



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:00 AM UTC

PDB ID : 1KOH / pdb_00001koh
Title : THE CRYSTAL STRUCTURE AND MUTATIONAL ANALYSIS OF A NOVEL RNA-BINDING DOMAIN FOUND IN THE HUMAN TAP NUCLEAR MRNA EXPORT FACTOR
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Deposited on : 2001-12-20
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

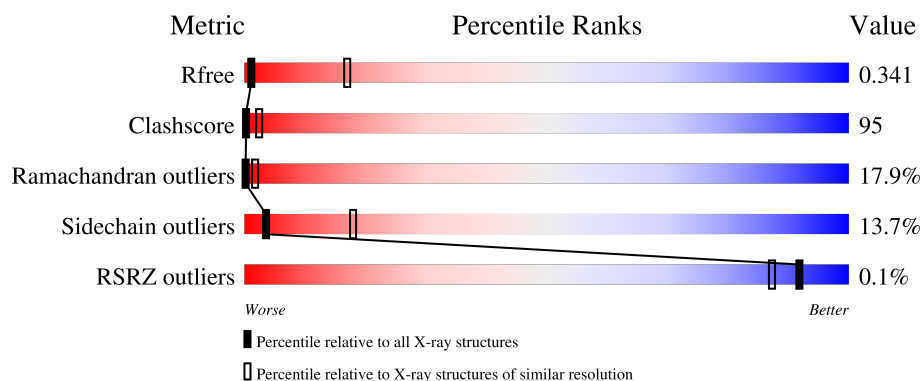
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	277	
1	B	277	
1	C	277	
1	D	277	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6854 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 TIP ASSOCIATING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2067	1305	365	393	4			
1	B	167	Total	C	N	O	S	0	0	0
			1337	839	235	260	3			
1	C	259	Total	C	N	O	S	0	0	0
			2076	1310	366	396	4			
1	D	172	Total	C	N	O	S	0	0	0
			1374	863	240	268	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	SER	CYS	engineered mutation	UNP Q9UBU9
A	252	SER	CYS	engineered mutation	UNP Q9UBU9
A	328	SER	CYS	engineered mutation	UNP Q9UBU9
B	143	SER	CYS	engineered mutation	UNP Q9UBU9
B	252	SER	CYS	engineered mutation	UNP Q9UBU9
B	328	SER	CYS	engineered mutation	UNP Q9UBU9
C	143	SER	CYS	engineered mutation	UNP Q9UBU9
C	252	SER	CYS	engineered mutation	UNP Q9UBU9
C	328	SER	CYS	engineered mutation	UNP Q9UBU9
D	143	SER	CYS	engineered mutation	UNP Q9UBU9
D	252	SER	CYS	engineered mutation	UNP Q9UBU9
D	328	SER	CYS	engineered mutation	UNP Q9UBU9

VAL	R158	D221	D282	R344	ASN	W216	L277	I338
ARG	A159	G222	M283	F345	THR	S217	L276	S339
ASP	Q160	S223	S284	P346	ARG	R218	L279	A340
ARG	F161	Q224	S285	K347	ALA	R219	L280	I341
ALA	F163	Q225	L286	L348	GLN	Y220	D281	R342
PRO	E164	A226	V287	L349	PHE	D221	W283	R344
E104	D165	L227	Q288	R350	PHE	G222	S284	F345
R105	A166	D228	K289	L351	VAL	S223	S285	P346
G106	S167	L229	A290	D352	GLU	Q224	L286	K347
G107	T168	G231	P291	L356	ASP	Q225	A226	D281
A108	S170	G232	N292	P359	ALA	A226	L227	L348
G109	A171	R233	K293	I360	THR	D228	Q288	R349
T110	A172	S234	L295	A361	ALA	L229	K289	R350
Q112	K173	D235	F362	ASP	THR	K230	P291	L351
	Y177	L238	N297	VAL	THR	K231	A290	D352
T115	K178	V239	L298	GLU	LYS	L232	Q225	L286
S116	L179	A240	S299	ALA	ASP	R233	A226	L227
K117	L180	Q241	G300	THR	THR	THR	L227	Q288
N118	D181	G242	N301	ALA	THR	ALA	Q288	K289
W119	R182	L243	K304	THR	THR	ALA	L227	A290
F120	E183	D244	S305	LEU	LEU	ALA	Q288	P291
K121	N184	V245	E306	PRO	PRO	ALA	L227	N292
I122	R185	L247	R307	PRO	PRO	ALA	Q288	K293
T123	R186	N248	E308			ALA	L227	L295
I124	R187	D310	L309			ALA	Q288	F362
P125	S188	R249	K311			ALA	L227	N297
Y126	I189	R250	T312			ALA	Q288	L298
G127	I190	S251	K313			ALA	L227	G300
R128	I191	S252	G314			ALA	Q288	A240
K129	N192	M253	L315			ALA	L227	D235
Y130	S193	A254	K316			ALA	Q288	N297
D131	S194	T255	L317			ALA	L227	L298
K132	A195	L257	E318			ALA	Q288	G300
A133	P196	R258	E319			ALA	L227	A240
W134		I259	L320			ALA	Q288	D235
L136		I260	W321			ALA	L227	N297
		E261	L322			ALA	Q288	L298
I139		E262	D323			ALA	L227	G300
Q140		N263	G324			ALA	Q288	A240
S141		I264	N325			ALA	L227	D235
K142		P265	S326			ALA	Q288	N297
S143		E266	L327			ALA	L227	L298
S144		L267	S328			ALA	Q288	G300
V145		S269	F331			ALA	L227	A240
P146		L270	R332			ALA	Q288	D235
F147		N271	D333			ALA	L227	N297
T148		L272	Q334			ALA	Q288	L298
P149		Q211	S335			ALA	L227	G300
K213		L212	T336			ALA	Q288	A240
I150		K214	Y337			ALA	L227	D235
E151		L215	I338			ALA	Q288	N297
F152		M216	S339			ALA	L227	L298
H153		S217	A340			ALA	Q288	G300
Y154		R218	I341			ALA	L227	A240
E155		K219	R342			ALA	Q288	D235
N156		L280	E343			ALA	L227	N297
T157		Y220				ALA	Q288	L298

● Molecule 1: TIP ASSOCIATING PROTEIN



VAL	ASN	W216	L277	I338
ARG	THR	S217	L276	S339
ARG	ARG	R218	L279	A340
ASP	ALA	R219	L280	I341
GLN	GLN	Y220	D281	R342
ALA	PHE	D221	W283	R344
PRO	PHE	G222	S284	F345
PRO	VAL	S223	S285	P346
GLU	GLU	Q224	L286	K347
GLY	ASP	Q225	A226	D281
GLY	ALA	A226	L227	L348
GLY	THR	D228	Q288	R349
THR	ALA	L229	K289	R350
THR	SER	K230	P291	L351
SER	ALA	L232	L293	D352
SER	LEU	R233	G294	G353
ASP	LYS	S234	L295	H354
ASP	THR	D235	L296	L356
THR	VAL	N297	L297	P357
THR	ASN	L298	L298	P358
LYS	TYR	D237	S299	P359
LYS	LYS	I360	I360	I360
TRP	ILE	V239	G300	A361
PHE	LEU	A240	N301	F362
LYS	ASP	Q241	E302	D363
ILE	ARG	N242	L303	V364
THR	GLU	L243	K304	E365
ILE	ASN	D244	S305	A366
PRO	ARG	V245	E306	P367
GLY	ARG	L246	R307	T368
GLY	ILE	L247	E308	T369
ARG	SER	N248	L309	L370
LYS	ILE	R249	D310	P371
LYS	ILE	R250	K311	P372
TYR	ILE	S251	L312	
ASP	ILE	S252	K313	
LYS	ASN	L253	G314	
ALA	SER	A254	L315	
TRP	SER	L255	K316	
LEU	ALA	T256	L317	
LEU	PRO	L257	E318	
SER	PRO	R258	E319	
MET	HIS	L259	L320	
ILE	THR	E260	W321	
GLN	SER	E261	D323	
SER	LYS	L201	G324	
LYS	LYS	N202	S325	
SER	SER	E203	S326	
VAL	VAL	L204	L327	
PRO	PRO	K205	E327	
PHE	PHE	P206	S328	
THR	THR	L267	D329	
PRO	PRO	S269	T330	
ILE	ILE	L270	F331	
GLU	GLU	N271	R332	
PHE	PHE	L272	S333	
HIS	HIS	S273	Q334	
TYR	TYR	N274	S335	
GLU	GLU	R275		
		R276		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	136.78Å 136.78Å 202.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.80 8.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	94.9 (8.00-3.80) 83.9 (8.00-3.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.66Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.275 , 0.355 0.265 , 0.341	Depositor DCC
R_{free} test set	575 reflections (2.73%)	wwPDB-VP
Wilson B-factor (Å ²)	133.4	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 117.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	6854	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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	0.59	0/2103	1.09	13/2840 (0.5%)
1	B	0.54	0/1354	1.15	19/1827 (1.0%)
1	C	0.49	0/2112	1.04	17/2852 (0.6%)
1	D	0.66	1/1393 (0.1%)	1.25	22/1882 (1.2%)
All	All	0.57	1/6962 (0.0%)	1.12	71/9401 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	371	PRO	CA-C	5.34	1.57	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	254	ALA	N-CA-C	-9.28	100.59	112.93
1	D	238	LEU	N-CA-C	-8.46	102.86	113.01
1	D	290	ALA	CA-C-N	8.29	130.20	119.84
1	D	290	ALA	C-N-CA	8.29	130.20	119.84
1	A	129	LYS	N-CA-C	-7.95	101.72	112.94
1	A	205	LYS	CA-C-N	7.93	129.75	119.84
1	A	205	LYS	C-N-CA	7.93	129.75	119.84
1	B	365	GLU	N-CA-C	-7.78	104.72	112.97
1	D	369	THR	N-CA-C	7.28	119.46	108.46
1	C	170	SER	N-CA-C	-7.06	103.60	111.71
1	B	240	ALA	N-CA-C	-6.94	103.71	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	ARG	N-CA-C	-6.94	103.91	112.38
1	D	305	SER	N-CA-C	6.88	119.01	108.42
1	C	148	THR	CA-C-N	6.86	127.80	120.11
1	C	148	THR	C-N-CA	6.86	127.80	120.11
1	B	209	VAL	N-CA-C	-6.81	103.67	110.62
1	B	246	VAL	N-CA-C	6.73	116.41	106.85
1	B	357	PRO	CA-C-N	6.70	127.28	120.38
1	B	357	PRO	C-N-CA	6.70	127.28	120.38
1	C	226	ALA	N-CA-C	6.68	123.41	114.12
1	A	223	SER	N-CA-C	-6.67	103.26	111.40
1	D	347	LYS	N-CA-C	-6.47	105.26	112.57
1	D	253	MET	N-CA-C	-6.44	105.41	113.20
1	B	208	GLN	N-CA-C	-6.42	105.09	113.12
1	B	282	ASP	N-CA-C	-6.34	104.30	111.14
1	B	312	ILE	CB-CA-C	-6.24	104.04	111.65
1	C	345	PHE	CA-C-N	6.21	127.61	119.84
1	C	345	PHE	C-N-CA	6.21	127.61	119.84
1	A	357	PRO	CA-C-N	6.20	126.77	120.38
1	A	357	PRO	C-N-CA	6.20	126.77	120.38
1	D	213	LYS	N-CA-C	-6.18	104.46	111.07
1	D	318	GLU	N-CA-C	-6.14	105.70	113.43
1	C	196	PRO	CA-C-N	6.12	126.09	120.21
1	C	196	PRO	C-N-CA	6.12	126.09	120.21
1	C	169	ALA	N-CA-C	-6.02	105.20	112.54
1	D	287	VAL	N-CA-C	-5.99	105.22	113.00
1	A	212	LEU	N-CA-C	-5.93	104.73	111.07
1	C	315	LEU	N-CA-C	5.91	118.28	109.59
1	D	212	LEU	N-CA-C	-5.80	104.87	111.14
1	D	357	PRO	CA-C-N	-5.77	114.43	120.38
1	D	357	PRO	C-N-CA	-5.77	114.43	120.38
1	C	307	ARG	N-CA-C	-5.76	100.81	109.79
1	D	295	ILE	N-CA-C	5.72	116.23	107.77
1	B	355	GLU	N-CA-C	-5.63	102.57	110.50
1	A	181	ASP	N-CA-C	5.56	122.65	110.80
1	A	175	VAL	N-CA-C	-5.55	106.42	112.80
1	B	238	LEU	N-CA-C	-5.55	106.44	113.43
1	C	173	LYS	N-CA-C	-5.54	105.14	111.07
1	A	358	PRO	N-CA-C	5.50	117.41	110.70
1	D	304	LYS	N-CA-C	5.46	118.75	111.75
1	C	219	ARG	N-CA-C	5.43	119.62	112.89
1	D	257	LEU	N-CA-C	-5.43	106.36	112.87
1	A	306	GLU	N-CA-C	-5.38	106.42	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	ILE	N-CA-C	-5.38	105.14	110.62
1	B	271	ASN	N-CA-C	5.37	116.12	108.54
1	B	358	PRO	N-CA-C	5.36	117.24	110.70
1	A	317	LEU	N-CA-C	5.35	117.83	108.52
1	D	210	GLU	N-CA-C	-5.34	106.72	113.18
1	C	244	ASP	N-CA-C	5.29	117.91	109.65
1	D	226	ALA	N-CA-C	5.29	118.05	109.79
1	C	155	GLU	N-CA-C	-5.28	106.61	112.57
1	C	196	PRO	N-CA-C	5.24	117.09	110.70
1	D	235	ASP	CA-C-N	5.23	126.38	119.84
1	D	235	ASP	C-N-CA	5.23	126.38	119.84
1	B	322	LEU	N-CA-C	-5.12	105.72	112.94
1	B	284	SER	N-CA-C	-5.12	106.87	113.01
1	C	331	PHE	N-CA-C	5.08	117.60	110.23
1	A	211	GLN	N-CA-C	-5.07	107.05	113.43
1	B	360	ILE	N-CA-C	-5.05	106.15	113.07
1	D	211	GLN	N-CA-C	-5.04	106.30	112.90
1	B	286	ILE	N-CA-C	-5.02	105.50	110.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	TYR	Sidechain

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	2067	0	2107	426	0
1	B	1337	0	1376	283	0
1	C	2076	0	2113	384	0
1	D	1374	0	1415	257	0
All	All	6854	0	7011	1316	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 95.

All (1316) 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:D:365:GLU:HG2	1:D:366:ALA:H	1.15	1.08
1:B:338:ILE:HA	1:B:341:ILE:HD11	1.30	1.08
1:A:334:GLN:HE21	1:A:334:GLN:HA	1.18	1.07
1:C:233:ARG:HH21	1:C:246:VAL:HG12	1.20	1.06
1:B:253:MET:HE3	1:B:283:MET:HB3	1.33	1.03
1:A:278:TYR:HD1	1:A:279:ARG:H	1.07	0.97
1:D:365:GLU:CG	1:D:366:ALA:H	1.71	0.96
1:B:295:ILE:HG23	1:B:319:GLU:HB3	1.46	0.96
1:C:306:GLU:HA	1:C:327:LEU:HD22	1.47	0.95
1:C:169:ALA:HA	1:C:172:LEU:HG	1.49	0.94
1:D:232:LEU:HG	1:D:245:VAL:HG21	1.47	0.94
1:C:158:ARG:HH22	1:C:207:GLU:HG3	1.32	0.94
1:C:105:ARG:HD2	1:C:106:GLY:N	1.83	0.94
1:A:306:GLU:HA	1:A:327:LEU:HD11	1.48	0.94
1:A:295:ILE:HG22	1:A:296:LEU:H	1.31	0.94
1:A:311:LYS:HE2	1:B:258:ARG:NH2	1.82	0.94
1:D:242:ASN:C	1:D:244:ASP:H	1.75	0.93
1:B:205:LYS:H	1:B:208:GLN:HE21	1.07	0.93
1:A:280:LEU:HD12	1:A:308:GLU:HB3	1.50	0.93
1:B:334:GLN:O	1:B:338:ILE:HG13	1.68	0.92
1:A:230:LYS:HG2	1:A:231:GLY:H	1.32	0.92
1:B:280:LEU:HD22	1:B:283:MET:HE2	1.50	0.92
1:D:358:PRO:HG2	1:D:360:ILE:O	1.70	0.92
1:A:297:ASN:HD22	1:A:298:LEU:H	1.13	0.91
1:A:147:PHE:HD1	1:A:148:THR:H	1.19	0.90
1:C:230:LYS:HG3	1:C:273:SER:HB3	1.52	0.90
1:B:351:LEU:HB2	1:B:356:LEU:HD11	1.52	0.90
1:C:320:LEU:HD12	1:C:321:TRP:H	1.37	0.89
1:D:360:ILE:HG21	1:D:365:GLU:HB3	1.54	0.89
1:A:200:ILE:HD12	1:A:200:ILE:H	1.36	0.89
1:C:319:GLU:HG3	1:C:350:ARG:HB2	1.54	0.89
1:D:201:LEU:HD12	1:D:243:ILE:HG23	1.55	0.89
1:A:277:LEU:HG	1:A:301:ASN:HD21	1.35	0.88
1:C:309:LEU:HD11	1:C:322:LEU:HD11	1.53	0.88
1:C:132:LYS:HA	1:C:136:LEU:HG	1.52	0.88
1:C:271:ASN:ND2	1:C:273:SER:H	1.70	0.88
1:D:271:ASN:C	1:D:271:ASN:HD22	1.81	0.88
1:B:296:LEU:HB3	1:B:320:LEU:HD12	1.54	0.88
1:D:293:LEU:HD23	1:D:315:LEU:HD13	1.56	0.88
1:B:306:GLU:HA	1:B:327:LEU:HD22	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:LEU:O	1:C:247:LEU:HD23	1.75	0.87
1:B:268:LEU:HA	1:B:293:LEU:HA	1.57	0.87
1:A:265:PRO:O	1:A:266:GLU:HG2	1.75	0.86
1:C:123:THR:HA	1:C:160:GLN:HG2	1.57	0.86
1:B:319:GLU:CD	1:B:350:ARG:HE	1.84	0.86
1:A:277:LEU:HG	1:A:301:ASN:ND2	1.91	0.85
1:B:205:LYS:H	1:B:208:GLN:NE2	1.75	0.85
1:D:319:GLU:OE2	1:D:350:ARG:HD2	1.76	0.85
1:C:271:ASN:C	1:C:271:ASN:HD22	1.83	0.85
1:C:232:LEU:HD13	1:C:247:LEU:HD12	1.59	0.85
1:B:271:ASN:HD21	1:B:273:SER:HB3	1.41	0.84
1:C:205:LYS:HB2	1:C:208:GLN:HG3	1.57	0.84
1:A:165:ASP:HB2	1:A:168:THR:OG1	1.77	0.84
1:B:274:ASN:ND2	1:B:300:GLY:HA3	1.93	0.83
1:B:342:ARG:HD2	1:B:348:LEU:HB3	1.59	0.83
1:C:118:ASN:HD22	1:C:120:PHE:HE1	1.26	0.83
1:C:278:TYR:HD1	1:C:279:ARG:N	1.77	0.83
1:B:277:LEU:HG	1:B:301:ASN:OD1	1.78	0.83
1:D:219:ARG:NH1	1:D:232:LEU:HD12	1.92	0.83
1:A:220:TYR:HB2	1:A:227:LEU:HD13	1.61	0.83
1:C:158:ARG:HD3	1:C:158:ARG:H	1.44	0.82
1:A:278:TYR:CE1	1:A:279:ARG:HG2	2.14	0.82
1:C:105:ARG:HD2	1:C:106:GLY:H	1.42	0.82
1:A:250:ARG:HG2	1:A:279:ARG:HH12	1.43	0.82
1:C:275:ASN:HB3	1:C:301:ASN:HD21	1.45	0.82
1:C:289:LYS:C	1:C:291:PRO:HD3	2.05	0.82
1:C:169:ALA:HA	1:C:172:LEU:CG	2.09	0.82
1:A:115:THR:HB	1:A:117:LYS:HG3	1.62	0.81
1:B:327:LEU:HD12	1:B:328:SER:N	1.94	0.81
1:C:223:SER:O	1:C:224:GLN:HB2	1.79	0.81
1:C:233:ARG:NH2	1:C:246:VAL:HG12	1.95	0.81
1:C:266:GLU:CD	1:C:266:GLU:H	1.87	0.81
1:D:294:LYS:HG2	1:D:318:GLU:HB2	1.58	0.81
1:D:344:ARG:H	1:D:344:ARG:HD3	1.44	0.81
1:C:294:LYS:C	1:C:295:ILE:HD12	2.04	0.81
1:A:250:ARG:HG2	1:A:279:ARG:NH1	1.95	0.81
1:C:116:SER:HB2	1:C:165:ASP:HA	1.60	0.81
1:D:327:LEU:O	1:D:327:LEU:HD12	1.81	0.81
1:A:278:TYR:HD1	1:A:279:ARG:N	1.78	0.81
1:C:126:TYR:HA	1:C:157:THR:HG22	1.63	0.81
1:D:295:ILE:HG23	1:D:319:GLU:HB3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HB3	1:A:208:GLN:HG3	1.63	0.80
1:D:261:GLU:HB2	1:D:289:LYS:HB3	1.61	0.80
1:B:299:SER:HB2	1:B:323:ASP:HB3	1.64	0.80
1:C:260:ILE:HA	1:C:264:ILE:HG13	1.62	0.80
1:A:174:ALA:O	1:A:178:LYS:HD2	1.81	0.80
1:B:327:LEU:HA	1:B:330:THR:HG23	1.63	0.80
1:B:212:LEU:HD21	1:B:256:THR:OG1	1.82	0.79
1:A:138:MET:HB3	1:A:179:ILE:HD12	1.65	0.79
1:A:320:LEU:HG	1:A:321:TRP:H	1.46	0.79
1:C:317:LEU:HD23	1:C:318:GLU:H	1.44	0.79
1:B:289:LYS:C	1:B:291:PRO:HD3	2.07	0.79
1:A:301:ASN:H	1:A:325:ASN:HD21	1.29	0.79
1:A:311:LYS:HE2	1:B:258:ARG:HH22	1.47	0.79
1:A:359:PRO:O	1:A:360:ILE:HG23	1.82	0.79
1:B:287:VAL:HG11	1:B:314:GLY:HA3	1.64	0.79
1:C:319:GLU:OE1	1:C:350:ARG:HG3	1.82	0.79
1:C:279:ARG:O	1:C:281:ASP:N	2.14	0.79
1:D:259:ILE:HD12	1:D:259:ILE:H	1.45	0.79
1:B:276:ARG:HG2	1:B:302:GLU:HG2	1.65	0.78
1:C:128:ARG:HD2	1:C:154:TYR:OH	1.82	0.78
1:B:227:LEU:HD22	1:B:260:ILE:HD11	1.66	0.78
1:C:149:PRO:HB3	1:C:161:PHE:CG	2.18	0.78
1:D:286:ILE:HG23	1:D:315:LEU:HD21	1.65	0.77
1:B:287:VAL:HG22	1:B:315:LEU:HB3	1.65	0.77
1:B:362:PHE:CD2	1:C:217:SER:HA	2.19	0.77
1:B:238:LEU:O	1:B:243:ILE:HG22	1.86	0.76
1:A:278:TYR:CD1	1:A:279:ARG:HG2	2.21	0.76
1:A:297:ASN:ND2	1:A:299:SER:H	1.83	0.76
1:A:277:LEU:O	1:A:277:LEU:HD12	1.86	0.76
1:D:335:SER:O	1:D:338:ILE:HG13	1.86	0.75
1:A:108:ALA:HA	1:A:116:SER:HB3	1.67	0.75
1:D:365:GLU:CG	1:D:366:ALA:N	2.46	0.75
1:A:297:ASN:O	1:A:298:LEU:HG	1.87	0.75
1:B:297:ASN:C	1:B:297:ASN:HD22	1.94	0.75
1:D:366:ALA:N	1:D:367:PRO:HD3	2.00	0.75
1:A:279:ARG:HH21	1:A:281:ASP:HB3	1.51	0.75
1:B:211:GLN:O	1:B:215:ILE:N	2.19	0.75
1:C:255:ALA:O	1:C:257:LEU:N	2.19	0.75
1:C:277:LEU:N	1:C:301:ASN:HD22	1.85	0.75
1:A:138:MET:C	1:A:140:GLN:H	1.92	0.75
1:C:280:LEU:HB2	1:C:308:GLU:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:NH2	1:A:281:ASP:HB3	2.01	0.75
1:A:230:LYS:HG2	1:A:231:GLY:N	2.02	0.74
1:D:317:LEU:HD12	1:D:345:PHE:CE2	2.22	0.74
1:C:130:TYR:O	1:C:135:LEU:HB2	1.86	0.74
1:C:235:ASP:H	1:C:239:VAL:HG23	1.52	0.74
1:D:365:GLU:HG2	1:D:366:ALA:N	1.98	0.74
1:B:265:PRO:O	1:B:267:LEU:N	2.17	0.74
1:A:295:ILE:HG22	1:A:296:LEU:N	2.02	0.74
1:A:115:THR:HG22	1:A:116:SER:H	1.52	0.74
1:A:297:ASN:HD21	1:A:299:SER:HB3	1.51	0.74
1:A:342:ARG:NH1	1:A:356:LEU:HD12	2.02	0.74
1:D:242:ASN:C	1:D:244:ASP:N	2.38	0.74
1:D:370:LEU:HD13	1:D:371:PRO:O	1.87	0.74
1:C:119:TRP:CD1	1:C:164:GLU:HA	2.22	0.74
1:C:360:ILE:HG22	1:C:361:ALA:H	1.52	0.74
1:D:287:VAL:HG11	1:D:314:GLY:HA3	1.69	0.74
1:D:310:ASP:HA	1:D:313:LYS:HB2	1.70	0.74
1:A:182:ARG:HG3	1:A:183:GLU:OE1	1.88	0.73
1:A:303:LEU:HB2	1:A:325:ASN:OD1	1.87	0.73
1:B:280:LEU:HD22	1:B:283:MET:CE	2.17	0.73
1:B:305:SER:C	1:B:307:ARG:H	1.96	0.73
1:A:195:ALA:HB1	1:A:199:THR:OG1	1.88	0.73
1:D:280:LEU:HD12	1:D:308:GLU:O	1.88	0.73
1:C:219:ARG:HH22	1:C:232:LEU:HA	1.52	0.73
1:D:230:LYS:HG3	1:D:273:SER:HG	1.53	0.73
1:A:209:VAL:C	1:A:211:GLN:H	1.96	0.73
1:A:220:TYR:C	1:A:220:TYR:CD2	2.67	0.73
1:B:216:MET:O	1:B:217:SER:C	2.32	0.73
1:C:296:LEU:HD13	1:C:298:LEU:HD11	1.69	0.73
1:C:309:LEU:HD12	1:C:345:PHE:HE1	1.54	0.73
1:A:110:THR:H	1:A:115:THR:HG21	1.53	0.73
1:B:233:ARG:HH21	1:B:244:ASP:HB3	1.54	0.73
1:D:326:SER:O	1:D:328:SER:N	2.21	0.73
1:A:298:LEU:O	1:A:301:ASN:HB2	1.89	0.72
1:B:204:LEU:HD11	1:B:252:SER:HA	1.70	0.72
1:B:253:MET:HE3	1:B:283:MET:CB	2.16	0.72
1:C:227:LEU:HD12	1:C:264:ILE:HD12	1.71	0.72
1:A:278:TYR:CD1	1:A:279:ARG:N	2.54	0.72
1:A:119:TRP:HH2	1:A:150:ILE:HG21	1.55	0.72
1:C:311:LYS:C	1:C:313:LYS:H	1.98	0.71
1:D:257:LEU:HD22	1:D:286:ILE:HG13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LYS:HA	1:B:317:LEU:HA	1.72	0.71
1:B:342:ARG:CD	1:B:348:LEU:HB3	2.19	0.71
1:C:163:VAL:HG12	1:C:164:GLU:H	1.55	0.71
1:C:310:ASP:O	1:C:313:LYS:HB3	1.90	0.71
1:A:318:GLU:O	1:A:319:GLU:HB2	1.87	0.71
1:C:169:ALA:CA	1:C:172:LEU:HG	2.20	0.71
1:D:344:ARG:HD3	1:D:344:ARG:N	2.05	0.71
1:A:180:LEU:HD12	1:A:186:ARG:NE	2.04	0.71
1:C:115:THR:HG22	1:C:116:SER:N	2.05	0.71
1:C:271:ASN:HA	1:C:297:ASN:HB3	1.71	0.71
1:B:271:ASN:ND2	1:B:297:ASN:HB3	2.06	0.71
1:D:242:ASN:O	1:D:244:ASP:N	2.23	0.71
1:B:315:LEU:HD23	1:B:315:LEU:O	1.91	0.71
1:B:327:LEU:HD12	1:B:327:LEU:C	2.15	0.71
1:A:162:PHE:HE1	1:A:197:PRO:HA	1.56	0.70
1:D:205:LYS:HD2	1:D:205:LYS:N	2.05	0.70
1:A:299:SER:O	1:A:301:ASN:N	2.24	0.70
1:A:301:ASN:N	1:A:325:ASN:HD21	1.89	0.70
1:C:182:ARG:HG3	1:C:183:GLU:HG3	1.73	0.70
1:C:312:ILE:O	1:C:315:LEU:HD12	1.90	0.70
1:B:296:LEU:HB2	1:B:317:LEU:HD22	1.73	0.70
1:D:338:ILE:HG21	1:D:356:LEU:HD22	1.73	0.70
1:C:226:ALA:O	1:C:227:LEU:C	2.35	0.70
1:A:346:PRO:C	1:A:348:LEU:H	2.00	0.69
1:A:162:PHE:CE1	1:A:197:PRO:HA	2.27	0.69
1:C:229:LEU:HB3	1:C:232:LEU:HD12	1.72	0.69
1:A:334:GLN:HA	1:A:334:GLN:NE2	2.00	0.69
1:C:118:ASN:HD21	1:C:166:ALA:HA	1.57	0.69
1:C:277:LEU:H	1:C:301:ASN:HD22	1.40	0.69
1:C:273:SER:O	1:C:274:ASN:C	2.36	0.69
1:B:234:SER:O	1:B:236:PRO:HD3	1.91	0.69
1:C:271:ASN:ND2	1:C:271:ASN:C	2.50	0.69
1:A:139:ILE:HG22	1:A:139:ILE:O	1.93	0.69
1:A:297:ASN:HD22	1:A:298:LEU:N	1.87	0.69
1:C:163:VAL:HG12	1:C:165:ASP:H	1.57	0.69
1:D:210:GLU:HG3	1:D:213:LYS:HE3	1.75	0.69
1:A:250:ARG:HG2	1:A:282:ASP:HB3	1.75	0.69
1:C:128:ARG:HB2	1:C:157:THR:HA	1.73	0.69
1:D:367:PRO:O	1:D:368:THR:C	2.36	0.69
1:C:308:GLU:O	1:C:310:ASP:N	2.26	0.69
1:D:257:LEU:HD23	1:D:260:ILE:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:VAL:O	1:B:288:GLN:HG2	1.93	0.69
1:C:158:ARG:NH2	1:C:206:PRO:HB2	2.07	0.69
1:B:271:ASN:ND2	1:B:273:SER:HB3	2.08	0.68
1:D:271:ASN:ND2	1:D:273:SER:H	1.90	0.68
1:D:358:PRO:C	1:D:360:ILE:H	2.00	0.68
1:A:251:SER:O	1:A:254:ALA:HB3	1.94	0.68
1:D:254:ALA:C	1:D:256:THR:H	2.00	0.68
1:D:237:ASP:HB2	1:D:239:VAL:HG22	1.75	0.68
1:A:163:VAL:HG12	1:A:164:GLU:H	1.59	0.68
1:A:199:THR:O	1:A:200:ILE:C	2.37	0.68
1:C:118:ASN:ND2	1:C:166:ALA:HA	2.09	0.68
1:C:201:LEU:O	1:C:203:GLU:N	2.27	0.68
1:C:320:LEU:HD12	1:C:321:TRP:N	2.09	0.68
1:D:219:ARG:NH2	1:D:236:PRO:HG3	2.09	0.68
1:A:147:PHE:O	1:A:148:THR:HG23	1.94	0.67
1:A:230:LYS:HE2	1:A:274:ASN:HD22	1.59	0.67
1:C:220:TYR:HE1	1:C:225:GLN:HA	1.58	0.67
1:C:278:TYR:CD1	1:C:279:ARG:N	2.61	0.67
1:B:299:SER:CB	1:B:323:ASP:HB3	2.23	0.67
1:C:227:LEU:HD12	1:C:264:ILE:CD1	2.24	0.67
1:A:301:ASN:H	1:A:325:ASN:ND2	1.91	0.67
1:D:264:ILE:HG22	1:D:267:LEU:HB2	1.77	0.67
1:A:229:LEU:HD23	1:A:232:LEU:HD13	1.76	0.67
1:A:294:LYS:O	1:A:317:LEU:HA	1.95	0.67
1:A:338:ILE:O	1:A:342:ARG:HB2	1.94	0.67
1:B:342:ARG:HA	1:B:345:PHE:O	1.94	0.67
1:D:294:LYS:CG	1:D:318:GLU:HB2	2.23	0.67
1:B:274:ASN:N	1:B:274:ASN:HD22	1.91	0.67
1:A:304:LYS:HA	1:A:326:SER:HB3	1.76	0.67
1:B:351:LEU:CB	1:B:356:LEU:HD11	2.25	0.67
1:C:124:ILE:HG12	1:C:189:ILE:HG23	1.77	0.67
1:A:235:ASP:O	1:A:239:VAL:HB	1.95	0.67
1:A:125:PRO:HG2	1:A:190:ILE:HD13	1.77	0.66
1:A:241:GLN:C	1:A:243:ILE:H	2.01	0.66
1:B:212:LEU:O	1:B:215:ILE:HG22	1.94	0.66
1:A:346:PRO:O	1:A:348:LEU:N	2.29	0.66
1:B:240:ALA:C	1:B:242:ASN:H	2.03	0.66
1:C:150:ILE:HD11	1:C:162:PHE:HB2	1.76	0.66
1:A:215:ILE:HG13	1:A:238:LEU:HD21	1.75	0.66
1:B:309:LEU:C	1:B:311:LYS:H	2.04	0.66
1:B:338:ILE:CA	1:B:341:ILE:HD11	2.17	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:PRO:C	1:B:238:LEU:H	2.04	0.66
1:D:241:GLN:O	1:D:241:GLN:HG2	1.94	0.66
1:D:201:LEU:HB2	1:D:243:ILE:HG23	1.77	0.66
1:A:279:ARG:NH2	1:A:282:ASP:H	1.93	0.66
1:B:225:GLN:HB2	1:B:268:LEU:HG	1.77	0.66
1:B:267:LEU:HD12	1:B:268:LEU:H	1.59	0.66
1:A:228:ASP:HA	1:A:271:ASN:HB3	1.77	0.65
1:B:287:VAL:O	1:B:287:VAL:HG12	1.95	0.65
1:C:258:ARG:NH2	1:D:307:ARG:NH2	2.43	0.65
1:C:263:ASN:C	1:C:265:PRO:HD3	2.21	0.65
1:D:235:ASP:C	1:D:237:ASP:H	2.02	0.65
1:D:358:PRO:CG	1:D:360:ILE:O	2.43	0.65
1:B:227:LEU:HD22	1:B:260:ILE:CD1	2.26	0.65
1:B:323:ASP:OD2	1:C:186:ARG:HD2	1.95	0.65
1:C:120:PHE:HA	1:C:193:SER:HA	1.79	0.65
1:C:177:TYR:HB3	1:C:186:ARG:HD3	1.79	0.65
1:C:337:TYR:HE2	1:C:351:LEU:HD21	1.61	0.65
1:A:297:ASN:HD21	1:A:299:SER:CB	2.10	0.65
1:B:280:LEU:H	1:B:308:GLU:CD	2.04	0.65
1:C:283:MET:O	1:C:286:ILE:HG22	1.97	0.65
1:D:230:LYS:HG3	1:D:273:SER:OG	1.96	0.65
1:D:264:ILE:HG22	1:D:264:ILE:O	1.95	0.65
1:B:354:HIS:CE1	1:C:126:TYR:HB2	2.31	0.65
1:A:334:GLN:HE21	1:A:334:GLN:CA	2.04	0.65
1:A:345:PHE:O	1:A:348:LEU:HB2	1.97	0.65
1:B:244:ASP:OD2	1:B:244:ASP:N	2.28	0.65
1:B:278:TYR:HB2	1:D:332:ARG:HH11	1.60	0.64
1:C:133:ALA:C	1:C:135:LEU:H	2.05	0.64
1:C:271:ASN:HD22	1:C:273:SER:H	1.43	0.64
1:A:238:LEU:HD12	1:A:238:LEU:H	1.61	0.64
1:A:261:GLU:OE1	1:A:289:LYS:HG2	1.97	0.64
1:C:271:ASN:HD21	1:C:273:SER:HB2	1.62	0.64
1:D:328:SER:C	1:D:330:THR:H	2.05	0.64
1:C:227:LEU:CD2	1:C:229:LEU:HG	2.27	0.64
1:C:305:SER:C	1:C:307:ARG:H	2.04	0.64
1:A:221:ASP:CG	1:A:223:SER:H	2.06	0.64
1:B:332:ARG:HH11	1:B:332:ARG:HG3	1.62	0.64
1:A:348:LEU:HD23	1:A:349:LEU:H	1.63	0.64
1:C:220:TYR:CE1	1:C:225:GLN:HA	2.32	0.64
1:C:266:GLU:CD	1:C:266:GLU:N	2.55	0.64
1:D:208:GLN:HA	1:D:211:GLN:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ILE:HG13	1:B:238:LEU:HD13	1.80	0.64
1:C:115:THR:HG22	1:C:116:SER:H	1.63	0.64
1:A:241:GLN:HB3	1:A:243:ILE:HG13	1.80	0.64
1:B:290:ALA:N	1:B:291:PRO:HD3	2.13	0.64
1:C:182:ARG:HG3	1:C:183:GLU:N	2.12	0.64
1:A:277:LEU:HG	1:A:301:ASN:CG	2.20	0.64
1:A:309:LEU:HD12	1:A:345:PHE:HE1	1.63	0.64
1:A:177:TYR:CE1	1:A:186:ARG:HG3	2.32	0.64
1:A:297:ASN:ND2	1:A:298:LEU:H	1.92	0.64
1:A:138:MET:O	1:A:140:GLN:N	2.27	0.63
1:A:172:LEU:HA	1:A:175:VAL:HG23	1.80	0.63
1:A:297:ASN:HD22	1:A:299:SER:H	1.44	0.63
1:B:338:ILE:HA	1:B:341:ILE:CD1	2.18	0.63
1:A:127:GLY:C	1:A:129:LYS:H	2.06	0.63
1:C:105:ARG:CD	1:C:106:GLY:H	2.12	0.63
1:D:219:ARG:NH1	1:D:232:LEU:CD1	2.62	0.63
1:B:287:VAL:CG2	1:B:315:LEU:H	2.11	0.63
1:B:302:GLU:HA	1:B:302:GLU:OE2	1.99	0.63
1:C:279:ARG:C	1:C:281:ASP:H	2.07	0.63
1:C:326:SER:C	1:C:328:SER:H	2.05	0.63
1:A:351:LEU:O	1:A:353:GLY:N	2.32	0.62
1:B:271:ASN:HD21	1:B:273:SER:CB	2.12	0.62
1:B:303:LEU:HD12	1:B:325:ASN:OD1	1.99	0.62
1:C:228:ASP:C	1:C:228:ASP:OD2	2.42	0.62
1:C:135:LEU:O	1:C:139:ILE:HG13	1.99	0.62
1:C:238:LEU:O	1:C:241:GLN:HG2	1.99	0.62
1:D:239:VAL:HG23	1:D:240:ALA:N	2.15	0.62
1:A:172:LEU:HB2	1:A:191:ILE:HD11	1.81	0.62
1:A:273:SER:HB3	1:A:299:SER:HB3	1.80	0.62
1:B:235:ASP:O	1:B:239:VAL:HG23	2.00	0.62
1:B:298:LEU:O	1:B:301:ASN:ND2	2.33	0.62
1:C:225:GLN:HB3	1:C:267:LEU:HA	1.80	0.62
1:C:258:ARG:O	1:C:261:GLU:HB3	1.99	0.62
1:C:271:ASN:HD22	1:C:272:LEU:N	1.97	0.62
1:A:277:LEU:CG	1:A:301:ASN:HD21	2.11	0.62
1:B:205:LYS:N	1:B:208:GLN:HE21	1.89	0.62
1:B:216:MET:O	1:B:219:ARG:N	2.31	0.62
1:B:305:SER:C	1:B:307:ARG:N	2.55	0.62
1:D:365:GLU:OE2	1:D:366:ALA:N	2.32	0.62
1:A:123:THR:HA	1:A:160:GLN:HB3	1.82	0.62
1:A:296:LEU:HD23	1:A:297:ASN:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LEU:HB2	1:B:308:GLU:OE1	2.00	0.62
1:B:325:ASN:O	1:B:326:SER:C	2.42	0.62
1:B:338:ILE:O	1:B:341:ILE:HD12	1.99	0.62
1:A:180:LEU:HD21	1:A:184:ASN:ND2	2.15	0.61
1:C:152:PHE:HA	1:C:160:GLN:O	2.00	0.61
1:C:323:ASP:OD1	1:C:352:ASP:HB3	1.99	0.61
1:C:251:SER:O	1:C:254:ALA:HB3	1.99	0.61
1:C:360:ILE:N	1:C:360:ILE:HD12	2.15	0.61
1:D:285:SER:O	1:D:288:GLN:HB2	2.00	0.61
1:B:227:LEU:CD2	1:B:260:ILE:HD11	2.29	0.61
1:A:289:LYS:C	1:A:291:PRO:HD3	2.25	0.61
1:D:264:ILE:N	1:D:265:PRO:HD3	2.15	0.61
1:A:283:MET:O	1:A:286:ILE:HG22	2.00	0.61
1:C:125:PRO:HD2	1:C:188:SER:O	2.00	0.61
1:A:283:MET:CE	1:A:286:ILE:HG21	2.31	0.61
1:A:306:GLU:HA	1:A:327:LEU:CD1	2.25	0.61
1:B:304:LYS:HD2	1:D:329:ASP:O	2.00	0.61
1:A:122:ILE:HG21	1:A:161:PHE:CE2	2.36	0.61
1:C:129:LYS:H	1:C:129:LYS:HD2	1.65	0.61
1:C:169:ALA:HB1	1:C:191:ILE:HG21	1.82	0.61
1:A:122:ILE:HG21	1:A:161:PHE:CZ	2.36	0.61
1:C:169:ALA:HB1	1:C:191:ILE:HG12	1.83	0.61
1:C:260:ILE:HA	1:C:264:ILE:CG1	2.30	0.61
1:A:309:LEU:HD21	1:A:322:LEU:HD11	1.83	0.61
1:A:337:TYR:HE2	1:A:351:LEU:HD21	1.65	0.61
1:B:296:LEU:O	1:B:320:LEU:HA	2.01	0.61
1:C:149:PRO:HB3	1:C:161:PHE:CB	2.31	0.61
1:B:304:LYS:HG3	1:D:332:ARG:NH2	2.16	0.61
1:B:309:LEU:O	1:B:311:LYS:N	2.33	0.61
1:A:332:ARG:CG	1:A:336:THR:HG21	2.31	0.60
1:C:257:LEU:O	1:C:258:ARG:C	2.44	0.60
1:A:277:LEU:HG	1:A:301:ASN:OD1	2.01	0.60
1:A:297:ASN:ND2	1:A:299:SER:HB3	2.15	0.60
1:A:309:LEU:HD12	1:A:345:PHE:CE1	2.36	0.60
1:C:195:ALA:HB1	1:C:196:PRO:CD	2.31	0.60
1:C:200:ILE:HG12	1:D:202:ASN:OD1	2.02	0.60
1:C:265:PRO:C	1:C:267:LEU:H	2.07	0.60
1:D:347:LYS:H	1:D:347:LYS:HD3	1.66	0.60
1:A:317:LEU:C	1:A:319:GLU:H	2.09	0.60
1:D:233:ARG:HH21	1:D:244:ASP:CB	2.14	0.60
1:A:238:LEU:HD23	1:A:243:ILE:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ASN:HA	1:C:321:TRP:HB2	1.82	0.60
1:C:305:SER:HB3	1:C:307:ARG:HG2	1.83	0.60
1:C:342:ARG:NH1	1:C:348:LEU:HB3	2.16	0.60
1:D:328:SER:C	1:D:330:THR:N	2.57	0.60
1:A:127:GLY:O	1:A:129:LYS:N	2.32	0.60
1:A:205:LYS:O	1:A:208:GLN:HG2	2.02	0.60
1:C:248:ASN:C	1:C:248:ASN:OD1	2.44	0.60
1:C:298:LEU:HD13	1:C:320:LEU:HD11	1.83	0.60
1:C:152:PHE:CE1	1:C:161:PHE:HD2	2.20	0.60
1:A:180:LEU:HD12	1:A:186:ARG:HE	1.65	0.60
1:A:194:SER:OG	1:A:195:ALA:N	2.31	0.60
1:C:338:ILE:HG23	1:C:356:LEU:HD13	1.84	0.60
1:D:219:ARG:HD3	1:D:228:ASP:O	2.02	0.60
1:A:278:TYR:HE1	1:A:279:ARG:HG2	1.67	0.60
1:C:264:ILE:O	1:C:267:LEU:HB2	2.01	0.60
1:D:233:ARG:HE	1:D:244:ASP:CG	2.10	0.60
1:D:256:THR:C	1:D:258:ARG:H	2.09	0.60
1:A:227:LEU:O	1:A:229:LEU:N	2.27	0.60
1:B:212:LEU:C	1:B:215:ILE:HG22	2.27	0.60
1:C:106:GLY:C	1:C:108:ALA:H	2.09	0.60
1:C:252:SER:C	1:C:254:ALA:N	2.60	0.60
1:D:297:ASN:C	1:D:297:ASN:HD22	2.09	0.60
1:C:283:MET:CE	1:C:286:ILE:HG21	2.32	0.59
1:C:308:GLU:C	1:C:310:ASP:N	2.58	0.59
1:D:233:ARG:O	1:D:233:ARG:HG3	1.99	0.59
1:A:241:GLN:C	1:A:243:ILE:N	2.60	0.59
1:A:296:LEU:HG	1:A:297:ASN:H	1.67	0.59
1:C:136:LEU:HD21	1:C:152:PHE:CE2	2.37	0.59
1:A:246:VAL:HG23	1:A:246:VAL:O	2.02	0.59
1:A:313:LYS:O	1:A:315:LEU:N	2.34	0.59
1:D:256:THR:C	1:D:258:ARG:N	2.59	0.59
1:B:236:PRO:O	1:B:238:LEU:N	2.35	0.59
1:B:322:LEU:HB2	1:B:337:TYR:OH	2.01	0.59
1:C:219:ARG:HH12	1:C:232:LEU:HG	1.68	0.59
1:A:204:LEU:HD11	1:A:245:VAL:HG12	1.82	0.59
1:C:327:LEU:HD12	1:C:327:LEU:C	2.27	0.59
1:D:317:LEU:O	1:D:347:LYS:HG2	2.03	0.59
1:A:145:VAL:HG23	1:A:146:PRO:O	2.03	0.59
1:D:261:GLU:O	1:D:265:PRO:HG3	2.02	0.59
1:D:341:ILE:HG22	1:D:348:LEU:HD22	1.84	0.59
1:D:208:GLN:O	1:D:211:GLN:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TYR:CD1	1:D:354:HIS:ND1	2.71	0.59
1:B:236:PRO:C	1:B:238:LEU:N	2.59	0.59
1:C:132:LYS:O	1:C:136:LEU:HB2	2.02	0.59
1:C:305:SER:C	1:C:307:ARG:N	2.61	0.59
1:D:257:LEU:HB3	1:D:289:LYS:HG3	1.85	0.59
1:B:327:LEU:C	1:B:329:ASP:H	2.11	0.59
1:C:280:LEU:HD22	1:C:312:ILE:HG21	1.85	0.59
1:B:354:HIS:HE1	1:C:126:TYR:HB2	1.67	0.59
1:C:180:LEU:HG	1:C:181:ASP:N	2.18	0.59
1:C:214:LEU:O	1:C:217:SER:N	2.25	0.59
1:C:241:GLN:NE2	1:C:244:ASP:HA	2.18	0.59
1:C:252:SER:C	1:C:254:ALA:H	2.09	0.59
1:C:280:LEU:HD22	1:C:312:ILE:CG2	2.33	0.59
1:C:331:PHE:CE2	1:C:337:TYR:HA	2.38	0.59
1:A:208:GLN:HA	1:A:211:GLN:OE1	2.03	0.58
1:B:287:VAL:HG22	1:B:315:LEU:H	1.68	0.58
1:C:213:LYS:HE3	1:C:263:ASN:ND2	2.19	0.58
1:C:229:LEU:HD22	1:C:232:LEU:HD12	1.84	0.58
1:A:303:LEU:O	1:A:327:LEU:HB2	2.03	0.58
1:B:281:ASP:OD1	1:B:311:LYS:HB3	2.03	0.58
1:A:250:ARG:NH2	1:A:282:ASP:HA	2.17	0.58
1:A:250:ARG:HH21	1:A:282:ASP:HA	1.68	0.58
1:B:276:ARG:C	1:B:277:LEU:HD23	2.28	0.58
1:B:295:ILE:HG23	1:B:319:GLU:CB	2.28	0.58
1:B:362:PHE:HD2	1:C:217:SER:HA	1.66	0.58
1:A:180:LEU:HD23	1:A:180:LEU:O	2.03	0.58
1:A:263:ASN:C	1:A:265:PRO:HD3	2.27	0.58
1:C:223:SER:O	1:C:224:GLN:CB	2.50	0.58
1:A:282:ASP:OD2	1:A:283:MET:N	2.37	0.58
1:B:215:ILE:HD11	1:B:235:ASP:OD2	2.02	0.58
1:C:289:LYS:O	1:C:291:PRO:HD3	2.02	0.58
1:C:337:TYR:CE2	1:C:351:LEU:HD21	2.38	0.58
1:D:219:ARG:HH22	1:D:236:PRO:HD3	1.69	0.58
1:A:301:ASN:N	1:A:325:ASN:ND2	2.50	0.58
1:A:320:LEU:CG	1:A:321:TRP:H	2.16	0.58
1:B:236:PRO:O	1:B:240:ALA:N	2.34	0.58
1:C:124:ILE:CG1	1:C:189:ILE:HG23	2.34	0.58
1:D:219:ARG:HH12	1:D:232:LEU:HA	1.67	0.58
1:D:327:LEU:O	1:D:327:LEU:CD1	2.49	0.58
1:A:163:VAL:HG12	1:A:164:GLU:N	2.17	0.58
1:A:172:LEU:HA	1:A:175:VAL:CG2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLY:HA2	1:A:324:GLY:HA3	1.84	0.58
1:B:240:ALA:C	1:B:242:ASN:N	2.59	0.58
1:B:337:TYR:O	1:B:341:ILE:HG13	2.04	0.58
1:D:289:LYS:C	1:D:291:PRO:HD3	2.29	0.58
1:A:330:THR:O	1:A:331:PHE:HD1	1.86	0.58
1:B:280:LEU:CD2	1:B:283:MET:HE2	2.29	0.58
1:C:286:ILE:HD11	1:C:290:ALA:HB2	1.86	0.58
1:D:233:ARG:HH21	1:D:244:ASP:HB3	1.68	0.58
1:D:235:ASP:HB3	1:D:236:PRO:HD3	1.84	0.58
1:D:363:ASP:OD1	1:D:364:VAL:HG23	2.04	0.58
1:D:269:SER:OG	1:D:295:ILE:HD12	2.03	0.57
1:D:201:LEU:CD1	1:D:243:ILE:HG23	2.31	0.57
1:D:233:ARG:HA	1:D:245:VAL:HG23	1.85	0.57
1:D:303:LEU:HB2	1:D:325:ASN:HB3	1.85	0.57
1:A:119:TRP:HZ3	1:A:162:PHE:HB2	1.70	0.57
1:C:307:ARG:O	1:C:308:GLU:HB2	2.04	0.57
1:D:212:LEU:HD13	1:D:245:VAL:HG11	1.85	0.57
1:D:271:ASN:HD22	1:D:272:LEU:N	2.01	0.57
1:A:179:ILE:HB	1:A:187:ILE:HB	1.86	0.57
1:A:323:ASP:C	1:A:325:ASN:H	2.12	0.57
1:A:351:LEU:HD23	1:A:352:ASP:HB2	1.86	0.57
1:C:125:PRO:HG2	1:C:188:SER:OG	2.04	0.57
1:D:224:GLN:O	1:D:225:GLN:HB2	2.04	0.57
1:D:201:LEU:HB2	1:D:243:ILE:CG2	2.34	0.57
1:B:219:ARG:O	1:B:220:TYR:HB2	2.04	0.57
1:B:280:LEU:HD12	1:B:308:GLU:O	2.05	0.57
1:C:158:ARG:NH2	1:C:207:GLU:HG3	2.11	0.57
1:C:296:LEU:HD22	1:C:298:LEU:CD1	2.34	0.57
1:A:272:LEU:HD23	1:A:275:ASN:HD22	1.69	0.57
1:A:286:ILE:HD11	1:A:293:LEU:CD2	2.35	0.57
1:B:236:PRO:HA	1:B:239:VAL:HB	1.85	0.57
1:B:309:LEU:C	1:B:311:LYS:N	2.60	0.57
1:C:116:SER:HA	1:C:166:ALA:HB2	1.87	0.57
1:A:225:GLN:HB3	1:A:268:LEU:H	1.70	0.57
1:B:237:ASP:O	1:B:241:GLN:HB2	2.04	0.57
1:C:309:LEU:HD12	1:C:345:PHE:CE1	2.39	0.57
1:A:213:LYS:HA	1:A:259:ILE:HD13	1.86	0.57
1:D:332:ARG:HE	1:D:332:ARG:HA	1.68	0.57
1:D:211:GLN:HA	1:D:214:LEU:HD23	1.87	0.57
1:D:215:ILE:O	1:D:218:LYS:N	2.38	0.57
1:A:258:ARG:O	1:A:262:GLU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ASN:HD22	1:B:300:GLY:HA3	1.70	0.56
1:C:130:TYR:O	1:C:135:LEU:HD22	2.04	0.56
1:D:366:ALA:N	1:D:367:PRO:CD	2.68	0.56
1:B:235:ASP:C	1:B:239:VAL:HG23	2.31	0.56
1:B:344:ARG:HG3	1:B:344:ARG:HH11	1.71	0.56
1:C:179:ILE:HG22	1:C:180:LEU:H	1.71	0.56
1:C:306:GLU:HG2	1:C:331:PHE:HE1	1.70	0.56
1:C:317:LEU:CD2	1:C:318:GLU:H	2.14	0.56
1:A:295:ILE:CG2	1:A:296:LEU:H	2.12	0.56
1:C:255:ALA:C	1:C:257:LEU:N	2.63	0.56
1:C:260:ILE:CG2	1:C:267:LEU:HD22	2.35	0.56
1:D:254:ALA:C	1:D:256:THR:N	2.60	0.56
1:D:363:ASP:OD1	1:D:364:VAL:N	2.37	0.56
1:B:208:GLN:HG2	1:B:243:ILE:CD1	2.36	0.56
1:C:307:ARG:O	1:C:308:GLU:CB	2.54	0.56
1:C:316:LYS:HG3	1:C:316:LYS:O	2.06	0.56
1:A:275:ASN:O	1:A:277:LEU:N	2.39	0.56
1:B:217:SER:O	1:B:218:LYS:C	2.47	0.56
1:C:270:LEU:O	1:C:270:LEU:HG	2.05	0.56
1:A:326:SER:C	1:A:328:SER:H	2.13	0.56
1:B:216:MET:CE	1:B:259:ILE:HG21	2.36	0.56
1:B:233:ARG:NH2	1:B:244:ASP:HB3	2.19	0.56
1:C:155:GLU:O	1:C:158:ARG:CZ	2.54	0.56
1:C:191:ILE:N	1:C:191:ILE:HD12	2.20	0.56
1:A:131:ASP:OD1	1:A:133:ALA:HB3	2.06	0.56
1:B:205:LYS:HG2	1:B:208:GLN:CG	2.36	0.56
1:C:345:PHE:O	1:C:348:LEU:HB2	2.06	0.56
1:B:205:LYS:O	1:B:208:GLN:HB2	2.06	0.56
1:C:264:ILE:N	1:C:265:PRO:HD3	2.21	0.56
1:C:346:PRO:C	1:C:348:LEU:H	2.13	0.56
1:C:152:PHE:CD1	1:C:161:PHE:HD2	2.24	0.56
1:C:271:ASN:HD21	1:C:273:SER:CB	2.18	0.56
1:D:365:GLU:C	1:D:367:PRO:HD3	2.31	0.56
1:A:277:LEU:HD12	1:A:277:LEU:C	2.31	0.55
1:C:132:LYS:CA	1:C:136:LEU:HG	2.33	0.55
1:C:216:MET:SD	1:C:259:ILE:HG21	2.46	0.55
1:D:211:GLN:HA	1:D:214:LEU:HB3	1.88	0.55
1:D:235:ASP:O	1:D:237:ASP:N	2.39	0.55
1:C:155:GLU:O	1:C:156:ASN:HB2	2.06	0.55
1:C:229:LEU:HD22	1:C:232:LEU:CD1	2.37	0.55
1:D:225:GLN:HE22	1:D:266:GLU:HG2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ARG:HH12	1:C:232:LEU:CG	2.18	0.55
1:A:122:ILE:O	1:A:123:THR:O	2.25	0.55
1:B:305:SER:O	1:B:307:ARG:N	2.39	0.55
1:C:205:LYS:N	1:C:208:GLN:OE1	2.29	0.55
1:A:119:TRP:CH2	1:A:150:ILE:HG21	2.40	0.55
1:A:296:LEU:CG	1:A:297:ASN:H	2.20	0.55
1:A:320:LEU:HG	1:A:321:TRP:N	2.20	0.55
1:A:320:LEU:CG	1:A:321:TRP:N	2.69	0.55
1:B:309:LEU:HB2	1:B:344:ARG:CD	2.37	0.55
1:C:181:ASP:OD1	1:C:185:ARG:O	2.24	0.55
1:D:225:GLN:NE2	1:D:266:GLU:HG2	2.22	0.55
1:A:258:ARG:HG2	1:A:262:GLU:OE2	2.07	0.55
1:B:215:ILE:HD13	1:B:215:ILE:O	2.07	0.55
1:B:296:LEU:HB3	1:B:320:LEU:CD1	2.33	0.55
1:A:175:VAL:C	1:A:178:LYS:HG3	2.31	0.55
1:B:204:LEU:HA	1:B:208:GLN:NE2	2.22	0.55
1:B:213:LYS:HB2	1:B:259:ILE:HD13	1.88	0.55
1:B:342:ARG:NH2	1:B:357:PRO:O	2.37	0.55
1:D:283:MET:HE2	1:D:312:ILE:HD13	1.89	0.55
1:C:342:ARG:HH11	1:C:348:LEU:HB3	1.72	0.55
1:D:358:PRO:C	1:D:360:ILE:N	2.65	0.55
1:A:255:ALA:O	1:A:258:ARG:N	2.40	0.54
1:B:229:LEU:HB3	1:B:232:LEU:HD11	1.89	0.54
1:B:325:ASN:O	1:B:328:SER:N	2.39	0.54
1:C:129:LYS:HD2	1:C:129:LYS:N	2.21	0.54
1:C:278:TYR:HD1	1:C:278:TYR:C	2.14	0.54
1:C:348:LEU:O	1:C:349:LEU:HG	2.07	0.54
1:C:278:TYR:CD1	1:C:278:TYR:C	2.85	0.54
1:D:210:GLU:HG3	1:D:213:LYS:CE	2.38	0.54
1:D:215:ILE:O	1:D:217:SER:N	2.40	0.54
1:B:349:LEU:O	1:B:356:LEU:N	2.35	0.54
1:C:247:LEU:HD23	1:C:247:LEU:C	2.32	0.54
1:C:258:ARG:HG3	1:C:258:ARG:HH11	1.71	0.54
1:C:322:LEU:O	1:C:325:ASN:ND2	2.40	0.54
1:A:216:MET:O	1:A:219:ARG:N	2.37	0.54
1:D:239:VAL:CG2	1:D:240:ALA:N	2.71	0.54
1:C:305:SER:CB	1:C:307:ARG:HD2	2.38	0.54
1:B:327:LEU:C	1:B:329:ASP:N	2.63	0.54
1:A:205:LYS:O	1:A:207:GLU:N	2.40	0.54
1:A:275:ASN:O	1:A:276:ARG:C	2.50	0.54
1:B:213:LYS:HA	1:B:216:MET:HE3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ILE:HG13	1:C:161:PHE:CE1	2.43	0.54
1:A:296:LEU:HD21	1:A:298:LEU:HG	1.87	0.54
1:A:343:GLU:HG3	1:A:344:ARG:N	2.21	0.54
1:B:205:LYS:HE3	1:B:208:GLN:HG3	1.89	0.54
1:A:153:HIS:NE2	1:A:160:GLN:HG3	2.22	0.54
1:C:180:LEU:HD11	1:C:184:ASN:HA	1.90	0.54
1:C:332:ARG:O	1:C:333:ASP:HB3	2.08	0.54
1:A:182:ARG:CG	1:A:183:GLU:H	2.21	0.54
1:A:215:ILE:CG2	1:A:238:LEU:HD11	2.38	0.54
1:D:327:LEU:O	1:D:327:LEU:CG	2.56	0.54
1:A:153:HIS:HD2	1:A:153:HIS:O	1.91	0.53
1:A:182:ARG:O	1:A:184:ASN:N	2.41	0.53
1:A:279:ARG:HH22	1:A:282:ASP:H	1.57	0.53
1:B:219:ARG:O	1:B:220:TYR:CB	2.56	0.53
1:D:240:ALA:O	1:D:241:GLN:HB3	2.07	0.53
1:D:303:LEU:HB2	1:D:325:ASN:CB	2.38	0.53
1:A:177:TYR:CG	1:A:177:TYR:O	2.62	0.53
1:A:228:ASP:C	1:A:230:LYS:H	2.16	0.53
1:B:267:LEU:HD11	1:B:269:SER:O	2.08	0.53
1:A:221:ASP:OD2	1:A:223:SER:HB2	2.07	0.53
1:A:229:LEU:HD23	1:A:229:LEU:O	2.08	0.53
1:A:317:LEU:HD13	1:A:320:LEU:HD12	1.90	0.53
1:A:347:LYS:O	1:A:349:LEU:HD12	2.09	0.53
1:B:274:ASN:ND2	1:B:299:SER:O	2.42	0.53
1:C:305:SER:HB3	1:C:307:ARG:HD2	1.91	0.53
1:D:300:GLY:H	1:D:324:GLY:HA3	1.74	0.53
1:A:110:THR:HG22	1:A:111:SER:N	2.24	0.53
1:A:190:ILE:HG22	1:A:190:ILE:O	2.08	0.53
1:B:235:ASP:OD1	1:B:238:LEU:HB2	2.09	0.53
1:C:132:LYS:HE2	1:C:152:PHE:HD2	1.73	0.53
1:C:308:GLU:O	1:C:309:LEU:C	2.51	0.53
1:C:342:ARG:HH22	1:C:356:LEU:HB2	1.72	0.53
1:A:183:GLU:O	1:A:184:ASN:CB	2.57	0.53
1:A:279:ARG:HH12	1:A:282:ASP:HB3	1.74	0.53
1:A:281:ASP:O	1:A:284:SER:HB3	2.08	0.53
1:B:267:LEU:HD21	1:B:270:LEU:HD13	1.91	0.53
1:B:287:VAL:HG11	1:B:314:GLY:CA	2.38	0.53
1:D:360:ILE:HG12	1:D:364:VAL:O	2.07	0.53
1:A:185:ARG:HD2	1:D:354:HIS:CD2	2.43	0.53
1:A:197:PRO:O	1:A:198:HIS:C	2.52	0.53
1:A:315:LEU:O	1:A:317:LEU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ASP:O	1:B:239:VAL:N	2.36	0.53
1:B:280:LEU:N	1:B:308:GLU:OE1	2.33	0.53
1:A:173:LYS:N	1:A:191:ILE:HD12	2.24	0.53
1:B:248:ASN:HB3	1:B:276:ARG:O	2.09	0.53
1:C:331:PHE:CD2	1:C:337:TYR:HA	2.43	0.53
1:D:215:ILE:C	1:D:217:SER:N	2.66	0.53
1:D:252:SER:HA	1:D:255:ALA:HB3	1.91	0.53
1:A:215:ILE:HG21	1:A:238:LEU:HD11	1.91	0.53
1:A:229:LEU:HD23	1:A:232:LEU:CD1	2.39	0.53
1:A:263:ASN:O	1:A:265:PRO:HD3	2.08	0.53
1:A:326:SER:C	1:A:328:SER:N	2.64	0.53
1:C:265:PRO:C	1:C:267:LEU:N	2.66	0.53
1:C:266:GLU:O	1:C:267:LEU:C	2.52	0.53
1:D:238:LEU:H	1:D:238:LEU:HD23	1.72	0.53
1:D:322:LEU:N	1:D:352:ASP:OD1	2.32	0.53
1:A:261:GLU:O	1:A:265:PRO:HG3	2.09	0.52
1:B:227:LEU:HD13	1:B:264:ILE:HD11	1.91	0.52
1:D:237:ASP:C	1:D:239:VAL:N	2.67	0.52
1:D:295:ILE:HG21	1:D:319:GLU:OE1	2.09	0.52
1:B:273:SER:HB3	1:B:297:ASN:ND2	2.25	0.52
1:B:322:LEU:HD11	1:B:341:ILE:CG2	2.39	0.52
1:C:169:ALA:HA	1:C:172:LEU:CB	2.38	0.52
1:C:265:PRO:O	1:C:267:LEU:N	2.43	0.52
1:D:287:VAL:HG13	1:D:315:LEU:N	2.25	0.52
1:A:241:GLN:O	1:A:243:ILE:HG13	2.09	0.52
1:C:105:ARG:CD	1:C:106:GLY:N	2.65	0.52
1:C:266:GLU:HA	1:C:292:ASN:OD1	2.09	0.52
1:C:297:ASN:ND2	1:C:297:ASN:O	2.42	0.52
1:D:303:LEU:HB2	1:D:325:ASN:ND2	2.24	0.52
1:A:122:ILE:O	1:A:123:THR:C	2.52	0.52
1:C:246:VAL:O	1:C:246:VAL:HG23	2.09	0.52
1:B:261:GLU:OE1	1:B:289:LYS:HD3	2.10	0.52
1:D:290:ALA:N	1:D:291:PRO:HD3	2.25	0.52
1:A:326:SER:O	1:A:328:SER:N	2.42	0.52
1:B:293:LEU:HD12	1:B:295:ILE:H	1.75	0.52
1:B:312:ILE:O	1:B:314:GLY:N	2.42	0.52
1:C:130:TYR:C	1:C:135:LEU:HB2	2.34	0.52
1:A:110:THR:C	1:A:112:GLN:H	2.18	0.52
1:C:168:THR:O	1:C:172:LEU:HG	2.10	0.52
1:C:271:ASN:HD21	1:C:273:SER:H	1.52	0.52
1:A:346:PRO:C	1:A:348:LEU:N	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:VAL:HG23	1:C:145:VAL:O	2.10	0.52
1:C:232:LEU:HD13	1:C:247:LEU:CD1	2.36	0.52
1:D:257:LEU:CD2	1:D:286:ILE:HG13	2.40	0.52
1:B:312:ILE:C	1:B:314:GLY:H	2.18	0.51
1:C:311:LYS:C	1:C:313:LYS:N	2.63	0.51
1:A:172:LEU:CB	1:A:191:ILE:HD11	2.41	0.51
1:A:173:LYS:CA	1:A:191:ILE:HD12	2.40	0.51
1:C:180:LEU:CD1	1:C:184:ASN:HA	2.40	0.51
1:C:219:ARG:HH12	1:C:232:LEU:CD1	2.22	0.51
1:C:306:GLU:HG2	1:C:331:PHE:CE1	2.45	0.51
1:D:243:ILE:HG22	1:D:243:ILE:O	2.09	0.51
1:A:147:PHE:CD1	1:A:148:THR:N	2.68	0.51
1:B:238:LEU:HD12	1:B:243:ILE:HG21	1.92	0.51
1:B:255:ALA:O	1:B:259:ILE:HG13	2.10	0.51
1:C:298:LEU:N	1:C:298:LEU:HD12	2.24	0.51
1:D:319:GLU:HG3	1:D:350:ARG:HB2	1.93	0.51
1:A:230:LYS:HE2	1:A:274:ASN:ND2	2.25	0.51
1:B:290:ALA:N	1:B:291:PRO:CD	2.71	0.51
1:B:327:LEU:HA	1:B:330:THR:CG2	2.38	0.51
1:C:255:ALA:C	1:C:257:LEU:H	2.17	0.51
1:D:235:ASP:C	1:D:237:ASP:N	2.68	0.51
1:D:279:ARG:HA	1:D:308:GLU:OE1	2.10	0.51
1:A:155:GLU:OE2	1:A:205:LYS:HE2	2.10	0.51
1:A:208:GLN:O	1:A:212:LEU:N	2.42	0.51
1:B:332:ARG:HH22	1:D:304:LYS:HG2	1.76	0.51
1:C:152:PHE:HD1	1:C:161:PHE:HB3	1.75	0.51
1:C:286:ILE:HD11	1:C:290:ALA:CB	2.40	0.51
1:A:328:SER:O	1:A:330:THR:N	2.43	0.51
1:B:364:VAL:HG13	1:B:364:VAL:O	2.10	0.51
1:C:246:VAL:O	1:C:248:ASN:N	2.44	0.51
1:A:279:ARG:NH1	1:A:282:ASP:OD1	2.44	0.51
1:A:322:LEU:HD21	1:A:327:LEU:HD13	1.92	0.51
1:A:348:LEU:HD21	1:A:350:ARG:O	2.10	0.51
1:B:215:ILE:HD13	1:B:215:ILE:C	2.36	0.51
1:D:204:LEU:C	1:D:205:LYS:HD2	2.35	0.51
1:A:236:PRO:HA	1:A:239:VAL:CG1	2.40	0.51
1:A:238:LEU:HB3	1:A:243:ILE:HG21	1.93	0.51
1:B:333:ASP:O	1:B:333:ASP:OD2	2.29	0.51
1:C:158:ARG:H	1:C:158:ARG:CD	2.22	0.51
1:C:320:LEU:HD21	1:C:322:LEU:HD11	1.92	0.51
1:D:342:ARG:NH1	1:D:348:LEU:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PRO:O	1:A:238:LEU:N	2.43	0.51
1:A:308:GLU:C	1:A:310:ASP:N	2.65	0.51
1:C:167:SER:HA	1:C:170:SER:HB2	1.93	0.51
1:D:322:LEU:O	1:D:323:ASP:C	2.51	0.51
1:A:246:VAL:HG23	1:A:249:ARG:HB3	1.92	0.51
1:C:179:ILE:HG22	1:C:180:LEU:N	2.25	0.51
1:D:303:LEU:N	1:D:303:LEU:HD22	2.26	0.51
1:A:327:LEU:HD23	1:A:327:LEU:O	2.11	0.50
1:B:204:LEU:CD1	1:B:252:SER:HA	2.41	0.50
1:B:271:ASN:C	1:B:273:SER:H	2.19	0.50
1:C:231:GLY:O	1:C:233:ARG:N	2.38	0.50
1:D:221:ASP:OD1	1:D:224:GLN:N	2.42	0.50
1:A:181:ASP:OD2	1:A:185:ARG:NH2	2.36	0.50
1:A:250:ARG:HD2	1:A:279:ARG:NH2	2.26	0.50
1:A:306:GLU:HG3	1:A:344:ARG:NH1	2.27	0.50
1:A:319:GLU:HG3	1:A:350:ARG:HD3	1.93	0.50
1:C:131:ASP:O	1:C:133:ALA:N	2.43	0.50
1:D:293:LEU:CD2	1:D:315:LEU:HD13	2.33	0.50
1:A:115:THR:HG22	1:A:116:SER:N	2.23	0.50
1:A:219:ARG:HH11	1:A:219:ARG:HG2	1.76	0.50
1:B:202:ASN:O	1:B:203:GLU:HB2	2.11	0.50
1:B:340:ALA:C	1:B:342:ARG:N	2.66	0.50
1:D:309:LEU:O	1:D:310:ASP:C	2.53	0.50
1:D:365:GLU:CD	1:D:366:ALA:H	2.20	0.50
1:A:132:LYS:HG3	1:A:152:PHE:CE2	2.46	0.50
1:A:306:GLU:HB2	1:A:327:LEU:HD21	1.93	0.50
1:B:342:ARG:NH1	1:B:348:LEU:O	2.44	0.50
1:D:295:ILE:HG23	1:D:319:GLU:CB	2.38	0.50
1:A:138:MET:HA	1:A:141:SER:OG	2.12	0.50
1:A:333:ASP:OD1	1:A:335:SER:HB2	2.11	0.50
1:B:229:LEU:C	1:B:231:GLY:H	2.19	0.50
1:C:169:ALA:HA	1:C:172:LEU:HB2	1.94	0.50
1:C:305:SER:CB	1:C:307:ARG:HG2	2.42	0.50
1:D:294:LYS:HE3	1:D:318:GLU:OE2	2.11	0.50
1:A:311:LYS:HE2	1:B:258:ARG:CZ	2.41	0.50
1:D:297:ASN:HA	1:D:321:TRP:HB2	1.94	0.50
1:B:209:VAL:C	1:B:211:GLN:N	2.69	0.50
1:B:237:ASP:O	1:B:241:GLN:NE2	2.45	0.50
1:B:274:ASN:ND2	1:B:274:ASN:N	2.59	0.50
1:B:324:GLY:HA2	1:C:177:TYR:CD1	2.46	0.50
1:B:360:ILE:HG23	1:C:214:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ARG:HD2	1:C:282:ASP:OD1	2.10	0.50
1:C:326:SER:C	1:C:328:SER:N	2.67	0.50
1:A:110:THR:N	1:A:115:THR:HG21	2.26	0.50
1:A:237:ASP:O	1:A:241:GLN:OE1	2.30	0.50
1:D:229:LEU:HD22	1:D:232:LEU:HD13	1.94	0.50
1:A:216:MET:O	1:A:220:TYR:N	2.38	0.50
1:B:228:ASP:C	1:B:229:LEU:HD23	2.37	0.50
1:B:305:SER:OG	1:B:307:ARG:HG2	2.12	0.50
1:B:324:GLY:O	1:B:325:ASN:ND2	2.45	0.50
1:C:227:LEU:HD21	1:C:229:LEU:HG	1.94	0.50
1:A:172:LEU:N	1:A:172:LEU:HD12	2.27	0.49
1:A:315:LEU:O	1:A:317:LEU:HG	2.12	0.49
1:D:225:GLN:HG3	1:D:268:LEU:HD12	1.94	0.49
1:A:238:LEU:HB3	1:A:243:ILE:CG2	2.42	0.49
1:B:212:LEU:HA	1:B:215:ILE:HG22	1.94	0.49
1:B:251:SER:O	1:B:254:ALA:HB3	2.12	0.49
1:C:216:MET:CG	1:C:227:LEU:HD11	2.42	0.49
1:D:219:ARG:NH2	1:D:236:PRO:CG	2.75	0.49
1:D:287:VAL:HA	1:D:315:LEU:HD23	1.93	0.49
1:D:329:ASP:OD1	1:D:329:ASP:N	2.30	0.49
1:D:338:ILE:O	1:D:339:SER:C	2.55	0.49
1:B:229:LEU:HB3	1:B:232:LEU:CD1	2.42	0.49
1:C:299:SER:OG	1:C:321:TRP:HB3	2.12	0.49
1:D:221:ASP:HB3	1:D:226:ALA:HB3	1.95	0.49
1:A:240:ALA:O	1:A:241:GLN:OE1	2.30	0.49
1:B:216:MET:HE3	1:B:259:ILE:HG21	1.93	0.49
1:B:266:GLU:CD	1:B:266:GLU:H	2.19	0.49
1:A:168:THR:O	1:A:169:ALA:C	2.54	0.49
1:A:127:GLY:C	1:A:129:LYS:N	2.71	0.49
1:A:158:ARG:NH2	1:A:205:LYS:HE3	2.27	0.49
1:A:182:ARG:C	1:A:184:ASN:N	2.70	0.49
1:A:200:ILE:H	1:A:200:ILE:CD1	2.15	0.49
1:A:305:SER:C	1:A:307:ARG:N	2.70	0.49
1:B:215:ILE:HG13	1:B:238:LEU:HD22	1.93	0.49
1:B:332:ARG:HG3	1:B:332:ARG:NH1	2.28	0.49
1:D:233:ARG:HH21	1:D:244:ASP:CG	2.21	0.49
1:A:123:THR:O	1:A:123:THR:HG22	2.12	0.49
1:C:168:THR:C	1:C:172:LEU:HG	2.37	0.49
1:C:322:LEU:O	1:C:325:ASN:HB2	2.13	0.49
1:D:266:GLU:N	1:D:266:GLU:OE1	2.45	0.49
1:A:115:THR:C	1:A:117:LYS:H	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ARG:NH2	1:A:246:VAL:HG12	2.27	0.49
1:B:308:GLU:HA	1:B:311:LYS:HE3	1.94	0.49
1:B:327:LEU:O	1:B:329:ASP:N	2.46	0.49
1:C:273:SER:HB2	1:C:297:ASN:HD21	1.78	0.49
1:A:130:TYR:CZ	1:A:187:ILE:HD11	2.48	0.49
1:B:362:PHE:CE2	1:C:217:SER:HA	2.48	0.49
1:D:232:LEU:HG	1:D:245:VAL:CG2	2.31	0.49
1:D:309:LEU:HB3	1:D:344:ARG:HG2	1.94	0.49
1:A:121:LYS:HE3	1:A:160:GLN:NE2	2.27	0.48
1:A:209:VAL:C	1:A:211:GLN:N	2.66	0.48
1:A:351:LEU:C	1:A:353:GLY:H	2.21	0.48
1:B:205:LYS:CE	1:B:208:GLN:HG3	2.43	0.48
1:D:297:ASN:ND2	1:D:321:TRP:HB2	2.28	0.48
1:A:221:ASP:O	1:A:225:GLN:HA	2.13	0.48
1:A:243:ILE:HG22	1:A:243:ILE:O	2.13	0.48
1:A:343:GLU:CG	1:A:344:ARG:N	2.76	0.48
1:B:221:ASP:OD1	1:B:221:ASP:O	2.31	0.48
1:B:243:ILE:O	1:B:243:ILE:HG23	2.12	0.48
1:C:283:MET:C	1:C:285:SER:H	2.21	0.48
1:C:315:LEU:C	1:C:317:LEU:H	2.21	0.48
1:D:235:ASP:C	1:D:235:ASP:OD2	2.56	0.48
1:D:236:PRO:C	1:D:237:ASP:CG	2.80	0.48
1:D:237:ASP:C	1:D:239:VAL:H	2.20	0.48
1:A:215:ILE:N	1:A:215:ILE:HD13	2.27	0.48
1:A:323:ASP:O	1:A:325:ASN:N	2.45	0.48
1:B:276:ARG:CZ	1:B:276:ARG:HB2	2.42	0.48
1:C:273:SER:HB2	1:C:297:ASN:ND2	2.29	0.48
1:A:306:GLU:CB	1:A:327:LEU:HD21	2.44	0.48
1:A:348:LEU:HD23	1:A:349:LEU:N	2.26	0.48
1:C:273:SER:O	1:C:275:ASN:HB2	2.13	0.48
1:A:362:PHE:O	1:A:362:PHE:CD1	2.67	0.48
1:C:225:GLN:HE21	1:C:266:GLU:HB2	1.79	0.48
1:C:275:ASN:C	1:C:301:ASN:ND2	2.71	0.48
1:D:271:ASN:C	1:D:271:ASN:ND2	2.54	0.48
1:A:199:THR:O	1:A:201:LEU:N	2.47	0.48
1:A:301:ASN:CA	1:A:325:ASN:HD21	2.26	0.48
1:D:355:GLU:OE1	1:D:355:GLU:O	2.32	0.48
1:A:138:MET:C	1:A:140:GLN:N	2.58	0.48
1:B:294:LYS:HB2	1:B:318:GLU:HG2	1.94	0.48
1:B:312:ILE:C	1:B:314:GLY:N	2.72	0.48
1:C:125:PRO:O	1:C:126:TYR:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:GLN:HE21	1:C:244:ASP:HA	1.77	0.48
1:D:370:LEU:CD1	1:D:371:PRO:O	2.59	0.48
1:A:308:GLU:O	1:A:310:ASP:N	2.47	0.48
1:B:269:SER:HB2	1:B:295:ILE:HD12	1.94	0.48
1:D:219:ARG:CZ	1:D:236:PRO:HG3	2.44	0.48
1:C:260:ILE:HG23	1:C:267:LEU:HD22	1.96	0.48
1:C:309:LEU:H	1:C:309:LEU:CD2	2.26	0.48
1:D:297:ASN:C	1:D:297:ASN:ND2	2.71	0.48
1:D:312:ILE:C	1:D:314:GLY:H	2.20	0.48
1:A:250:ARG:CG	1:A:282:ASP:HB3	2.41	0.48
1:A:322:LEU:HD23	1:A:322:LEU:O	2.14	0.48
1:B:216:MET:HE1	1:B:259:ILE:HB	1.96	0.48
1:C:199:THR:HG23	1:C:200:ILE:H	1.78	0.48
1:C:219:ARG:HH12	1:C:232:LEU:HD12	1.79	0.48
1:D:246:VAL:HG23	1:D:249:ARG:HG3	1.96	0.48
1:A:128:ARG:HB2	1:A:154:TYR:HD2	1.79	0.47
1:A:338:ILE:O	1:A:342:ARG:CB	2.62	0.47
1:C:195:ALA:HB1	1:C:196:PRO:HD2	1.96	0.47
1:D:249:ARG:HG3	1:D:249:ARG:HH11	1.78	0.47
1:A:137:SER:O	1:A:140:GLN:HB3	2.14	0.47
1:A:267:LEU:HD11	1:A:269:SER:O	2.14	0.47
1:B:344:ARG:HG3	1:B:344:ARG:NH1	2.26	0.47
1:C:296:LEU:HD22	1:C:298:LEU:HD12	1.95	0.47
1:A:261:GLU:CD	1:A:289:LYS:HG2	2.39	0.47
1:B:212:LEU:CA	1:B:215:ILE:HG22	2.43	0.47
1:B:264:ILE:O	1:B:265:PRO:C	2.56	0.47
1:C:155:GLU:HB3	1:C:158:ARG:NE	2.30	0.47
1:C:280:LEU:CB	1:C:308:GLU:HB3	2.41	0.47
1:D:235:ASP:O	1:D:237:ASP:OD1	2.32	0.47
1:B:274:ASN:HD22	1:B:274:ASN:H	1.60	0.47
1:C:131:ASP:C	1:C:135:LEU:HB3	2.39	0.47
1:C:162:PHE:N	1:C:162:PHE:CD1	2.82	0.47
1:B:277:LEU:H	1:B:301:ASN:HB3	1.80	0.47
1:C:283:MET:HE2	1:C:286:ILE:HG21	1.95	0.47
1:C:312:ILE:O	1:C:315:LEU:HB2	2.14	0.47
1:C:319:GLU:CD	1:C:350:ARG:HG3	2.39	0.47
1:D:207:GLU:HG3	1:D:208:GLN:HG3	1.96	0.47
1:D:246:VAL:C	1:D:248:ASN:N	2.71	0.47
1:A:191:ILE:O	1:A:192:ASN:OD1	2.32	0.47
1:A:196:PRO:O	1:A:197:PRO:C	2.57	0.47
1:A:320:LEU:O	1:A:321:TRP:CD1	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:TYR:HB3	1:C:134:TRP:CE3	2.50	0.47
1:D:370:LEU:HD22	1:D:371:PRO:N	2.29	0.47
1:A:119:TRP:C	1:A:120:PHE:CD1	2.92	0.47
1:A:119:TRP:CG	1:A:196:PRO:HA	2.48	0.47
1:A:230:LYS:CG	1:A:231:GLY:H	2.13	0.47
1:A:274:ASN:HA	1:A:300:GLY:O	2.14	0.47
1:A:283:MET:HE2	1:A:286:ILE:HG21	1.95	0.47
1:A:296:LEU:CG	1:A:297:ASN:N	2.78	0.47
1:A:297:ASN:O	1:A:298:LEU:CG	2.60	0.47
1:A:308:GLU:C	1:A:310:ASP:H	2.23	0.47
1:B:206:PRO:C	1:B:208:GLN:N	2.69	0.47
1:C:133:ALA:C	1:C:135:LEU:N	2.72	0.47
1:C:252:SER:O	1:C:254:ALA:N	2.47	0.47
1:C:296:LEU:HD23	1:C:297:ASN:H	1.80	0.47
1:C:323:ASP:HB3	1:C:352:ASP:CG	2.40	0.47
1:A:125:PRO:HD2	1:A:188:SER:O	2.15	0.47
1:B:276:ARG:HA	1:B:301:ASN:HA	1.97	0.47
1:B:333:ASP:O	1:B:334:GLN:C	2.57	0.47
1:C:177:TYR:CE1	1:C:188:SER:HB3	2.50	0.47
1:D:246:VAL:O	1:D:248:ASN:N	2.48	0.47
1:D:351:LEU:HB2	1:D:356:LEU:HD11	1.96	0.47
1:A:321:TRP:O	1:A:322:LEU:HB2	2.15	0.47
1:B:206:PRO:C	1:B:208:GLN:H	2.23	0.47
1:B:280:LEU:CB	1:B:308:GLU:OE1	2.63	0.47
1:C:130:TYR:HE2	1:C:181:ASP:CG	2.23	0.47
1:D:312:ILE:C	1:D:314:GLY:N	2.73	0.47
1:A:204:LEU:HB3	1:A:208:GLN:CG	2.42	0.47
1:D:268:LEU:HA	1:D:293:LEU:HA	1.97	0.47
1:A:254:ALA:O	1:A:255:ALA:C	2.58	0.46
1:A:334:GLN:O	1:A:338:ILE:HG13	2.15	0.46
1:A:362:PHE:O	1:A:362:PHE:HD1	1.98	0.46
1:C:139:ILE:O	1:C:141:SER:N	2.48	0.46
1:D:213:LYS:HG3	1:D:259:ILE:HG21	1.96	0.46
1:D:232:LEU:O	1:D:236:PRO:HD2	2.15	0.46
1:A:119:TRP:CH2	1:A:197:PRO:HD3	2.50	0.46
1:A:180:LEU:HD12	1:A:186:ARG:CZ	2.45	0.46
1:A:297:ASN:C	1:A:298:LEU:HG	2.39	0.46
1:A:299:SER:O	1:A:300:GLY:C	2.57	0.46
1:A:320:LEU:HD23	1:A:321:TRP:N	2.30	0.46
1:B:205:LYS:N	1:B:208:GLN:NE2	2.55	0.46
1:C:149:PRO:HB3	1:C:161:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:GLU:C	1:C:310:ASP:H	2.22	0.46
1:D:280:LEU:C	1:D:282:ASP:N	2.71	0.46
1:A:292:ASN:O	1:A:293:LEU:C	2.58	0.46
1:A:303:LEU:O	1:A:325:ASN:HB3	2.16	0.46
1:A:330:THR:O	1:A:331:PHE:CD1	2.67	0.46
1:B:326:SER:OG	1:B:327:LEU:N	2.49	0.46
1:B:338:ILE:O	1:B:342:ARG:HB2	2.15	0.46
1:A:152:PHE:O	1:A:153:HIS:HB3	2.16	0.46
1:A:252:SER:C	1:A:254:ALA:N	2.73	0.46
1:A:317:LEU:CD1	1:A:320:LEU:HD12	2.45	0.46
1:A:322:LEU:CD2	1:A:327:LEU:HD13	2.45	0.46
1:A:252:SER:O	1:A:254:ALA:N	2.49	0.46
1:A:323:ASP:N	1:A:352:ASP:OD1	2.45	0.46
1:B:332:ARG:NH2	1:D:304:LYS:HG2	2.31	0.46
1:C:169:ALA:CB	1:C:191:ILE:HG21	2.44	0.46
1:C:230:LYS:CG	1:C:273:SER:HB3	2.35	0.46
1:A:131:ASP:C	1:A:133:ALA:N	2.71	0.46
1:A:230:LYS:O	1:A:231:GLY:C	2.58	0.46
1:A:342:ARG:NH1	1:A:356:LEU:CD1	2.78	0.46
1:C:130:TYR:HD1	1:C:135:LEU:HD13	1.79	0.46
1:C:235:ASP:H	1:C:239:VAL:CG2	2.27	0.46
1:A:205:LYS:H	1:A:208:GLN:NE2	2.13	0.46
1:C:283:MET:C	1:C:285:SER:N	2.71	0.46
1:D:208:GLN:O	1:D:211:GLN:N	2.47	0.46
1:A:162:PHE:HE1	1:A:198:HIS:H	1.64	0.46
1:B:208:GLN:HG2	1:B:243:ILE:HD11	1.98	0.46
1:B:271:ASN:ND2	1:B:273:SER:CB	2.75	0.46
1:B:342:ARG:HG3	1:B:345:PHE:O	2.16	0.46
1:C:283:MET:HE3	1:C:286:ILE:HG21	1.98	0.46
1:C:319:GLU:HG3	1:C:350:ARG:CB	2.36	0.46
1:C:332:ARG:O	1:C:333:ASP:CB	2.64	0.46
1:C:342:ARG:HH22	1:C:356:LEU:CB	2.28	0.46
1:D:246:VAL:CG2	1:D:249:ARG:HG3	2.45	0.46
1:D:328:SER:O	1:D:330:THR:N	2.49	0.46
1:A:123:THR:HA	1:A:160:GLN:CB	2.46	0.46
1:A:208:GLN:O	1:A:211:GLN:HB3	2.16	0.46
1:B:276:ARG:O	1:B:277:LEU:HD23	2.16	0.46
1:B:294:LYS:CA	1:B:317:LEU:HA	2.42	0.46
1:C:299:SER:O	1:C:301:ASN:N	2.40	0.46
1:A:182:ARG:C	1:A:184:ASN:H	2.24	0.46
1:A:212:LEU:O	1:A:214:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HG	1:A:229:LEU:HB2	1.98	0.46
1:A:283:MET:O	1:A:283:MET:HG3	2.15	0.46
1:A:309:LEU:H	1:A:309:LEU:CD2	2.28	0.46
1:A:320:LEU:CD2	1:A:321:TRP:O	2.64	0.46
1:B:211:GLN:O	1:B:212:LEU:C	2.58	0.46
1:B:351:LEU:HB2	1:B:356:LEU:CD1	2.36	0.46
1:D:215:ILE:O	1:D:216:MET:C	2.59	0.46
1:D:219:ARG:HH11	1:D:232:LEU:CD1	2.29	0.46
1:D:338:ILE:O	1:D:342:ARG:N	2.45	0.46
1:A:306:GLU:HG3	1:A:344:ARG:HH12	1.81	0.45
1:B:366:ALA:HB1	1:B:367:PRO:CD	2.46	0.45
1:C:199:THR:HG23	1:C:200:ILE:N	2.32	0.45
1:C:253:MET:HG3	1:C:253:MET:O	2.15	0.45
1:C:341:ILE:HG22	1:C:348:LEU:HD22	1.97	0.45
1:D:259:ILE:HD12	1:D:259:ILE:N	2.23	0.45
1:D:259:ILE:H	1:D:259:ILE:CD1	2.23	0.45
1:A:305:SER:C	1:A:307:ARG:H	2.24	0.45
1:A:351:LEU:C	1:A:353:GLY:N	2.74	0.45
1:B:230:LYS:O	1:B:230:LYS:HG2	2.16	0.45
1:D:314:GLY:O	1:D:315:LEU:O	2.33	0.45
1:A:143:SER:O	1:A:144:SER:C	2.57	0.45
1:A:153:HIS:O	1:A:153:HIS:CD2	2.69	0.45
1:A:280:LEU:HG	1:A:303:LEU:HD21	1.98	0.45
1:A:311:LYS:HD2	1:B:258:ARG:HH12	1.81	0.45
1:B:216:MET:HE1	1:B:259:ILE:HD12	1.98	0.45
1:C:177:TYR:CZ	1:C:188:SER:HB3	2.51	0.45
1:C:204:LEU:HA	1:C:208:GLN:OE1	2.16	0.45
1:D:213:LYS:CG	1:D:259:ILE:HG21	2.46	0.45
1:A:126:TYR:CG	1:D:354:HIS:ND1	2.84	0.45
1:A:290:ALA:N	1:A:291:PRO:HD3	2.31	0.45
1:C:125:PRO:O	1:C:127:GLY:N	2.49	0.45
1:C:296:LEU:H	1:C:317:LEU:HD21	1.80	0.45
1:C:323:ASP:O	1:C:324:GLY:C	2.60	0.45
1:D:219:ARG:HH12	1:D:232:LEU:HD12	1.78	0.45
1:D:339:SER:O	1:D:342:ARG:HB3	2.17	0.45
1:A:313:LYS:C	1:A:315:LEU:H	2.24	0.45
1:A:351:LEU:HD23	1:A:351:LEU:C	2.42	0.45
1:B:364:VAL:C	1:B:366:ALA:H	2.23	0.45
1:C:211:GLN:O	1:C:215:ILE:HG13	2.16	0.45
1:C:216:MET:HE3	1:C:216:MET:HB2	1.76	0.45
1:C:342:ARG:CZ	1:C:359:PRO:HG3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASP:OD1	1:A:181:ASP:C	2.59	0.45
1:A:279:ARG:HH22	1:A:282:ASP:N	2.15	0.45
1:A:323:ASP:HB3	1:A:352:ASP:CG	2.41	0.45
1:C:171:ALA:C	1:C:173:LYS:N	2.73	0.45
1:C:342:ARG:HD2	1:C:346:PRO:O	2.17	0.45
1:D:314:GLY:O	1:D:315:LEU:C	2.59	0.45
1:A:121:LYS:HE3	1:A:160:GLN:HE22	1.82	0.45
1:A:200:ILE:HD12	1:A:200:ILE:N	2.18	0.45
1:B:216:MET:CE	1:B:259:ILE:HD12	2.46	0.45
1:B:236:PRO:O	1:B:239:VAL:N	2.50	0.45
1:C:327:LEU:HD12	1:C:327:LEU:O	2.16	0.45
1:C:340:ALA:O	1:C:343:GLU:HB3	2.16	0.45
1:A:124:ILE:CD1	1:A:135:LEU:HD21	2.47	0.45
1:A:306:GLU:C	1:A:308:GLU:H	2.25	0.45
1:B:280:LEU:HG	1:B:303:LEU:CD2	2.47	0.45
1:B:293:LEU:HD12	1:B:294:LYS:N	2.31	0.45
1:B:340:ALA:C	1:B:342:ARG:H	2.24	0.45
1:D:276:ARG:HA	1:D:302:GLU:HG2	1.98	0.45
1:B:337:TYR:O	1:B:337:TYR:HD1	2.00	0.45
1:C:109:GLY:O	1:C:110:THR:C	2.59	0.45
1:C:227:LEU:C	1:C:227:LEU:HD23	2.41	0.45
1:C:248:ASN:CB	1:C:277:LEU:HD23	2.46	0.45
1:D:249:ARG:HG3	1:D:249:ARG:NH1	2.32	0.45
1:A:220:TYR:HA	1:A:227:LEU:HA	1.98	0.45
1:B:211:GLN:NE2	1:B:214:LEU:HB3	2.32	0.45
1:C:224:GLN:O	1:C:225:GLN:O	2.34	0.45
1:C:258:ARG:HG2	1:C:262:GLU:OE2	2.17	0.45
1:C:305:SER:O	1:C:307:ARG:N	2.50	0.45
1:C:316:LYS:O	1:C:317:LEU:O	2.35	0.45
1:D:250:ARG:HA	1:D:282:ASP:OD2	2.17	0.45
1:B:267:LEU:HD12	1:B:268:LEU:N	2.27	0.44
1:A:212:LEU:C	1:A:214:LEU:N	2.72	0.44
1:A:299:SER:C	1:A:301:ASN:N	2.75	0.44
1:A:309:LEU:H	1:A:309:LEU:HD22	1.83	0.44
1:B:327:LEU:C	1:B:327:LEU:CD1	2.87	0.44
1:C:180:LEU:CG	1:C:181:ASP:N	2.80	0.44
1:A:220:TYR:CD1	1:A:264:ILE:HD13	2.52	0.44
1:A:276:ARG:CB	1:A:276:ARG:NH2	2.80	0.44
1:A:348:LEU:CD2	1:A:350:ARG:O	2.65	0.44
1:B:305:SER:HB2	1:D:330:THR:O	2.17	0.44
1:C:203:GLU:HA	1:C:251:SER:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ASP:C	1:C:335:SER:N	2.74	0.44
1:D:349:LEU:O	1:D:356:LEU:HB2	2.16	0.44
1:A:121:LYS:HE2	1:A:160:GLN:CD	2.42	0.44
1:A:238:LEU:HD23	1:A:243:ILE:CG2	2.46	0.44
1:A:317:LEU:C	1:A:319:GLU:N	2.74	0.44
1:B:205:LYS:HG2	1:B:208:GLN:CD	2.43	0.44
1:B:232:LEU:N	1:B:232:LEU:HD12	2.32	0.44
1:D:220:TYR:CD2	1:D:221:ASP:N	2.85	0.44
1:D:247:LEU:C	1:D:249:ARG:H	2.26	0.44
1:D:283:MET:CE	1:D:312:ILE:HG21	2.47	0.44
1:B:312:ILE:O	1:B:315:LEU:HD22	2.17	0.44
1:C:216:MET:HG2	1:C:227:LEU:HD11	2.00	0.44
1:C:337:TYR:O	1:C:338:ILE:C	2.58	0.44
1:D:216:MET:HE3	1:D:216:MET:HB2	1.87	0.44
1:D:280:LEU:C	1:D:282:ASP:H	2.25	0.44
1:D:310:ASP:OD1	1:D:344:ARG:CD	2.65	0.44
1:D:360:ILE:CG2	1:D:365:GLU:HB3	2.36	0.44
1:D:365:GLU:CD	1:D:366:ALA:N	2.75	0.44
1:A:205:LYS:H	1:A:208:GLN:CD	2.25	0.44
1:A:268:LEU:HD12	1:A:292:ASN:HB3	2.00	0.44
1:B:213:LYS:CB	1:B:259:ILE:HD13	2.47	0.44
1:B:227:LEU:HG	1:B:228:ASP:N	2.33	0.44
1:B:277:LEU:HG	1:B:301:ASN:CG	2.41	0.44
1:B:323:ASP:N	1:B:352:ASP:OD1	2.50	0.44
1:B:323:ASP:HA	1:C:177:TYR:CE2	2.52	0.44
1:B:325:ASN:HD22	1:B:325:ASN:HA	1.57	0.44
1:C:273:SER:O	1:C:274:ASN:O	2.35	0.44
1:A:172:LEU:CA	1:A:175:VAL:HG23	2.47	0.44
1:A:193:SER:O	1:A:194:SER:HB2	2.18	0.44
1:B:342:ARG:HD3	1:B:348:LEU:HB3	2.00	0.44
1:B:360:ILE:HG23	1:C:214:LEU:CD1	2.48	0.44
1:B:362:PHE:HB3	1:C:220:TYR:HD2	1.82	0.44
1:C:219:ARG:NH1	1:C:229:LEU:HA	2.33	0.44
1:D:233:ARG:CA	1:D:245:VAL:HG23	2.47	0.44
1:D:241:GLN:O	1:D:242:ASN:C	2.61	0.44
1:A:119:TRP:CZ2	1:A:197:PRO:HD3	2.53	0.44
1:A:280:LEU:HD12	1:A:308:GLU:CB	2.34	0.44
1:B:212:LEU:HA	1:B:215:ILE:CG2	2.47	0.44
1:B:257:LEU:C	1:B:259:ILE:N	2.73	0.44
1:C:122:ILE:HG23	1:C:124:ILE:HG13	1.99	0.44
1:C:205:LYS:HB3	1:C:206:PRO:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:ILE:C	1:D:288:GLN:N	2.75	0.44
1:D:303:LEU:HB2	1:D:325:ASN:HD22	1.82	0.44
1:A:119:TRP:CZ3	1:A:197:PRO:HD3	2.53	0.43
1:A:317:LEU:HD12	1:A:345:PHE:CD1	2.53	0.43
1:B:266:GLU:CD	1:B:266:GLU:N	2.76	0.43
1:B:354:HIS:ND1	1:C:126:TYR:CG	2.83	0.43
1:C:122:ILE:CG2	1:C:124:ILE:HG13	2.48	0.43
1:C:123:THR:O	1:C:124:ILE:O	2.36	0.43
1:C:265:PRO:HB2	1:C:266:GLU:OE2	2.18	0.43
1:D:211:GLN:CA	1:D:214:LEU:HB3	2.48	0.43
1:D:294:LYS:HD3	1:D:318:GLU:CD	2.42	0.43
1:D:358:PRO:O	1:D:360:ILE:N	2.51	0.43
1:A:250:ARG:CG	1:A:279:ARG:NH1	2.75	0.43
1:B:211:GLN:O	1:B:214:LEU:N	2.51	0.43
1:B:216:MET:HE1	1:B:259:ILE:CB	2.48	0.43
1:C:182:ARG:HG3	1:C:183:GLU:H	1.83	0.43
1:A:299:SER:OG	1:A:300:GLY:N	2.49	0.43
1:A:332:ARG:HB2	1:A:336:THR:CG2	2.49	0.43
1:B:205:LYS:O	1:B:209:VAL:N	2.48	0.43
1:B:327:LEU:CD1	1:B:328:SER:N	2.75	0.43
1:C:105:ARG:O	1:C:109:GLY:O	2.36	0.43
1:C:241:GLN:C	1:C:243:ILE:H	2.26	0.43
1:D:297:ASN:ND2	1:D:321:TRP:CB	2.81	0.43
1:A:109:GLY:HA2	1:A:117:LYS:HG2	1.99	0.43
1:A:249:ARG:HG3	1:A:251:SER:HB3	1.99	0.43
1:C:118:ASN:CG	1:C:166:ALA:HA	2.44	0.43
1:C:131:ASP:O	1:C:132:LYS:C	2.61	0.43
1:D:212:LEU:HG	1:D:216:MET:HE3	2.00	0.43
1:A:276:ARG:HB2	1:A:276:ARG:HH21	1.84	0.43
1:A:343:GLU:CD	1:A:343:GLU:C	2.87	0.43
1:C:255:ALA:O	1:C:258:ARG:N	2.52	0.43
1:C:271:ASN:ND2	1:C:297:ASN:HD22	2.17	0.43
1:C:332:ARG:CZ	1:C:332:ARG:HB3	2.49	0.43
1:A:256:THR:O	1:A:260:ILE:HG13	2.19	0.43
1:B:287:VAL:C	1:B:288:GLN:HG2	2.43	0.43
1:C:231:GLY:C	1:C:233:ARG:H	2.23	0.43
1:C:277:LEU:HG	1:C:301:ASN:ND2	2.34	0.43
1:D:331:PHE:CD1	1:D:331:PHE:N	2.86	0.43
1:A:131:ASP:HB3	1:A:134:TRP:CB	2.47	0.43
1:A:230:LYS:CE	1:A:274:ASN:HD22	2.28	0.43
1:A:250:ARG:O	1:A:254:ALA:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ARG:O	1:B:254:ALA:HB2	2.18	0.43
1:C:132:LYS:O	1:C:136:LEU:N	2.52	0.43
1:C:147:PHE:CD2	1:C:168:THR:HG23	2.53	0.43
1:D:206:PRO:O	1:D:209:VAL:HG12	2.19	0.43
1:A:108:ALA:CA	1:A:116:SER:HB3	2.41	0.43
1:A:119:TRP:CD2	1:A:196:PRO:HA	2.53	0.43
1:A:204:LEU:CD1	1:A:245:VAL:HG12	2.49	0.43
1:A:241:GLN:O	1:A:243:ILE:N	2.52	0.43
1:C:152:PHE:CD1	1:C:161:PHE:HB3	2.52	0.43
1:D:201:LEU:CB	1:D:243:ILE:HG23	2.48	0.43
1:A:232:LEU:HD22	1:A:247:LEU:HD11	1.99	0.43
1:B:304:LYS:HA	1:B:326:SER:OG	2.19	0.43
1:C:212:LEU:C	1:C:214:LEU:N	2.76	0.43
1:D:220:TYR:CD2	1:D:220:TYR:C	2.96	0.43
1:D:249:ARG:O	1:D:251:SER:O	2.36	0.43
1:D:303:LEU:N	1:D:303:LEU:CD2	2.82	0.43
1:D:323:ASP:OD1	1:D:323:ASP:O	2.37	0.43
1:A:121:LYS:CE	1:A:160:GLN:NE2	2.82	0.43
1:A:337:TYR:CE2	1:A:351:LEU:HD21	2.50	0.43
1:C:224:GLN:O	1:C:268:LEU:HB2	2.19	0.43
1:C:255:ALA:O	1:C:256:THR:C	2.62	0.43
1:D:219:ARG:O	1:D:227:LEU:HD12	2.19	0.43
1:D:321:TRP:CZ2	1:D:353:GLY:HA2	2.54	0.43
1:A:153:HIS:CD2	1:A:160:GLN:HG3	2.53	0.42
1:A:180:LEU:HD21	1:A:184:ASN:HD22	1.82	0.42
1:A:270:LEU:O	1:A:271:ASN:C	2.62	0.42
1:B:216:MET:HE1	1:B:259:ILE:HG21	2.00	0.42
1:B:238:LEU:HG	1:B:243:ILE:HG23	2.01	0.42
1:C:235:ASP:O	1:C:239:VAL:HG23	2.18	0.42
1:A:208:GLN:HA	1:A:211:GLN:HB3	2.01	0.42
1:B:220:TYR:O	1:B:222:GLY:N	2.50	0.42
1:B:304:LYS:CG	1:D:332:ARG:NH2	2.83	0.42
1:C:116:SER:HA	1:C:166:ALA:CB	2.49	0.42
1:C:258:ARG:HG3	1:C:258:ARG:NH1	2.34	0.42
1:C:360:ILE:HD12	1:C:360:ILE:H	1.85	0.42
1:D:305:SER:HA	1:D:327:LEU:CB	2.50	0.42
1:D:309:LEU:O	1:D:311:LYS:N	2.52	0.42
1:A:220:TYR:HD2	1:A:220:TYR:O	2.01	0.42
1:A:287:VAL:HG11	1:B:288:GLN:HE22	1.84	0.42
1:C:185:ARG:O	1:C:186:ARG:C	2.62	0.42
1:C:219:ARG:HH11	1:C:229:LEU:CD2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:PRO:HB2	1:C:266:GLU:CD	2.44	0.42
1:C:271:ASN:ND2	1:C:297:ASN:ND2	2.68	0.42
1:A:173:LYS:N	1:A:191:ILE:CD1	2.82	0.42
1:A:208:GLN:C	1:A:211:GLN:HB3	2.44	0.42
1:A:320:LEU:HD13	1:A:345:PHE:CD1	2.55	0.42
1:C:106:GLY:C	1:C:108:ALA:N	2.75	0.42
1:C:163:VAL:HG12	1:C:164:GLU:N	2.29	0.42
1:A:131:ASP:HB3	1:A:134:TRP:HB3	2.02	0.42
1:A:233:ARG:O	1:A:235:ASP:N	2.52	0.42
1:A:306:GLU:C	1:A:308:GLU:N	2.77	0.42
1:C:192:ASN:O	1:C:193:SER:OG	2.34	0.42
1:C:212:LEU:O	1:C:213:LYS:C	2.63	0.42
1:C:260:ILE:HG21	1:C:267:LEU:CD2	2.49	0.42
1:D:260:ILE:HG23	1:D:267:LEU:HD22	2.01	0.42
1:A:333:ASP:CG	1:A:335:SER:HB2	2.44	0.42
1:B:287:VAL:HG21	1:B:315:LEU:H	1.83	0.42
1:B:298:LEU:O	1:B:299:SER:C	2.61	0.42
1:B:330:THR:HB	1:D:305:SER:HB2	2.02	0.42
1:B:338:ILE:O	1:B:341:ILE:CD1	2.66	0.42
1:B:354:HIS:CD2	1:B:354:HIS:N	2.87	0.42
1:B:357:PRO:HA	1:B:358:PRO:HD3	1.73	0.42
1:C:360:ILE:N	1:C:360:ILE:CD1	2.81	0.42
1:A:119:TRP:CE2	1:A:197:PRO:HD3	2.54	0.42
1:A:202:ASN:O	1:A:203:GLU:HB2	2.19	0.42
1:A:255:ALA:O	1:A:257:LEU:N	2.53	0.42
1:B:220:TYR:CE1	1:B:225:GLN:HA	2.55	0.42
1:B:317:LEU:HD13	1:B:320:LEU:HB2	2.01	0.42
1:C:148:THR:HA	1:C:149:PRO:HD3	1.78	0.42
1:C:228:ASP:OD2	1:C:228:ASP:O	2.38	0.42
1:D:221:ASP:OD1	1:D:223:SER:N	2.53	0.42
1:D:360:ILE:CG2	1:D:361:ALA:N	2.80	0.42
1:A:180:LEU:HD23	1:A:180:LEU:C	2.44	0.42
1:A:261:GLU:OE2	1:A:289:LYS:HA	2.20	0.42
1:A:323:ASP:HB3	1:A:352:ASP:OD1	2.20	0.42
1:B:206:PRO:O	1:B:209:VAL:N	2.53	0.42
1:B:220:TYR:CE2	1:B:264:ILE:HG21	2.54	0.42
1:B:280:LEU:HG	1:B:303:LEU:HD21	2.02	0.42
1:B:360:ILE:HG22	1:B:360:ILE:O	2.20	0.42
1:C:280:LEU:HD12	1:C:308:GLU:CB	2.50	0.42
1:C:298:LEU:HD12	1:C:298:LEU:H	1.84	0.42
1:D:232:LEU:C	1:D:234:SER:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:CG	1:A:183:GLU:OE1	2.64	0.42
1:A:214:LEU:HD22	1:D:361:ALA:H	1.85	0.42
1:A:292:ASN:O	1:A:294:LYS:HG2	2.20	0.42
1:B:224:GLN:O	1:B:225:GLN:C	2.62	0.42
1:B:271:ASN:HD22	1:B:297:ASN:HB3	1.83	0.42
1:C:121:LYS:HB3	1:C:192:ASN:HB2	2.01	0.42
1:C:169:ALA:HB1	1:C:191:ILE:CG2	2.50	0.42
1:B:306:GLU:OE1	1:B:344:ARG:NH2	2.53	0.42
1:C:145:VAL:O	1:C:145:VAL:CG2	2.67	0.42
1:C:231:GLY:O	1:C:235:ASP:OD1	2.38	0.42
1:D:231:GLY:HA2	1:D:274:ASN:O	2.19	0.42
1:D:306:GLU:OE2	1:D:340:ALA:HB1	2.20	0.42
1:D:309:LEU:C	1:D:311:LYS:N	2.77	0.42
1:A:117:LYS:NZ	1:A:117:LYS:HB3	2.35	0.41
1:A:140:GLN:C	1:A:142:LYS:N	2.77	0.41
1:A:295:ILE:CG2	1:A:296:LEU:N	2.73	0.41
1:B:287:VAL:HG22	1:B:315:LEU:N	2.34	0.41
1:C:248:ASN:OD1	1:C:249:ARG:N	2.53	0.41
1:C:277:LEU:H	1:C:301:ASN:HB3	1.83	0.41
1:A:317:LEU:O	1:A:319:GLU:N	2.44	0.41
1:A:348:LEU:CD2	1:A:349:LEU:N	2.83	0.41
1:C:232:LEU:O	1:C:232:LEU:HD23	2.20	0.41
1:C:280:LEU:HD12	1:C:308:GLU:HB3	2.02	0.41
1:C:317:LEU:HB2	1:C:345:PHE:CD2	2.55	0.41
1:D:282:ASP:N	1:D:282:ASP:OD1	2.50	0.41
1:A:119:TRP:CE3	1:A:162:PHE:HB3	2.55	0.41
1:A:278:TYR:HD1	1:A:279:ARG:HG2	1.80	0.41
1:A:296:LEU:CD2	1:A:297:ASN:N	2.82	0.41
1:B:287:VAL:CG2	1:B:315:LEU:N	2.82	0.41
1:C:105:ARG:HD2	1:C:106:GLY:CA	2.48	0.41
1:C:130:TYR:OH	1:C:187:ILE:HG12	2.20	0.41
1:C:219:ARG:HH11	1:C:229:LEU:HD23	1.85	0.41
1:D:356:LEU:HA	1:D:357:PRO:HD3	1.91	0.41
1:A:139:ILE:O	1:A:139:ILE:CG2	2.64	0.41
1:A:277:LEU:O	1:A:301:ASN:OD1	2.36	0.41
1:B:205:LYS:O	1:B:209:VAL:HG23	2.20	0.41
1:B:235:ASP:C	1:B:235:ASP:OD1	2.63	0.41
1:B:249:ARG:O	1:B:251:SER:N	2.54	0.41
1:C:150:ILE:H	1:C:161:PHE:HB2	1.84	0.41
1:A:213:LYS:CA	1:A:259:ILE:HD13	2.50	0.41
1:B:215:ILE:HG23	1:B:216:MET:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:PHE:HB3	1:C:191:ILE:CG2	2.50	0.41
1:C:156:ASN:N	1:C:156:ASN:HD22	2.17	0.41
1:C:336:THR:HA	1:C:339:SER:OG	2.20	0.41
1:D:238:LEU:HD23	1:D:238:LEU:N	2.34	0.41
1:D:260:ILE:HG22	1:D:260:ILE:O	2.19	0.41
1:D:275:ASN:C	1:D:277:LEU:N	2.78	0.41
1:A:109:GLY:HA2	1:A:117:LYS:CG	2.50	0.41
1:A:235:ASP:O	1:A:236:PRO:O	2.38	0.41
1:A:296:LEU:CD2	1:A:298:LEU:HG	2.51	0.41
1:B:280:LEU:HD21	1:B:303:LEU:HD21	2.02	0.41
1:B:309:LEU:HB2	1:B:344:ARG:HD2	2.02	0.41
1:C:115:THR:CG2	1:C:116:SER:H	2.24	0.41
1:C:181:ASP:OD2	1:C:185:ARG:HB2	2.21	0.41
1:C:193:SER:CB	1:D:276:ARG:HH22	2.33	0.41
1:C:276:ARG:HG2	1:C:276:ARG:HH21	1.86	0.41
1:C:317:LEU:CD2	1:C:319:GLU:H	2.32	0.41
1:C:360:ILE:O	1:C:361:ALA:HB2	2.20	0.41
1:D:211:GLN:CA	1:D:214:LEU:HD23	2.50	0.41
1:D:229:LEU:HB2	1:D:272:LEU:HD23	2.03	0.41
1:D:310:ASP:OD1	1:D:344:ARG:HD2	2.20	0.41
1:D:334:GLN:O	1:D:334:GLN:HG3	2.19	0.41
1:A:212:LEU:O	1:A:213:LYS:C	2.62	0.41
1:A:304:LYS:NZ	1:A:304:LYS:HB3	2.35	0.41
1:A:331:PHE:HE2	1:A:340:ALA:CB	2.34	0.41
1:C:132:LYS:HE2	1:C:152:PHE:CD2	2.52	0.41
1:C:167:SER:HA	1:C:170:SER:CB	2.50	0.41
1:C:231:GLY:C	1:C:233:ARG:N	2.78	0.41
1:C:272:LEU:O	1:C:273:SER:O	2.39	0.41
1:C:342:ARG:NH1	1:C:348:LEU:C	2.78	0.41
1:D:215:ILE:C	1:D:217:SER:H	2.28	0.41
1:D:335:SER:O	1:D:338:ILE:CG1	2.64	0.41
1:A:110:THR:C	1:A:112:GLN:N	2.77	0.41
1:A:187:ILE:HG22	1:A:189:ILE:HD12	2.02	0.41
1:A:187:ILE:HG22	1:A:189:ILE:CD1	2.51	0.41
1:A:278:TYR:HA	1:A:302:GLU:O	2.20	0.41
1:C:105:ARG:CG	1:C:106:GLY:H	2.33	0.41
1:C:124:ILE:HG12	1:C:189:ILE:HG12	2.03	0.41
1:D:295:ILE:HA	1:D:319:GLU:O	2.20	0.41
1:A:131:ASP:O	1:A:132:LYS:C	2.64	0.41
1:A:204:LEU:HA	1:A:208:GLN:OE1	2.21	0.41
1:A:241:GLN:HB3	1:A:243:ILE:CG1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:MET:O	1:A:257:LEU:HG	2.20	0.41
1:B:246:VAL:HG23	1:B:246:VAL:O	2.20	0.41
1:B:319:GLU:OE1	1:B:350:ARG:NE	2.44	0.41
1:C:168:THR:O	1:C:172:LEU:N	2.49	0.41
1:C:258:ARG:O	1:C:261:GLU:CB	2.69	0.41
1:D:210:GLU:HG3	1:D:213:LYS:NZ	2.36	0.41
1:D:273:SER:HA	1:D:299:SER:O	2.20	0.41
1:A:205:LYS:N	1:A:208:GLN:CD	2.79	0.41
1:A:344:ARG:C	1:A:346:PRO:HD3	2.46	0.41
1:B:321:TRP:CH2	1:B:353:GLY:HA2	2.56	0.41
1:A:230:LYS:O	1:A:232:LEU:HD12	2.21	0.40
1:A:274:ASN:O	1:A:276:ARG:N	2.54	0.40
1:A:276:ARG:NH2	1:A:276:ARG:HB3	2.37	0.40
1:A:304:LYS:O	1:A:327:LEU:HA	2.20	0.40
1:A:319:GLU:HG2	1:A:350:ARG:HB2	2.04	0.40
1:A:357:PRO:HA	1:A:358:PRO:HD3	1.89	0.40
1:B:289:LYS:C	1:B:291:PRO:CD	2.88	0.40
1:B:316:LYS:HB2	1:B:316:LYS:HE3	1.86	0.40
1:C:278:TYR:CE1	1:C:279:ARG:HB2	2.56	0.40
1:C:317:LEU:HD23	1:C:318:GLU:N	2.22	0.40
1:D:246:VAL:C	1:D:248:ASN:H	2.29	0.40
1:D:321:TRP:CZ2	1:D:353:GLY:CA	3.04	0.40
1:A:192:ASN:HD21	1:D:332:ARG:HA	1.85	0.40
1:C:221:ASP:OD2	1:C:223:SER:O	2.38	0.40
1:D:250:ARG:NH2	1:D:281:ASP:OD2	2.49	0.40
1:D:339:SER:O	1:D:343:GLU:N	2.52	0.40
1:A:229:LEU:HD21	1:A:247:LEU:HD11	2.02	0.40
1:D:201:LEU:CG	1:D:243:ILE:HG23	2.51	0.40
1:D:335:SER:HA	1:D:338:ILE:HD11	2.03	0.40
1:A:158:ARG:HH12	1:A:206:PRO:HG2	1.86	0.40
1:A:173:LYS:HB2	1:A:191:ILE:HD12	2.03	0.40
1:A:298:LEU:O	1:A:299:SER:O	2.39	0.40
1:A:306:GLU:CA	1:A:327:LEU:HD11	2.34	0.40
1:B:281:ASP:OD1	1:B:311:LYS:HD2	2.22	0.40
1:B:295:ILE:HA	1:B:319:GLU:O	2.21	0.40
1:B:360:ILE:HD11	1:C:210:GLU:OE1	2.21	0.40
1:C:201:LEU:O	1:C:202:ASN:C	2.64	0.40
1:C:275:ASN:O	1:C:276:ARG:C	2.64	0.40
1:D:210:GLU:O	1:D:214:LEU:HB3	2.21	0.40
1:A:235:ASP:HA	1:A:236:PRO:HD3	1.98	0.40
1:A:283:MET:HE3	1:A:286:ILE:HG21	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ASN:CB	1:A:325:ASN:HD21	2.35	0.40
1:B:208:GLN:HG2	1:B:243:ILE:HD12	2.03	0.40
1:B:341:ILE:HD13	1:B:348:LEU:CD2	2.52	0.40
1:C:322:LEU:O	1:C:323:ASP:O	2.39	0.40
1:D:254:ALA:O	1:D:256:THR:N	2.54	0.40

There are no symmetry-related clashes.

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	256/277 (92%)	137 (54%)	60 (23%)	59 (23%)	0	0
1	B	165/277 (60%)	98 (59%)	38 (23%)	29 (18%)	0	2
1	C	257/277 (93%)	133 (52%)	74 (29%)	50 (20%)	0	1
1	D	170/277 (61%)	110 (65%)	46 (27%)	14 (8%)	0	10
All	All	848/1108 (76%)	478 (56%)	218 (26%)	152 (18%)	0	2

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	ASP
1	A	123	THR
1	A	139	ILE
1	A	148	THR
1	A	182	ARG
1	A	200	ILE
1	A	201	LEU
1	A	206	PRO
1	A	228	ASP
1	A	231	GLY

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Mol	Chain	Res	Type
1	A	241	GLN
1	A	275	ASN
1	A	299	SER
1	A	300	GLY
1	A	314	GLY
1	A	319	GLU
1	A	322	LEU
1	A	330	THR
1	A	347	LYS
1	A	352	ASP
1	A	358	PRO
1	A	360	ILE
1	A	361	ALA
1	B	217	SER
1	B	220	TYR
1	B	234	SER
1	B	266	GLU
1	B	323	ASP
1	C	124	ILE
1	C	126	TYR
1	C	129	LYS
1	C	132	LYS
1	C	140	GLN
1	C	143	SER
1	C	164	GLU
1	C	179	ILE
1	C	202	ASN
1	C	227	LEU
1	C	256	THR
1	C	273	SER
1	C	280	LEU
1	C	301	ASN
1	C	317	LEU
1	C	323	ASP
1	C	333	ASP
1	D	315	LEU
1	D	327	LEU
1	D	367	PRO
1	A	128	ARG
1	A	183	GLU
1	A	184	ASN
1	A	198	HIS

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Mol	Chain	Res	Type
1	A	226	ALA
1	A	236	PRO
1	A	266	GLU
1	A	276	ARG
1	A	298	LEU
1	A	329	ASP
1	B	204	LEU
1	B	225	GLN
1	B	227	LEU
1	B	250	ARG
1	B	292	ASN
1	B	293	LEU
1	B	301	ASN
1	B	310	ASP
1	B	313	LYS
1	B	326	SER
1	B	361	ALA
1	C	110	THR
1	C	130	TYR
1	C	141	SER
1	C	224	GLN
1	C	247	LEU
1	C	267	LEU
1	C	274	ASN
1	C	300	GLY
1	C	309	LEU
1	C	318	GLU
1	C	326	SER
1	C	361	ALA
1	D	216	MET
1	D	236	PRO
1	D	243	ILE
1	D	293	LEU
1	A	233	ARG
1	A	237	ASP
1	A	240	ALA
1	A	253	MET
1	A	256	THR
1	A	309	LEU
1	A	324	GLY
1	A	327	LEU
1	A	328	SER

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Mol	Chain	Res	Type
1	A	346	PRO
1	B	219	ARG
1	B	237	ASP
1	B	274	ASN
1	B	275	ASN
1	B	306	GLU
1	C	111	SER
1	C	125	PRO
1	C	133	ALA
1	C	134	TRP
1	C	156	ASN
1	C	163	VAL
1	C	182	ARG
1	C	225	GLN
1	C	266	GLU
1	C	299	SER
1	C	319	GLU
1	C	338	ILE
1	C	347	LYS
1	D	247	LEU
1	D	291	PRO
1	A	118	ASN
1	A	210	GLU
1	A	229	LEU
1	A	230	LYS
1	A	318	GLU
1	B	230	LYS
1	B	276	ARG
1	B	287	VAL
1	B	291	PRO
1	B	328	SER
1	C	112	GLN
1	C	118	ASN
1	C	233	ARG
1	C	234	SER
1	C	253	MET
1	C	304	LYS
1	D	204	LEU
1	D	230	LYS
1	D	237	ASP
1	D	240	ALA
1	A	197	PRO

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Mol	Chain	Res	Type
1	A	213	LYS
1	A	291	PRO
1	A	337	TYR
1	A	341	ILE
1	B	263	ASN
1	B	265	PRO
1	B	288	GLN
1	C	265	PRO
1	C	308	GLU
1	A	107	GLY
1	A	207	GLU
1	A	342	ARG
1	A	357	PRO
1	A	286	ILE
1	A	359	PRO
1	D	359	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	232/249 (93%)	195 (84%)	37 (16%)	2	14
1	B	153/249 (61%)	134 (88%)	19 (12%)	4	21
1	C	233/249 (94%)	213 (91%)	20 (9%)	10	33
1	D	158/249 (64%)	128 (81%)	30 (19%)	1	10
All	All	776/996 (78%)	670 (86%)	106 (14%)	3	18

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ARG
1	A	122	ILE
1	A	123	THR
1	A	142	LYS
1	A	145	VAL

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Mol	Chain	Res	Type
1	A	148	THR
1	A	157	THR
1	A	168	THR
1	A	182	ARG
1	A	187	ILE
1	A	190	ILE
1	A	197	PRO
1	A	200	ILE
1	A	206	PRO
1	A	215	ILE
1	A	219	ARG
1	A	220	TYR
1	A	228	ASP
1	A	241	GLN
1	A	251	SER
1	A	262	GLU
1	A	278	TYR
1	A	285	SER
1	A	299	SER
1	A	302	GLU
1	A	304	LYS
1	A	306	GLU
1	A	312	ILE
1	A	319	GLU
1	A	322	LEU
1	A	334	GLN
1	A	343	GLU
1	A	348	LEU
1	A	349	LEU
1	A	355	GLU
1	A	356	LEU
1	A	357	PRO
1	B	215	ILE
1	B	241	GLN
1	B	244	ASP
1	B	266	GLU
1	B	274	ASN
1	B	281	ASP
1	B	293	LEU
1	B	294	LYS
1	B	297	ASN
1	B	306	GLU

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Mol	Chain	Res	Type
1	B	308	GLU
1	B	315	LEU
1	B	317	LEU
1	B	319	GLU
1	B	325	ASN
1	B	334	GLN
1	B	341	ILE
1	B	342	ARG
1	B	363	ASP
1	C	126	TYR
1	C	130	TYR
1	C	155	GLU
1	C	163	VAL
1	C	201	LEU
1	C	228	ASP
1	C	243	ILE
1	C	264	ILE
1	C	271	ASN
1	C	274	ASN
1	C	278	TYR
1	C	285	SER
1	C	288	GLN
1	C	296	LEU
1	C	307	ARG
1	C	309	LEU
1	C	317	LEU
1	C	325	ASN
1	C	349	LEU
1	C	360	ILE
1	D	202	ASN
1	D	212	LEU
1	D	214	LEU
1	D	218	LYS
1	D	233	ARG
1	D	237	ASP
1	D	245	VAL
1	D	251	SER
1	D	253	MET
1	D	258	ARG
1	D	259	ILE
1	D	266	GLU
1	D	271	ASN

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Mol	Chain	Res	Type
1	D	294	LYS
1	D	295	ILE
1	D	302	GLU
1	D	307	ARG
1	D	325	ASN
1	D	327	LEU
1	D	329	ASP
1	D	330	THR
1	D	338	ILE
1	D	344	ARG
1	D	347	LYS
1	D	355	GLU
1	D	358	PRO
1	D	360	ILE
1	D	362	PHE
1	D	365	GLU
1	D	370	LEU

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

Mol	Chain	Res	Type
1	A	184	ASN
1	A	192	ASN
1	A	241	GLN
1	A	263	ASN
1	A	274	ASN
1	A	275	ASN
1	A	297	ASN
1	A	325	ASN
1	A	334	GLN
1	B	208	GLN
1	B	241	GLN
1	B	263	ASN
1	B	271	ASN
1	B	274	ASN
1	B	288	GLN
1	B	297	ASN
1	C	112	GLN
1	C	156	ASN
1	C	225	GLN
1	C	271	ASN
1	C	288	GLN

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Mol	Chain	Res	Type
1	C	301	ASN
1	D	211	GLN
1	D	225	GLN
1	D	271	ASN
1	D	297	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	258/277 (93%)	-0.51	0 100 100	47, 81, 120, 130	0
1	B	167/277 (60%)	-0.59	0 100 100	46, 83, 111, 120	0
1	C	259/277 (93%)	-0.47	0 100 100	58, 104, 142, 148	0
1	D	172/277 (62%)	-0.53	1 (0%) 85 68	46, 72, 111, 122	0
All	All	856/1108 (77%)	-0.52	1 (0%) 92 87	46, 84, 138, 148	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	371	PRO	2.7

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.