	2.27	0.45
1:B:215:LYS:O	1:B:219:VAL:HG23	2.16	0.45
1:B:252:ASP:O	1:B:253:LEU:HB2	2.16	0.45
1:B:658:ASP:O	1:B:661:SER:OG	2.26	0.45
1:A:289:ILE:CG2	1:A:301:ILE:HB	2.45	0.45
1:A:344:THR:HG22	1:A:396:ARG:HB2	1.99	0.45
1:A:635:GLU:O	1:A:642:VAL:HG22	2.17	0.45
1:B:203:GLU:HA	1:B:206:LEU:CD2	2.36	0.45
1:B:336:THR:HG22	1:B:368:GLU:CB	2.46	0.45
1:B:345:THR:HG22	1:B:398:ILE:HG22	1.98	0.45
1:B:466:LEU:O	1:B:470:PHE:O	2.35	0.45
1:B:507:TYR:O	1:B:581:ALA:HB1	2.17	0.45
1:A:440:VAL:HG13	1:A:440:VAL:O	2.17	0.45
1:A:526:VAL:CG1	1:A:527:ASN:H	2.29	0.45
1:A:573:HIS:CG	1:A:576:ASP:HB2	2.52	0.45
1:A:639:ASN:OD1	1:A:639:ASN:C	2.59	0.45
1:A:653:PHE:C	1:A:655:TYR:H	2.25	0.45
1:B:352:VAL:O	1:B:353:ALA:O	2.35	0.45
1:B:497:PHE:CG	1:B:584:ILE:HG21	2.51	0.45
1:B:542:VAL:HA	1:B:582:PHE:O	2.16	0.45
1:A:34:TYR:O	1:A:34:TYR:HD1	1.98	0.45
1:A:259:PHE:CE2	1:A:275:ALA:HB1	2.52	0.45
1:A:649:LEU:C	1:A:649:LEU:HD22	2.42	0.45
1:A:649:LEU:O	1:A:652:MET:HB3	2.16	0.45
1:B:450:ILE:HG13	1:B:450:ILE:O	2.16	0.45
1:A:38:ARG:C	1:A:39:ILE:CG2	2.89	0.45
1:A:99:ARG:CD	1:A:289:ILE:HD12	2.47	0.45
1:A:240:GLU:O	1:A:241:GLU:C	2.59	0.45
1:A:381:LYS:HB2	1:A:381:LYS:NZ	2.31	0.45
1:A:486:THR:OG1	1:A:561:VAL:O	2.32	0.45
1:A:655:TYR:CD1	1:A:655:TYR:C	2.94	0.45
1:A:681:LYS:H	1:A:681:LYS:CD	2.30	0.45
1:B:628:ARG:NH1	1:B:648:PRO:HB2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:THR:CB	1:A:398:ILE:HD12	2.47	0.45
1:A:301:ILE:HD13	1:A:301:ILE:HA	1.84	0.45
1:A:443:HIS:ND1	1:A:450:ILE:CD1	2.80	0.45
1:A:623:ASP:O	1:A:626:ALA:HB3	2.17	0.45
1:B:120:THR:O	1:B:123:ARG:HB2	2.17	0.45
1:B:496:LYS:CE	1:B:509:HIS:ND1	2.80	0.45
1:A:469:GLU:O	1:A:470:PHE:HD1	1.98	0.44
1:B:19:ALA:CB	1:B:107:VAL:HG13	2.46	0.44
1:B:69:VAL:CG2	1:B:314:PHE:HZ	2.30	0.44
1:B:78:ARG:NE	1:B:357:ARG:HH21	2.14	0.44
1:B:156:ARG:HB3	1:B:666:ARG:NH1	2.30	0.44
1:B:170:ARG:O	1:B:171:GLU:C	2.60	0.44
1:B:631:ILE:HD12	1:B:631:ILE:N	2.31	0.44
1:B:647:VAL:CG2	1:B:652:MET:SD	3.05	0.44
1:A:384:ILE:HB	1:A:385:THR:H	1.39	0.44
1:A:539:ILE:O	1:A:542:VAL:HB	2.16	0.44
1:A:588:MET:C	1:A:590:ILE:N	2.73	0.44
1:A:614:GLU:OE1	1:A:641:GLN:HG3	2.16	0.44
1:B:18:ALA:HB1	1:B:121:VAL:CG1	2.47	0.44
1:B:123:ARG:O	1:B:126:GLU:HB3	2.18	0.44
1:B:168:ILE:O	1:B:174:PHE:HA	2.16	0.44
1:B:413:ILE:HA	1:B:480:GLN:O	2.17	0.44
1:B:458:HIS:ND1	1:B:458:HIS:C	2.72	0.44
1:B:494:GLU:HB2	1:B:511:LYS:HG2	1.99	0.44
1:B:678:GLU:HB3	1:B:679:VAL:H	1.49	0.44
1:A:78:ARG:CZ	1:A:357:ARG:HH21	2.31	0.44
1:A:203:GLU:HA	1:A:206:LEU:HB2	1.98	0.44
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.81	0.44
1:B:76:ASP:O	1:B:76:ASP:CG	2.60	0.44
1:A:122:TRP:O	1:A:123:ARG:C	2.61	0.44
1:A:147:TRP:O	1:A:151:ARG:N	2.40	0.44
1:A:228:MET:O	1:A:231:TYR:N	2.50	0.44
1:A:411:VAL:CA	1:A:453:GLY:HA2	2.47	0.44
1:A:458:HIS:CA	1:A:461:ILE:HG13	2.47	0.44
1:A:460:GLU:HA	1:A:463:VAL:HB	1.99	0.44
1:A:608:VAL:HG21	1:A:652:MET:HE2	1.99	0.44
1:A:624:LEU:O	1:A:627:ARG:HB2	2.17	0.44
1:B:96:ARG:C	1:B:98:MET:N	2.72	0.44
1:B:109:ASP:OD1	1:B:111:SER:CB	2.63	0.44
1:B:140:ASP:HA	1:B:171:GLU:O	2.17	0.44
1:B:293:THR:O	1:B:294:PRO:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ASP:O	1:B:411:VAL:CG2	2.65	0.44
1:B:414:GLU:CB	1:B:452:SER:HB2	2.47	0.44
1:B:612:THR:HG21	1:B:620:VAL:CG2	2.41	0.44
1:A:208:GLN:O	1:A:211:GLU:HB3	2.18	0.44
1:A:228:MET:O	1:A:229:LEU:C	2.59	0.44
1:A:314:PHE:C	1:A:385:THR:HG23	2.42	0.44
1:A:391:GLY:O	1:A:394:ALA:N	2.51	0.44
1:A:517:LEU:HD12	1:A:563:ILE:O	2.17	0.44
1:A:669:PHE:CE2	1:A:671:MET:HE2	2.52	0.44
1:B:35:TYR:O	1:B:36:THR:C	2.61	0.44
1:B:444:PRO:HD3	1:B:551:GLN:OE1	2.18	0.44
1:B:525:PHE:HE2	1:B:546:ILE:HD12	1.83	0.44
1:A:121:VAL:O	1:A:122:TRP:C	2.60	0.44
1:A:554:PRO:HG2	1:A:594:VAL:CG1	2.48	0.44
1:A:625:ASN:HD22	1:A:625:ASN:HA	1.60	0.44
1:B:20:HIS:CG	1:B:21:ILE:N	2.85	0.44
1:B:146:LEU:C	1:B:146:LEU:CD2	2.90	0.44
1:B:301:ILE:HD13	1:B:301:ILE:HA	1.84	0.44
1:B:504:ARG:HG2	1:B:504:ARG:NH1	2.32	0.44
1:B:622:GLY:O	1:B:623:ASP:C	2.61	0.44
1:B:671:MET:C	1:B:672:PHE:HD1	2.26	0.44
1:A:26:THR:O	1:A:27:THR:C	2.59	0.44
1:A:85:PRO:CG	1:A:94:VAL:HG22	2.48	0.44
1:A:201:ILE:O	1:A:202:PRO:C	2.61	0.44
1:A:271:LEU:O	1:A:272:LEU:C	2.61	0.44
1:A:427:ALA:HA	1:A:470:PHE:HD2	1.71	0.44
1:A:595:GLN:HE21	1:A:595:GLN:HB3	1.51	0.44
1:A:680:PRO:O	1:A:681:LYS:C	2.59	0.44
1:B:16:GLY:O	1:B:104:ALA:HA	2.18	0.44
1:B:203:GLU:HA	1:B:206:LEU:HB2	2.00	0.44
1:B:333:GLY:O	1:B:371:ALA:HB2	2.17	0.44
1:B:435:ASP:O	1:B:438:PHE:CE2	2.70	0.44
1:B:616:TYR:HE2	1:B:666:ARG:HD3	1.83	0.44
1:A:242:LEU:O	1:A:243:VAL:C	2.61	0.44
1:A:308:PRO:HB2	1:A:394:ALA:HB1	1.99	0.44
1:A:493:VAL:HG21	1:A:589:ALA:O	2.18	0.44
1:A:525:PHE:HB3	1:B:197:ARG:CB	2.48	0.44
1:A:604:PRO:HG2	1:A:649:LEU:CB	2.47	0.44
1:B:118:SER:HA	1:B:121:VAL:CG2	2.48	0.44
1:B:487:ILE:HD12	1:B:489:LYS:O	2.17	0.44
1:B:511:LYS:HD2	1:B:569:ASP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:LEU:O	1:B:652:MET:CB	2.66	0.44
1:A:74:TRP:CD2	1:A:273:LEU:HD13	2.52	0.44
1:A:247:ARG:HG3	1:A:279:TYR:O	2.18	0.44
1:A:605:ILE:HD13	1:A:677:GLN:HB3	1.98	0.44
1:A:632:LEU:HD23	1:A:645:ALA:HA	1.99	0.44
1:A:652:MET:O	1:A:655:TYR:HB2	2.17	0.44
1:B:85:PRO:O	1:B:87:HIS:N	2.51	0.44
1:B:166:LEU:HD21	1:B:208:GLN:HG2	2.00	0.44
1:B:181:LEU:HD21	1:B:243:VAL:CG2	2.36	0.44
1:B:510:VAL:HB	1:B:567:LEU:HD11	1.99	0.44
1:B:592:GLU:O	1:B:594:VAL:N	2.51	0.44
1:A:241:GLU:O	1:A:245:ALA:CB	2.65	0.43
1:A:290:LYS:HE2	1:A:298:VAL:HG11	2.00	0.43
1:A:357:ARG:HG3	1:A:357:ARG:NH1	2.27	0.43
1:A:441:SER:HB3	1:A:450:ILE:HG13	2.00	0.43
1:A:620:VAL:C	1:A:622:GLY:H	2.25	0.43
1:B:220:ALA:O	1:B:221:ALA:O	2.36	0.43
1:B:644:ARG:H	1:B:644:ARG:HG3	1.68	0.43
1:B:688:ILE:C	1:B:689:LYS:HZ2	2.25	0.43
1:A:20:HIS:CG	1:A:21:ILE:H	2.36	0.43
1:B:218:GLU:HG3	1:B:231:TYR:CE2	2.53	0.43
1:B:309:LEU:C	1:B:309:LEU:CD2	2.85	0.43
1:A:20:HIS:CG	1:A:21:ILE:N	2.86	0.43
1:A:274:ASP:O	1:A:277:VAL:HG13	2.19	0.43
1:A:336:THR:HG22	1:A:368:GLU:CB	2.48	0.43
1:A:490:PRO:HG3	1:A:516:PRO:HD3	2.00	0.43
1:B:9:LEU:HD12	1:B:12:LEU:HD13	2.01	0.43
1:B:33:LEU:HD21	1:B:81:ILE:HD12	2.01	0.43
1:B:485:GLU:O	1:B:560:VAL:HA	2.19	0.43
1:A:523:PHE:CZ	1:A:525:PHE:HB2	2.53	0.43
1:A:525:PHE:CD1	1:A:525:PHE:C	2.96	0.43
1:A:677:GLN:C	1:A:678:GLU:O	2.61	0.43
1:B:135:PHE:HE2	1:B:137:ASN:ND2	2.16	0.43
1:B:441:SER:HG	1:B:450:ILE:HD11	1.84	0.43
1:A:464:ASP:C	1:A:466:LEU:H	2.26	0.43
1:A:534:ILE:HG23	1:A:582:PHE:CE2	2.54	0.43
1:A:573:HIS:CB	1:A:576:ASP:HB2	2.48	0.43
1:A:669:PHE:O	1:A:670:VAL:HG23	2.17	0.43
1:B:312:LEU:HD21	1:B:386:GLY:HA2	2.00	0.43
1:B:575:VAL:HG23	1:B:576:ASP:N	2.32	0.43
1:A:309:LEU:CG	1:A:310:ALA:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:THR:HG23	1:A:388:THR:HB	1.99	0.43
1:A:456:GLU:C	1:A:458:HIS:N	2.76	0.43
1:A:554:PRO:HG2	1:A:594:VAL:CB	2.45	0.43
1:B:92:ILE:N	1:B:92:ILE:CD1	2.81	0.43
1:A:94:VAL:HG11	1:A:124:GLN:OE1	2.18	0.43
1:B:228:MET:O	1:B:231:TYR:HB3	2.19	0.43
1:B:448:GLN:O	1:B:449:THR:OG1	2.31	0.43
1:B:459:LEU:H	1:B:459:LEU:CD1	2.27	0.43
1:B:558:PHE:O	1:B:559:PRO:O	2.36	0.43
1:B:592:GLU:HG3	1:B:593:ALA:N	2.33	0.43
1:B:682:GLN:CD	1:B:682:GLN:H	2.26	0.43
1:A:14:ASN:OD1	1:A:80:ASN:HB2	2.18	0.43
1:A:218:GLU:O	1:A:221:ALA:CB	2.66	0.43
1:A:224:ASP:O	1:A:225:GLU:C	2.62	0.43
1:A:485:GLU:O	1:A:560:VAL:HG13	2.19	0.43
1:A:573:HIS:O	1:A:574:GLU:C	2.62	0.43
1:A:616:TYR:O	1:A:620:VAL:HG23	2.19	0.43
1:A:655:TYR:CE1	1:A:659:LEU:HB2	2.54	0.43
1:B:329:ARG:HH11	1:B:329:ARG:HG2	1.84	0.43
1:B:384:ILE:HB	1:B:385:THR:H	1.42	0.43
1:B:441:SER:HB3	1:B:450:ILE:CD1	2.49	0.43
1:B:542:VAL:CG2	1:B:582:PHE:HB3	2.49	0.43
1:B:608:VAL:HG23	1:B:647:VAL:HG12	2.00	0.43
1:B:663:THR:C	1:B:665:GLY:H	2.26	0.43
1:A:178:ILE:HG22	1:A:179:ASP:N	2.33	0.43
1:B:11:ARG:NH1	1:B:11:ARG:CG	2.73	0.43
1:B:165:GLN:HE21	1:B:165:GLN:HB3	1.55	0.43
1:B:224:ASP:O	1:B:225:GLU:C	2.62	0.43
1:B:384:ILE:H	1:B:384:ILE:HG13	1.64	0.43
1:A:96:ARG:NH2	1:A:386:GLY:HA3	2.33	0.43
1:A:220:ALA:HB1	1:A:227:ILE:CD1	2.49	0.43
1:A:224:ASP:O	1:A:227:ILE:HB	2.19	0.43
1:A:616:TYR:C	1:A:618:GLY:N	2.75	0.43
1:A:649:LEU:HD22	1:A:649:LEU:O	2.19	0.43
1:B:118:SER:HA	1:B:121:VAL:HG23	2.01	0.43
1:B:125:ALA:O	1:B:126:GLU:C	2.62	0.43
1:B:681:LYS:N	1:B:681:LYS:CD	2.76	0.43
1:A:195:ASP:C	1:A:196:ILE:HG22	2.43	0.42
1:A:302:HIS:O	1:A:332:SER:HB2	2.18	0.42
1:A:304:ASP:HA	1:A:305:PRO:HD3	1.82	0.42
1:A:457:LEU:CA	1:A:460:GLU:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ASP:HA	1:B:267:LYS:NZ	2.34	0.42
1:B:326:THR:HB	1:B:377:VAL:HG13	2.01	0.42
1:B:441:SER:HB3	1:B:450:ILE:CG1	2.48	0.42
1:B:525:PHE:CZ	1:B:543:GLN:HG3	2.55	0.42
1:B:646:PHE:HA	1:B:646:PHE:HD1	1.72	0.42
1:A:292:THR:CG2	1:A:398:ILE:HD12	2.49	0.42
1:A:342:TYR:HE1	1:A:347:GLY:O	2.02	0.42
1:B:6:GLU:CD	1:B:7:TYR:H	2.26	0.42
1:B:181:LEU:HD11	1:B:242:LEU:HB3	2.00	0.42
1:B:493:VAL:HG21	1:B:593:ALA:HB2	2.01	0.42
1:B:620:VAL:C	1:B:622:GLY:H	2.25	0.42
1:A:346:LYS:C	1:A:348:ARG:H	2.27	0.42
1:A:357:ARG:HH11	1:A:357:ARG:CG	2.28	0.42
1:A:69:VAL:CG2	1:A:314:PHE:HZ	2.32	0.42
1:A:286:ILE:CG2	1:A:287:PRO:N	2.82	0.42
1:A:461:ILE:O	1:A:465:ARG:CG	2.66	0.42
1:A:504:ARG:HG2	1:A:504:ARG:NH1	2.33	0.42
1:A:679:VAL:HG22	1:A:683:VAL:CG2	2.49	0.42
1:B:169:GLY:O	1:B:174:PHE:HA	2.19	0.42
1:B:549:ALA:C	1:B:551:GLN:N	2.78	0.42
1:A:127:LYS:HB2	1:A:637:ARG:CZ	2.48	0.42
1:A:231:TYR:C	1:A:231:TYR:CD1	2.96	0.42
1:A:286:ILE:HG22	1:A:287:PRO:N	2.33	0.42
1:A:496:LYS:HG2	1:A:509:HIS:ND1	2.35	0.42
1:A:522:GLY:HA3	1:B:194:THR:C	2.43	0.42
1:B:319:ASP:HB3	1:B:322:VAL:HG22	2.01	0.42
1:B:458:HIS:O	1:B:461:ILE:CB	2.66	0.42
1:B:677:GLN:O	1:B:678:GLU:O	2.37	0.42
1:A:25:LYS:NZ	1:A:84:THR:CB	2.82	0.42
1:A:98:MET:C	1:A:100:VAL:N	2.77	0.42
1:A:681:LYS:N	1:A:681:LYS:CD	2.82	0.42
1:B:496:LYS:HE3	1:B:509:HIS:CE1	2.54	0.42
1:B:513:LYS:HG3	1:B:568:TYR:CE1	2.54	0.42
1:A:74:TRP:O	1:A:75:LYS:C	2.63	0.42
1:A:140:ASP:HA	1:A:171:GLU:C	2.44	0.42
1:A:632:LEU:CD2	1:A:645:ALA:HA	2.50	0.42
1:A:669:PHE:CG	1:A:670:VAL:N	2.87	0.42
1:B:15:ILE:HD13	1:B:276:VAL:HG11	2.02	0.42
1:B:89:ASP:HB2	1:B:90:PHE:H	1.53	0.42
1:B:282:SER:O	1:B:283:PRO:C	2.63	0.42
1:B:319:ASP:OD1	1:B:320:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:LEU:HD23	1:B:399:LEU:HA	1.87	0.42
1:B:413:ILE:CD1	1:B:454:MET:O	2.54	0.42
1:B:457:LEU:CB	1:B:460:GLU:HB2	2.50	0.42
1:B:467:LYS:HE3	1:B:467:LYS:HB3	1.69	0.42
1:B:515:GLU:HB3	1:B:516:PRO:CD	2.49	0.42
1:B:561:VAL:O	1:B:562:ASP:C	2.63	0.42
1:B:607:ARG:O	1:B:671:MET:HB2	2.20	0.42
1:A:22:ASP:O	1:A:23:ALA:C	2.61	0.42
1:A:385:THR:C	1:A:387:ASP:N	2.78	0.42
1:A:480:GLN:HE22	1:A:558:PHE:HZ	1.66	0.42
1:B:128:TYR:O	1:B:129:LYS:HB3	2.20	0.42
1:B:146:LEU:HD23	1:B:146:LEU:C	2.45	0.42
1:B:157:LEU:CD1	1:B:157:LEU:N	2.83	0.42
1:B:459:LEU:O	1:B:463:VAL:N	2.49	0.42
1:B:499:ARG:HG3	1:B:500:GLN:N	2.34	0.42
1:A:31:ARG:NH2	1:A:34:TYR:CD2	2.88	0.42
1:A:357:ARG:HD3	1:A:364:GLU:OE2	2.20	0.42
1:A:427:ALA:CB	1:A:470:PHE:HD2	2.32	0.42
1:B:272:LEU:O	1:B:276:VAL:HG23	2.20	0.42
1:B:416:LYS:HG2	1:B:449:THR:CG2	2.50	0.42
1:B:444:PRO:HA	1:B:448:GLN:HG3	2.01	0.42
1:B:663:THR:C	1:B:665:GLY:N	2.77	0.42
1:A:247:ARG:NH1	1:A:251:ILE:CD1	2.83	0.42
1:A:260:LEU:C	1:A:260:LEU:CD2	2.93	0.42
1:A:603:GLU:CD	1:A:648:PRO:HB3	2.44	0.42
1:B:165:GLN:HG3	1:B:260:LEU:HD11	2.00	0.42
1:B:293:THR:O	1:B:296:GLY:O	2.38	0.42
1:B:545:GLY:N	1:B:583:LYS:HG3	2.35	0.42
1:A:5:VAL:CG1	1:A:6:GLU:H	2.01	0.41
1:A:166:LEU:HD23	1:A:208:GLN:HG2	2.02	0.41
1:A:448:GLN:O	1:A:449:THR:HB	2.20	0.41
1:A:448:GLN:O	1:A:449:THR:OG1	2.38	0.41
1:A:493:VAL:CG2	1:A:593:ALA:HB2	2.50	0.41
1:A:499:ARG:HG3	1:A:501:THR:H	1.85	0.41
1:A:608:VAL:CG1	1:A:609:GLU:N	2.83	0.41
1:A:27:THR:O	1:A:31:ARG:HG2	2.20	0.41
1:A:292:THR:HG22	1:A:398:ILE:CD1	2.50	0.41
1:A:319:ASP:CG	1:A:320:PRO:HD2	2.45	0.41
1:A:493:VAL:HB	1:A:494:GLU:H	1.55	0.41
1:A:528:ALA:HB3	1:A:568:TYR:HA	2.02	0.41
1:A:585:ALA:HA	1:A:588:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:GLY:O	1:A:639:ASN:C	2.61	0.41
1:A:682:GLN:CD	1:A:682:GLN:H	2.28	0.41
1:B:31:ARG:O	1:B:35:TYR:HD1	2.03	0.41
1:B:182:ARG:C	1:B:184:LYS:HG2	2.45	0.41
1:B:268:GLY:O	1:B:269:VAL:C	2.63	0.41
1:B:272:LEU:O	1:B:272:LEU:HD23	2.20	0.41
1:A:188:TYR:HB2	1:A:267:LYS:HD3	2.00	0.41
1:A:507:TYR:O	1:A:577:SER:HA	2.20	0.41
1:A:686:LYS:HG3	1:A:687:LEU:N	2.34	0.41
1:B:35:TYR:O	1:B:38:ARG:HG3	2.20	0.41
1:B:201:ILE:O	1:B:202:PRO:C	2.62	0.41
1:B:352:VAL:O	1:B:353:ALA:C	2.63	0.41
1:B:554:PRO:HG2	1:B:594:VAL:CB	2.44	0.41
1:B:679:VAL:O	1:B:680:PRO:C	2.63	0.41
1:A:31:ARG:O	1:A:34:TYR:N	2.53	0.41
1:B:119:GLU:O	1:B:123:ARG:HG2	2.19	0.41
1:B:221:ALA:O	1:B:223:PHE:N	2.53	0.41
1:B:309:LEU:HD23	1:B:390:VAL:HA	2.02	0.41
1:B:486:THR:HG22	1:B:487:ILE:N	2.35	0.41
1:B:573:HIS:HB3	1:B:576:ASP:HB2	2.02	0.41
1:B:612:THR:O	1:B:613:PRO:C	2.62	0.41
1:B:631:ILE:H	1:B:631:ILE:CD1	2.34	0.41
1:A:74:TRP:CZ2	1:A:75:LYS:HE3	2.54	0.41
1:A:152:THR:O	1:A:153:MET:C	2.64	0.41
1:A:178:ILE:HD12	1:A:201:ILE:HG13	2.02	0.41
1:A:178:ILE:CD1	1:A:185:ALA:HB2	2.51	0.41
1:A:286:ILE:HD12	1:A:286:ILE:N	2.35	0.41
1:A:442:THR:OG1	1:A:443:HIS:N	2.45	0.41
1:A:457:LEU:HG	1:A:460:GLU:CG	2.50	0.41
1:A:511:LYS:HD2	1:A:569:ASP:HB3	2.03	0.41
1:A:658:ASP:O	1:A:659:LEU:C	2.62	0.41
1:B:680:PRO:HB2	1:B:682:GLN:NE2	2.25	0.41
1:A:337:SER:OG	1:A:354:ARG:HA	2.20	0.41
1:A:556:ILE:HG13	1:A:558:PHE:CD1	2.55	0.41
1:A:560:VAL:O	1:A:561:VAL:HG13	2.20	0.41
1:A:617:MET:HE3	1:A:617:MET:HB3	1.83	0.41
1:B:127:LYS:HE2	1:B:637:ARG:NH2	2.36	0.41
1:B:346:LYS:O	1:B:348:ARG:N	2.52	0.41
1:B:416:LYS:C	1:B:416:LYS:CD	2.92	0.41
1:A:205:TYR:O	1:A:207:ASP:N	2.53	0.41
1:A:325:LEU:CD2	1:A:378:VAL:HG23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:MET:HB3	1:A:458:HIS:CD2	2.55	0.41
1:A:477:GLY:O	1:A:478:LYS:C	2.62	0.41
1:B:238:THR:OG1	1:B:241:GLU:HB2	2.21	0.41
1:B:342:TYR:CD1	1:B:342:TYR:C	2.98	0.41
1:B:598:ASP:N	1:B:599:PRO:CD	2.84	0.41
1:A:181:LEU:HD11	1:A:242:LEU:HB3	2.02	0.41
1:A:352:VAL:HG13	1:A:352:VAL:O	2.20	0.41
1:B:242:LEU:HA	1:B:242:LEU:HD12	1.76	0.41
1:B:496:LYS:HE2	1:B:509:HIS:ND1	2.36	0.41
1:A:322:VAL:HB	1:A:378:VAL:CG2	2.50	0.41
1:A:340:TYR:CZ	1:A:351:ARG:HB2	2.55	0.41
1:A:527:ASN:OD1	1:A:529:ILE:HB	2.20	0.41
1:A:573:HIS:C	1:A:575:VAL:H	2.29	0.41
1:A:659:LEU:HD12	1:A:659:LEU:HA	1.83	0.41
1:A:685:GLU:O	1:A:689:LYS:NZ	2.53	0.41
1:B:97:SER:C	1:B:100:VAL:HG22	2.46	0.41
1:B:190:ASN:HD21	1:B:195:ASP:HB2	1.86	0.41
1:B:220:ALA:HB1	1:B:227:ILE:CD1	2.51	0.41
1:B:330:VAL:HB	1:B:371:ALA:HA	2.03	0.41
1:B:335:LEU:HD21	1:B:355:LEU:HD21	2.03	0.41
1:B:606:MET:CE	1:B:671:MET:HG3	2.51	0.41
1:B:648:PRO:O	1:B:651:GLU:N	2.48	0.41
1:A:119:GLU:OE2	1:A:123:ARG:NH1	2.54	0.41
1:A:221:ALA:HB1	1:A:228:MET:CG	2.41	0.41
1:A:290:LYS:HE2	1:A:298:VAL:CG1	2.51	0.41
1:B:327:PHE:CD1	1:B:376:ALA:HB2	2.55	0.41
1:A:573:HIS:ND1	1:A:576:ASP:CB	2.77	0.40
1:B:138:LYS:C	1:B:140:ASP:N	2.79	0.40
1:B:216:LEU:O	1:B:216:LEU:HD12	2.21	0.40
1:B:228:MET:C	1:B:230:LYS:N	2.78	0.40
1:B:269:VAL:HG23	1:B:270:GLN:OE1	2.21	0.40
1:B:496:LYS:HG3	1:B:509:HIS:ND1	2.35	0.40
1:B:609:GLU:N	1:B:670:VAL:O	2.52	0.40
1:A:25:LYS:HZ1	1:A:84:THR:CB	2.34	0.40
1:A:101:LEU:H	1:A:101:LEU:CD2	2.33	0.40
1:A:309:LEU:C	1:A:309:LEU:CD2	2.91	0.40
1:A:309:LEU:HD11	1:A:335:LEU:HB2	2.03	0.40
1:A:584:ILE:C	1:A:586:GLY:N	2.77	0.40
1:B:512:ILE:HD12	1:B:514:VAL:HG22	2.02	0.40
1:A:507:TYR:CE1	1:A:572:TYR:HA	2.56	0.40
1:B:157:LEU:C	1:B:639:ASN:HD22	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:VAL:CB	1:B:453:GLY:HA2	2.43	0.40
1:B:443:HIS:HB2	1:B:450:ILE:HD13	2.03	0.40
1:B:602:LEU:HD12	1:B:678:GLU:CA	2.44	0.40
1:A:385:THR:HG22	1:A:386:GLY:H	1.86	0.40
1:A:385:THR:O	1:A:387:ASP:N	2.54	0.40
1:A:449:THR:O	1:A:449:THR:HG22	2.21	0.40
1:A:590:ILE:HG22	1:A:591:LYS:N	2.35	0.40
1:B:459:LEU:O	1:B:462:ILE:N	2.55	0.40
1:B:534:ILE:CD1	1:B:582:PHE:HE2	2.34	0.40
1:A:101:LEU:HD23	1:A:101:LEU:N	2.33	0.40
1:A:205:TYR:O	1:A:206:LEU:C	2.64	0.40
1:A:517:LEU:O	1:A:518:PRO:C	2.64	0.40
1:B:122:TRP:CZ2	1:B:159:ALA:HB2	2.56	0.40
1:B:321:TYR:C	1:B:323:GLY:H	2.29	0.40
1:B:362:HIS:O	1:B:362:HIS:CD2	2.75	0.40
1:B:454:MET:HB3	1:B:458:HIS:NE2	2.36	0.40
1:B:464:ASP:C	1:B:466:LEU:H	2.28	0.40
1:B:485:GLU:OE2	1:B:556:ILE:HG12	2.21	0.40
1:B:542:VAL:C	1:B:544:LYS:N	2.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	620/691 (90%)	446 (72%)	114 (18%)	60 (10%)	0	7
1	B	620/691 (90%)	437 (70%)	117 (19%)	66 (11%)	0	6
All	All	1240/1382 (90%)	883 (71%)	231 (19%)	126 (10%)	0	7

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	91	THR
1	A	92	ILE
1	A	93	GLU
1	A	104	ALA
1	A	196	ILE
1	A	206	LEU
1	A	233	GLU
1	A	353	ALA
1	A	362	HIS
1	A	410	ASP
1	A	427	ALA
1	A	435	ASP
1	A	442	THR
1	A	443	HIS
1	A	449	THR
1	A	457	LEU
1	A	555	LEU
1	A	574	GLU
1	A	617	MET
1	A	678	GLU
1	B	38	ARG
1	B	69	VAL
1	B	91	THR
1	B	92	ILE
1	B	93	GLU
1	B	104	ALA
1	B	139	MET
1	B	196	ILE
1	B	233	GLU
1	B	353	ALA
1	B	362	HIS
1	B	410	ASP
1	B	427	ALA
1	B	435	ASP
1	B	443	HIS
1	B	449	THR
1	B	457	LEU
1	B	555	LEU
1	B	592	GLU
1	B	617	MET
1	B	678	GLU
1	A	6	GLU

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Mol	Chain	Res	Type
1	A	69	VAL
1	A	113	GLY
1	A	142	THR
1	A	174	PHE
1	A	297	GLU
1	A	345	THR
1	A	393	ASP
1	A	455	GLY
1	A	467	LYS
1	A	468	ARG
1	A	501	THR
1	A	532	GLY
1	A	591	LYS
1	A	639	ASN
1	A	654	GLY
1	A	681	LYS
1	B	6	GLU
1	B	86	GLY
1	B	88	VAL
1	B	113	GLY
1	B	174	PHE
1	B	222	ASP
1	B	297	GLU
1	B	345	THR
1	B	393	ASP
1	B	415	PRO
1	B	442	THR
1	B	468	ARG
1	B	501	THR
1	B	532	GLY
1	B	574	GLU
1	B	593	ALA
1	A	88	VAL
1	A	112	GLN
1	A	139	MET
1	A	322	VAL
1	A	347	GLY
1	A	415	PRO
1	A	634	MET
1	B	171	GLU
1	B	206	LEU
1	B	412	ALA

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Mol	Chain	Res	Type
1	B	550	MET
1	B	559	PRO
1	B	634	MET
1	B	652	MET
1	A	75	LYS
1	A	171	GLU
1	A	242	LEU
1	A	392	GLU
1	A	454	MET
1	A	652	MET
1	B	240	GLU
1	B	347	GLY
1	B	373	ASP
1	B	639	ASN
1	B	649	LEU
1	A	19	ALA
1	A	368	GLU
1	A	478	LYS
1	A	627	ARG
1	B	19	ALA
1	B	75	LYS
1	B	142	THR
1	B	144	ALA
1	B	151	ARG
1	B	238	THR
1	B	241	GLU
1	B	539	ILE
1	A	384	ILE
1	B	126	GLU
1	B	253	LEU
1	B	322	VAL
1	B	554	PRO
1	A	411	VAL
1	B	384	ILE
1	A	86	GLY
1	A	32	ILE
1	A	269	VAL
1	B	283	PRO
1	B	561	VAL
1	B	648	PRO
1	B	590	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	534/582 (92%)	432 (81%)	102 (19%)	1	9
1	B	534/582 (92%)	431 (81%)	103 (19%)	1	9
All	All	1068/1164 (92%)	863 (81%)	205 (19%)	1	9

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	TYR
1	A	11	ARG
1	A	12	LEU
1	A	26	THR
1	A	34	TYR
1	A	36	THR
1	A	38	ARG
1	A	39	ILE
1	A	72	CYS
1	A	83	ASP
1	A	84	THR
1	A	89	ASP
1	A	92	ILE
1	A	93	GLU
1	A	96	ARG
1	A	99	ARG
1	A	102	ASP
1	A	107	VAL
1	A	115	GLU
1	A	126	GLU
1	A	129	LYS
1	A	130	VAL
1	A	156	ARG
1	A	166	LEU
1	A	191	ASP
1	A	196	ILE
1	A	201	ILE

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Mol	Chain	Res	Type
1	A	204	GLU
1	A	206	LEU
1	A	226	ASN
1	A	228	MET
1	A	229	LEU
1	A	242	LEU
1	A	248	LYS
1	A	252	ASP
1	A	260	LEU
1	A	265	LYS
1	A	269	VAL
1	A	277	VAL
1	A	293	THR
1	A	298	VAL
1	A	300	GLU
1	A	312	LEU
1	A	321	TYR
1	A	322	VAL
1	A	348	ARG
1	A	350	GLU
1	A	357	ARG
1	A	365	GLU
1	A	367	GLU
1	A	369	LEU
1	A	370	LYS
1	A	374	LEU
1	A	377	VAL
1	A	381	LYS
1	A	384	ILE
1	A	389	LEU
1	A	396	ARG
1	A	398	ILE
1	A	415	PRO
1	A	435	ASP
1	A	440	VAL
1	A	458	HIS
1	A	464	ASP
1	A	466	LEU
1	A	468	ARG
1	A	501	THR
1	A	506	GLN
1	A	510	VAL

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Mol	Chain	Res	Type
1	A	514	VAL
1	A	519	ARG
1	A	524	GLU
1	A	543	GLN
1	A	554	PRO
1	A	572	TYR
1	A	574	GLU
1	A	580	MET
1	A	595	GLN
1	A	602	LEU
1	A	612	THR
1	A	614	GLU
1	A	619	ASP
1	A	623	ASP
1	A	625	ASN
1	A	631	ILE
1	A	632	LEU
1	A	634	MET
1	A	641	GLN
1	A	643	ILE
1	A	644	ARG
1	A	647	VAL
1	A	649	LEU
1	A	660	ARG
1	A	664	GLN
1	A	672	PHE
1	A	678	GLU
1	A	679	VAL
1	A	681	LYS
1	A	682	GLN
1	A	683	VAL
1	A	686	LYS
1	A	689	LYS
1	B	7	TYR
1	B	12	LEU
1	B	26	THR
1	B	34	TYR
1	B	36	THR
1	B	38	ARG
1	B	39	ILE
1	B	72	CYS
1	B	83	ASP

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Mol	Chain	Res	Type
1	B	84	THR
1	B	89	ASP
1	B	92	ILE
1	B	93	GLU
1	B	96	ARG
1	B	97	SER
1	B	99	ARG
1	B	107	VAL
1	B	126	GLU
1	B	129	LYS
1	B	130	VAL
1	B	131	PRO
1	B	146	LEU
1	B	156	ARG
1	B	166	LEU
1	B	167	PRO
1	B	184	LYS
1	B	191	ASP
1	B	192	LEU
1	B	196	ILE
1	B	206	LEU
1	B	226	ASN
1	B	229	LEU
1	B	242	LEU
1	B	248	LYS
1	B	252	ASP
1	B	260	LEU
1	B	265	LYS
1	B	269	VAL
1	B	277	VAL
1	B	283	PRO
1	B	293	THR
1	B	300	GLU
1	B	301	ILE
1	B	312	LEU
1	B	321	TYR
1	B	322	VAL
1	B	335	LEU
1	B	348	ARG
1	B	350	GLU
1	B	352	VAL
1	B	357	ARG

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Mol	Chain	Res	Type
1	B	365	GLU
1	B	367	GLU
1	B	369	LEU
1	B	370	LYS
1	B	377	VAL
1	B	378	VAL
1	B	381	LYS
1	B	384	ILE
1	B	389	LEU
1	B	396	ARG
1	B	398	ILE
1	B	415	PRO
1	B	435	ASP
1	B	440	VAL
1	B	458	HIS
1	B	459	LEU
1	B	464	ASP
1	B	466	LEU
1	B	468	ARG
1	B	501	THR
1	B	506	GLN
1	B	517	LEU
1	B	518	PRO
1	B	519	ARG
1	B	524	GLU
1	B	561	VAL
1	B	572	TYR
1	B	574	GLU
1	B	580	MET
1	B	595	GLN
1	B	598	ASP
1	B	602	LEU
1	B	612	THR
1	B	614	GLU
1	B	619	ASP
1	B	623	ASP
1	B	625	ASN
1	B	634	MET
1	B	643	ILE
1	B	644	ARG
1	B	646	PHE
1	B	649	LEU

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Mol	Chain	Res	Type
1	B	660	ARG
1	B	664	GLN
1	B	670	VAL
1	B	678	GLU
1	B	679	VAL
1	B	681	LYS
1	B	682	GLN
1	B	683	VAL
1	B	686	LYS
1	B	689	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	190	ASN
1	A	208	GLN
1	A	266	ASN
1	A	343	ASN
1	A	426	GLN
1	A	448	GLN
1	A	480	GLN
1	A	506	GLN
1	A	543	GLN
1	A	595	GLN
1	A	625	ASN
1	A	630	GLN
1	A	664	GLN
1	A	682	GLN
1	B	77	HIS
1	B	117	GLN
1	B	208	GLN
1	B	343	ASN
1	B	426	GLN
1	B	448	GLN
1	B	480	GLN
1	B	506	GLN
1	B	595	GLN
1	B	625	ASN
1	B	664	GLN
1	B	677	GLN
1	B	682	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	632/691 (91%)	0.13	15 (2%) 59 41	0, 11, 91, 189	0
1	B	632/691 (91%)	0.24	13 (2%) 63 44	0, 13, 95, 192	0
All	All	1264/1382 (91%)	0.19	28 (2%) 62 44	0, 12, 94, 192	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	398	ILE	3.6
1	A	39	ILE	3.1
1	A	348	ARG	3.0
1	B	39	ILE	3.0
1	A	317	MET	2.9
1	A	379	GLY	2.8
1	A	90	PHE	2.7
1	B	439	ARG	2.7
1	B	396	ARG	2.6
1	A	234	GLY	2.5
1	B	233	GLU	2.5
1	A	396	ARG	2.5
1	A	532	GLY	2.4
1	A	294	PRO	2.4
1	B	532	GLY	2.4
1	B	234	GLY	2.3
1	A	88	VAL	2.3
1	B	90	PHE	2.2
1	A	449	THR	2.2
1	A	468	ARG	2.2
1	B	92	ILE	2.1
1	B	504	ARG	2.1
1	A	233	GLU	2.1
1	A	99	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	505	GLY	2.1
1	B	468	ARG	2.1
1	B	295	GLU	2.1
1	A	16	GLY	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 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.