



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:28 pm BST

PDB ID : 1QZX
Title : Crystal structure of the complete core of archaeal SRP and implications for inter-domain communication
Authors : Rosendal, K.R.; Wild, K.; Montoya, G.; Sinning, I.
Deposited on : 2003-09-18
Resolution : 4.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

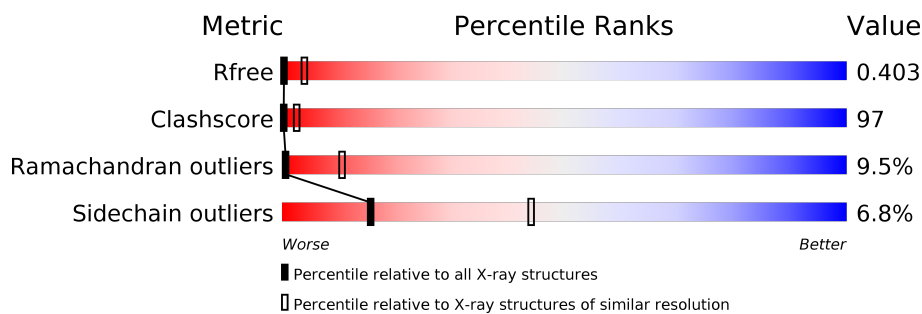
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	440	
1	B	440	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6698 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 Signal recognition 54 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3349	2142	565	628	14			
1	B	425	Total	C	N	O	S	0	0	0
			3349	2142	565	628	14			

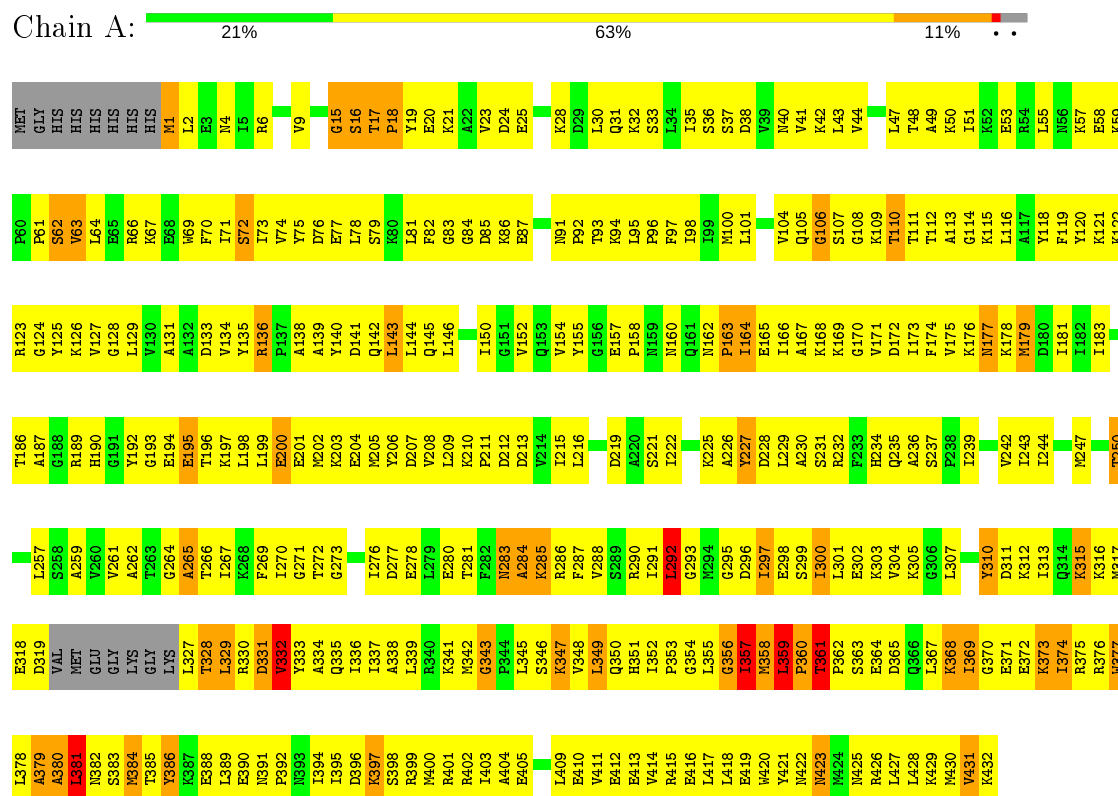
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP Q97ZE7
A	-6	GLY	-	EXPRESSION TAG	UNP Q97ZE7
A	-5	HIS	-	EXPRESSION TAG	UNP Q97ZE7
A	-4	HIS	-	EXPRESSION TAG	UNP Q97ZE7
A	-3	HIS	-	EXPRESSION TAG	UNP Q97ZE7
A	-2	HIS	-	EXPRESSION TAG	UNP Q97ZE7
A	-1	HIS	-	EXPRESSION TAG	UNP Q97ZE7
A	0	HIS	-	EXPRESSION TAG	UNP Q97ZE7
B	-7	MET	-	EXPRESSION TAG	UNP Q97ZE7
B	-6	GLY	-	EXPRESSION TAG	UNP Q97ZE7
B	-5	HIS	-	EXPRESSION TAG	UNP Q97ZE7
B	-4	HIS	-	EXPRESSION TAG	UNP Q97ZE7
B	-3	HIS	-	EXPRESSION TAG	UNP Q97ZE7
B	-2	HIS	-	EXPRESSION TAG	UNP Q97ZE7
B	-1	HIS	-	EXPRESSION TAG	UNP Q97ZE7
B	0	HIS	-	EXPRESSION TAG	UNP Q97ZE7

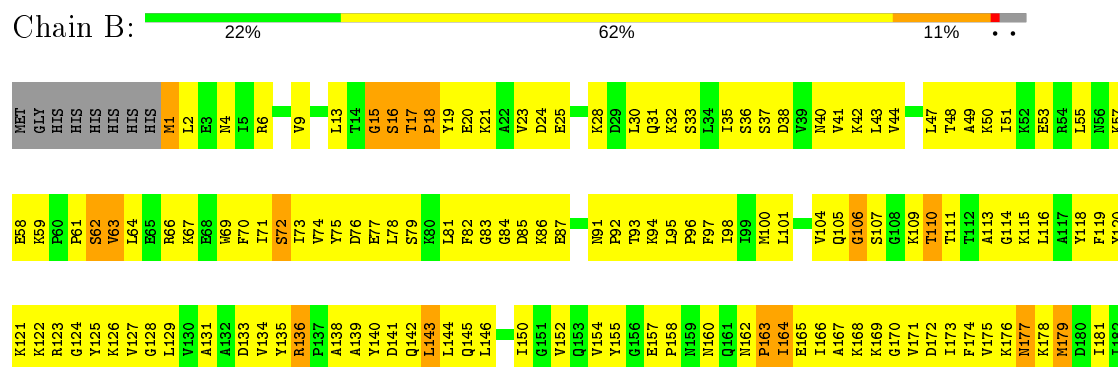
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Signal recognition 54 kDa protein



- Molecule 1: Signal recognition 54 kDa protein



K316	K317	E318	D319	VAL	MET	GLU	GLY	LYS	GLY	LYS	L327	T328	L329	R330	D331	Y332	Y333	A334	Q335	I336	I337	A338	I339	R340	K341	G342	G343	F344	I345	S346	K347	V348	L349	Q350	R351	I352	P353	G354	L355	G356	I357	M358	L359	P360	T361	P362	S363	E364	D365	Q366	L367	K368	I369	G370	E371	E372	K373	I374	R375
R376	W377	L378	A379	A380	I381	N382	S383	T384	T385	K386	K387	E388	L389	E390	N391	P392	N393	I394	L395	D396	K397	S398	R399	M400	R401	R402	I403	A404	E405		L409	E410	V411	E412	E413	V414	R415	E416	L417	L418	E419	W420	Y421	M422	N423	N424	N425	R426	L427	L428	K429	M430	V431	K432					
I183		T186	A187	R188	R189	H190	G191	Y192	G193	E194	E195	T196	K197	L198	L199	E200	E201	M202	K203	E204	M205	Y206	D207	V208	L209	K210	P211	D212	D213	V214	I215	L216		D219	A220	S221	I222		K225	A226	Y227	D228	L229	A230	S231	R232	F233	H234	Q235	A236	S237	P238	I239		V242	I243	L244		M247
	T250		L257	S258	A259	V260	V261	A262	T263	G264	A265	T266	I267	K268	F269	I270	G271	T272	G273		I276	D277	E278	I279	E280	T281	F282	N283	A284	K285	R286	F287	V288	S289	R290	I291	L292	G293	M294	G295	D296	I297	E298	S299	I300	L301	E302	K303	V304	K305	G306	L307		Y310	D311	K312	I313	Q314	K315

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	197.91Å 197.91Å 64.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.00 38.81 – 4.00	Depositor EDS
% Data completeness (in resolution range)	89.0 (40.00-4.00) 97.9 (38.81-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 3.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.313 , 0.383 0.404 , 0.403	Depositor DCC
R_{free} test set	725 reflections (6.88%)	wwPDB-VP
Wilson B-factor (Å ²)	171.1	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.428 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	6698	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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	0.71	5/3399 (0.1%)	0.88	4/4569 (0.1%)
1	B	0.71	5/3399 (0.1%)	0.88	4/4569 (0.1%)
All	All	0.71	10/6798 (0.1%)	0.88	8/9138 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	THR	CB-CG2	-6.78	1.29	1.52
1	B	361	THR	CB-CG2	-6.78	1.29	1.52
1	B	227	TYR	CD2-CE2	-5.99	1.30	1.39
1	A	227	TYR	CD2-CE2	-5.96	1.30	1.39
1	A	361	THR	CA-CB	5.92	1.68	1.53
1	B	361	THR	CA-CB	5.91	1.68	1.53
1	B	360	PRO	N-CD	5.33	1.55	1.47
1	A	360	PRO	N-CD	5.33	1.55	1.47
1	A	360	PRO	C-N	-5.15	1.22	1.34
1	B	360	PRO	C-N	-5.13	1.22	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	LEU	CA-CB-CG	-5.79	101.99	115.30
1	B	292	LEU	CA-CB-CG	-5.77	102.03	115.30
1	B	361	THR	N-CA-CB	5.21	120.20	110.30
1	A	361	THR	N-CA-CB	5.20	120.19	110.30
1	B	332	VAL	N-CA-C	-5.16	97.06	111.00
1	A	332	VAL	N-CA-C	-5.16	97.07	111.00
1	B	359	LEU	CB-CA-C	5.02	119.74	110.20
1	A	359	LEU	CB-CA-C	5.02	119.74	110.20

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	3349	0	3486	713	43
1	B	3349	0	3486	708	43
All	All	6698	0	6972	1324	43

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 97.

All (1324) 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:362:PRO:HD3	1:B:367:LEU:CD2	1.43	1.47
1:B:190:HIS:CD2	1:B:197:LYS:HD2	1.49	1.45
1:A:190:HIS:CD2	1:A:197:LYS:HD2	1.49	1.44
1:A:362:PRO:HD3	1:A:367:LEU:CD2	1.43	1.43
1:B:359:LEU:CG	1:B:360:PRO:HD3	1.49	1.42
1:A:359:LEU:CG	1:A:360:PRO:HD3	1.49	1.39
1:A:362:PRO:CD	1:A:367:LEU:HD21	1.54	1.38
1:B:362:PRO:CD	1:B:367:LEU:HD21	1.54	1.38
1:A:361:THR:HA	1:A:367:LEU:CD1	1.54	1.36
1:A:385:THR:HG21	1:B:382:ASN:O	1.25	1.35
1:A:382:ASN:O	1:B:385:THR:HG21	1.27	1.34
1:B:361:THR:HA	1:B:367:LEU:CD1	1.54	1.34
1:A:361:THR:CA	1:A:367:LEU:HD11	1.62	1.28
1:B:361:THR:CA	1:B:367:LEU:HD11	1.62	1.27
1:A:164:ILE:CD1	1:A:208:VAL:HG21	1.66	1.24
1:B:164:ILE:CD1	1:B:208:VAL:HG21	1.66	1.24
1:B:92:PRO:HB2	1:B:97:PHE:CE2	1.75	1.21
1:B:359:LEU:CD1	1:B:360:PRO:HD3	1.70	1.20
1:A:92:PRO:HB2	1:A:97:PHE:CE2	1.75	1.20
1:A:359:LEU:CD1	1:A:360:PRO:HD3	1.70	1.20
1:A:2:LEU:HD22	1:A:291:ILE:HG21	1.23	1.17
1:B:356:GLY:O	1:B:357:ILE:HG13	1.47	1.14
1:B:164:ILE:HD11	1:B:208:VAL:HG21	1.20	1.13
1:A:190:HIS:CD2	1:A:197:LYS:CD	2.31	1.13
1:B:359:LEU:HG	1:B:360:PRO:HD3	1.15	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:HG	1:A:360:PRO:HD3	1.15	1.13
1:B:190:HIS:CD2	1:B:197:LYS:CD	2.31	1.13
1:B:194:GLU:HB3	1:B:197:LYS:CE	1.80	1.11
1:A:129:LEU:HD13	1:A:143:LEU:HD21	1.29	1.11
1:A:194:GLU:HB3	1:A:197:LYS:CE	1.80	1.11
1:B:2:LEU:HD22	1:B:291:ILE:HG21	1.23	1.11
1:B:17:THR:HG22	1:B:18:PRO:CD	1.81	1.10
1:A:356:GLY:O	1:A:357:ILE:HG13	1.47	1.10
1:A:17:THR:HG22	1:A:18:PRO:CD	1.82	1.10
1:A:194:GLU:HB3	1:A:197:LYS:HE3	1.16	1.10
1:A:164:ILE:HD11	1:A:208:VAL:CG2	1.82	1.09
1:B:164:ILE:HD11	1:B:208:VAL:CG2	1.82	1.08
1:B:129:LEU:HD13	1:B:143:LEU:HD21	1.29	1.08
1:B:359:LEU:HG	1:B:360:PRO:CD	1.84	1.07
1:A:164:ILE:HD11	1:A:208:VAL:HG21	1.20	1.07
1:A:17:THR:CG2	1:A:18:PRO:HD2	1.83	1.07
1:A:359:LEU:HG	1:A:360:PRO:CD	1.84	1.07
1:A:126:LYS:HE3	1:B:364:GLU:OE2	1.54	1.07
1:B:17:THR:CG2	1:B:18:PRO:HD2	1.83	1.07
1:B:190:HIS:CG	1:B:197:LYS:HD2	1.88	1.07
1:B:194:GLU:HB3	1:B:197:LYS:HE3	1.16	1.07
1:A:122:LYS:O	1:B:359:LEU:HD13	1.55	1.06
1:A:190:HIS:CG	1:A:197:LYS:HD2	1.88	1.06
1:B:409:LEU:HD13	1:B:413:GLU:OE1	1.56	1.06
1:B:157:GLU:HB3	1:B:160:ASN:ND2	1.70	1.06
1:A:364:GLU:OE2	1:B:126:LYS:HE3	1.56	1.05
1:A:157:GLU:HB3	1:A:160:ASN:ND2	1.69	1.05
1:B:378:LEU:HA	1:B:381:LEU:HD12	1.39	1.05
1:A:409:LEU:HD13	1:A:413:GLU:OE1	1.56	1.05
1:A:348:VAL:O	1:A:352:ILE:HG13	1.56	1.05
1:A:378:LEU:HA	1:A:381:LEU:HD12	1.39	1.04
1:A:359:LEU:HD13	1:B:122:LYS:O	1.57	1.04
1:B:194:GLU:CB	1:B:197:LYS:HE3	1.87	1.04
1:B:348:VAL:O	1:B:352:ILE:HG13	1.56	1.04
1:A:329:LEU:HD22	1:A:392:PRO:HB3	1.40	1.03
1:A:385:THR:HG21	1:B:382:ASN:C	1.79	1.03
1:A:359:LEU:CG	1:A:360:PRO:CD	2.36	1.03
1:A:194:GLU:CB	1:A:197:LYS:HE3	1.87	1.03
1:B:157:GLU:HB3	1:B:160:ASN:HD22	1.18	1.03
1:B:303:LYS:O	1:B:307:LEU:HG	1.59	1.02
1:A:382:ASN:C	1:B:385:THR:HG21	1.79	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LEU:CG	1:B:360:PRO:CD	2.36	1.02
1:B:61:PRO:HD2	1:B:64:LEU:HD12	1.40	1.02
1:A:303:LYS:O	1:A:307:LEU:HG	1.59	1.02
1:A:157:GLU:HB3	1:A:160:ASN:HD22	1.18	1.01
1:B:361:THR:HG23	1:B:362:PRO:HD2	1.40	1.01
1:B:383:SER:HB3	1:B:403:ILE:HG23	1.41	1.01
1:A:383:SER:HB3	1:A:403:ILE:HG23	1.41	1.00
1:A:402:ARG:HD3	1:B:402:ARG:HD3	1.37	1.00
1:B:378:LEU:HA	1:B:381:LEU:CD1	1.91	1.00
1:A:378:LEU:HA	1:A:381:LEU:CD1	1.91	0.99
1:A:359:LEU:HD12	1:A:360:PRO:HD3	1.42	0.99
1:A:361:THR:HG23	1:A:362:PRO:HD2	1.40	0.99
1:A:61:PRO:HD2	1:A:64:LEU:HD12	1.40	0.99
1:B:329:LEU:HD22	1:B:392:PRO:HB3	1.40	0.99
1:B:359:LEU:HD12	1:B:360:PRO:HD3	1.42	0.98
1:A:385:THR:HA	1:B:384:MET:O	1.64	0.97
1:A:384:MET:O	1:B:385:THR:HA	1.64	0.97
1:A:385:THR:CG2	1:B:382:ASN:O	2.11	0.97
1:A:382:ASN:O	1:B:385:THR:CG2	2.12	0.97
1:A:1:MET:SD	1:A:37:SER:CB	2.55	0.95
1:B:164:ILE:CG1	1:B:208:VAL:HG21	1.97	0.95
1:B:1:MET:SD	1:B:37:SER:CB	2.55	0.95
1:A:164:ILE:CG1	1:A:208:VAL:HG21	1.97	0.95
1:A:301:LEU:HG	1:A:305:LYS:HD2	1.49	0.95
1:A:397:LYS:HA	1:A:400:MET:HE3	1.49	0.94
1:A:335:GLN:O	1:A:339:LEU:HD22	1.66	0.94
1:B:75:TYR:CD2	1:B:297:ILE:HG23	2.02	0.94
1:B:94:LYS:N	1:B:97:PHE:CZ	2.36	0.94
1:A:75:TYR:CD2	1:A:297:ILE:HG23	2.02	0.94
1:A:72:SER:HB2	1:A:300:ILE:HD11	1.48	0.94
1:B:301:LEU:HG	1:B:305:LYS:HD2	1.49	0.94
1:A:94:LYS:N	1:A:97:PHE:CZ	2.36	0.93
1:A:15:GLY:HA2	1:A:67:LYS:NZ	1.83	0.93
1:B:72:SER:HB2	1:B:300:ILE:HD11	1.48	0.93
1:B:335:GLN:O	1:B:339:LEU:HD22	1.66	0.93
1:B:15:GLY:HA2	1:B:67:LYS:NZ	1.83	0.93
1:B:200:GLU:CD	1:B:201:GLU:N	2.23	0.93
1:B:397:LYS:HA	1:B:400:MET:HE3	1.49	0.92
1:B:197:LYS:O	1:B:200:GLU:OE1	1.87	0.92
1:A:200:GLU:CD	1:A:201:GLU:N	2.23	0.92
1:B:157:GLU:CB	1:B:160:ASN:HD22	1.82	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LYS:O	1:A:200:GLU:OE1	1.87	0.92
1:B:15:GLY:HA2	1:B:67:LYS:HZ3	1.34	0.92
1:B:297:ILE:O	1:B:300:ILE:HB	1.69	0.92
1:A:327:LEU:HD12	1:A:391:ASN:OD1	1.70	0.91
1:A:297:ILE:O	1:A:300:ILE:HB	1.69	0.91
1:B:221:SER:HA	1:B:250:THR:HG21	1.53	0.91
1:A:221:SER:HA	1:A:250:THR:HG21	1.53	0.91
1:A:349:LEU:HA	1:A:352:ILE:HB	1.53	0.91
1:B:327:LEU:HD12	1:B:391:ASN:OD1	1.70	0.91
1:B:295:GLY:HA2	1:B:298:GLU:HB2	1.52	0.91
1:A:157:GLU:CB	1:A:160:ASN:HD22	1.82	0.91
1:B:317:MET:SD	1:B:328:THR:OG1	2.29	0.91
1:B:362:PRO:CD	1:B:367:LEU:CD2	2.27	0.91
1:A:331:ASP:O	1:A:332:VAL:HG23	1.71	0.90
1:A:301:LEU:HD11	1:A:305:LYS:HE3	1.51	0.90
1:A:317:MET:SD	1:A:328:THR:OG1	2.29	0.90
1:B:301:LEU:HD11	1:B:305:LYS:HE3	1.51	0.90
1:A:281:THR:HG21	1:B:315:LYS:NZ	1.86	0.90
1:A:295:GLY:HA2	1:A:298:GLU:HB2	1.52	0.90
1:B:361:THR:OG1	1:B:367:LEU:HG	1.70	0.90
1:B:331:ASP:O	1:B:332:VAL:HG23	1.71	0.90
1:B:349:LEU:HA	1:B:352:ILE:HB	1.53	0.90
1:A:85:ASP:CG	1:A:285:LYS:HD3	1.92	0.90
1:A:2:LEU:HD22	1:A:291:ILE:HD13	1.51	0.89
1:B:2:LEU:HD22	1:B:291:ILE:HD13	1.51	0.89
1:B:85:ASP:CG	1:B:285:LYS:HD3	1.92	0.89
1:A:361:THR:OG1	1:A:367:LEU:HG	1.70	0.89
1:A:362:PRO:CD	1:A:367:LEU:CD2	2.27	0.89
1:A:315:LYS:NZ	1:B:281:THR:HG21	1.87	0.89
1:A:329:LEU:CD2	1:A:392:PRO:HB3	2.03	0.89
1:B:329:LEU:CD2	1:B:392:PRO:HB3	2.03	0.89
1:B:17:THR:HG22	1:B:18:PRO:HD2	0.92	0.88
1:B:1:MET:SD	1:B:37:SER:HB3	2.15	0.87
1:B:118:TYR:HE2	1:B:277:ASP:HB3	1.40	0.87
1:A:167:ALA:HB1	1:A:209:LEU:HD11	1.57	0.87
1:A:118:TYR:HE2	1:A:277:ASP:HB3	1.40	0.87
1:A:150:ILE:HG13	1:A:152:VAL:HG23	1.56	0.87
1:A:359:LEU:CB	1:A:360:PRO:CD	2.53	0.87
1:B:167:ALA:HB1	1:B:209:LEU:HD11	1.57	0.87
1:A:86:LYS:HE2	1:A:266:THR:HG23	1.56	0.86
1:B:359:LEU:CB	1:B:360:PRO:CD	2.53	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:HB3	1:B:242:VAL:HG22	1.56	0.86
1:A:2:LEU:CD2	1:A:291:ILE:HG21	2.06	0.86
1:A:383:SER:CB	1:A:403:ILE:HG23	2.06	0.86
1:B:150:ILE:HG13	1:B:152:VAL:HG23	1.56	0.86
1:A:216:LEU:HB3	1:A:242:VAL:HG22	1.56	0.86
1:A:359:LEU:HD12	1:A:360:PRO:CD	2.06	0.86
1:B:2:LEU:HD22	1:B:291:ILE:CG2	2.05	0.85
1:B:86:LYS:HE2	1:B:266:THR:HG23	1.56	0.85
1:B:383:SER:CB	1:B:403:ILE:HG23	2.06	0.85
1:B:359:LEU:HD12	1:B:360:PRO:CD	2.06	0.85
1:A:1:MET:SD	1:A:37:SER:HB3	2.15	0.85
1:A:402:ARG:CZ	1:B:402:ARG:HG2	2.07	0.85
1:B:381:LEU:N	1:B:381:LEU:HD23	1.92	0.85
1:B:422:ASN:O	1:B:426:ARG:HG3	1.77	0.84
1:A:2:LEU:HD22	1:A:291:ILE:CG2	2.05	0.84
1:A:402:ARG:HG2	1:B:402:ARG:CZ	2.07	0.84
1:A:95:LEU:HD23	1:A:97:PHE:CE1	2.12	0.84
1:B:372:GLU:O	1:B:374:ILE:N	2.10	0.84
1:A:123:ARG:CZ	1:B:318:GLU:OE1	2.26	0.84
1:A:381:LEU:N	1:A:381:LEU:HD23	1.92	0.84
1:A:422:ASN:O	1:A:426:ARG:HG3	1.77	0.84
1:B:417:LEU:HB3	1:B:421:TYR:HE1	1.41	0.84
1:B:95:LEU:HD23	1:B:97:PHE:CE1	2.12	0.84
1:A:310:TYR:OH	1:A:355:LEU:HD23	1.78	0.84
1:A:69:TRP:O	1:A:73:ILE:HG13	1.78	0.84
1:A:417:LEU:HB3	1:A:421:TYR:HE1	1.41	0.84
1:A:17:THR:HG22	1:A:18:PRO:HD2	0.92	0.83
1:A:200:GLU:OE2	1:A:201:GLU:HA	1.78	0.83
1:A:164:ILE:HG23	1:A:165:GLU:N	1.94	0.83
1:A:372:GLU:O	1:A:374:ILE:N	2.10	0.83
1:B:164:ILE:HG23	1:B:165:GLU:N	1.94	0.83
1:B:69:TRP:O	1:B:73:ILE:HG13	1.78	0.83
1:B:2:LEU:CD2	1:B:291:ILE:HG21	2.06	0.83
1:A:372:GLU:C	1:A:374:ILE:H	1.78	0.83
1:B:310:TYR:OH	1:B:355:LEU:HD23	1.78	0.83
1:A:318:GLU:OE1	1:B:123:ARG:CZ	2.26	0.82
1:A:92:PRO:HB2	1:A:97:PHE:CZ	2.14	0.82
1:B:92:PRO:HB2	1:B:97:PHE:CZ	2.14	0.82
1:B:418:LEU:HA	1:B:421:TYR:HD1	1.44	0.82
1:A:418:LEU:HA	1:A:421:TYR:HD1	1.43	0.82
1:A:313:ILE:HD11	1:A:331:ASP:OD1	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:GLU:OE2	1:B:201:GLU:HA	1.78	0.81
1:B:380:ALA:HA	1:B:383:SER:HB2	1.61	0.81
1:A:55:LEU:HD13	1:A:55:LEU:O	1.80	0.81
1:B:164:ILE:CD1	1:B:208:VAL:CG2	2.51	0.81
1:A:15:GLY:HA2	1:A:67:LYS:HZ3	1.40	0.81
1:A:2:LEU:CD2	1:A:291:ILE:HD13	2.11	0.81
1:B:55:LEU:HD13	1:B:55:LEU:O	1.80	0.81
1:B:100:MET:HE3	1:B:205:MET:O	1.80	0.81
1:A:380:ALA:HA	1:A:383:SER:HB2	1.61	0.81
1:B:2:LEU:CD2	1:B:291:ILE:HD13	2.11	0.81
1:B:75:TYR:HD2	1:B:297:ILE:HG23	1.45	0.81
1:A:378:LEU:O	1:A:381:LEU:HG	1.81	0.80
1:A:176:LYS:O	1:A:178:LYS:N	2.14	0.80
1:B:176:LYS:O	1:B:178:LYS:N	2.15	0.80
1:A:6:ARG:HG3	1:A:292:LEU:HD23	1.62	0.80
1:B:372:GLU:C	1:B:374:ILE:H	1.78	0.80
1:B:313:ILE:HD11	1:B:331:ASP:OD1	1.80	0.80
1:B:359:LEU:CB	1:B:360:PRO:HD3	2.11	0.80
1:A:75:TYR:HD2	1:A:297:ILE:HG23	1.45	0.80
1:B:378:LEU:O	1:B:381:LEU:HG	1.81	0.80
1:B:394:ILE:HG22	1:B:399:ARG:NH1	1.96	0.80
1:B:346:SER:O	1:B:348:VAL:N	2.15	0.80
1:B:6:ARG:HG3	1:B:292:LEU:HD23	1.62	0.80
1:A:359:LEU:CB	1:A:360:PRO:HD3	2.11	0.80
1:A:346:SER:O	1:A:348:VAL:N	2.15	0.80
1:A:129:LEU:CD1	1:A:143:LEU:HD21	2.11	0.80
1:A:163:PRO:HG2	1:A:164:ILE:H	1.47	0.79
1:B:199:LEU:HD23	1:B:202:MET:SD	2.23	0.79
1:B:94:LYS:N	1:B:97:PHE:HZ	1.81	0.79
1:A:417:LEU:HB3	1:A:421:TYR:CE1	2.18	0.79
1:A:199:LEU:HD23	1:A:202:MET:SD	2.23	0.78
1:B:272:THR:HG21	1:B:280:GLU:OE2	1.82	0.78
1:B:417:LEU:HB3	1:B:421:TYR:CE1	2.18	0.78
1:A:172:ASP:O	1:A:176:LYS:HG3	1.83	0.78
1:A:272:THR:HG21	1:A:280:GLU:OE2	1.82	0.78
1:B:172:ASP:O	1:B:176:LYS:HG3	1.83	0.78
1:A:94:LYS:N	1:A:97:PHE:HZ	1.81	0.78
1:A:100:MET:HE3	1:A:205:MET:O	1.83	0.78
1:A:394:ILE:HG22	1:A:399:ARG:NH1	1.96	0.78
1:B:129:LEU:CD1	1:B:143:LEU:HD21	2.11	0.78
1:A:124:GLY:HA3	1:B:359:LEU:CA	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:HIS:CE1	1:A:265:ALA:CB	2.67	0.78
1:B:163:PRO:HG2	1:B:164:ILE:H	1.47	0.78
1:B:82:PHE:C	1:B:261:VAL:HG21	2.04	0.78
1:A:402:ARG:HD3	1:B:402:ARG:CD	2.14	0.78
1:A:384:MET:HE2	1:A:389:LEU:HD23	1.66	0.77
1:B:234:HIS:CE1	1:B:265:ALA:CB	2.67	0.77
1:A:82:PHE:C	1:A:261:VAL:HG21	2.04	0.77
1:A:299:SER:O	1:A:303:LYS:HG2	1.85	0.77
1:A:222:ILE:HG21	1:A:226:ALA:HB2	1.68	0.76
1:A:396:ASP:O	1:A:400:MET:HG3	1.86	0.76
1:B:299:SER:O	1:B:303:LYS:HG2	1.85	0.76
1:B:222:ILE:HG21	1:B:226:ALA:HB2	1.67	0.76
1:B:194:GLU:HB3	1:B:197:LYS:CD	2.16	0.76
1:A:402:ARG:CD	1:B:402:ARG:HD3	2.14	0.76
1:A:87:GLU:HG3	1:B:315:LYS:HZ1	1.50	0.76
1:B:396:ASP:O	1:B:400:MET:HG3	1.86	0.76
1:A:361:THR:OG1	1:A:367:LEU:CG	2.34	0.76
1:A:383:SER:O	1:A:403:ILE:HG12	1.85	0.76
1:A:124:GLY:HA3	1:B:359:LEU:HA	1.68	0.76
1:B:383:SER:O	1:B:403:ILE:HG12	1.85	0.76
1:A:194:GLU:HB3	1:A:197:LYS:CD	2.16	0.76
1:A:359:LEU:CA	1:B:124:GLY:HA3	2.16	0.76
1:B:200:GLU:OE2	1:B:201:GLU:CA	2.33	0.75
1:A:200:GLU:OE2	1:A:201:GLU:CA	2.34	0.75
1:B:234:HIS:CE1	1:B:265:ALA:HB1	2.22	0.75
1:A:356:GLY:O	1:A:357:ILE:CG1	2.32	0.75
1:A:234:HIS:CE1	1:A:265:ALA:HB1	2.22	0.75
1:A:329:LEU:CD1	1:A:421:TYR:HB3	2.17	0.75
1:A:402:ARG:HG2	1:B:402:ARG:NH2	2.02	0.75
1:B:361:THR:OG1	1:B:367:LEU:CG	2.34	0.75
1:A:122:LYS:O	1:B:359:LEU:CD1	2.33	0.74
1:B:222:ILE:CG2	1:B:226:ALA:HB2	2.17	0.74
1:B:335:GLN:HB3	1:B:355:LEU:HD22	1.70	0.74
1:B:92:PRO:HB2	1:B:97:PHE:CD2	2.22	0.74
1:A:335:GLN:HB3	1:A:355:LEU:HD22	1.70	0.74
1:A:359:LEU:HA	1:B:124:GLY:HA3	1.68	0.74
1:A:382:ASN:CA	1:B:385:THR:HG21	2.18	0.74
1:B:118:TYR:CE2	1:B:277:ASP:HB3	2.22	0.74
1:A:349:LEU:HD22	1:A:371:GLU:HG2	1.70	0.74
1:A:402:ARG:NH2	1:B:402:ARG:HG2	2.03	0.74
1:B:329:LEU:CD1	1:B:421:TYR:HB3	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LEU:HD22	1:B:392:PRO:CB	2.17	0.74
1:B:378:LEU:O	1:B:380:ALA:O	2.06	0.74
1:A:164:ILE:HG23	1:A:165:GLU:H	1.50	0.74
1:A:118:TYR:CE2	1:A:277:ASP:HB3	2.22	0.74
1:A:222:ILE:CG2	1:A:226:ALA:HB2	2.17	0.74
1:A:92:PRO:HB2	1:A:97:PHE:CD2	2.22	0.74
1:A:384:MET:CE	1:A:389:LEU:HD23	2.18	0.73
1:A:206:TYR:OH	1:A:239:ILE:HD11	1.88	0.73
1:A:362:PRO:HD3	1:A:367:LEU:HD23	1.66	0.73
1:A:378:LEU:O	1:A:380:ALA:O	2.06	0.73
1:B:200:GLU:OE2	1:B:201:GLU:N	2.22	0.73
1:B:164:ILE:HG23	1:B:165:GLU:H	1.50	0.73
1:A:382:ASN:HA	1:B:385:THR:CG2	2.18	0.73
1:A:385:THR:CG2	1:B:382:ASN:HA	2.19	0.73
1:B:346:SER:C	1:B:348:VAL:H	1.92	0.73
1:A:346:SER:C	1:A:348:VAL:H	1.92	0.73
1:B:206:TYR:OH	1:B:239:ILE:HD11	1.88	0.73
1:B:356:GLY:O	1:B:357:ILE:CG1	2.31	0.73
1:A:402:ARG:HB3	1:B:402:ARG:NH1	2.04	0.73
1:A:373:LYS:HE3	1:A:377:TRP:CH2	2.24	0.73
1:A:385:THR:HG21	1:B:382:ASN:CA	2.19	0.73
1:B:349:LEU:HD22	1:B:371:GLU:HG2	1.70	0.72
1:A:318:GLU:CD	1:B:123:ARG:NH1	2.43	0.72
1:A:95:LEU:HD23	1:A:97:PHE:CD1	2.24	0.72
1:B:174:PHE:O	1:B:179:MET:HB2	1.90	0.72
1:A:123:ARG:NH1	1:B:318:GLU:CD	2.42	0.72
1:A:155:TYR:CD2	1:A:170:GLY:HA2	2.24	0.72
1:A:342:MET:O	1:A:348:VAL:HG21	1.90	0.72
1:B:155:TYR:CD2	1:B:170:GLY:HA2	2.24	0.72
1:B:373:LYS:HE3	1:B:377:TRP:CH2	2.24	0.72
1:B:384:MET:HE2	1:B:389:LEU:HD23	1.69	0.72
1:B:383:SER:HB3	1:B:403:ILE:CG2	2.19	0.72
1:A:372:GLU:O	1:A:374:ILE:HG22	1.88	0.72
1:B:95:LEU:HD23	1:B:97:PHE:CD1	2.24	0.72
1:A:281:THR:HG21	1:B:315:LYS:CE	2.19	0.72
1:A:357:ILE:O	1:A:358:MET:HB2	1.88	0.72
1:B:164:ILE:HG13	1:B:208:VAL:HG21	1.70	0.72
1:B:342:MET:O	1:B:348:VAL:HG21	1.90	0.72
1:A:83:GLY:N	1:A:261:VAL:HG11	2.05	0.72
1:B:234:HIS:NE2	1:B:265:ALA:HB2	2.04	0.72
1:B:372:GLU:O	1:B:374:ILE:HG22	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ARG:NH1	1:B:318:GLU:OE2	2.23	0.72
1:B:334:ALA:O	1:B:337:ILE:HG22	1.90	0.72
1:A:200:GLU:OE2	1:A:201:GLU:N	2.22	0.72
1:A:234:HIS:NE2	1:A:265:ALA:HB2	2.04	0.72
1:B:329:LEU:HD11	1:B:421:TYR:HB3	1.72	0.72
1:B:384:MET:CE	1:B:389:LEU:HD23	2.18	0.72
1:B:362:PRO:HD3	1:B:367:LEU:HD23	1.66	0.71
1:A:329:LEU:HD11	1:A:421:TYR:HB3	1.72	0.71
1:A:334:ALA:O	1:A:337:ILE:HG22	1.90	0.71
1:A:42:LYS:O	1:A:42:LYS:HD3	1.91	0.71
1:A:164:ILE:HG13	1:A:208:VAL:HG21	1.70	0.71
1:B:357:ILE:O	1:B:358:MET:HB2	1.88	0.71
1:A:301:LEU:HD21	1:A:305:LYS:NZ	2.06	0.71
1:A:329:LEU:HD22	1:A:392:PRO:CB	2.17	0.71
1:A:359:LEU:CD1	1:B:122:LYS:O	2.35	0.71
1:A:169:LYS:O	1:A:173:ILE:HG13	1.91	0.71
1:A:174:PHE:O	1:A:179:MET:HB2	1.90	0.71
1:B:385:THR:HG22	1:B:386:TYR:N	2.05	0.71
1:B:403:ILE:HG22	1:B:414:VAL:HG21	1.73	0.71
1:A:134:VAL:HA	1:A:140:TYR:HE1	1.55	0.71
1:B:134:VAL:HA	1:B:140:TYR:HE1	1.55	0.71
1:A:432:LYS:HE2	1:B:277:ASP:HB2	1.72	0.71
1:B:83:GLY:N	1:B:261:VAL:HG11	2.05	0.71
1:A:318:GLU:OE2	1:B:123:ARG:NH1	2.24	0.70
1:B:355:LEU:O	1:B:356:GLY:C	2.29	0.70
1:A:403:ILE:HG22	1:A:414:VAL:HG21	1.73	0.70
1:A:355:LEU:O	1:A:356:GLY:C	2.30	0.70
1:A:402:ARG:NH1	1:B:402:ARG:HB3	2.05	0.70
1:A:402:ARG:CG	1:B:402:ARG:CZ	2.70	0.70
1:A:402:ARG:CZ	1:B:402:ARG:CG	2.70	0.70
1:A:179:MET:HA	1:A:179:MET:CE	2.21	0.70
1:A:63:VAL:HG12	1:A:63:VAL:O	1.92	0.70
1:B:169:LYS:O	1:B:173:ILE:HG13	1.91	0.70
1:B:301:LEU:O	1:B:305:LYS:HD2	1.92	0.70
1:A:176:LYS:C	1:A:178:LYS:H	1.96	0.70
1:B:42:LYS:HD3	1:B:42:LYS:O	1.91	0.70
1:A:200:GLU:CD	1:A:200:GLU:C	2.51	0.69
1:A:277:ASP:HB2	1:B:432:LYS:HE2	1.73	0.69
1:A:303:LYS:HG3	1:A:304:VAL:H	1.57	0.69
1:A:315:LYS:HZ3	1:B:281:THR:HG21	1.55	0.69
1:B:303:LYS:HG3	1:B:304:VAL:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:THR:HG22	1:A:386:TYR:N	2.05	0.69
1:B:136:ARG:HD3	1:B:139:ALA:HB2	1.74	0.69
1:B:200:GLU:CD	1:B:200:GLU:C	2.51	0.69
1:A:247:MET:CE	1:A:270:ILE:HD11	2.23	0.69
1:A:301:LEU:O	1:A:305:LYS:HD2	1.92	0.69
1:B:301:LEU:HD21	1:B:305:LYS:NZ	2.06	0.69
1:B:397:LYS:CA	1:B:400:MET:HE3	2.23	0.69
1:B:176:LYS:C	1:B:178:LYS:H	1.96	0.69
1:B:401:ARG:O	1:B:405:GLU:HG2	1.92	0.69
1:B:179:MET:CE	1:B:179:MET:HA	2.21	0.69
1:B:78:LEU:O	1:B:81:LEU:HB3	1.93	0.69
1:A:315:LYS:CE	1:B:281:THR:HG21	2.21	0.69
1:B:310:TYR:HA	1:B:335:GLN:HE22	1.57	0.69
1:B:384:MET:HA	1:B:388:GLU:OE1	1.92	0.69
1:A:401:ARG:O	1:A:405:GLU:HG2	1.92	0.69
1:B:361:THR:HG23	1:B:362:PRO:CD	2.20	0.69
1:B:369:ILE:HG22	1:B:370:GLY:H	1.58	0.69
1:A:369:ILE:HG22	1:A:370:GLY:H	1.58	0.68
1:A:78:LEU:O	1:A:81:LEU:HB3	1.93	0.68
1:A:300:ILE:O	1:A:303:LYS:HG2	1.93	0.68
1:A:384:MET:HA	1:A:388:GLU:OE1	1.92	0.68
1:A:315:LYS:HZ1	1:B:87:GLU:HG3	1.57	0.68
1:A:310:TYR:HA	1:A:335:GLN:HE22	1.58	0.68
1:B:100:MET:CE	1:B:205:MET:O	2.42	0.68
1:B:235:GLN:O	1:B:237:SER:N	2.27	0.68
1:B:300:ILE:O	1:B:303:LYS:HG2	1.93	0.68
1:B:247:MET:CE	1:B:270:ILE:HD11	2.23	0.68
1:A:412:GLU:OE1	1:A:415:ARG:HD2	1.93	0.68
1:B:302:GLU:OE1	1:B:341:LYS:HE3	1.94	0.68
1:A:136:ARG:HD3	1:A:139:ALA:HB2	1.74	0.68
1:A:190:HIS:CD2	1:A:194:GLU:OE1	2.47	0.68
1:A:383:SER:HB3	1:A:403:ILE:CG2	2.19	0.68
1:A:394:ILE:O	1:A:399:ARG:NH1	2.27	0.68
1:B:63:VAL:HG12	1:B:63:VAL:O	1.92	0.68
1:A:234:HIS:CE1	1:A:265:ALA:HB2	2.30	0.67
1:A:409:LEU:HB3	1:A:413:GLU:CD	2.14	0.67
1:A:378:LEU:HA	1:A:381:LEU:HD11	1.76	0.67
1:A:397:LYS:HA	1:A:400:MET:CE	2.24	0.67
1:B:361:THR:OG1	1:B:367:LEU:CD1	2.42	0.67
1:B:394:ILE:O	1:B:399:ARG:NH1	2.27	0.67
1:B:412:GLU:OE1	1:B:415:ARG:HD2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:MET:CE	1:A:205:MET:O	2.42	0.67
1:B:378:LEU:HA	1:B:381:LEU:HD11	1.76	0.67
1:B:397:LYS:HA	1:B:400:MET:CE	2.24	0.67
1:A:235:GLN:O	1:A:237:SER:N	2.27	0.67
1:A:302:GLU:OE1	1:A:341:LYS:HE3	1.94	0.67
1:B:374:ILE:C	1:B:376:ARG:H	1.96	0.67
1:B:190:HIS:CD2	1:B:194:GLU:OE1	2.47	0.67
1:B:374:ILE:HG23	1:B:375:ARG:H	1.60	0.67
1:B:373:LYS:HE3	1:B:377:TRP:CZ3	2.30	0.67
1:A:373:LYS:HE3	1:A:377:TRP:CZ3	2.30	0.67
1:B:369:ILE:HG22	1:B:370:GLY:N	2.10	0.67
1:B:409:LEU:HB3	1:B:413:GLU:CD	2.14	0.67
1:A:397:LYS:CA	1:A:400:MET:HE3	2.23	0.67
1:A:361:THR:OG1	1:A:367:LEU:CD1	2.42	0.67
1:B:234:HIS:CE1	1:B:265:ALA:HB2	2.30	0.67
1:B:247:MET:HE2	1:B:257:LEU:HD21	1.77	0.67
1:A:95:LEU:CD2	1:A:97:PHE:HE1	2.08	0.66
1:B:75:TYR:OH	1:B:292:LEU:HD12	1.95	0.66
1:B:301:LEU:HG	1:B:305:LYS:CD	2.24	0.66
1:A:369:ILE:HG22	1:A:370:GLY:N	2.10	0.66
1:A:94:LYS:C	1:A:97:PHE:CZ	2.69	0.66
1:A:374:ILE:C	1:A:376:ARG:H	1.96	0.66
1:A:374:ILE:HG23	1:A:375:ARG:H	1.60	0.66
1:B:378:LEU:O	1:B:379:ALA:C	2.34	0.66
1:A:280:GLU:OE1	1:A:290:ARG:NH2	2.28	0.66
1:A:1:MET:O	1:A:4:ASN:N	2.28	0.66
1:B:190:HIS:HD2	1:B:194:GLU:OE1	1.79	0.66
1:A:348:VAL:HG12	1:A:352:ILE:HD11	1.77	0.66
1:A:31:GLN:HG3	1:A:48:THR:HG21	1.78	0.66
1:B:118:TYR:HE2	1:B:277:ASP:CB	2.09	0.66
1:B:95:LEU:CD2	1:B:97:PHE:HE1	2.08	0.66
1:B:119:PHE:CZ	1:B:123:ARG:NH2	2.64	0.66
1:B:276:ILE:HG23	1:B:277:ASP:N	2.10	0.66
1:A:348:VAL:O	1:A:352:ILE:CG1	2.39	0.66
1:B:1:MET:O	1:B:4:ASN:N	2.28	0.66
1:B:31:GLN:HG3	1:B:48:THR:HG21	1.78	0.66
1:B:361:THR:CA	1:B:367:LEU:CD1	2.44	0.66
1:B:379:ALA:O	1:B:380:ALA:O	2.14	0.66
1:A:164:ILE:CG2	1:A:165:GLU:H	2.09	0.65
1:B:280:GLU:OE1	1:B:290:ARG:NH2	2.28	0.65
1:A:119:PHE:CZ	1:A:123:ARG:NH2	2.64	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ILE:HG23	1:A:277:ASP:N	2.10	0.65
1:A:361:THR:HG23	1:A:362:PRO:CD	2.20	0.65
1:A:373:LYS:HA	1:A:376:ARG:HG3	1.78	0.65
1:B:373:LYS:HA	1:B:376:ARG:HG3	1.78	0.65
1:B:409:LEU:CD1	1:B:413:GLU:OE1	2.41	0.65
1:A:301:LEU:HG	1:A:305:LYS:CD	2.24	0.65
1:B:301:LEU:HD21	1:B:305:LYS:HZ1	1.62	0.65
1:B:348:VAL:HG12	1:B:352:ILE:HD11	1.77	0.65
1:B:94:LYS:C	1:B:97:PHE:CZ	2.69	0.65
1:A:190:HIS:HD2	1:A:194:GLU:OE1	1.79	0.65
1:A:339:LEU:HD22	1:A:339:LEU:H	1.62	0.65
1:B:423:ASN:O	1:B:427:LEU:HG	1.97	0.65
1:A:75:TYR:OH	1:A:292:LEU:HD12	1.95	0.64
1:A:310:TYR:O	1:A:313:ILE:HG22	1.97	0.64
1:A:53:GLU:HG3	1:A:57:LYS:HE3	1.79	0.64
1:B:53:GLU:HG3	1:B:57:LYS:HE3	1.79	0.64
1:A:297:ILE:O	1:A:300:ILE:CB	2.45	0.64
1:A:423:ASN:O	1:A:427:LEU:HG	1.97	0.64
1:B:164:ILE:CG2	1:B:165:GLU:N	2.59	0.64
1:A:378:LEU:O	1:A:379:ALA:C	2.34	0.64
1:A:379:ALA:O	1:A:380:ALA:O	2.15	0.64
1:A:21:LYS:HD3	1:A:25:GLU:OE2	1.97	0.64
1:A:2:LEU:HD13	1:A:291:ILE:HG23	1.79	0.64
1:A:359:LEU:HA	1:B:124:GLY:CA	2.28	0.64
1:B:167:ALA:HB1	1:B:209:LEU:HD21	1.79	0.64
1:A:86:LYS:CE	1:A:266:THR:HG23	2.28	0.64
1:A:361:THR:CA	1:A:367:LEU:CD1	2.44	0.64
1:B:21:LYS:HD3	1:B:25:GLU:OE2	1.97	0.64
1:A:124:GLY:CA	1:B:359:LEU:HA	2.27	0.64
1:B:288:VAL:O	1:B:291:ILE:HG12	1.97	0.64
1:B:310:TYR:O	1:B:313:ILE:HG22	1.98	0.64
1:A:87:GLU:OE2	1:B:315:LYS:HD2	1.98	0.64
1:B:335:GLN:O	1:B:339:LEU:CD2	2.45	0.64
1:A:385:THR:CA	1:B:384:MET:O	2.44	0.64
1:B:164:ILE:CG2	1:B:165:GLU:H	2.09	0.64
1:A:167:ALA:HB1	1:A:209:LEU:HD21	1.79	0.64
1:B:176:LYS:C	1:B:178:LYS:N	2.51	0.64
1:A:119:PHE:CZ	1:A:123:ARG:NE	2.66	0.63
1:A:95:LEU:CD2	1:A:97:PHE:CE1	2.82	0.63
1:A:129:LEU:HD13	1:A:143:LEU:CD2	2.18	0.63
1:A:288:VAL:O	1:A:291:ILE:HG12	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:MET:O	1:B:385:THR:CA	2.44	0.63
1:A:281:THR:HG21	1:B:315:LYS:HZ3	1.63	0.63
1:A:385:THR:CG2	1:B:382:ASN:C	2.63	0.63
1:A:335:GLN:O	1:A:339:LEU:CD2	2.45	0.63
1:A:87:GLU:HG3	1:B:315:LYS:NZ	2.14	0.63
1:B:196:THR:OG1	1:B:232:ARG:NH1	2.32	0.63
1:B:244:ILE:O	1:B:271:GLY:N	2.24	0.63
1:B:339:LEU:HD22	1:B:339:LEU:H	1.62	0.63
1:A:247:MET:HE1	1:A:257:LEU:HD21	1.81	0.63
1:B:372:GLU:C	1:B:374:ILE:N	2.52	0.63
1:A:118:TYR:HE2	1:A:277:ASP:CB	2.09	0.63
1:B:362:PRO:HD3	1:B:367:LEU:HD21	0.68	0.63
1:A:69:TRP:NE1	1:A:73:ILE:HD11	2.14	0.63
1:B:119:PHE:HZ	1:B:123:ARG:NH2	1.95	0.63
1:B:2:LEU:HD13	1:B:291:ILE:HG23	1.79	0.63
1:B:362:PRO:O	1:B:363:SER:C	2.36	0.63
1:A:33:SER:O	1:A:36:SER:HB2	1.99	0.63
1:B:85:ASP:OD1	1:B:285:LYS:HD3	1.99	0.63
1:B:348:VAL:O	1:B:352:ILE:CG1	2.39	0.63
1:B:9:VAL:HG13	1:B:71:ILE:CD1	2.28	0.63
1:A:167:ALA:CB	1:A:209:LEU:HD21	2.29	0.62
1:A:9:VAL:HG13	1:A:71:ILE:CD1	2.28	0.62
1:B:357:ILE:HD12	1:B:358:MET:H	1.64	0.62
1:A:379:ALA:HB2	1:A:409:LEU:HD11	1.80	0.62
1:B:379:ALA:HB2	1:B:409:LEU:HD11	1.80	0.62
1:A:164:ILE:CD1	1:A:208:VAL:CG2	2.51	0.62
1:B:33:SER:O	1:B:36:SER:HB2	1.99	0.62
1:B:359:LEU:HB3	1:B:360:PRO:HD2	1.81	0.62
1:B:69:TRP:NE1	1:B:73:ILE:HD11	2.14	0.62
1:A:196:THR:OG1	1:A:232:ARG:NH1	2.32	0.62
1:A:119:PHE:HZ	1:A:123:ARG:NH2	1.95	0.62
1:A:376:ARG:O	1:A:377:TRP:C	2.38	0.62
1:B:283:ASN:C	1:B:283:ASN:HD22	2.03	0.62
1:B:379:ALA:CB	1:B:409:LEU:HD11	2.30	0.62
1:A:362:PRO:HD3	1:A:367:LEU:HD21	0.68	0.62
1:A:283:ASN:HD22	1:A:283:ASN:C	2.03	0.62
1:A:357:ILE:HD12	1:A:358:MET:H	1.64	0.62
1:B:1:MET:SD	1:B:37:SER:HB2	2.40	0.62
1:A:291:ILE:O	1:A:292:LEU:HB2	2.00	0.62
1:A:315:LYS:NZ	1:B:87:GLU:HG3	2.14	0.62
1:A:75:TYR:O	1:A:76:ASP:C	2.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:HIS:O	1:B:353:PRO:HD3	2.00	0.62
1:A:244:ILE:O	1:A:271:GLY:N	2.24	0.62
1:A:82:PHE:O	1:A:261:VAL:HG21	1.99	0.62
1:A:315:LYS:HD2	1:B:87:GLU:OE2	2.00	0.62
1:A:379:ALA:CB	1:A:409:LEU:HD11	2.30	0.61
1:B:167:ALA:CB	1:B:209:LEU:HD21	2.29	0.61
1:A:359:LEU:HB3	1:A:360:PRO:HD2	1.81	0.61
1:B:119:PHE:CZ	1:B:123:ARG:NE	2.66	0.61
1:B:75:TYR:O	1:B:76:ASP:C	2.38	0.61
1:A:351:HIS:O	1:A:353:PRO:HD3	2.00	0.61
1:B:129:LEU:HD13	1:B:143:LEU:CD2	2.18	0.61
1:A:382:ASN:C	1:B:385:THR:CG2	2.64	0.61
1:A:85:ASP:OD1	1:A:285:LYS:HD3	1.99	0.61
1:B:297:ILE:O	1:B:300:ILE:CB	2.45	0.61
1:B:394:ILE:CG2	1:B:399:ARG:NH1	2.63	0.61
1:A:194:GLU:CA	1:A:197:LYS:HE3	2.30	0.61
1:A:329:LEU:HD11	1:A:421:TYR:CB	2.31	0.61
1:A:394:ILE:CG2	1:A:399:ARG:HH12	2.14	0.61
1:A:394:ILE:CG2	1:A:399:ARG:NH1	2.64	0.61
1:B:242:VAL:CG1	1:B:243:ILE:N	2.64	0.61
1:A:394:ILE:HG22	1:A:394:ILE:O	2.00	0.61
1:B:116:LEU:HD11	1:B:120:TYR:CE2	2.36	0.61
1:B:380:ALA:C	1:B:381:LEU:HG	2.21	0.61
1:A:380:ALA:C	1:A:381:LEU:HG	2.21	0.61
1:B:82:PHE:O	1:B:261:VAL:HG21	2.00	0.61
1:B:273:GLY:HA3	1:B:278:GLU:OE1	2.00	0.61
1:B:291:ILE:O	1:B:292:LEU:HB2	2.00	0.61
1:A:87:GLU:HB3	1:B:312:LYS:HE2	1.82	0.61
1:B:300:ILE:HD13	1:B:303:LYS:CE	2.31	0.61
1:B:394:ILE:O	1:B:394:ILE:HG22	2.00	0.61
1:A:247:MET:HE1	1:A:270:ILE:HD11	1.82	0.60
1:A:273:GLY:HA3	1:A:278:GLU:OE1	2.00	0.60
1:B:377:TRP:CE3	1:B:377:TRP:HA	2.35	0.60
1:B:6:ARG:HA	1:B:292:LEU:HD21	1.83	0.60
1:A:176:LYS:C	1:A:178:LYS:N	2.51	0.60
1:A:6:ARG:HA	1:A:292:LEU:HD21	1.83	0.60
1:A:328:THR:HG23	1:A:331:ASP:OD2	2.01	0.60
1:A:377:TRP:HA	1:A:377:TRP:CE3	2.35	0.60
1:A:91:ASN:ND2	1:B:357:ILE:HG21	2.16	0.60
1:A:234:HIS:CD2	1:A:265:ALA:HB2	2.36	0.60
1:A:402:ARG:CD	1:B:402:ARG:CD	2.78	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:MET:HE2	1:B:257:LEU:CD2	2.31	0.60
1:B:378:LEU:HD23	1:B:378:LEU:C	2.22	0.60
1:B:378:LEU:CA	1:B:381:LEU:CD1	2.76	0.60
1:B:376:ARG:O	1:B:377:TRP:C	2.38	0.60
1:B:301:LEU:CD1	1:B:305:LYS:HE3	2.28	0.60
1:A:116:LEU:HD11	1:A:120:TYR:CE2	2.36	0.60
1:A:300:ILE:HD13	1:A:303:LYS:CE	2.31	0.60
1:A:30:LEU:HD23	1:A:48:THR:HG22	1.84	0.60
1:A:378:LEU:HD23	1:A:378:LEU:C	2.22	0.60
1:A:327:LEU:HB2	1:A:390:GLU:O	2.01	0.60
1:B:122:LYS:C	1:B:124:GLY:H	2.05	0.60
1:B:234:HIS:CD2	1:B:265:ALA:HB2	2.36	0.60
1:B:329:LEU:HD11	1:B:421:TYR:CB	2.31	0.60
1:A:119:PHE:HZ	1:A:123:ARG:HH21	1.48	0.60
1:B:327:LEU:HB2	1:B:390:GLU:O	2.01	0.60
1:A:378:LEU:CA	1:A:381:LEU:CD1	2.76	0.60
1:B:328:THR:HG23	1:B:331:ASP:OD2	2.01	0.60
1:B:394:ILE:CG2	1:B:399:ARG:HH12	2.14	0.60
1:B:194:GLU:CA	1:B:197:LYS:HE3	2.30	0.60
1:A:123:ARG:NH2	1:B:318:GLU:OE1	2.35	0.59
1:A:276:ILE:CG2	1:A:277:ASP:N	2.65	0.59
1:B:85:ASP:OD1	1:B:285:LYS:CD	2.50	0.59
1:A:302:GLU:OE1	1:A:341:LYS:HG3	2.02	0.59
1:A:382:ASN:CA	1:B:385:THR:CG2	2.79	0.59
1:A:122:LYS:C	1:A:124:GLY:H	2.05	0.59
1:A:85:ASP:OD1	1:A:285:LYS:CD	2.50	0.59
1:A:312:LYS:HE2	1:B:87:GLU:HB3	1.83	0.59
1:A:41:VAL:O	1:A:41:VAL:HG12	2.02	0.59
1:A:242:VAL:CG1	1:A:243:ILE:N	2.64	0.59
1:A:372:GLU:C	1:A:374:ILE:N	2.52	0.59
1:A:385:THR:CG2	1:B:382:ASN:CA	2.79	0.59
1:B:276:ILE:CG2	1:B:277:ASP:N	2.65	0.59
1:A:377:TRP:CA	1:A:377:TRP:CE3	2.85	0.59
1:B:302:GLU:OE1	1:B:341:LYS:HG3	2.02	0.59
1:B:30:LEU:HD23	1:B:48:THR:HG22	1.84	0.59
1:A:331:ASP:O	1:A:332:VAL:CG2	2.49	0.59
1:A:357:ILE:HG21	1:B:91:ASN:ND2	2.18	0.59
1:B:86:LYS:CE	1:B:266:THR:HG23	2.28	0.59
1:B:348:VAL:CG1	1:B:352:ILE:HD11	2.33	0.59
1:B:346:SER:C	1:B:348:VAL:N	2.55	0.59
1:A:362:PRO:O	1:A:363:SER:C	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ASP:O	1:B:332:VAL:CG2	2.49	0.59
1:A:318:GLU:OE1	1:B:123:ARG:NH2	2.36	0.58
1:B:109:LYS:O	1:B:110:THR:CB	2.51	0.58
1:B:377:TRP:CA	1:B:377:TRP:CE3	2.85	0.58
1:B:318:GLU:O	1:B:319:ASP:OD1	2.22	0.58
1:B:418:LEU:HA	1:B:421:TYR:CD1	2.34	0.58
1:B:41:VAL:HG12	1:B:41:VAL:O	2.02	0.58
1:A:109:LYS:O	1:A:110:THR:CB	2.51	0.58
1:B:377:TRP:HE3	1:B:377:TRP:N	2.02	0.58
1:B:100:MET:CE	1:B:209:LEU:HD12	2.34	0.58
1:A:2:LEU:HB3	1:A:291:ILE:CG2	2.34	0.58
1:A:335:GLN:HB3	1:A:355:LEU:CD2	2.33	0.58
1:A:409:LEU:CD1	1:A:413:GLU:OE1	2.41	0.58
1:A:346:SER:C	1:A:348:VAL:N	2.55	0.57
1:B:335:GLN:HB3	1:B:355:LEU:CD2	2.33	0.57
1:A:301:LEU:O	1:A:305:LYS:HB2	2.04	0.57
1:B:131:ALA:O	1:B:140:TYR:HE2	1.87	0.57
1:A:123:ARG:O	1:B:358:MET:O	2.22	0.57
1:B:359:LEU:HB3	1:B:360:PRO:CD	2.33	0.57
1:A:1:MET:SD	1:A:37:SER:HB2	2.40	0.57
1:B:199:LEU:CD2	1:B:202:MET:SD	2.92	0.57
1:A:402:ARG:CD	1:B:402:ARG:NE	2.68	0.57
1:A:402:ARG:NE	1:B:402:ARG:NE	2.51	0.57
1:A:359:LEU:HB3	1:A:360:PRO:CD	2.33	0.57
1:A:367:LEU:O	1:A:368:LYS:HB2	2.04	0.57
1:B:359:LEU:CD1	1:B:360:PRO:CD	2.60	0.57
1:A:87:GLU:HG2	1:B:312:LYS:HG2	1.86	0.57
1:B:118:TYR:OH	1:B:122:LYS:HE3	2.04	0.57
1:B:2:LEU:HB3	1:B:291:ILE:CG2	2.34	0.57
1:A:299:SER:O	1:A:303:LYS:N	2.37	0.57
1:A:300:ILE:HG22	1:A:301:LEU:N	2.20	0.57
1:A:348:VAL:CG1	1:A:352:ILE:HD11	2.33	0.57
1:B:367:LEU:O	1:B:368:LYS:HB2	2.04	0.57
1:A:199:LEU:CD2	1:A:202:MET:SD	2.92	0.57
1:A:377:TRP:N	1:A:377:TRP:HE3	2.02	0.57
1:B:301:LEU:O	1:B:305:LYS:HB2	2.04	0.57
1:B:283:ASN:O	1:B:284:ALA:C	2.42	0.57
1:A:361:THR:OG1	1:A:367:LEU:HD12	2.04	0.56
1:B:369:ILE:CG2	1:B:370:GLY:H	2.18	0.56
1:A:100:MET:CE	1:A:209:LEU:HD12	2.34	0.56
1:A:402:ARG:NE	1:B:402:ARG:CD	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:SER:O	1:B:303:LYS:N	2.37	0.56
1:A:283:ASN:O	1:A:284:ALA:C	2.42	0.56
1:A:318:GLU:OE1	1:B:123:ARG:NH1	2.39	0.56
1:A:318:GLU:O	1:A:319:ASP:OD1	2.21	0.56
1:B:300:ILE:HG22	1:B:301:LEU:N	2.20	0.56
1:B:361:THR:OG1	1:B:367:LEU:HD12	2.04	0.56
1:B:77:GLU:O	1:B:78:LEU:C	2.41	0.56
1:A:118:TYR:OH	1:A:122:LYS:HE3	2.04	0.56
1:A:116:LEU:HD11	1:A:120:TYR:HE2	1.69	0.56
1:A:300:ILE:HD13	1:A:303:LYS:HE3	1.88	0.56
1:A:342:MET:O	1:A:343:GLY:O	2.23	0.56
1:A:131:ALA:O	1:A:140:TYR:HE2	1.87	0.56
1:B:116:LEU:HD11	1:B:120:TYR:HE2	1.69	0.56
1:A:358:MET:O	1:B:123:ARG:O	2.23	0.56
1:A:143:LEU:HD13	1:A:154:VAL:HG13	1.88	0.56
1:A:301:LEU:CD1	1:A:305:LYS:HE3	2.28	0.56
1:B:427:LEU:O	1:B:431:VAL:HG23	2.06	0.56
1:B:95:LEU:CD2	1:B:97:PHE:CE1	2.82	0.56
1:A:135:TYR:CD1	1:A:189:ARG:CZ	2.88	0.56
1:A:293:GLY:HA3	1:A:296:ASP:OD2	2.06	0.56
1:B:293:GLY:HA3	1:B:296:ASP:OD2	2.06	0.56
1:B:347:LYS:O	1:B:347:LYS:HG3	2.06	0.56
1:A:312:LYS:HG2	1:B:87:GLU:HG2	1.87	0.56
1:A:427:LEU:O	1:A:431:VAL:HG23	2.05	0.56
1:B:135:TYR:CD1	1:B:189:ARG:CZ	2.88	0.56
1:B:1:MET:CG	1:B:37:SER:HB3	2.36	0.56
1:B:300:ILE:HD13	1:B:303:LYS:HE3	1.88	0.56
1:B:380:ALA:C	1:B:381:LEU:CG	2.74	0.56
1:A:347:LYS:HG3	1:A:347:LYS:O	2.06	0.56
1:A:385:THR:CG2	1:A:386:TYR:N	2.69	0.56
1:A:293:GLY:O	1:A:296:ASP:N	2.32	0.55
1:A:369:ILE:CG2	1:A:370:GLY:H	2.18	0.55
1:B:219:ASP:OD1	1:B:221:SER:OG	2.23	0.55
1:B:95:LEU:HD23	1:B:97:PHE:HE1	1.63	0.55
1:B:247:MET:HE2	1:B:270:ILE:HD11	1.89	0.55
1:A:219:ASP:OD1	1:A:221:SER:OG	2.23	0.55
1:A:123:ARG:NH1	1:B:318:GLU:OE1	2.39	0.55
1:B:342:MET:O	1:B:343:GLY:O	2.24	0.55
1:B:376:ARG:O	1:B:379:ALA:N	2.40	0.55
1:B:425:ASN:O	1:B:429:LYS:HG3	2.06	0.55
1:B:427:LEU:O	1:B:428:LEU:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:TYR:CD2	1:B:297:ILE:CG2	2.85	0.55
1:A:376:ARG:O	1:A:379:ALA:N	2.40	0.55
1:A:379:ALA:HB3	1:A:417:LEU:HD11	1.88	0.55
1:B:293:GLY:O	1:B:296:ASP:N	2.32	0.55
1:A:51:ILE:HD13	1:A:74:VAL:HG22	1.88	0.55
1:B:85:ASP:OD1	1:B:285:LYS:CE	2.54	0.55
1:A:416:GLU:O	1:A:417:LEU:C	2.45	0.55
1:B:267:ILE:HG22	1:B:267:ILE:O	2.07	0.55
1:A:409:LEU:HB3	1:A:413:GLU:OE1	2.07	0.55
1:A:85:ASP:OD1	1:A:285:LYS:CE	2.54	0.55
1:B:379:ALA:HB3	1:B:417:LEU:HD11	1.88	0.54
1:B:143:LEU:HD13	1:B:154:VAL:HG13	1.88	0.54
1:B:329:LEU:O	1:B:329:LEU:HG	2.07	0.54
1:B:385:THR:CG2	1:B:386:TYR:N	2.69	0.54
1:A:300:ILE:HD13	1:A:303:LYS:HZ2	1.72	0.54
1:A:40:ASN:HD22	1:A:42:LYS:CB	2.20	0.54
1:B:129:LEU:HD23	1:B:183:ILE:HB	1.89	0.54
1:B:416:GLU:O	1:B:417:LEU:C	2.45	0.54
1:A:247:MET:HE1	1:A:257:LEU:CD2	2.37	0.54
1:A:270:ILE:HG23	1:A:270:ILE:O	2.08	0.54
1:A:1:MET:CG	1:A:37:SER:HB3	2.36	0.54
1:A:77:GLU:O	1:A:78:LEU:C	2.41	0.54
1:B:75:TYR:CE2	1:B:297:ILE:HG23	2.42	0.54
1:A:129:LEU:HD23	1:A:183:ILE:HB	1.89	0.54
1:A:163:PRO:O	1:A:164:ILE:C	2.46	0.54
1:A:221:SER:CA	1:A:250:THR:HG21	2.33	0.54
1:B:361:THR:CB	1:B:367:LEU:HG	2.38	0.54
1:A:329:LEU:HG	1:A:329:LEU:O	2.07	0.54
1:B:28:LYS:O	1:B:32:LYS:HD3	2.07	0.54
1:B:361:THR:HA	1:B:367:LEU:HD11	0.66	0.54
1:B:369:ILE:HA	1:B:373:LYS:HG2	1.89	0.54
1:A:101:LEU:HD12	1:A:113:ALA:HB2	1.90	0.54
1:A:267:ILE:O	1:A:267:ILE:HG22	2.07	0.54
1:A:336:ILE:HD11	1:A:377:TRP:HD1	1.73	0.54
1:A:425:ASN:O	1:A:429:LYS:HG3	2.06	0.54
1:B:409:LEU:HB3	1:B:413:GLU:OE1	2.07	0.54
1:A:369:ILE:HA	1:A:373:LYS:HG2	1.89	0.54
1:B:190:HIS:HB3	1:B:194:GLU:HB2	1.89	0.54
1:B:101:LEU:HD12	1:B:113:ALA:HB2	1.90	0.54
1:A:247:MET:HG3	1:A:270:ILE:HD11	1.90	0.54
1:A:28:LYS:O	1:A:32:LYS:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLY:CA	1:A:296:ASP:OD2	2.56	0.54
1:A:75:TYR:CE2	1:A:297:ILE:HG23	2.42	0.54
1:A:385:THR:HG23	1:B:384:MET:O	2.08	0.54
1:B:155:TYR:CE1	1:B:173:ILE:HD12	2.43	0.54
1:B:94:LYS:N	1:B:97:PHE:CE2	2.68	0.54
1:A:359:LEU:CD1	1:A:360:PRO:CD	2.60	0.53
1:A:403:ILE:CG2	1:A:414:VAL:HG21	2.38	0.53
1:B:105:GLN:O	1:B:106:GLY:O	2.26	0.53
1:B:162:ASN:O	1:B:166:ILE:HG13	2.08	0.53
1:B:209:LEU:O	1:B:210:LYS:C	2.46	0.53
1:B:381:LEU:N	1:B:381:LEU:CD2	2.62	0.53
1:B:403:ILE:CG2	1:B:414:VAL:HG21	2.37	0.53
1:B:51:ILE:HD13	1:B:74:VAL:HG22	1.88	0.53
1:A:105:GLN:O	1:A:106:GLY:O	2.26	0.53
1:A:19:TYR:CD2	1:A:66:ARG:NH2	2.76	0.53
1:A:361:THR:CB	1:A:367:LEU:HG	2.38	0.53
1:B:380:ALA:O	1:B:381:LEU:CB	2.56	0.53
1:B:380:ALA:O	1:B:381:LEU:HG	2.08	0.53
1:B:40:ASN:HD22	1:B:42:LYS:CB	2.20	0.53
1:A:380:ALA:C	1:A:381:LEU:CG	2.74	0.53
1:A:380:ALA:O	1:A:382:ASN:OD1	2.26	0.53
1:A:427:LEU:O	1:A:428:LEU:C	2.45	0.53
1:B:270:ILE:HG23	1:B:270:ILE:O	2.08	0.53
1:B:336:ILE:HD11	1:B:377:TRP:HD1	1.73	0.53
1:A:162:ASN:O	1:A:166:ILE:HG13	2.08	0.53
1:B:118:TYR:CZ	1:B:122:LYS:HE3	2.44	0.53
1:B:19:TYR:CD2	1:B:66:ARG:NH2	2.76	0.53
1:B:247:MET:HG3	1:B:270:ILE:HD11	1.91	0.53
1:B:343:GLY:O	1:B:348:VAL:HG21	2.09	0.53
1:A:9:VAL:HG13	1:A:71:ILE:HD12	1.90	0.53
1:B:310:TYR:CZ	1:B:355:LEU:HD23	2.44	0.53
1:B:1:MET:HG2	1:B:37:SER:HB3	1.91	0.53
1:B:75:TYR:OH	1:B:292:LEU:CD1	2.55	0.53
1:A:380:ALA:O	1:A:381:LEU:HG	2.08	0.53
1:B:380:ALA:O	1:B:382:ASN:OD1	2.26	0.53
1:B:9:VAL:HG13	1:B:71:ILE:HD12	1.90	0.53
1:A:23:VAL:O	1:A:24:ASP:C	2.46	0.53
1:B:155:TYR:CD2	1:B:170:GLY:CA	2.91	0.53
1:A:190:HIS:HB3	1:A:194:GLU:HB2	1.89	0.53
1:A:394:ILE:HG22	1:A:399:ARG:CZ	2.39	0.53
1:A:155:TYR:CE1	1:A:173:ILE:HD12	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ALA:HB1	1:A:209:LEU:CD1	2.36	0.53
1:A:300:ILE:O	1:A:303:LYS:CG	2.57	0.53
1:A:75:TYR:OH	1:A:292:LEU:CD1	2.55	0.53
1:B:163:PRO:O	1:B:164:ILE:C	2.46	0.53
1:B:167:ALA:HB1	1:B:209:LEU:CD1	2.36	0.53
1:B:293:GLY:CA	1:B:296:ASP:OD2	2.56	0.53
1:A:380:ALA:O	1:A:381:LEU:CB	2.56	0.53
1:A:70:PHE:O	1:A:71:ILE:C	2.46	0.53
1:B:300:ILE:O	1:B:303:LYS:CG	2.57	0.53
1:A:15:GLY:HA2	1:A:67:LYS:HZ2	1.71	0.52
1:B:70:PHE:O	1:B:71:ILE:C	2.46	0.52
1:A:155:TYR:CD2	1:A:170:GLY:CA	2.91	0.52
1:A:299:SER:O	1:A:303:LYS:CG	2.56	0.52
1:B:23:VAL:O	1:B:24:ASP:C	2.45	0.52
1:B:431:VAL:O	1:B:432:LYS:HB2	2.09	0.52
1:A:313:ILE:CD1	1:A:331:ASP:OD1	2.56	0.52
1:B:143:LEU:O	1:B:143:LEU:HD22	2.10	0.52
1:B:394:ILE:HG22	1:B:399:ARG:CZ	2.39	0.52
1:A:372:GLU:C	1:A:374:ILE:HG22	2.30	0.52
1:B:345:LEU:HG	1:B:346:SER:H	1.74	0.52
1:B:362:PRO:CD	1:B:367:LEU:HD23	2.33	0.52
1:B:64:LEU:HD11	1:B:303:LYS:HZ3	1.73	0.52
1:A:1:MET:HG2	1:A:37:SER:HB3	1.91	0.52
1:A:343:GLY:O	1:A:348:VAL:HG21	2.09	0.52
1:A:357:ILE:O	1:A:358:MET:CB	2.57	0.52
1:A:377:TRP:CZ3	1:A:417:LEU:CD2	2.93	0.52
1:A:75:TYR:CE1	1:A:292:LEU:HD12	2.44	0.52
1:B:428:LEU:O	1:B:431:VAL:HG23	2.10	0.52
1:A:310:TYR:CZ	1:A:355:LEU:HD23	2.44	0.52
1:B:225:LYS:C	1:B:227:TYR:H	2.12	0.52
1:B:75:TYR:HD2	1:B:297:ILE:CG2	2.19	0.52
1:A:100:MET:HE3	1:A:209:LEU:HD12	1.90	0.52
1:A:384:MET:O	1:B:385:THR:HG23	2.09	0.52
1:A:428:LEU:O	1:A:431:VAL:HG23	2.10	0.52
1:B:372:GLU:C	1:B:374:ILE:HG22	2.30	0.52
1:A:118:TYR:CZ	1:A:122:LYS:HE3	2.44	0.52
1:A:209:LEU:O	1:A:210:LYS:C	2.46	0.52
1:B:295:GLY:HA2	1:B:298:GLU:CB	2.33	0.52
1:B:361:THR:CG2	1:B:365:ASP:O	2.58	0.52
1:B:374:ILE:HG23	1:B:375:ARG:N	2.24	0.52
1:A:225:LYS:C	1:A:227:TYR:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:HB3	1:A:389:LEU:O	2.10	0.51
1:A:58:GLU:O	1:A:69:TRP:NE1	2.43	0.51
1:B:377:TRP:CZ3	1:B:417:LEU:CD2	2.93	0.51
1:A:164:ILE:CG2	1:A:165:GLU:N	2.59	0.51
1:A:133:ASP:OD1	1:A:187:ALA:HB2	2.09	0.51
1:A:190:HIS:CG	1:A:197:LYS:CD	2.79	0.51
1:A:283:ASN:ND2	1:A:283:ASN:C	2.62	0.51
1:B:133:ASP:OD1	1:B:187:ALA:HB2	2.09	0.51
1:A:329:LEU:HD11	1:A:421:TYR:CG	2.45	0.51
1:A:75:TYR:HD2	1:A:297:ILE:CG2	2.19	0.51
1:B:329:LEU:HD11	1:B:421:TYR:CG	2.45	0.51
1:B:83:GLY:HA2	1:B:261:VAL:HG13	1.92	0.51
1:A:361:THR:CG2	1:A:365:ASP:O	2.58	0.51
1:A:417:LEU:O	1:A:421:TYR:CD1	2.64	0.51
1:A:431:VAL:O	1:A:432:LYS:HB2	2.09	0.51
1:B:75:TYR:CE1	1:B:292:LEU:HD12	2.44	0.51
1:A:225:LYS:C	1:A:227:TYR:N	2.64	0.51
1:A:380:ALA:HB1	1:A:384:MET:SD	2.51	0.51
1:A:40:ASN:ND2	1:A:42:LYS:CB	2.73	0.51
1:B:417:LEU:O	1:B:421:TYR:CD1	2.64	0.51
1:A:143:LEU:HD22	1:A:143:LEU:O	2.10	0.51
1:B:144:LEU:HD23	1:B:154:VAL:HB	1.91	0.51
1:B:168:LYS:HE3	1:B:208:VAL:HG13	1.93	0.51
1:A:259:ALA:O	1:A:262:ALA:HB3	2.11	0.51
1:A:346:SER:O	1:A:349:LEU:N	2.43	0.51
1:A:310:TYR:OH	1:A:355:LEU:HA	2.11	0.51
1:A:361:THR:HA	1:A:367:LEU:HD11	0.66	0.51
1:A:374:ILE:HG23	1:A:375:ARG:N	2.24	0.51
1:A:40:ASN:HB3	1:A:43:LEU:HG	1.92	0.51
1:A:53:GLU:CG	1:A:57:LYS:HE3	2.40	0.51
1:B:225:LYS:C	1:B:227:TYR:N	2.64	0.51
1:B:283:ASN:C	1:B:283:ASN:ND2	2.62	0.51
1:B:310:TYR:OH	1:B:355:LEU:HA	2.11	0.51
1:B:374:ILE:C	1:B:376:ARG:N	2.64	0.51
1:B:53:GLU:CG	1:B:57:LYS:HE3	2.40	0.51
1:A:163:PRO:HG2	1:A:164:ILE:N	2.22	0.51
1:A:295:GLY:HA2	1:A:298:GLU:CB	2.33	0.51
1:B:380:ALA:HB1	1:B:384:MET:SD	2.51	0.51
1:B:330:ARG:HB3	1:B:389:LEU:O	2.10	0.51
1:B:40:ASN:HB3	1:B:43:LEU:HG	1.92	0.51
1:A:168:LYS:HE3	1:A:208:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:SER:O	1:B:303:LYS:CG	2.56	0.51
1:A:384:MET:O	1:B:385:THR:CB	2.59	0.50
1:A:63:VAL:CG1	1:A:63:VAL:O	2.59	0.50
1:A:75:TYR:CD2	1:A:297:ILE:CG2	2.85	0.50
1:B:301:LEU:O	1:B:301:LEU:HG	2.11	0.50
1:B:40:ASN:ND2	1:B:42:LYS:CB	2.73	0.50
1:B:61:PRO:O	1:B:62:SER:C	2.48	0.50
1:A:114:GLY:O	1:A:115:LYS:C	2.49	0.50
1:A:301:LEU:HG	1:A:301:LEU:O	2.11	0.50
1:A:61:PRO:O	1:A:62:SER:C	2.48	0.50
1:B:131:ALA:HB2	1:B:143:LEU:HD12	1.92	0.50
1:A:195:GLU:O	1:A:196:THR:C	2.49	0.50
1:A:345:LEU:HG	1:A:346:SER:H	1.74	0.50
1:A:6:ARG:HG3	1:A:292:LEU:CD2	2.37	0.50
1:A:83:GLY:HA2	1:A:261:VAL:HG13	1.92	0.50
1:B:369:ILE:CG2	1:B:370:GLY:N	2.75	0.50
1:A:420:TRP:O	1:A:423:ASN:N	2.45	0.50
1:B:6:ARG:HG3	1:B:292:LEU:CD2	2.37	0.50
1:A:119:PHE:CE1	1:A:123:ARG:NE	2.73	0.50
1:B:101:LEU:HD23	1:B:215:ILE:HB	1.94	0.50
1:B:374:ILE:HD13	1:B:374:ILE:C	2.31	0.50
1:A:101:LEU:HD23	1:A:215:ILE:HB	1.94	0.50
1:A:144:LEU:HD23	1:A:154:VAL:HB	1.91	0.50
1:A:359:LEU:CB	1:A:360:PRO:HD2	2.36	0.50
1:A:369:ILE:CG2	1:A:370:GLY:N	2.75	0.50
1:B:346:SER:O	1:B:349:LEU:N	2.43	0.50
1:B:420:TRP:O	1:B:423:ASN:N	2.45	0.50
1:A:243:ILE:HG12	1:A:269:PHE:HB2	1.94	0.50
1:A:374:ILE:C	1:A:374:ILE:HD13	2.31	0.50
1:B:374:ILE:HD13	1:B:375:ARG:N	2.27	0.50
1:A:123:ARG:C	1:B:358:MET:O	2.50	0.50
1:B:115:LYS:O	1:B:118:TYR:HB3	2.12	0.50
1:B:349:LEU:HA	1:B:352:ILE:CB	2.36	0.50
1:A:374:ILE:HD13	1:A:375:ARG:N	2.27	0.50
1:B:259:ALA:O	1:B:262:ALA:HB3	2.11	0.49
1:B:87:GLU:OE1	1:B:283:ASN:OD1	2.30	0.49
1:A:244:ILE:HB	1:A:270:ILE:HG13	1.94	0.49
1:A:385:THR:CB	1:B:384:MET:O	2.60	0.49
1:A:418:LEU:HA	1:A:421:TYR:CD1	2.34	0.49
1:A:131:ALA:HB2	1:A:143:LEU:HD12	1.92	0.49
1:A:374:ILE:C	1:A:376:ARG:N	2.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLY:O	1:B:115:LYS:C	2.49	0.49
1:B:195:GLU:O	1:B:196:THR:C	2.49	0.49
1:B:58:GLU:O	1:B:69:TRP:NE1	2.44	0.49
1:B:243:ILE:HG12	1:B:269:PHE:HB2	1.94	0.49
1:A:300:ILE:HA	1:A:303:LYS:HE3	1.94	0.49
1:B:200:GLU:OE2	1:B:200:GLU:C	2.49	0.49
1:B:300:ILE:HD13	1:B:303:LYS:HZ2	1.77	0.49
1:A:281:THR:CB	1:B:315:LYS:HD3	2.42	0.49
1:A:115:LYS:O	1:A:118:TYR:HB3	2.12	0.49
1:A:200:GLU:OE1	1:A:201:GLU:N	2.46	0.49
1:A:40:ASN:HD22	1:A:42:LYS:H	1.61	0.49
1:B:63:VAL:O	1:B:63:VAL:CG1	2.59	0.49
1:A:242:VAL:HG12	1:A:243:ILE:N	2.27	0.49
1:B:357:ILE:O	1:B:358:MET:CB	2.57	0.49
1:B:377:TRP:N	1:B:377:TRP:CE3	2.81	0.49
1:A:349:LEU:O	1:A:352:ILE:N	2.43	0.48
1:B:163:PRO:CG	1:B:164:ILE:H	2.23	0.48
1:A:127:VAL:HA	1:A:181:ILE:O	2.14	0.48
1:B:100:MET:HE2	1:B:209:LEU:HD12	1.95	0.48
1:B:244:ILE:HB	1:B:270:ILE:HG13	1.94	0.48
1:A:207:ASP:OD1	1:A:207:ASP:C	2.52	0.48
1:B:207:ASP:OD1	1:B:207:ASP:C	2.52	0.48
1:B:100:MET:HE3	1:B:209:LEU:HD12	1.95	0.48
1:B:242:VAL:HG12	1:B:243:ILE:N	2.27	0.48
1:A:215:ILE:HG21	1:A:243:ILE:CD1	2.43	0.48
1:A:358:MET:O	1:B:123:ARG:C	2.52	0.48
1:B:300:ILE:HA	1:B:303:LYS:HE3	1.94	0.48
1:B:330:ARG:HB3	1:B:389:LEU:HB3	1.95	0.48
1:A:200:GLU:C	1:A:200:GLU:OE2	2.49	0.48
1:A:87:GLU:OE1	1:A:283:ASN:OD1	2.30	0.48
1:B:107:SER:OG	1:B:109:LYS:HB2	2.13	0.48
1:B:168:LYS:CE	1:B:208:VAL:HG13	2.44	0.48
1:A:432:LYS:HE2	1:B:277:ASP:CB	2.40	0.48
1:A:108:GLY:O	1:A:112:THR:OG1	2.25	0.48
1:A:234:HIS:NE2	1:A:265:ALA:CB	2.75	0.48
1:A:362:PRO:HD2	1:A:367:LEU:CD2	2.38	0.48
1:A:432:LYS:HE2	1:B:277:ASP:OD2	2.14	0.48
1:B:396:ASP:C	1:B:396:ASP:OD1	2.52	0.48
1:A:20:GLU:O	1:A:24:ASP:OD2	2.32	0.48
1:B:164:ILE:HD11	1:B:208:VAL:HG22	1.88	0.48
1:A:107:SER:OG	1:A:109:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ASN:HD22	1:B:42:LYS:H	1.61	0.48
1:B:430:MET:HA	1:B:430:MET:HE3	1.95	0.48
1:A:277:ASP:OD2	1:B:432:LYS:HE2	2.14	0.48
1:A:168:LYS:CE	1:A:208:VAL:HG13	2.44	0.48
1:A:373:LYS:HE3	1:A:377:TRP:HH2	1.78	0.48
1:B:194:GLU:O	1:B:197:LYS:HG2	2.14	0.48
1:B:215:ILE:HG21	1:B:243:ILE:CD1	2.43	0.48
1:B:303:LYS:C	1:B:307:LEU:HG	2.31	0.48
1:B:370:GLY:O	1:B:373:LYS:HB3	2.14	0.48
1:A:315:LYS:HD3	1:B:281:THR:CB	2.44	0.47
1:A:377:TRP:N	1:A:377:TRP:CE3	2.81	0.47
1:B:127:VAL:HA	1:B:181:ILE:O	2.14	0.47
1:A:194:GLU:HA	1:A:197:LYS:HE3	1.96	0.47
1:A:194:GLU:O	1:A:197:LYS:HG2	2.14	0.47
1:A:376:ARG:O	1:A:379:ALA:CB	2.62	0.47
1:A:417:LEU:C	1:A:421:TYR:CD1	2.88	0.47
1:A:430:MET:HA	1:A:430:MET:HE3	1.96	0.47
1:A:291:ILE:O	1:A:292:LEU:CB	2.62	0.47
1:A:74:VAL:O	1:A:75:TYR:C	2.53	0.47
1:B:177:ASN:O	1:B:178:LYS:HB2	2.14	0.47
1:A:383:SER:HB3	1:A:403:ILE:CA	2.44	0.47
1:A:70:PHE:O	1:A:73:ILE:N	2.47	0.47
1:B:163:PRO:HG2	1:B:164:ILE:N	2.22	0.47
1:B:247:MET:SD	1:B:270:ILE:HD11	2.55	0.47
1:A:277:ASP:CB	1:B:432:LYS:HE2	2.41	0.47
1:B:221:SER:CA	1:B:250:THR:HG21	2.33	0.47
1:B:302:GLU:CD	1:B:341:LYS:HE3	2.35	0.47
1:B:300:ILE:HD13	1:B:303:LYS:NZ	2.29	0.47
1:B:417:LEU:C	1:B:421:TYR:CD1	2.88	0.47
1:A:141:ASP:O	1:A:145:GLN:HG3	2.15	0.47
1:B:376:ARG:O	1:B:379:ALA:CB	2.62	0.47
1:B:383:SER:HB3	1:B:403:ILE:CA	2.44	0.47
1:A:98:ILE:HD13	1:A:171:VAL:HG11	1.97	0.47
1:A:177:ASN:O	1:A:178:LYS:HB2	2.14	0.47
1:A:302:GLU:HB3	1:A:341:LYS:HB3	1.97	0.47
1:B:194:GLU:HA	1:B:197:LYS:HE3	1.96	0.47
1:B:200:GLU:OE1	1:B:201:GLU:N	2.46	0.47
1:B:20:GLU:O	1:B:24:ASP:OD2	2.32	0.47
1:A:247:MET:SD	1:A:270:ILE:HD11	2.55	0.47
1:A:334:ALA:HA	1:A:337:ILE:HG22	1.97	0.47
1:A:370:GLY:O	1:A:373:LYS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:CA	1:A:421:TYR:HD1	2.21	0.47
1:B:61:PRO:O	1:B:62:SER:O	2.33	0.47
1:A:317:MET:CE	1:A:328:THR:HB	2.45	0.47
1:A:61:PRO:O	1:A:62:SER:O	2.33	0.47
1:B:98:ILE:HD13	1:B:171:VAL:HG11	1.97	0.47
1:A:362:PRO:CD	1:A:367:LEU:HD23	2.33	0.47
1:B:302:GLU:HB3	1:B:341:LYS:HB3	1.97	0.47
1:A:85:ASP:OD1	1:A:285:LYS:HE2	2.15	0.47
1:A:300:ILE:HD13	1:A:303:LYS:NZ	2.29	0.47
1:A:302:GLU:CD	1:A:341:LYS:HE3	2.34	0.47
1:B:235:GLN:C	1:B:237:SER:H	2.18	0.47
1:B:367:LEU:O	1:B:368:LYS:CB	2.63	0.47
1:A:115:LYS:HG2	1:A:276:ILE:O	2.14	0.46
1:A:235:GLN:C	1:A:237:SER:H	2.18	0.46
1:A:330:ARG:HB3	1:A:389:LEU:HB3	1.95	0.46
1:B:115:LYS:HG2	1:B:276:ILE:O	2.14	0.46
1:B:190:HIS:CG	1:B:197:LYS:CD	2.79	0.46
1:B:378:LEU:O	1:B:381:LEU:CG	2.60	0.46
1:B:40:ASN:ND2	1:B:42:LYS:H	2.13	0.46
1:A:119:PHE:CZ	1:A:123:ARG:CZ	2.98	0.46
1:A:135:TYR:CE1	1:A:189:ARG:NE	2.83	0.46
1:A:301:LEU:HD21	1:A:305:LYS:HZ1	1.77	0.46
1:A:367:LEU:O	1:A:368:LYS:CB	2.63	0.46
1:A:417:LEU:C	1:A:421:TYR:CE1	2.89	0.46
1:A:40:ASN:ND2	1:A:42:LYS:HB2	2.31	0.46
1:B:300:ILE:HA	1:B:303:LYS:HG2	1.97	0.46
1:B:317:MET:CE	1:B:328:THR:HB	2.45	0.46
1:B:334:ALA:CA	1:B:337:ILE:HG22	2.46	0.46
1:A:94:LYS:N	1:A:97:PHE:CE2	2.68	0.46
1:B:119:PHE:CE1	1:B:123:ARG:NE	2.74	0.46
1:B:230:ALA:O	1:B:231:SER:C	2.54	0.46
1:B:74:VAL:O	1:B:75:TYR:C	2.53	0.46
1:B:85:ASP:OD1	1:B:285:LYS:HE2	2.15	0.46
1:A:317:MET:SD	1:A:328:THR:CB	3.04	0.46
1:A:40:ASN:ND2	1:A:42:LYS:H	2.13	0.46
1:B:207:ASP:O	1:B:210:LYS:HG3	2.16	0.46
1:B:313:ILE:CD1	1:B:331:ASP:OD1	2.56	0.46
1:B:336:ILE:HG13	1:B:377:TRP:HB3	1.98	0.46
1:B:379:ALA:C	1:B:380:ALA:O	2.52	0.46
1:A:109:LYS:O	1:A:110:THR:HB	2.16	0.46
1:A:163:PRO:CG	1:A:164:ILE:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ALA:O	1:A:231:SER:C	2.54	0.46
1:A:215:ILE:CG2	1:A:243:ILE:HG13	2.46	0.46
1:A:300:ILE:HA	1:A:303:LYS:HG2	1.97	0.46
1:B:270:ILE:O	1:B:270:ILE:CG2	2.64	0.46
1:B:298:GLU:O	1:B:302:GLU:HG2	2.16	0.46
1:A:193:GLY:N	1:A:195:GLU:OE2	2.42	0.46
1:A:334:ALA:CA	1:A:337:ILE:HG22	2.46	0.46
1:A:361:THR:HG23	1:A:367:LEU:HG	1.98	0.46
1:A:361:THR:CB	1:A:367:LEU:CD1	2.93	0.46
1:B:141:ASP:O	1:B:145:GLN:HG3	2.15	0.46
1:B:362:PRO:HD2	1:B:367:LEU:CD2	2.38	0.46
1:B:417:LEU:C	1:B:421:TYR:CE1	2.89	0.46
1:A:270:ILE:CG2	1:A:270:ILE:O	2.63	0.46
1:A:300:ILE:C	1:A:302:GLU:N	2.69	0.46
1:A:301:LEU:O	1:A:305:LYS:CD	2.61	0.46
1:A:303:LYS:C	1:A:307:LEU:HG	2.31	0.46
1:B:135:TYR:CE1	1:B:189:ARG:NE	2.83	0.46
1:B:9:VAL:HG11	1:B:292:LEU:HD13	1.98	0.46
1:B:397:LYS:O	1:B:398:SER:C	2.53	0.46
1:A:125:TYR:CD2	1:B:358:MET:SD	3.09	0.46
1:A:336:ILE:HG13	1:A:377:TRP:HB3	1.98	0.46
1:B:303:LYS:O	1:B:307:LEU:CG	2.49	0.46
1:A:330:ARG:CB	1:A:389:LEU:HB3	2.46	0.46
1:A:300:ILE:CD1	1:A:303:LYS:HZ2	2.28	0.46
1:B:298:GLU:C	1:B:300:ILE:N	2.67	0.46
1:B:310:TYR:HA	1:B:335:GLN:NE2	2.29	0.46
1:B:334:ALA:HA	1:B:337:ILE:HG22	1.97	0.46
1:B:361:THR:CB	1:B:367:LEU:CD1	2.93	0.46
1:B:378:LEU:CA	1:B:381:LEU:HD11	2.45	0.46
1:A:122:LYS:C	1:A:124:GLY:N	2.70	0.45
1:A:75:TYR:CZ	1:A:292:LEU:HD12	2.50	0.45
1:B:307:LEU:N	1:B:307:LEU:HD23	2.31	0.45
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.61	0.45
1:A:396:ASP:C	1:A:396:ASP:OD1	2.52	0.45
1:B:392:PRO:O	1:B:395:ILE:HG13	2.16	0.45
1:A:378:LEU:O	1:A:381:LEU:CG	2.60	0.45
1:B:2:LEU:HD13	1:B:291:ILE:CG2	2.46	0.45
1:B:94:LYS:O	1:B:96:PRO:O	2.34	0.45
1:B:119:PHE:CZ	1:B:123:ARG:CZ	2.98	0.45
1:B:215:ILE:CG2	1:B:243:ILE:HG13	2.46	0.45
1:B:301:LEU:O	1:B:305:LYS:CD	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ASN:ND2	1:B:42:LYS:HB2	2.31	0.45
1:B:70:PHE:O	1:B:73:ILE:N	2.47	0.45
1:A:235:GLN:C	1:A:237:SER:N	2.70	0.45
1:A:307:LEU:HD23	1:A:307:LEU:N	2.31	0.45
1:A:335:GLN:O	1:A:338:ALA:HB3	2.17	0.45
1:B:2:LEU:HD11	1:B:288:VAL:HA	1.98	0.45
1:B:75:TYR:CZ	1:B:292:LEU:HD12	2.50	0.45
1:A:207:ASP:O	1:A:210:LYS:HG3	2.16	0.45
1:A:298:GLU:O	1:A:302:GLU:HG2	2.16	0.45
1:A:349:LEU:HA	1:A:352:ILE:CB	2.36	0.45
1:A:392:PRO:O	1:A:395:ILE:HG13	2.17	0.45
1:A:93:THR:O	1:A:93:THR:HG22	2.16	0.45
1:A:9:VAL:HG11	1:A:292:LEU:HD13	1.98	0.45
1:B:109:LYS:O	1:B:110:THR:HB	2.16	0.45
1:B:111:THR:HG22	1:B:115:LYS:HE3	1.98	0.45
1:B:116:LEU:HA	1:B:116:LEU:HD12	1.70	0.45
1:B:212:ASP:O	1:B:213:ASP:OD1	2.35	0.45
1:B:335:GLN:O	1:B:338:ALA:HB3	2.17	0.45
1:B:93:THR:O	1:B:93:THR:HG22	2.16	0.45
1:A:2:LEU:HD11	1:A:288:VAL:HA	1.98	0.45
1:A:417:LEU:CB	1:A:421:TYR:HE1	2.21	0.45
1:B:300:ILE:CA	1:B:303:LYS:HG2	2.47	0.45
1:B:317:MET:SD	1:B:328:THR:CB	3.04	0.45
1:A:125:TYR:CG	1:B:358:MET:SD	3.10	0.45
1:B:391:ASN:O	1:B:392:PRO:C	2.55	0.45
1:A:164:ILE:HD11	1:A:208:VAL:HG22	1.88	0.45
1:A:168:LYS:HG3	1:A:172:ASP:OD2	2.17	0.45
1:A:94:LYS:O	1:A:96:PRO:O	2.34	0.45
1:B:300:ILE:C	1:B:302:GLU:H	2.19	0.45
1:B:300:ILE:HA	1:B:303:LYS:CD	2.47	0.45
1:B:40:ASN:HD22	1:B:42:LYS:HB3	1.82	0.45
1:A:336:ILE:HD11	1:A:377:TRP:CD1	2.52	0.45
1:A:397:LYS:O	1:A:398:SER:C	2.53	0.45
1:A:50:LYS:HD3	1:A:77:GLU:OE1	2.17	0.45
1:A:94:LYS:CA	1:A:97:PHE:CZ	3.00	0.45
1:B:301:LEU:O	1:B:305:LYS:CG	2.65	0.45
1:B:330:ARG:CB	1:B:389:LEU:HB3	2.46	0.45
1:B:372:GLU:O	1:B:374:ILE:CG2	2.62	0.45
1:A:100:MET:HE2	1:A:209:LEU:HD12	2.00	0.44
1:A:300:ILE:CA	1:A:303:LYS:HG2	2.47	0.44
1:A:300:ILE:C	1:A:302:GLU:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LYS:HG3	1:A:373:LYS:O	2.17	0.44
1:B:373:LYS:O	1:B:373:LYS:HG3	2.17	0.44
1:A:212:ASP:O	1:A:213:ASP:OD1	2.35	0.44
1:A:300:ILE:HA	1:A:303:LYS:CD	2.47	0.44
1:A:301:LEU:O	1:A:305:LYS:CG	2.65	0.44
1:A:335:GLN:OE1	1:A:335:GLN:HA	2.17	0.44
1:B:207:ASP:OD1	1:B:210:LYS:NZ	2.50	0.44
1:B:234:HIS:NE2	1:B:265:ALA:CB	2.75	0.44
1:B:418:LEU:CA	1:B:421:TYR:HD1	2.22	0.44
1:A:157:GLU:OE2	1:A:169:LYS:HD2	2.17	0.44
1:A:336:ILE:HA	1:A:339:LEU:HD23	1.99	0.44
1:B:150:ILE:HG13	1:B:152:VAL:CG2	2.39	0.44
1:B:168:LYS:HG3	1:B:172:ASP:OD2	2.17	0.44
1:B:30:LEU:HD23	1:B:48:THR:CG2	2.47	0.44
1:B:349:LEU:O	1:B:352:ILE:N	2.43	0.44
1:B:361:THR:HG23	1:B:367:LEU:HG	1.98	0.44
1:B:47:LEU:CD1	1:B:77:GLU:HB3	2.48	0.44
1:A:298:GLU:C	1:A:300:ILE:N	2.67	0.44
1:B:192:TYR:HE1	1:B:229:LEU:HD23	1.83	0.44
1:B:23:VAL:HG13	1:B:70:PHE:CZ	2.53	0.44
1:B:336:ILE:HA	1:B:339:LEU:HD23	1.99	0.44
1:A:111:THR:HG22	1:A:115:LYS:HE3	1.98	0.44
1:A:198:LEU:O	1:A:201:GLU:HB3	2.18	0.44
1:A:53:GLU:O	1:A:57:LYS:HG3	2.18	0.44
1:A:47:LEU:CD1	1:A:77:GLU:HB3	2.48	0.44
1:B:157:GLU:OE2	1:B:169:LYS:HD2	2.17	0.44
1:B:333:TYR:O	1:B:334:ALA:C	2.55	0.44
1:B:53:GLU:O	1:B:57:LYS:HG3	2.18	0.44
1:A:378:LEU:CA	1:A:381:LEU:HD11	2.45	0.44
1:A:71:ILE:O	1:A:74:VAL:HB	2.18	0.44
1:B:94:LYS:CA	1:B:97:PHE:CZ	3.00	0.44
1:A:302:GLU:CD	1:A:341:LYS:CD	2.86	0.44
1:A:40:ASN:HD22	1:A:42:LYS:HB3	1.82	0.44
1:A:402:ARG:CB	1:B:402:ARG:NH1	2.79	0.44
1:B:410:GLU:HG2	1:B:411:VAL:N	2.33	0.44
1:A:23:VAL:HG13	1:A:70:PHE:CZ	2.53	0.44
1:B:164:ILE:O	1:B:165:GLU:C	2.56	0.44
1:B:291:ILE:O	1:B:292:LEU:CB	2.62	0.44
1:B:300:ILE:C	1:B:302:GLU:N	2.69	0.44
1:B:335:GLN:OE1	1:B:335:GLN:HA	2.17	0.44
1:B:361:THR:HA	1:B:367:LEU:CG	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LYS:HD3	1:B:77:GLU:OE1	2.17	0.44
1:A:164:ILE:O	1:A:165:GLU:C	2.56	0.44
1:A:303:LYS:HG3	1:A:304:VAL:N	2.30	0.44
1:A:348:VAL:HG12	1:A:352:ILE:CD1	2.45	0.44
1:B:298:GLU:O	1:B:299:SER:C	2.56	0.44
1:B:69:TRP:CD1	1:B:73:ILE:HD11	2.53	0.44
1:A:207:ASP:OD1	1:A:210:LYS:NZ	2.50	0.43
1:A:244:ILE:HG13	1:A:267:ILE:HD13	1.99	0.43
1:B:122:LYS:C	1:B:124:GLY:N	2.70	0.43
1:B:198:LEU:O	1:B:201:GLU:HB3	2.18	0.43
1:A:64:LEU:HD11	1:A:303:LYS:HZ3	1.83	0.43
1:A:41:VAL:CG1	1:A:41:VAL:O	2.65	0.43
1:A:69:TRP:CD1	1:A:73:ILE:HD11	2.53	0.43
1:B:302:GLU:CD	1:B:341:LYS:CD	2.86	0.43
1:B:71:ILE:O	1:B:74:VAL:HB	2.18	0.43
1:B:78:LEU:O	1:B:79:SER:C	2.56	0.43
1:A:109:LYS:HE2	1:A:186:THR:O	2.18	0.43
1:A:176:LYS:O	1:A:177:ASN:C	2.56	0.43
1:A:176:LYS:O	1:A:178:LYS:HG2	2.18	0.43
1:A:104:VAL:HG21	1:A:192:TYR:CE2	2.53	0.43
1:A:298:GLU:O	1:A:299:SER:C	2.56	0.43
1:A:2:LEU:HD23	1:A:2:LEU:HA	1.79	0.43
1:A:349:LEU:HA	1:A:352:ILE:HD12	2.00	0.43
1:A:372:GLU:O	1:A:374:ILE:CG2	2.62	0.43
1:B:41:VAL:CG1	1:B:41:VAL:O	2.65	0.43
1:A:2:LEU:HD13	1:A:291:ILE:CG2	2.46	0.43
1:B:235:GLN:C	1:B:237:SER:N	2.70	0.43
1:B:349:LEU:HA	1:B:352:ILE:HD12	2.00	0.43
1:A:163:PRO:O	1:A:166:ILE:N	2.52	0.43
1:A:199:LEU:HA	1:A:202:MET:SD	2.59	0.43
1:A:410:GLU:HG2	1:A:411:VAL:N	2.33	0.43
1:A:83:GLY:HA2	1:A:261:VAL:CG1	2.48	0.43
1:B:131:ALA:O	1:B:140:TYR:CE2	2.69	0.43
1:A:192:TYR:HE1	1:A:229:LEU:HD23	1.83	0.43
1:B:119:PHE:HZ	1:B:123:ARG:HH21	1.48	0.43
1:B:244:ILE:HG13	1:B:267:ILE:HD13	1.99	0.43
1:B:293:GLY:O	1:B:296:ASP:HB2	2.18	0.43
1:B:2:LEU:HA	1:B:2:LEU:HD23	1.79	0.43
1:B:403:ILE:HG22	1:B:414:VAL:CG2	2.45	0.43
1:B:417:LEU:CB	1:B:421:TYR:HE1	2.21	0.43
1:A:293:GLY:O	1:A:296:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLN:O	1:B:106:GLY:C	2.56	0.43
1:B:163:PRO:O	1:B:166:ILE:N	2.52	0.43
1:B:302:GLU:CD	1:B:341:LYS:HD2	2.39	0.43
1:A:247:MET:HG3	1:A:270:ILE:CD1	2.48	0.43
1:A:291:ILE:HG13	1:A:291:ILE:O	2.19	0.43
1:A:301:LEU:HD21	1:A:305:LYS:HZ2	1.83	0.43
1:A:358:MET:SD	1:B:125:TYR:CD2	3.12	0.43
1:B:199:LEU:HA	1:B:202:MET:SD	2.59	0.43
1:B:2:LEU:HB3	1:B:291:ILE:HG22	2.01	0.43
1:B:336:ILE:HD11	1:B:377:TRP:CD1	2.52	0.43
1:B:348:VAL:HG12	1:B:352:ILE:CD1	2.45	0.43
1:B:109:LYS:HE2	1:B:186:THR:O	2.18	0.43
1:B:247:MET:HG3	1:B:270:ILE:CD1	2.48	0.43
1:B:291:ILE:O	1:B:291:ILE:HG13	2.19	0.43
1:B:303:LYS:HG3	1:B:304:VAL:N	2.30	0.43
1:A:131:ALA:O	1:A:140:TYR:CE2	2.69	0.43
1:A:175:VAL:HG12	1:A:175:VAL:O	2.19	0.43
1:B:127:VAL:HG12	1:B:128:GLY:N	2.34	0.43
1:B:146:LEU:HD22	1:B:276:ILE:HD13	2.00	0.43
1:B:210:LYS:N	1:B:211:PRO:CD	2.82	0.43
1:A:124:GLY:HA3	1:B:359:LEU:N	2.34	0.42
1:A:219:ASP:CG	1:A:221:SER:HG	2.19	0.42
1:A:333:TYR:O	1:A:334:ALA:C	2.55	0.42
1:A:391:ASN:O	1:A:392:PRO:C	2.55	0.42
1:B:104:VAL:HG21	1:B:192:TYR:CE2	2.53	0.42
1:B:163:PRO:CG	1:B:164:ILE:N	2.82	0.42
1:A:403:ILE:HG22	1:A:414:VAL:CG2	2.45	0.42
1:B:176:LYS:O	1:B:178:LYS:HG2	2.18	0.42
1:B:40:ASN:O	1:B:44:VAL:HG23	2.19	0.42
1:A:302:GLU:CD	1:A:341:LYS:HD2	2.39	0.42
1:B:107:SER:C	1:B:109:LYS:N	2.71	0.42
1:B:335:GLN:CB	1:B:355:LEU:HD22	2.46	0.42
1:A:37:SER:O	1:A:38:ASP:HB3	2.19	0.42
1:B:157:GLU:HB2	1:B:160:ASN:HD22	1.77	0.42
1:B:83:GLY:HA2	1:B:261:VAL:CG1	2.48	0.42
1:A:210:LYS:N	1:A:211:PRO:CD	2.82	0.42
1:B:383:SER:O	1:B:384:MET:HG3	2.20	0.42
1:A:222:ILE:HD12	1:A:222:ILE:HA	1.93	0.42
1:A:299:SER:C	1:A:303:LYS:HE3	2.40	0.42
1:A:2:LEU:HB3	1:A:291:ILE:HG22	2.01	0.42
1:A:30:LEU:HD23	1:A:48:THR:CG2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:SER:O	1:A:384:MET:HG3	2.20	0.42
1:A:72:SER:OG	1:A:73:ILE:N	2.53	0.42
1:A:76:ASP:O	1:A:79:SER:HB3	2.19	0.42
1:B:302:GLU:CD	1:B:341:LYS:CE	2.88	0.42
1:B:368:LYS:O	1:B:369:ILE:HB	2.20	0.42
1:A:310:TYR:OH	1:A:354:GLY:O	2.37	0.42
1:A:358:MET:SD	1:B:125:TYR:CG	3.13	0.42
1:A:376:ARG:O	1:A:379:ALA:HB3	2.19	0.42
1:B:283:ASN:HD21	1:B:285:LYS:HG2	1.85	0.42
1:A:146:LEU:HD22	1:A:276:ILE:HD13	2.00	0.42
1:A:334:ALA:C	1:A:337:ILE:HG22	2.40	0.42
1:A:383:SER:HB2	1:A:403:ILE:HG23	1.97	0.42
1:A:40:ASN:O	1:A:44:VAL:HG23	2.19	0.42
1:B:35:ILE:O	1:B:36:SER:C	2.57	0.42
1:B:37:SER:O	1:B:38:ASP:HB3	2.20	0.42
1:A:167:ALA:C	1:A:209:LEU:HD21	2.40	0.42
1:A:227:TYR:O	1:A:228:ASP:C	2.57	0.42
1:A:303:LYS:O	1:A:307:LEU:CG	2.49	0.42
1:B:13:LEU:HD23	1:B:13:LEU:HA	1.84	0.42
1:A:283:ASN:HD21	1:A:285:LYS:HG2	1.85	0.42
1:B:227:TYR:O	1:B:228:ASP:C	2.57	0.42
1:B:76:ASP:O	1:B:79:SER:HB3	2.19	0.42
1:A:105:GLN:O	1:A:106:GLY:C	2.56	0.41
1:A:302:GLU:CD	1:A:341:LYS:CE	2.88	0.41
1:B:121:LYS:O	1:B:124:GLY:N	2.52	0.41
1:B:202:MET:O	1:B:203:LYS:C	2.59	0.41
1:B:347:LYS:HD2	1:B:350:GLN:HE21	1.84	0.41
1:A:127:VAL:HG12	1:A:128:GLY:N	2.34	0.41
1:B:20:GLU:OE1	1:B:20:GLU:HA	2.20	0.41
1:B:298:GLU:O	1:B:300:ILE:N	2.54	0.41
1:B:377:TRP:CA	1:B:377:TRP:HE3	2.33	0.41
1:A:284:ALA:O	1:A:286:ARG:N	2.52	0.41
1:B:113:ALA:O	1:B:129:LEU:HD21	2.21	0.41
1:B:116:LEU:HD23	1:B:183:ILE:HD13	2.03	0.41
1:B:64:LEU:CD1	1:B:303:LYS:HZ3	2.33	0.41
1:A:138:ALA:O	1:A:142:GLN:HB2	2.20	0.41
1:A:116:LEU:HD23	1:A:183:ILE:HD13	2.03	0.41
1:A:1:MET:SD	1:A:37:SER:OG	2.79	0.41
1:A:379:ALA:C	1:A:380:ALA:O	2.52	0.41
1:A:381:LEU:HB2	1:A:382:ASN:H	1.54	0.41
1:B:299:SER:C	1:B:303:LYS:HE3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ALA:C	1:B:337:ILE:HG22	2.39	0.41
1:B:373:LYS:HE3	1:B:377:TRP:HH2	1.78	0.41
1:B:383:SER:HB3	1:B:403:ILE:HA	2.03	0.41
1:A:350:GLN:HG3	1:A:351:HIS:CD2	2.56	0.41
1:B:138:ALA:O	1:B:142:GLN:HB2	2.20	0.41
1:B:15:GLY:HA2	1:B:67:LYS:HZ2	1.78	0.41
1:B:284:ALA:O	1:B:286:ARG:N	2.52	0.41
1:B:350:GLN:HG3	1:B:351:HIS:CD2	2.56	0.41
1:B:376:ARG:O	1:B:379:ALA:HB3	2.19	0.41
1:A:368:LYS:O	1:A:369:ILE:HB	2.20	0.41
1:A:381:LEU:N	1:A:381:LEU:CD2	2.62	0.41
1:B:219:ASP:CG	1:B:221:SER:HG	2.21	0.41
1:B:244:ILE:HG21	1:B:257:LEU:CD1	2.51	0.41
1:A:107:SER:C	1:A:109:LYS:N	2.71	0.41
1:A:202:MET:O	1:A:203:LYS:C	2.58	0.41
1:A:333:TYR:O	1:A:337:ILE:HG22	2.21	0.41
1:A:402:ARG:NH1	1:B:402:ARG:CB	2.79	0.41
1:B:383:SER:HB2	1:B:403:ILE:HG23	1.97	0.41
1:A:143:LEU:HA	1:A:143:LEU:HD23	1.81	0.41
1:A:335:GLN:CB	1:A:355:LEU:HD22	2.46	0.41
1:A:379:ALA:HB1	1:A:409:LEU:HD11	2.03	0.41
1:A:430:MET:CE	1:A:430:MET:HA	2.50	0.41
1:B:168:LYS:HE3	1:B:208:VAL:CG1	2.51	0.41
1:A:116:LEU:HD12	1:A:116:LEU:HA	1.70	0.41
1:A:284:ALA:O	1:A:287:PHE:N	2.54	0.41
1:A:347:LYS:HD2	1:A:350:GLN:HE21	1.84	0.41
1:A:78:LEU:O	1:A:79:SER:C	2.56	0.41
1:B:175:VAL:HG12	1:B:175:VAL:O	2.19	0.41
1:B:300:ILE:CD1	1:B:303:LYS:HZ2	2.33	0.41
1:A:113:ALA:O	1:A:129:LEU:HD21	2.20	0.41
1:A:131:ALA:HB1	1:A:140:TYR:CD2	2.56	0.41
1:A:157:GLU:HB2	1:A:160:ASN:HD22	1.77	0.41
1:A:20:GLU:HA	1:A:20:GLU:OE1	2.20	0.41
1:B:167:ALA:C	1:B:209:LEU:HD21	2.40	0.41
1:A:168:LYS:HE3	1:A:208:VAL:CG1	2.51	0.41
1:A:179:MET:HA	1:A:179:MET:HE1	1.99	0.41
1:A:310:TYR:HA	1:A:335:GLN:NE2	2.29	0.41
1:A:47:LEU:C	1:A:49:ALA:H	2.24	0.41
1:B:264:GLY:O	1:B:265:ALA:O	2.39	0.41
1:B:381:LEU:HB2	1:B:382:ASN:H	1.53	0.41
1:A:347:LYS:CG	1:A:347:LYS:O	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:MET:O	1:A:432:LYS:N	2.55	0.40
1:B:131:ALA:HB1	1:B:140:TYR:CD2	2.56	0.40
1:B:6:ARG:CA	1:B:292:LEU:HD21	2.51	0.40
1:B:377:TRP:O	1:B:381:LEU:HD11	2.22	0.40
1:B:423:ASN:O	1:B:423:ASN:ND2	2.55	0.40
1:A:119:PHE:CE1	1:A:123:ARG:NH2	2.88	0.40
1:A:121:LYS:O	1:A:124:GLY:N	2.52	0.40
1:A:264:GLY:O	1:A:265:ALA:O	2.39	0.40
1:A:281:THR:HG21	1:B:315:LYS:HZ2	1.77	0.40
1:A:35:ILE:O	1:A:36:SER:C	2.57	0.40
1:A:383:SER:HB3	1:A:403:ILE:HA	2.03	0.40
1:A:420:TRP:O	1:A:421:TYR:C	2.60	0.40
1:B:127:VAL:HG13	1:B:181:ILE:O	2.22	0.40
1:B:312:LYS:O	1:B:315:LYS:N	2.54	0.40
1:B:331:ASP:O	1:B:332:VAL:CB	2.70	0.40
1:A:298:GLU:O	1:A:300:ILE:N	2.54	0.40
1:A:377:TRP:O	1:A:381:LEU:HD11	2.21	0.40
1:A:397:LYS:N	1:A:400:MET:CE	2.85	0.40
1:A:419:GLU:HG3	1:A:419:GLU:O	2.21	0.40
1:B:329:LEU:HD22	1:B:392:PRO:CG	2.51	0.40
1:B:349:LEU:N	1:B:352:ILE:HD12	2.37	0.40
1:B:380:ALA:O	1:B:381:LEU:CG	2.70	0.40
1:B:47:LEU:C	1:B:49:ALA:H	2.24	0.40
1:A:127:VAL:HG13	1:A:181:ILE:O	2.22	0.40
1:A:313:ILE:HG21	1:A:335:GLN:NE2	2.37	0.40
1:B:333:TYR:O	1:B:337:ILE:HG22	2.21	0.40
1:B:83:GLY:CA	1:B:261:VAL:CG1	3.00	0.40
1:B:430:MET:HA	1:B:430:MET:CE	2.51	0.40

All (43) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:PRO:CB	1:B:362:PRO:CA[8_454]	1.18	1.02
1:A:362:PRO:CA	1:B:360:PRO:CB[8_454]	1.24	0.96
1:A:200:GLU:CB	1:B:203:LYS:CB[6_555]	1.41	0.79
1:A:203:LYS:CB	1:B:200:GLU:CB[6_555]	1.45	0.75
1:A:360:PRO:CB	1:B:362:PRO:CB[8_454]	1.57	0.63
1:A:362:PRO:CB	1:B:360:PRO:CB[8_454]	1.69	0.51
1:A:362:PRO:C	1:B:360:PRO:CB[8_454]	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:PRO:CB	1:B:362:PRO:C[8_454]	1.79	0.41
1:A:367:LEU:CD1	1:B:367:LEU:CD2[8_454]	1.83	0.37
1:A:207:ASP:CB	1:B:196:THR:CB[6_555]	1.85	0.35
1:A:196:THR:CB	1:B:207:ASP:CB[6_555]	1.85	0.35
1:A:200:GLU:O	1:B:200:GLU:O[6_555]	1.89	0.31
1:A:204:GLU:CB	1:B:197:LYS:CA[6_555]	1.90	0.30
1:A:367:LEU:CD2	1:B:367:LEU:CD1[8_454]	1.90	0.30
1:A:207:ASP:CB	1:B:196:THR:CG2[6_555]	1.92	0.28
1:A:197:LYS:CA	1:B:204:GLU:CB[6_555]	1.92	0.28
1:A:196:THR:CG2	1:B:207:ASP:CB[6_555]	1.93	0.27
1:A:204:GLU:N	1:B:200:GLU:CG[6_555]	2.03	0.17
1:A:200:GLU:CG	1:B:204:GLU:N[6_555]	2.03	0.17
1:A:41:VAL:CG1	1:B:41:VAL:CG1[6_554]	2.04	0.16
1:A:207:ASP:OD2	1:B:196:THR:OG1[6_555]	2.04	0.16
1:A:360:PRO:CA	1:B:362:PRO:CA[8_454]	2.04	0.16
1:A:196:THR:OG1	1:B:207:ASP:OD2[6_555]	2.07	0.13
1:A:207:ASP:CG	1:B:196:THR:OG1[6_555]	2.10	0.10
1:A:362:PRO:CA	1:B:360:PRO:CA[8_454]	2.10	0.10
1:A:207:ASP:OD2	1:B:196:THR:CB[6_555]	2.12	0.08
1:A:363:SER:N	1:B:360:PRO:CB[8_454]	2.12	0.08
1:A:196:THR:OG1	1:B:207:ASP:CG[6_555]	2.13	0.07
1:A:196:THR:CB	1:B:207:ASP:OD2[6_555]	2.13	0.07
1:A:204:GLU:CA	1:B:197:LYS:CA[6_555]	2.14	0.06
1:A:197:LYS:CA	1:B:204:GLU:CA[6_555]	2.14	0.06
1:A:200:GLU:C	1:B:200:GLU:O[6_555]	2.15	0.05
1:A:200:GLU:O	1:B:200:GLU:C[6_555]	2.15	0.05
1:A:200:GLU:CG	1:B:200:GLU:O[6_555]	2.16	0.04
1:A:204:GLU:CB	1:B:197:LYS:CB[6_555]	2.16	0.04
1:A:197:LYS:CB	1:B:204:GLU:CB[6_555]	2.16	0.04
1:A:200:GLU:O	1:B:200:GLU:CG[6_555]	2.17	0.03
1:A:200:GLU:CA	1:B:203:LYS:CB[6_555]	2.17	0.03
1:A:204:GLU:CB	1:B:200:GLU:OE1[6_555]	2.19	0.01
1:A:200:GLU:OE2	1:B:200:GLU:OE2[6_555]	2.19	0.01
1:A:200:GLU:OE1	1:B:204:GLU:CB[6_555]	2.19	0.01
1:A:200:GLU:CB	1:B:203:LYS:CA[6_555]	2.19	0.01
1:A:203:LYS:CB	1:B:200:GLU:CA[6_555]	2.19	0.01

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	421/440 (96%)	294 (70%)	87 (21%)	40 (10%)	0	10
1	B	421/440 (96%)	293 (70%)	88 (21%)	40 (10%)	0	10
All	All	842/880 (96%)	587 (70%)	175 (21%)	80 (10%)	0	10

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	VAL
1	A	236	ALA
1	A	265	ALA
1	A	332	VAL
1	A	343	GLY
1	A	347	LYS
1	A	357	ILE
1	A	358	MET
1	A	359	LEU
1	A	369	ILE
1	A	373	LYS
1	A	379	ALA
1	A	380	ALA
1	B	63	VAL
1	B	236	ALA
1	B	265	ALA
1	B	332	VAL
1	B	343	GLY
1	B	347	LYS
1	B	357	ILE
1	B	358	MET
1	B	359	LEU
1	B	369	ILE
1	B	373	LYS
1	B	379	ALA

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Mol	Chain	Res	Type
1	B	380	ALA
1	A	15	GLY
1	A	16	SER
1	A	62	SER
1	A	106	GLY
1	A	110	THR
1	A	177	ASN
1	A	179	MET
1	A	284	ALA
1	A	292	LEU
1	A	300	ILE
1	A	329	LEU
1	A	356	GLY
1	A	368	LYS
1	A	404	ALA
1	B	15	GLY
1	B	16	SER
1	B	62	SER
1	B	106	GLY
1	B	110	THR
1	B	177	ASN
1	B	179	MET
1	B	284	ALA
1	B	292	LEU
1	B	300	ILE
1	B	329	LEU
1	B	356	GLY
1	B	368	LYS
1	B	404	ALA
1	A	195	GLU
1	A	316	LYS
1	B	195	GLU
1	B	316	LYS
1	A	84	GLY
1	A	285	LYS
1	A	315	LYS
1	A	397	LYS
1	B	84	GLY
1	B	285	LYS
1	B	315	LYS
1	B	397	LYS
1	A	18	PRO

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Mol	Chain	Res	Type
1	A	361	THR
1	A	381	LEU
1	A	431	VAL
1	B	18	PRO
1	B	361	THR
1	B	381	LEU
1	B	431	VAL
1	A	158	PRO
1	A	164	ILE
1	B	158	PRO
1	B	164	ILE
1	A	163	PRO
1	B	163	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	365/377 (97%)	340 (93%)	25 (7%)	16	44
1	B	365/377 (97%)	340 (93%)	25 (7%)	16	44
All	All	730/754 (97%)	680 (93%)	50 (7%)	16	44

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	16	SER
1	A	17	THR
1	A	59	LYS
1	A	72	SER
1	A	136	ARG
1	A	143	LEU
1	A	200	GLU
1	A	250	THR
1	A	283	ASN

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Mol	Chain	Res	Type
1	A	297	ILE
1	A	310	TYR
1	A	311	ASP
1	A	328	THR
1	A	331	ASP
1	A	349	LEU
1	A	357	ILE
1	A	359	LEU
1	A	361	THR
1	A	374	ILE
1	A	377	TRP
1	A	381	LEU
1	A	384	MET
1	A	386	TYR
1	A	423	ASN
1	B	1	MET
1	B	16	SER
1	B	17	THR
1	B	59	LYS
1	B	72	SER
1	B	136	ARG
1	B	143	LEU
1	B	200	GLU
1	B	250	THR
1	B	283	ASN
1	B	297	ILE
1	B	310	TYR
1	B	311	ASP
1	B	328	THR
1	B	331	ASP
1	B	349	LEU
1	B	357	ILE
1	B	359	LEU
1	B	361	THR
1	B	374	ILE
1	B	377	TRP
1	B	381	LEU
1	B	384	MET
1	B	386	TYR
1	B	423	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	31	GLN
1	A	40	ASN
1	A	91	ASN
1	A	148	ASN
1	A	160	ASN
1	A	190	HIS
1	A	224	GLN
1	A	234	HIS
1	A	235	GLN
1	A	283	ASN
1	A	350	GLN
1	A	351	HIS
1	B	4	ASN
1	B	31	GLN
1	B	40	ASN
1	B	91	ASN
1	B	148	ASN
1	B	160	ASN
1	B	190	HIS
1	B	224	GLN
1	B	234	HIS
1	B	235	GLN
1	B	283	ASN
1	B	350	GLN
1	B	351	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.