Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2024 – 03:13 PM EST

PDB ID	:	1HT2
Title	:	Nucleotide-Dependent Conformational Changes in a Protease-Associated ATPase HslU
Authors	:	Wang, J.; Song, J.J.; Seong, I.S.; Franklin, M.C.; Kamtekar, S.; Eom, S.H.; Chung, C.H.
Deposited on	:	2000-12-27
Resolution	:	2.80 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:

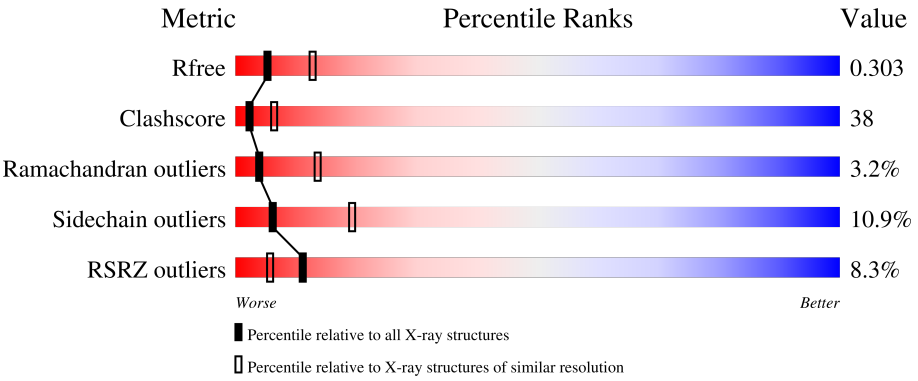
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	175	57% 37% 5%
1	B	175	6% 43% 47% 9%
1	C	175	2% 50% 42% 7%
1	D	175	7% 43% 49% 7%

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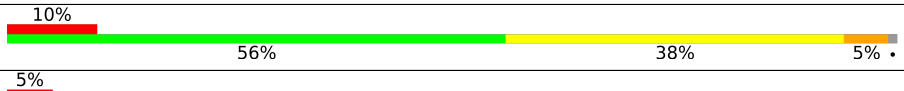
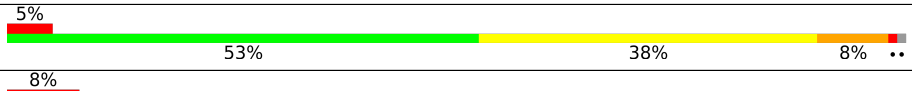
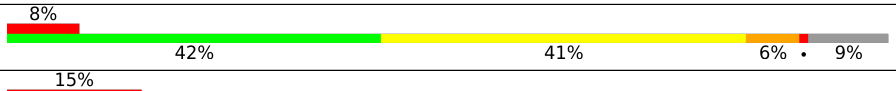
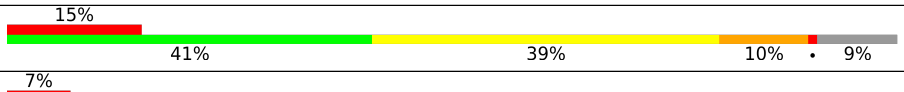
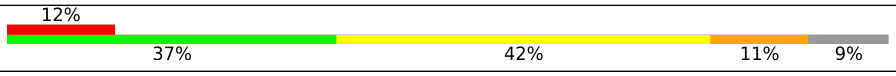
Mol	Chain	Length	Quality of chain
1	I	175	
1	J	175	
1	K	175	
1	L	175	
2	E	449	
2	F	449	
2	G	449	
2	H	449	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23636 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 HEAT SHOCK LOCUS HSLV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	B	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	C	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	D	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	I	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	J	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	K	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	L	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			

- Molecule 2 is a protein called HEAT SHOCK LOCUS HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	408	Total	C	N	O	S	0	0	0
			3226	2014	577	625	10			
2	F	408	Total	C	N	O	S	0	0	0
			3226	2014	577	625	10			
2	G	408	Total	C	N	O	S	0	0	0
			3226	2014	577	625	10			
2	H	408	Total	C	N	O	S	0	0	0
			3226	2014	577	625	10			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP P0A6H5

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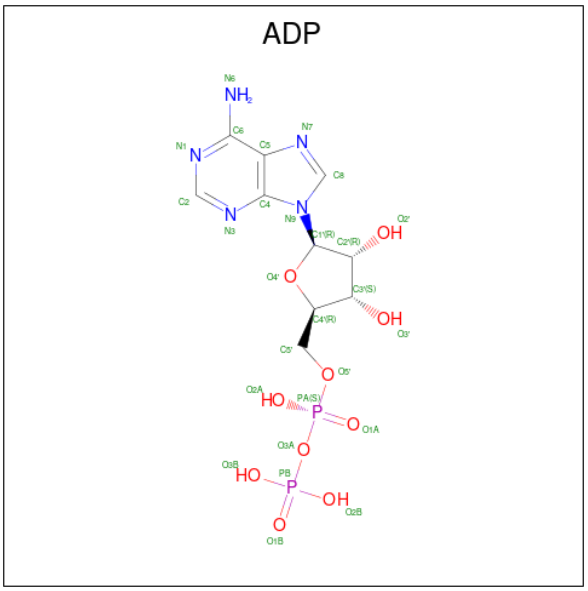
Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP P0A6H5
E	-3	HIS	-	expression tag	UNP P0A6H5
E	-2	HIS	-	expression tag	UNP P0A6H5
E	-1	HIS	-	expression tag	UNP P0A6H5
E	0	HIS	-	expression tag	UNP P0A6H5
E	1	HIS	-	expression tag	UNP P0A6H5
F	-5	HIS	-	expression tag	UNP P0A6H5
F	-4	HIS	-	expression tag	UNP P0A6H5
F	-3	HIS	-	expression tag	UNP P0A6H5
F	-2	HIS	-	expression tag	UNP P0A6H5
F	-1	HIS	-	expression tag	UNP P0A6H5
F	0	HIS	-	expression tag	UNP P0A6H5
F	1	HIS	-	expression tag	UNP P0A6H5
G	-5	HIS	-	expression tag	UNP P0A6H5
G	-4	HIS	-	expression tag	UNP P0A6H5
G	-3	HIS	-	expression tag	UNP P0A6H5
G	-2	HIS	-	expression tag	UNP P0A6H5
G	-1	HIS	-	expression tag	UNP P0A6H5
G	0	HIS	-	expression tag	UNP P0A6H5
G	1	HIS	-	expression tag	UNP P0A6H5
H	-5	HIS	-	expression tag	UNP P0A6H5
H	-4	HIS	-	expression tag	UNP P0A6H5
H	-3	HIS	-	expression tag	UNP P0A6H5
H	-2	HIS	-	expression tag	UNP P0A6H5
H	-1	HIS	-	expression tag	UNP P0A6H5
H	0	HIS	-	expression tag	UNP P0A6H5
H	1	HIS	-	expression tag	UNP P0A6H5

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



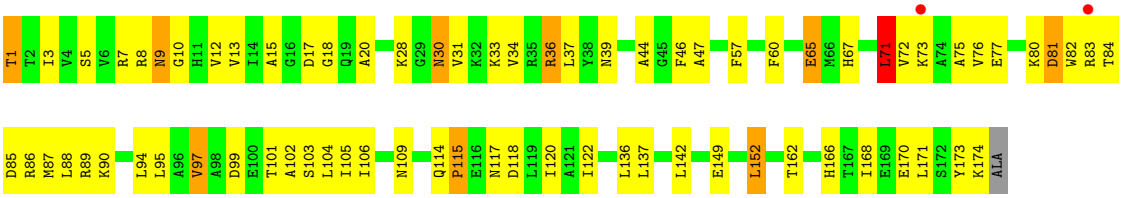
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots (i)

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

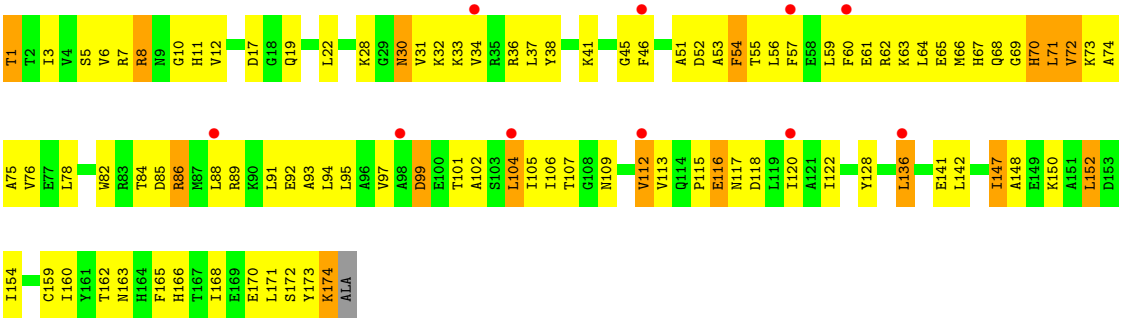
• Molecule 1: HEAT SHOCK LOCUS HSLV

Chain A:



• Molecule 1: HEAT SHOCK LOCUS HSLV

Chain B:

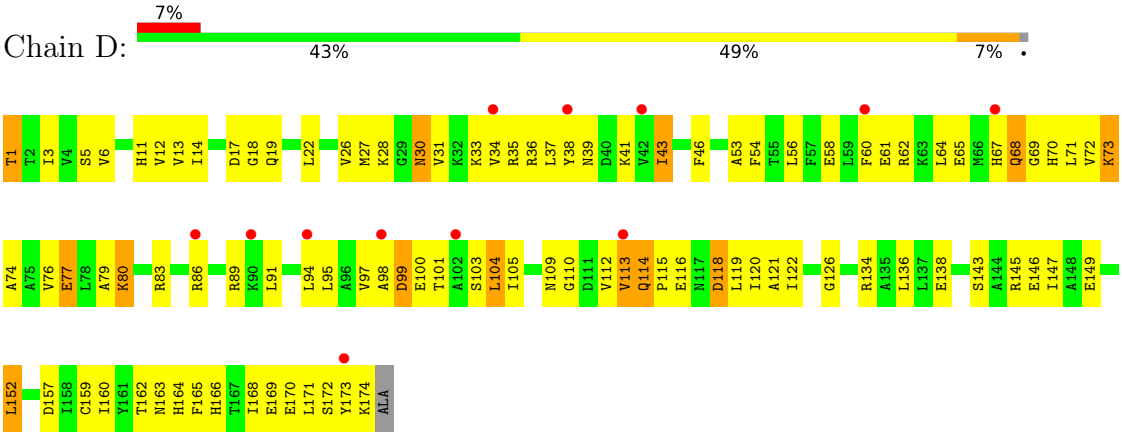


• Molecule 1: HEAT SHOCK LOCUS HSLV

Chain C:

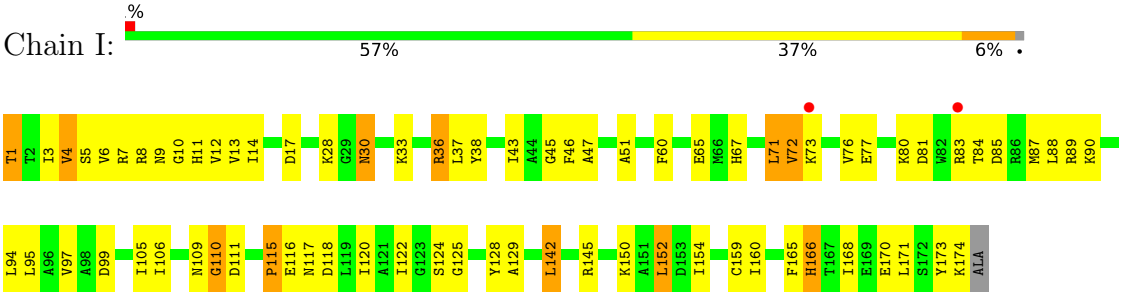
• Molecule 1: HEAT SHOCK LOCUS HSLV

Chain D:



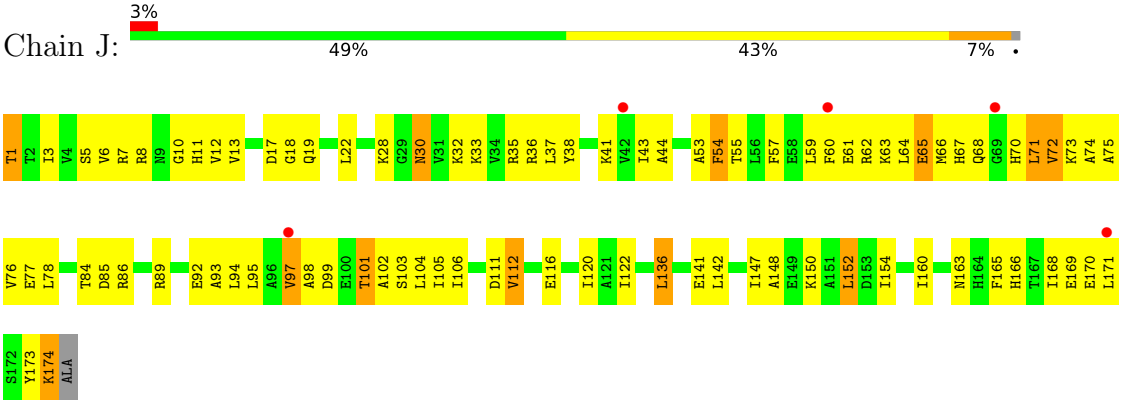
• Molecule 1: HEAT SHOCK LOCUS HSLV

Chain I:



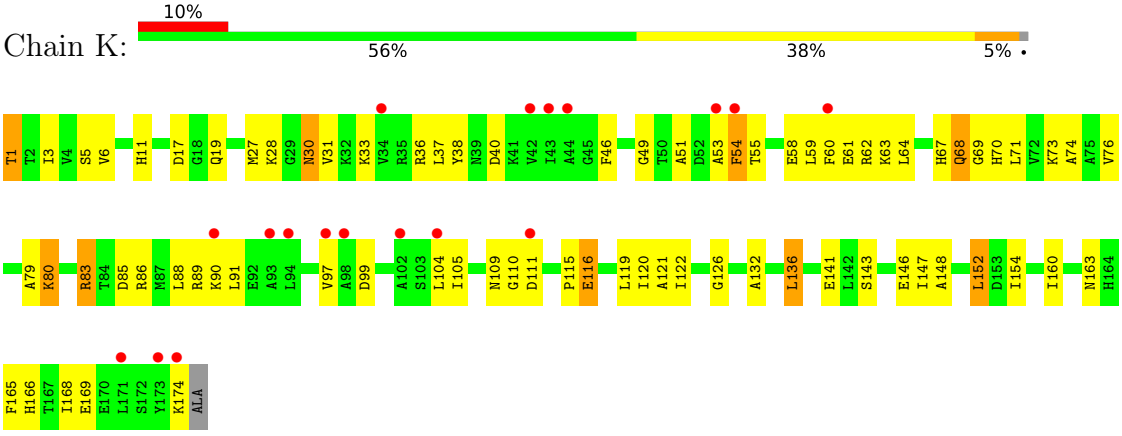
• Molecule 1: HEAT SHOCK LOCUS HSLV

Chain J:



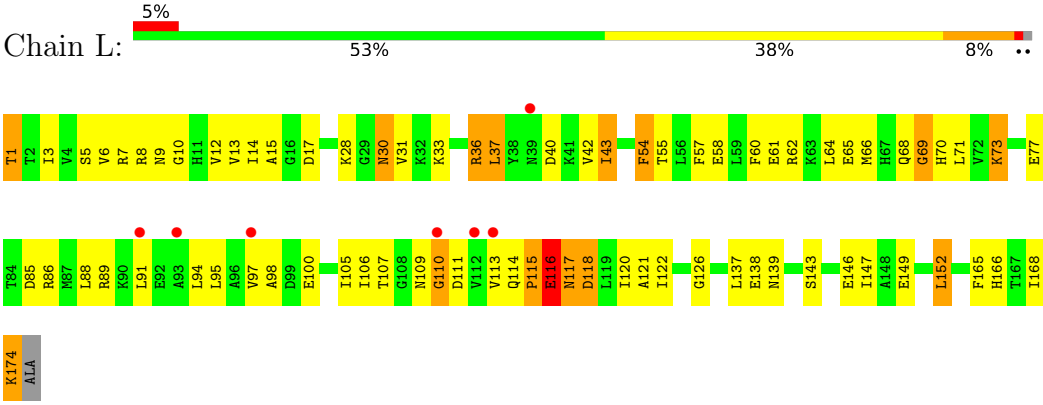
• Molecule 1: HEAT SHOCK LOCUS HSLV

Chain K:



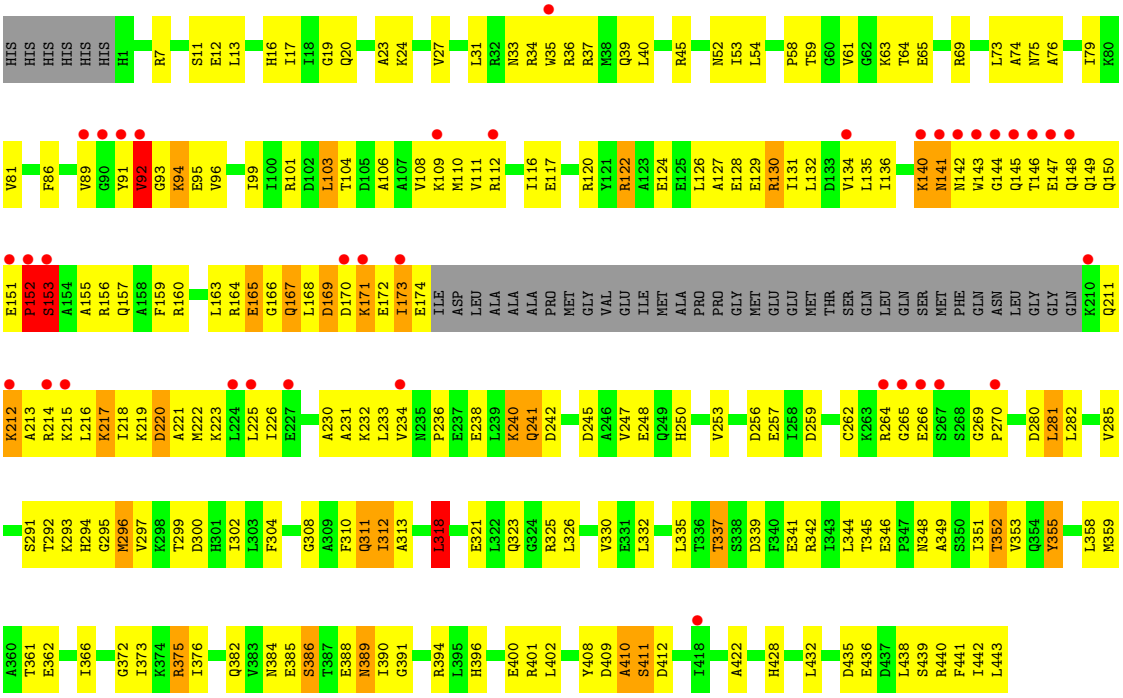
• Molecule 1: HEAT SHOCK LOCUS HSLV

Chain L:



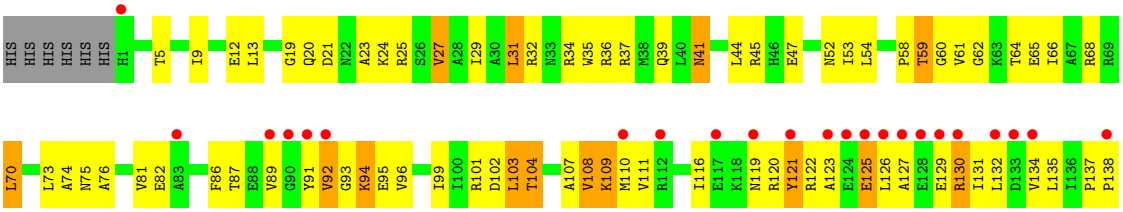
• Molecule 2: HEAT SHOCK LOCUS HSLU

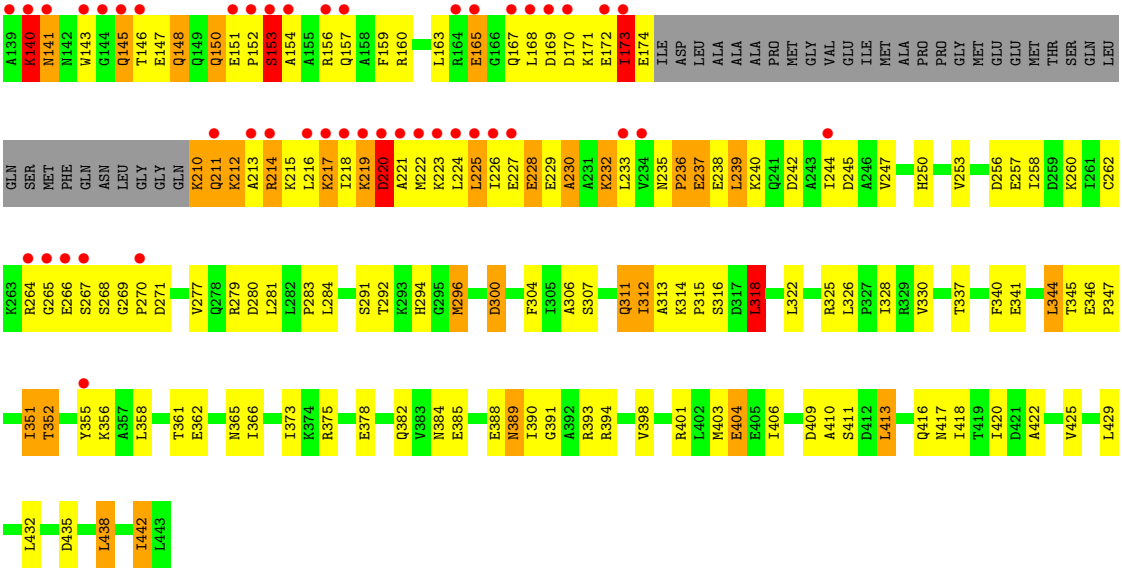
Chain E:



• Molecule 2: HEAT SHOCK LOCUS HSLU

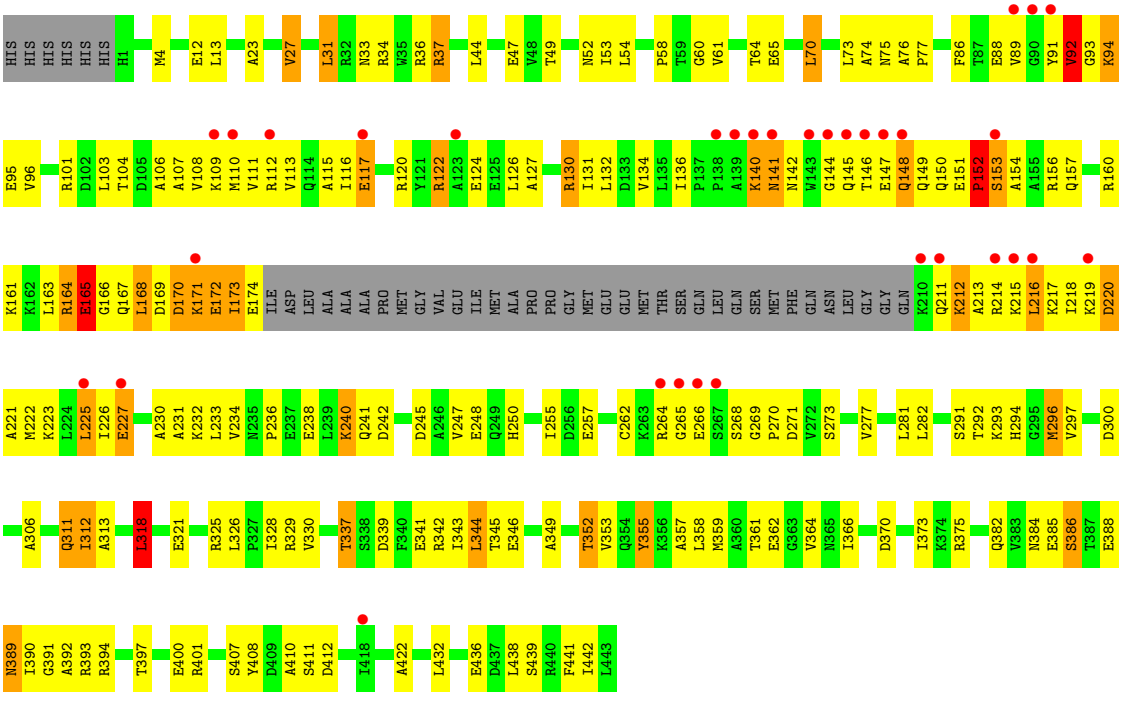
Chain F:





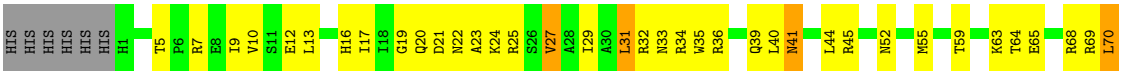
• Molecule 2: HEAT SHOCK LOCUS HSLU

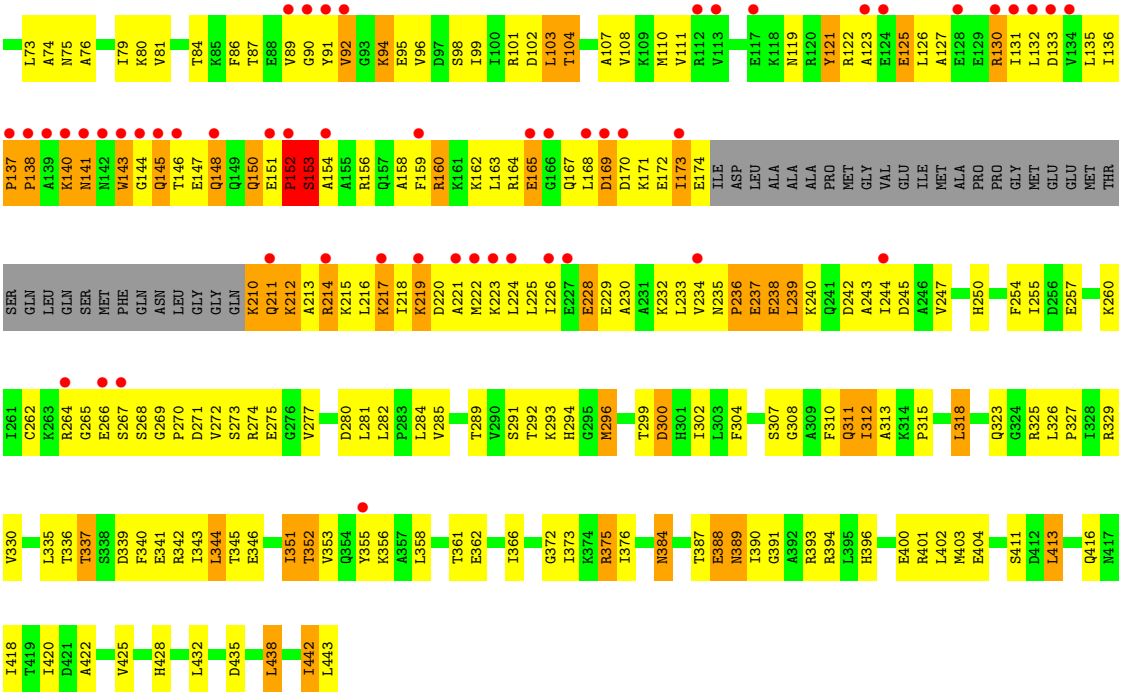
Chain G:



• Molecule 2: HEAT SHOCK LOCUS HSLU

Chain H:




L73 A74 N75 A76 I79 K80 V81 T84 K85 F86 T87 E88 V89 G90 Y91 V92 G93 K94 E95 V96 D97 S98 I99 I100 R101 D102 L103 T104 A107 V108 K109 M110 V111 R112 V113 E117 K118 N119 R120 Y121 R122 A123 E124 E125 L126 A127 E128 E129 R130 I131 L132 D133 V134 L135 I136
P137 P138 A139 K140 N141 N142 W143 G144 Q145 T146 E147 Q148 Q149 Q150 E151 P152 S153 A154 A155 R156 Q157 A158 F159 R160 K161 K162 L163 R164 E165 G166 Q167 L168 D169 D170 K171 E172 I173 E174 ILE ASP LEU ALA ALA ALA PRO MET GLY VAL GLU ILE MET ALA PRO PRO GLY MET GLU GLU MET THR
SER GLN LEU GLN SER MET PHE GLN ASN LEU GLY GLY GLN K210 Q211 K212 A213 R214 K215 L216 K217 I218 K219 D220 A221 M222 K223 L224 L225 I226 E227 E228 E229 A230 A231 K232 L233 V234 N235 P236 E237 E238 L239 K240 Q241 D242 A243 I244 D245 A246 V247 H250 F254 I255 D256 E257 K260
I261 C262 K263 R264 G265 E266 S267 S268 G269 P270 D271 V272 S273 R274 E275 G276 V277 D280 L281 L282 P283 L284 V285 T289 V290 S291 T292 K293 H294 G295 M296 T299 D300 H301 I302 L303 F304 S307 G308 A309 F310 Q311 I312 A313 K314 P315 L318 Q323 G324 R325 L326 P327 I328 R329
V330 L335 T336 T337 S338 D339 F340 E341 R342 I343 L344 T345 E346 I351 T352 V353 Q354 Y355 K356 A357 L358 T361 E362 I366 G372 I373 K374 R375 I376 N384 T387 E388 N389 I390 G391 A392 R393 R394 L395 H396 E400 R401 L402 M403 E404 S411 D412 L413 Q416 N417
I418 T419 I420 D421 A422 V425 H428 L432 D435 L438 I442 L443

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 1 2	Depositor
Cell constants a, b, c, α, β, γ	172.02Å 172.02Å 276.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.62 – 2.80 29.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.5 (29.62-2.80) 92.5 (29.62-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.49 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.262 , 0.310 0.254 , 0.303	Depositor DCC
R_{free} test set	12111 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å^2)	67.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23636	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3765e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	0.45	0/1345	0.72	0/1817
1	B	0.41	0/1345	0.67	0/1817
1	C	0.39	0/1345	0.67	0/1817
1	D	0.34	0/1345	0.62	0/1817
1	I	0.45	0/1345	0.73	0/1817
1	J	0.41	0/1345	0.67	0/1817
1	K	0.32	0/1345	0.60	0/1817
1	L	0.34	0/1345	0.63	0/1817
2	E	0.44	0/3266	0.71	5/4400 (0.1%)
2	F	0.44	0/3266	0.71	4/4400 (0.1%)
2	G	0.43	1/3266 (0.0%)	0.69	3/4400 (0.1%)
2	H	0.45	1/3266 (0.0%)	0.70	2/4400 (0.0%)
All	All	0.42	2/23824 (0.0%)	0.68	14/32136 (0.0%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	152	PRO	CA-C	-6.59	1.39	1.52
2	G	152	PRO	CA-C	-5.91	1.41	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	152	PRO	CA-N-CD	-6.83	101.94	111.50
2	E	152	PRO	CA-N-CD	-6.78	102.02	111.50
2	F	220	ASP	CB-CA-C	-6.51	97.38	110.40
2	G	318	LEU	CA-CB-CG	6.31	129.80	115.30
2	E	153	SER	C-N-CA	6.07	136.87	121.70
2	F	153	SER	CB-CA-C	5.86	121.24	110.10
2	H	153	SER	CB-CA-C	5.75	121.02	110.10
2	E	318	LEU	CA-CB-CG	5.73	128.47	115.30
2	E	153	SER	CB-CA-C	5.52	120.59	110.10
2	F	318	LEU	CA-CB-CG	5.46	127.86	115.30
2	F	153	SER	C-N-CA	5.45	135.32	121.70
2	H	152	PRO	CA-N-CD	-5.30	104.07	111.50
2	E	152	PRO	C-N-CA	-5.24	108.60	121.70
2	G	152	PRO	C-N-CA	-5.04	109.10	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	128	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	1328	0	1348	94	0
1	B	1328	0	1348	105	0
1	C	1328	0	1348	82	0
1	D	1328	0	1348	108	1
1	I	1328	0	1348	75	0
1	J	1328	0	1348	102	0
1	K	1328	0	1348	74	1
1	L	1328	0	1348	92	0
2	E	3226	0	3293	267	1
2	F	3226	0	3293	290	1
2	G	3226	0	3293	309	0
2	H	3226	0	3293	348	0
3	E	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	27	0	12	3	0
3	G	27	0	12	2	0
3	H	27	0	12	3	0
All	All	23636	0	24004	1831	3

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 38.

All (1831) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:152:PRO:O	2:G:154:ALA:CA	1.76	1.33
2:G:152:PRO:O	2:G:153:SER:C	1.74	1.22
2:G:152:PRO:C	2:G:154:ALA:N	1.72	1.22
2:E:174:GLU:HB3	2:E:211:GLN:HG3	1.30	1.10
2:G:109:LYS:HB2	2:H:296:MET:HG2	1.32	1.10
2:H:216:LEU:HG	2:H:221:ALA:HB2	1.32	1.09
1:I:80:LYS:HA	1:I:83:ARG:HH12	1.12	1.09
2:G:174:GLU:HB3	2:G:211:GLN:HG3	1.34	1.08
2:G:109:LYS:HD3	2:H:296:MET:HB3	1.31	1.08
1:L:83:ARG:NH1	1:L:83:ARG:HB3	1.66	1.08
2:G:168:LEU:HG	2:G:219:LYS:HD3	1.30	1.07
2:G:152:PRO:HB2	2:G:156:ARG:HB2	1.37	1.06
1:C:83:ARG:HB3	1:C:83:ARG:NH1	1.72	1.05
1:L:83:ARG:HB3	1:L:83:ARG:HH11	1.12	1.03
2:E:212:LYS:HD3	2:E:216:LEU:HD21	1.41	1.03
2:G:130:ARG:HD2	2:G:225:LEU:HD11	1.38	1.03
1:A:13:VAL:HG12	1:A:170:GLU:HG3	1.41	1.01
2:H:150:GLN:O	2:H:153:SER:HB2	1.61	1.00
1:K:105:ILE:HD11	1:K:120:ILE:HG23	1.41	1.00
2:E:312:ILE:H	2:E:312:ILE:HD13	1.27	1.00
2:F:122:ARG:HH11	2:F:126:LEU:HD23	1.27	1.00
2:E:152:PRO:HB2	2:E:156:ARG:HB2	1.43	0.99
2:H:351:ILE:HD13	2:H:351:ILE:H	1.27	0.98
2:G:220:ASP:HA	2:G:223:LYS:HD2	1.43	0.98
1:B:65:GLU:HG2	2:F:143:TRP:CD1	1.97	0.97
2:G:92:VAL:HG21	2:H:92:VAL:HG13	1.42	0.97
2:G:88:GLU:HB3	2:H:90:GLY:HA2	1.44	0.96
2:H:123:ALA:HA	2:H:127:ALA:HB3	1.46	0.96
2:G:170:ASP:HA	2:G:217:LYS:HA	1.44	0.96
2:F:132:LEU:HD11	2:F:160:ARG:HG3	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:92:VAL:HG21	2:H:92:VAL:CG1	1.94	0.96
1:I:80:LYS:HA	1:I:83:ARG:NH1	1.81	0.95
1:A:80:LYS:HA	1:A:83:ARG:NH1	1.81	0.95
2:G:94:LYS:HA	2:G:94:LYS:HE2	1.49	0.95
2:H:312:ILE:HD13	2:H:312:ILE:H	1.31	0.95
1:B:65:GLU:HB3	2:F:143:TRP:HA	1.47	0.95
2:H:135:LEU:HD23	2:H:171:LYS:HE2	1.46	0.95
2:G:103:LEU:HD22	2:G:247:VAL:HG22	1.48	0.94
1:A:80:LYS:HA	1:A:83:ARG:HH12	1.29	0.94
2:F:94:LYS:HE2	2:F:94:LYS:HA	1.48	0.93
2:H:172:GLU:HB3	2:H:215:LYS:HD2	1.51	0.93
2:H:132:LEU:HD11	2:H:160:ARG:HG3	1.50	0.91
1:D:83:ARG:NH1	1:D:83:ARG:HB3	1.86	0.91
1:J:71:LEU:HB2	1:J:99:ASP:OD2	1.71	0.91
2:F:351:ILE:H	2:F:351:ILE:HD13	1.35	0.91
2:G:130:ARG:NH2	2:G:130:ARG:HB2	1.85	0.91
2:F:59:THR:HG22	2:F:393:ARG:NH2	1.84	0.90
1:B:65:GLU:OE1	2:F:143:TRP:CD1	2.25	0.90
2:H:122:ARG:HH11	2:H:126:LEU:HD23	1.34	0.90
1:I:85:ASP:O	1:I:89:ARG:HB2	1.70	0.90
1:D:83:ARG:HB3	1:D:83:ARG:HH11	1.37	0.89
2:E:94:LYS:HE2	2:E:94:LYS:HA	1.52	0.89
2:H:94:LYS:HE2	2:H:94:LYS:HA	1.53	0.88
1:D:105:ILE:HD11	1:D:120:ILE:HG21	1.54	0.88
2:E:299:THR:HA	2:E:302:ILE:HD13	1.55	0.87
2:G:344:LEU:O	2:G:352:THR:HB	1.73	0.87
1:I:10:GLY:HA3	1:I:174:LYS:HA	1.55	0.87
2:G:64:THR:HB	3:G:2450:ADP:O2A	1.74	0.87
2:H:216:LEU:CG	2:H:221:ALA:HB2	2.05	0.87
1:B:104:LEU:HD12	1:B:112:VAL:HG12	1.57	0.86
2:E:344:LEU:O	2:E:352:THR:HB	1.75	0.86
1:K:105:ILE:HD11	1:K:120:ILE:CG2	2.05	0.86
1:L:174:LYS:HA	1:L:174:LYS:NZ	1.90	0.86
1:I:1:THR:HB	1:I:33:LYS:HZ3	1.39	0.86
2:H:312:ILE:H	2:H:312:ILE:CD1	1.89	0.86
2:G:397:THR:HG22	2:H:327:PRO:HA	1.58	0.85
1:B:65:GLU:OE1	2:F:143:TRP:CG	2.29	0.85
2:E:132:LEU:HD11	2:E:160:ARG:HG3	1.58	0.85
1:D:152:LEU:HD13	1:D:166:HIS:ND1	1.91	0.84
1:I:47:ALA:HB3	1:I:94:LEU:HB2	1.58	0.84
2:G:312:ILE:H	2:G:312:ILE:HD13	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASP:O	1:A:89:ARG:HB2	1.76	0.84
1:B:17:ASP:HA	1:B:165:PHE:O	1.78	0.84
2:F:91:TYR:O	2:F:92:VAL:HG13	1.78	0.84
1:C:83:ARG:HB3	1:C:83:ARG:HH11	1.34	0.84
2:H:132:LEU:HA	2:H:135:LEU:HD12	1.58	0.84
1:B:65:GLU:CG	2:F:143:TRP:CD1	2.60	0.84
2:F:59:THR:HG22	2:F:393:ARG:HH21	1.42	0.84
2:E:130:ARG:HB2	2:E:130:ARG:NH2	1.92	0.84
2:E:214:ARG:HD3	2:E:216:LEU:HD22	1.59	0.83
2:H:174:GLU:HA	2:H:213:ALA:H	1.43	0.83
1:B:72:VAL:O	1:B:76:VAL:HG23	1.78	0.83
2:E:64:THR:HB	3:E:450:ADP:O2A	1.78	0.83
2:F:123:ALA:HA	2:F:127:ALA:HB3	1.59	0.83
2:G:362:GLU:OE2	2:H:32:ARG:NH2	2.08	0.83
2:E:131:ILE:HD11	2:E:218:ILE:HG12	1.61	0.83
2:G:91:TYR:HB2	2:H:90:GLY:O	1.78	0.82
2:F:103:LEU:HD13	2:F:247:VAL:HG22	1.61	0.82
1:J:72:VAL:O	1:J:76:VAL:HG23	1.79	0.82
2:G:220:ASP:O	2:G:223:LYS:N	2.10	0.82
2:E:145:GLN:HB2	2:E:148:GLN:HB2	1.62	0.82
2:G:361:THR:HG22	2:H:35:TRP:CZ3	2.15	0.82
1:A:10:GLY:HA2	1:A:173:TYR:CE1	2.15	0.82
2:F:173:ILE:HG12	2:F:212:LYS:HD2	1.59	0.82
2:F:171:LYS:NZ	2:F:218:ILE:HD11	1.94	0.81
2:E:312:ILE:H	2:E:312:ILE:CD1	1.93	0.81
2:F:312:ILE:HD13	2:F:312:ILE:H	1.46	0.81
2:H:173:ILE:HG12	2:H:212:LYS:HD2	1.63	0.81
1:D:71:LEU:HD21	1:D:97:VAL:HG11	1.62	0.80
1:K:152:LEU:HD13	1:K:166:HIS:ND1	1.96	0.80
1:D:43:ILE:HD13	1:D:43:ILE:H	1.46	0.80
2:H:171:LYS:NZ	2:H:218:ILE:HD11	1.96	0.80
2:F:64:THR:HB	3:F:1450:ADP:O2A	1.82	0.80
2:H:131:ILE:HD11	2:H:218:ILE:HD13	1.64	0.80
2:E:150:GLN:O	2:E:153:SER:HB2	1.82	0.79
1:L:1:THR:HB	1:L:33:LYS:HZ3	1.47	0.79
2:F:27:VAL:HG13	2:F:70:LEU:HG	1.62	0.79
2:E:173:ILE:HG12	2:E:212:LYS:HD2	1.64	0.79
2:E:389:ASN:ND2	2:E:391:GLY:H	1.80	0.79
1:I:10:GLY:HA2	1:I:173:TYR:CE1	2.18	0.79
2:G:92:VAL:HG11	2:H:92:VAL:CG1	2.12	0.79
2:G:211:GLN:HG2	2:G:212:LYS:H	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:62:ARG:O	1:L:66:MET:HB2	1.82	0.79
2:H:345:THR:CG2	2:H:373:ILE:HD13	2.13	0.79
2:E:152:PRO:HB3	2:E:156:ARG:H	1.48	0.79
1:D:105:ILE:HD11	1:D:120:ILE:CG2	2.13	0.79
2:H:384:ASN:ND2	2:H:394:ARG:HE	1.80	0.79
2:H:389:ASN:ND2	2:H:391:GLY:H	1.81	0.79
2:E:389:ASN:HD22	2:E:389:ASN:C	1.83	0.78
2:F:224:LEU:O	2:F:228:GLU:HB2	1.83	0.78
1:L:13:VAL:HG12	1:L:170:GLU:HG3	1.64	0.78
1:J:57:PHE:O	1:J:61:GLU:HG3	1.83	0.78
2:G:147:GLU:HA	2:G:150:GLN:HG3	1.66	0.78
2:F:172:GLU:HB3	2:F:215:LYS:HD2	1.64	0.78
2:H:91:TYR:O	2:H:92:VAL:HG13	1.83	0.78
1:B:65:GLU:HG2	2:F:143:TRP:HD1	1.46	0.77
2:F:223:LYS:HA	2:F:226:ILE:HG12	1.64	0.77
2:H:132:LEU:HD23	2:H:135:LEU:HD12	1.66	0.77
2:E:211:GLN:HG2	2:E:212:LYS:H	1.49	0.76
1:A:10:GLY:HA3	1:A:174:LYS:HA	1.65	0.76
1:B:105:ILE:HD11	1:B:120:ILE:HG23	1.68	0.76
2:G:109:LYS:CD	2:H:296:MET:HB3	2.13	0.76
2:F:257:GLU:HB2	2:F:260:LYS:HG3	1.68	0.76
2:F:148:GLN:OE1	2:F:151:GLU:HG3	1.85	0.76
2:H:103:LEU:HD13	2:H:247:VAL:HG22	1.68	0.76
1:B:170:GLU:HG2	1:B:171:LEU:H	1.51	0.75
2:G:142:ASN:HB2	2:G:149:GLN:HE22	1.51	0.75
2:H:217:LYS:HB2	2:H:217:LYS:NZ	2.01	0.75
1:L:30:ASN:H	1:L:30:ASN:HD22	1.31	0.75
1:D:54:PHE:O	1:D:58:GLU:HB2	1.86	0.75
2:H:64:THR:HB	3:H:3450:ADP:O2A	1.85	0.75
1:L:105:ILE:HD11	1:L:120:ILE:HG23	1.68	0.75
2:E:130:ARG:HD2	2:E:225:LEU:HD11	1.67	0.75
1:J:104:LEU:HD12	1:J:112:VAL:HG12	1.68	0.75
1:B:1:THR:HB	1:B:33:LYS:NZ	2.01	0.75
2:G:152:PRO:CB	2:G:156:ARG:HB2	2.16	0.74
2:E:384:ASN:ND2	2:E:394:ARG:HE	1.85	0.74
1:J:1:THR:HB	1:J:33:LYS:NZ	2.03	0.74
2:G:291:SER:HA	2:G:296:MET:HE2	1.69	0.74
2:E:174:GLU:HA	2:E:213:ALA:H	1.51	0.74
2:G:136:ILE:O	2:G:136:ILE:HG22	1.88	0.74
1:I:83:ARG:HG2	1:I:83:ARG:HH11	1.52	0.74
2:G:152:PRO:O	2:G:154:ALA:N	0.59	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:130:ARG:HH21	2:H:229:GLU:HG3	1.50	0.74
1:B:60:PHE:CD1	1:B:78:LEU:HD22	2.23	0.74
2:E:104:THR:HG21	2:E:292:THR:HG21	1.69	0.74
1:L:64:LEU:HB3	1:L:69:GLY:HA2	1.69	0.74
2:F:384:ASN:ND2	2:F:394:ARG:HE	1.85	0.74
1:B:57:PHE:O	1:B:61:GLU:HG3	1.88	0.73
2:G:168:LEU:HA	2:G:219:LYS:HB3	1.68	0.73
2:H:108:VAL:HA	2:H:111:VAL:HG22	1.68	0.73
1:L:138:GLU:C	1:L:139:ASN:HD22	1.90	0.73
2:G:145:GLN:HB2	2:G:148:GLN:HB2	1.70	0.73
2:H:130:ARG:HG2	2:H:225:LEU:HD11	1.70	0.73
1:B:28:LYS:HZ2	1:B:30:ASN:HD21	1.36	0.73
2:F:122:ARG:NH1	2:F:126:LEU:HD23	2.02	0.73
1:C:85:ASP:HB3	1:C:88:LEU:HB2	1.69	0.73
2:H:356:LYS:HG3	2:H:366:ILE:HG22	1.71	0.73
2:G:389:ASN:ND2	2:G:391:GLY:H	1.86	0.73
2:E:167:GLN:NE2	2:E:168:LEU:HG	2.04	0.73
1:J:19:GLN:HB2	1:J:163:ASN:ND2	2.03	0.73
2:H:147:GLU:O	2:H:151:GLU:HG2	1.89	0.73
1:D:3:ILE:HB	1:D:122:ILE:HG12	1.71	0.72
1:L:30:ASN:H	1:L:30:ASN:ND2	1.87	0.72
1:L:115:PRO:HG3	1:L:120:ILE:HG12	1.68	0.72
1:B:36:ARG:O	1:B:37:LEU:HD23	1.88	0.72
1:C:136:LEU:HB3	1:C:147:ILE:HD12	1.72	0.72
2:H:219:LYS:HA	2:H:219:LYS:HE3	1.71	0.72
1:B:86:ARG:HA	1:B:89:ARG:NE	2.03	0.72
2:F:356:LYS:HG3	2:F:366:ILE:HG22	1.70	0.72
2:G:312:ILE:H	2:G:312:ILE:CD1	2.02	0.72
2:H:232:LYS:H	2:H:232:LYS:HD2	1.54	0.72
2:H:220:ASP:O	2:H:224:LEU:HD23	1.88	0.72
2:G:91:TYR:HD1	2:H:91:TYR:CD2	2.06	0.72
1:K:71:LEU:HG	1:K:99:ASP:OD1	1.88	0.72
1:L:152:LEU:HD13	1:L:166:HIS:CE1	2.24	0.72
2:E:124:GLU:HA	2:E:127:ALA:HB3	1.72	0.72
2:E:167:GLN:HE22	2:E:168:LEU:HG	1.54	0.72
1:D:71:LEU:HD21	1:D:97:VAL:CG1	2.19	0.72
1:D:79:ALA:HB1	1:D:110:GLY:HA2	1.69	0.72
1:J:152:LEU:HD13	1:J:166:HIS:ND1	2.05	0.72
2:E:91:TYR:O	2:E:92:VAL:HG13	1.89	0.72
2:F:81:VAL:HG11	2:F:99:ILE:HG12	1.72	0.72
2:G:362:GLU:HG2	2:G:410:ALA:HB1	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:171:LYS:HG3	2:E:218:ILE:HD11	1.72	0.71
2:H:242:ASP:HA	2:H:245:ASP:OD1	1.90	0.71
2:G:389:ASN:HD22	2:G:389:ASN:C	1.92	0.71
2:E:140:LYS:O	2:E:141:ASN:HB2	1.90	0.71
1:D:115:PRO:HG3	1:D:120:ILE:HG12	1.71	0.71
1:J:5:SER:HB3	1:J:120:ILE:HD13	1.72	0.71
2:G:361:THR:CG2	2:H:35:TRP:CZ3	2.74	0.71
2:G:124:GLU:HA	2:G:127:ALA:HB3	1.73	0.71
2:G:153:SER:O	2:G:157:GLN:NE2	2.23	0.71
1:L:174:LYS:HA	1:L:174:LYS:HZ3	1.53	0.71
2:G:92:VAL:CG2	2:H:91:TYR:C	2.59	0.71
1:B:28:LYS:NZ	1:B:30:ASN:HD21	1.88	0.70
2:F:108:VAL:HG21	2:F:294:HIS:HD2	1.56	0.70
1:J:105:ILE:HD11	1:J:120:ILE:HG23	1.73	0.70
1:K:64:LEU:HD23	1:K:74:ALA:CB	2.20	0.70
2:F:242:ASP:HA	2:F:245:ASP:OD1	1.90	0.70
2:G:130:ARG:HB2	2:G:130:ARG:HH21	1.54	0.70
2:H:344:LEU:O	2:H:352:THR:HB	1.90	0.70
1:B:63:LYS:HA	1:B:66:MET:HE3	1.72	0.70
2:F:312:ILE:H	2:F:312:ILE:CD1	2.04	0.70
1:D:14:ILE:HD13	1:D:43:ILE:CG1	2.22	0.70
2:F:174:GLU:HA	2:F:213:ALA:H	1.56	0.70
1:I:1:THR:HB	1:I:33:LYS:NZ	2.05	0.70
1:L:43:ILE:HD13	1:L:43:ILE:H	1.57	0.70
1:B:1:THR:HB	1:B:33:LYS:HZ3	1.56	0.70
2:G:91:TYR:HD1	2:H:91:TYR:CE2	2.09	0.70
2:E:165:GLU:HG2	2:E:166:GLY:H	1.55	0.69
2:F:344:LEU:O	2:F:352:THR:HB	1.92	0.69
1:D:6:VAL:HG21	1:D:147:ILE:HG22	1.74	0.69
2:G:91:TYR:O	2:G:92:VAL:HG13	1.91	0.69
2:H:217:LYS:O	2:H:221:ALA:N	2.13	0.69
2:G:174:GLU:HA	2:G:212:LYS:HB3	1.73	0.69
2:F:217:LYS:HB2	2:F:217:LYS:NZ	2.07	0.69
2:H:174:GLU:HB3	2:H:211:GLN:HB2	1.74	0.69
2:E:293:LYS:HG3	2:E:294:HIS:CD2	2.28	0.69
1:J:104:LEU:CD1	1:J:112:VAL:HG12	2.22	0.69
1:A:71:LEU:HD23	1:A:99:ASP:OD2	1.92	0.69
2:H:27:VAL:HG13	2:H:70:LEU:HG	1.75	0.69
2:H:148:GLN:HA	2:H:151:GLU:HG3	1.72	0.69
1:B:86:ARG:HA	1:B:89:ARG:CZ	2.23	0.69
1:I:8:ARG:HG2	1:I:9:ASN:ND2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:86:ARG:HA	1:J:89:ARG:CZ	2.23	0.69
1:K:86:ARG:HA	1:K:89:ARG:NH1	2.06	0.69
2:E:170:ASP:HA	2:E:217:LYS:HA	1.73	0.69
1:J:141:GLU:HA	1:J:141:GLU:OE2	1.93	0.69
2:E:312:ILE:HG12	2:E:313:ALA:H	1.58	0.69
2:G:91:TYR:CD1	2:H:91:TYR:CE2	2.81	0.69
1:B:104:LEU:CD1	1:B:112:VAL:HG12	2.22	0.69
2:E:359:MET:HG3	2:E:366:ILE:HG13	1.75	0.69
2:G:359:MET:HG3	2:G:366:ILE:HG13	1.74	0.69
1:B:65:GLU:CD	2:F:143:TRP:CD1	2.65	0.68
2:E:337:THR:O	2:E:341:GLU:HG3	1.92	0.68
2:G:345:THR:HG21	2:G:373:ILE:HD13	1.74	0.68
2:H:236:PRO:HG2	2:H:237:GLU:H	1.58	0.68
2:H:389:ASN:HD22	2:H:391:GLY:H	1.41	0.68
2:E:214:ARG:HG2	2:E:215:LYS:N	2.08	0.68
1:I:77:GLU:O	1:I:80:LYS:HB2	1.93	0.68
2:H:223:LYS:HA	2:H:226:ILE:HG12	1.76	0.68
2:F:264:ARG:NE	2:F:265:GLY:H	1.91	0.68
2:F:375:ARG:CZ	2:F:422:ALA:HB1	2.23	0.68
2:H:235:ASN:HB2	2:H:236:PRO:HD2	1.73	0.68
2:F:108:VAL:C	2:F:110:MET:H	1.96	0.68
1:I:10:GLY:HA2	1:I:173:TYR:CZ	2.29	0.68
2:E:122:ARG:CZ	2:E:126:LEU:HD21	2.24	0.68
2:H:375:ARG:CZ	2:H:422:ALA:HB1	2.23	0.68
2:G:152:PRO:HB2	2:G:156:ARG:CB	2.21	0.68
2:E:291:SER:HA	2:E:296:MET:HE2	1.76	0.68
1:D:28:LYS:HD3	1:D:31:VAL:HG22	1.74	0.68
2:H:135:LEU:HB3	2:H:159:PHE:CD2	2.28	0.68
1:K:73:LYS:HA	1:K:76:VAL:HG12	1.76	0.68
2:G:359:MET:CE	2:H:36:ARG:NH1	2.57	0.67
2:E:174:GLU:CB	2:E:211:GLN:HG3	2.18	0.67
2:G:173:ILE:HD13	2:G:173:ILE:N	2.09	0.67
1:A:1:THR:HB	1:A:33:LYS:HZ3	1.59	0.67
2:H:96:VAL:HG11	2:H:281:LEU:HD12	1.75	0.67
2:G:147:GLU:HG3	2:G:150:GLN:NE2	2.10	0.67
1:C:11:HIS:NE2	1:C:174:LYS:HE2	2.08	0.67
1:J:86:ARG:HA	1:J:89:ARG:NE	2.09	0.67
1:B:152:LEU:HD13	1:B:166:HIS:ND1	2.10	0.67
2:E:216:LEU:HD23	2:E:216:LEU:H	1.60	0.67
2:F:163:LEU:HD11	2:F:222:MET:CE	2.24	0.67
2:F:82:GLU:HB3	2:F:257:GLU:OE2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:153:SER:HA	2:G:157:GLN:HG3	1.75	0.67
2:F:216:LEU:HD11	2:F:221:ALA:HA	1.76	0.67
2:G:130:ARG:CD	2:G:225:LEU:HD11	2.20	0.67
2:G:140:LYS:O	2:G:141:ASN:HB2	1.95	0.67
2:G:384:ASN:ND2	2:G:394:ARG:HE	1.92	0.67
2:F:152:PRO:HB2	2:F:156:ARG:HB2	1.77	0.67
1:C:152:LEU:HD13	1:C:166:HIS:CE1	2.29	0.67
1:D:73:LYS:NZ	1:D:77:GLU:HG2	2.09	0.67
1:J:85:ASP:O	1:J:89:ARG:HG3	1.95	0.66
2:G:89:VAL:HG12	2:G:93:GLY:HA3	1.77	0.66
1:A:65:GLU:CD	2:E:141:ASN:HB3	2.15	0.66
1:C:10:GLY:HA2	1:C:173:TYR:CE1	2.30	0.66
2:F:223:LYS:HD2	2:F:223:LYS:N	2.09	0.66
1:B:19:GLN:HB2	1:B:163:ASN:ND2	2.11	0.66
2:E:136:ILE:HG22	2:E:136:ILE:O	1.95	0.66
1:C:79:ALA:HB1	1:C:110:GLY:HA2	1.78	0.66
2:F:135:LEU:CD2	2:F:171:LYS:HE2	2.25	0.66
1:A:28:LYS:NZ	1:A:30:ASN:ND2	2.43	0.66
2:F:130:ARG:HD2	2:F:225:LEU:HD11	1.77	0.66
2:F:389:ASN:ND2	2:F:391:GLY:H	1.93	0.66
1:J:8:ARG:NH1	1:J:142:LEU:O	2.26	0.66
1:K:27:MET:SD	1:L:113:VAL:HG21	2.35	0.66
2:E:211:GLN:HG2	2:E:212:LYS:N	2.11	0.66
2:F:174:GLU:HA	2:F:212:LYS:HB3	1.76	0.66
2:F:291:SER:HA	2:F:296:MET:HE2	1.77	0.66
2:G:173:ILE:HG12	2:G:212:LYS:HD2	1.76	0.66
2:H:130:ARG:HG2	2:H:225:LEU:CD1	2.26	0.66
2:H:130:ARG:NH2	2:H:229:GLU:HG3	2.10	0.66
1:A:65:GLU:OE1	2:E:141:ASN:CB	2.44	0.66
2:E:103:LEU:HD22	2:E:247:VAL:HG22	1.78	0.66
2:E:122:ARG:O	2:E:126:LEU:HD23	1.96	0.66
2:F:211:GLN:HE21	2:F:212:LYS:H	1.43	0.66
2:F:362:GLU:HG2	2:F:410:ALA:CB	2.25	0.66
2:F:151:GLU:HB2	2:F:152:PRO:CD	2.26	0.66
1:J:36:ARG:O	1:J:37:LEU:HD23	1.95	0.66
1:B:62:ARG:HA	1:B:65:GLU:HG3	1.77	0.65
2:G:174:GLU:HB3	2:G:211:GLN:CG	2.20	0.65
2:E:52:ASN:HB2	2:E:325:ARG:O	1.97	0.65
1:C:73:LYS:HA	1:C:76:VAL:HG12	1.78	0.65
2:G:92:VAL:HG21	2:H:91:TYR:C	2.15	0.65
2:G:293:LYS:HG3	2:G:294:HIS:CD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:345:THR:CG2	2:E:373:ILE:HD13	2.27	0.65
1:J:28:LYS:NZ	1:J:30:ASN:HD21	1.94	0.65
2:H:223:LYS:HA	2:H:226:ILE:CG1	2.27	0.65
1:J:1:THR:HB	1:J:33:LYS:HZ3	1.60	0.65
1:J:28:LYS:HZ2	1:J:30:ASN:HD21	1.44	0.65
2:H:108:VAL:C	2:H:110:MET:H	1.98	0.65
1:B:28:LYS:NZ	1:B:30:ASN:ND2	2.44	0.65
2:G:92:VAL:HG11	2:H:92:VAL:HG12	1.76	0.65
2:F:89:VAL:HG11	2:F:94:LYS:O	1.97	0.65
2:F:130:ARG:CD	2:F:225:LEU:HD11	2.27	0.65
2:H:168:LEU:O	2:H:217:LYS:HD2	1.97	0.65
2:H:148:GLN:OE1	2:H:151:GLU:HG3	1.97	0.65
2:H:219:LYS:O	2:H:223:LYS:HD3	1.96	0.65
2:H:229:GLU:HA	2:H:232:LYS:HD3	1.78	0.65
1:K:168:ILE:N	1:K:168:ILE:HD12	2.12	0.65
2:F:145:GLN:HB2	2:F:148:GLN:HG2	1.78	0.64
2:F:210:LYS:HD3	2:F:210:LYS:N	2.12	0.64
1:D:30:ASN:H	1:D:30:ASN:HD22	1.45	0.64
1:J:168:ILE:H	1:J:168:ILE:HD12	1.63	0.64
2:G:92:VAL:CG2	2:H:92:VAL:HG13	2.23	0.64
2:H:389:ASN:HD22	2:H:389:ASN:C	2.01	0.64
2:G:361:THR:HG21	2:H:36:ARG:HA	1.79	0.64
1:K:115:PRO:HG3	1:K:120:ILE:HG12	1.80	0.64
1:A:1:THR:HB	1:A:33:LYS:NZ	2.11	0.64
1:J:17:ASP:HA	1:J:165:PHE:O	1.98	0.64
2:G:152:PRO:HB3	2:G:156:ARG:H	1.63	0.64
1:L:91:LEU:HD12	1:L:91:LEU:O	1.98	0.64
1:I:152:LEU:HD13	1:I:166:HIS:CE1	2.32	0.64
2:G:142:ASN:CB	2:G:149:GLN:HE22	2.10	0.64
2:E:147:GLU:HA	2:E:150:GLN:HG3	1.80	0.64
2:E:173:ILE:HD13	2:E:173:ILE:N	2.12	0.64
2:E:174:GLU:HB3	2:E:211:GLN:CG	2.19	0.64
1:D:17:ASP:HA	1:D:165:PHE:O	1.97	0.64
1:D:30:ASN:HD22	1:D:30:ASN:N	1.95	0.64
2:G:112:ARG:HG3	2:G:112:ARG:HH11	1.62	0.64
1:I:168:ILE:N	1:I:168:ILE:HD12	2.13	0.64
2:H:145:GLN:HB2	2:H:148:GLN:HG2	1.80	0.64
2:H:214:ARG:HE	2:H:216:LEU:HB3	1.61	0.64
2:F:127:ALA:HA	2:F:130:ARG:NH2	2.13	0.64
2:F:132:LEU:HA	2:F:135:LEU:HD12	1.80	0.64
1:C:30:ASN:HD22	1:C:30:ASN:H	1.43	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:GLN:HB2	1:D:163:ASN:ND2	2.12	0.64
2:H:232:LYS:HD2	2:H:232:LYS:N	2.11	0.64
1:K:168:ILE:HD12	1:K:168:ILE:H	1.63	0.64
1:L:79:ALA:HB1	1:L:110:GLY:HA2	1.80	0.64
2:F:123:ALA:HA	2:F:127:ALA:CB	2.27	0.64
2:E:116:ILE:O	2:E:120:ARG:HB2	1.98	0.64
1:D:34:VAL:HG12	1:D:169:GLU:HG3	1.80	0.64
2:G:122:ARG:CZ	2:G:126:LEU:HD21	2.28	0.64
2:H:167:GLN:O	2:H:168:LEU:HB3	1.98	0.64
1:A:7:ARG:HB2	1:A:12:VAL:HG23	1.80	0.63
1:A:84:THR:HG23	1:A:85:ASP:H	1.63	0.63
1:A:88:LEU:H	1:A:88:LEU:HD12	1.63	0.63
1:C:28:LYS:HD2	1:D:113:VAL:HG13	1.79	0.63
1:I:67:HIS:CD2	1:I:73:LYS:HD2	2.33	0.63
2:G:408:TYR:HB2	2:H:29:ILE:HD11	1.80	0.63
2:E:152:PRO:HB2	2:E:156:ARG:CB	2.25	0.63
2:E:311:GLN:CA	2:E:311:GLN:HE21	2.11	0.63
2:E:375:ARG:CZ	2:E:422:ALA:HB1	2.27	0.63
2:F:147:GLU:O	2:F:151:GLU:HG2	1.99	0.63
2:F:236:PRO:HG2	2:F:237:GLU:H	1.64	0.63
2:F:132:LEU:HD11	2:F:160:ARG:CG	2.27	0.63
2:F:235:ASN:HB2	2:F:236:PRO:HD2	1.81	0.63
1:C:83:ARG:HB3	1:C:83:ARG:CZ	2.29	0.63
2:H:174:GLU:HA	2:H:212:LYS:HB3	1.81	0.63
1:K:83:ARG:HH11	1:K:83:ARG:HG3	1.63	0.63
1:J:28:LYS:NZ	1:J:30:ASN:ND2	2.47	0.63
1:K:36:ARG:O	1:K:37:LEU:HD23	1.98	0.63
1:A:67:HIS:HD2	1:A:73:LYS:HD2	1.62	0.63
2:F:41:ASN:HD22	2:F:41:ASN:C	2.02	0.63
2:F:96:VAL:HG11	2:F:281:LEU:HD12	1.80	0.63
1:I:8:ARG:O	1:I:11:HIS:HB2	1.99	0.63
2:H:312:ILE:HD13	2:H:312:ILE:N	2.08	0.63
2:F:132:LEU:HD23	2:F:135:LEU:HD12	1.80	0.63
2:H:315:PRO:O	2:H:318:LEU:HB2	1.99	0.63
1:L:6:VAL:HG21	1:L:147:ILE:HG22	1.79	0.63
2:G:88:GLU:CB	2:H:90:GLY:HA2	2.25	0.63
2:G:375:ARG:CZ	2:G:422:ALA:HB1	2.29	0.63
2:F:27:VAL:CG1	2:F:70:LEU:HG	2.30	0.62
1:I:36:ARG:HB3	1:I:36:ARG:HH11	1.63	0.62
2:F:131:ILE:HD13	2:F:222:MET:HE1	1.80	0.62
2:F:147:GLU:CG	2:F:150:GLN:NE2	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:211:GLN:NE2	2:F:212:LYS:H	1.97	0.62
1:A:65:GLU:CD	2:E:141:ASN:CB	2.68	0.62
2:F:31:LEU:HD11	2:F:74:ALA:HB2	1.81	0.62
2:F:101:ARG:O	2:F:104:THR:HB	1.99	0.62
1:D:37:LEU:HD11	1:D:60:PHE:HD2	1.63	0.62
1:L:95:LEU:HB2	1:L:106:ILE:HB	1.81	0.62
2:F:401:ARG:NH2	2:F:442:ILE:HG13	2.15	0.62
2:G:359:MET:HE2	2:H:36:ARG:NH1	2.14	0.62
2:H:123:ALA:HA	2:H:127:ALA:CB	2.24	0.62
1:B:28:LYS:HD3	1:B:31:VAL:HG22	1.82	0.62
2:F:108:VAL:HG21	2:F:294:HIS:CD2	2.34	0.62
1:J:86:ARG:HA	1:J:89:ARG:NH1	2.14	0.62
2:G:170:ASP:HB3	2:G:217:LYS:HD3	1.81	0.62
1:K:28:LYS:HE2	1:K:30:ASN:ND2	2.15	0.62
1:L:152:LEU:HD13	1:L:166:HIS:ND1	2.13	0.62
2:E:130:ARG:HB2	2:E:130:ARG:CZ	2.30	0.62
2:E:389:ASN:HD22	2:E:391:GLY:H	1.46	0.62
1:A:65:GLU:OE1	2:E:141:ASN:HB3	2.00	0.62
2:G:231:ALA:C	2:G:233:LEU:H	2.03	0.62
2:E:312:ILE:HD13	2:E:312:ILE:N	2.09	0.62
2:E:312:ILE:HG12	2:E:313:ALA:N	2.14	0.62
2:F:219:LYS:O	2:F:223:LYS:HD3	2.00	0.62
2:G:362:GLU:HG2	2:G:410:ALA:CB	2.30	0.62
2:H:239:LEU:HD23	2:H:240:LYS:N	2.14	0.62
1:B:46:PHE:CE2	1:B:53:ALA:HB2	2.35	0.61
2:F:129:GLU:HB2	2:F:130:ARG:NH1	2.15	0.61
2:E:140:LYS:H	2:E:140:LYS:HD3	1.66	0.61
1:I:87:MET:CE	1:J:84:THR:HA	2.30	0.61
2:H:221:ALA:O	2:H:225:LEU:HD23	2.00	0.61
1:L:55:THR:O	1:L:58:GLU:HB3	2.00	0.61
2:H:81:VAL:HG11	2:H:99:ILE:HG12	1.82	0.61
2:F:362:GLU:HG2	2:F:410:ALA:HB1	1.80	0.61
2:G:140:LYS:HD3	2:G:140:LYS:H	1.65	0.61
2:H:19:GLY:O	2:H:24:LYS:HE3	2.00	0.61
2:H:20:GLN:O	2:H:24:LYS:HG3	2.00	0.61
1:D:38:TYR:HE1	1:D:65:GLU:HB3	1.64	0.61
1:D:86:ARG:HA	1:D:89:ARG:CZ	2.30	0.61
1:B:168:ILE:HD12	1:B:168:ILE:N	2.15	0.61
2:E:293:LYS:HG3	2:E:294:HIS:HD2	1.65	0.61
2:G:108:VAL:HG21	2:G:294:HIS:ND1	2.16	0.61
2:G:148:GLN:HA	2:G:151:GLU:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:393:ARG:HG2	2:H:393:ARG:HH11	1.65	0.61
1:A:8:ARG:NH1	1:A:142:LEU:O	2.23	0.61
1:L:1:THR:HB	1:L:33:LYS:NZ	2.16	0.61
1:A:88:LEU:H	1:A:88:LEU:CD1	2.13	0.61
2:E:152:PRO:CB	2:E:156:ARG:H	2.13	0.61
2:F:116:ILE:O	2:F:120:ARG:HB2	2.01	0.61
2:F:170:ASP:HA	2:F:217:LYS:HA	1.81	0.61
2:G:345:THR:HG22	2:G:352:THR:HG21	1.82	0.61
2:H:123:ALA:CA	2:H:127:ALA:HB3	2.25	0.61
1:C:95:LEU:HB2	1:C:106:ILE:HB	1.83	0.60
1:A:105:ILE:CD1	1:A:120:ILE:HG23	2.30	0.60
1:B:65:GLU:OE1	2:F:143:TRP:CD2	2.55	0.60
1:D:13:VAL:HG12	1:D:170:GLU:HA	1.82	0.60
1:D:86:ARG:HA	1:D:89:ARG:NH1	2.15	0.60
2:H:262:CYS:SG	2:H:318:LEU:HD13	2.41	0.60
1:J:168:ILE:HD12	1:J:168:ILE:N	2.16	0.60
2:G:109:LYS:HB2	2:H:296:MET:CG	2.21	0.60
2:G:214:ARG:NH2	2:H:233:LEU:HD13	2.16	0.60
2:G:242:ASP:HA	2:G:245:ASP:OD1	2.02	0.60
2:G:359:MET:HE1	2:H:36:ARG:HH12	1.66	0.60
2:H:127:ALA:HA	2:H:130:ARG:NH2	2.15	0.60
1:J:19:GLN:HB2	1:J:163:ASN:HD22	1.65	0.60
2:H:63:LYS:HE2	2:H:307:SER:OG	2.01	0.60
2:F:312:ILE:HG12	2:F:313:ALA:N	2.15	0.60
2:H:108:VAL:HG21	2:H:294:HIS:HD2	1.67	0.60
2:H:375:ARG:HB3	2:H:425:VAL:HG11	1.83	0.60
1:B:70:HIS:HE1	1:B:72:VAL:HB	1.67	0.60
1:C:55:THR:O	1:C:58:GLU:HB3	2.02	0.60
1:D:14:ILE:HD13	1:D:43:ILE:HG13	1.83	0.60
2:H:25:ARG:O	2:H:29:ILE:HG12	2.02	0.60
2:H:132:LEU:HD23	2:H:135:LEU:CD1	2.31	0.60
2:H:211:GLN:NE2	2:H:212:LYS:H	2.00	0.60
2:F:212:LYS:NZ	2:F:212:LYS:HB2	2.17	0.60
2:G:389:ASN:HD22	2:G:391:GLY:H	1.49	0.60
2:E:168:LEU:HA	2:E:219:LYS:HB3	1.84	0.60
2:F:19:GLY:O	2:F:24:LYS:HE3	2.02	0.60
2:F:130:ARG:CG	2:F:225:LEU:HD11	2.32	0.60
1:C:94:LEU:CD2	1:C:107:THR:HG22	2.31	0.60
1:D:14:ILE:HD13	1:D:43:ILE:HG12	1.83	0.60
2:G:219:LYS:O	2:G:223:LYS:HE3	2.01	0.60
2:H:291:SER:HA	2:H:296:MET:HE2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:136:LEU:HB3	1:K:147:ILE:HD12	1.82	0.60
2:E:33:ASN:ND2	2:E:36:ARG:HD2	2.17	0.60
2:E:168:LEU:HD23	2:E:219:LYS:HB3	1.82	0.60
2:F:86:PHE:O	2:F:89:VAL:HG22	2.02	0.60
1:I:14:ILE:HD12	1:I:43:ILE:HG13	1.84	0.60
2:H:311:GLN:NE2	2:H:311:GLN:HA	2.17	0.60
1:L:174:LYS:HA	1:L:174:LYS:HZ2	1.65	0.60
1:A:77:GLU:O	1:A:80:LYS:HB2	2.01	0.60
2:F:147:GLU:HG2	2:F:150:GLN:NE2	2.16	0.60
2:F:229:GLU:OE2	2:F:232:LYS:HD2	2.02	0.60
2:G:88:GLU:HB3	2:H:90:GLY:CA	2.25	0.60
2:G:131:ILE:HD11	2:G:218:ILE:HG12	1.83	0.60
2:H:337:THR:O	2:H:341:GLU:HG3	2.02	0.60
2:E:131:ILE:HD11	2:E:218:ILE:CG1	2.30	0.59
2:E:432:LEU:H	2:E:432:LEU:HD12	1.67	0.59
2:F:12:GLU:HG2	2:F:73:LEU:CD1	2.32	0.59
1:I:105:ILE:CD1	1:I:120:ILE:HG23	2.31	0.59
2:G:142:ASN:HB2	2:G:149:GLN:NE2	2.15	0.59
2:G:174:GLU:HA	2:G:213:ALA:H	1.67	0.59
2:H:218:ILE:O	2:H:222:MET:HB3	2.02	0.59
2:E:33:ASN:HD22	2:E:36:ARG:HD2	1.66	0.59
2:E:130:ARG:CD	2:E:225:LEU:HD11	2.33	0.59
2:F:59:THR:CG2	2:F:393:ARG:HH21	2.13	0.59
1:I:83:ARG:NH1	1:I:83:ARG:HG2	2.17	0.59
2:G:153:SER:CA	2:G:157:GLN:HG3	2.32	0.59
2:H:212:LYS:HB2	2:H:212:LYS:NZ	2.18	0.59
1:L:30:ASN:HD22	1:L:30:ASN:N	1.96	0.59
2:H:311:GLN:CA	2:H:311:GLN:HE21	2.15	0.59
2:G:174:GLU:C	2:G:211:GLN:HB2	2.22	0.59
2:H:108:VAL:HG21	2:H:294:HIS:CD2	2.36	0.59
2:H:264:ARG:NE	2:H:265:GLY:H	1.99	0.59
2:H:169:ASP:O	2:H:218:ILE:HG13	2.02	0.59
1:A:39:ASN:OD1	2:E:143:TRP:CZ2	2.55	0.59
2:F:340:PHE:O	2:F:344:LEU:HD22	2.03	0.59
2:F:389:ASN:HD22	2:F:391:GLY:H	1.51	0.59
1:J:38:TYR:HB2	1:J:64:LEU:CD1	2.33	0.59
2:G:311:GLN:CA	2:G:311:GLN:HE21	2.15	0.59
2:G:312:ILE:HG12	2:G:313:ALA:N	2.18	0.59
2:F:351:ILE:HD13	2:F:351:ILE:N	2.13	0.59
1:J:6:VAL:HG12	1:J:7:ARG:N	2.17	0.59
2:G:152:PRO:O	2:G:154:ALA:C	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:335:LEU:HD22	2:H:339:ASP:HB3	1.84	0.59
1:L:10:GLY:HA2	1:L:173:TYR:CZ	2.38	0.59
2:E:174:GLU:HA	2:E:212:LYS:HB3	1.83	0.59
2:F:65:GLU:HG3	3:F:1450:ADP:H2'	1.84	0.59
1:I:17:ASP:HA	1:I:165:PHE:O	2.03	0.59
1:J:62:ARG:HA	1:J:65:GLU:HG3	1.83	0.59
2:H:12:GLU:HG2	2:H:73:LEU:HD11	1.84	0.59
2:F:218:ILE:C	2:F:220:ASP:H	2.06	0.59
1:J:98:ALA:CB	1:J:103:SER:HB3	2.33	0.59
1:K:54:PHE:O	1:K:58:GLU:HB2	2.02	0.59
2:E:89:VAL:HG12	2:E:93:GLY:HA3	1.84	0.58
2:E:96:VAL:HG11	2:E:281:LEU:HD12	1.85	0.58
2:F:130:ARG:HH21	2:F:229:GLU:HG3	1.67	0.58
1:L:8:ARG:NH2	1:L:137:LEU:HD12	2.18	0.58
1:L:83:ARG:HH11	1:L:83:ARG:CB	2.01	0.58
2:F:366:ILE:HD12	2:F:418:ILE:HB	1.84	0.58
1:C:100:GLU:OE2	1:C:173:TYR:HB2	2.04	0.58
1:D:14:ILE:HD11	1:D:98:ALA:HB3	1.84	0.58
2:G:145:GLN:C	2:G:147:GLU:H	2.05	0.58
1:L:57:PHE:O	1:L:61:GLU:HG2	2.02	0.58
1:B:86:ARG:HA	1:B:89:ARG:NH1	2.18	0.58
2:E:124:GLU:HA	2:E:127:ALA:CB	2.33	0.58
2:E:142:ASN:HB2	2:E:149:GLN:HE22	1.67	0.58
2:E:362:GLU:HG2	2:E:410:ALA:HB1	1.84	0.58
2:F:131:ILE:HD11	2:F:218:ILE:HD13	1.83	0.58
2:H:401:ARG:NH2	2:H:442:ILE:HG13	2.18	0.58
1:A:90:LYS:NZ	1:B:89:ARG:NH2	2.51	0.58
2:G:58:PRO:HG2	2:G:61:VAL:HG11	1.84	0.58
2:G:116:ILE:O	2:G:120:ARG:HB2	2.03	0.58
2:E:89:VAL:HA	2:E:93:GLY:N	2.17	0.58
2:E:382:GLN:O	2:E:386:SER:HB3	2.03	0.58
1:L:143:SER:OG	1:L:146:GLU:HG3	2.03	0.58
1:B:115:PRO:HG3	1:B:120:ILE:HG12	1.85	0.58
1:D:159:CYS:HB3	1:D:162:THR:HB	1.84	0.58
1:L:14:ILE:HD12	1:L:43:ILE:HG12	1.85	0.58
2:F:389:ASN:HD22	2:F:389:ASN:C	2.06	0.58
2:G:389:ASN:HD22	2:G:390:ILE:N	2.02	0.58
1:L:15:ALA:HB1	1:L:152:LEU:HD12	1.86	0.58
1:A:149:GLU:HG2	1:A:168:ILE:HD11	1.85	0.58
2:E:132:LEU:HD11	2:E:160:ARG:CG	2.32	0.58
1:C:30:ASN:H	1:C:30:ASN:ND2	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:LYS:HA	1:D:76:VAL:HG12	1.85	0.58
2:G:217:LYS:HG3	2:G:219:LYS:HZ1	1.69	0.58
2:H:345:THR:HG21	2:H:373:ILE:HD13	1.85	0.58
1:K:59:LEU:HD11	1:K:63:LYS:HE2	1.86	0.58
1:B:141:GLU:HA	1:B:141:GLU:OE2	2.04	0.58
1:D:67:HIS:CD2	1:D:73:LYS:HE2	2.38	0.58
1:I:117:ASN:O	1:I:118:ASP:HB2	2.03	0.58
2:E:222:MET:O	2:E:226:ILE:HG12	2.04	0.57
2:F:76:ALA:HB1	2:F:250:HIS:O	2.03	0.57
2:F:123:ALA:CA	2:F:127:ALA:HB3	2.33	0.57
2:H:52:ASN:HB2	2:H:325:ARG:O	2.04	0.57
2:H:351:ILE:H	2:H:351:ILE:CD1	2.07	0.57
1:L:64:LEU:O	1:L:69:GLY:N	2.36	0.57
1:A:67:HIS:CD2	1:A:73:LYS:HD2	2.38	0.57
2:F:311:GLN:HE21	2:F:311:GLN:CA	2.17	0.57
2:F:413:LEU:O	2:F:416:GLN:HG3	2.03	0.57
1:D:170:GLU:HG2	1:D:171:LEU:H	1.69	0.57
2:G:31:LEU:HD12	2:G:70:LEU:CD2	2.34	0.57
2:G:92:VAL:HG21	2:H:92:VAL:CA	2.34	0.57
2:E:172:GLU:HG3	2:E:214:ARG:O	2.05	0.57
2:E:389:ASN:ND2	2:E:389:ASN:C	2.56	0.57
2:G:131:ILE:O	2:G:134:VAL:HG12	2.04	0.57
1:A:10:GLY:HA3	1:A:174:LYS:CA	2.33	0.57
1:A:12:VAL:HG12	1:A:171:LEU:HB3	1.86	0.57
1:B:159:CYS:HB3	1:B:162:THR:HB	1.87	0.57
2:F:218:ILE:C	2:F:220:ASP:N	2.57	0.57
1:J:38:TYR:CD2	1:J:41:LYS:HD2	2.39	0.57
1:J:60:PHE:CD1	1:J:78:LEU:HD22	2.39	0.57
2:G:170:ASP:CB	2:G:217:LYS:HD3	2.34	0.57
1:A:37:LEU:HD21	1:A:57:PHE:HB3	1.86	0.57
2:E:131:ILE:CD1	2:E:218:ILE:HG12	2.31	0.57
2:F:140:LYS:O	2:F:141:ASN:HB3	2.05	0.57
2:F:151:GLU:CB	2:F:152:PRO:CD	2.82	0.57
2:G:122:ARG:NH1	2:G:126:LEU:HD21	2.20	0.57
1:B:60:PHE:HD1	1:B:78:LEU:HD22	1.69	0.57
1:C:71:LEU:HD12	1:C:104:LEU:HD21	1.86	0.57
2:F:108:VAL:C	2:F:110:MET:N	2.58	0.57
2:F:223:LYS:HA	2:F:226:ILE:CG1	2.31	0.57
2:F:258:ILE:HG22	2:F:307:SER:O	2.05	0.57
2:G:257:GLU:HG3	2:G:257:GLU:O	2.05	0.57
2:H:211:GLN:HE21	2:H:212:LYS:H	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:130:ARG:HB2	2:G:130:ARG:CZ	2.35	0.57
2:G:145:GLN:HG3	2:G:148:GLN:HG3	1.87	0.57
2:G:240:LYS:HE3	2:G:294:HIS:O	2.04	0.57
2:H:145:GLN:CA	2:H:145:GLN:HE21	2.17	0.57
2:H:432:LEU:HD12	2:H:432:LEU:N	2.18	0.57
1:A:86:ARG:HA	1:A:89:ARG:NH2	2.20	0.57
1:C:10:GLY:HA2	1:C:173:TYR:CZ	2.39	0.57
1:D:28:LYS:NZ	1:D:30:ASN:ND2	2.52	0.57
2:G:293:LYS:HG3	2:G:294:HIS:HD2	1.68	0.57
2:H:103:LEU:O	2:H:107:ALA:HB2	2.04	0.57
2:E:145:GLN:HG3	2:E:148:GLN:HG3	1.86	0.57
2:F:145:GLN:HB2	2:F:148:GLN:CG	2.35	0.57
1:C:7:ARG:HB2	1:C:12:VAL:HG23	1.87	0.57
1:D:46:PHE:CE2	1:D:53:ALA:HB2	2.39	0.57
1:I:4:VAL:HG11	1:I:129:ALA:HB1	1.86	0.57
2:G:312:ILE:HG12	2:G:313:ALA:H	1.69	0.57
2:G:441:PHE:HA	2:H:315:PRO:HG2	1.87	0.57
2:H:168:LEU:HD12	2:H:217:LYS:HD2	1.87	0.57
1:A:65:GLU:OE1	2:E:141:ASN:HB2	2.05	0.56
2:H:171:LYS:HZ2	2:H:218:ILE:HD11	1.67	0.56
2:F:52:ASN:HB2	2:F:325:ARG:O	2.05	0.56
1:C:105:ILE:HD11	1:C:120:ILE:HG23	1.87	0.56
1:B:8:ARG:NH1	1:B:142:LEU:O	2.39	0.56
2:E:170:ASP:HB3	2:E:217:LYS:HD3	1.87	0.56
2:F:89:VAL:HA	2:F:92:VAL:O	2.05	0.56
1:I:88:LEU:CD1	1:I:88:LEU:H	2.18	0.56
2:G:27:VAL:HG13	2:G:70:LEU:HG	1.88	0.56
2:G:174:GLU:CB	2:G:211:GLN:HG3	2.21	0.56
2:G:269:GLY:N	2:G:270:PRO:HD2	2.21	0.56
1:L:28:LYS:HD3	1:L:31:VAL:HG22	1.88	0.56
1:A:88:LEU:HD12	1:A:88:LEU:N	2.21	0.56
1:B:152:LEU:HD13	1:B:166:HIS:CE1	2.40	0.56
2:G:122:ARG:NE	2:G:126:LEU:HD21	2.21	0.56
2:F:168:LEU:O	2:F:217:LYS:HD2	2.04	0.56
1:D:68:GLN:O	1:D:70:HIS:N	2.38	0.56
2:G:4:MET:HE1	2:G:73:LEU:HD11	1.88	0.56
2:G:147:GLU:HA	2:G:150:GLN:CG	2.34	0.56
2:E:148:GLN:HA	2:E:151:GLU:HG2	1.87	0.56
2:F:211:GLN:HE21	2:F:212:LYS:N	2.03	0.56
1:J:63:LYS:HA	1:J:66:MET:HE3	1.86	0.56
2:G:86:PHE:O	2:G:89:VAL:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:88:GLU:CD	2:H:90:GLY:HA3	2.26	0.56
2:G:89:VAL:HG12	2:G:93:GLY:CA	2.35	0.56
2:G:211:GLN:HG2	2:G:212:LYS:N	2.18	0.56
2:H:228:GLU:O	2:H:232:LYS:HE2	2.05	0.56
2:H:351:ILE:HD13	2:H:351:ILE:N	2.10	0.56
2:E:257:GLU:HG3	2:E:257:GLU:O	2.06	0.56
1:I:150:LYS:O	1:I:154:ILE:HG12	2.04	0.56
1:J:59:LEU:HG	1:J:78:LEU:HD13	1.88	0.56
1:K:86:ARG:HA	1:K:89:ARG:HH12	1.69	0.56
2:E:86:PHE:O	2:E:89:VAL:HG22	2.05	0.56
2:E:131:ILE:HD11	2:E:218:ILE:CD1	2.35	0.56
1:C:136:LEU:HB3	1:C:147:ILE:CD1	2.35	0.56
1:J:120:ILE:HD12	1:J:120:ILE:N	2.21	0.56
1:J:98:ALA:HB2	1:J:103:SER:HB3	1.87	0.56
2:G:312:ILE:HD13	2:G:312:ILE:N	2.18	0.56
2:H:108:VAL:C	2:H:110:MET:N	2.58	0.56
2:H:244:ILE:HD11	2:H:294:HIS:O	2.06	0.56
2:E:109:LYS:HG3	2:E:109:LYS:O	2.05	0.55
2:E:311:GLN:NE2	2:E:311:GLN:HA	2.21	0.55
2:H:389:ASN:HD22	2:H:390:ILE:N	2.03	0.55
2:F:32:ARG:O	2:F:36:ARG:HG3	2.06	0.55
2:G:60:GLY:N	2:G:393:ARG:NH2	2.54	0.55
2:E:108:VAL:C	2:E:110:MET:H	2.09	0.55
2:E:108:VAL:HG21	2:E:294:HIS:ND1	2.22	0.55
2:F:130:ARG:HG2	2:F:225:LEU:HD11	1.88	0.55
2:G:37:ARG:HB3	2:G:37:ARG:HH11	1.72	0.55
2:G:89:VAL:HA	2:G:93:GLY:N	2.22	0.55
2:G:92:VAL:HG21	2:H:92:VAL:N	2.20	0.55
2:H:312:ILE:HG12	2:H:313:ALA:N	2.21	0.55
2:F:151:GLU:HB2	2:F:152:PRO:HD2	1.88	0.55
1:I:33:LYS:HA	1:I:46:PHE:CE1	2.41	0.55
2:G:52:ASN:HB2	2:G:325:ARG:O	2.06	0.55
1:L:109:ASN:O	1:L:110:GLY:C	2.45	0.55
2:E:130:ARG:CG	2:E:225:LEU:HD11	2.36	0.55
2:E:160:ARG:HH12	2:E:164:ARG:HH22	1.52	0.55
1:A:149:GLU:OE1	1:A:168:ILE:HD11	2.06	0.55
1:B:150:LYS:O	1:B:154:ILE:HG12	2.07	0.55
2:E:211:GLN:O	2:E:212:LYS:HB2	2.06	0.55
2:E:242:ASP:HA	2:E:245:ASP:OD1	2.06	0.55
2:H:64:THR:HG21	2:H:68:ARG:NH1	2.21	0.55
2:E:212:LYS:CD	2:E:216:LEU:HD21	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:171:LYS:HZ2	2:F:218:ILE:HD11	1.72	0.55
1:I:105:ILE:HD11	1:I:120:ILE:HG23	1.89	0.55
1:L:8:ARG:HG2	1:L:9:ASN:ND2	2.22	0.55
1:A:87:MET:HE3	1:B:84:THR:O	2.06	0.55
2:E:441:PHE:CZ	2:F:314:LYS:HG2	2.42	0.55
1:L:83:ARG:HB3	1:L:83:ARG:CZ	2.36	0.55
1:A:33:LYS:HA	1:A:46:PHE:CE1	2.42	0.55
2:E:151:GLU:CB	2:E:152:PRO:CD	2.84	0.55
2:F:219:LYS:C	2:F:223:LYS:HD3	2.27	0.55
1:K:51:ALA:HB3	1:L:110:GLY:O	2.07	0.55
1:B:72:VAL:O	1:B:75:ALA:HB3	2.07	0.54
2:H:151:GLU:HB2	2:H:152:PRO:CD	2.37	0.54
1:K:86:ARG:HG3	1:K:89:ARG:HH22	1.71	0.54
2:F:174:GLU:C	2:F:211:GLN:HB2	2.28	0.54
1:J:59:LEU:HD12	1:J:59:LEU:O	2.06	0.54
2:H:41:ASN:HD22	2:H:41:ASN:C	2.10	0.54
2:H:211:GLN:HE21	2:H:212:LYS:N	2.05	0.54
2:E:134:VAL:HG13	2:E:171:LYS:HD3	1.88	0.54
2:E:152:PRO:CB	2:E:156:ARG:HB2	2.29	0.54
2:E:165:GLU:HG2	2:E:166:GLY:N	2.23	0.54
2:F:390:ILE:O	2:F:393:ARG:HB2	2.07	0.54
1:D:86:ARG:HA	1:D:89:ARG:NH2	2.22	0.54
2:G:131:ILE:CD1	2:G:218:ILE:HG12	2.37	0.54
2:E:103:LEU:HD13	2:E:247:VAL:HG13	1.90	0.54
2:F:389:ASN:HD22	2:F:390:ILE:N	2.05	0.54
2:G:442:ILE:O	2:G:442:ILE:HG22	2.07	0.54
2:H:217:LYS:HB2	2:H:217:LYS:HZ3	1.72	0.54
2:H:362:GLU:HG3	2:H:411:SER:HA	1.88	0.54
1:L:37:LEU:HB2	1:L:61:GLU:OE1	2.07	0.54
1:D:143:SER:OG	1:D:146:GLU:HG3	2.06	0.54
1:J:71:LEU:HD11	1:J:104:LEU:HD21	1.90	0.54
2:H:174:GLU:CA	2:H:212:LYS:HB3	2.38	0.54
2:E:147:GLU:HA	2:E:150:GLN:CG	2.36	0.54
2:E:212:LYS:HB2	2:E:212:LYS:NZ	2.21	0.54
2:G:147:GLU:CA	2:G:150:GLN:HG3	2.37	0.54
2:G:264:ARG:CZ	2:G:265:GLY:H	2.20	0.54
2:H:122:ARG:NH1	2:H:126:LEU:HD23	2.12	0.54
2:G:132:LEU:HB3	2:G:156:ARG:NH1	2.23	0.54
2:G:145:GLN:O	2:G:147:GLU:N	2.41	0.54
2:H:89:VAL:HG11	2:H:94:LYS:O	2.07	0.54
2:H:135:LEU:CD2	2:H:171:LYS:HE2	2.29	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5:SER:HB3	1:K:120:ILE:HB	1.89	0.54
2:F:135:LEU:HD23	2:F:171:LYS:HE2	1.89	0.54
1:C:43:ILE:O	1:C:43:ILE:HG13	2.08	0.54
1:C:149:GLU:CD	1:C:168:ILE:HD11	2.27	0.54
1:J:13:VAL:HG12	1:J:170:GLU:HG3	1.90	0.54
2:G:127:ALA:HA	2:G:130:ARG:HH22	1.73	0.54
2:G:168:LEU:HD12	2:G:219:LYS:HB3	1.89	0.54
2:H:12:GLU:HG2	2:H:73:LEU:CD1	2.38	0.54
2:H:167:GLN:NE2	2:H:219:LYS:NZ	2.56	0.54
2:H:413:LEU:O	2:H:416:GLN:HG3	2.08	0.54
1:B:3:ILE:HB	1:B:122:ILE:HG12	1.90	0.54
2:F:345:THR:HG22	2:F:352:THR:HG21	1.89	0.54
2:F:432:LEU:N	2:F:432:LEU:HD12	2.22	0.54
1:C:91:LEU:HD12	1:C:91:LEU:O	2.07	0.54
1:D:70:HIS:CE1	1:D:72:VAL:HB	2.43	0.54
2:H:96:VAL:HG21	2:H:280:ASP:HB3	1.90	0.54
2:H:210:LYS:N	2:H:210:LYS:HD3	2.23	0.54
1:K:64:LEU:HD23	1:K:74:ALA:HB3	1.89	0.54
1:A:28:LYS:HZ3	1:A:30:ASN:ND2	2.05	0.53
2:E:335:LEU:HD22	2:E:339:ASP:HB3	1.90	0.53
2:F:167:GLN:O	2:F:168:LEU:HB3	2.07	0.53
1:D:30:ASN:N	1:D:30:ASN:ND2	2.55	0.53
2:G:134:VAL:CG1	2:G:171:LYS:HD3	2.38	0.53
2:G:359:MET:HE1	2:H:36:ARG:NH1	2.21	0.53
2:H:340:PHE:O	2:H:344:LEU:HD22	2.07	0.53
1:L:30:ASN:ND2	1:L:30:ASN:N	2.50	0.53
1:L:73:LYS:HZ2	1:L:77:GLU:HG2	1.73	0.53
1:B:10:GLY:HA2	1:B:173:TYR:CZ	2.43	0.53
2:E:134:VAL:CG1	2:E:171:LYS:HD3	2.39	0.53
2:F:239:LEU:HD23	2:F:240:LYS:N	2.23	0.53
1:D:43:ILE:HD12	1:D:171:LEU:HD22	1.91	0.53
1:D:73:LYS:HZ2	1:D:77:GLU:HG2	1.71	0.53
1:D:99:ASP:OD1	1:D:101:THR:N	2.40	0.53
1:I:10:GLY:HA3	1:I:174:LYS:CA	2.34	0.53
1:I:109:ASN:O	1:I:110:GLY:C	2.46	0.53
1:J:3:ILE:HB	1:J:122:ILE:HG12	1.91	0.53
1:J:70:HIS:HE1	1:J:72:VAL:HB	1.73	0.53
1:B:86:ARG:HA	1:B:89:ARG:HE	1.72	0.53
2:E:217:LYS:HG3	2:E:219:LYS:NZ	2.23	0.53
2:E:441:PHE:CE2	2:F:314:LYS:HG2	2.44	0.53
2:G:268:SER:HA	2:G:271:ASP:OD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:ASN:ND2	2:H:36:ARG:HD2	2.24	0.53
2:H:119:ASN:ND2	2:H:233:LEU:HD23	2.24	0.53
2:H:420:ILE:N	2:H:420:ILE:HD12	2.24	0.53
1:L:68:GLN:O	1:L:70:HIS:N	2.41	0.53
2:E:34:ARG:CZ	2:E:250:HIS:HA	2.38	0.53
2:F:173:ILE:HD13	2:F:173:ILE:N	2.23	0.53
1:C:64:LEU:HB3	1:C:69:GLY:HA2	1.90	0.53
1:I:125:GLY:HA2	1:I:128:TYR:CD2	2.43	0.53
1:K:115:PRO:HB2	1:K:119:LEU:O	2.08	0.53
1:A:13:VAL:CG1	1:A:170:GLU:HG3	2.29	0.53
2:E:58:PRO:HG2	2:E:61:VAL:HG11	1.91	0.53
2:F:269:GLY:N	2:F:270:PRO:HD2	2.22	0.53
2:F:315:PRO:O	2:F:318:LEU:HB2	2.08	0.53
2:H:223:LYS:N	2:H:223:LYS:HD2	2.23	0.53
1:K:148:ALA:O	1:K:152:LEU:HB2	2.09	0.53
1:I:80:LYS:O	1:I:84:THR:HG22	2.09	0.53
1:I:87:MET:HE3	1:J:84:THR:O	2.09	0.53
1:J:71:LEU:CD1	1:J:104:LEU:HD21	2.37	0.53
2:G:349:ALA:CB	2:H:44:LEU:HD23	2.39	0.53
2:H:91:TYR:O	2:H:92:VAL:HG22	2.08	0.53
2:H:145:GLN:C	2:H:147:GLU:H	2.12	0.53
2:H:255:ILE:HD11	2:H:304:PHE:HD2	1.74	0.53
1:K:17:ASP:HA	1:K:165:PHE:O	2.09	0.53
1:K:91:LEU:HD12	1:K:91:LEU:O	2.09	0.53
1:A:10:GLY:HA2	1:A:173:TYR:CD1	2.42	0.53
1:B:104:LEU:HD23	1:B:104:LEU:N	2.23	0.53
2:F:103:LEU:CD1	2:F:247:VAL:HG13	2.38	0.53
2:G:432:LEU:HD12	2:G:432:LEU:N	2.23	0.53
1:K:83:ARG:HG3	1:K:109:ASN:O	2.09	0.53
1:L:6:VAL:HG21	1:L:147:ILE:CG2	2.38	0.53
1:L:10:GLY:HA2	1:L:173:TYR:CE1	2.43	0.53
2:E:81:VAL:HG11	2:E:99:ILE:HG12	1.90	0.53
2:E:361:THR:HG21	2:F:36:ARG:HA	1.90	0.53
2:E:432:LEU:HD12	2:E:432:LEU:N	2.22	0.53
2:F:41:ASN:HD21	2:F:44:LEU:H	1.57	0.53
1:J:95:LEU:H	1:J:95:LEU:HD12	1.74	0.53
2:G:94:LYS:HA	2:G:94:LYS:CE	2.30	0.53
2:H:5:THR:O	2:H:9:ILE:HG12	2.09	0.53
2:H:358:LEU:O	2:H:361:THR:HB	2.08	0.53
1:L:58:GLU:O	1:L:61:GLU:HB2	2.09	0.53
1:C:152:LEU:HD13	1:C:166:HIS:ND1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:LEU:HD13	1:D:95:LEU:HD11	1.91	0.53
1:D:83:ARG:HD3	1:D:109:ASN:O	2.09	0.53
1:D:115:PRO:HG3	1:D:120:ILE:CG1	2.39	0.53
2:G:104:THR:HG21	2:G:292:THR:HG21	1.91	0.53
1:K:30:ASN:HD22	1:K:30:ASN:H	1.57	0.53
1:B:136:LEU:HB3	1:B:147:ILE:CD1	2.39	0.53
2:F:54:LEU:HD12	2:F:306:ALA:HB3	1.90	0.53
2:F:103:LEU:O	2:F:107:ALA:HB2	2.09	0.53
2:F:375:ARG:HB3	2:F:425:VAL:HG11	1.91	0.53
1:D:115:PRO:HB2	1:D:119:LEU:O	2.09	0.53
1:J:53:ALA:C	1:J:55:THR:H	2.11	0.53
1:L:36:ARG:HB3	1:L:36:ARG:HH11	1.74	0.53
2:F:89:VAL:HA	2:F:92:VAL:C	2.30	0.52
1:I:88:LEU:H	1:I:88:LEU:HD12	1.74	0.52
2:G:132:LEU:HD11	2:G:160:ARG:CG	2.39	0.52
2:H:21:ASP:O	2:H:24:LYS:HB2	2.08	0.52
2:H:122:ARG:HA	2:H:122:ARG:NE	2.25	0.52
1:L:54:PHE:O	1:L:58:GLU:HB2	2.09	0.52
2:E:372:GLY:O	2:E:376:ILE:HG13	2.09	0.52
2:F:5:THR:O	2:F:9:ILE:HG12	2.08	0.52
2:F:147:GLU:HG3	2:F:150:GLN:NE2	2.24	0.52
1:I:67:HIS:HD2	1:I:73:LYS:HD2	1.71	0.52
1:J:10:GLY:HA2	1:J:173:TYR:CZ	2.43	0.52
2:G:150:GLN:O	2:G:153:SER:HB2	2.09	0.52
2:G:168:LEU:HA	2:G:219:LYS:CB	2.39	0.52
2:H:160:ARG:HG2	2:H:160:ARG:HH11	1.74	0.52
2:F:73:LEU:HG	2:F:73:LEU:O	2.10	0.52
1:I:28:LYS:NZ	1:I:30:ASN:ND2	2.58	0.52
2:G:92:VAL:HG21	2:H:91:TYR:O	2.09	0.52
2:G:127:ALA:HA	2:G:130:ARG:NH2	2.24	0.52
1:L:28:LYS:NZ	1:L:30:ASN:ND2	2.57	0.52
2:F:12:GLU:HG2	2:F:73:LEU:HD13	1.92	0.52
1:D:36:ARG:C	1:D:37:LEU:HD23	2.30	0.52
1:I:90:LYS:NZ	1:J:89:ARG:NH2	2.58	0.52
2:F:256:ASP:O	2:F:257:GLU:HG2	2.10	0.52
1:D:64:LEU:HD23	1:D:74:ALA:CB	2.40	0.52
1:I:5:SER:HB2	1:I:14:ILE:HG12	1.92	0.52
2:G:89:VAL:HG12	2:G:93:GLY:C	2.29	0.52
2:G:147:GLU:CG	2:G:150:GLN:NE2	2.73	0.52
1:A:152:LEU:HD13	1:A:166:HIS:CE1	2.45	0.52
2:H:152:PRO:HB2	2:H:156:ARG:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:3:ILE:HD11	1:K:46:PHE:O	2.10	0.52
1:K:28:LYS:HD3	1:K:31:VAL:HG22	1.92	0.52
1:B:38:TYR:HB2	1:B:64:LEU:HD12	1.92	0.52
2:E:269:GLY:N	2:E:270:PRO:HD2	2.25	0.52
2:F:119:ASN:ND2	2:F:233:LEU:HD23	2.24	0.52
2:H:396:HIS:O	2:H:400:GLU:HB2	2.10	0.52
1:K:83:ARG:HB3	1:K:83:ARG:CZ	2.40	0.52
2:E:311:GLN:CA	2:E:311:GLN:NE2	2.73	0.52
2:E:401:ARG:HG2	2:E:443:LEU:HD21	1.91	0.52
2:F:153:SER:HA	2:F:157:GLN:H	1.74	0.52
2:H:173:ILE:N	2:H:173:ILE:HD13	2.25	0.52
2:H:269:GLY:N	2:H:270:PRO:HD2	2.23	0.52
2:H:366:ILE:HD11	2:H:420:ILE:HD11	1.92	0.52
1:K:19:GLN:HB2	1:K:163:ASN:ND2	2.24	0.52
1:K:91:LEU:HB3	1:L:83:ARG:HE	1.74	0.52
2:F:108:VAL:HA	2:F:111:VAL:HG22	1.91	0.52
1:C:8:ARG:HG2	1:C:9:ASN:ND2	2.25	0.52
2:G:34:ARG:CZ	2:G:250:HIS:HA	2.39	0.52
1:A:37:LEU:CD2	1:A:57:PHE:HB3	2.40	0.51
2:E:214:ARG:HG2	2:E:215:LYS:H	1.76	0.51
2:F:262:CYS:SG	2:F:318:LEU:HD13	2.50	0.51
2:G:212:LYS:HB2	2:G:212:LYS:NZ	2.25	0.51
2:F:312:ILE:HG12	2:F:313:ALA:H	1.75	0.51
1:I:115:PRO:HG3	1:I:120:ILE:HG12	1.92	0.51
1:K:71:LEU:C	1:K:71:LEU:HD13	2.31	0.51
2:E:94:LYS:HA	2:E:94:LYS:CE	2.32	0.51
1:D:94:LEU:HD13	1:D:122:ILE:HB	1.93	0.51
1:J:72:VAL:O	1:J:75:ALA:HB3	2.10	0.51
1:L:73:LYS:NZ	1:L:77:GLU:HG2	2.24	0.51
2:E:153:SER:O	2:E:157:GLN:NE2	2.43	0.51
1:D:43:ILE:HD13	1:D:98:ALA:O	2.10	0.51
1:D:100:GLU:OE2	1:D:173:TYR:HB2	2.11	0.51
1:D:170:GLU:HG2	1:D:171:LEU:N	2.25	0.51
2:G:401:ARG:NH2	2:H:329:ARG:O	2.42	0.51
2:H:35:TRP:O	2:H:39:GLN:HG2	2.10	0.51
2:H:255:ILE:N	2:H:255:ILE:HD12	2.26	0.51
1:L:62:ARG:HA	1:L:65:GLU:CG	2.41	0.51
2:E:217:LYS:HB3	2:E:219:LYS:HZ3	1.75	0.51
1:D:18:GLY:C	1:D:163:ASN:HD21	2.12	0.51
2:G:86:PHE:HA	2:G:89:VAL:HG13	1.93	0.51
2:G:117:GLU:OE2	2:G:120:ARG:NH2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:389:ASN:ND2	2:G:389:ASN:C	2.64	0.51
2:H:95:GLU:H	2:H:95:GLU:CD	2.14	0.51
2:H:311:GLN:NE2	2:H:311:GLN:CA	2.74	0.51
1:A:28:LYS:HD2	1:B:113:VAL:CG1	2.40	0.51
2:E:76:ALA:HB1	2:E:250:HIS:O	2.11	0.51
2:E:362:GLU:HG2	2:E:410:ALA:CB	2.40	0.51
2:F:54:LEU:CD1	2:F:306:ALA:HB3	2.41	0.51
2:F:174:GLU:HB3	2:F:211:GLN:HB2	1.90	0.51
1:I:87:MET:CE	1:J:84:THR:HG23	2.40	0.51
1:J:95:LEU:HD12	1:J:95:LEU:N	2.25	0.51
2:G:349:ALA:HB1	2:H:44:LEU:HD23	1.91	0.51
2:G:358:LEU:HD22	2:H:36:ARG:HB2	1.93	0.51
2:F:174:GLU:CA	2:F:212:LYS:HB3	2.40	0.51
2:G:122:ARG:O	2:G:126:LEU:HD23	2.11	0.51
2:G:124:GLU:HA	2:G:127:ALA:CB	2.41	0.51
2:G:412:ASP:CG	2:H:7:ARG:HE	2.14	0.51
2:H:150:GLN:O	2:H:153:SER:CB	2.48	0.51
2:H:339:ASP:O	2:H:343:ILE:HG13	2.10	0.51
1:B:59:LEU:HD12	1:B:59:LEU:O	2.11	0.51
2:E:130:ARG:HB2	2:E:130:ARG:HH21	1.71	0.51
1:I:36:ARG:O	1:I:37:LEU:HD23	2.11	0.51
1:J:18:GLY:HA2	1:J:33:LYS:HE3	1.91	0.51
2:G:358:LEU:HD23	2:H:36:ARG:HB3	1.92	0.51
1:K:85:ASP:O	1:K:89:ARG:HB2	2.11	0.51
2:F:280:ASP:O	2:F:283:PRO:HD2	2.09	0.51
2:F:292:THR:C	2:F:294:HIS:H	2.14	0.51
2:G:91:TYR:C	2:G:92:VAL:HG22	2.31	0.51
2:G:112:ARG:HG3	2:G:112:ARG:NH1	2.26	0.51
2:H:31:LEU:HD11	2:H:74:ALA:HB2	1.93	0.51
2:H:217:LYS:O	2:H:220:ASP:HB2	2.11	0.51
1:L:36:ARG:HH12	1:L:40:ASP:C	2.14	0.51
1:A:86:ARG:HA	1:A:89:ARG:CZ	2.41	0.51
2:E:23:ALA:HA	2:E:330:VAL:HG21	1.92	0.51
2:E:171:LYS:HB2	2:E:218:ILE:HG13	1.93	0.51
2:E:401:ARG:HD2	2:E:432:LEU:CD2	2.41	0.51
2:F:20:GLN:O	2:F:24:LYS:HG3	2.10	0.51
1:C:36:ARG:HD3	1:C:40:ASP:OD1	2.10	0.51
1:I:81:ASP:HA	1:I:84:THR:CG2	2.41	0.51
1:J:170:GLU:HG2	1:J:171:LEU:H	1.76	0.51
1:A:36:ARG:HB3	1:A:36:ARG:HH11	1.76	0.50
1:B:60:PHE:CE2	1:B:97:VAL:HG21	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:312:ILE:HD13	2:F:312:ILE:N	2.21	0.50
2:G:355:TYR:CE2	2:G:400:GLU:OE2	2.64	0.50
1:A:39:ASN:OD1	2:E:143:TRP:CH2	2.65	0.50
1:A:65:GLU:CG	2:E:141:ASN:HB3	2.41	0.50
2:E:128:GLU:O	2:E:131:ILE:HG22	2.11	0.50
2:E:408:TYR:HA	2:F:29:ILE:CD1	2.40	0.50
1:D:28:LYS:HG2	1:D:30:ASN:ND2	2.26	0.50
2:G:357:ALA:HB1	2:H:40:LEU:HD22	1.93	0.50
2:H:217:LYS:HB2	2:H:217:LYS:HZ2	1.76	0.50
2:H:345:THR:HG21	2:H:373:ILE:CD1	2.41	0.50
1:K:83:ARG:HH11	1:K:83:ARG:CG	2.21	0.50
2:E:89:VAL:HG12	2:E:93:GLY:CA	2.41	0.50
2:E:122:ARG:NE	2:E:126:LEU:HD21	2.27	0.50
2:E:230:ALA:O	2:E:233:LEU:HB3	2.10	0.50
2:F:34:ARG:CZ	2:F:250:HIS:HA	2.41	0.50
2:F:351:ILE:H	2:F:351:ILE:CD1	2.14	0.50
1:D:13:VAL:C	1:D:14:ILE:HD12	2.32	0.50
2:G:442:ILE:O	2:G:442:ILE:CG2	2.59	0.50
1:B:92:GLU:O	1:B:93:ALA:HB2	2.11	0.50
2:G:151:GLU:CB	2:G:152:PRO:CD	2.89	0.50
2:H:211:GLN:O	2:H:212:LYS:HB2	2.11	0.50
2:H:216:LEU:CD2	2:H:221:ALA:HB2	2.41	0.50
2:F:346:GLU:HB2	2:F:347:PRO:HD3	1.94	0.50
2:G:92:VAL:CG2	2:H:92:VAL:N	2.74	0.50
2:G:355:TYR:HH	2:G:400:GLU:CD	2.15	0.50
2:H:145:GLN:HE21	2:H:145:GLN:HA	1.77	0.50
2:F:148:GLN:HA	2:F:151:GLU:CG	2.42	0.50
1:C:77:GLU:O	1:C:80:LYS:HB3	2.11	0.50
1:C:105:ILE:CD1	1:C:120:ILE:HG23	2.42	0.50
1:D:28:LYS:HZ3	1:D:30:ASN:HD21	1.59	0.50
2:H:76:ALA:HB1	2:H:250:HIS:O	2.11	0.50
1:K:58:GLU:HG3	1:K:62:ARG:NH2	2.27	0.50
1:A:5:SER:HB3	1:A:120:ILE:HB	1.92	0.50
1:A:84:THR:HG23	1:A:85:ASP:N	2.26	0.50
2:F:135:LEU:HD22	2:F:159:PHE:CD2	2.47	0.50
1:C:143:SER:O	1:C:147:ILE:HG12	2.11	0.50
1:J:1:THR:HB	1:J:33:LYS:HZ2	1.76	0.50
2:H:23:ALA:HA	2:H:330:VAL:HG21	1.93	0.50
2:H:101:ARG:O	2:H:104:THR:HB	2.11	0.50
2:H:235:ASN:HB2	2:H:236:PRO:CD	2.42	0.50
1:L:86:ARG:HA	1:L:89:ARG:HH12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:117:ASN:O	1:L:118:ASP:HB2	2.10	0.50
1:A:28:LYS:HE3	1:B:113:VAL:HG13	1.93	0.50
1:B:38:TYR:HB2	1:B:64:LEU:CD1	2.40	0.50
2:F:95:GLU:CD	2:F:95:GLU:H	2.15	0.50
2:H:41:ASN:ND2	2:H:44:LEU:HB2	2.27	0.50
2:H:167:GLN:CD	2:H:219:LYS:HZ1	2.14	0.50
2:E:91:TYR:C	2:E:92:VAL:HG22	2.32	0.50
2:F:221:ALA:O	2:F:225:LEU:HD23	2.12	0.50
1:C:8:ARG:NH1	1:C:142:LEU:O	2.45	0.50
1:C:10:GLY:HA3	1:C:174:LYS:HA	1.93	0.50
1:D:91:LEU:HD12	1:D:91:LEU:O	2.12	0.50
1:D:145:ARG:NH1	1:D:168:ILE:HD12	2.27	0.50
2:G:109:LYS:HD3	2:H:296:MET:O	2.12	0.50
2:G:147:GLU:HG3	2:G:150:GLN:CD	2.32	0.50
1:A:103:SER:OG	1:A:118:ASP:HB3	2.12	0.49
2:F:235:ASN:OD1	2:F:238:GLU:HB2	2.12	0.49
1:D:73:LYS:HZ1	1:D:77:GLU:HG2	1.76	0.49
2:H:94:LYS:NZ	2:H:101:ARG:HH12	2.10	0.49
1:L:85:ASP:HB3	1:L:88:LEU:HB2	1.93	0.49
2:E:108:VAL:C	2:E:110:MET:N	2.63	0.49
2:E:152:PRO:HB3	2:E:155:ALA:HB3	1.94	0.49
1:I:88:LEU:HD12	1:I:88:LEU:N	2.26	0.49
1:J:6:VAL:HG12	1:J:7:ARG:H	1.75	0.49
1:J:10:GLY:HA2	1:J:173:TYR:CE1	2.46	0.49
2:G:77:PRO:HB2	2:G:103:LEU:HD21	1.94	0.49
2:H:131:ILE:HG21	2:H:222:MET:HE1	1.93	0.49
2:H:151:GLU:CB	2:H:152:PRO:CD	2.91	0.49
1:K:105:ILE:HD12	1:K:122:ILE:HG21	1.94	0.49
1:B:53:ALA:O	1:B:55:THR:N	2.45	0.49
2:E:167:GLN:OE1	2:E:168:LEU:N	2.46	0.49
2:E:318:LEU:O	2:E:323:GLN:NE2	2.44	0.49
2:F:108:VAL:O	2:F:110:MET:N	2.45	0.49
1:I:4:VAL:CG1	1:I:129:ALA:HB1	2.42	0.49
1:I:30:ASN:ND2	1:I:30:ASN:H	2.11	0.49
1:I:84:THR:HG23	1:I:85:ASP:H	1.76	0.49
2:G:382:GLN:O	2:G:386:SER:HB3	2.12	0.49
2:H:270:PRO:O	2:H:274:ARG:HD2	2.11	0.49
1:L:37:LEU:HD13	1:L:57:PHE:HB3	1.93	0.49
1:A:18:GLY:HA2	1:A:33:LYS:HE3	1.94	0.49
2:E:95:GLU:OE1	2:E:101:ARG:NH1	2.43	0.49
2:E:382:GLN:HA	2:E:382:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:25:ARG:O	2:F:29:ILE:HG12	2.13	0.49
1:C:12:VAL:HG12	1:C:171:LEU:HB3	1.95	0.49
1:C:28:LYS:HG2	1:C:30:ASN:ND2	2.27	0.49
1:J:28:LYS:HZ1	1:J:30:ASN:ND2	2.10	0.49
2:G:108:VAL:C	2:G:110:MET:H	2.16	0.49
2:H:352:THR:HG22	2:H:353:VAL:N	2.27	0.49
1:B:71:LEU:HB2	1:B:99:ASP:OD1	2.12	0.49
2:E:89:VAL:HG12	2:E:93:GLY:C	2.32	0.49
2:F:74:ALA:O	2:F:75:ASN:C	2.51	0.49
2:F:384:ASN:HD21	2:F:390:ILE:HG12	1.77	0.49
1:J:136:LEU:HB3	1:J:147:ILE:CD1	2.42	0.49
2:G:103:LEU:HD13	2:G:247:VAL:HG13	1.93	0.49
2:G:362:GLU:HG3	2:G:411:SER:HA	1.95	0.49
2:H:135:LEU:HD13	2:H:159:PHE:HB3	1.94	0.49
2:H:345:THR:CG2	2:H:373:ILE:CD1	2.88	0.49
2:H:393:ARG:HG2	2:H:393:ARG:NH1	2.27	0.49
1:B:65:GLU:OE1	2:F:143:TRP:CE2	2.65	0.49
2:E:163:LEU:O	2:E:163:LEU:HG	2.12	0.49
2:E:151:GLU:HB2	2:E:152:PRO:HD2	1.95	0.49
2:F:140:LYS:HD3	2:F:140:LYS:H	1.78	0.49
2:F:345:THR:CG2	2:F:373:ILE:HD13	2.43	0.49
1:D:36:ARG:O	1:D:37:LEU:HB3	2.13	0.49
2:H:147:GLU:CG	2:H:150:GLN:NE2	2.75	0.49
2:H:432:LEU:HD12	2:H:432:LEU:H	1.77	0.49
2:H:435:ASP:CG	2:H:438:LEU:HB2	2.32	0.49
1:L:86:ARG:HA	1:L:89:ARG:NH1	2.28	0.49
1:A:65:GLU:HG3	2:E:141:ASN:HB3	1.94	0.49
1:A:103:SER:O	1:A:104:LEU:HB3	2.13	0.49
2:E:282:LEU:HD11	2:E:321:GLU:HB3	1.94	0.49
1:D:12:VAL:O	1:D:12:VAL:HG13	2.13	0.49
1:I:90:LYS:HZ1	1:J:89:ARG:NH2	2.11	0.49
2:G:31:LEU:HD12	2:G:70:LEU:HD22	1.95	0.49
2:G:131:ILE:HD11	2:G:218:ILE:CD1	2.43	0.49
2:G:136:ILE:O	2:G:136:ILE:CG2	2.60	0.49
2:G:145:GLN:C	2:G:147:GLU:N	2.66	0.49
2:G:248:GLU:HG2	2:G:297:VAL:HG13	1.95	0.49
2:H:257:GLU:HB2	2:H:260:LYS:HG3	1.95	0.49
2:H:292:THR:C	2:H:294:HIS:H	2.16	0.49
2:E:355:TYR:HE2	2:E:400:GLU:OE2	1.94	0.49
2:F:132:LEU:HD23	2:F:135:LEU:CD1	2.41	0.49
2:F:232:LYS:HZ2	2:F:232:LYS:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:ILE:HB	1:D:122:ILE:CG1	2.41	0.49
1:I:5:SER:HB3	1:I:120:ILE:HB	1.94	0.49
1:J:53:ALA:O	1:J:55:THR:N	2.46	0.49
2:H:384:ASN:HD21	2:H:390:ILE:HG12	1.77	0.49
1:B:64:LEU:HD23	1:B:74:ALA:CB	2.43	0.49
2:E:217:LYS:CB	2:E:219:LYS:HZ3	2.26	0.49
1:J:35:ARG:O	1:J:169:GLU:HG3	2.13	0.49
2:H:108:VAL:HA	2:H:111:VAL:CG2	2.41	0.49
2:H:164:ARG:O	2:H:165:GLU:HB3	2.13	0.49
1:A:104:LEU:HD12	1:A:104:LEU:O	2.13	0.48
2:E:145:GLN:C	2:E:147:GLU:H	2.16	0.48
1:I:109:ASN:HD22	1:I:109:ASN:N	2.09	0.48
2:H:64:THR:CG2	2:H:68:ARG:NH1	2.76	0.48
1:L:43:ILE:HG12	1:L:43:ILE:O	2.13	0.48
1:A:47:ALA:HB3	1:A:94:LEU:HB2	1.95	0.48
2:E:147:GLU:O	2:E:150:GLN:HG3	2.13	0.48
2:E:171:LYS:HE3	2:E:172:GLU:N	2.27	0.48
2:E:362:GLU:OE1	2:F:36:ARG:NE	2.46	0.48
1:C:5:SER:HB3	1:C:120:ILE:HB	1.95	0.48
1:C:83:ARG:HH11	1:C:83:ARG:CB	2.17	0.48
2:G:132:LEU:HD11	2:G:160:ARG:HG2	1.96	0.48
2:G:168:LEU:HG	2:G:219:LYS:CD	2.21	0.48
2:H:170:ASP:HB3	2:H:217:LYS:HD3	1.95	0.48
2:E:256:ASP:O	2:E:257:GLU:HG2	2.12	0.48
2:F:132:LEU:CD1	2:F:160:ARG:HG3	2.31	0.48
1:C:60:PHE:CZ	1:C:97:VAL:HG11	2.48	0.48
2:G:95:GLU:H	2:G:95:GLU:CD	2.15	0.48
1:L:5:SER:HB3	1:L:120:ILE:HB	1.94	0.48
2:E:311:GLN:HE21	2:E:311:GLN:HA	1.77	0.48
2:E:362:GLU:HG3	2:E:411:SER:HA	1.95	0.48
2:G:231:ALA:C	2:G:233:LEU:N	2.67	0.48
2:G:355:TYR:HE2	2:G:400:GLU:OE2	1.96	0.48
1:A:105:ILE:HD11	1:A:120:ILE:HG23	1.95	0.48
2:F:153:SER:HB3	2:F:157:GLN:HG3	1.95	0.48
1:C:64:LEU:O	1:C:69:GLY:N	2.39	0.48
1:C:71:LEU:HD11	1:C:97:VAL:HG12	1.94	0.48
1:J:12:VAL:HG12	1:J:171:LEU:HB3	1.95	0.48
2:G:211:GLN:O	2:G:212:LYS:HB2	2.13	0.48
2:G:212:LYS:C	2:G:214:ARG:H	2.15	0.48
1:A:117:ASN:O	1:A:118:ASP:HB2	2.13	0.48
1:B:70:HIS:CE1	1:B:72:VAL:HB	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:86:PHE:HB2	2:F:277:VAL:HG13	1.94	0.48
2:F:240:LYS:O	2:F:244:ILE:HD13	2.14	0.48
2:F:279:ARG:O	2:F:283:PRO:HD3	2.14	0.48
1:J:44:ALA:HB2	1:J:97:VAL:HG23	1.96	0.48
2:G:408:TYR:CB	2:H:29:ILE:HD11	2.43	0.48
2:H:34:ARG:CZ	2:H:250:HIS:HA	2.44	0.48
2:H:140:LYS:O	2:H:141:ASN:HB3	2.14	0.48
2:H:318:LEU:O	2:H:323:GLN:NE2	2.45	0.48
1:K:49:GLY:HA2	1:L:111:ASP:OD1	2.14	0.48
1:A:20:ALA:HB2	1:A:31:VAL:HG21	1.94	0.48
2:E:299:THR:HA	2:E:302:ILE:CD1	2.38	0.48
2:F:311:GLN:NE2	2:F:311:GLN:HA	2.29	0.48
2:G:361:THR:HG22	2:H:35:TRP:HZ3	1.74	0.48
2:G:361:THR:HG23	2:H:39:GLN:HG3	1.96	0.48
2:H:103:LEU:HD13	2:H:247:VAL:CG2	2.42	0.48
1:K:85:ASP:HB3	1:K:88:LEU:HB2	1.94	0.48
1:L:71:LEU:HD21	1:L:97:VAL:CG1	2.44	0.48
1:L:94:LEU:CD2	1:L:107:THR:HG22	2.44	0.48
2:E:442:ILE:O	2:E:442:ILE:CG2	2.62	0.48
2:F:366:ILE:HD11	2:F:406:ILE:HD13	1.95	0.48
1:C:30:ASN:HD22	1:C:30:ASN:N	2.04	0.48
1:C:83:ARG:O	1:C:83:ARG:HG2	2.13	0.48
1:D:17:ASP:O	1:D:33:LYS:HD2	2.14	0.48
1:D:71:LEU:HD13	1:D:71:LEU:C	2.34	0.48
1:I:95:LEU:HB2	1:I:106:ILE:HB	1.95	0.48
1:I:109:ASN:N	1:I:109:ASN:ND2	2.62	0.48
2:E:240:LYS:HE3	2:E:294:HIS:O	2.13	0.48
1:J:3:ILE:HB	1:J:122:ILE:CG1	2.43	0.48
2:G:31:LEU:HD12	2:G:70:LEU:HD21	1.96	0.48
2:H:267:SER:O	2:H:271:ASP:OD2	2.32	0.48
1:A:99:ASP:C	1:A:99:ASP:OD1	2.52	0.48
1:B:59:LEU:HG	1:B:78:LEU:CD1	2.44	0.48
1:B:174:LYS:N	1:B:174:LYS:HD2	2.29	0.48
2:E:112:ARG:HH11	2:E:112:ARG:HG3	1.78	0.48
2:E:345:THR:HG21	2:E:373:ILE:HD13	1.95	0.48
2:F:152:PRO:CB	2:F:156:ARG:HB2	2.43	0.48
2:H:89:VAL:HA	2:H:92:VAL:C	2.34	0.48
1:B:1:THR:HB	1:B:33:LYS:HZ2	1.77	0.47
1:B:5:SER:HB3	1:B:120:ILE:HB	1.95	0.47
2:E:130:ARG:HG2	2:E:225:LEU:HD11	1.95	0.47
1:D:28:LYS:HZ2	1:D:30:ASN:ND2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:60:PHE:CE2	1:I:97:VAL:HG21	2.49	0.47
2:G:221:ALA:O	2:G:225:LEU:HD23	2.14	0.47
2:G:222:MET:O	2:G:226:ILE:HG12	2.14	0.47
2:H:23:ALA:HB1	2:H:55:MET:HE2	1.96	0.47
2:H:122:ARG:HA	2:H:122:ARG:CZ	2.43	0.47
1:K:17:ASP:O	1:K:33:LYS:HD2	2.14	0.47
1:B:65:GLU:OE1	2:F:143:TRP:NE1	2.47	0.47
2:E:170:ASP:CB	2:E:217:LYS:HD3	2.45	0.47
2:F:23:ALA:HA	2:F:330:VAL:HG21	1.97	0.47
2:F:163:LEU:HD11	2:F:222:MET:HE1	1.94	0.47
1:I:77:GLU:HA	1:I:80:LYS:HD2	1.97	0.47
2:G:407:SER:OG	2:H:29:ILE:HG23	2.13	0.47
2:H:272:VAL:HA	2:H:275:GLU:HB2	1.96	0.47
1:K:136:LEU:HB3	1:K:147:ILE:CD1	2.43	0.47
1:A:115:PRO:HG3	1:A:120:ILE:HG12	1.96	0.47
1:B:38:TYR:CD2	1:B:41:LYS:HD2	2.49	0.47
1:B:105:ILE:HG22	1:B:106:ILE:N	2.29	0.47
1:B:170:GLU:CG	1:B:171:LEU:H	2.22	0.47
2:E:142:ASN:CB	2:E:149:GLN:HE22	2.27	0.47
1:D:94:LEU:HB3	1:D:122:ILE:HD12	1.96	0.47
2:G:116:ILE:O	2:G:116:ILE:HG22	2.14	0.47
2:H:103:LEU:CD1	2:H:247:VAL:HG13	2.44	0.47
1:L:105:ILE:CD1	1:L:120:ILE:HG23	2.41	0.47
2:E:401:ARG:HD2	2:E:432:LEU:HD21	1.96	0.47
2:F:134:VAL:HG21	2:F:172:GLU:O	2.15	0.47
1:D:36:ARG:NH1	1:D:43:ILE:HG22	2.29	0.47
1:D:99:ASP:HA	1:D:171:LEU:CD2	2.45	0.47
1:J:98:ALA:HB2	1:J:103:SER:CB	2.45	0.47
1:K:11:HIS:HE1	1:K:174:LYS:NZ	2.11	0.47
1:A:80:LYS:O	1:A:81:ASP:C	2.52	0.47
2:F:235:ASN:ND2	2:F:238:GLU:OE1	2.47	0.47
2:G:408:TYR:CA	2:H:29:ILE:HD11	2.45	0.47
2:H:27:VAL:CG1	2:H:70:LEU:HG	2.43	0.47
2:H:86:PHE:HB2	2:H:277:VAL:HG13	1.95	0.47
2:F:216:LEU:HG	2:F:221:ALA:HB2	1.96	0.47
2:F:219:LYS:HA	2:F:219:LYS:HE3	1.95	0.47
2:F:365:ASN:ND2	2:F:417:ASN:OD1	2.47	0.47
1:C:149:GLU:OE1	1:C:166:HIS:CD2	2.67	0.47
1:D:174:LYS:HA	1:D:174:LYS:HZ2	1.80	0.47
2:G:108:VAL:C	2:G:110:MET:N	2.67	0.47
2:H:133:ASP:O	2:H:137:PRO:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:167:GLN:NE2	2:H:219:LYS:HZ2	2.12	0.47
1:A:83:ARG:HG2	1:A:83:ARG:HH11	1.80	0.47
2:E:131:ILE:O	2:E:134:VAL:HG12	2.14	0.47
2:E:348:ASN:O	2:E:349:ALA:HB3	2.15	0.47
2:F:41:ASN:ND2	2:F:44:LEU:HB2	2.30	0.47
2:F:62:GLY:O	2:F:66:ILE:HG13	2.15	0.47
2:F:435:ASP:CG	2:F:438:LEU:HB2	2.35	0.47
1:C:1:THR:N	1:C:161:TYR:O	2.47	0.47
1:C:67:HIS:N	1:C:67:HIS:ND1	2.62	0.47
1:I:8:ARG:NH1	1:I:142:LEU:O	2.48	0.47
2:G:76:ALA:HB1	2:G:250:HIS:O	2.15	0.47
2:G:214:ARG:HG2	2:G:215:LYS:N	2.28	0.47
2:G:217:LYS:HB3	2:G:219:LYS:HZ3	1.80	0.47
2:G:358:LEU:CD2	2:H:36:ARG:HB3	2.44	0.47
2:H:94:LYS:NZ	2:H:98:SER:HB3	2.29	0.47
2:H:147:GLU:HG3	2:H:150:GLN:NE2	2.30	0.47
2:H:356:LYS:CG	2:H:366:ILE:HG22	2.42	0.47
2:H:393:ARG:NH2	3:H:3450:ADP:O1B	2.47	0.47
1:K:68:GLN:O	1:K:70:HIS:N	2.48	0.47
1:K:132:ALA:HB2	1:K:154:ILE:HG21	1.97	0.47
1:L:8:ARG:HH21	1:L:137:LEU:HD12	1.80	0.47
1:B:51:ALA:O	1:B:52:ASP:C	2.52	0.47
2:E:432:LEU:H	2:E:432:LEU:CD1	2.27	0.47
1:I:33:LYS:O	1:I:45:GLY:HA2	2.15	0.47
1:J:30:ASN:C	1:J:30:ASN:HD22	2.17	0.47
2:G:74:ALA:O	2:G:75:ASN:C	2.53	0.47
2:G:382:GLN:HA	2:G:382:GLN:NE2	2.30	0.47
2:H:65:GLU:HG3	3:H:3450:ADP:H2'	1.97	0.47
1:K:6:VAL:HG21	1:K:147:ILE:HG22	1.96	0.47
1:K:36:ARG:NE	1:K:169:GLU:OE1	2.47	0.47
1:L:36:ARG:HB3	1:L:36:ARG:NH1	2.30	0.47
1:B:12:VAL:HG12	1:B:171:LEU:HB3	1.97	0.47
2:E:132:LEU:HB3	2:E:156:ARG:NH1	2.29	0.47
2:E:171:LYS:HB3	2:E:172:GLU:H	1.53	0.47
2:E:173:ILE:HG12	2:E:212:LYS:CD	2.42	0.47
2:E:259:ASP:HB3	2:E:310:PHE:CZ	2.50	0.47
2:F:96:VAL:CG1	2:F:281:LEU:HD12	2.45	0.47
1:D:28:LYS:CD	1:D:31:VAL:HG22	2.45	0.47
2:G:165:GLU:HG2	2:G:166:GLY:N	2.29	0.47
2:G:345:THR:CG2	2:G:373:ILE:HD13	2.43	0.47
2:H:219:LYS:HA	2:H:223:LYS:HZ3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:121:ALA:HB1	1:K:126:GLY:O	2.15	0.47
1:A:90:LYS:HZ2	1:B:89:ARG:NH2	2.12	0.47
2:E:153:SER:HA	2:E:157:GLN:HG3	1.97	0.47
2:F:60:GLY:H	2:F:393:ARG:NH2	2.12	0.47
2:F:358:LEU:O	2:F:361:THR:HB	2.14	0.47
1:I:3:ILE:HB	1:I:122:ILE:HG12	1.97	0.47
2:G:217:LYS:HG3	2:G:219:LYS:NZ	2.30	0.47
2:H:145:GLN:HA	2:H:145:GLN:NE2	2.30	0.47
1:K:55:THR:O	1:K:58:GLU:HB3	2.15	0.47
1:L:37:LEU:N	1:L:37:LEU:HD23	2.30	0.46
2:F:135:LEU:HD13	2:F:159:PHE:HD2	1.79	0.46
1:D:5:SER:HB3	1:D:120:ILE:HB	1.96	0.46
1:J:60:PHE:CE2	1:J:97:VAL:HG21	2.50	0.46
2:H:131:ILE:HG23	2:H:132:LEU:N	2.31	0.46
2:H:135:LEU:HD13	2:H:159:PHE:HD2	1.80	0.46
2:H:236:PRO:O	2:H:238:GLU:N	2.47	0.46
1:L:12:VAL:O	1:L:12:VAL:HG13	2.15	0.46
1:A:149:GLU:CG	1:A:168:ILE:HD11	2.46	0.46
2:F:102:ASP:C	2:F:104:THR:H	2.18	0.46
2:F:148:GLN:HA	2:F:151:GLU:HG3	1.96	0.46
1:D:3:ILE:O	1:D:121:ALA:HA	2.15	0.46
2:G:220:ASP:O	2:G:221:ALA:C	2.53	0.46
2:G:311:GLN:HE21	2:G:311:GLN:HA	1.80	0.46
2:H:167:GLN:CD	2:H:219:LYS:NZ	2.68	0.46
2:H:172:GLU:O	2:H:173:ILE:HG23	2.15	0.46
1:L:168:ILE:HG22	1:L:169:GLU:N	2.29	0.46
2:E:409:ASP:O	2:E:410:ALA:C	2.54	0.46
2:G:60:GLY:H	2:G:393:ARG:HH22	1.62	0.46
2:G:109:LYS:O	2:G:113:VAL:HG23	2.15	0.46
2:G:171:LYS:HA	2:G:171:LYS:NZ	2.30	0.46
2:H:366:ILE:HG13	2:H:420:ILE:HD13	1.97	0.46
1:K:71:LEU:HD21	1:K:97:VAL:CG1	2.45	0.46
1:A:80:LYS:O	1:A:82:TRP:N	2.49	0.46
1:A:149:GLU:HG2	1:A:168:ILE:CD1	2.46	0.46
2:E:240:LYS:HD3	2:E:241:GLN:N	2.29	0.46
2:F:130:ARG:NH2	2:F:229:GLU:HG3	2.31	0.46
1:J:99:ASP:OD1	1:J:101:THR:HB	2.16	0.46
1:K:73:LYS:HA	1:K:76:VAL:CG1	2.44	0.46
1:C:117:ASN:O	1:C:118:ASP:HB2	2.15	0.46
1:D:46:PHE:HA	1:D:94:LEU:O	2.16	0.46
2:G:91:TYR:O	2:G:92:VAL:HG22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:358:LEU:CD2	2:H:36:ARG:CB	2.93	0.46
2:H:163:LEU:HD11	2:H:222:MET:CE	2.45	0.46
1:B:3:ILE:HB	1:B:122:ILE:CG1	2.45	0.46
2:E:221:ALA:O	2:E:225:LEU:HD23	2.15	0.46
2:E:389:ASN:HD22	2:E:390:ILE:N	2.12	0.46
1:K:80:LYS:HD2	1:K:80:LYS:C	2.36	0.46
1:A:80:LYS:O	1:A:84:THR:HG22	2.15	0.46
1:A:90:LYS:HZ1	1:B:89:ARG:NH2	2.13	0.46
2:E:234:VAL:O	2:E:236:PRO:HD3	2.15	0.46
2:E:442:ILE:O	2:E:442:ILE:HG22	2.15	0.46
2:F:147:GLU:HG2	2:F:150:GLN:HE21	1.79	0.46
2:F:163:LEU:HD11	2:F:222:MET:HE3	1.98	0.46
2:F:217:LYS:HG3	2:F:218:ILE:H	1.81	0.46
1:C:28:LYS:HE2	1:D:114:GLN:O	2.16	0.46
1:D:83:ARG:HH11	1:D:83:ARG:CB	2.17	0.46
2:H:86:PHE:O	2:H:89:VAL:HG22	2.16	0.46
2:F:53:ILE:HG12	2:F:328:ILE:HB	1.97	0.46
2:F:145:GLN:CA	2:F:145:GLN:HE21	2.28	0.46
2:F:223:LYS:N	2:F:223:LYS:CD	2.79	0.46
2:F:362:GLU:HG2	2:F:410:ALA:C	2.36	0.46
2:G:92:VAL:CG2	2:H:92:VAL:CG1	2.80	0.46
2:H:312:ILE:HG12	2:H:313:ALA:H	1.81	0.46
2:H:372:GLY:O	2:H:376:ILE:HG13	2.16	0.46
1:A:17:ASP:CB	1:A:162:THR:HG23	2.46	0.46
2:E:352:THR:HG22	2:E:353:VAL:N	2.31	0.46
1:C:36:ARG:HH12	1:C:40:ASP:C	2.19	0.46
2:G:95:GLU:OE1	2:G:101:ARG:NH1	2.47	0.46
1:A:17:ASP:HB3	1:A:162:THR:HG23	1.98	0.45
2:E:436:GLU:O	2:E:439:SER:HB2	2.16	0.45
2:F:169:ASP:O	2:F:218:ILE:HG13	2.15	0.45
1:D:62:ARG:O	1:D:65:GLU:HG2	2.16	0.45
1:D:105:ILE:HD12	1:D:122:ILE:HG21	1.98	0.45
2:H:17:ILE:HD12	2:H:17:ILE:N	2.31	0.45
1:K:86:ARG:HA	1:K:89:ARG:CZ	2.47	0.45
1:B:95:LEU:HD12	1:B:95:LEU:N	2.31	0.45
2:E:147:GLU:CA	2:E:150:GLN:HG3	2.46	0.45
2:E:308:GLY:HA3	2:E:310:PHE:CE2	2.51	0.45
2:F:236:PRO:O	2:F:238:GLU:N	2.49	0.45
2:G:262:CYS:SG	2:G:318:LEU:HD13	2.55	0.45
2:F:122:ARG:CZ	2:F:122:ARG:HA	2.46	0.45
2:F:212:LYS:HB2	2:F:212:LYS:HZ2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:90:LYS:NZ	1:L:89:ARG:CZ	2.80	0.45
1:L:89:ARG:NH1	1:L:89:ARG:HB3	2.31	0.45
1:L:100:GLU:OE2	1:L:173:TYR:HB2	2.16	0.45
2:E:95:GLU:H	2:E:95:GLU:CD	2.20	0.45
2:F:171:LYS:O	2:F:172:GLU:HB3	2.17	0.45
2:F:398:VAL:HG13	2:F:429:LEU:HD13	1.97	0.45
1:C:22:LEU:HD23	1:C:22:LEU:C	2.36	0.45
1:J:148:ALA:O	1:J:152:LEU:HB2	2.15	0.45
2:H:135:LEU:O	2:H:136:ILE:HD13	2.17	0.45
2:F:233:LEU:HD12	2:F:233:LEU:O	2.17	0.45
1:I:51:ALA:CB	1:J:111:ASP:OD2	2.65	0.45
1:J:71:LEU:HD13	1:J:71:LEU:C	2.37	0.45
1:J:86:ARG:HA	1:J:89:ARG:HE	1.82	0.45
2:G:311:GLN:HA	2:G:311:GLN:NE2	2.31	0.45
1:K:73:LYS:O	1:K:76:VAL:HG12	2.16	0.45
1:A:10:GLY:HA2	1:A:173:TYR:CZ	2.51	0.45
1:A:95:LEU:HB2	1:A:106:ILE:HB	1.99	0.45
2:E:86:PHE:HA	2:E:89:VAL:HG13	1.98	0.45
2:E:169:ASP:O	2:E:218:ILE:CG1	2.65	0.45
2:E:312:ILE:CG1	2:E:313:ALA:H	2.27	0.45
2:F:41:ASN:ND2	2:F:44:LEU:H	2.14	0.45
2:F:96:VAL:HG12	2:F:284:LEU:HD11	1.97	0.45
2:F:119:ASN:HD21	2:F:233:LEU:HD23	1.81	0.45
2:F:121:TYR:O	2:F:125:GLU:HB2	2.17	0.45
2:F:160:ARG:HG2	2:F:160:ARG:HH11	1.82	0.45
1:J:136:LEU:HB3	1:J:147:ILE:HD12	1.97	0.45
2:G:54:LEU:HD12	2:G:306:ALA:HB3	1.98	0.45
2:G:88:GLU:CD	2:H:90:GLY:CA	2.85	0.45
2:G:173:ILE:HD11	2:G:221:ALA:HB1	1.98	0.45
2:G:358:LEU:HD22	2:H:36:ARG:CB	2.46	0.45
1:K:58:GLU:O	1:K:61:GLU:HB2	2.16	0.45
1:L:62:ARG:HA	1:L:65:GLU:HG2	1.98	0.45
1:B:38:TYR:CE2	1:B:41:LYS:HD2	2.52	0.45
2:E:214:ARG:CG	2:E:215:LYS:N	2.79	0.45
2:E:264:ARG:NE	2:E:265:GLY:H	2.15	0.45
2:E:402:LEU:HD12	2:E:428:HIS:HB2	1.98	0.45
1:I:87:MET:HE1	1:J:84:THR:HA	1.98	0.45
1:J:94:LEU:HB3	1:J:122:ILE:HD12	1.98	0.45
2:G:153:SER:N	2:G:156:ARG:HB3	2.32	0.45
2:G:227:GLU:O	2:G:230:ALA:N	2.49	0.45
2:G:230:ALA:O	2:G:233:LEU:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:64:LEU:CB	1:L:69:GLY:HA2	2.43	0.45
2:F:311:GLN:CA	2:F:311:GLN:NE2	2.80	0.45
2:F:312:ILE:CG1	2:F:313:ALA:N	2.78	0.45
1:C:7:ARG:O	1:C:8:ARG:HB2	2.17	0.45
1:C:11:HIS:CE1	1:C:174:LYS:HE2	2.52	0.45
1:I:85:ASP:OD1	1:I:88:LEU:HD13	2.17	0.45
1:J:60:PHE:HB2	1:J:78:LEU:HD22	1.97	0.45
1:J:70:HIS:CE1	1:J:72:VAL:HB	2.51	0.45
2:G:216:LEU:CD1	2:G:221:ALA:HB2	2.47	0.45
2:H:308:GLY:HA3	2:H:310:PHE:CE2	2.52	0.45
1:K:58:GLU:HG3	1:K:62:ARG:HH21	1.82	0.45
2:E:126:LEU:O	2:E:130:ARG:NH2	2.45	0.45
2:E:134:VAL:HG22	2:E:134:VAL:O	2.17	0.45
1:D:73:LYS:O	1:D:76:VAL:HG12	2.17	0.45
1:J:104:LEU:HD23	1:J:104:LEU:N	2.31	0.45
2:G:171:LYS:HG3	2:G:218:ILE:HD11	1.98	0.45
2:E:53:ILE:HG22	2:E:54:LEU:N	2.32	0.45
2:E:65:GLU:O	2:E:69:ARG:HG2	2.17	0.45
2:E:96:VAL:HG21	2:E:280:ASP:HB3	1.99	0.45
2:E:384:ASN:HD21	2:E:390:ILE:HG12	1.82	0.45
1:C:8:ARG:O	1:C:11:HIS:HB2	2.16	0.45
1:I:17:ASP:O	1:I:33:LYS:HD2	2.17	0.45
2:G:140:LYS:O	2:G:141:ASN:CB	2.63	0.45
1:L:89:ARG:NH1	1:L:89:ARG:CB	2.80	0.45
1:A:34:VAL:HG13	1:A:44:ALA:O	2.17	0.44
1:A:71:LEU:O	1:A:75:ALA:N	2.49	0.44
2:E:89:VAL:HA	2:E:93:GLY:HA3	1.99	0.44
2:F:211:GLN:O	2:F:212:LYS:HB2	2.17	0.44
1:I:72:VAL:O	1:I:76:VAL:HG23	2.18	0.44
2:G:23:ALA:HA	2:G:330:VAL:HG21	1.99	0.44
2:G:109:LYS:O	2:G:109:LYS:HG3	2.17	0.44
2:G:130:ARG:HD2	2:G:225:LEU:CD1	2.27	0.44
1:A:30:ASN:HD22	1:A:30:ASN:C	2.20	0.44
2:E:262:CYS:SG	2:E:318:LEU:HD13	2.57	0.44
2:F:135:LEU:HB3	2:F:159:PHE:CD2	2.52	0.44
2:F:345:THR:CG2	2:F:373:ILE:CD1	2.95	0.44
1:C:156:GLY:HA2	1:C:162:THR:HG22	1.99	0.44
1:I:8:ARG:HG2	1:I:9:ASN:CG	2.38	0.44
2:G:152:PRO:O	2:G:154:ALA:CB	2.58	0.44
2:E:19:GLY:O	2:E:24:LYS:HE3	2.17	0.44
1:C:20:ALA:HB2	1:C:31:VAL:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:GLU:C	1:C:118:ASP:H	2.21	0.44
1:D:28:LYS:HZ3	1:D:30:ASN:ND2	2.15	0.44
1:D:98:ALA:HA	1:D:103:SER:HA	2.00	0.44
1:D:99:ASP:HA	1:D:171:LEU:HD23	1.99	0.44
1:J:66:MET:C	1:J:67:HIS:ND1	2.70	0.44
2:H:255:ILE:HD12	2:H:255:ILE:H	1.80	0.44
1:K:73:LYS:CA	1:K:76:VAL:HG12	2.47	0.44
1:A:28:LYS:NZ	1:A:30:ASN:HD21	2.12	0.44
2:E:89:VAL:HA	2:E:93:GLY:CA	2.48	0.44
2:E:216:LEU:HD23	2:E:216:LEU:N	2.31	0.44
2:E:248:GLU:HG2	2:E:297:VAL:HG13	1.99	0.44
2:E:264:ARG:CZ	2:E:265:GLY:H	2.30	0.44
2:E:408:TYR:HD1	2:F:29:ILE:HD11	1.82	0.44
2:F:217:LYS:HB2	2:F:217:LYS:HZ2	1.80	0.44
2:F:362:GLU:HG3	2:F:411:SER:HA	2.00	0.44
1:D:41:LYS:O	1:D:171:LEU:HD21	2.16	0.44
1:D:73:LYS:HD2	1:D:76:VAL:CG1	2.47	0.44
2:G:153:SER:C	2:G:157:GLN:HG3	2.37	0.44
2:G:165:GLU:HG2	2:G:166:GLY:H	1.82	0.44
2:H:158:ALA:HB1	2:H:162:LYS:NZ	2.33	0.44
2:H:167:GLN:CG	2:H:219:LYS:HZ1	2.31	0.44
2:E:35:TRP:O	2:E:39:GLN:HG2	2.17	0.44
2:F:21:ASP:O	2:F:24:LYS:HB2	2.17	0.44
2:F:150:GLN:O	2:F:153:SER:HB2	2.18	0.44
1:C:121:ALA:HB1	1:C:126:GLY:O	2.18	0.44
1:D:70:HIS:HE1	1:D:72:VAL:HB	1.83	0.44
1:D:168:ILE:HG22	1:D:169:GLU:N	2.32	0.44
1:I:85:ASP:CG	1:I:88:LEU:HD13	2.37	0.44
2:G:362:GLU:HB3	2:G:364:VAL:HG23	2.00	0.44
2:G:408:TYR:CE1	2:H:10:VAL:HG21	2.52	0.44
2:H:119:ASN:OD1	2:H:234:VAL:HG23	2.16	0.44
2:H:121:TYR:O	2:H:125:GLU:HB2	2.18	0.44
1:B:59:LEU:HG	1:B:78:LEU:HD13	1.99	0.44
1:B:65:GLU:CD	2:F:143:TRP:NE1	2.71	0.44
1:B:65:GLU:O	2:F:143:TRP:O	2.35	0.44
2:E:145:GLN:HB2	2:E:148:GLN:CB	2.39	0.44
2:E:220:ASP:HA	2:E:223:LYS:HD2	1.98	0.44
2:E:342:ARG:NH2	2:E:346:GLU:OE2	2.40	0.44
2:F:172:GLU:O	2:F:173:ILE:HG23	2.18	0.44
1:D:11:HIS:HA	1:D:171:LEU:O	2.17	0.44
1:J:62:ARG:O	1:J:66:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:145:GLN:HB2	2:H:148:GLN:CG	2.46	0.44
2:H:214:ARG:NE	2:H:216:LEU:HB3	2.32	0.44
2:H:282:LEU:HD12	2:H:282:LEU:HA	1.76	0.44
2:H:299:THR:O	2:H:302:ILE:HG12	2.18	0.44
2:H:356:LYS:HG3	2:H:366:ILE:CG2	2.46	0.44
2:F:41:ASN:O	2:F:45:ARG:HG3	2.17	0.44
2:F:268:SER:HA	2:F:271:ASP:OD2	2.16	0.44
2:F:345:THR:HG21	2:F:373:ILE:CD1	2.47	0.44
2:G:34:ARG:NH2	2:G:250:HIS:HA	2.32	0.44
2:H:16:HIS:HB2	2:H:17:ILE:HD12	1.99	0.44
2:H:151:GLU:HB2	2:H:152:PRO:HD2	1.99	0.44
1:A:60:PHE:CE2	1:A:97:VAL:HG21	2.53	0.44
2:E:219:LYS:O	2:E:223:LYS:HG3	2.18	0.44
2:F:174:GLU:HB3	2:F:211:GLN:NE2	2.33	0.44
1:C:34:VAL:HB	1:C:167:THR:HG22	1.99	0.44
1:I:84:THR:HG23	1:I:85:ASP:N	2.32	0.44
1:J:92:GLU:O	1:J:93:ALA:HB2	2.17	0.44
2:H:96:VAL:HG12	2:H:284:LEU:HD11	2.00	0.44
2:H:167:GLN:OE1	2:H:168:LEU:N	2.51	0.44
1:K:79:ALA:HB1	1:K:110:GLY:HA2	2.00	0.44
1:K:115:PRO:HG3	1:K:120:ILE:CG1	2.47	0.44
1:L:60:PHE:CZ	1:L:97:VAL:HG11	2.53	0.44
1:A:1:THR:HA	1:A:17:ASP:OD1	2.18	0.44
1:A:15:ALA:HB1	1:A:152:LEU:HD12	2.00	0.44
1:A:72:VAL:O	1:A:76:VAL:HG23	2.18	0.44
1:J:37:LEU:HD11	1:J:57:PHE:CD1	2.53	0.44
1:J:38:TYR:HB2	1:J:64:LEU:HD12	1.99	0.44
2:G:171:LYS:HB3	2:G:172:GLU:H	1.48	0.44
2:G:255:ILE:HD13	2:G:281:LEU:HD21	2.00	0.44
2:G:436:GLU:O	2:G:439:SER:HB2	2.17	0.44
2:H:102:ASP:C	2:H:104:THR:H	2.21	0.44
2:H:127:ALA:HB1	2:H:229:GLU:HB3	1.99	0.44
1:K:91:LEU:HB3	1:L:83:ARG:NE	2.32	0.44
1:K:143:SER:OG	1:K:146:GLU:HG3	2.18	0.44
1:L:149:GLU:OE1	1:L:166:HIS:CD2	2.71	0.44
2:F:47:GLU:OE1	2:F:47:GLU:HA	2.18	0.43
1:D:157:ASP:OD2	1:D:164:HIS:NE2	2.37	0.43
2:G:47:GLU:OE1	2:G:47:GLU:HA	2.18	0.43
2:G:53:ILE:HA	2:G:328:ILE:HB	2.00	0.43
2:G:126:LEU:N	2:G:126:LEU:HD22	2.33	0.43
2:G:311:GLN:CA	2:G:311:GLN:NE2	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:432:LEU:H	2:H:432:LEU:CD1	2.30	0.43
1:L:89:ARG:CB	1:L:89:ARG:HH11	2.31	0.43
1:A:88:LEU:CD1	1:A:88:LEU:N	2.80	0.43
2:E:91:TYR:O	2:E:92:VAL:HG22	2.18	0.43
2:E:122:ARG:NH1	2:E:126:LEU:HD21	2.33	0.43
2:E:169:ASP:O	2:E:218:ILE:HG13	2.18	0.43
2:E:401:ARG:CZ	2:E:442:ILE:HG23	2.48	0.43
2:H:103:LEU:O	2:H:103:LEU:HD22	2.18	0.43
1:K:60:PHE:CZ	1:K:97:VAL:HG11	2.53	0.43
1:L:37:LEU:HD23	1:L:37:LEU:H	1.83	0.43
1:B:7:ARG:NE	1:B:118:ASP:OD2	2.48	0.43
2:E:12:GLU:HG2	2:E:73:LEU:HD11	2.00	0.43
2:E:74:ALA:O	2:E:75:ASN:C	2.56	0.43
2:F:58:PRO:HG2	2:F:61:VAL:HG11	2.00	0.43
2:F:170:ASP:HB3	2:F:217:LYS:HD3	2.00	0.43
1:D:115:PRO:HG2	1:D:118:ASP:HA	2.00	0.43
2:H:220:ASP:O	2:H:224:LEU:N	2.44	0.43
1:L:17:ASP:HA	1:L:165:PHE:O	2.18	0.43
1:B:148:ALA:O	1:B:152:LEU:HB2	2.19	0.43
2:E:358:LEU:O	2:E:361:THR:HB	2.17	0.43
2:F:60:GLY:N	2:F:393:ARG:NH2	2.66	0.43
2:F:214:ARG:O	2:F:214:ARG:HD3	2.19	0.43
1:C:15:ALA:HB1	1:C:152:LEU:HD12	2.00	0.43
1:D:11:HIS:HE1	1:D:172:SER:OG	2.01	0.43
1:D:104:LEU:HD22	1:D:112:VAL:HG12	2.00	0.43
1:J:64:LEU:HD23	1:J:74:ALA:CB	2.48	0.43
2:G:106:ALA:O	2:G:110:MET:HB2	2.18	0.43
2:G:257:GLU:O	2:G:257:GLU:CG	2.65	0.43
2:G:273:SER:O	2:G:277:VAL:HG23	2.18	0.43
2:H:65:GLU:O	2:H:69:ARG:HG2	2.18	0.43
1:A:28:LYS:HZ1	1:A:30:ASN:ND2	2.12	0.43
2:E:63:LYS:HG2	2:E:332:LEU:HD13	2.00	0.43
2:E:79:ILE:CG2	2:E:103:LEU:HG	2.48	0.43
2:E:174:GLU:C	2:E:211:GLN:HB2	2.39	0.43
2:F:129:GLU:HB2	2:F:130:ARG:HH11	1.83	0.43
2:F:236:PRO:C	2:F:238:GLU:H	2.22	0.43
1:C:112:VAL:HG12	1:C:112:VAL:O	2.18	0.43
1:I:12:VAL:HG12	1:I:171:LEU:HB3	2.00	0.43
2:H:96:VAL:CG1	2:H:281:LEU:HD12	2.45	0.43
2:H:140:LYS:H	2:H:140:LYS:HD3	1.83	0.43
2:H:296:MET:HA	2:H:296:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:28:LYS:CE	1:K:30:ASN:ND2	2.81	0.43
1:K:83:ARG:CG	1:K:83:ARG:NH1	2.80	0.43
2:E:20:GLN:O	2:E:24:LYS:HG3	2.18	0.43
2:E:292:THR:HB	2:E:295:GLY:O	2.18	0.43
2:F:91:TYR:O	2:F:92:VAL:HG22	2.19	0.43
2:F:322:LEU:HD12	2:F:322:LEU:HA	1.77	0.43
2:F:341:GLU:O	2:F:344:LEU:HB2	2.19	0.43
1:D:13:VAL:HG11	1:D:145:ARG:HB2	1.99	0.43
1:I:109:ASN:O	1:I:111:ASP:N	2.51	0.43
1:J:65:GLU:HB3	2:H:143:TRP:HA	2.00	0.43
2:G:134:VAL:HG13	2:G:171:LYS:HD3	1.99	0.43
2:G:173:ILE:HG12	2:G:212:LYS:CD	2.45	0.43
2:G:282:LEU:HD11	2:G:321:GLU:HB3	2.00	0.43
2:G:384:ASN:HD21	2:G:390:ILE:HG12	1.84	0.43
2:H:94:LYS:HA	2:H:94:LYS:CE	2.35	0.43
1:B:99:ASP:OD1	1:B:101:THR:HB	2.18	0.43
1:B:99:ASP:OD2	1:B:101:THR:N	2.29	0.43
2:F:159:PHE:O	2:F:163:LEU:HB2	2.18	0.43
2:F:227:GLU:O	2:F:228:GLU:C	2.56	0.43
2:F:267:SER:O	2:F:271:ASP:OD2	2.35	0.43
2:F:312:ILE:CG1	2:F:313:ALA:H	2.31	0.43
2:F:388:GLU:N	2:F:388:GLU:OE2	2.52	0.43
1:C:28:LYS:NZ	1:C:30:ASN:ND2	2.67	0.43
2:G:96:VAL:HG11	2:G:281:LEU:HD12	2.00	0.43
2:G:212:LYS:HB2	2:G:212:LYS:HZ2	1.84	0.43
2:G:231:ALA:O	2:G:233:LEU:N	2.51	0.43
2:G:292:THR:HG22	2:G:293:LYS:N	2.34	0.43
2:G:342:ARG:NH2	2:G:346:GLU:OE2	2.37	0.43
2:G:384:ASN:HD22	2:G:384:ASN:HA	1.61	0.43
2:H:122:ARG:HH21	2:H:122:ARG:HG2	1.84	0.43
1:K:3:ILE:HB	1:K:122:ILE:CG1	2.49	0.43
1:K:46:PHE:CD2	1:K:53:ALA:HB2	2.54	0.43
1:A:101:THR:O	1:A:102:ALA:HB2	2.18	0.43
2:E:140:LYS:O	2:E:141:ASN:CB	2.65	0.43
2:F:102:ASP:C	2:F:104:THR:N	2.71	0.43
1:C:86:ARG:HA	1:C:89:ARG:NH2	2.34	0.43
2:G:108:VAL:O	2:G:110:MET:N	2.52	0.43
2:G:165:GLU:O	2:G:167:GLN:HG3	2.18	0.43
2:H:224:LEU:O	2:H:228:GLU:HB2	2.19	0.43
2:H:236:PRO:C	2:H:238:GLU:H	2.22	0.43
2:F:35:TRP:O	2:F:39:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:123:ALA:HB2	2:F:229:GLU:O	2.19	0.43
2:F:214:ARG:HE	2:F:216:LEU:HB3	1.84	0.43
1:I:145:ARG:NE	1:I:170:GLU:OE1	2.44	0.43
1:J:60:PHE:HD1	1:J:78:LEU:HD22	1.81	0.43
2:G:174:GLU:HG3	2:G:213:ALA:HA	2.01	0.43
2:H:111:VAL:HG21	2:H:243:ALA:HB2	2.01	0.43
2:H:136:ILE:HD11	2:H:159:PHE:CZ	2.54	0.43
2:H:223:LYS:C	2:H:225:LEU:H	2.21	0.43
2:H:366:ILE:HD12	2:H:418:ILE:HB	2.00	0.43
1:A:102:ALA:HB1	1:A:114:GLN:OE1	2.19	0.43
2:E:16:HIS:HB2	2:E:17:ILE:HD12	2.00	0.43
2:F:403:MET:SD	2:F:420:ILE:HD13	2.59	0.43
1:C:36:ARG:NH1	1:C:40:ASP:CA	2.82	0.43
1:D:28:LYS:HG2	1:D:30:ASN:HD22	1.82	0.43
1:D:37:LEU:HB2	1:D:61:GLU:OE1	2.19	0.43
2:G:54:LEU:HB3	2:G:329:ARG:HD3	2.01	0.43
2:G:65:GLU:HA	2:G:65:GLU:OE2	2.19	0.43
2:G:89:VAL:HA	2:G:92:VAL:C	2.40	0.43
2:G:337:THR:O	2:G:341:GLU:HG3	2.19	0.43
2:H:108:VAL:O	2:H:110:MET:N	2.51	0.43
1:K:86:ARG:HG3	1:K:89:ARG:NH2	2.34	0.43
1:C:36:ARG:NH1	1:C:40:ASP:HB3	2.34	0.42
1:C:85:ASP:CB	1:C:88:LEU:HD12	2.49	0.42
1:J:67:HIS:CD2	1:J:73:LYS:HD2	2.54	0.42
2:G:164:ARG:HA	2:G:164:ARG:HH11	1.83	0.42
2:H:79:ILE:HG21	2:H:103:LEU:HB2	2.00	0.42
2:F:264:ARG:HE	2:F:265:GLY:H	1.64	0.42
1:C:168:ILE:HG22	1:C:169:GLU:N	2.34	0.42
1:D:152:LEU:HB3	1:D:166:HIS:CE1	2.54	0.42
2:G:145:GLN:HB2	2:G:148:GLN:CB	2.44	0.42
2:G:151:GLU:HB2	2:G:152:PRO:HD2	2.01	0.42
1:A:109:ASN:N	1:A:109:ASN:HD22	2.16	0.42
2:E:116:ILE:O	2:E:116:ILE:HG22	2.18	0.42
2:E:296:MET:HE2	2:E:296:MET:HA	2.00	0.42
2:E:435:ASP:OD1	2:E:438:LEU:HB2	2.19	0.42
2:F:125:GLU:C	2:F:127:ALA:H	2.22	0.42
2:F:135:LEU:HD22	2:F:159:PHE:CE2	2.54	0.42
1:C:37:LEU:HB3	1:C:61:GLU:OE1	2.19	0.42
1:D:121:ALA:HB1	1:D:126:GLY:O	2.18	0.42
2:G:170:ASP:HB3	2:G:217:LYS:CD	2.47	0.42
2:G:358:LEU:O	2:G:361:THR:HB	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:392:ALA:HB3	3:G:2450:ADP:C8	2.55	0.42
1:K:30:ASN:ND2	1:K:30:ASN:H	2.17	0.42
1:L:14:ILE:HD12	1:L:43:ILE:O	2.19	0.42
1:L:116:GLU:C	1:L:118:ASP:H	2.22	0.42
2:E:217:LYS:O	2:E:221:ALA:N	2.36	0.42
2:E:351:ILE:HD13	2:E:396:HIS:ND1	2.34	0.42
1:D:43:ILE:H	1:D:43:ILE:CD1	2.24	0.42
2:G:140:LYS:HD3	2:G:140:LYS:N	2.33	0.42
2:H:174:GLU:C	2:H:212:LYS:HB3	2.40	0.42
2:E:108:VAL:HA	2:E:111:VAL:HG22	2.01	0.42
1:C:67:HIS:O	1:C:68:GLN:C	2.57	0.42
1:D:22:LEU:HD12	1:D:27:MET:CE	2.49	0.42
1:J:70:HIS:ND1	1:J:73:LYS:HB2	2.34	0.42
2:G:163:LEU:HG	2:G:163:LEU:O	2.19	0.42
2:H:84:THR:C	2:H:86:PHE:H	2.22	0.42
2:H:312:ILE:CG1	2:H:313:ALA:N	2.82	0.42
1:K:38:TYR:HB2	1:K:64:LEU:CD1	2.50	0.42
1:K:67:HIS:O	1:K:68:GLN:C	2.57	0.42
2:E:232:LYS:NZ	2:E:232:LYS:HB3	2.33	0.42
1:J:32:LYS:HE3	1:J:32:LYS:HB2	1.78	0.42
1:J:59:LEU:HD11	1:J:63:LYS:HE2	2.02	0.42
1:J:150:LYS:O	1:J:154:ILE:HG12	2.18	0.42
2:G:33:ASN:ND2	2:G:36:ARG:HD2	2.35	0.42
1:B:11:HIS:CE1	1:B:172:SER:OG	2.73	0.42
1:B:32:LYS:HE3	1:B:32:LYS:HB2	1.78	0.42
2:E:231:ALA:C	2:E:233:LEU:N	2.73	0.42
2:F:264:ARG:CZ	2:F:265:GLY:H	2.31	0.42
1:D:134:ARG:HD2	1:D:138:GLU:OE1	2.19	0.42
2:G:216:LEU:HD12	2:G:216:LEU:O	2.19	0.42
2:G:293:LYS:C	2:G:294:HIS:HD2	2.23	0.42
2:G:349:ALA:HB1	2:H:44:LEU:CD2	2.50	0.42
2:H:96:VAL:CG1	2:H:99:ILE:HD12	2.49	0.42
2:H:147:GLU:HG2	2:H:150:GLN:NE2	2.35	0.42
2:H:432:LEU:N	2:H:432:LEU:CD1	2.83	0.42
1:K:141:GLU:OE2	1:K:141:GLU:HA	2.20	0.42
1:A:28:LYS:HD2	1:B:113:VAL:HG13	2.01	0.42
1:A:86:ARG:HG2	1:A:89:ARG:HH22	1.85	0.42
1:B:104:LEU:HB2	1:B:113:VAL:O	2.19	0.42
1:B:117:ASN:O	1:B:118:ASP:HB2	2.19	0.42
2:E:40:LEU:O	2:E:45:ARG:NH1	2.53	0.42
2:E:217:LYS:HG3	2:E:219:LYS:HZ1	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:8:ARG:O	1:J:11:HIS:HB2	2.20	0.42
1:B:53:ALA:O	1:B:56:LEU:N	2.53	0.42
2:E:151:GLU:C	2:E:153:SER:N	2.71	0.42
1:I:6:VAL:HG12	1:I:7:ARG:N	2.35	0.42
2:G:366:ILE:HD13	2:G:366:ILE:HA	1.92	0.42
1:L:89:ARG:HH11	1:L:89:ARG:HB2	1.84	0.42
1:B:6:VAL:HG12	1:B:7:ARG:N	2.34	0.42
2:E:299:THR:CA	2:E:302:ILE:HD13	2.38	0.42
2:F:151:GLU:CB	2:F:152:PRO:HD3	2.50	0.42
1:D:1:THR:HB	1:D:33:LYS:NZ	2.35	0.42
1:J:63:LYS:HD2	1:J:77:GLU:HB3	2.01	0.42
2:G:214:ARG:HD3	2:G:216:LEU:HD23	2.02	0.42
2:H:32:ARG:O	2:H:36:ARG:HG3	2.20	0.42
2:H:40:LEU:O	2:H:45:ARG:NH1	2.52	0.42
2:H:94:LYS:HZ1	2:H:101:ARG:HH12	1.68	0.42
2:H:342:ARG:O	2:H:346:GLU:HB2	2.20	0.42
1:A:99:ASP:OD1	1:A:101:THR:N	2.36	0.41
2:E:173:ILE:N	2:E:173:ILE:CD1	2.82	0.41
1:C:95:LEU:N	1:C:95:LEU:HD12	2.35	0.41
1:C:114:GLN:O	1:C:115:PRO:O	2.38	0.41
2:G:92:VAL:CG1	2:H:92:VAL:CG1	2.93	0.41
2:G:161:LYS:O	2:G:164:ARG:HB2	2.19	0.41
2:G:174:GLU:OE2	2:G:213:ALA:HA	2.19	0.41
2:G:349:ALA:CB	2:H:44:LEU:CD2	2.98	0.41
2:H:218:ILE:C	2:H:220:ASP:N	2.73	0.41
2:H:257:GLU:HB2	2:H:260:LYS:CG	2.50	0.41
2:E:257:GLU:O	2:E:257:GLU:CG	2.63	0.41
2:E:408:TYR:CB	2:F:29:ILE:HD11	2.50	0.41
1:C:44:ALA:HB1	1:C:57:PHE:CE1	2.55	0.41
1:D:43:ILE:HD13	1:D:43:ILE:N	2.25	0.41
1:D:160:ILE:HD13	1:D:160:ILE:HA	1.86	0.41
2:G:131:ILE:HD11	2:G:218:ILE:CG1	2.49	0.41
2:H:74:ALA:O	2:H:75:ASN:C	2.58	0.41
2:H:80:LYS:HG3	2:H:254:PHE:HD1	1.85	0.41
2:H:135:LEU:HB3	2:H:159:PHE:HD2	1.80	0.41
2:H:285:VAL:HG12	2:H:304:PHE:CD1	2.55	0.41
2:H:289:THR:CG2	2:H:296:MET:HG3	2.50	0.41
2:E:106:ALA:O	2:E:110:MET:HB2	2.20	0.41
2:E:214:ARG:CD	2:E:216:LEU:HD22	2.41	0.41
2:E:231:ALA:C	2:E:233:LEU:H	2.22	0.41
1:C:73:LYS:HD2	1:C:76:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:89:VAL:HA	2:G:93:GLY:HA3	2.02	0.41
2:G:400:GLU:HG3	2:H:327:PRO:HB2	2.02	0.41
2:H:148:GLN:HA	2:H:151:GLU:CG	2.44	0.41
2:H:389:ASN:ND2	2:H:389:ASN:C	2.72	0.41
2:F:168:LEU:HD12	2:F:217:LYS:HG2	2.02	0.41
2:F:212:LYS:O	2:F:213:ALA:HB3	2.20	0.41
2:F:311:GLN:HE21	2:F:311:GLN:HA	1.83	0.41
1:C:8:ARG:NH2	1:C:137:LEU:HD12	2.35	0.41
1:C:73:LYS:HA	1:C:73:LYS:HD2	1.92	0.41
1:I:38:TYR:HE1	1:I:65:GLU:HG2	1.85	0.41
2:G:91:TYR:CE1	2:H:91:TYR:CE2	3.09	0.41
2:H:41:ASN:HD21	2:H:44:LEU:HB2	1.84	0.41
2:H:89:VAL:HA	2:H:92:VAL:O	2.20	0.41
2:H:269:GLY:N	2:H:270:PRO:CD	2.84	0.41
2:H:355:TYR:CE1	2:H:403:MET:HE3	2.56	0.41
1:L:42:VAL:HG13	1:L:98:ALA:O	2.21	0.41
2:F:109:LYS:HG3	2:F:109:LYS:O	2.19	0.41
2:F:167:GLN:OE1	2:F:168:LEU:N	2.53	0.41
2:F:223:LYS:HD2	2:F:223:LYS:H	1.84	0.41
1:J:101:THR:HG22	1:J:102:ALA:N	2.34	0.41
2:G:408:TYR:HE1	2:H:10:VAL:HG21	1.85	0.41
2:H:387:THR:OG1	2:H:388:GLU:N	2.53	0.41
1:L:3:ILE:HB	1:L:122:ILE:HG12	2.02	0.41
1:L:121:ALA:HB1	1:L:126:GLY:O	2.20	0.41
1:A:173:TYR:O	1:A:174:LYS:C	2.58	0.41
1:B:28:LYS:HZ1	1:B:30:ASN:ND2	2.17	0.41
1:B:73:LYS:HA	1:B:76:VAL:HG23	2.03	0.41
1:B:85:ASP:O	1:B:86:ARG:C	2.59	0.41
2:E:296:MET:HA	2:E:296:MET:CE	2.50	0.41
2:E:312:ILE:CG1	2:E:313:ALA:N	2.81	0.41
2:F:89:VAL:HG12	2:F:93:GLY:HA3	2.02	0.41
2:F:103:LEU:HD13	2:F:247:VAL:CG2	2.43	0.41
1:C:152:LEU:HD22	1:C:166:HIS:CE1	2.56	0.41
1:J:105:ILE:HG22	1:J:106:ILE:N	2.35	0.41
2:G:12:GLU:HG2	2:G:73:LEU:CD1	2.51	0.41
2:G:113:VAL:C	2:G:115:ALA:H	2.23	0.41
2:G:147:GLU:O	2:G:150:GLN:HG3	2.21	0.41
1:K:71:LEU:HD21	1:K:97:VAL:HG12	2.02	0.41
1:B:17:ASP:HB2	1:B:163:ASN:OD1	2.20	0.41
1:B:88:LEU:HD12	1:B:91:LEU:HD11	2.03	0.41
1:B:170:GLU:HG2	1:B:171:LEU:N	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:94:LYS:HA	2:F:94:LYS:CE	2.29	0.41
2:F:375:ARG:HA	2:F:378:GLU:HB2	2.02	0.41
2:F:384:ASN:HD21	2:F:394:ARG:HE	1.62	0.41
2:F:403:MET:O	2:F:404:GLU:C	2.59	0.41
1:C:99:ASP:HA	1:C:171:LEU:HD22	2.01	0.41
2:H:236:PRO:CG	2:H:237:GLU:H	2.32	0.41
2:H:247:VAL:O	2:H:302:ILE:HD13	2.21	0.41
2:H:268:SER:HA	2:H:271:ASP:OD2	2.20	0.41
1:L:6:VAL:HG12	1:L:7:ARG:N	2.36	0.41
1:B:101:THR:HG22	1:B:102:ALA:N	2.35	0.41
2:E:352:THR:CG2	2:E:353:VAL:N	2.84	0.41
2:F:96:VAL:HG21	2:F:280:ASP:HB3	2.03	0.41
2:F:217:LYS:CG	2:F:218:ILE:H	2.31	0.41
2:F:432:LEU:N	2:F:432:LEU:CD1	2.83	0.41
1:J:99:ASP:OD1	1:J:101:THR:N	2.53	0.41
1:J:174:LYS:HD2	1:J:174:LYS:N	2.36	0.41
2:G:107:ALA:O	2:G:111:VAL:HG22	2.20	0.41
2:G:148:GLN:OE1	2:G:151:GLU:HG3	2.21	0.41
2:G:173:ILE:N	2:G:173:ILE:CD1	2.79	0.41
2:G:212:LYS:HD3	2:G:216:LEU:HD11	2.02	0.41
2:H:443:LEU:HD23	2:H:443:LEU:HA	1.94	0.41
1:K:1:THR:HB	1:K:33:LYS:HZ3	1.86	0.41
1:A:3:ILE:HB	1:A:122:ILE:HG12	2.03	0.41
1:A:71:LEU:HD11	1:A:97:VAL:HG13	2.02	0.41
1:B:6:VAL:HG21	1:B:147:ILE:HG22	2.02	0.41
2:E:135:LEU:HB3	2:E:159:PHE:CD2	2.55	0.41
2:E:168:LEU:HD22	2:E:219:LYS:HD3	2.02	0.41
2:E:174:GLU:CA	2:E:212:LYS:HB3	2.51	0.41
2:E:285:VAL:HG12	2:E:304:PHE:CD1	2.56	0.41
2:E:408:TYR:CD1	2:F:29:ILE:HD11	2.55	0.41
2:F:41:ASN:C	2:F:41:ASN:ND2	2.72	0.41
2:F:145:GLN:C	2:F:147:GLU:H	2.23	0.41
1:C:152:LEU:HD22	1:C:166:HIS:HE1	1.86	0.41
1:D:64:LEU:HA	1:D:74:ALA:HB2	2.03	0.41
1:D:149:GLU:CD	1:D:168:ILE:HD11	2.41	0.41
1:J:38:TYR:HB2	1:J:64:LEU:HD13	2.03	0.41
2:G:27:VAL:CG1	2:G:70:LEU:HG	2.51	0.41
2:G:92:VAL:CG2	2:H:91:TYR:O	2.69	0.41
2:G:226:ILE:O	2:G:230:ALA:HB2	2.20	0.41
2:H:145:GLN:H	2:H:148:GLN:HB2	1.86	0.41
2:H:402:LEU:HD12	2:H:428:HIS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TRP:CH2	1:A:95:LEU:HD13	2.56	0.41
2:E:292:THR:C	2:E:294:HIS:H	2.24	0.41
1:C:59:LEU:HD23	1:C:78:LEU:HD12	2.03	0.41
1:D:80:LYS:HD2	1:D:80:LYS:O	2.21	0.41
1:I:28:LYS:HZ1	1:I:30:ASN:ND2	2.18	0.41
1:I:88:LEU:CD1	1:I:88:LEU:N	2.82	0.41
1:J:12:VAL:CG1	1:J:171:LEU:HB3	2.50	0.41
1:J:53:ALA:C	1:J:55:THR:N	2.75	0.41
1:J:59:LEU:HD12	1:J:59:LEU:C	2.40	0.41
2:H:145:GLN:CA	2:H:145:GLN:NE2	2.84	0.41
2:H:174:GLU:HB3	2:H:211:GLN:NE2	2.36	0.41
2:H:220:ASP:C	2:H:224:LEU:HD23	2.42	0.41
2:H:223:LYS:C	2:H:225:LEU:N	2.74	0.41
2:H:293:LYS:HG3	2:H:294:HIS:CE1	2.56	0.41
1:L:28:LYS:HG2	1:L:30:ASN:ND2	2.36	0.41
1:A:109:ASN:N	1:A:109:ASN:ND2	2.69	0.40
1:B:71:LEU:O	1:B:72:VAL:C	2.60	0.40
2:E:65:GLU:HG3	3:E:450:ADP:H2'	2.02	0.40
2:E:440:ARG:HB3	2:F:316:SER:OG	2.20	0.40
2:F:61:VAL:C	3:F:1450:ADP:N7	2.74	0.40
2:F:384:ASN:ND2	2:F:390:ILE:H	2.19	0.40
1:C:28:LYS:HG2	1:C:30:ASN:HD22	1.86	0.40
2:G:167:GLN:OE1	2:G:168:LEU:N	2.53	0.40
2:G:312:ILE:CG1	2:G:313:ALA:N	2.84	0.40
2:H:235:ASN:OD1	2:H:238:GLU:HB2	2.20	0.40
2:H:270:PRO:O	2:H:273:SER:HB3	2.21	0.40
2:H:336:THR:H	2:H:339:ASP:HB2	1.86	0.40
1:A:83:ARG:NH1	1:A:83:ARG:HG2	2.36	0.40
1:B:34:VAL:HA	1:B:45:GLY:HA2	2.03	0.40
2:E:149:GLN:C	2:E:151:GLU:H	2.25	0.40
2:E:151:GLU:HB2	2:E:152:PRO:CD	2.51	0.40
2:E:215:LYS:HG3	2:E:215:LYS:O	2.21	0.40
2:E:240:LYS:HD3	2:E:240:LYS:C	2.41	0.40
2:E:253:VAL:HB	2:E:304:PHE:CD2	2.56	0.40
2:F:108:VAL:HG12	2:F:109:LYS:N	2.35	0.40
2:F:122:ARG:HA	2:F:122:ARG:NE	2.36	0.40
1:C:109:ASN:O	1:C:110:GLY:C	2.60	0.40
1:D:60:PHE:CZ	1:D:97:VAL:HG11	2.56	0.40
1:I:30:ASN:HD22	1:I:30:ASN:C	2.25	0.40
1:I:171:LEU:HD12	1:I:171:LEU:HA	1.93	0.40
2:H:384:ASN:HD22	2:H:384:ASN:HA	1.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:85:ASP:CB	1:L:88:LEU:HD12	2.52	0.40
1:L:114:GLN:O	1:L:115:PRO:O	2.39	0.40
1:B:66:MET:O	1:B:67:HIS:ND1	2.54	0.40
2:E:128:GLU:O	2:E:129:GLU:C	2.60	0.40
2:E:220:ASP:O	2:E:221:ALA:C	2.59	0.40
2:F:253:VAL:HB	2:F:304:PHE:CD2	2.57	0.40
1:C:62:ARG:HA	1:C:65:GLU:OE2	2.21	0.40
1:C:105:ILE:HD12	1:C:122:ILE:CG2	2.52	0.40
2:G:131:ILE:HG21	2:G:222:MET:HE3	2.03	0.40
2:G:339:ASP:O	2:G:343:ILE:HG13	2.22	0.40
2:G:408:TYR:CE1	2:H:25:ARG:HG2	2.55	0.40
2:H:22:ASN:HD22	2:H:22:ASN:HA	1.66	0.40
2:H:160:ARG:HG2	2:H:160:ARG:NH1	2.36	0.40
2:H:168:LEU:HD12	2:H:217:LYS:CD	2.49	0.40
2:H:366:ILE:HG13	2:H:420:ILE:CD1	2.51	0.40
1:B:94:LEU:HB3	1:B:122:ILE:HD12	2.03	0.40
1:B:107:THR:C	1:B:109:ASN:N	2.75	0.40
1:B:168:ILE:N	1:B:168:ILE:CD1	2.84	0.40
2:E:108:VAL:O	2:E:110:MET:N	2.55	0.40
2:E:355:TYR:CE2	2:E:400:GLU:OE2	2.73	0.40
2:F:168:LEU:O	2:F:168:LEU:HG	2.21	0.40
1:D:26:VAL:HG12	1:D:28:LYS:O	2.22	0.40
1:I:13:VAL:HG12	1:I:170:GLU:HG3	2.03	0.40
1:I:124:SER:HB3	1:I:159:CYS:SG	2.62	0.40
1:J:6:VAL:CG1	1:J:7:ARG:N	2.83	0.40
1:J:43:ILE:HG12	1:J:98:ALA:O	2.21	0.40
2:G:145:GLN:HG3	2:G:148:GLN:CG	2.50	0.40
2:G:234:VAL:O	2:G:236:PRO:HD3	2.22	0.40
1:A:137:LEU:HD23	1:A:137:LEU:O	2.22	0.40
1:B:66:MET:C	1:B:67:HIS:ND1	2.75	0.40
1:B:107:THR:O	1:B:109:ASN:N	2.54	0.40
2:E:145:GLN:C	2:E:147:GLU:N	2.75	0.40
2:F:12:GLU:HG2	2:F:73:LEU:HD11	2.02	0.40
2:F:219:LYS:HA	2:F:223:LYS:HZ3	1.86	0.40
2:F:229:GLU:O	2:F:230:ALA:HB2	2.22	0.40
2:G:432:LEU:HD12	2:G:432:LEU:H	1.87	0.40
1:L:88:LEU:O	1:L:91:LEU:HG	2.22	0.40
1:L:95:LEU:HD12	1:L:95:LEU:N	2.36	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:7:ARG:NH2	2:F:409:ASP:OD2[2_665]	2.01	0.19
1:K:160:ILE:CG2	1:K:160:ILE:CG2[4_666]	2.04	0.16
1:D:160:ILE:CG2	1:D:160:ILE:CG2[6_577]	2.19	0.01

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	172/175 (98%)	152 (88%)	16 (9%)	4 (2%)	6 21
1	B	172/175 (98%)	137 (80%)	25 (14%)	10 (6%)	1 4
1	C	172/175 (98%)	150 (87%)	17 (10%)	5 (3%)	4 15
1	D	172/175 (98%)	145 (84%)	23 (13%)	4 (2%)	6 21
1	I	172/175 (98%)	147 (86%)	20 (12%)	5 (3%)	4 15
1	J	172/175 (98%)	140 (81%)	26 (15%)	6 (4%)	3 12
1	K	172/175 (98%)	146 (85%)	23 (13%)	3 (2%)	9 29
1	L	172/175 (98%)	149 (87%)	18 (10%)	5 (3%)	4 15
2	E	404/449 (90%)	348 (86%)	47 (12%)	9 (2%)	6 22
2	F	404/449 (90%)	344 (85%)	43 (11%)	17 (4%)	3 9
2	G	404/449 (90%)	344 (85%)	48 (12%)	12 (3%)	4 15
2	H	404/449 (90%)	343 (85%)	45 (11%)	16 (4%)	3 9
All	All	2992/3196 (94%)	2545 (85%)	351 (12%)	96 (3%)	4 13

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	71	LEU
1	B	72	VAL
1	B	116	GLU
2	E	92	VAL
2	E	144	GLY

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Mol	Chain	Res	Type
2	E	153	SER
2	E	212	LYS
2	F	92	VAL
2	F	153	SER
2	F	165	GLU
2	F	212	LYS
2	F	237	GLU
1	C	116	GLU
1	D	69	GLY
1	J	116	GLU
2	G	92	VAL
2	G	144	GLY
2	G	146	THR
2	G	153	SER
2	G	212	LYS
2	H	92	VAL
2	H	153	SER
2	H	165	GLU
2	H	212	LYS
2	H	236	PRO
2	H	237	GLU
1	L	116	GLU
1	A	9	ASN
1	B	54	PHE
2	E	165	GLU
2	E	410	ALA
2	F	230	ALA
2	F	236	PRO
2	F	300	ASP
1	D	68	GLN
1	D	113	VAL
1	J	54	PHE
2	G	165	GLU
2	G	170	ASP
2	H	138	PRO
2	H	154	ALA
2	H	228	GLU
2	H	230	ALA
2	H	300	ASP
1	K	68	GLN
1	K	69	GLY
1	K	116	GLU

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Mol	Chain	Res	Type
1	L	69	GLY
1	A	115	PRO
1	B	68	GLN
2	E	141	ASN
2	E	146	THR
2	F	138	PRO
1	C	115	PRO
1	C	117	ASN
1	I	71	LEU
1	I	115	PRO
1	J	71	LEU
1	J	101	THR
2	G	141	ASN
2	G	227	GLU
2	G	232	LYS
2	H	143	TRP
2	H	146	THR
1	L	115	PRO
1	A	71	LEU
1	A	81	ASP
1	B	70	HIS
2	E	217	LYS
2	F	109	LYS
2	F	125	GLU
2	F	137	PRO
1	I	110	GLY
1	I	142	LEU
1	J	68	GLN
2	G	44	LEU
2	G	172	GLU
2	H	125	GLU
1	L	117	ASN
2	F	140	LYS
2	F	228	GLU
1	D	99	ASP
2	H	137	PRO
1	B	69	GLY
1	B	82	TRP
1	B	86	ARG
2	F	146	THR
2	F	154	ALA
1	C	40	ASP

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Mol	Chain	Res	Type
1	L	110	GLY
1	C	69	GLY
2	H	144	GLY
2	F	173	ILE
1	J	72	VAL
1	B	147	ILE
1	I	72	VAL

5.3.2 Protein sidechains (i)

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	136/136 (100%)	127 (93%)	9 (7%)	16 44
1	B	136/136 (100%)	123 (90%)	13 (10%)	8 24
1	C	136/136 (100%)	125 (92%)	11 (8%)	11 33
1	D	136/136 (100%)	122 (90%)	14 (10%)	7 21
1	I	136/136 (100%)	126 (93%)	10 (7%)	13 37
1	J	136/136 (100%)	125 (92%)	11 (8%)	11 33
1	K	136/136 (100%)	125 (92%)	11 (8%)	11 33
1	L	136/136 (100%)	125 (92%)	11 (8%)	11 33
2	E	350/383 (91%)	310 (89%)	40 (11%)	5 18
2	F	350/383 (91%)	300 (86%)	50 (14%)	3 10
2	G	350/383 (91%)	306 (87%)	44 (13%)	4 14
2	H	350/383 (91%)	302 (86%)	48 (14%)	3 11
All	All	2488/2620 (95%)	2216 (89%)	272 (11%)	6 19

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	9	ASN
1	A	30	ASN

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Mol	Chain	Res	Type
1	A	36	ARG
1	A	65	GLU
1	A	71	LEU
1	A	97	VAL
1	A	136	LEU
1	A	152	LEU
1	B	1	THR
1	B	8	ARG
1	B	22	LEU
1	B	30	ASN
1	B	54	PHE
1	B	99	ASP
1	B	104	LEU
1	B	112	VAL
1	B	116	GLU
1	B	136	LEU
1	B	152	LEU
1	B	160	ILE
1	B	174	LYS
2	E	11	SER
2	E	13	LEU
2	E	27	VAL
2	E	31	LEU
2	E	37	ARG
2	E	59	THR
2	E	92	VAL
2	E	94	LYS
2	E	103	LEU
2	E	117	GLU
2	E	122	ARG
2	E	130	ARG
2	E	140	LYS
2	E	152	PRO
2	E	167	GLN
2	E	169	ASP
2	E	171	LYS
2	E	173	ILE
2	E	220	ASP
2	E	238	GLU
2	E	240	LYS
2	E	241	GLN
2	E	266	GLU

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Mol	Chain	Res	Type
2	E	281	LEU
2	E	296	MET
2	E	300	ASP
2	E	311	GLN
2	E	312	ILE
2	E	318	LEU
2	E	326	LEU
2	E	337	THR
2	E	352	THR
2	E	355	TYR
2	E	375	ARG
2	E	385	GLU
2	E	386	SER
2	E	388	GLU
2	E	389	ASN
2	E	411	SER
2	E	412	ASP
2	F	13	LEU
2	F	27	VAL
2	F	31	LEU
2	F	37	ARG
2	F	41	ASN
2	F	59	THR
2	F	68	ARG
2	F	70	LEU
2	F	87	THR
2	F	94	LYS
2	F	103	LEU
2	F	104	THR
2	F	108	VAL
2	F	121	TYR
2	F	130	ARG
2	F	140	LYS
2	F	141	ASN
2	F	145	GLN
2	F	148	GLN
2	F	150	GLN
2	F	165	GLU
2	F	173	ILE
2	F	210	LYS
2	F	211	GLN
2	F	214	ARG

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Mol	Chain	Res	Type
2	F	217	LYS
2	F	219	LYS
2	F	220	ASP
2	F	225	LEU
2	F	232	LYS
2	F	239	LEU
2	F	266	GLU
2	F	296	MET
2	F	300	ASP
2	F	311	GLN
2	F	312	ILE
2	F	318	LEU
2	F	326	LEU
2	F	337	THR
2	F	344	LEU
2	F	351	ILE
2	F	352	THR
2	F	355	TYR
2	F	382	GLN
2	F	385	GLU
2	F	389	ASN
2	F	404	GLU
2	F	413	LEU
2	F	438	LEU
2	F	442	ILE
1	C	1	THR
1	C	30	ASN
1	C	36	ARG
1	C	37	LEU
1	C	54	PHE
1	C	67	HIS
1	C	71	LEU
1	C	81	ASP
1	C	87	MET
1	C	99	ASP
1	C	152	LEU
1	D	1	THR
1	D	30	ASN
1	D	35	ARG
1	D	39	ASN
1	D	43	ILE
1	D	73	LYS

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Mol	Chain	Res	Type
1	D	77	GLU
1	D	80	LYS
1	D	104	LEU
1	D	114	GLN
1	D	116	GLU
1	D	118	ASP
1	D	136	LEU
1	D	152	LEU
1	I	1	THR
1	I	4	VAL
1	I	30	ASN
1	I	36	ARG
1	I	71	LEU
1	I	99	ASP
1	I	116	GLU
1	I	152	LEU
1	I	160	ILE
1	I	166	HIS
1	J	1	THR
1	J	22	LEU
1	J	30	ASN
1	J	54	PHE
1	J	65	GLU
1	J	97	VAL
1	J	112	VAL
1	J	136	LEU
1	J	152	LEU
1	J	160	ILE
1	J	174	LYS
2	G	13	LEU
2	G	27	VAL
2	G	31	LEU
2	G	37	ARG
2	G	49	THR
2	G	70	LEU
2	G	92	VAL
2	G	94	LYS
2	G	117	GLU
2	G	122	ARG
2	G	130	ARG
2	G	140	LYS
2	G	148	GLN

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Mol	Chain	Res	Type
2	G	152	PRO
2	G	164	ARG
2	G	165	GLU
2	G	168	LEU
2	G	169	ASP
2	G	171	LYS
2	G	173	ILE
2	G	216	LEU
2	G	220	ASP
2	G	225	LEU
2	G	238	GLU
2	G	240	LYS
2	G	241	GLN
2	G	266	GLU
2	G	296	MET
2	G	300	ASP
2	G	311	GLN
2	G	312	ILE
2	G	318	LEU
2	G	326	LEU
2	G	337	THR
2	G	344	LEU
2	G	352	THR
2	G	353	VAL
2	G	355	TYR
2	G	370	ASP
2	G	385	GLU
2	G	386	SER
2	G	388	GLU
2	G	389	ASN
2	G	438	LEU
2	H	13	LEU
2	H	27	VAL
2	H	31	LEU
2	H	41	ASN
2	H	59	THR
2	H	70	LEU
2	H	87	THR
2	H	94	LYS
2	H	103	LEU
2	H	104	THR
2	H	121	TYR

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Mol	Chain	Res	Type
2	H	130	ARG
2	H	138	PRO
2	H	140	LYS
2	H	141	ASN
2	H	145	GLN
2	H	148	GLN
2	H	150	GLN
2	H	152	PRO
2	H	160	ARG
2	H	169	ASP
2	H	173	ILE
2	H	210	LYS
2	H	211	GLN
2	H	214	ARG
2	H	217	LYS
2	H	219	LYS
2	H	238	GLU
2	H	239	LEU
2	H	266	GLU
2	H	296	MET
2	H	300	ASP
2	H	311	GLN
2	H	312	ILE
2	H	318	LEU
2	H	326	LEU
2	H	337	THR
2	H	344	LEU
2	H	351	ILE
2	H	352	THR
2	H	375	ARG
2	H	384	ASN
2	H	388	GLU
2	H	389	ASN
2	H	404	GLU
2	H	413	LEU
2	H	438	LEU
2	H	442	ILE
1	K	1	THR
1	K	30	ASN
1	K	40	ASP
1	K	54	PHE
1	K	80	LYS

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Mol	Chain	Res	Type
1	K	83	ARG
1	K	104	LEU
1	K	111	ASP
1	K	116	GLU
1	K	136	LEU
1	K	152	LEU
1	L	1	THR
1	L	30	ASN
1	L	36	ARG
1	L	37	LEU
1	L	43	ILE
1	L	54	PHE
1	L	73	LYS
1	L	116	GLU
1	L	118	ASP
1	L	152	LEU
1	L	174	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	39	ASN
1	A	109	ASN
1	A	166	HIS
1	B	11	HIS
1	B	30	ASN
1	B	109	ASN
1	B	130	GLN
2	E	22	ASN
2	E	33	ASN
2	E	75	ASN
2	E	114	GLN
2	E	141	ASN
2	E	149	GLN
2	E	150	GLN
2	E	241	GLN
2	E	294	HIS
2	E	311	GLN
2	E	348	ASN
2	E	382	GLN
2	E	384	ASN

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Mol	Chain	Res	Type
2	E	389	ASN
2	E	416	GLN
2	E	428	HIS
2	F	22	ASN
2	F	41	ASN
2	F	75	ASN
2	F	114	GLN
2	F	119	ASN
2	F	141	ASN
2	F	142	ASN
2	F	145	GLN
2	F	149	GLN
2	F	150	GLN
2	F	211	GLN
2	F	311	GLN
2	F	348	ASN
2	F	384	ASN
2	F	389	ASN
2	F	416	GLN
1	C	9	ASN
1	C	30	ASN
1	D	11	HIS
1	D	30	ASN
1	D	114	GLN
1	I	9	ASN
1	I	30	ASN
1	I	39	ASN
1	I	109	ASN
1	J	30	ASN
1	J	109	ASN
1	J	130	GLN
2	G	22	ASN
2	G	33	ASN
2	G	75	ASN
2	G	114	GLN
2	G	149	GLN
2	G	150	GLN
2	G	241	GLN
2	G	294	HIS
2	G	311	GLN
2	G	348	ASN
2	G	382	GLN

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Mol	Chain	Res	Type
2	G	384	ASN
2	G	389	ASN
2	G	416	GLN
2	G	428	HIS
2	H	22	ASN
2	H	33	ASN
2	H	41	ASN
2	H	75	ASN
2	H	114	GLN
2	H	119	ASN
2	H	142	ASN
2	H	145	GLN
2	H	149	GLN
2	H	150	GLN
2	H	167	GLN
2	H	211	GLN
2	H	311	GLN
2	H	348	ASN
2	H	384	ASN
2	H	389	ASN
2	H	416	GLN
2	H	428	HIS
1	K	30	ASN
1	K	39	ASN
1	K	114	GLN
1	L	9	ASN
1	L	11	HIS
1	L	30	ASN
1	L	114	GLN
1	L	139	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ADP	H	3450	-	24,29,29	1.59	5 (20%)	29,45,45	1.27	4 (13%)
3	ADP	G	2450	-	24,29,29	1.65	6 (25%)	29,45,45	1.28	5 (17%)
3	ADP	F	1450	-	24,29,29	1.50	3 (12%)	29,45,45	1.24	3 (10%)
3	ADP	E	450	-	24,29,29	1.69	7 (29%)	29,45,45	1.28	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	H	3450	-	-	3/12/32/32	0/3/3/3
3	ADP	G	2450	-	-	3/12/32/32	0/3/3/3
3	ADP	F	1450	-	-	3/12/32/32	0/3/3/3
3	ADP	E	450	-	-	3/12/32/32	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	450	ADP	C8-N7	-4.30	1.27	1.34
3	H	3450	ADP	C8-N7	-4.26	1.27	1.34
3	G	2450	ADP	C8-N7	-4.12	1.27	1.34
3	F	1450	ADP	C8-N7	-4.02	1.27	1.34
3	G	2450	ADP	C2'-C1'	2.99	1.58	1.53
3	H	3450	ADP	C4-N3	2.77	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	3450	ADP	C2-N3	2.74	1.36	1.32
3	E	450	ADP	C2-N3	2.65	1.36	1.32
3	E	450	ADP	C2'-C1'	2.55	1.57	1.53
3	G	2450	ADP	C4-N3	2.55	1.39	1.35
3	G	2450	ADP	C2-N3	2.53	1.36	1.32
3	E	450	ADP	C4-N3	2.50	1.39	1.35
3	F	1450	ADP	C2-N3	2.50	1.36	1.32
3	F	1450	ADP	C4-N3	2.47	1.39	1.35
3	E	450	ADP	PA-O1A	-2.34	1.42	1.50
3	E	450	ADP	O4'-C1'	2.32	1.44	1.41
3	H	3450	ADP	O4'-C1'	2.22	1.44	1.41
3	G	2450	ADP	O4'-C1'	2.19	1.44	1.41
3	H	3450	ADP	PA-O1A	-2.07	1.43	1.50
3	E	450	ADP	PA-O2A	-2.05	1.45	1.55
3	G	2450	ADP	PA-O2A	-2.02	1.45	1.55

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2450	ADP	C2'-C3'-C4'	3.21	108.88	102.64
3	H	3450	ADP	C2'-C3'-C4'	3.20	108.86	102.64
3	E	450	ADP	C3'-C2'-C1'	3.17	105.74	100.98
3	E	450	ADP	C2'-C3'-C4'	3.12	108.70	102.64
3	H	3450	ADP	C3'-C2'-C1'	3.10	105.64	100.98
3	F	1450	ADP	C2'-C3'-C4'	3.07	108.61	102.64
3	F	1450	ADP	C3'-C2'-C1'	3.03	105.54	100.98
3	G	2450	ADP	C3'-C2'-C1'	2.86	105.28	100.98
3	H	3450	ADP	N3-C2-N1	-2.45	124.86	128.68
3	F	1450	ADP	N3-C2-N1	-2.35	125.00	128.68
3	G	2450	ADP	N3-C2-N1	-2.30	125.08	128.68
3	E	450	ADP	N3-C2-N1	-2.22	125.20	128.68
3	E	450	ADP	O2A-PA-O1A	2.21	123.19	112.24
3	H	3450	ADP	O2A-PA-O1A	2.15	122.86	112.24
3	G	2450	ADP	O3B-PB-O3A	2.09	111.64	104.64
3	G	2450	ADP	O2A-PA-O1A	2.05	122.37	112.24

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	450	ADP	O4'-C4'-C5'-O5'
3	F	1450	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	G	2450	ADP	O4'-C4'-C5'-O5'
3	H	3450	ADP	O4'-C4'-C5'-O5'
3	H	3450	ADP	C3'-C4'-C5'-O5'
3	F	1450	ADP	C3'-C4'-C5'-O5'
3	G	2450	ADP	C3'-C4'-C5'-O5'
3	H	3450	ADP	C4'-C5'-O5'-PA
3	E	450	ADP	C4'-C5'-O5'-PA
3	G	2450	ADP	C4'-C5'-O5'-PA
3	F	1450	ADP	C4'-C5'-O5'-PA
3	E	450	ADP	C3'-C4'-C5'-O5'

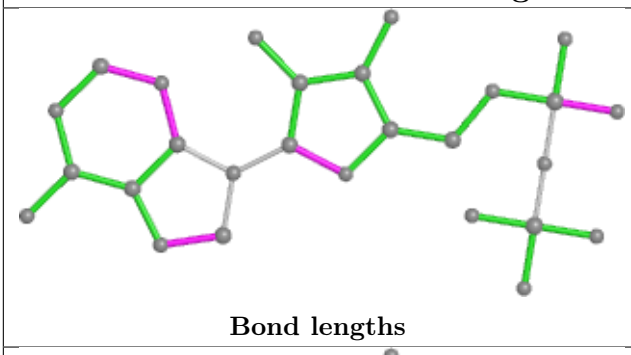
There are no ring outliers.

4 monomers are involved in 10 short contacts:

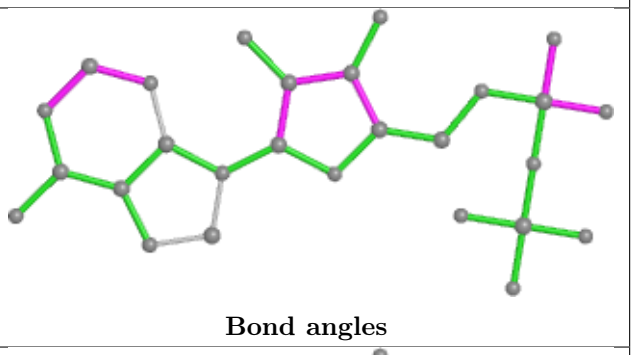
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	3450	ADP	3	0
3	G	2450	ADP	2	0
3	F	1450	ADP	3	0
3	E	450	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

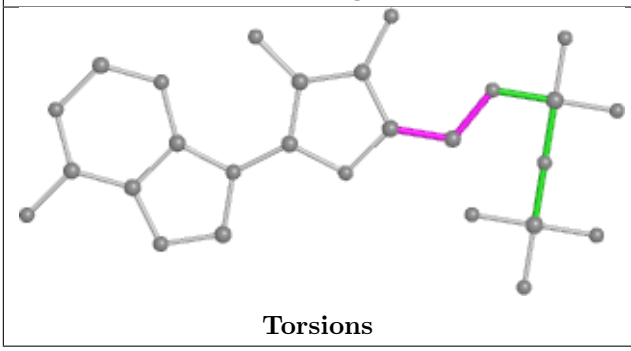
Ligand ADP H 3450



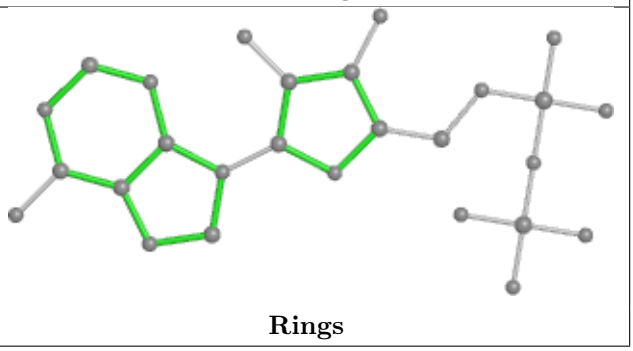
Bond lengths



Bond angles

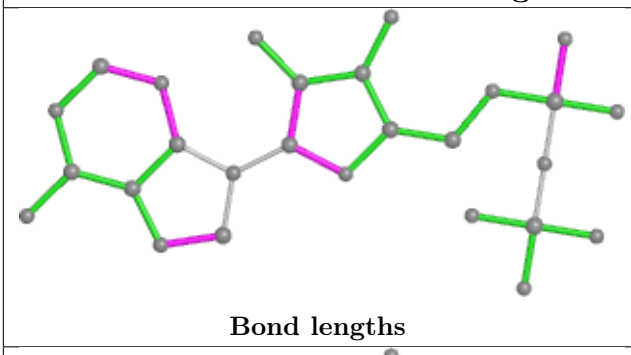


Torsions

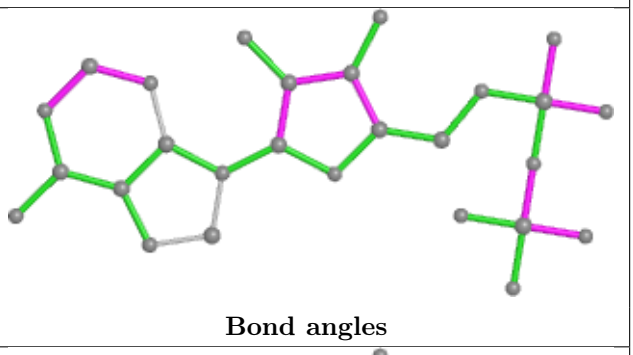


Rings

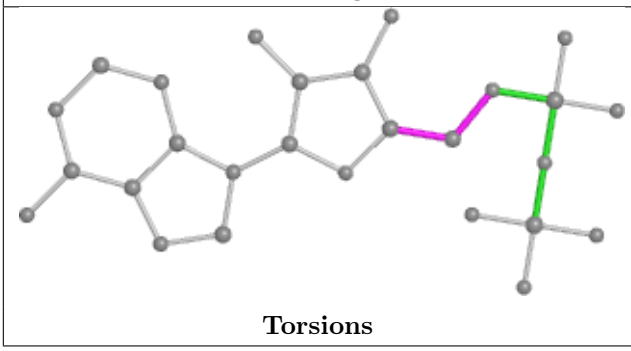
Ligand ADP G 2450



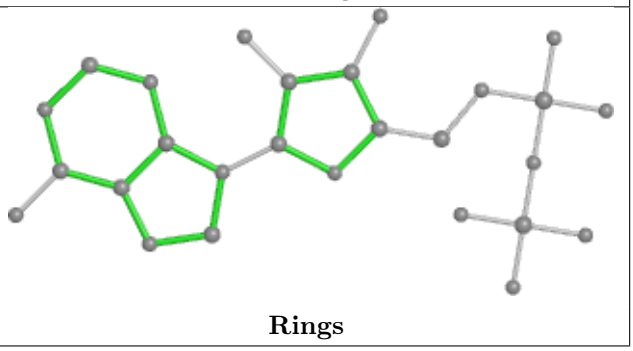
Bond lengths



Bond angles

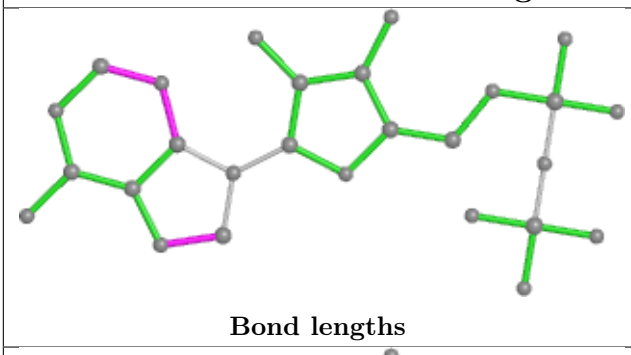


Torsions

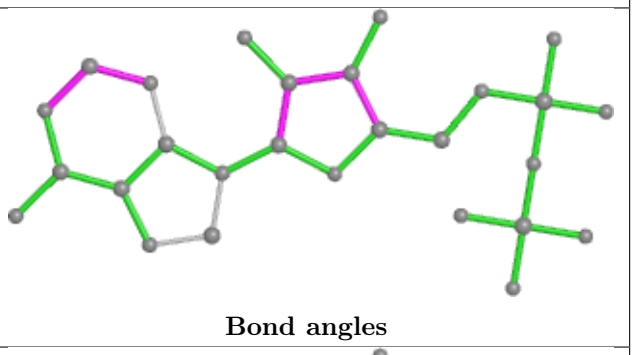


Rings

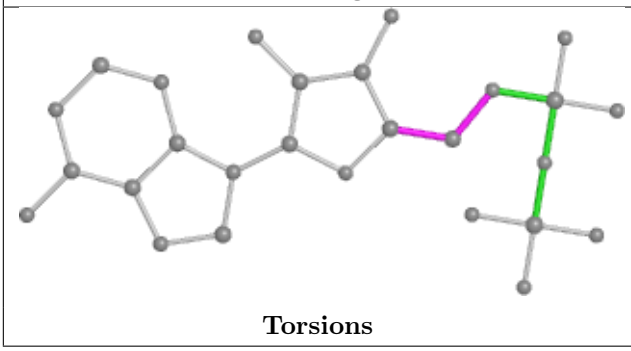
Ligand ADP F 1450



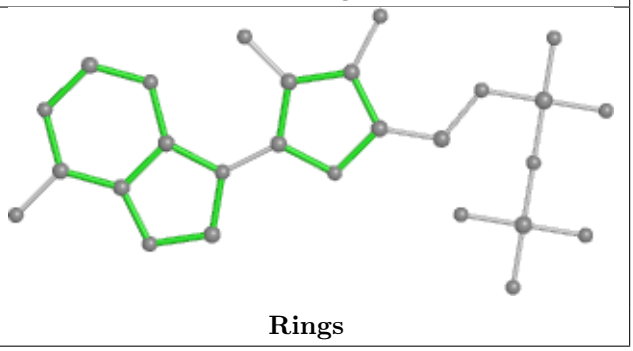
Bond lengths



Bond angles

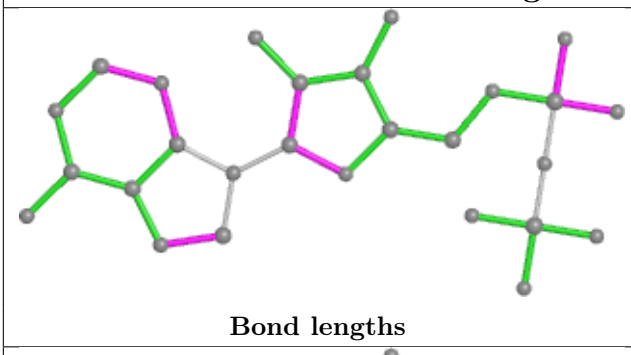


Torsions

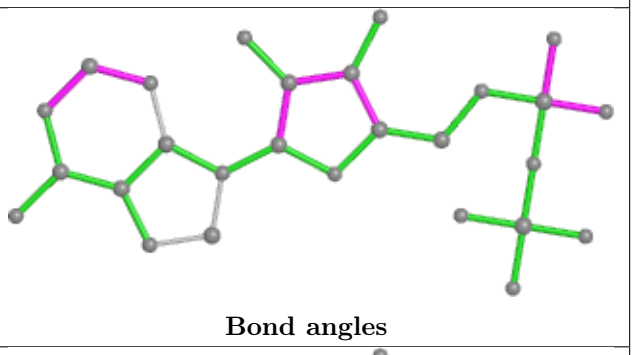


Rings

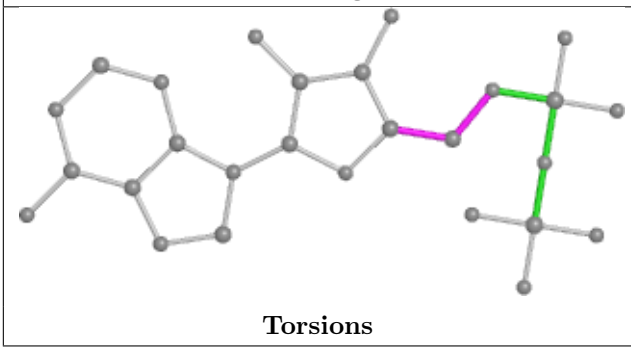
Ligand ADP E 450



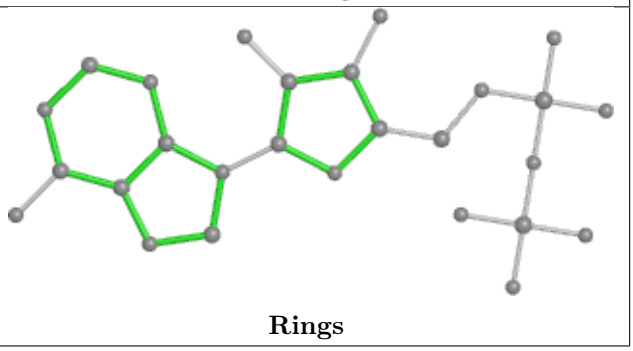
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	174/175 (99%)	0.44	2 (1%) 80 75	33, 58, 91, 99	0
1	B	174/175 (99%)	0.52	10 (5%) 23 15	38, 70, 101, 102	0
1	C	174/175 (99%)	0.39	3 (1%) 70 63	51, 68, 98, 101	0
1	D	174/175 (99%)	0.58	12 (6%) 16 10	54, 87, 101, 102	0
1	I	174/175 (99%)	0.46	2 (1%) 80 75	29, 56, 89, 97	0
1	J	174/175 (99%)	0.55	5 (2%) 51 41	36, 70, 100, 102	0
1	K	174/175 (99%)	0.70	18 (10%) 6 3	62, 95, 102, 102	0
1	L	174/175 (99%)	0.51	8 (4%) 32 22	57, 80, 102, 102	0
2	E	408/449 (90%)	0.62	37 (9%) 9 5	32, 59, 102, 102	0
2	F	408/449 (90%)	0.93	68 (16%) 1 1	35, 61, 102, 102	0
2	G	408/449 (90%)	0.61	33 (8%) 12 6	35, 62, 102, 102	0
2	H	408/449 (90%)	0.79	52 (12%) 3 2	35, 63, 102, 102	0
All	All	3024/3196 (94%)	0.63	250 (8%) 11 6	29, 66, 102, 102	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	144	GLY	11.3
2	F	144	GLY	10.2
2	F	90	GLY	10.2
2	F	146	THR	9.2
2	F	141	ASN	7.5
2	G	90	GLY	7.4
2	H	141	ASN	7.2
2	F	153	SER	6.9
2	E	144	GLY	6.4
2	H	168	LEU	6.4
2	F	89	VAL	6.0

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Mol	Chain	Res	Type	RSRZ
2	E	143	TRP	5.8
2	H	140	LYS	5.8
2	F	165	GLU	5.5
2	H	145	GLN	5.4
2	H	144	GLY	5.4
2	E	140	LYS	5.4
2	H	226	ILE	5.3
2	H	143	TRP	5.1
2	H	134	VAL	5.1
2	F	133	ASP	5.1
2	F	226	ILE	5.0
2	G	153	SER	4.9
2	F	222	MET	4.9
2	G	140	LYS	4.9
2	F	132	LEU	4.7
2	H	154	ALA	4.7
2	F	91	TYR	4.7
2	E	148	GLN	4.7
2	F	173	ILE	4.7
2	F	267	SER	4.6
2	H	123	ALA	4.6
2	F	123	ALA	4.6
2	G	267	SER	4.5
2	H	91	TYR	4.5
2	H	146	THR	4.5
2	G	89	VAL	4.5
2	F	134	VAL	4.5
2	F	138	PRO	4.4
2	E	145	GLN	4.4
2	E	267	SER	4.4
1	K	93	ALA	4.4
2	F	264	ARG	4.4
2	F	169	ASP	4.3
2	H	152	PRO	4.3
2	H	131	ILE	4.2
2	H	221	ALA	4.2
2	E	264	ARG	4.1
1	B	60	PHE	4.1
2	F	219	LYS	4.1
2	H	170	ASP	4.1
2	G	148	GLN	4.0
2	F	168	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
2	F	211	GLN	3.9
2	H	89	VAL	3.9
2	F	221	ALA	3.8
2	H	165	GLU	3.8
2	F	151	GLU	3.8
2	F	145	GLN	3.8
2	F	143	TRP	3.8
1	K	42	VAL	3.8
1	K	174	LYS	3.7
2	H	132	LEU	3.7
2	G	143	TRP	3.7
1	K	44	ALA	3.7
2	F	233	LEU	3.7
2	H	173	ILE	3.7
2	E	215	LYS	3.6
2	G	117	GLU	3.6
2	F	266	GLU	3.5
1	K	53	ALA	3.5
2	H	222	MET	3.5
2	E	173	ILE	3.5
2	E	89	VAL	3.4
2	E	92	VAL	3.4
2	G	91	TYR	3.4
2	E	134	VAL	3.4
2	G	215	LYS	3.4
2	H	211	GLN	3.4
1	K	94	LEU	3.4
2	H	264	ARG	3.4
2	G	145	GLN	3.4
2	F	139	ALA	3.4
1	L	93	ALA	3.4
1	A	83	ARG	3.3
2	H	113	VAL	3.3
1	J	42	VAL	3.3
2	G	265	GLY	3.3
2	G	214	ARG	3.2
2	G	123	ALA	3.2
2	F	119	ASN	3.2
2	F	128	GLU	3.2
2	E	265	GLY	3.2
2	F	172	GLU	3.2
2	H	92	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	219	LYS	3.1
2	H	166	GLY	3.1
2	G	171	LYS	3.1
2	G	216	LEU	3.1
1	J	60	PHE	3.1
1	K	43	ILE	3.1
2	E	91	TYR	3.1
2	E	210	LYS	3.1
2	H	224	LEU	3.1
2	F	154	ALA	3.1
1	D	60	PHE	3.1
2	F	216	LEU	3.1
2	G	146	THR	3.1
1	C	93	ALA	3.0
1	D	173	TYR	3.0
2	F	92	VAL	3.0
2	E	212	LYS	3.0
2	E	141	ASN	3.0
1	L	112	VAL	3.0
1	B	98	ALA	3.0
2	E	214	ARG	3.0
1	L	113	VAL	3.0
2	F	117	GLU	2.9
2	H	137	PRO	2.9
2	H	267	SER	2.9
2	F	170	ASP	2.9
2	F	213	ALA	2.9
2	F	355	TYR	2.9
2	F	124	GLU	2.9
2	H	138	PRO	2.9
2	H	128	GLU	2.9
1	D	86	ARG	2.8
2	F	1	HIS	2.8
2	F	265	GLY	2.8
1	D	90	LYS	2.8
1	L	78	LEU	2.8
2	H	90	GLY	2.8
1	C	91	LEU	2.8
2	G	227	GLU	2.8
2	F	234	VAL	2.8
2	G	210	LYS	2.7
2	F	214	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	G	264	ARG	2.7
1	B	57	PHE	2.7
2	E	227	GLU	2.7
2	E	90	GLY	2.7
2	G	141	ASN	2.7
1	D	38	TYR	2.7
2	E	224	LEU	2.7
2	H	117	GLU	2.7
1	I	83	ARG	2.6
1	K	98	ALA	2.6
2	F	225	LEU	2.6
2	G	112	ARG	2.6
1	D	98	ALA	2.6
2	F	112	ARG	2.6
1	K	97	VAL	2.6
2	E	109	LYS	2.6
2	E	142	ASN	2.6
2	E	270	PRO	2.6
2	F	167	GLN	2.5
2	E	152	PRO	2.5
2	E	225	LEU	2.5
2	H	112	ARG	2.5
1	K	111	ASP	2.5
1	K	34	VAL	2.5
1	B	46	PHE	2.5
1	K	60	PHE	2.5
2	H	223	LYS	2.5
2	E	112	ARG	2.5
1	L	110	GLY	2.5
1	K	90	LYS	2.5
2	H	130	ARG	2.5
2	H	266	GLU	2.5
2	G	418	ILE	2.5
1	K	104	LEU	2.4
2	F	164	ARG	2.4
2	F	270	PRO	2.4
2	H	234	VAL	2.4
2	F	152	PRO	2.4
2	E	151	GLU	2.4
2	F	140	LYS	2.4
1	K	171	LEU	2.4
2	F	121	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	227	GLU	2.4
1	J	69	GLY	2.4
1	B	104	LEU	2.4
1	D	42	VAL	2.4
2	H	124	GLU	2.4
2	E	146	THR	2.4
2	G	147	GLU	2.3
1	K	173	TYR	2.3
1	B	136	LEU	2.3
2	F	218	ILE	2.3
2	G	219	LYS	2.3
2	F	130	ARG	2.3
2	F	125	GLU	2.3
2	F	244	ILE	2.3
2	H	151	GLU	2.3
2	E	266	GLU	2.3
2	H	133	ASP	2.3
2	H	227	GLU	2.3
1	D	102	ALA	2.3
2	E	234	VAL	2.3
1	I	73	LYS	2.3
2	E	147	GLU	2.3
2	F	83	ALA	2.3
1	B	112	VAL	2.2
1	A	73	LYS	2.2
2	F	110	MET	2.2
2	G	266	GLU	2.2
1	L	39	ASN	2.2
2	G	138	PRO	2.2
2	G	211	GLN	2.2
2	H	142	ASN	2.2
1	K	54	PHE	2.2
2	H	139	ALA	2.2
1	C	89	ARG	2.2
2	G	139	ALA	2.2
2	F	157	GLN	2.2
2	H	214	ARG	2.2
2	H	217	LYS	2.2
2	F	129	GLU	2.2
2	F	223	LYS	2.2
1	B	88	LEU	2.1
2	E	170	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	225	LEU	2.1
2	F	156	ARG	2.1
1	J	97	VAL	2.1
1	J	171	LEU	2.1
2	F	220	ASP	2.1
1	B	120	ILE	2.1
1	K	102	ALA	2.1
2	E	418	ILE	2.1
2	H	244	ILE	2.1
2	E	153	SER	2.1
1	L	91	LEU	2.1
2	F	224	LEU	2.1
2	G	110	MET	2.1
2	H	148	GLN	2.1
2	H	355	TYR	2.1
1	D	34	VAL	2.1
1	D	113	VAL	2.1
1	L	97	VAL	2.1
2	F	126	LEU	2.1
1	B	34	VAL	2.1
2	F	217	LYS	2.0
1	D	94	LEU	2.0
2	H	159	PHE	2.0
2	G	109	LYS	2.0
1	D	67	HIS	2.0
2	E	171	LYS	2.0
2	H	169	ASP	2.0
2	F	127	ALA	2.0
2	E	35	TRP	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 monosaccharides in this entry.

6.4 Ligands

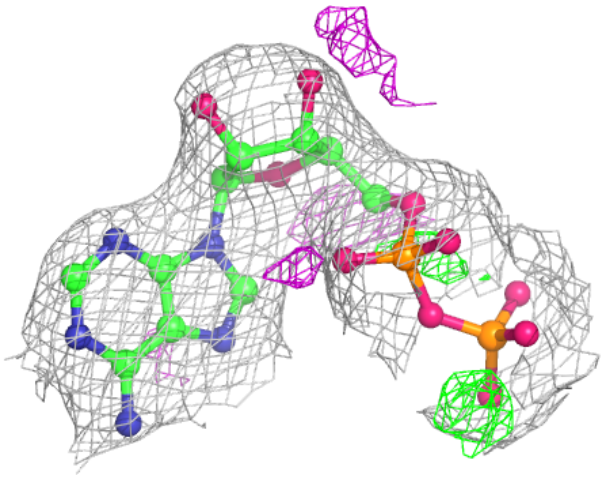
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

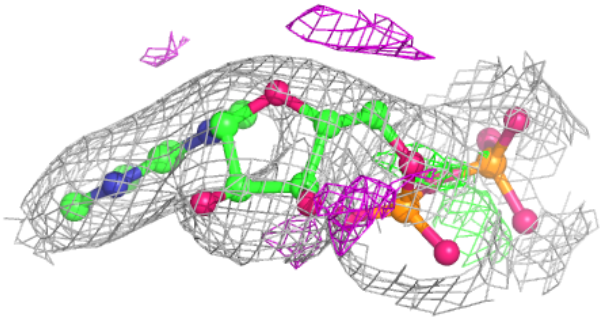
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	E	450	27/27	0.96	0.26	46,50,60,62	0
3	ADP	F	1450	27/27	0.96	0.26	45,50,57,59	0
3	ADP	G	2450	27/27	0.96	0.24	43,51,61,61	0
3	ADP	H	3450	27/27	0.96	0.26	53,55,58,61	0

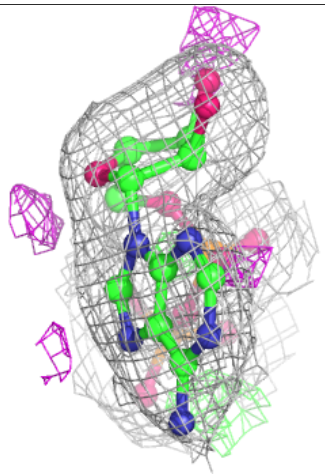
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP E 450:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

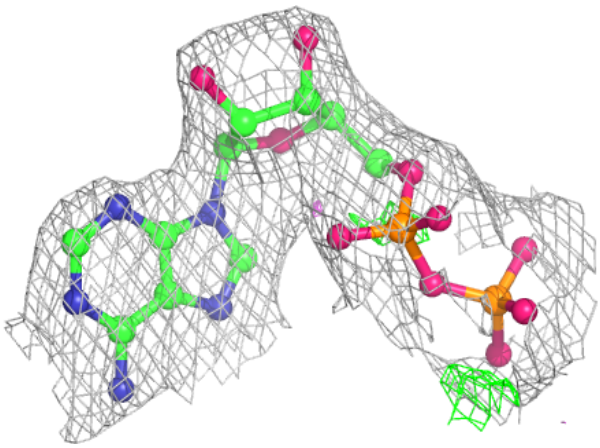


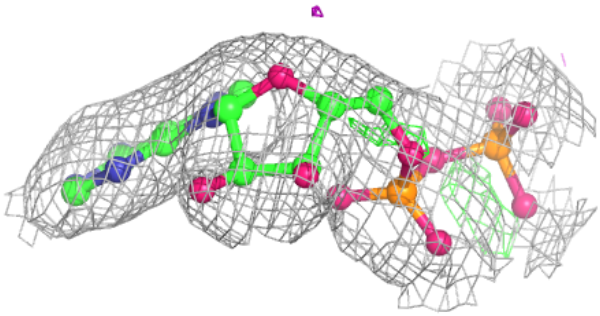


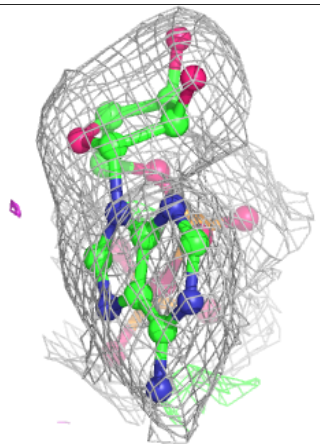


Electron density around ADP F 1450:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

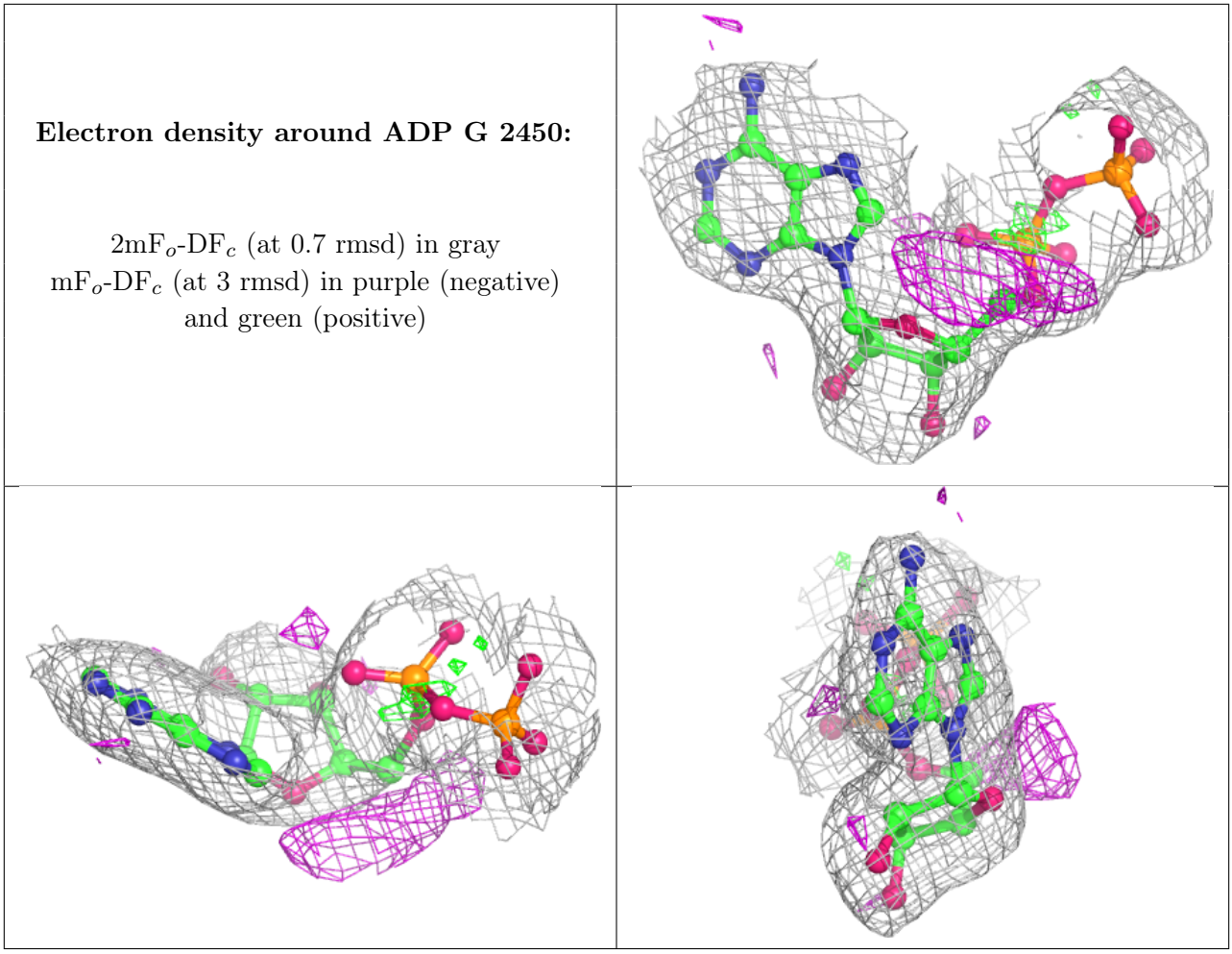






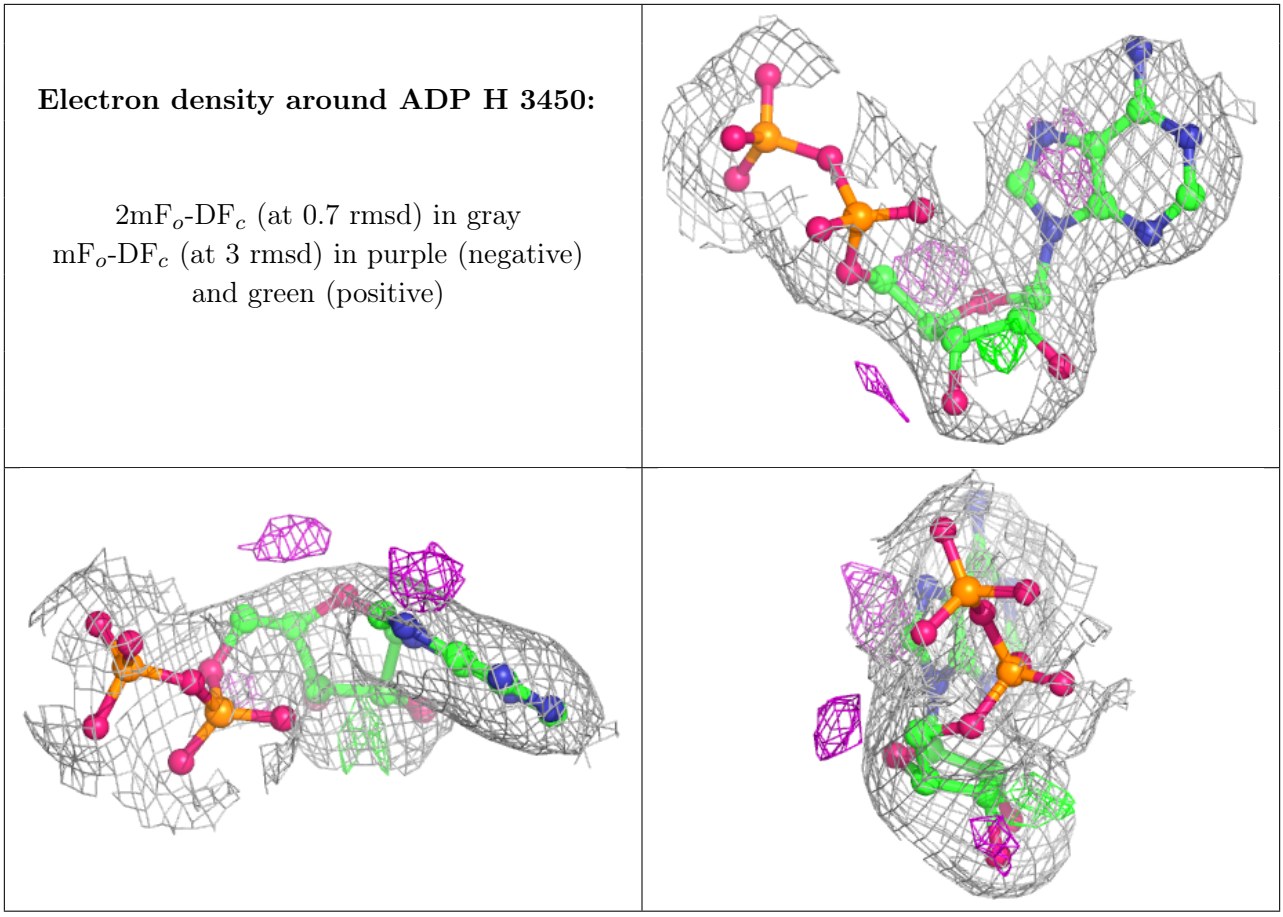
Electron density around ADP G 2450:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ADP H 3450:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.