



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:08 am BST

PDB ID : 1NJ8
Title : Crystal Structure of Prolyl-tRNA Synthetase from Methanocaldococcus
janaschii
Authors : Kamtekar, S.; Kennedy, W.D.; Wang, J.; Stathopoulos, C.; Soll, D.; Steitz,
T.A.
Deposited on : 2002-12-30
Resolution : 3.20 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

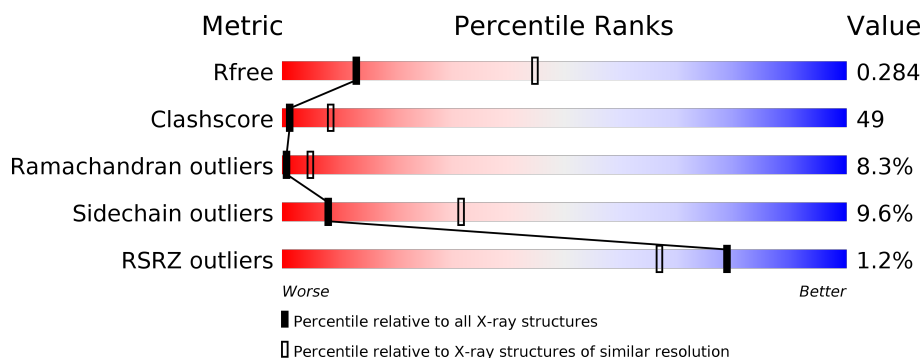
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	459	<div> <div>2%</div> <div> <div></div> <div>31%</div> <div>56%</div> <div>12%</div> <div>..</div> </div> </div>
1	B	459	<div> <div>%</div> <div> <div></div> <div>31%</div> <div>57%</div> <div>10%</div> <div>..</div> </div> </div>
1	C	459	<div> <div>%</div> <div> <div></div> <div>29%</div> <div>58%</div> <div>12%</div> <div>..</div> </div> </div>
1	D	459	<div> <div>2%</div> <div> <div></div> <div>31%</div> <div>58%</div> <div>10%</div> <div>.</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15182 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 Proline-tRNA Synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3772	2447	614	698	13			
1	B	456	Total	C	N	O	S	0	0	0
			3772	2447	614	698	13			
1	C	456	Total	C	N	O	S	0	0	0
			3772	2447	614	698	13			
1	D	456	Total	C	N	O	S	0	0	0
			3772	2447	614	698	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q58635
A	-2	SER	-	EXPRESSION TAG	UNP Q58635
A	-1	HIS	-	EXPRESSION TAG	UNP Q58635
A	0	MET	-	EXPRESSION TAG	UNP Q58635
A	1	LEU	MET	CLONING ARTIFACT	UNP Q58635
B	-3	GLY	-	EXPRESSION TAG	UNP Q58635
B	-2	SER	-	EXPRESSION TAG	UNP Q58635
B	-1	HIS	-	EXPRESSION TAG	UNP Q58635
B	0	MET	-	EXPRESSION TAG	UNP Q58635
B	1	LEU	MET	CLONING ARTIFACT	UNP Q58635
C	-3	GLY	-	EXPRESSION TAG	UNP Q58635
C	-2	SER	-	EXPRESSION TAG	UNP Q58635
C	-1	HIS	-	EXPRESSION TAG	UNP Q58635
C	0	MET	-	EXPRESSION TAG	UNP Q58635
C	1	LEU	MET	CLONING ARTIFACT	UNP Q58635
D	-3	GLY	-	EXPRESSION TAG	UNP Q58635
D	-2	SER	-	EXPRESSION TAG	UNP Q58635
D	-1	HIS	-	EXPRESSION TAG	UNP Q58635
D	0	MET	-	EXPRESSION TAG	UNP Q58635
D	1	LEU	MET	CLONING ARTIFACT	UNP Q58635

- Molecule 2 is water.

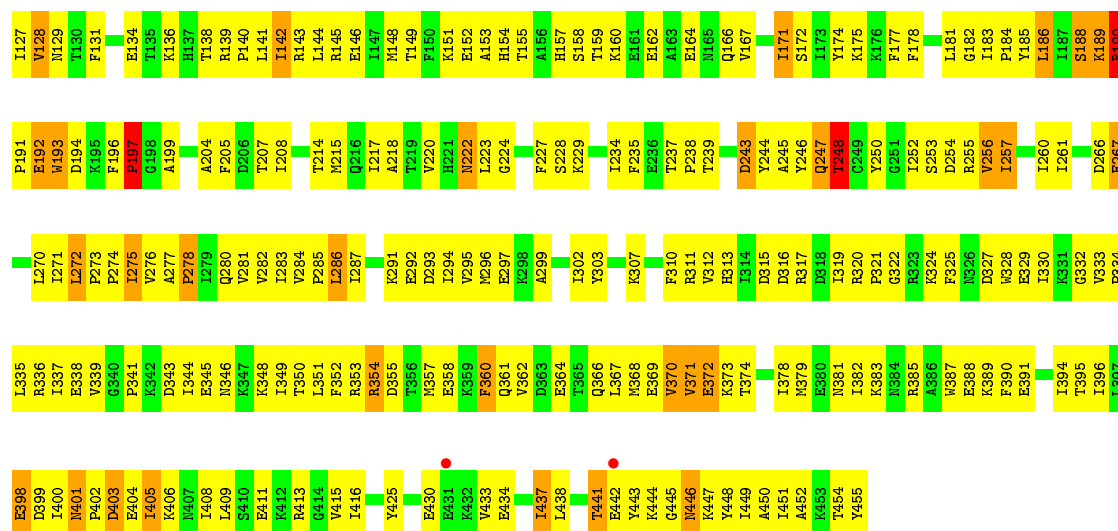
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	35	Total 35	O 35	0	0
2	B	16	Total 16	O 16	0	0
2	C	25	Total 25	O 25	0	0
2	D	18	Total 18	O 18	0	0

3 Residue-property plots

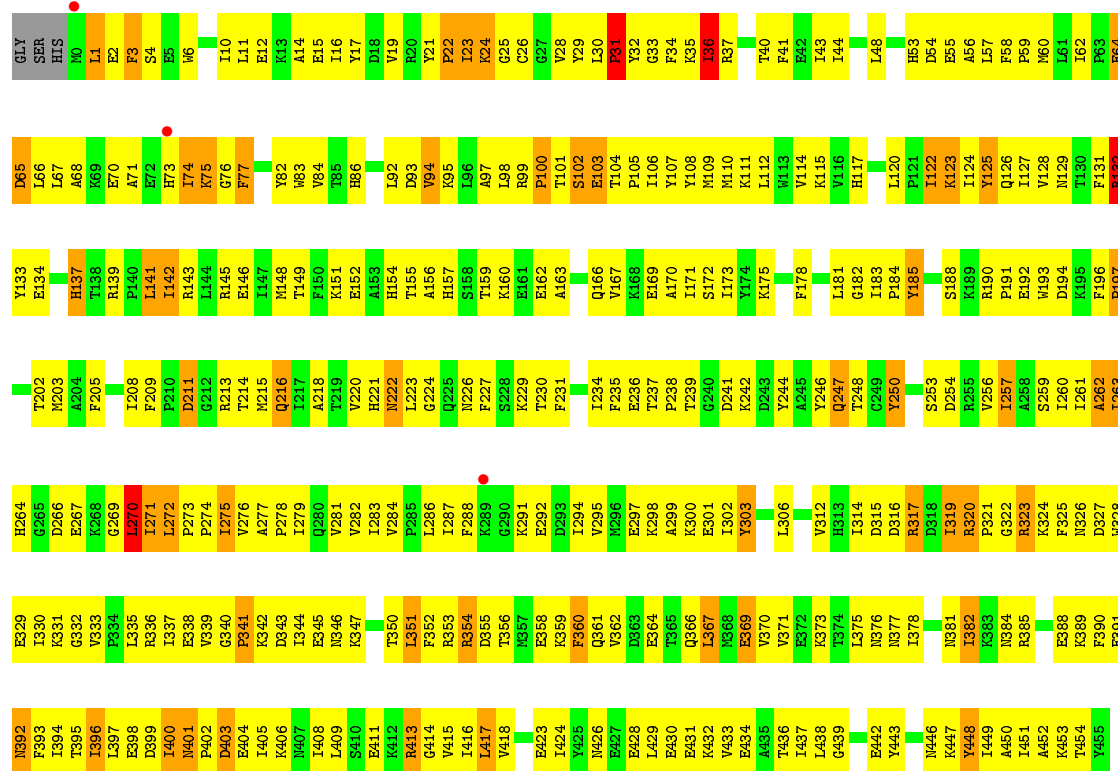
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Proline-tRNA Synthetase

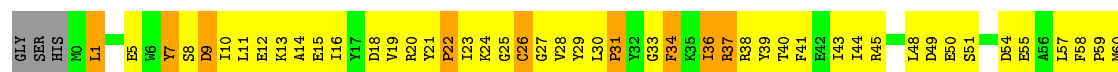




• Molecule 1: Proline-tRNA Synthetase



• Molecule 1: Proline-tRNA Synthetase



T395	T396	T397	E398	D399	I400	M401	P402	D403	E404	I405	K406	M407	I408	L409	E410	E411	K412	R413	G414	V415	I416		Y425		L426	E430	E431	K432	V433	V434	A435	T436	L437	L438		T441	E442	Y443	K444	G445	M446	K447	Y448	I449	A450	I451	A452	K453	T454	Y455												
V333	P334	L335	R336	I337	E338	V339	G340	P341	K342	D343	I344	F345	I346	K347	K348	T349	T350	L351	F352	R353	K354	D355	T356	K357	E358	K359	F360	Q361	V362	D363	E364	T365	Q366	L367	K368	K369	V370	V371	E372	K373	T374		I378	K379	E380	I381	I382	K383	M384	K385	K386	W387	E388	K389	F390	E391	M392	F393				
A262		D266	E267		L270	I271	L272	P273	P274	I275	V276	A277	P278	I279	Q280	V281	V282	I283	V284	T285	L286	I287		K291	E292	I293	L294	V295	M296	E297		T302	Y303		K307		F310	K311	V312	K313	I314	D315	D316	K317	D318	I319	K320	K321	G322	K323	K324	F325	M326	K327	K328	E329	I330	K331	G332			
K190	P191	E192	W193	D194	K195	F196	P197	G198	A199		T202	W203	A204	P205	D206	T207	L208		T214	M215	Q216	I217	A218	T219	V220	H221	N222	L223	G224	Q225	N226	P227	S228	K229		I234	F235	E236	T237	P238		D243	Y244	A245	Y246	Q247	T248	C249	G251	L252	S253	D254	R255	V256	I257		L260	T261				
L61	Q126	I127	V128	M129	T130	F131		E134	T135	K136	H137	T138	R139	P140	L141	I142	R143	L144	R145	E146	M147	M148	T149	F150		K151	E152	A153	H154	T155	A156	H157	S158	T159	K160	E161	E162	A163	E164	M165	Q166	V167		Y107	Y108	M109	M110	K111	L112	W113	V114	K115	V116	H117	T118	D119	L120	P121	I122	K123	I124	Y125

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.94Å 104.84Å 91.75Å 90.00° 93.63° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 29.81 – 3.16	Depositor EDS
% Data completeness (in resolution range)	87.0 (20.00-3.20) 84.9 (29.81-3.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	720.88 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.301 0.223 , 0.284	Depositor DCC
R_{free} test set	2974 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	67.4	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15182	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.44	0/3860	0.71	3/5213 (0.1%)
1	B	0.40	0/3860	0.63	0/5213
1	C	0.44	0/3860	0.70	3/5213 (0.1%)
1	D	0.39	0/3860	0.63	0/5213
All	All	0.42	0/15440	0.67	6/20852 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	ARG	NE-CZ-NH2	-11.57	114.52	120.30
1	C	320	ARG	NE-CZ-NH1	-11.40	114.60	120.30
1	C	320	ARG	NE-CZ-NH2	11.27	125.94	120.30
1	A	320	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	C	320	ARG	CD-NE-CZ	5.36	131.10	123.60
1	A	320	ARG	CD-NE-CZ	5.23	130.93	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3772	0	3804	386	2
1	B	3772	0	3804	353	0
1	C	3772	0	3804	409	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3772	0	3804	363	1
2	A	35	0	0	2	0
2	B	16	0	0	1	0
2	C	25	0	0	6	0
2	D	18	0	0	3	0
All	All	15182	0	15216	1472	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

All (1472) 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:275:ILE:HD12	1:B:275:ILE:H	1.06	1.14
1:D:275:ILE:H	1:D:275:ILE:HD12	1.08	1.11
1:B:48:LEU:HD11	1:B:151:LYS:HD2	1.32	1.10
1:D:48:LEU:HD11	1:D:151:LYS:HD2	1.34	1.07
1:A:337:ILE:HG12	1:A:351:LEU:HD12	1.36	1.02
1:A:396:ILE:HD12	1:A:396:ILE:H	1.22	1.02
1:B:16:ILE:HD13	1:B:261:ILE:HD11	1.41	1.01
1:C:337:ILE:HG12	1:C:351:LEU:HD12	1.39	1.00
1:A:71:ALA:HA	1:A:75:LYS:HE2	1.42	1.00
1:C:71:ALA:HA	1:C:75:LYS:HE2	1.43	0.99
1:D:16:ILE:HD13	1:D:261:ILE:HD11	1.44	0.99
1:B:58:PHE:H	1:B:126:GLN:HE22	1.03	0.98
1:D:18:ASP:HB2	1:D:30:LEU:HD11	1.43	0.97
1:C:396:ILE:H	1:C:396:ILE:HD12	1.24	0.97
1:D:99:ARG:NH2	1:D:128:VAL:HB	1.79	0.97
1:D:58:PHE:H	1:D:126:GLN:HE22	1.07	0.96
1:B:10:ILE:HD11	1:B:270:LEU:HB2	1.48	0.96
1:D:10:ILE:HD11	1:D:270:LEU:HB2	1.48	0.95
1:B:18:ASP:HB2	1:B:30:LEU:HD11	1.48	0.95
1:D:286:LEU:H	1:D:286:LEU:HD12	1.29	0.95
1:B:99:ARG:NH2	1:B:128:VAL:HB	1.83	0.93
1:C:430:GLU:HG3	1:C:437:ILE:HG12	1.51	0.92
1:B:286:LEU:HD12	1:B:286:LEU:H	1.32	0.92
1:A:430:GLU:HG3	1:A:437:ILE:HG12	1.51	0.91
1:D:141:LEU:H	1:D:144:LEU:HD21	1.35	0.91
1:D:83:TRP:CE3	1:D:95:LYS:HE2	2.03	0.91
1:D:271:ILE:HG12	1:D:354:ARG:NH1	1.85	0.91
1:D:190:ARG:HH11	1:D:204:ALA:HB3	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:TYR:HD2	1:D:84:VAL:HG11	1.35	0.90
1:B:141:LEU:H	1:B:144:LEU:HD21	1.36	0.90
1:B:275:ILE:H	1:B:275:ILE:CD1	1.82	0.90
1:D:403:ASP:HA	1:D:406:LYS:HD3	1.51	0.90
1:B:190:ARG:HH11	1:B:204:ALA:HB3	1.36	0.90
1:B:83:TRP:CE3	1:B:95:LYS:HE2	2.06	0.89
1:D:275:ILE:H	1:D:275:ILE:CD1	1.84	0.88
1:B:362:VAL:HG11	1:B:370:VAL:HG21	1.56	0.88
1:B:271:ILE:HG12	1:B:354:ARG:NH1	1.87	0.88
1:B:403:ASP:HA	1:B:406:LYS:HD3	1.53	0.88
1:A:82:TYR:HD2	1:B:84:VAL:HG11	1.37	0.87
1:D:127:ILE:HG12	1:D:151:LYS:HG3	1.57	0.87
1:A:10:ILE:HD11	1:A:270:LEU:N	1.90	0.87
1:B:127:ILE:HG12	1:B:151:LYS:HG3	1.57	0.87
1:D:362:VAL:HG11	1:D:370:VAL:HG21	1.57	0.87
1:A:360:PHE:HD2	1:A:360:PHE:H	1.22	0.86
1:A:101:THR:HG23	1:A:102:SER:H	1.41	0.86
1:C:101:THR:HG23	1:C:102:SER:H	1.41	0.85
1:C:306:LEU:HD21	1:C:371:VAL:HG21	1.55	0.85
1:D:336:ARG:HB3	1:D:352:PHE:HB3	1.57	0.85
1:C:360:PHE:H	1:C:360:PHE:HD2	1.22	0.85
1:C:256:VAL:HG23	1:C:257:ILE:H	1.42	0.85
1:C:275:ILE:H	1:C:275:ILE:HD12	1.41	0.85
1:B:275:ILE:HD12	1:B:275:ILE:N	1.91	0.84
1:B:389:LYS:NZ	1:B:389:LYS:HB3	1.93	0.84
1:B:58:PHE:H	1:B:126:GLN:NE2	1.74	0.84
1:C:10:ILE:HD11	1:C:270:LEU:N	1.94	0.83
1:A:70:GLU:HG2	1:A:77:PHE:CE2	2.13	0.83
1:D:275:ILE:HD12	1:D:275:ILE:N	1.93	0.83
1:B:336:ARG:HB3	1:B:352:PHE:HB3	1.59	0.82
1:D:389:LYS:HB3	1:D:389:LYS:NZ	1.95	0.82
1:A:275:ILE:HD12	1:A:275:ILE:H	1.43	0.82
1:D:167:VAL:HG13	1:D:220:VAL:HG11	1.61	0.81
1:A:282:VAL:HG23	1:A:333:VAL:HG11	1.61	0.81
1:A:306:LEU:HD21	1:A:371:VAL:HG21	1.60	0.81
1:A:256:VAL:HG23	1:A:257:ILE:H	1.46	0.81
1:C:55:GLU:HB2	1:C:125:TYR:CZ	2.16	0.81
1:C:70:GLU:HG2	1:C:77:PHE:CE2	2.15	0.80
1:B:413:ARG:HB2	1:B:413:ARG:NH1	1.96	0.80
1:D:413:ARG:NH1	1:D:413:ARG:HB2	1.96	0.80
1:B:286:LEU:HD11	1:B:338:GLU:HB3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:VAL:HG13	1:B:220:VAL:HG11	1.62	0.79
1:A:106:ILE:HD12	1:A:154:HIS:CD2	2.18	0.79
1:D:58:PHE:H	1:D:126:GLN:NE2	1.80	0.79
1:D:33:GLY:O	1:D:36:ILE:HG22	1.83	0.79
1:B:33:GLY:O	1:B:36:ILE:HG22	1.83	0.79
1:D:405:ILE:O	1:D:408:ILE:HG22	1.83	0.79
1:A:55:GLU:HB2	1:A:125:TYR:CZ	2.18	0.79
1:A:275:ILE:HD12	1:A:275:ILE:N	1.97	0.79
1:A:99:ARG:NH2	1:A:128:VAL:HB	1.98	0.79
1:D:36:ILE:HA	1:D:278:PRO:HG3	1.64	0.78
1:A:10:ILE:HD11	1:A:270:LEU:H	1.48	0.78
1:C:371:VAL:O	1:C:375:LEU:HB2	1.83	0.78
1:C:353:ARG:HB3	1:C:355:ASP:OD2	1.83	0.78
1:A:371:VAL:O	1:A:375:LEU:HB2	1.84	0.77
1:A:223:LEU:HD13	1:A:227:PHE:CD2	2.18	0.77
1:C:64:GLU:HG2	1:C:95:LYS:HB2	1.65	0.77
1:C:106:ILE:HD12	1:C:154:HIS:CD2	2.19	0.77
1:C:99:ARG:NH2	1:C:128:VAL:HB	2.00	0.77
1:B:405:ILE:O	1:B:408:ILE:HG22	1.85	0.77
1:D:286:LEU:HD11	1:D:338:GLU:HB3	1.68	0.76
1:A:32:TYR:O	1:A:36:ILE:HG22	1.84	0.76
1:C:275:ILE:N	1:C:275:ILE:HD12	1.99	0.76
1:B:155:THR:OG1	1:B:248:THR:HG23	1.84	0.76
1:D:208:ILE:HG12	1:D:214:THR:HG22	1.66	0.76
1:A:102:SER:HB3	1:A:152:GLU:OE2	1.85	0.75
1:D:283:ILE:HD12	1:D:283:ILE:N	2.01	0.75
1:B:283:ILE:N	1:B:283:ILE:HD12	2.01	0.75
1:C:181:LEU:HB3	1:C:183:ILE:CD1	2.16	0.75
1:D:155:THR:OG1	1:D:248:THR:HG23	1.85	0.75
1:D:16:ILE:HD13	1:D:261:ILE:CD1	2.16	0.75
1:A:22:PRO:HD3	1:B:108:TYR:CE2	2.21	0.75
1:B:16:ILE:HD13	1:B:261:ILE:CD1	2.15	0.75
1:A:159:THR:HG23	1:A:162:GLU:H	1.51	0.75
1:A:397:LEU:HD21	1:A:404:GLU:OE2	1.87	0.75
1:A:64:GLU:HG2	1:A:95:LYS:HB2	1.67	0.75
1:C:75:LYS:O	1:C:77:PHE:N	2.20	0.75
1:A:175:LYS:HG2	1:A:185:TYR:OH	1.86	0.75
1:D:349:ILE:HG22	1:D:362:VAL:O	1.87	0.75
1:B:208:ILE:HG12	1:B:214:THR:HG22	1.67	0.74
1:B:40:THR:HG21	1:B:257:ILE:HG22	1.68	0.74
1:C:159:THR:HG23	1:C:162:GLU:H	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:TYR:O	1:C:36:ILE:HG22	1.86	0.74
1:C:10:ILE:HD11	1:C:270:LEU:H	1.53	0.74
1:B:344:ILE:HD12	1:B:345:GLU:N	2.01	0.74
1:C:222:ASN:HD22	1:C:223:LEU:N	1.85	0.74
1:B:349:ILE:HG22	1:B:362:VAL:O	1.87	0.74
1:C:282:VAL:HG23	1:C:333:VAL:HG11	1.68	0.74
1:D:344:ILE:HD12	1:D:345:GLU:N	2.01	0.74
1:A:75:LYS:O	1:A:77:PHE:N	2.21	0.74
1:B:1:LEU:HD12	1:B:1:LEU:H	1.52	0.74
1:B:36:ILE:HA	1:B:278:PRO:HG3	1.69	0.74
1:D:127:ILE:HG12	1:D:151:LYS:CG	2.17	0.73
1:D:335:LEU:HD11	1:D:374:THR:HG21	1.69	0.73
1:B:127:ILE:HG12	1:B:151:LYS:CG	2.17	0.73
1:C:181:LEU:HB3	1:C:183:ILE:HD13	1.69	0.73
1:A:181:LEU:HB3	1:A:183:ILE:CD1	2.19	0.73
1:A:273:PRO:HG3	1:A:382:ILE:HD11	1.71	0.73
1:C:175:LYS:HG2	1:C:185:TYR:OH	1.88	0.73
1:D:10:ILE:CD1	1:D:270:LEU:HB2	2.19	0.73
1:D:24:LYS:HG3	1:D:138:THR:HG23	1.70	0.73
1:A:222:ASN:HD22	1:A:223:LEU:N	1.86	0.72
1:B:10:ILE:CD1	1:B:270:LEU:HB2	2.19	0.72
1:A:329:GLU:HG3	1:A:354:ARG:CD	2.19	0.72
1:A:92:LEU:C	1:A:94:VAL:H	1.92	0.72
1:A:101:THR:O	1:A:102:SER:HB2	1.88	0.72
1:A:353:ARG:HB3	1:A:355:ASP:OD2	1.88	0.72
1:D:1:LEU:HD12	1:D:1:LEU:H	1.53	0.72
1:D:40:THR:HG21	1:D:257:ILE:HG22	1.70	0.72
1:C:101:THR:O	1:C:102:SER:HB2	1.89	0.72
1:C:22:PRO:HD3	1:D:108:TYR:CE2	2.24	0.72
1:C:92:LEU:C	1:C:94:VAL:H	1.91	0.72
1:B:281:VAL:HB	1:B:312:VAL:HG12	1.69	0.71
1:C:275:ILE:H	1:C:275:ILE:CD1	2.02	0.71
1:D:127:ILE:HA	1:D:151:LYS:HA	1.71	0.71
1:D:270:LEU:O	1:D:332:GLY:HA2	1.90	0.71
1:A:100:PRO:HG2	1:A:101:THR:H	1.56	0.71
1:B:181:LEU:HB3	1:B:183:ILE:HD12	1.72	0.71
1:B:24:LYS:HG3	1:B:138:THR:HG23	1.71	0.71
1:C:223:LEU:HD13	1:C:227:PHE:CD2	2.25	0.71
1:C:295:VAL:HG13	1:C:339:VAL:HG12	1.73	0.71
1:C:329:GLU:HG3	1:C:354:ARG:CD	2.20	0.71
1:D:182:GLY:HA2	1:D:383:LYS:HG3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LEU:HD21	1:A:416:ILE:HG12	1.73	0.71
1:B:127:ILE:HA	1:B:151:LYS:HA	1.72	0.71
1:C:100:PRO:HG2	1:C:101:THR:H	1.56	0.71
1:A:401:ASN:HD22	1:A:401:ASN:C	1.94	0.71
1:B:43:ILE:HD11	1:B:275:ILE:HG21	1.73	0.71
1:C:256:VAL:HG23	1:C:257:ILE:N	2.05	0.71
1:C:397:LEU:HD21	1:C:404:GLU:OE2	1.91	0.71
1:A:275:ILE:CD1	1:A:275:ILE:H	2.03	0.70
1:A:101:THR:HG23	1:A:102:SER:N	2.06	0.70
1:B:102:SER:HB3	1:B:152:GLU:OE1	1.91	0.70
1:A:378:ILE:O	1:A:382:ILE:HG23	1.92	0.70
1:C:48:LEU:O	1:C:53:HIS:HB2	1.91	0.70
1:D:178:PHE:HE2	1:D:256:VAL:HG12	1.55	0.70
1:A:295:VAL:HG13	1:A:339:VAL:HG12	1.74	0.70
1:C:273:PRO:HG3	1:C:382:ILE:HD11	1.74	0.70
1:D:281:VAL:HB	1:D:312:VAL:HG12	1.73	0.70
1:C:102:SER:HB3	1:C:152:GLU:OE2	1.91	0.70
1:D:181:LEU:HB3	1:D:183:ILE:HD12	1.74	0.70
1:A:36:ILE:HD13	1:A:36:ILE:O	1.92	0.69
1:B:182:GLY:HA2	1:B:383:LYS:HG3	1.74	0.69
1:C:378:ILE:O	1:C:382:ILE:HG23	1.92	0.69
1:C:401:ASN:C	1:C:401:ASN:HD22	1.95	0.69
1:A:342:LYS:O	1:A:342:LYS:HD3	1.92	0.69
1:B:253:SER:O	1:B:256:VAL:HG22	1.91	0.69
1:B:272:LEU:HD11	1:B:278:PRO:HD2	1.73	0.69
1:B:48:LEU:CD1	1:B:151:LYS:HD2	2.18	0.69
1:C:35:LYS:C	1:C:37:ARG:H	1.94	0.69
1:B:270:LEU:O	1:B:332:GLY:HA2	1.92	0.69
1:D:24:LYS:HG3	1:D:138:THR:CG2	2.23	0.69
1:B:276:VAL:O	1:B:278:PRO:HD3	1.93	0.69
1:C:36:ILE:O	1:C:36:ILE:HD13	1.93	0.69
1:A:396:ILE:H	1:A:396:ILE:CD1	1.97	0.69
1:D:102:SER:HB3	1:D:152:GLU:OE1	1.93	0.69
1:A:181:LEU:HB3	1:A:183:ILE:HD13	1.74	0.68
1:C:405:ILE:HA	1:C:408:ILE:HG22	1.75	0.68
1:A:110:MET:O	1:A:114:VAL:HG23	1.93	0.68
1:A:256:VAL:HG23	1:A:257:ILE:N	2.07	0.68
1:A:48:LEU:O	1:A:53:HIS:HB2	1.92	0.68
1:B:190:ARG:NH2	1:B:438:LEU:HD22	2.08	0.68
1:C:101:THR:HG23	1:C:102:SER:N	2.08	0.68
1:C:254:ASP:O	1:C:257:ILE:HG23	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:ILE:H	1:C:396:ILE:CD1	2.02	0.68
1:D:190:ARG:NH2	1:D:438:LEU:HD22	2.07	0.68
1:D:207:THR:CG2	1:D:215:MET:HB3	2.23	0.68
1:D:43:ILE:HD11	1:D:275:ILE:HG21	1.75	0.68
1:A:156:ALA:HB2	1:A:247:GLN:HE22	1.58	0.68
1:A:405:ILE:HA	1:A:408:ILE:HG22	1.75	0.68
1:A:329:GLU:HG3	1:A:354:ARG:HD2	1.75	0.68
1:C:342:LYS:HD3	1:C:342:LYS:O	1.94	0.68
1:C:142:ILE:HG23	1:C:215:MET:HE2	1.74	0.68
1:C:178:PHE:CZ	1:C:218:ALA:HB2	2.29	0.68
1:D:140:PRO:O	1:D:142:ILE:HD12	1.93	0.68
1:B:181:LEU:HB3	1:B:183:ILE:CD1	2.24	0.68
1:B:343:ASP:HB3	1:B:348:LYS:O	1.94	0.68
1:C:110:MET:O	1:C:114:VAL:HG23	1.94	0.68
1:A:178:PHE:CZ	1:A:218:ALA:HB2	2.29	0.67
1:D:343:ASP:HB3	1:D:348:LYS:O	1.94	0.67
1:B:335:LEU:HD11	1:B:374:THR:HG21	1.74	0.67
1:C:409:LEU:HD21	1:C:416:ILE:HG12	1.77	0.67
1:D:205:PHE:HB2	1:D:218:ALA:HB3	1.76	0.67
1:C:443:TYR:H	1:C:448:TYR:HE1	1.43	0.67
1:D:151:LYS:HE2	1:D:151:LYS:O	1.95	0.67
1:A:67:LEU:HD11	1:A:77:PHE:HE2	1.60	0.67
1:B:24:LYS:HG3	1:B:138:THR:CG2	2.25	0.67
1:D:48:LEU:CD1	1:D:151:LYS:HD2	2.19	0.67
1:D:253:SER:O	1:D:256:VAL:HG22	1.93	0.67
1:D:272:LEU:HD11	1:D:278:PRO:HD2	1.74	0.67
1:B:101:THR:HG23	1:B:103:GLU:HG2	1.75	0.67
1:B:413:ARG:HB2	1:B:413:ARG:HH11	1.59	0.66
1:C:156:ALA:HB2	1:C:247:GLN:HE22	1.60	0.66
1:A:288:PHE:O	1:A:292:GLU:HG3	1.96	0.66
1:A:326:ASN:O	1:A:330:ILE:HG13	1.95	0.66
1:D:413:ARG:HB2	1:D:413:ARG:HH11	1.59	0.66
1:A:48:LEU:HD11	1:A:151:LYS:HD2	1.77	0.66
1:A:74:ILE:HG22	1:A:74:ILE:O	1.96	0.66
1:A:92:LEU:O	1:A:94:VAL:HG23	1.94	0.66
1:C:270:LEU:O	1:C:271:ILE:HG13	1.96	0.66
1:B:205:PHE:HB2	1:B:218:ALA:HB3	1.77	0.66
1:C:48:LEU:HD11	1:C:151:LYS:HD2	1.77	0.66
1:B:167:VAL:HG13	1:B:220:VAL:CG1	2.26	0.66
1:C:10:ILE:CD1	1:C:270:LEU:HD13	2.25	0.66
1:D:167:VAL:HG13	1:D:220:VAL:CG1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ARG:HB2	1:C:413:ARG:NH1	2.10	0.66
1:C:92:LEU:O	1:C:94:VAL:HG23	1.95	0.66
1:B:178:PHE:HE2	1:B:256:VAL:HG12	1.61	0.66
1:C:288:PHE:O	1:C:292:GLU:HG3	1.96	0.66
1:D:181:LEU:HB3	1:D:183:ILE:CD1	2.25	0.66
1:A:413:ARG:HB2	1:A:413:ARG:NH1	2.11	0.66
1:C:397:LEU:HD23	1:C:399:ASP:O	1.96	0.66
1:C:35:LYS:O	1:C:37:ARG:N	2.26	0.66
1:A:338:GLU:HB2	1:A:350:THR:HG23	1.78	0.65
1:A:353:ARG:O	1:A:355:ASP:N	2.30	0.65
1:B:207:THR:CG2	1:B:215:MET:HB3	2.26	0.65
1:C:329:GLU:HG3	1:C:354:ARG:HD2	1.77	0.65
1:B:140:PRO:O	1:B:142:ILE:HD12	1.96	0.65
1:C:353:ARG:O	1:C:355:ASP:N	2.30	0.65
1:D:353:ARG:HD3	1:D:358:GLU:OE2	1.96	0.65
1:A:142:ILE:HG23	1:A:215:MET:HE2	1.77	0.65
1:B:353:ARG:HD3	1:B:358:GLU:OE2	1.96	0.65
1:C:73:HIS:O	1:C:74:ILE:HG13	1.96	0.65
1:B:389:LYS:HB3	1:B:389:LYS:HZ3	1.62	0.65
1:C:353:ARG:C	1:C:355:ASP:H	2.00	0.65
1:D:445:GLY:O	1:D:447:LYS:N	2.30	0.65
1:B:151:LYS:O	1:B:151:LYS:HE2	1.97	0.65
1:A:443:TYR:H	1:A:448:TYR:HE1	1.45	0.65
1:D:36:ILE:CA	1:D:278:PRO:HG3	2.26	0.65
1:A:35:LYS:C	1:A:37:ARG:H	1.99	0.65
1:A:73:HIS:O	1:A:74:ILE:HG13	1.97	0.65
1:D:101:THR:HG23	1:D:103:GLU:HG2	1.77	0.65
1:D:283:ILE:HA	1:D:337:ILE:HB	1.78	0.65
1:B:283:ILE:HD12	1:B:283:ILE:H	1.62	0.64
1:C:16:ILE:HD11	1:C:270:LEU:HD21	1.79	0.64
1:C:74:ILE:O	1:C:74:ILE:HG22	1.98	0.64
1:B:445:GLY:O	1:B:447:LYS:N	2.31	0.64
1:C:82:TYR:CD2	1:D:84:VAL:HG11	2.26	0.64
1:B:415:VAL:HA	1:B:452:ALA:HB2	1.79	0.64
1:C:67:LEU:HD11	1:C:77:PHE:HE2	1.63	0.64
1:B:149:THR:HB	1:B:254:ASP:OD2	1.97	0.64
1:C:395:THR:HB	1:C:416:ILE:CD1	2.28	0.64
1:D:291:LYS:HB3	1:D:294:ILE:HG21	1.78	0.64
1:A:397:LEU:HD23	1:A:399:ASP:O	1.98	0.64
1:B:291:LYS:HB3	1:B:294:ILE:HG21	1.78	0.64
1:B:396:ILE:N	1:B:396:ILE:HD12	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:GLU:HB2	1:C:350:THR:HG23	1.80	0.64
1:D:220:VAL:HA	1:D:250:TYR:HB3	1.80	0.63
1:D:16:ILE:HD11	1:D:270:LEU:HD22	1.80	0.63
1:A:70:GLU:HG2	1:A:77:PHE:CZ	2.32	0.63
1:D:178:PHE:CE2	1:D:256:VAL:HG12	2.33	0.63
1:D:286:LEU:H	1:D:286:LEU:CD1	2.09	0.63
1:D:214:THR:OG1	1:D:454:THR:HG22	1.98	0.63
1:C:369:GLU:HG3	1:C:370:VAL:N	2.12	0.63
1:D:276:VAL:O	1:D:278:PRO:HD3	1.97	0.63
1:D:415:VAL:HA	1:D:452:ALA:HB2	1.80	0.63
1:A:337:ILE:HG12	1:A:351:LEU:CD1	2.20	0.63
1:C:10:ILE:C	1:C:12:GLU:H	2.02	0.63
1:B:142:ILE:HG22	1:B:143:ARG:N	2.13	0.63
1:B:64:GLU:HG2	1:B:83:TRP:CH2	2.33	0.63
1:D:396:ILE:N	1:D:396:ILE:HD12	2.14	0.63
1:A:58:PHE:H	1:A:126:GLN:HE22	1.46	0.63
1:B:214:THR:OG1	1:B:454:THR:HG22	1.99	0.63
1:B:220:VAL:HA	1:B:250:TYR:HB3	1.81	0.63
1:C:354:ARG:O	1:C:354:ARG:NE	2.32	0.63
1:D:350:THR:HA	1:D:361:GLN:HG2	1.81	0.63
1:A:55:GLU:HA	1:A:125:TYR:O	1.99	0.62
1:C:127:ILE:O	1:C:127:ILE:HG22	1.99	0.62
1:C:36:ILE:HG13	1:C:272:LEU:HD22	1.81	0.62
1:C:178:PHE:HZ	1:C:218:ALA:HB2	1.63	0.62
1:C:326:ASN:O	1:C:330:ILE:HG13	1.99	0.62
1:A:10:ILE:C	1:A:12:GLU:H	2.02	0.62
1:A:328:TRP:CZ3	1:A:331:LYS:HD2	2.35	0.62
1:C:58:PHE:HD1	1:C:126:GLN:NE2	1.97	0.62
1:D:283:ILE:HD12	1:D:283:ILE:H	1.64	0.62
1:A:178:PHE:HZ	1:A:218:ALA:HB2	1.62	0.62
1:A:353:ARG:C	1:A:355:ASP:H	2.03	0.62
1:B:178:PHE:CE2	1:B:217:ILE:HD12	2.35	0.62
1:A:82:TYR:CD2	1:B:84:VAL:HG11	2.28	0.62
1:C:323:ARG:O	1:C:327:ASP:N	2.25	0.62
1:D:190:ARG:HH21	1:D:438:LEU:HD22	1.64	0.62
1:C:10:ILE:HD13	1:C:270:LEU:HD13	1.82	0.62
1:D:389:LYS:HB3	1:D:389:LYS:HZ3	1.65	0.62
1:D:64:GLU:HG2	1:D:83:TRP:CH2	2.34	0.62
1:B:127:ILE:HG12	1:B:151:LYS:CB	2.29	0.62
1:C:58:PHE:H	1:C:126:GLN:HE22	1.48	0.62
1:C:360:PHE:N	1:C:360:PHE:HD2	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:ILE:HG12	1:D:151:LYS:CB	2.29	0.62
1:D:149:THR:HB	1:D:254:ASP:OD2	1.99	0.62
1:A:215:MET:HA	2:A:460:HOH:O	1.98	0.62
1:A:65:ASP:O	1:A:68:ALA:HB3	1.99	0.62
1:B:379:MET:O	1:B:382:ILE:HG12	2.00	0.62
1:C:208:ILE:HD11	1:C:415:VAL:HG12	1.81	0.62
1:C:1:LEU:HD13	1:C:6:TRP:HB2	1.81	0.62
1:C:70:GLU:HG2	1:C:77:PHE:CZ	2.34	0.62
1:D:379:MET:O	1:D:382:ILE:HG12	2.00	0.62
1:A:224:GLY:O	1:A:246:TYR:HA	2.00	0.62
1:A:254:ASP:O	1:A:257:ILE:HG23	2.00	0.62
1:A:395:THR:HB	1:A:416:ILE:CD1	2.30	0.62
1:A:1:LEU:HD13	1:A:6:TRP:HB2	1.81	0.62
1:B:291:LYS:HD2	1:B:291:LYS:N	2.14	0.62
1:D:142:ILE:HG22	1:D:143:ARG:N	2.13	0.62
1:A:369:GLU:HG3	1:A:370:VAL:N	2.14	0.61
1:B:322:GLY:HA2	1:B:325:PHE:HD2	1.63	0.61
1:D:191:PRO:HB2	1:D:193:TRP:CZ3	2.35	0.61
1:A:360:PHE:HD2	1:A:360:PHE:N	1.97	0.61
1:B:58:PHE:N	1:B:126:GLN:HE22	1.88	0.61
1:B:274:PRO:HD2	1:B:379:MET:HB2	1.81	0.61
1:A:142:ILE:HG22	1:A:143:ARG:N	2.13	0.61
1:A:328:TRP:HZ3	1:A:331:LYS:HD2	1.64	0.61
1:C:48:LEU:HD22	1:C:53:HIS:CD2	2.36	0.61
1:A:36:ILE:HG13	1:A:272:LEU:HD22	1.83	0.61
1:B:270:LEU:HB3	1:B:330:ILE:O	2.00	0.61
1:A:354:ARG:NE	1:A:354:ARG:O	2.33	0.61
1:A:48:LEU:HD22	1:A:53:HIS:CD2	2.36	0.61
1:B:16:ILE:HD11	1:B:270:LEU:HD22	1.82	0.61
1:B:36:ILE:CA	1:B:278:PRO:HG3	2.29	0.61
1:B:283:ILE:HA	1:B:337:ILE:HB	1.82	0.61
1:A:127:ILE:O	1:A:127:ILE:HG22	2.01	0.61
1:A:223:LEU:HD13	1:A:227:PHE:HD2	1.62	0.61
1:A:323:ARG:O	1:A:327:ASP:N	2.26	0.61
1:C:190:ARG:NH2	1:C:216:GLN:HE21	1.99	0.61
1:B:272:LEU:CD1	1:B:277:ALA:HA	2.29	0.61
1:B:286:LEU:CD1	1:B:286:LEU:H	2.11	0.61
1:A:211:ASP:OD2	1:A:213:ARG:HB2	2.01	0.61
1:B:373:LYS:HB2	1:B:373:LYS:NZ	2.16	0.61
1:B:123:LYS:HA	1:B:155:THR:HG22	1.82	0.61
1:B:178:PHE:CE2	1:B:256:VAL:HG12	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:LYS:NZ	1:D:373:LYS:HB2	2.16	0.61
1:A:21:TYR:HB3	1:A:26:CYS:O	2.00	0.61
1:A:270:LEU:O	1:A:271:ILE:HG13	2.01	0.61
1:B:43:ILE:HD11	1:B:275:ILE:CG2	2.31	0.61
1:C:211:ASP:OD2	1:C:213:ARG:HB2	2.01	0.61
1:D:256:VAL:HG23	1:D:257:ILE:H	1.66	0.61
1:C:337:ILE:HG12	1:C:351:LEU:CD1	2.23	0.60
1:C:55:GLU:HA	1:C:125:TYR:O	2.01	0.60
1:D:291:LYS:N	1:D:291:LYS:HD2	2.15	0.60
1:B:41:PHE:CE2	1:B:149:THR:HG22	2.36	0.60
1:C:157:HIS:CD2	1:C:163:ALA:HA	2.36	0.60
1:D:274:PRO:HD2	1:D:379:MET:HB2	1.83	0.60
1:B:190:ARG:HH21	1:B:438:LEU:HD22	1.65	0.60
1:D:43:ILE:HD11	1:D:275:ILE:CG2	2.31	0.60
1:D:322:GLY:HA2	1:D:325:PHE:HD2	1.64	0.60
1:B:191:PRO:HB2	1:B:193:TRP:CZ3	2.36	0.60
1:C:60:MET:HE1	1:C:129:ASN:OD1	2.01	0.60
1:C:55:GLU:HB2	1:C:125:TYR:CE1	2.35	0.60
1:A:55:GLU:HB2	1:A:125:TYR:CE1	2.35	0.60
1:B:75:LYS:O	1:B:77:PHE:HB3	2.02	0.60
1:D:237:THR:CG2	1:D:243:ASP:HB2	2.32	0.60
1:D:270:LEU:HB3	1:D:330:ILE:O	2.02	0.60
1:A:236:GLU:HG3	1:A:242:LYS:HE2	1.84	0.60
1:A:59:PRO:HG2	1:B:21:TYR:CD1	2.36	0.60
1:B:30:LEU:O	1:B:33:GLY:N	2.34	0.60
1:C:21:TYR:HB3	1:C:26:CYS:O	2.01	0.60
1:C:373:LYS:NZ	1:C:373:LYS:HB2	2.16	0.60
1:B:355:ASP:OD1	1:B:378:ILE:HA	2.00	0.60
1:C:124:ILE:HA	2:C:476:HOH:O	2.01	0.60
1:D:178:PHE:CE2	1:D:217:ILE:HD12	2.37	0.60
1:C:110:MET:HE2	1:C:122:ILE:HG13	1.82	0.60
1:A:320:ARG:NH1	1:A:322:GLY:HA3	2.17	0.60
1:B:237:THR:CG2	1:B:243:ASP:HB2	2.32	0.60
1:B:350:THR:HA	1:B:361:GLN:HG2	1.84	0.60
1:C:142:ILE:HG22	1:C:143:ARG:N	2.15	0.60
1:A:157:HIS:CD2	1:A:163:ALA:HA	2.37	0.59
1:A:275:ILE:CD1	1:A:275:ILE:N	2.65	0.59
1:A:388:GLU:OE1	1:C:108:TYR:HE1	1.85	0.59
1:D:104:THR:N	1:D:105:PRO:HD2	2.17	0.59
1:D:29:TYR:HE2	1:D:257:ILE:CD1	2.15	0.59
1:B:285:PRO:O	1:B:287:ILE:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:LYS:HA	1:D:244:TYR:CD2	2.37	0.59
1:B:196:PHE:CD1	1:B:197:PRO:HD2	2.37	0.59
1:A:190:ARG:NH2	1:A:216:GLN:HE21	2.00	0.59
1:C:328:TRP:HZ3	1:C:331:LYS:HD2	1.67	0.59
1:C:325:PHE:HB3	1:C:336:ARG:NH2	2.17	0.59
1:D:196:PHE:CD1	1:D:197:PRO:HD2	2.37	0.59
1:D:385:ARG:O	1:D:388:GLU:HB3	2.02	0.59
1:A:10:ILE:HD13	1:A:270:LEU:HD13	1.85	0.59
1:A:396:ILE:HD12	1:A:396:ILE:N	2.06	0.59
1:C:299:ALA:HB1	1:C:314:ILE:HD13	1.84	0.59
1:C:328:TRP:CZ3	1:C:331:LYS:HD2	2.38	0.59
1:A:102:SER:HB3	1:A:152:GLU:CD	2.22	0.59
1:B:229:LYS:HA	1:B:244:TYR:CD2	2.38	0.59
1:C:236:GLU:HG3	1:C:242:LYS:HE2	1.85	0.59
1:D:355:ASP:OD1	1:D:378:ILE:HA	2.02	0.59
1:A:401:ASN:C	1:A:401:ASN:ND2	2.53	0.59
1:A:66:LEU:H	1:A:66:LEU:HD12	1.67	0.59
1:B:127:ILE:CG1	1:B:151:LYS:HG3	2.32	0.59
1:D:60:MET:HA	1:D:99:ARG:HD3	1.85	0.59
1:D:75:LYS:O	1:D:77:PHE:HB3	2.03	0.59
1:A:60:MET:HE1	1:A:129:ASN:OD1	2.02	0.59
1:B:69:LYS:C	1:B:71:ALA:H	2.04	0.59
1:D:41:PHE:CE2	1:D:149:THR:HG22	2.38	0.59
1:D:69:LYS:C	1:D:71:ALA:H	2.05	0.59
1:A:284:VAL:O	1:A:286:LEU:HD12	2.02	0.59
1:C:102:SER:HB3	1:C:152:GLU:CD	2.23	0.59
1:A:10:ILE:CD1	1:A:270:LEU:HD13	2.33	0.59
1:B:256:VAL:HG23	1:B:257:ILE:H	1.68	0.59
1:C:350:THR:HB	1:C:361:GLN:HG2	1.85	0.59
1:C:65:ASP:O	1:C:68:ALA:HB3	2.02	0.59
1:D:58:PHE:N	1:D:126:GLN:HE22	1.90	0.59
1:D:92:LEU:C	1:D:94:VAL:H	2.07	0.58
1:A:114:VAL:HG22	1:A:122:ILE:HD11	1.85	0.58
1:B:116:VAL:HG23	1:B:118:THR:HB	1.84	0.58
1:C:59:PRO:HG2	1:D:21:TYR:CD1	2.38	0.58
1:D:123:LYS:HA	1:D:155:THR:HG22	1.84	0.58
1:D:127:ILE:CG1	1:D:151:LYS:HG3	2.32	0.58
1:D:67:LEU:O	1:D:70:GLU:HB3	2.02	0.58
1:B:266:ASP:CG	1:B:271:ILE:HD11	2.23	0.58
1:C:395:THR:HB	1:C:416:ILE:HD12	1.86	0.58
1:D:282:VAL:HG23	1:D:333:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:THR:HG23	1:B:243:ASP:HB2	1.86	0.58
1:C:114:VAL:HG22	1:C:122:ILE:HD11	1.86	0.58
1:A:58:PHE:H	1:A:126:GLN:NE2	2.00	0.58
1:A:350:THR:HB	1:A:361:GLN:HG2	1.86	0.58
1:A:430:GLU:C	1:A:432:LYS:H	2.04	0.58
1:B:385:ARG:O	1:B:388:GLU:HB3	2.03	0.58
1:B:399:ASP:OD2	1:B:401:ASN:HB2	2.03	0.58
1:C:401:ASN:ND2	1:C:401:ASN:C	2.54	0.58
1:D:190:ARG:NH1	1:D:204:ALA:HB3	2.14	0.58
1:D:389:LYS:HZ2	1:D:389:LYS:HB3	1.68	0.58
1:B:67:LEU:O	1:B:70:GLU:HB3	2.02	0.58
1:B:29:TYR:HE2	1:B:257:ILE:CD1	2.17	0.58
1:B:402:PRO:HG2	1:B:403:ASP:H	1.67	0.58
1:A:373:LYS:NZ	1:A:373:LYS:HB2	2.18	0.58
1:A:184:PRO:HB3	1:A:390:PHE:CG	2.39	0.58
1:B:181:LEU:HD22	1:B:260:ILE:HD11	1.86	0.58
1:C:351:LEU:HB2	1:C:360:PHE:CE2	2.38	0.58
1:D:399:ASP:OD2	1:D:401:ASN:HB2	2.04	0.58
1:A:110:MET:HE2	1:A:122:ILE:HG13	1.85	0.58
1:A:344:ILE:HD12	1:A:345:GLU:N	2.19	0.58
1:A:54:ASP:O	1:A:124:ILE:HG13	2.04	0.58
1:B:175:LYS:HG3	1:B:185:TYR:OH	2.04	0.58
1:C:284:VAL:O	1:C:286:LEU:HD12	2.03	0.58
1:C:54:ASP:O	1:C:124:ILE:HG13	2.04	0.58
1:D:266:ASP:CG	1:D:271:ILE:HD11	2.24	0.58
1:C:159:THR:HG23	1:C:162:GLU:HB2	1.85	0.57
1:D:116:VAL:HG23	1:D:118:THR:HB	1.85	0.57
1:A:437:ILE:HG22	1:A:439:GLY:H	1.69	0.57
1:C:205:PHE:HB2	1:C:218:ALA:HB3	1.85	0.57
1:C:224:GLY:O	1:C:246:TYR:HA	2.04	0.57
1:C:184:PRO:HB3	1:C:390:PHE:CG	2.39	0.57
1:A:229:LYS:HA	1:A:244:TYR:CD2	2.40	0.57
1:A:298:LYS:O	1:A:302:ILE:HG13	2.04	0.57
1:C:396:ILE:HD12	1:C:396:ILE:N	2.07	0.57
1:C:41:PHE:O	1:C:44:ILE:HG22	2.04	0.57
1:D:402:PRO:HG2	1:D:403:ASP:H	1.68	0.57
1:A:34:PHE:O	1:A:37:ARG:HB3	2.04	0.57
1:D:237:THR:HG23	1:D:243:ASP:HB2	1.87	0.57
1:D:395:THR:HB	1:D:416:ILE:CD1	2.33	0.57
1:A:331:LYS:NZ	2:A:485:HOH:O	2.27	0.57
1:B:190:ARG:NH1	1:B:204:ALA:HB3	2.14	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ILE:HD12	1:C:234:ILE:C	2.25	0.57
1:C:391:GLU:HA	1:C:394:ILE:HD12	1.84	0.57
1:A:123:LYS:HA	1:A:155:THR:HA	1.87	0.57
1:A:351:LEU:HB2	1:A:360:PHE:CE2	2.38	0.57
1:C:58:PHE:H	1:C:126:GLN:NE2	2.02	0.57
1:D:18:ASP:CB	1:D:30:LEU:HD11	2.29	0.57
1:D:92:LEU:O	1:D:94:VAL:N	2.38	0.57
1:B:104:THR:N	1:B:105:PRO:HD2	2.20	0.57
1:C:222:ASN:C	1:C:222:ASN:HD22	2.05	0.57
1:A:35:LYS:O	1:A:37:ARG:N	2.35	0.57
1:B:122:ILE:O	1:B:122:ILE:HG13	2.05	0.57
1:B:60:MET:HA	1:B:99:ARG:HD3	1.87	0.57
1:C:319:ILE:HG13	1:C:320:ARG:N	2.20	0.57
1:D:449:ILE:O	1:D:449:ILE:HG22	2.04	0.57
1:A:234:ILE:C	1:A:234:ILE:HD12	2.25	0.57
1:A:405:ILE:HG23	1:A:416:ILE:HG21	1.86	0.57
1:D:272:LEU:CD1	1:D:277:ALA:HA	2.34	0.57
1:A:319:ILE:HG13	1:A:320:ARG:N	2.20	0.56
1:A:395:THR:HB	1:A:416:ILE:HD12	1.88	0.56
1:B:353:ARG:HB3	1:B:355:ASP:OD2	2.03	0.56
1:B:395:THR:HG21	1:B:408:ILE:HD11	1.87	0.56
1:C:430:GLU:C	1:C:432:LYS:H	2.06	0.56
1:D:175:LYS:HG3	1:D:185:TYR:OH	2.05	0.56
1:D:395:THR:HG21	1:D:408:ILE:HD11	1.87	0.56
1:A:41:PHE:HD2	1:A:127:ILE:HD13	1.70	0.56
1:A:430:GLU:HG3	1:A:437:ILE:CG1	2.31	0.56
1:C:123:LYS:HA	1:C:155:THR:HA	1.87	0.56
1:C:344:ILE:HD12	1:C:345:GLU:N	2.20	0.56
1:A:29:TYR:HE1	1:A:148:MET:HB2	1.70	0.56
1:A:325:PHE:HB3	1:A:336:ARG:NH2	2.19	0.56
1:B:282:VAL:HG23	1:B:333:VAL:HG11	1.87	0.56
1:B:64:GLU:HG2	1:B:83:TRP:HH2	1.70	0.56
1:C:196:PHE:CG	1:C:197:PRO:HD2	2.40	0.56
1:D:141:LEU:N	1:D:144:LEU:HD21	2.14	0.56
1:D:215:MET:HE3	1:D:455:TYR:HB2	1.87	0.56
1:A:286:LEU:HD12	1:A:286:LEU:N	2.20	0.56
1:D:270:LEU:O	1:D:332:GLY:CA	2.52	0.56
1:A:196:PHE:CG	1:A:197:PRO:HD2	2.40	0.56
1:A:205:PHE:HB2	1:A:218:ALA:HB3	1.86	0.56
1:A:381:ASN:HD21	1:A:385:ARG:CZ	2.18	0.56
1:B:92:LEU:C	1:B:94:VAL:H	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:GLU:HA	1:A:394:ILE:HD12	1.87	0.56
1:C:298:LYS:O	1:C:302:ILE:HG13	2.06	0.56
1:D:122:ILE:HG13	1:D:122:ILE:O	2.05	0.56
1:D:207:THR:HG22	1:D:215:MET:HB3	1.87	0.56
1:D:353:ARG:HB3	1:D:355:ASP:OD2	2.04	0.56
1:A:156:ALA:HB2	1:A:247:GLN:NE2	2.20	0.56
1:C:29:TYR:HE1	1:C:148:MET:HB2	1.71	0.56
1:C:169:GLU:O	1:C:173:ILE:HG12	2.06	0.56
1:C:430:GLU:HG3	1:C:437:ILE:CG1	2.32	0.56
1:D:295:VAL:C	1:D:297:GLU:H	2.08	0.56
1:D:229:LYS:HA	1:D:244:TYR:CE2	2.41	0.56
1:A:223:LEU:HD13	1:A:227:PHE:CE2	2.41	0.56
1:A:302:ILE:HG23	1:A:367:LEU:HD21	1.88	0.56
1:A:394:ILE:HG12	1:A:415:VAL:CG1	2.34	0.56
1:B:99:ARG:HD2	1:B:102:SER:HB2	1.86	0.56
1:B:196:PHE:CG	1:B:197:PRO:HD2	2.40	0.56
1:C:229:LYS:HA	1:C:244:TYR:CD2	2.41	0.56
1:D:64:GLU:HG2	1:D:83:TRP:HH2	1.71	0.56
1:D:5:GLU:O	1:D:9:ASP:HB2	2.05	0.56
1:B:74:ILE:HG22	1:B:74:ILE:O	2.06	0.56
1:C:262:ALA:O	1:C:264:HIS:N	2.38	0.56
1:D:127:ILE:HG12	1:D:151:LYS:HB2	1.88	0.56
1:B:295:VAL:C	1:B:297:GLU:H	2.08	0.56
1:B:413:ARG:CB	1:B:413:ARG:HH11	2.18	0.56
1:C:101:THR:HG21	1:C:103:GLU:OE1	2.06	0.56
1:C:286:LEU:HD12	1:C:286:LEU:N	2.21	0.56
1:A:190:ARG:HG3	1:A:194:ASP:OD2	2.05	0.55
1:C:190:ARG:HG3	1:C:194:ASP:OD2	2.05	0.55
1:C:92:LEU:O	1:C:93:ASP:HB2	2.05	0.55
1:A:58:PHE:HD1	1:A:126:GLN:NE2	2.03	0.55
1:A:159:THR:HG23	1:A:162:GLU:HB2	1.88	0.55
1:A:294:ILE:HG23	1:A:295:VAL:N	2.21	0.55
1:B:322:GLY:HA2	1:B:325:PHE:CD2	2.42	0.55
1:A:266:ASP:CG	1:A:354:ARG:HH22	2.09	0.55
1:C:417:LEU:HA	1:C:449:ILE:O	2.07	0.55
1:A:120:LEU:HD13	1:A:157:HIS:C	2.27	0.55
1:B:127:ILE:HG12	1:B:151:LYS:HB2	1.88	0.55
1:B:19:VAL:HG11	1:B:140:PRO:HG3	1.88	0.55
1:C:127:ILE:HG12	1:C:151:LYS:CB	2.36	0.55
1:D:181:LEU:HD22	1:D:260:ILE:HD11	1.89	0.55
1:D:285:PRO:O	1:D:287:ILE:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:TYR:HE1	1:A:148:MET:CB	2.19	0.55
1:C:437:ILE:HG22	1:C:439:GLY:H	1.72	0.55
1:B:229:LYS:HA	1:B:244:TYR:CE2	2.42	0.55
1:D:196:PHE:CG	1:D:197:PRO:HD2	2.41	0.55
1:D:413:ARG:HH11	1:D:413:ARG:CB	2.19	0.55
1:A:220:VAL:HG22	1:A:250:TYR:HB3	1.88	0.55
1:A:41:PHE:CD2	1:A:127:ILE:HD13	2.42	0.55
1:B:159:THR:HG23	1:B:162:GLU:H	1.72	0.55
1:C:394:ILE:HG12	1:C:415:VAL:CG1	2.36	0.55
1:D:19:VAL:HG11	1:D:140:PRO:HG3	1.89	0.55
1:D:390:PHE:CE2	1:D:394:ILE:HD11	2.42	0.55
1:D:74:ILE:HG22	1:D:74:ILE:O	2.07	0.55
1:A:155:THR:OG1	1:A:248:THR:HG22	2.05	0.55
1:C:196:PHE:CD2	1:C:197:PRO:HD2	2.41	0.55
1:B:141:LEU:N	1:B:144:LEU:HD21	2.16	0.55
1:B:346:ASN:O	1:B:348:LYS:HG3	2.06	0.55
1:C:53:HIS:CE1	1:C:250:TYR:HH	2.23	0.55
1:C:62:ILE:HD13	1:C:105:PRO:HD3	1.89	0.55
1:D:188:SER:HB3	1:D:438:LEU:O	2.07	0.55
1:A:417:LEU:HD12	1:A:450:ALA:HA	1.89	0.55
1:A:62:ILE:HD13	1:A:105:PRO:HD3	1.89	0.55
1:B:449:ILE:HG22	1:B:449:ILE:O	2.07	0.55
1:C:223:LEU:HD13	1:C:227:PHE:HD2	1.69	0.55
1:D:10:ILE:HD11	1:D:270:LEU:CB	2.32	0.55
1:D:134:GLU:H	1:D:145:ARG:HD2	1.71	0.55
1:D:159:THR:HG23	1:D:162:GLU:H	1.72	0.55
1:A:169:GLU:O	1:A:172:SER:HB3	2.07	0.54
1:A:417:LEU:HA	1:A:449:ILE:O	2.07	0.54
1:C:169:GLU:O	1:C:172:SER:HB3	2.07	0.54
1:C:302:ILE:HG23	1:C:367:LEU:HD21	1.89	0.54
1:D:322:GLY:HA2	1:D:325:PHE:CD2	2.42	0.54
1:C:247:GLN:HA	1:C:247:GLN:HE21	1.72	0.54
1:D:99:ARG:HD2	1:D:102:SER:HB2	1.88	0.54
1:A:299:ALA:HB1	1:A:314:ILE:HD13	1.90	0.54
1:B:215:MET:HE3	1:B:455:TYR:HB2	1.89	0.54
1:C:60:MET:SD	1:D:60:MET:SD	3.04	0.54
1:A:222:ASN:HD22	1:A:222:ASN:C	2.08	0.54
1:B:125:TYR:CB	1:B:153:ALA:HA	2.37	0.54
1:B:86:HIS:ND1	1:B:91:GLN:HA	2.22	0.54
1:D:272:LEU:HD11	1:D:278:PRO:CD	2.36	0.54
1:A:17:TYR:CE2	1:A:19:VAL:HG12	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:PHE:CE1	1:A:215:MET:SD	3.01	0.54
1:C:17:TYR:CE2	1:C:19:VAL:HG12	2.42	0.54
1:C:156:ALA:HB2	1:C:247:GLN:NE2	2.22	0.54
1:C:294:ILE:HG23	1:C:295:VAL:N	2.23	0.54
1:C:397:LEU:HB2	1:C:418:VAL:HG12	1.89	0.54
1:A:167:VAL:HG13	1:A:220:VAL:HG11	1.89	0.54
1:A:190:ARG:HH21	1:A:216:GLN:HE21	1.55	0.54
1:A:25:GLY:HA3	1:A:145:ARG:HB2	1.89	0.54
1:B:389:LYS:HZ2	1:B:389:LYS:HB3	1.69	0.54
1:B:395:THR:HB	1:B:416:ILE:CD1	2.36	0.54
1:C:120:LEU:HD13	1:C:157:HIS:C	2.27	0.54
1:C:127:ILE:HG12	1:C:151:LYS:HB2	1.89	0.54
1:D:274:PRO:CD	1:D:379:MET:HB2	2.36	0.54
1:B:92:LEU:O	1:B:94:VAL:N	2.41	0.54
1:C:272:LEU:HD12	1:C:272:LEU:O	2.08	0.54
1:A:196:PHE:CD2	1:A:197:PRO:HD2	2.42	0.54
1:C:124:ILE:N	1:C:154:HIS:O	2.41	0.54
1:C:159:THR:CG2	1:C:162:GLU:HB2	2.37	0.54
1:C:167:VAL:HG13	1:C:220:VAL:HG11	1.89	0.54
1:D:125:TYR:CB	1:D:153:ALA:HA	2.37	0.54
1:D:286:LEU:N	1:D:286:LEU:HD12	2.12	0.54
1:A:430:GLU:CG	1:A:437:ILE:HG12	2.29	0.54
1:B:325:PHE:CD1	1:B:336:ARG:HD3	2.43	0.54
1:C:190:ARG:HH21	1:C:216:GLN:HE21	1.55	0.54
1:D:30:LEU:O	1:D:33:GLY:N	2.41	0.54
1:C:92:LEU:C	1:C:94:VAL:N	2.60	0.54
1:A:400:ILE:HD13	1:A:424:ILE:HD11	1.89	0.53
1:C:430:GLU:CG	1:C:437:ILE:HG12	2.31	0.53
1:D:335:LEU:HD11	1:D:374:THR:CG2	2.38	0.53
1:D:86:HIS:ND1	1:D:91:GLN:HA	2.23	0.53
1:A:92:LEU:C	1:A:94:VAL:N	2.61	0.53
1:A:92:LEU:O	1:A:93:ASP:HB2	2.07	0.53
1:C:381:ASN:HD21	1:C:385:ARG:CZ	2.22	0.53
1:C:266:ASP:CG	1:C:354:ARG:HH22	2.11	0.53
1:D:10:ILE:O	1:D:11:LEU:C	2.47	0.53
1:D:402:PRO:C	1:D:404:GLU:N	2.61	0.53
1:A:262:ALA:O	1:A:264:HIS:N	2.41	0.53
1:C:25:GLY:HA3	1:C:145:ARG:HB2	1.90	0.53
1:B:18:ASP:CB	1:B:30:LEU:HD11	2.32	0.53
1:C:209:PHE:CE1	1:C:215:MET:SD	3.02	0.53
1:C:320:ARG:NH1	1:C:322:GLY:HA3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:THR:HG21	1:A:103:GLU:OE1	2.09	0.53
1:A:247:GLN:HE21	1:A:247:GLN:HA	1.74	0.53
1:B:402:PRO:C	1:B:404:GLU:N	2.62	0.53
1:B:66:LEU:C	1:B:68:ALA:H	2.12	0.53
1:C:417:LEU:HD12	1:C:450:ALA:HA	1.90	0.53
1:C:99:ARG:O	1:C:99:ARG:HG3	2.09	0.53
1:D:196:PHE:HB3	1:D:199:ALA:HB3	1.89	0.53
1:D:346:ASN:O	1:D:348:LYS:HG3	2.08	0.53
1:A:155:THR:OG1	1:A:248:THR:CG2	2.56	0.53
1:A:267:GLU:N	1:A:267:GLU:OE2	2.42	0.53
1:B:10:ILE:O	1:B:11:LEU:C	2.47	0.53
1:B:270:LEU:O	1:B:332:GLY:CA	2.56	0.53
1:C:112:LEU:HB3	1:D:20:ARG:NH2	2.23	0.53
1:C:41:PHE:CD2	1:C:127:ILE:HD13	2.44	0.53
1:D:402:PRO:O	1:D:404:GLU:N	2.42	0.53
1:A:401:ASN:HD22	1:A:402:PRO:N	2.06	0.53
1:B:234:ILE:C	1:B:234:ILE:HD12	2.29	0.53
1:C:215:MET:HA	2:C:468:HOH:O	2.08	0.53
1:A:397:LEU:HB2	1:A:418:VAL:HG12	1.91	0.53
1:B:160:LYS:HA	1:B:246:TYR:CD2	2.44	0.53
1:C:34:PHE:O	1:C:37:ARG:HB3	2.09	0.53
1:D:75:LYS:O	1:D:76:GLY:C	2.46	0.53
1:B:45:ARG:O	1:B:48:LEU:HB2	2.08	0.52
1:C:267:GLU:OE2	1:C:267:GLU:N	2.42	0.52
1:A:41:PHE:O	1:A:44:ILE:HG22	2.09	0.52
1:B:175:LYS:HG3	1:B:185:TYR:CZ	2.44	0.52
1:B:142:ILE:HA	1:B:255:ARG:HD3	1.91	0.52
1:B:272:LEU:HD12	1:B:277:ALA:HA	1.90	0.52
1:B:446:ASN:HB2	1:B:448:TYR:CE1	2.45	0.52
1:C:202:THR:HG23	1:C:221:HIS:ND1	2.24	0.52
1:C:66:LEU:HD12	1:C:66:LEU:H	1.74	0.52
1:A:114:VAL:HG22	1:A:122:ILE:CD1	2.39	0.52
1:A:16:ILE:HD11	1:A:270:LEU:HD21	1.91	0.52
1:B:274:PRO:CD	1:B:379:MET:HB2	2.38	0.52
1:C:405:ILE:HG23	1:C:416:ILE:HG21	1.90	0.52
1:D:215:MET:HE3	1:D:215:MET:HA	1.89	0.52
1:D:234:ILE:HD12	1:D:234:ILE:C	2.29	0.52
1:B:5:GLU:O	1:B:9:ASP:HB2	2.09	0.52
1:B:134:GLU:H	1:B:145:ARG:HD2	1.74	0.52
1:A:1:LEU:H	1:A:1:LEU:HD12	1.75	0.52
1:A:272:LEU:CD1	1:A:277:ALA:HA	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:SER:HB3	1:B:438:LEU:O	2.10	0.52
1:B:196:PHE:HB3	1:B:199:ALA:HB3	1.90	0.52
1:C:29:TYR:HE1	1:C:148:MET:CB	2.22	0.52
1:C:184:PRO:HB3	1:C:390:PHE:CD2	2.44	0.52
1:C:10:ILE:HD11	1:C:270:LEU:HD13	1.92	0.52
1:A:270:LEU:O	1:A:354:ARG:NH1	2.42	0.52
1:B:390:PHE:CE2	1:B:394:ILE:HD11	2.45	0.52
1:C:256:VAL:CG2	1:C:257:ILE:H	2.19	0.52
1:D:171:ILE:HG23	1:D:205:PHE:HZ	1.75	0.52
1:A:253:SER:O	1:A:256:VAL:HG22	2.09	0.52
1:C:344:ILE:HD12	1:C:344:ILE:C	2.30	0.52
1:C:298:LYS:HG3	1:C:344:ILE:HG21	1.90	0.52
1:D:55:GLU:HA	1:D:125:TYR:O	2.10	0.52
1:A:316:ASP:O	1:A:317:ARG:O	2.27	0.52
1:B:396:ILE:H	1:B:396:ILE:HD12	1.74	0.52
1:B:430:GLU:CG	1:B:437:ILE:HG12	2.40	0.52
1:B:430:GLU:HG3	1:B:437:ILE:HG12	1.92	0.52
1:C:114:VAL:HG22	1:C:122:ILE:CD1	2.40	0.52
1:C:262:ALA:O	1:C:263:ILE:C	2.48	0.52
1:C:381:ASN:HD21	1:C:385:ARG:NH2	2.08	0.52
1:D:283:ILE:CD1	1:D:283:ILE:N	2.71	0.52
1:A:344:ILE:HD12	1:A:344:ILE:C	2.30	0.52
1:B:171:ILE:HG23	1:B:205:PHE:HZ	1.75	0.52
1:B:283:ILE:N	1:B:283:ILE:CD1	2.71	0.52
1:C:401:ASN:HD22	1:C:402:PRO:N	2.07	0.52
1:D:325:PHE:CD1	1:D:336:ARG:HD3	2.45	0.52
1:D:401:ASN:O	1:D:404:GLU:HB3	2.10	0.52
1:D:402:PRO:C	1:D:404:GLU:H	2.13	0.52
1:A:271:ILE:O	1:A:272:LEU:O	2.28	0.51
1:B:272:LEU:HD11	1:B:278:PRO:CD	2.39	0.51
1:C:1:LEU:HD12	1:C:1:LEU:H	1.75	0.51
1:D:381:ASN:O	1:D:385:ARG:HG2	2.10	0.51
1:D:66:LEU:C	1:D:68:ALA:H	2.13	0.51
1:A:400:ILE:HG22	1:A:418:VAL:HG21	1.93	0.51
1:B:215:MET:HA	1:B:215:MET:HE3	1.90	0.51
1:B:75:LYS:O	1:B:76:GLY:C	2.47	0.51
1:D:105:PRO:HG2	1:D:106:ILE:H	1.75	0.51
1:D:396:ILE:HD12	1:D:396:ILE:H	1.75	0.51
1:B:223:LEU:HD13	1:B:227:PHE:CD2	2.46	0.51
1:C:385:ARG:NH1	1:C:385:ARG:HG3	2.25	0.51
1:C:64:GLU:CG	1:C:95:LYS:HB2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:PRO:O	1:D:344:ILE:HG13	2.10	0.51
1:A:159:THR:CG2	1:A:162:GLU:HB2	2.40	0.51
1:A:208:ILE:HD11	1:A:415:VAL:HG12	1.92	0.51
1:B:106:ILE:O	1:B:110:MET:HG3	2.10	0.51
1:C:223:LEU:HD13	1:C:227:PHE:CE2	2.45	0.51
1:D:175:LYS:HG3	1:D:185:TYR:CZ	2.45	0.51
1:A:298:LYS:HG3	1:A:344:ILE:HG21	1.92	0.51
1:A:409:LEU:CD2	1:A:416:ILE:HG12	2.40	0.51
1:B:207:THR:HG22	1:B:215:MET:HB3	1.92	0.51
1:B:302:ILE:HG23	1:B:367:LEU:HD21	1.92	0.51
1:B:381:ASN:O	1:B:385:ARG:HG2	2.11	0.51
1:B:416:ILE:O	1:B:450:ALA:HA	2.10	0.51
1:B:44:ILE:HG12	1:B:151:LYS:HD3	1.92	0.51
1:A:127:ILE:HG12	1:A:151:LYS:CB	2.41	0.51
1:B:178:PHE:CZ	1:B:217:ILE:HD12	2.45	0.51
1:C:272:LEU:CD1	1:C:277:ALA:HA	2.40	0.51
1:D:160:LYS:HA	1:D:246:TYR:CD2	2.45	0.51
1:A:23:ILE:O	1:A:24:LYS:O	2.28	0.51
1:B:57:LEU:HA	1:B:126:GLN:HE21	1.76	0.51
1:B:66:LEU:O	1:B:68:ALA:N	2.42	0.51
1:B:66:LEU:C	1:B:68:ALA:N	2.64	0.51
1:C:35:LYS:C	1:C:37:ARG:N	2.63	0.51
1:C:41:PHE:HD2	1:C:127:ILE:HD13	1.75	0.51
1:D:430:GLU:CG	1:D:437:ILE:HG12	2.41	0.51
1:D:430:GLU:HG3	1:D:437:ILE:HG12	1.93	0.51
1:A:112:LEU:HB3	1:B:20:ARG:NH2	2.26	0.51
1:A:184:PRO:HB3	1:A:390:PHE:CD2	2.45	0.51
1:A:99:ARG:HG3	1:A:99:ARG:O	2.11	0.51
1:D:114:VAL:HG12	1:D:235:PHE:HB3	1.92	0.51
1:D:44:ILE:HG12	1:D:151:LYS:HD3	1.92	0.51
1:B:55:GLU:HA	1:B:125:TYR:O	2.11	0.51
1:B:402:PRO:O	1:B:404:GLU:N	2.44	0.51
1:D:353:ARG:O	1:D:357:MET:N	2.43	0.51
1:D:360:PHE:HD2	1:D:360:PHE:H	1.59	0.51
1:B:360:PHE:HD2	1:B:360:PHE:H	1.59	0.51
1:B:402:PRO:C	1:B:404:GLU:H	2.14	0.51
1:C:253:SER:O	1:C:256:VAL:HG22	2.10	0.51
1:A:56:ALA:HB3	1:A:124:ILE:HD11	1.93	0.50
1:B:295:VAL:O	1:B:297:GLU:N	2.44	0.50
1:D:295:VAL:O	1:D:297:GLU:N	2.44	0.50
1:B:443:TYR:O	1:B:444:LYS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:HD12	1:A:269:GLY:HA2	1.92	0.50
1:A:328:TRP:HA	1:A:328:TRP:CE3	2.46	0.50
1:C:112:LEU:HB3	1:D:20:ARG:HH21	1.75	0.50
1:D:45:ARG:O	1:D:48:LEU:HB2	2.10	0.50
1:D:66:LEU:C	1:D:68:ALA:N	2.64	0.50
1:A:124:ILE:N	1:A:154:HIS:O	2.44	0.50
1:A:175:LYS:HG2	1:A:185:TYR:CZ	2.46	0.50
1:A:98:LEU:HD11	1:B:61:LEU:HD21	1.93	0.50
1:C:385:ARG:HH11	1:C:385:ARG:HG3	1.77	0.50
1:D:106:ILE:O	1:D:110:MET:HG3	2.10	0.50
1:A:160:LYS:HB2	1:A:246:TYR:CE2	2.46	0.50
1:B:10:ILE:HA	1:B:13:LYS:HB3	1.93	0.50
1:D:378:ILE:O	1:D:382:ILE:HG23	2.11	0.50
1:A:430:GLU:C	1:A:432:LYS:N	2.64	0.50
1:C:220:VAL:HG22	1:C:250:TYR:HB3	1.93	0.50
1:C:400:ILE:HD13	1:C:424:ILE:HD11	1.93	0.50
1:A:48:LEU:CD1	1:A:151:LYS:HD2	2.41	0.50
1:A:205:PHE:CD1	1:A:218:ALA:HB3	2.47	0.50
1:A:266:ASP:OD2	1:A:354:ARG:NH2	2.45	0.50
1:A:66:LEU:HB3	1:A:104:THR:CG2	2.42	0.50
1:B:401:ASN:O	1:B:404:GLU:HB3	2.12	0.50
1:A:381:ASN:HD21	1:A:385:ARG:NH2	2.10	0.50
1:A:385:ARG:NH1	1:A:385:ARG:HG3	2.27	0.50
1:A:388:GLU:O	1:A:392:ASN:HB2	2.12	0.50
1:B:237:THR:HB	1:B:238:PRO:HD2	1.94	0.50
1:D:178:PHE:CZ	1:D:217:ILE:HD12	2.46	0.50
1:A:405:ILE:O	1:A:408:ILE:HG22	2.12	0.49
1:D:157:HIS:NE2	1:D:166:GLN:HG2	2.27	0.49
1:D:237:THR:HB	1:D:238:PRO:HD2	1.94	0.49
1:A:131:PHE:CE2	1:A:146:GLU:HG3	2.47	0.49
1:A:428:GLU:O	1:A:431:GLU:N	2.45	0.49
1:B:229:LYS:HG2	1:B:244:TYR:CD2	2.46	0.49
1:C:272:LEU:HD11	1:C:277:ALA:HA	1.93	0.49
1:C:353:ARG:C	1:C:355:ASP:N	2.63	0.49
1:C:3:PHE:O	1:C:6:TRP:N	2.45	0.49
1:A:188:SER:O	1:A:203:MET:HA	2.12	0.49
1:A:202:THR:HG23	1:A:221:HIS:ND1	2.28	0.49
1:C:102:SER:O	1:C:106:ILE:HG13	2.13	0.49
1:C:56:ALA:HB3	1:C:124:ILE:HD11	1.94	0.49
1:D:10:ILE:HA	1:D:13:LYS:HB3	1.94	0.49
1:D:134:GLU:H	1:D:145:ARG:CD	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:LYS:O	1:D:190:ARG:C	2.51	0.49
1:D:284:VAL:O	1:D:286:LEU:HD12	2.11	0.49
1:B:223:LEU:HB2	1:B:247:GLN:HB2	1.94	0.49
1:B:353:ARG:O	1:B:357:MET:N	2.44	0.49
1:C:160:LYS:HB2	1:C:246:TYR:CE2	2.47	0.49
1:D:443:TYR:O	1:D:444:LYS:HB2	2.12	0.49
1:D:446:ASN:HB2	1:D:448:TYR:CE1	2.48	0.49
1:D:71:ALA:HB2	1:D:77:PHE:CE2	2.47	0.49
1:A:223:LEU:HB2	1:A:247:GLN:HB2	1.94	0.49
1:A:191:PRO:HD3	1:A:439:GLY:HA2	1.92	0.49
1:B:272:LEU:HD11	1:B:277:ALA:HA	1.94	0.49
1:C:74:ILE:O	1:C:75:LYS:O	2.31	0.49
1:D:437:ILE:HG23	1:D:451:ILE:HG12	1.93	0.49
1:A:343:ASP:OD1	1:A:350:THR:HG22	2.13	0.49
1:B:16:ILE:HD11	1:B:270:LEU:CD2	2.43	0.49
1:B:275:ILE:HD11	1:B:379:MET:HG2	1.94	0.49
1:C:178:PHE:O	1:C:182:GLY:N	2.46	0.49
1:C:205:PHE:CD1	1:C:218:ALA:HB3	2.47	0.49
1:D:295:VAL:C	1:D:297:GLU:N	2.65	0.49
1:A:149:THR:HB	1:A:254:ASP:OD2	2.13	0.49
1:A:429:LEU:O	1:A:432:LYS:HB3	2.12	0.49
1:B:171:ILE:HG23	1:B:205:PHE:CZ	2.48	0.49
1:B:295:VAL:C	1:B:297:GLU:N	2.66	0.49
1:C:294:ILE:O	1:C:297:GLU:HB3	2.12	0.49
1:D:141:LEU:HA	1:D:144:LEU:HD11	1.94	0.49
1:D:332:GLY:O	1:D:333:VAL:C	2.49	0.49
1:D:416:ILE:O	1:D:450:ALA:HA	2.12	0.49
1:D:66:LEU:O	1:D:68:ALA:N	2.45	0.49
1:B:11:LEU:O	1:B:16:ILE:HB	2.12	0.49
1:B:71:ALA:HB2	1:B:77:PHE:CE2	2.47	0.49
1:D:16:ILE:HD11	1:D:270:LEU:CD2	2.43	0.49
1:D:275:ILE:HD11	1:D:379:MET:HG2	1.94	0.49
1:D:272:LEU:HD12	1:D:277:ALA:HA	1.93	0.49
1:D:335:LEU:CD1	1:D:378:ILE:HD11	2.43	0.49
1:C:400:ILE:HG22	1:C:418:VAL:HG21	1.95	0.49
1:A:272:LEU:HD11	1:A:277:ALA:HA	1.94	0.49
1:A:283:ILE:HG22	1:A:314:ILE:HG23	1.95	0.49
1:A:385:ARG:HH11	1:A:385:ARG:HG3	1.78	0.49
1:B:58:PHE:N	1:B:126:GLN:NE2	2.55	0.49
1:C:66:LEU:HB3	1:C:104:THR:CG2	2.43	0.49
1:C:237:THR:C	1:C:239:THR:H	2.17	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ILE:CD1	1:C:270:LEU:HD21	2.41	0.49
1:C:302:ILE:HG22	1:C:306:LEU:HD12	1.94	0.49
1:C:328:TRP:CE3	1:C:328:TRP:HA	2.47	0.49
1:C:409:LEU:CD2	1:C:416:ILE:HG12	2.42	0.49
1:A:114:VAL:CG2	1:A:122:ILE:HD11	2.42	0.48
1:A:262:ALA:O	1:A:263:ILE:C	2.51	0.48
1:A:74:ILE:O	1:A:75:LYS:O	2.31	0.48
1:B:114:VAL:HG22	1:B:120:LEU:HD21	1.94	0.48
1:D:11:LEU:O	1:D:16:ILE:HB	2.13	0.48
1:B:114:VAL:HG12	1:B:235:PHE:HB3	1.95	0.48
1:C:175:LYS:HG2	1:C:185:TYR:CZ	2.47	0.48
1:C:271:ILE:O	1:C:272:LEU:O	2.31	0.48
1:C:316:ASP:O	1:C:317:ARG:O	2.30	0.48
1:C:430:GLU:C	1:C:432:LYS:N	2.66	0.48
1:C:98:LEU:HD11	1:D:61:LEU:HD21	1.95	0.48
1:A:30:LEU:O	1:A:31:PRO:C	2.51	0.48
1:B:19:VAL:HG11	1:B:140:PRO:CG	2.43	0.48
1:C:114:VAL:CG2	1:C:122:ILE:HD11	2.42	0.48
1:C:428:GLU:O	1:C:431:GLU:N	2.47	0.48
1:D:222:ASN:HD22	1:D:222:ASN:C	2.15	0.48
1:D:280:GLN:OE1	1:D:311:ARG:HG3	2.14	0.48
1:A:169:GLU:O	1:A:173:ILE:HG12	2.13	0.48
1:B:141:LEU:HA	1:B:144:LEU:HD11	1.95	0.48
1:B:378:ILE:O	1:B:382:ILE:HG23	2.13	0.48
1:C:274:PRO:HD2	1:C:275:ILE:HD12	1.95	0.48
1:A:306:LEU:HB2	1:A:312:VAL:HG11	1.94	0.48
1:B:108:TYR:O	1:B:111:LYS:HB3	2.13	0.48
1:B:119:ASP:O	1:B:120:LEU:HD23	2.13	0.48
1:B:332:GLY:O	1:B:333:VAL:C	2.51	0.48
1:B:341:PRO:O	1:B:344:ILE:HG13	2.13	0.48
1:C:188:SER:O	1:C:203:MET:HA	2.13	0.48
1:D:57:LEU:HA	1:D:126:GLN:HE21	1.78	0.48
1:A:256:VAL:CG2	1:A:257:ILE:H	2.23	0.48
1:B:437:ILE:HG23	1:B:451:ILE:HG12	1.95	0.48
1:C:343:ASP:OD1	1:C:350:THR:HG22	2.14	0.48
1:D:284:VAL:HG11	1:D:325:PHE:CE1	2.49	0.48
1:A:208:ILE:HG13	1:A:390:PHE:HE1	1.79	0.48
1:A:36:ILE:O	1:A:36:ILE:CD1	2.60	0.48
1:B:189:LYS:O	1:B:190:ARG:C	2.52	0.48
1:C:321:PRO:O	1:C:324:LYS:HB2	2.14	0.48
1:C:350:THR:C	1:C:351:LEU:HD13	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:LYS:HG2	1:D:244:TYR:CD2	2.48	0.48
1:D:70:GLU:O	1:D:70:GLU:HG3	2.12	0.48
1:B:131:PHE:CE2	1:B:146:GLU:HG3	2.48	0.48
1:B:222:ASN:HD22	1:B:222:ASN:C	2.17	0.48
1:C:48:LEU:CD1	1:C:151:LYS:HD2	2.43	0.48
1:A:294:ILE:O	1:A:297:GLU:HB3	2.14	0.48
1:A:401:ASN:OD1	1:A:404:GLU:HB2	2.14	0.48
1:B:286:LEU:HD11	1:B:338:GLU:CB	2.41	0.48
1:C:281:VAL:O	1:C:312:VAL:HA	2.14	0.48
1:D:99:ARG:HH21	1:D:129:ASN:H	1.60	0.48
1:A:277:ALA:C	1:A:279:ILE:N	2.65	0.48
1:A:66:LEU:HD12	1:A:66:LEU:N	2.29	0.48
1:B:39:TYR:CD2	1:B:311:ARG:NH1	2.81	0.48
1:A:60:MET:SD	1:B:60:MET:SD	3.11	0.48
1:C:102:SER:C	1:C:105:PRO:HD2	2.34	0.48
1:C:266:ASP:OD2	1:C:354:ARG:NH2	2.47	0.48
1:A:291:LYS:HB3	1:A:294:ILE:CG2	2.43	0.47
1:A:415:VAL:HA	1:A:452:ALA:HB2	1.96	0.47
1:D:223:LEU:HB2	1:D:247:GLN:HB2	1.95	0.47
1:A:237:THR:C	1:A:239:THR:H	2.18	0.47
1:A:112:LEU:HB3	1:B:20:ARG:HH21	1.79	0.47
1:C:401:ASN:O	1:C:404:GLU:HB3	2.14	0.47
1:C:191:PRO:HD3	1:C:439:GLY:HA2	1.94	0.47
1:D:63:PRO:HA	1:D:96:LEU:HD23	1.96	0.47
1:A:171:ILE:O	1:A:175:LYS:HB2	2.14	0.47
1:B:280:GLN:OE1	1:B:311:ARG:HG3	2.15	0.47
1:C:129:ASN:OD1	1:D:60:MET:HE3	2.13	0.47
1:C:30:LEU:O	1:C:31:PRO:C	2.53	0.47
1:D:171:ILE:HG23	1:D:205:PHE:CZ	2.50	0.47
1:B:104:THR:HB	1:B:105:PRO:CD	2.44	0.47
1:C:155:THR:OG1	1:C:248:THR:HG22	2.13	0.47
1:C:36:ILE:O	1:C:36:ILE:CD1	2.61	0.47
1:D:302:ILE:HG23	1:D:367:LEU:HD21	1.96	0.47
1:A:141:LEU:HD13	1:A:257:ILE:HG12	1.95	0.47
1:B:157:HIS:NE2	1:B:166:GLN:HG2	2.30	0.47
1:C:388:GLU:O	1:C:392:ASN:HB2	2.14	0.47
1:D:319:ILE:HG13	1:D:320:ARG:N	2.29	0.47
1:A:53:HIS:CE1	1:A:250:TYR:HH	2.25	0.47
1:A:350:THR:C	1:A:351:LEU:HD13	2.34	0.47
1:A:3:PHE:O	1:A:6:TRP:N	2.47	0.47
1:B:25:GLY:HA2	2:B:461:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:LYS:HB3	1:C:294:ILE:CG2	2.44	0.47
1:D:112:LEU:HD22	1:D:112:LEU:N	2.30	0.47
1:D:282:VAL:HG11	1:D:328:TRP:CD1	2.50	0.47
1:A:257:ILE:O	1:A:261:ILE:HG13	2.15	0.47
1:A:355:ASP:OD2	1:A:356:THR:N	2.46	0.47
1:A:35:LYS:C	1:A:37:ARG:N	2.67	0.47
1:A:60:MET:HA	1:A:99:ARG:NH1	2.30	0.47
1:B:158:SER:HA	1:B:235:PHE:CZ	2.50	0.47
1:B:222:ASN:HD22	1:B:224:GLY:H	1.62	0.47
1:B:284:VAL:O	1:B:286:LEU:HD12	2.13	0.47
1:B:367:LEU:O	1:B:369:GLU:N	2.48	0.47
1:D:19:VAL:HG11	1:D:140:PRO:CG	2.44	0.47
1:D:406:LYS:O	1:D:409:LEU:HB2	2.15	0.47
1:D:68:ALA:C	1:D:70:GLU:N	2.68	0.47
1:A:272:LEU:O	1:A:272:LEU:HD12	2.15	0.47
1:A:346:ASN:O	1:A:347:LYS:HB2	2.13	0.47
1:A:43:ILE:HD11	1:A:275:ILE:HG22	1.97	0.47
1:B:134:GLU:H	1:B:145:ARG:CD	2.27	0.47
1:B:319:ILE:HG13	1:B:320:ARG:N	2.30	0.47
1:C:208:ILE:HD11	1:C:415:VAL:CG1	2.45	0.47
1:C:277:ALA:C	1:C:279:ILE:N	2.66	0.47
1:C:364:GLU:O	1:C:364:GLU:HG2	2.14	0.47
1:C:366:GLN:HA	1:C:366:GLN:HE21	1.80	0.47
1:D:142:ILE:HA	1:D:255:ARG:HD3	1.97	0.47
1:C:111:LYS:HG2	1:C:112:LEU:HD12	1.97	0.47
1:A:171:ILE:HD11	1:A:203:MET:HG3	1.96	0.47
1:C:131:PHE:CE2	1:C:146:GLU:HG3	2.50	0.47
1:C:117:HIS:CD2	1:C:238:PRO:HA	2.50	0.47
1:C:405:ILE:O	1:C:408:ILE:HG22	2.15	0.47
1:D:313:HIS:HD2	1:D:328:TRP:CZ2	2.33	0.47
1:A:111:LYS:HG2	1:A:112:LEU:HD12	1.97	0.47
1:A:356:THR:OG1	1:A:358:GLU:HG2	2.15	0.47
1:B:159:THR:HG23	1:B:162:GLU:HB2	1.95	0.47
1:B:196:PHE:O	1:B:197:PRO:C	2.53	0.47
1:B:325:PHE:CE1	1:B:338:GLU:HG2	2.50	0.47
1:B:387:TRP:O	1:B:388:GLU:C	2.54	0.47
1:C:66:LEU:HB3	1:C:104:THR:HG22	1.97	0.47
1:D:271:ILE:HG12	1:D:354:ARG:HH12	1.74	0.47
1:A:205:PHE:N	1:A:205:PHE:CD1	2.83	0.46
1:A:64:GLU:CG	1:A:95:LYS:HB2	2.42	0.46
1:C:346:ASN:O	1:C:347:LYS:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ARG:HB2	1:C:413:ARG:CZ	2.46	0.46
1:D:114:VAL:CG1	1:D:235:PHE:HB3	2.45	0.46
1:D:33:GLY:O	1:D:36:ILE:CG2	2.60	0.46
1:D:387:TRP:O	1:D:388:GLU:C	2.54	0.46
1:A:248:THR:HG23	1:A:248:THR:O	2.15	0.46
1:A:401:ASN:O	1:A:404:GLU:HB3	2.16	0.46
1:B:30:LEU:O	1:B:31:PRO:C	2.53	0.46
1:C:171:ILE:HD11	1:C:203:MET:HG3	1.97	0.46
1:C:205:PHE:CD1	1:C:205:PHE:N	2.83	0.46
1:C:306:LEU:HB2	1:C:312:VAL:HG11	1.97	0.46
1:C:54:ASP:HB2	2:C:476:HOH:O	2.15	0.46
1:D:171:ILE:O	1:D:172:SER:C	2.54	0.46
1:D:92:LEU:C	1:D:94:VAL:N	2.69	0.46
1:A:37:ARG:NE	1:A:149:THR:OG1	2.48	0.46
1:A:120:LEU:HD13	1:A:157:HIS:O	2.15	0.46
1:A:340:GLY:O	1:A:344:ILE:HG23	2.16	0.46
1:A:364:GLU:HG2	1:A:364:GLU:O	2.14	0.46
1:A:306:LEU:HD22	1:A:371:VAL:HG11	1.96	0.46
1:C:223:LEU:HB2	1:C:247:GLN:HB2	1.97	0.46
1:C:43:ILE:HD11	1:C:275:ILE:HG22	1.97	0.46
1:A:58:PHE:N	1:A:126:GLN:HE22	2.13	0.46
1:A:117:HIS:CD2	1:A:238:PRO:HA	2.50	0.46
1:B:101:THR:O	1:B:103:GLU:N	2.48	0.46
1:C:360:PHE:CD2	1:C:360:PHE:N	2.68	0.46
1:D:140:PRO:HA	2:D:457:HOH:O	2.14	0.46
1:D:158:SER:HA	1:D:235:PHE:CZ	2.51	0.46
1:B:284:VAL:HG11	1:B:325:PHE:CE1	2.51	0.46
1:B:336:ARG:NH1	1:B:338:GLU:OE2	2.46	0.46
1:B:64:GLU:O	1:B:65:ASP:C	2.54	0.46
1:C:104:THR:HB	1:C:105:PRO:HD3	1.97	0.46
1:D:65:ASP:O	1:D:68:ALA:HB3	2.15	0.46
1:A:132:ARG:O	1:A:134:GLU:N	2.48	0.46
1:A:413:ARG:HB2	1:A:413:ARG:CZ	2.46	0.46
1:B:291:LYS:CB	1:B:294:ILE:HG21	2.45	0.46
1:B:68:ALA:C	1:B:70:GLU:N	2.69	0.46
1:C:126:GLN:HG3	1:C:128:VAL:HG22	1.97	0.46
1:C:102:SER:HB3	1:C:152:GLU:OE1	2.16	0.46
1:D:100:PRO:HG2	1:D:101:THR:H	1.80	0.46
1:B:191:PRO:HB3	1:B:425:TYR:OH	2.16	0.46
1:B:49:ASP:C	1:B:51:SER:H	2.20	0.46
1:B:63:PRO:HA	1:B:96:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:VAL:HB	1:C:312:VAL:HG12	1.98	0.46
1:C:340:GLY:O	1:C:344:ILE:HG23	2.16	0.46
1:D:119:ASP:O	1:D:120:LEU:HD23	2.16	0.46
1:D:291:LYS:CB	1:D:294:ILE:HG21	2.45	0.46
1:A:281:VAL:O	1:A:312:VAL:HA	2.16	0.46
1:B:189:LYS:HG2	1:B:189:LYS:O	2.16	0.46
1:D:223:LEU:HD13	1:D:227:PHE:CD2	2.51	0.46
1:D:66:LEU:HB3	1:D:104:THR:CG2	2.44	0.46
1:C:84:VAL:HG11	1:D:82:TYR:CD2	2.51	0.46
1:A:271:ILE:O	1:A:272:LEU:C	2.53	0.46
1:B:159:THR:CG2	1:B:162:GLU:HB2	2.45	0.46
1:B:33:GLY:O	1:B:36:ILE:CG2	2.62	0.46
1:B:70:GLU:O	1:B:70:GLU:HG3	2.15	0.46
1:C:132:ARG:O	1:C:134:GLU:N	2.49	0.46
1:C:271:ILE:O	1:C:272:LEU:C	2.53	0.46
1:C:401:ASN:OD1	1:C:404:GLU:HB2	2.16	0.46
1:C:415:VAL:HA	1:C:452:ALA:HB2	1.98	0.46
1:D:99:ARG:HH21	1:D:128:VAL:HB	1.76	0.46
1:A:353:ARG:C	1:A:355:ASP:N	2.66	0.45
1:B:29:TYR:HE2	1:B:257:ILE:HD11	1.81	0.45
1:C:112:LEU:HD12	1:C:112:LEU:N	2.32	0.45
1:C:149:THR:HB	1:C:254:ASP:OD2	2.16	0.45
1:C:37:ARG:NE	1:C:149:THR:OG1	2.48	0.45
1:C:373:LYS:HB2	1:C:373:LYS:HZ2	1.79	0.45
1:C:108:TYR:CE2	1:D:22:PRO:HD3	2.51	0.45
1:D:272:LEU:HA	1:D:273:PRO:HD3	1.82	0.45
1:D:64:GLU:O	1:D:65:ASP:C	2.55	0.45
1:A:127:ILE:HG12	1:A:151:LYS:HB2	1.97	0.45
1:A:360:PHE:CD2	1:A:360:PHE:N	2.68	0.45
1:A:405:ILE:CA	1:A:408:ILE:HG22	2.43	0.45
1:B:114:VAL:CG1	1:B:235:PHE:HB3	2.46	0.45
1:A:31:PRO:HG3	1:B:54:ASP:HB3	1.99	0.45
1:B:69:LYS:C	1:B:71:ALA:N	2.69	0.45
1:C:320:ARG:CZ	1:C:322:GLY:HA3	2.45	0.45
1:C:351:LEU:N	1:C:351:LEU:HD13	2.31	0.45
1:D:153:ALA:HB3	1:D:250:TYR:CE1	2.51	0.45
1:A:102:SER:O	1:A:106:ILE:HG13	2.16	0.45
1:A:126:GLN:HG3	1:A:128:VAL:HG22	1.98	0.45
1:A:211:ASP:CG	1:A:213:ARG:HB2	2.36	0.45
1:A:235:PHE:C	1:A:235:PHE:CD1	2.89	0.45
1:A:406:LYS:HB3	1:A:433:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:TYR:CD2	1:B:22:PRO:HD2	2.50	0.45
1:B:99:ARG:HG3	1:B:99:ARG:O	2.16	0.45
1:C:64:GLU:OE2	1:C:64:GLU:HA	2.15	0.45
1:D:29:TYR:HE2	1:D:257:ILE:HD11	1.82	0.45
1:A:112:LEU:HD12	1:A:112:LEU:N	2.32	0.45
1:A:366:GLN:O	1:A:370:VAL:HG23	2.16	0.45
1:C:58:PHE:N	1:C:126:GLN:HE22	2.14	0.45
1:C:211:ASP:CG	1:C:213:ARG:HB2	2.36	0.45
1:C:155:THR:OG1	1:C:248:THR:CG2	2.64	0.45
1:D:367:LEU:O	1:D:369:GLU:N	2.50	0.45
1:A:283:ILE:O	1:A:314:ILE:HG23	2.16	0.45
1:A:191:PRO:HD3	1:A:439:GLY:CA	2.47	0.45
1:B:37:ARG:HA	1:B:40:THR:HB	1.99	0.45
1:C:107:TYR:N	1:C:107:TYR:CD2	2.83	0.45
1:C:141:LEU:HD13	1:C:257:ILE:HG12	1.97	0.45
1:C:196:PHE:CG	1:C:197:PRO:CD	2.99	0.45
1:C:306:LEU:HD22	1:C:371:VAL:HG11	1.97	0.45
1:C:191:PRO:HD3	1:C:439:GLY:CA	2.47	0.45
1:C:56:ALA:HB1	1:D:29:TYR:O	2.17	0.45
1:D:159:THR:HG23	1:D:162:GLU:HB2	1.97	0.45
1:D:266:ASP:OD1	1:D:271:ILE:HD11	2.17	0.45
1:D:272:LEU:HD11	1:D:277:ALA:HA	1.98	0.45
1:D:277:ALA:O	1:D:278:PRO:C	2.55	0.45
1:A:108:TYR:CE2	1:B:22:PRO:HD3	2.51	0.45
1:A:286:LEU:HD12	1:A:286:LEU:H	1.82	0.45
1:A:351:LEU:N	1:A:351:LEU:HD13	2.31	0.45
1:A:60:MET:HG3	1:A:99:ARG:HG2	1.97	0.45
1:B:112:LEU:HD22	1:B:112:LEU:N	2.32	0.45
1:B:171:ILE:O	1:B:172:SER:C	2.55	0.45
1:B:41:PHE:CE1	1:B:256:VAL:HG21	2.52	0.45
1:C:405:ILE:CA	1:C:408:ILE:HG22	2.43	0.45
1:D:11:LEU:HD12	1:D:11:LEU:HA	1.74	0.45
1:D:286:LEU:HD11	1:D:338:GLU:CB	2.43	0.45
1:D:336:ARG:NH1	1:D:338:GLU:OE2	2.48	0.45
1:D:387:TRP:O	1:D:391:GLU:HG3	2.17	0.45
1:A:266:ASP:O	1:A:269:GLY:N	2.36	0.45
1:A:338:GLU:HB2	1:A:350:THR:CG2	2.45	0.45
1:A:405:ILE:HD13	1:A:451:ILE:CD1	2.46	0.45
1:B:23:ILE:O	1:B:26:CYS:HB2	2.15	0.45
1:B:60:MET:HG3	1:B:99:ARG:HG2	1.99	0.45
1:C:10:ILE:HD12	1:C:269:GLY:HA2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:MET:HA	1:C:99:ARG:NH1	2.32	0.45
1:D:131:PHE:CE2	1:D:146:GLU:HG3	2.51	0.45
1:D:196:PHE:O	1:D:197:PRO:C	2.55	0.45
1:D:222:ASN:HD22	1:D:224:GLY:H	1.65	0.45
1:D:292:GLU:N	1:D:292:GLU:CD	2.70	0.45
1:A:428:GLU:O	1:A:432:LYS:N	2.50	0.45
1:C:104:THR:N	1:C:105:PRO:HD2	2.32	0.45
1:C:62:ILE:CD1	1:C:105:PRO:HD3	2.46	0.45
1:C:256:VAL:O	1:C:260:ILE:N	2.45	0.45
1:C:430:GLU:O	1:C:434:GLU:N	2.50	0.45
1:D:252:ILE:HG13	1:D:252:ILE:O	2.17	0.45
1:D:30:LEU:O	1:D:31:PRO:C	2.54	0.45
1:D:37:ARG:O	1:D:37:ARG:HG2	2.16	0.45
1:A:60:MET:SD	1:A:131:PHE:HE1	2.40	0.45
1:B:141:LEU:HD13	1:B:257:ILE:HD11	1.98	0.45
1:B:283:ILE:CD1	1:B:283:ILE:H	2.28	0.45
1:B:292:GLU:CD	1:B:292:GLU:N	2.71	0.45
1:B:335:LEU:CD1	1:B:378:ILE:HD11	2.47	0.45
1:B:65:ASP:O	1:B:68:ALA:HB3	2.17	0.45
1:C:157:HIS:HB3	1:C:162:GLU:HB3	1.99	0.45
1:C:256:VAL:HG23	1:C:257:ILE:HG22	1.99	0.45
1:D:351:LEU:HD22	1:D:351:LEU:N	2.32	0.45
1:D:350:THR:CA	1:D:361:GLN:HG2	2.46	0.45
1:A:428:GLU:O	1:A:429:LEU:C	2.56	0.45
1:C:306:LEU:CD2	1:C:371:VAL:HG21	2.39	0.45
1:B:153:ALA:HB3	1:B:250:TYR:CE1	2.52	0.44
1:B:405:ILE:O	1:B:406:LYS:C	2.55	0.44
1:C:235:PHE:C	1:C:235:PHE:CD1	2.90	0.44
1:D:223:LEU:O	1:D:224:GLY:C	2.55	0.44
1:D:405:ILE:O	1:D:406:LYS:C	2.54	0.44
1:D:191:PRO:HB3	1:D:425:TYR:OH	2.17	0.44
1:D:451:ILE:O	1:D:452:ALA:HB2	2.16	0.44
1:C:31:PRO:HG3	1:D:54:ASP:HB3	1.99	0.44
1:A:134:GLU:HA	1:A:134:GLU:OE1	2.16	0.44
1:A:157:HIS:NE2	1:A:166:GLN:HG2	2.33	0.44
1:A:295:VAL:O	1:A:298:LYS:N	2.50	0.44
1:A:302:ILE:HG22	1:A:306:LEU:HD12	1.98	0.44
1:B:387:TRP:O	1:B:391:GLU:HG3	2.17	0.44
1:C:283:ILE:HG22	1:C:314:ILE:HG23	1.99	0.44
1:C:55:GLU:N	2:C:477:HOH:O	2.50	0.44
1:D:159:THR:CG2	1:D:162:GLU:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:THR:HG21	2:D:464:HOH:O	2.16	0.44
1:A:403:ASP:HA	1:A:406:LYS:HD3	1.98	0.44
1:A:402:PRO:O	1:A:406:LYS:HG2	2.17	0.44
1:A:64:GLU:HA	1:A:64:GLU:OE2	2.17	0.44
1:B:11:LEU:HD12	1:B:11:LEU:HA	1.74	0.44
1:B:92:LEU:C	1:B:94:VAL:N	2.71	0.44
1:C:120:LEU:HD13	1:C:157:HIS:O	2.17	0.44
1:C:338:GLU:HB2	1:C:350:THR:CG2	2.45	0.44
1:C:56:ALA:CA	1:D:34:PHE:HD1	2.29	0.44
1:C:100:PRO:CG	1:C:101:THR:H	2.27	0.44
1:C:300:LYS:O	1:C:301:GLU:C	2.54	0.44
1:C:55:GLU:OE1	1:D:38:ARG:NH2	2.47	0.44
1:D:282:VAL:HG11	1:D:328:TRP:NE1	2.33	0.44
1:D:325:PHE:CE1	1:D:338:GLU:HG2	2.52	0.44
1:A:66:LEU:HB3	1:A:104:THR:HG22	2.00	0.44
1:A:62:ILE:CD1	1:A:105:PRO:HD3	2.47	0.44
1:A:67:LEU:HD11	1:A:77:PHE:CE2	2.48	0.44
1:B:100:PRO:HG2	1:B:101:THR:H	1.82	0.44
1:B:223:LEU:O	1:B:224:GLY:C	2.56	0.44
1:B:252:ILE:O	1:B:252:ILE:HG13	2.17	0.44
1:B:313:HIS:HD2	1:B:328:TRP:CZ2	2.35	0.44
1:B:343:ASP:O	1:B:348:LYS:N	2.47	0.44
1:B:406:LYS:O	1:B:409:LEU:HB2	2.17	0.44
1:C:23:ILE:O	1:C:24:LYS:O	2.35	0.44
1:A:191:PRO:C	1:A:193:TRP:H	2.21	0.44
1:A:56:ALA:HB1	1:B:29:TYR:O	2.18	0.44
1:B:103:GLU:O	1:B:104:THR:C	2.55	0.44
1:B:23:ILE:O	1:B:24:LYS:C	2.54	0.44
1:C:319:ILE:CG1	1:C:320:ARG:N	2.80	0.44
1:C:83:TRP:CE3	1:C:97:ALA:HB2	2.53	0.44
1:D:69:LYS:C	1:D:71:ALA:N	2.70	0.44
1:A:196:PHE:CG	1:A:197:PRO:CD	3.00	0.44
1:A:83:TRP:CE3	1:A:97:ALA:HB2	2.53	0.44
1:B:177:PHE:CZ	1:B:181:LEU:HD11	2.53	0.44
1:B:270:LEU:HG	1:B:272:LEU:HD23	1.98	0.44
1:B:367:LEU:C	1:B:369:GLU:N	2.71	0.44
1:C:86:HIS:CD2	2:C:460:HOH:O	2.71	0.44
1:D:104:THR:HB	1:D:105:PRO:CD	2.48	0.44
1:D:114:VAL:HG22	1:D:120:LEU:HD21	1.98	0.44
1:D:123:LYS:HG2	1:D:155:THR:HG22	2.00	0.44
1:D:183:ILE:HA	1:D:184:PRO:HD3	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:ASP:O	1:D:348:LYS:N	2.48	0.44
1:A:100:PRO:CG	1:A:101:THR:H	2.28	0.44
1:A:178:PHE:O	1:A:182:GLY:N	2.51	0.44
1:A:274:PRO:HD2	1:A:275:ILE:HD12	1.99	0.44
1:A:214:THR:HG23	1:A:453:LYS:O	2.17	0.44
1:B:364:GLU:C	1:B:366:GLN:N	2.71	0.44
1:C:36:ILE:O	1:C:36:ILE:CG1	2.66	0.44
1:D:103:GLU:O	1:D:104:THR:C	2.55	0.44
1:D:174:TYR:O	1:D:177:PHE:HB3	2.18	0.44
1:D:21:TYR:CD2	1:D:22:PRO:HD2	2.52	0.44
1:D:141:LEU:HD13	1:D:257:ILE:HD11	1.99	0.44
1:D:273:PRO:HB3	1:D:379:MET:SD	2.57	0.44
1:A:319:ILE:CG1	1:A:320:ARG:N	2.81	0.44
1:C:270:LEU:O	1:C:354:ARG:NH1	2.51	0.44
1:C:355:ASP:OD2	1:C:356:THR:N	2.49	0.44
1:C:384:ASN:O	1:C:385:ARG:C	2.55	0.44
1:D:101:THR:O	1:D:103:GLU:N	2.50	0.44
1:D:108:TYR:O	1:D:111:LYS:HB3	2.18	0.44
1:A:115:LYS:O	1:A:235:PHE:HA	2.18	0.43
1:A:21:TYR:CG	1:B:59:PRO:HG2	2.53	0.43
1:A:321:PRO:O	1:A:324:LYS:HB2	2.18	0.43
1:A:366:GLN:HA	1:A:366:GLN:HE21	1.83	0.43
1:A:448:TYR:N	1:A:448:TYR:CD1	2.86	0.43
1:C:279:ILE:O	1:C:333:VAL:HG13	2.18	0.43
1:C:405:ILE:HD13	1:C:451:ILE:CD1	2.47	0.43
1:D:189:LYS:O	1:D:189:LYS:HG2	2.18	0.43
1:D:37:ARG:HA	1:D:40:THR:HB	2.00	0.43
1:A:102:SER:C	1:A:105:PRO:HD2	2.39	0.43
1:A:102:SER:HB3	1:A:152:GLU:OE1	2.18	0.43
1:B:266:ASP:OD1	1:B:271:ILE:HD11	2.18	0.43
1:C:191:PRO:C	1:C:193:TRP:H	2.22	0.43
1:C:286:LEU:HD12	1:C:286:LEU:H	1.83	0.43
1:C:428:GLU:O	1:C:432:LYS:N	2.52	0.43
1:D:291:LYS:N	1:D:292:GLU:OE2	2.51	0.43
1:B:398:GLU:OE1	1:B:399:ASP:N	2.51	0.43
1:C:10:ILE:C	1:C:12:GLU:N	2.70	0.43
1:C:448:TYR:N	1:C:448:TYR:CD1	2.86	0.43
1:C:214:THR:HG23	1:C:453:LYS:O	2.17	0.43
1:D:207:THR:HG23	1:D:215:MET:HB3	1.99	0.43
1:D:60:MET:HG3	1:D:99:ARG:HG2	2.00	0.43
1:D:91:GLN:HG2	1:D:93:ASP:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:HIS:HB3	1:A:162:GLU:HB3	2.00	0.43
1:A:373:LYS:HZ2	1:A:373:LYS:HB2	1.81	0.43
1:A:437:ILE:HG22	1:A:439:GLY:N	2.32	0.43
1:A:55:GLU:OE1	1:B:38:ARG:NH2	2.49	0.43
1:B:183:ILE:HA	1:B:184:PRO:HD3	1.75	0.43
1:B:291:LYS:N	1:B:292:GLU:OE2	2.51	0.43
1:B:335:LEU:HD11	1:B:374:THR:CG2	2.45	0.43
1:C:127:ILE:HA	1:C:151:LYS:HA	2.00	0.43
1:C:248:THR:HG23	1:C:248:THR:O	2.18	0.43
1:D:186:LEU:HD21	1:D:441:THR:OG1	2.17	0.43
1:D:82:TYR:HB2	1:D:98:LEU:HB2	1.99	0.43
1:A:16:ILE:HG21	1:A:261:ILE:HD11	2.01	0.43
1:A:36:ILE:O	1:A:36:ILE:CG1	2.66	0.43
1:C:105:PRO:O	1:C:109:MET:HG2	2.18	0.43
1:C:157:HIS:NE2	1:C:166:GLN:HG2	2.34	0.43
1:C:142:ILE:CG2	1:C:215:MET:HE2	2.47	0.43
1:C:429:LEU:O	1:C:432:LYS:HB3	2.18	0.43
1:D:261:ILE:HG22	1:D:262:ALA:N	2.33	0.43
1:D:351:LEU:HB2	1:D:360:PHE:CE2	2.53	0.43
1:A:283:ILE:O	1:A:314:ILE:HA	2.19	0.43
1:A:300:LYS:O	1:A:301:GLU:C	2.55	0.43
1:B:82:TYR:HB2	1:B:98:LEU:HB2	2.00	0.43
1:C:208:ILE:HG21	1:C:414:GLY:HA2	2.00	0.43
1:C:226:ASN:HD22	1:C:226:ASN:N	2.16	0.43
1:C:295:VAL:O	1:C:298:LYS:N	2.51	0.43
1:D:58:PHE:N	1:D:126:GLN:NE2	2.59	0.43
1:A:24:LYS:NZ	1:A:137:HIS:CD2	2.86	0.43
1:A:320:ARG:C	1:A:322:GLY:N	2.69	0.43
1:A:59:PRO:HG2	1:B:21:TYR:CE1	2.54	0.43
1:A:71:ALA:HA	1:A:75:LYS:CE	2.31	0.43
1:B:272:LEU:HA	1:B:273:PRO:HD3	1.85	0.43
1:B:315:ASP:OD2	1:B:324:LYS:HD3	2.19	0.43
1:C:362:VAL:HG21	1:C:370:VAL:HG21	2.01	0.43
1:D:360:PHE:CD2	1:D:360:PHE:N	2.84	0.43
1:D:367:LEU:C	1:D:369:GLU:N	2.72	0.43
1:A:10:ILE:C	1:A:12:GLU:N	2.70	0.43
1:A:341:PRO:C	1:A:343:ASP:N	2.71	0.43
1:B:104:THR:HB	1:B:105:PRO:HD3	2.01	0.43
1:B:207:THR:HG23	1:B:215:MET:HB3	1.99	0.43
1:B:286:LEU:HD12	1:B:286:LEU:N	2.15	0.43
1:C:16:ILE:HD13	1:C:261:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:ILE:O	1:C:261:ILE:HG13	2.19	0.43
1:C:36:ILE:O	1:C:40:THR:OG1	2.36	0.43
1:C:406:LYS:HB3	1:C:433:VAL:O	2.18	0.43
1:D:41:PHE:CE1	1:D:256:VAL:HG21	2.54	0.43
1:D:315:ASP:OD2	1:D:324:LYS:HD3	2.19	0.43
1:A:211:ASP:OD1	1:A:213:ARG:HB2	2.19	0.43
1:B:360:PHE:N	1:B:360:PHE:CD2	2.84	0.43
1:D:283:ILE:H	1:D:283:ILE:CD1	2.30	0.43
1:D:49:ASP:C	1:D:51:SER:H	2.22	0.43
1:A:279:ILE:O	1:A:333:VAL:HG13	2.19	0.43
1:A:351:LEU:O	1:A:359:LYS:HG3	2.19	0.43
1:B:36:ILE:O	1:B:36:ILE:HD13	2.18	0.43
1:B:40:THR:HG22	1:B:41:PHE:CD1	2.54	0.43
1:C:376:ASN:O	1:C:377:ASN:C	2.57	0.43
1:A:281:VAL:HB	1:A:312:VAL:HG12	2.01	0.42
1:A:84:VAL:HG11	1:B:82:TYR:CD2	2.54	0.42
1:C:190:ARG:HH21	1:C:216:GLN:NE2	2.15	0.42
1:C:208:ILE:CD1	1:C:415:VAL:HG12	2.49	0.42
1:A:341:PRO:C	1:A:343:ASP:H	2.22	0.42
1:A:376:ASN:O	1:A:377:ASN:C	2.57	0.42
1:A:60:MET:HA	1:A:99:ARG:HH11	1.83	0.42
1:B:10:ILE:HD11	1:B:270:LEU:CB	2.33	0.42
1:B:91:GLN:HG2	1:B:93:ASP:H	1.84	0.42
1:C:370:VAL:O	1:C:371:VAL:C	2.57	0.42
1:D:23:ILE:O	1:D:26:CYS:HB2	2.19	0.42
1:A:405:ILE:HD13	1:A:451:ILE:HD12	2.02	0.42
1:A:74:ILE:O	1:A:74:ILE:CG2	2.67	0.42
1:B:105:PRO:HG2	1:B:106:ILE:H	1.84	0.42
1:B:10:ILE:O	1:B:12:GLU:N	2.52	0.42
1:B:125:TYR:HB2	1:B:153:ALA:HA	2.01	0.42
1:B:271:ILE:HG12	1:B:354:ARG:HH12	1.76	0.42
1:B:350:THR:CA	1:B:361:GLN:HG2	2.48	0.42
1:C:269:GLY:O	1:C:270:LEU:O	2.37	0.42
1:C:33:GLY:HA2	1:C:36:ILE:CG2	2.49	0.42
1:C:403:ASP:HA	1:C:406:LYS:HD3	1.99	0.42
1:C:57:LEU:HD23	1:D:148:MET:HB3	1.99	0.42
1:C:71:ALA:HA	1:C:75:LYS:CE	2.31	0.42
1:D:321:PRO:HG3	2:D:469:HOH:O	2.18	0.42
1:C:84:VAL:HG21	1:D:98:LEU:HD11	2.00	0.42
1:B:433:VAL:O	1:B:434:GLU:C	2.58	0.42
1:C:92:LEU:O	1:C:94:VAL:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:MET:HG3	1:C:99:ARG:HG2	1.99	0.42
1:D:63:PRO:HG2	1:D:66:LEU:HD13	2.01	0.42
1:A:362:VAL:HG22	1:A:363:ASP:N	2.34	0.42
1:B:66:LEU:HB3	1:B:104:THR:CG2	2.48	0.42
1:B:99:ARG:HH21	1:B:129:ASN:H	1.66	0.42
1:C:99:ARG:HH21	1:C:129:ASN:H	1.67	0.42
1:C:211:ASP:OD1	1:C:213:ARG:HB2	2.20	0.42
1:D:177:PHE:CZ	1:D:181:LEU:HD11	2.55	0.42
1:D:364:GLU:C	1:D:366:GLN:N	2.73	0.42
1:A:125:TYR:C	1:A:125:TYR:CD1	2.92	0.42
1:A:279:ILE:HD13	1:A:313:HIS:HB3	2.01	0.42
1:B:192:GLU:O	1:B:194:ASP:N	2.53	0.42
1:C:101:THR:CG2	1:C:102:SER:H	2.14	0.42
1:C:256:VAL:O	1:C:259:SER:N	2.53	0.42
1:D:398:GLU:OE1	1:D:399:ASP:N	2.52	0.42
1:A:107:TYR:CD2	1:A:107:TYR:N	2.87	0.42
1:A:105:PRO:O	1:A:109:MET:HG2	2.19	0.42
1:A:127:ILE:HA	1:A:151:LYS:HA	2.01	0.42
1:A:405:ILE:HA	1:A:408:ILE:CG2	2.47	0.42
1:A:92:LEU:O	1:A:94:VAL:N	2.52	0.42
1:B:152:GLU:O	1:B:152:GLU:HG3	2.19	0.42
1:B:247:GLN:C	1:B:248:THR:HG22	2.40	0.42
1:C:142:ILE:HD13	1:C:215:MET:HE1	2.00	0.42
1:C:356:THR:OG1	1:C:358:GLU:HG2	2.19	0.42
1:C:37:ARG:HA	1:C:40:THR:HB	2.02	0.42
1:D:34:PHE:CE2	1:D:37:ARG:NH1	2.87	0.42
1:A:101:THR:CG2	1:A:102:SER:H	2.12	0.42
1:A:104:THR:N	1:A:105:PRO:HD2	2.35	0.42
1:B:228:SER:OG	1:B:245:ALA:O	2.30	0.42
1:B:277:ALA:O	1:B:278:PRO:C	2.59	0.42
1:B:373:LYS:HB2	1:B:373:LYS:HZ2	1.85	0.42
1:C:2:GLU:HG3	1:C:3:PHE:N	2.35	0.42
1:C:341:PRO:C	1:C:343:ASP:H	2.22	0.42
1:C:341:PRO:C	1:C:343:ASP:N	2.72	0.42
1:D:247:GLN:C	1:D:248:THR:HG22	2.40	0.42
1:D:39:TYR:CD2	1:D:311:ARG:NH1	2.87	0.42
1:A:283:ILE:HB	1:A:314:ILE:HG12	2.01	0.42
1:B:351:LEU:HD22	1:B:351:LEU:N	2.35	0.42
1:C:14:ALA:O	1:C:15:GLU:HB2	2.19	0.42
1:C:402:PRO:O	1:C:406:LYS:HG2	2.20	0.42
1:D:191:PRO:HB3	1:D:425:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:O	1:A:40:THR:OG1	2.37	0.42
1:A:56:ALA:CA	1:B:34:PHE:HD1	2.32	0.42
1:B:416:ILE:HA	1:B:416:ILE:HD13	1.89	0.42
1:C:58:PHE:CD1	1:C:126:GLN:NE2	2.83	0.42
1:C:284:VAL:HG11	1:C:325:PHE:HE1	1.84	0.42
1:C:335:LEU:HD12	1:C:352:PHE:O	2.20	0.42
1:C:428:GLU:O	1:C:429:LEU:C	2.58	0.42
1:C:437:ILE:HG22	1:C:439:GLY:N	2.34	0.42
1:D:270:LEU:HG	1:D:272:LEU:HD23	2.00	0.42
1:D:355:ASP:OD2	1:D:355:ASP:N	2.53	0.42
1:D:385:ARG:HG3	1:D:385:ARG:HH11	1.85	0.42
1:A:104:THR:HB	1:A:105:PRO:HD3	2.01	0.41
1:A:37:ARG:HA	1:A:40:THR:HB	2.02	0.41
1:B:344:ILE:C	1:B:344:ILE:HD12	2.39	0.41
1:C:222:ASN:ND2	1:C:222:ASN:C	2.72	0.41
1:C:56:ALA:HA	1:D:34:PHE:HD1	1.85	0.41
1:C:59:PRO:HA	1:D:148:MET:HE3	2.01	0.41
1:A:112:LEU:O	1:A:113:TRP:HD1	2.03	0.41
1:A:151:LYS:HE2	1:A:151:LYS:O	2.19	0.41
1:B:107:TYR:C	1:B:109:MET:N	2.73	0.41
1:C:99:ARG:HA	1:C:100:PRO:HD2	1.95	0.41
1:D:39:TYR:O	1:D:40:THR:C	2.58	0.41
1:A:103:GLU:HB2	1:A:107:TYR:CE1	2.55	0.41
1:B:10:ILE:C	1:B:12:GLU:N	2.73	0.41
1:A:21:TYR:CD2	1:B:59:PRO:HG2	2.55	0.41
1:C:125:TYR:CD1	1:C:125:TYR:C	2.93	0.41
1:C:134:GLU:OE1	1:C:134:GLU:HA	2.19	0.41
1:C:405:ILE:HA	1:C:408:ILE:CG2	2.47	0.41
1:C:66:LEU:HD12	1:C:66:LEU:N	2.36	0.41
1:D:82:TYR:OH	1:D:145:ARG:NH1	2.51	0.41
1:A:103:GLU:HG2	1:A:104:THR:N	2.36	0.41
1:A:107:TYR:HB3	1:A:233:ILE:HD11	2.02	0.41
1:A:35:LYS:HZ3	1:A:38:ARG:NH2	2.18	0.41
1:A:57:LEU:HD23	1:B:148:MET:HB3	2.01	0.41
1:B:178:PHE:CD2	1:B:217:ILE:HD12	2.55	0.41
1:B:351:LEU:HB2	1:B:360:PHE:CE2	2.54	0.41
1:B:34:PHE:CE2	1:B:37:ARG:NH1	2.88	0.41
1:C:405:ILE:HD13	1:C:451:ILE:HD12	2.03	0.41
1:D:373:LYS:HZ2	1:D:373:LYS:HB2	1.86	0.41
1:D:415:VAL:HG23	1:D:452:ALA:HB2	2.02	0.41
1:D:416:ILE:HA	1:D:416:ILE:HD13	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LYS:O	1:A:231:PHE:N	2.54	0.41
1:B:106:ILE:HG22	1:B:106:ILE:O	2.20	0.41
1:B:139:ARG:HB2	1:B:143:ARG:H	1.84	0.41
1:C:170:ALA:O	1:C:173:ILE:N	2.53	0.41
1:C:171:ILE:O	1:C:175:LYS:HB2	2.20	0.41
1:C:282:VAL:HG11	1:C:328:TRP:CD1	2.56	0.41
1:C:60:MET:HA	1:C:99:ARG:HH11	1.84	0.41
1:D:139:ARG:HB2	1:D:143:ARG:H	1.84	0.41
1:D:310:PHE:CZ	1:D:372:GLU:HA	2.56	0.41
1:C:287:ILE:O	1:C:287:ILE:HG13	2.21	0.41
1:C:320:ARG:C	1:C:322:GLY:N	2.70	0.41
1:C:67:LEU:HD11	1:C:77:PHE:CE2	2.50	0.41
1:A:190:ARG:HH21	1:A:216:GLN:NE2	2.17	0.41
1:B:324:LYS:O	1:B:325:PHE:C	2.59	0.41
1:B:325:PHE:HD1	1:B:336:ARG:HD3	1.81	0.41
1:B:39:TYR:O	1:B:40:THR:C	2.59	0.41
1:B:45:ARG:HE	1:B:127:ILE:HD12	1.85	0.41
1:C:229:LYS:O	1:C:231:PHE:N	2.54	0.41
1:C:274:PRO:HD2	1:C:275:ILE:CD1	2.51	0.41
1:A:127:ILE:HG12	1:A:151:LYS:HG3	2.03	0.41
1:A:384:ASN:O	1:A:385:ARG:C	2.58	0.41
1:C:103:GLU:HG2	1:C:104:THR:N	2.36	0.41
1:C:55:GLU:HB3	2:C:477:HOH:O	2.20	0.41
1:D:14:ALA:O	1:D:15:GLU:HB2	2.20	0.41
1:D:125:TYR:HB2	1:D:153:ALA:HA	2.02	0.41
1:D:192:GLU:O	1:D:194:ASP:N	2.54	0.41
1:D:225:GLN:O	1:D:226:ASN:C	2.58	0.41
1:A:43:ILE:O	1:A:47:LEU:HG	2.20	0.41
1:B:310:PHE:CZ	1:B:372:GLU:HA	2.56	0.41
1:B:355:ASP:OD2	1:B:355:ASP:N	2.54	0.41
1:B:415:VAL:HG23	1:B:452:ALA:HB2	2.02	0.41
1:B:186:LEU:HD21	1:B:441:THR:OG1	2.20	0.41
1:C:16:ILE:HG21	1:C:261:ILE:HD11	2.03	0.41
1:C:270:LEU:HB3	1:C:332:GLY:HA3	2.02	0.41
1:D:190:ARG:HB2	1:D:202:THR:O	2.21	0.41
1:A:16:ILE:HD13	1:A:261:ILE:HD11	2.03	0.41
1:A:353:ARG:NH2	1:A:377:ASN:OD1	2.54	0.41
1:B:124:ILE:O	1:B:154:HIS:N	2.54	0.41
1:B:174:TYR:O	1:B:177:PHE:HB3	2.21	0.41
1:B:223:LEU:HD13	1:B:227:PHE:HD2	1.86	0.41
1:C:24:LYS:NZ	1:C:137:HIS:CD2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ILE:CG2	1:C:74:ILE:O	2.69	0.41
1:D:107:TYR:C	1:D:109:MET:N	2.74	0.41
1:A:142:ILE:CG2	1:A:215:MET:HE2	2.49	0.41
1:A:436:THR:O	1:A:436:THR:HG22	2.20	0.41
1:B:297:GLU:C	1:B:299:ALA:N	2.74	0.41
1:C:99:ARG:CZ	1:C:128:VAL:HB	2.51	0.41
1:C:257:ILE:HA	1:C:260:ILE:HD12	2.03	0.41
1:D:163:ALA:O	1:D:166:GLN:N	2.52	0.41
1:D:256:VAL:HG23	1:D:257:ILE:N	2.34	0.41
1:D:328:TRP:HA	1:D:328:TRP:CE3	2.55	0.41
1:B:222:ASN:ND2	1:B:224:GLY:H	2.19	0.40
1:B:329:GLU:HG2	1:B:354:ARG:NE	2.36	0.40
1:D:152:GLU:HG3	1:D:152:GLU:O	2.21	0.40
1:D:324:LYS:O	1:D:325:PHE:C	2.60	0.40
1:D:36:ILE:O	1:D:36:ILE:HD13	2.20	0.40
1:C:21:TYR:CG	1:D:59:PRO:HG2	2.56	0.40
1:A:256:VAL:O	1:A:259:SER:N	2.55	0.40
1:A:287:ILE:HG13	1:A:287:ILE:O	2.21	0.40
1:B:237:THR:C	1:B:239:THR:H	2.24	0.40
1:B:37:ARG:O	1:B:37:ARG:HG2	2.21	0.40
1:B:191:PRO:HB3	1:B:425:TYR:CE2	2.56	0.40
1:C:115:LYS:O	1:C:235:PHE:HA	2.21	0.40
1:C:60:MET:SD	1:C:131:PHE:HE1	2.44	0.40
1:D:189:LYS:O	1:D:190:ARG:O	2.39	0.40
1:D:228:SER:OG	1:D:245:ALA:O	2.30	0.40
1:D:7:TYR:O	1:D:8:SER:C	2.58	0.40
1:A:10:ILE:CD1	1:A:270:LEU:N	2.75	0.40
1:B:32:TYR:CE1	1:B:278:PRO:HB2	2.57	0.40
1:C:190:ARG:HH12	1:C:438:LEU:HD22	1.85	0.40
1:C:205:PHE:CG	1:C:218:ALA:HB3	2.56	0.40
1:D:202:THR:O	1:D:202:THR:HG22	2.21	0.40
1:D:208:ILE:HD11	1:D:415:VAL:HG12	2.03	0.40
1:D:405:ILE:O	1:D:408:ILE:N	2.54	0.40
1:D:397:LEU:HD13	1:D:416:ILE:HG23	2.02	0.40
1:A:66:LEU:H	1:A:66:LEU:CD1	2.32	0.40
1:B:370:VAL:O	1:B:371:VAL:C	2.60	0.40
1:C:191:PRO:HB2	1:C:193:TRP:CE3	2.56	0.40
1:C:351:LEU:O	1:C:359:LYS:HG3	2.21	0.40
1:C:432:LYS:HA	1:C:432:LYS:HD2	1.91	0.40
1:D:157:HIS:HD1	1:D:162:GLU:HG2	1.87	0.40
1:D:23:ILE:O	1:D:24:LYS:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:PHE:HD2	1:D:360:PHE:N	2.19	0.40
1:A:107:TYR:O	1:A:108:TYR:C	2.60	0.40
1:A:24:LYS:HZ3	1:A:137:HIS:CD2	2.40	0.40
1:C:107:TYR:C	1:C:109:MET:N	2.73	0.40
1:C:139:ARG:HH11	1:C:139:ARG:HG2	1.87	0.40
1:C:237:THR:C	1:C:239:THR:N	2.75	0.40
1:C:276:VAL:O	1:C:278:PRO:HD3	2.22	0.40
1:C:395:THR:HG21	1:C:408:ILE:HD11	2.03	0.40
1:D:10:ILE:O	1:D:12:GLU:N	2.55	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:NH1	1:C:323:ARG:NH1[2_646]	1.95	0.25
1:A:293:ASP:OD1	1:D:392:ASN:OD1[1_554]	2.10	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	454/459 (99%)	331 (73%)	84 (18%)	39 (9%)	1	4
1	B	454/459 (99%)	313 (69%)	104 (23%)	37 (8%)	1	5
1	C	454/459 (99%)	330 (73%)	85 (19%)	39 (9%)	1	4
1	D	454/459 (99%)	312 (69%)	107 (24%)	35 (8%)	1	6
All	All	1816/1836 (99%)	1286 (71%)	380 (21%)	150 (8%)	1	5

All (150) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	A	74	ILE
1	A	75	LYS
1	A	76	GLY
1	A	102	SER
1	A	262	ALA
1	A	263	ILE
1	A	270	LEU
1	A	272	LEU
1	A	317	ARG
1	A	354	ARG
1	B	102	SER
1	B	316	ASP
1	B	446	ASN
1	C	36	ILE
1	C	74	ILE
1	C	75	LYS
1	C	76	GLY
1	C	102	SER
1	C	262	ALA
1	C	263	ILE
1	C	270	LEU
1	C	272	LEU
1	C	317	ARG
1	C	354	ARG
1	D	93	ASP
1	D	102	SER
1	D	190	ARG
1	D	316	ASP
1	D	446	ASN
1	A	65	ASP
1	A	271	ILE
1	A	303	TYR
1	A	423	GLU
1	B	22	PRO
1	B	27	GLY
1	B	76	GLY
1	B	93	ASP
1	B	190	ARG
1	B	248	THR
1	B	317	ARG
1	C	65	ASP
1	C	230	THR

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Mol	Chain	Res	Type
1	C	271	ILE
1	C	303	TYR
1	C	423	GLU
1	D	22	PRO
1	D	27	GLY
1	D	76	GLY
1	D	95	LYS
1	D	193	TRP
1	D	248	THR
1	D	317	ARG
1	D	334	PRO
1	A	4	SER
1	A	11	LEU
1	A	22	PRO
1	A	24	LYS
1	A	31	PRO
1	A	123	LYS
1	A	132	ARG
1	A	133	TYR
1	A	197	PRO
1	A	230	THR
1	A	411	GLU
1	B	65	ASP
1	B	95	LYS
1	B	188	SER
1	B	193	TRP
1	B	267	GLU
1	B	296	MET
1	B	307	LYS
1	B	334	PRO
1	B	368	MET
1	B	411	GLU
1	C	4	SER
1	C	11	LEU
1	C	22	PRO
1	C	24	LYS
1	C	123	LYS
1	C	132	ARG
1	C	133	TYR
1	C	197	PRO
1	C	241	ASP
1	C	411	GLU

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Mol	Chain	Res	Type
1	C	436	THR
1	D	65	ASP
1	D	188	SER
1	D	267	GLU
1	D	296	MET
1	D	368	MET
1	D	411	GLU
1	A	3	PHE
1	A	192	GLU
1	A	241	ASP
1	A	436	THR
1	B	7	TYR
1	B	50	GLU
1	B	67	LEU
1	B	100	PRO
1	B	136	LYS
1	B	400	ILE
1	C	3	PHE
1	C	31	PRO
1	C	100	PRO
1	C	192	GLU
1	D	7	TYR
1	D	100	PRO
1	D	189	LYS
1	D	307	LYS
1	D	400	ILE
1	D	403	ASP
1	A	100	PRO
1	A	248	THR
1	A	341	PRO
1	A	367	LEU
1	A	400	ILE
1	B	189	LYS
1	B	403	ASP
1	C	141	LEU
1	C	341	PRO
1	C	367	LEU
1	C	400	ILE
1	D	50	GLU
1	D	67	LEU
1	D	136	LYS
1	A	77	PHE

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Mol	Chain	Res	Type
1	C	77	PHE
1	A	23	ILE
1	A	142	ILE
1	B	25	GLY
1	B	171	ILE
1	B	405	ILE
1	C	23	ILE
1	D	25	GLY
1	D	405	ILE
1	A	319	ILE
1	B	74	ILE
1	B	371	VAL
1	C	142	ILE
1	D	74	ILE
1	D	171	ILE
1	D	371	VAL
1	B	142	ILE
1	C	319	ILE
1	D	142	ILE
1	D	370	VAL
1	B	128	VAL
1	B	197	PRO
1	B	370	VAL

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	412/414 (100%)	373 (90%)	39 (10%)	8	32
1	B	412/414 (100%)	373 (90%)	39 (10%)	8	32
1	C	412/414 (100%)	370 (90%)	42 (10%)	7	29
1	D	412/414 (100%)	374 (91%)	38 (9%)	9	33
All	All	1648/1656 (100%)	1490 (90%)	158 (10%)	8	32

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	28	VAL
1	A	36	ILE
1	A	64	GLU
1	A	94	VAL
1	A	103	GLU
1	A	122	ILE
1	A	125	TYR
1	A	132	ARG
1	A	137	HIS
1	A	211	ASP
1	A	216	GLN
1	A	222	ASN
1	A	250	TYR
1	A	257	ILE
1	A	270	LEU
1	A	275	ILE
1	A	303	TYR
1	A	315	ASP
1	A	323	ARG
1	A	351	LEU
1	A	360	PHE
1	A	369	GLU
1	A	382	ILE
1	A	389	LYS
1	A	392	ASN
1	A	393	PHE
1	A	396	ILE
1	A	398	GLU
1	A	401	ASN
1	A	403	ASP
1	A	413	ARG
1	A	417	LEU
1	A	426	ASN
1	A	442	GLU
1	A	446	ASN
1	A	447	LYS
1	A	448	TYR
1	A	454	THR
1	B	1	LEU
1	B	26	CYS
1	B	28	VAL
1	B	31	PRO

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Mol	Chain	Res	Type
1	B	34	PHE
1	B	36	ILE
1	B	37	ARG
1	B	77	PHE
1	B	78	GLU
1	B	124	ILE
1	B	164	GLU
1	B	186	LEU
1	B	190	ARG
1	B	192	GLU
1	B	197	PRO
1	B	222	ASN
1	B	243	ASP
1	B	247	GLN
1	B	248	THR
1	B	256	VAL
1	B	257	ILE
1	B	267	GLU
1	B	272	LEU
1	B	275	ILE
1	B	278	PRO
1	B	286	LEU
1	B	293	ASP
1	B	303	TYR
1	B	321	PRO
1	B	327	ASP
1	B	339	VAL
1	B	354	ARG
1	B	360	PHE
1	B	372	GLU
1	B	398	GLU
1	B	401	ASN
1	B	437	ILE
1	B	441	THR
1	B	442	GLU
1	C	1	LEU
1	C	28	VAL
1	C	31	PRO
1	C	36	ILE
1	C	64	GLU
1	C	94	VAL
1	C	103	GLU

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Mol	Chain	Res	Type
1	C	122	ILE
1	C	125	TYR
1	C	132	ARG
1	C	137	HIS
1	C	185	TYR
1	C	211	ASP
1	C	216	GLN
1	C	222	ASN
1	C	247	GLN
1	C	250	TYR
1	C	257	ILE
1	C	270	LEU
1	C	275	ILE
1	C	303	TYR
1	C	315	ASP
1	C	323	ARG
1	C	351	LEU
1	C	360	PHE
1	C	369	GLU
1	C	382	ILE
1	C	389	LYS
1	C	392	ASN
1	C	393	PHE
1	C	396	ILE
1	C	398	GLU
1	C	401	ASN
1	C	403	ASP
1	C	413	ARG
1	C	417	LEU
1	C	426	ASN
1	C	442	GLU
1	C	446	ASN
1	C	447	LYS
1	C	448	TYR
1	C	454	THR
1	D	1	LEU
1	D	9	ASP
1	D	26	CYS
1	D	28	VAL
1	D	31	PRO
1	D	34	PHE
1	D	36	ILE

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Mol	Chain	Res	Type
1	D	37	ARG
1	D	77	PHE
1	D	78	GLU
1	D	124	ILE
1	D	164	GLU
1	D	186	LEU
1	D	190	ARG
1	D	192	GLU
1	D	197	PRO
1	D	222	ASN
1	D	243	ASP
1	D	247	GLN
1	D	248	THR
1	D	256	VAL
1	D	257	ILE
1	D	267	GLU
1	D	272	LEU
1	D	275	ILE
1	D	286	LEU
1	D	303	TYR
1	D	321	PRO
1	D	327	ASP
1	D	339	VAL
1	D	354	ARG
1	D	360	PHE
1	D	372	GLU
1	D	398	GLU
1	D	401	ASN
1	D	437	ILE
1	D	441	THR
1	D	442	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	126	GLN
1	A	137	HIS
1	A	216	GLN
1	A	222	ASN
1	A	225	GLN
1	A	226	ASN

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Mol	Chain	Res	Type
1	A	247	GLN
1	A	366	GLN
1	A	381	ASN
1	A	384	ASN
1	A	401	ASN
1	B	46	ASN
1	B	126	GLN
1	B	137	HIS
1	B	216	GLN
1	B	222	ASN
1	B	225	GLN
1	B	226	ASN
1	B	247	GLN
1	B	313	HIS
1	B	366	GLN
1	B	384	ASN
1	B	401	ASN
1	B	446	ASN
1	C	46	ASN
1	C	126	GLN
1	C	137	HIS
1	C	216	GLN
1	C	222	ASN
1	C	225	GLN
1	C	226	ASN
1	C	247	GLN
1	C	366	GLN
1	C	381	ASN
1	C	384	ASN
1	C	401	ASN
1	D	46	ASN
1	D	126	GLN
1	D	137	HIS
1	D	216	GLN
1	D	222	ASN
1	D	225	GLN
1	D	226	ASN
1	D	247	GLN
1	D	313	HIS
1	D	346	ASN
1	D	366	GLN
1	D	384	ASN

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Mol	Chain	Res	Type
1	D	401	ASN
1	D	446	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	456/459 (99%)	-0.45	7 (1%) 73 61	10, 49, 112, 140	0
1	B	456/459 (99%)	-0.30	4 (0%) 84 75	17, 69, 129, 144	0
1	C	456/459 (99%)	-0.44	3 (0%) 87 81	11, 49, 111, 140	0
1	D	456/459 (99%)	-0.25	8 (1%) 68 55	16, 69, 129, 144	0
All	All	1824/1836 (99%)	-0.36	22 (1%) 79 67	10, 58, 122, 144	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	HIS	6.3
1	B	74	ILE	4.7
1	C	73	HIS	4.5
1	D	74	ILE	4.0
1	B	73	HIS	3.7
1	D	73	HIS	3.3
1	C	289	LYS	3.2
1	D	435	ALA	3.2
1	C	0	MET	2.9
1	B	442	GLU	2.8
1	A	87	GLY	2.8
1	A	89	LYS	2.5
1	A	74	ILE	2.3
1	D	135	THR	2.2
1	A	90	THR	2.2
1	D	411	GLU	2.2
1	D	432	LYS	2.1
1	A	289	LYS	2.1
1	D	429	LEU	2.1
1	B	431	GLU	2.1
1	A	0	MET	2.0
1	D	433	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.