Full wwPDB X-ray Structure Validation Report (i)

Aug 14, 2023 – 10:59 PM EDT

PDB ID	:	1R4N
Title	:	APPBP1-UBA3-NEDD8, an E1-ubiquitin-like protein complex with ATP
Authors	:	Walden, H.; Podgorski, M.S.; Holton, J.M.; Schulman, B.A.
Deposited on	:	2003-10-07
Resolution	:	3.60 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 (i) 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 (1)) were used in the production of this report:

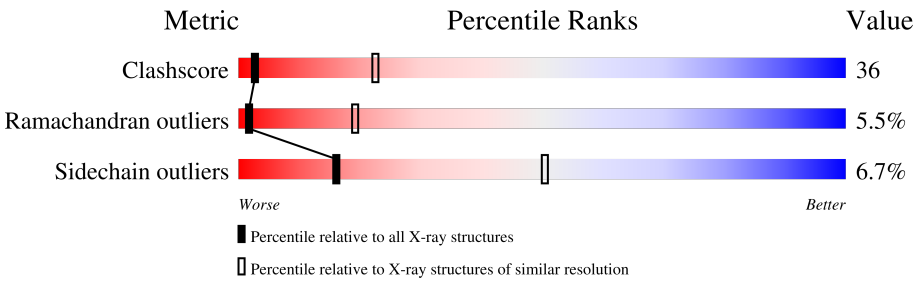
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.60 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))
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	529	50% 41% 6% • •
1	C	529	49% 43% 5% • •
1	E	529	50% 41% 5% • •
1	G	529	52% 39% 6% • •
2	B	431	44% 42% 9% • •
2	D	431	45% 41% 9% • •
2	F	431	46% 40% 9% • •
2	H	431	45% 43% 8% • •

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Mol	Chain	Length	Quality of chain
3	I	76	42% 54% •
3	J	76	39% 54% 7%
3	K	76	39% 55% 5%
3	L	76	42% 53% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATP	H	8	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 31744 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 amyloid beta precursor protein-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	516	4105	2602	699	789	15	0	0	0
1	C	516	4105	2602	699	789	15	0	0	0
1	E	516	4105	2602	699	789	15	0	0	0
1	G	516	4105	2602	699	789	15	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP Q13564
A	?	-	GLU	deletion	UNP Q13564
A	?	-	ASN	deletion	UNP Q13564
A	?	-	GLY	deletion	UNP Q13564
A	?	-	ALA	deletion	UNP Q13564
C	?	-	ASN	deletion	UNP Q13564
C	?	-	GLU	deletion	UNP Q13564
C	?	-	ASN	deletion	UNP Q13564
C	?	-	GLY	deletion	UNP Q13564
C	?	-	ALA	deletion	UNP Q13564
E	?	-	ASN	deletion	UNP Q13564
E	?	-	GLU	deletion	UNP Q13564
E	?	-	ASN	deletion	UNP Q13564
E	?	-	GLY	deletion	UNP Q13564
E	?	-	ALA	deletion	UNP Q13564
G	?	-	ASN	deletion	UNP Q13564
G	?	-	GLU	deletion	UNP Q13564
G	?	-	ASN	deletion	UNP Q13564
G	?	-	GLY	deletion	UNP Q13564
G	?	-	ALA	deletion	UNP Q13564

- Molecule 2 is a protein called ubiquitin-activating enzyme E1C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	418	3199	2038	549	595	17	0	0	0
2	D	418	3199	2038	549	595	17	0	0	0
2	F	418	3199	2038	549	595	17	0	0	0
2	H	418	3199	2038	549	595	17	0	0	0

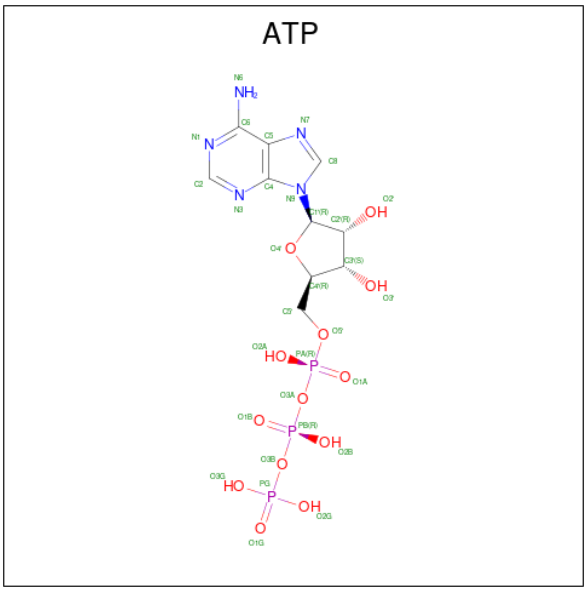
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	150	ALA	CYS	engineered mutation	UNP Q8TBC4
D	150	ALA	CYS	engineered mutation	UNP Q8TBC4
F	150	ALA	CYS	engineered mutation	UNP Q8TBC4
H	150	ALA	CYS	engineered mutation	UNP Q8TBC4

- Molecule 3 is a protein called Ubiquitin-like protein NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	76	600	378	104	116	2	0	0	0
3	J	76	600	378	104	116	2	0	0	0
3	K	76	600	378	104	116	2	0	0	0
3	L	76	600	378	104	116	2	0	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	B	1	31	10	5	13	3	0	0
4	D	1	31	10	5	13	3	0	0
4	F	1	31	10	5	13	3	0	0
4	H	1	31	10	5	13	3	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	J	1	1	1	0	0
5	F	1	1	1	0	0
5	H	2	2	2	0	0

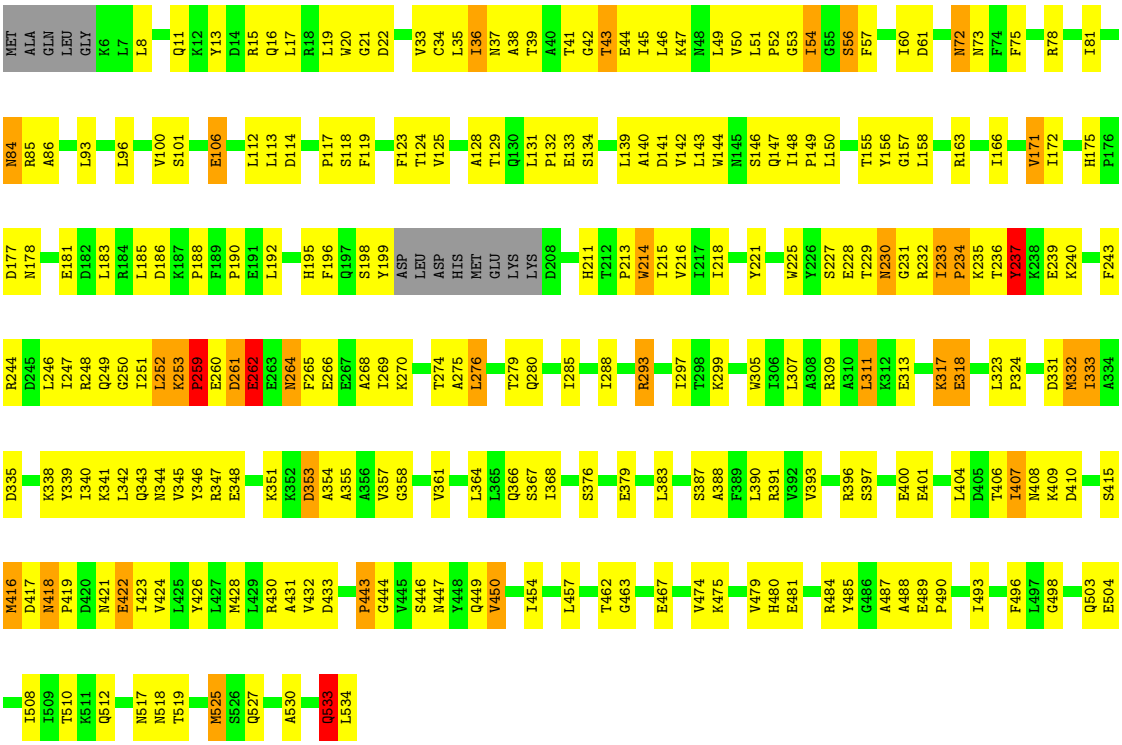
3 Residue-property plots (i)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

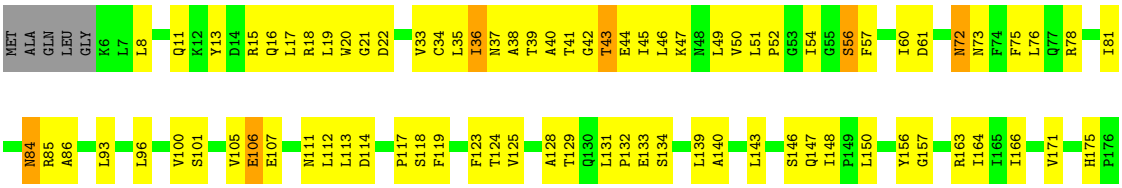
• Molecule 1: amyloid beta precursor protein-binding protein 1

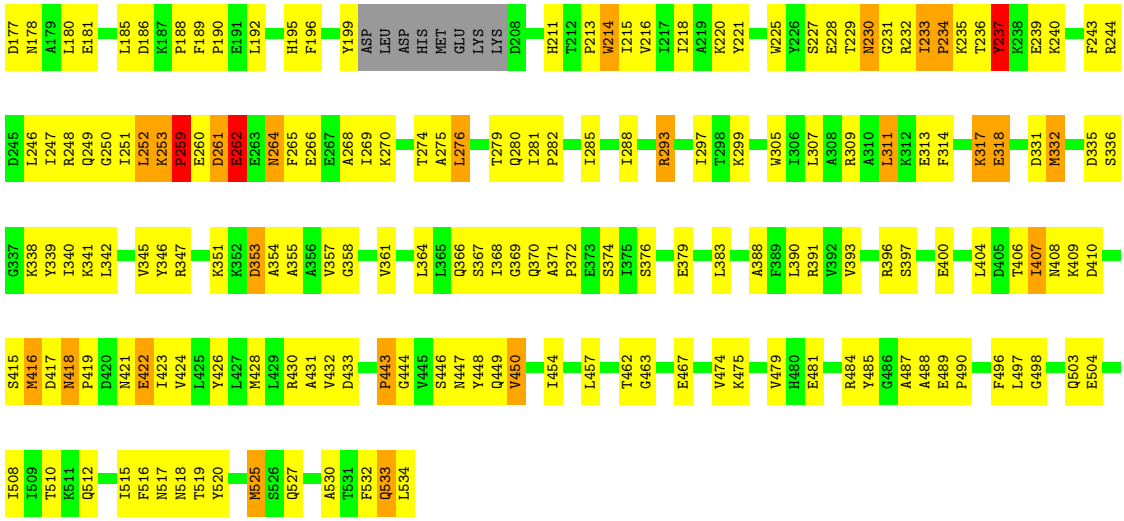
Chain A: 50% 41% 6% • •



• Molecule 1: amyloid beta precursor protein-binding protein 1

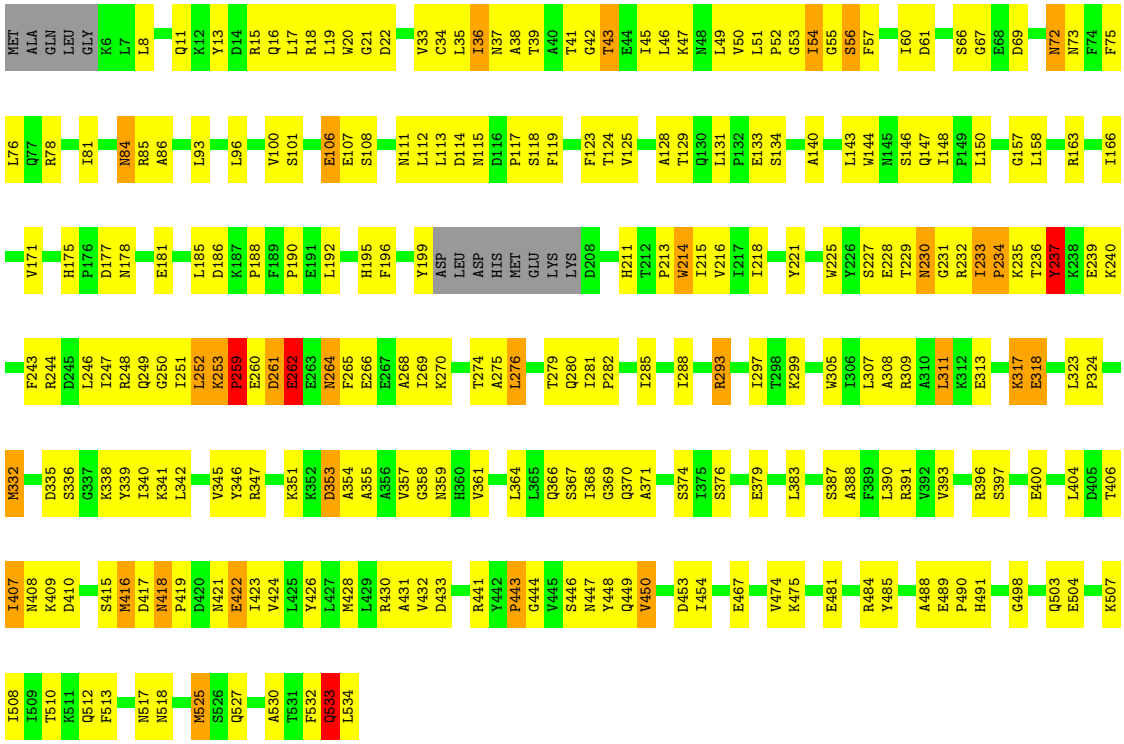
Chain C: 49% 43% 5% • •





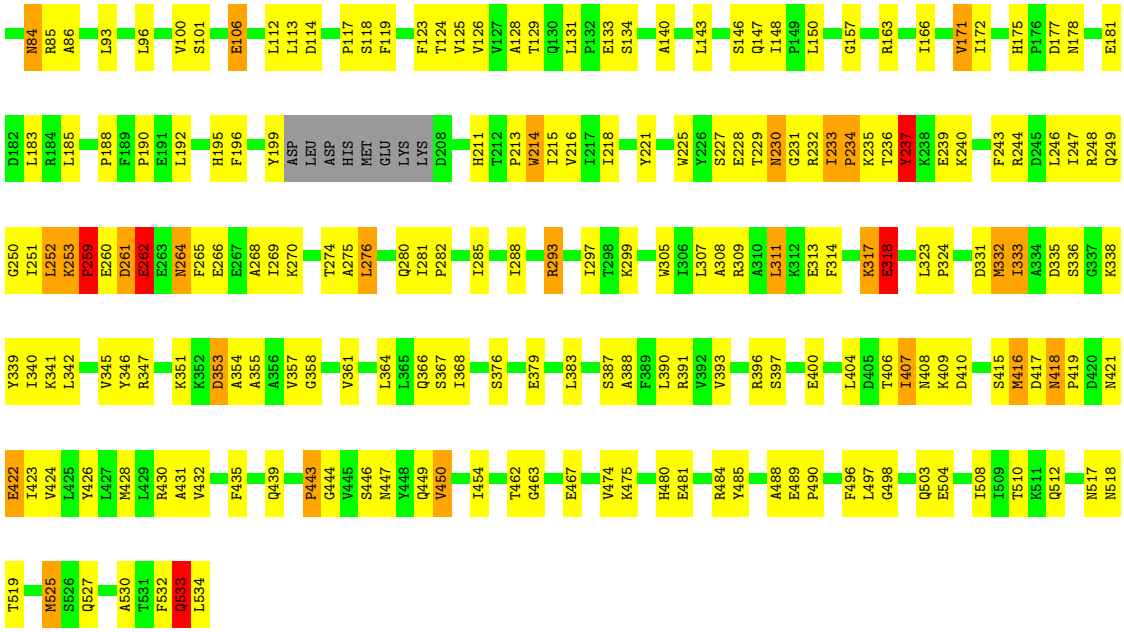
• Molecule 1: amyloid beta precursor protein-binding protein 1

Chain E:



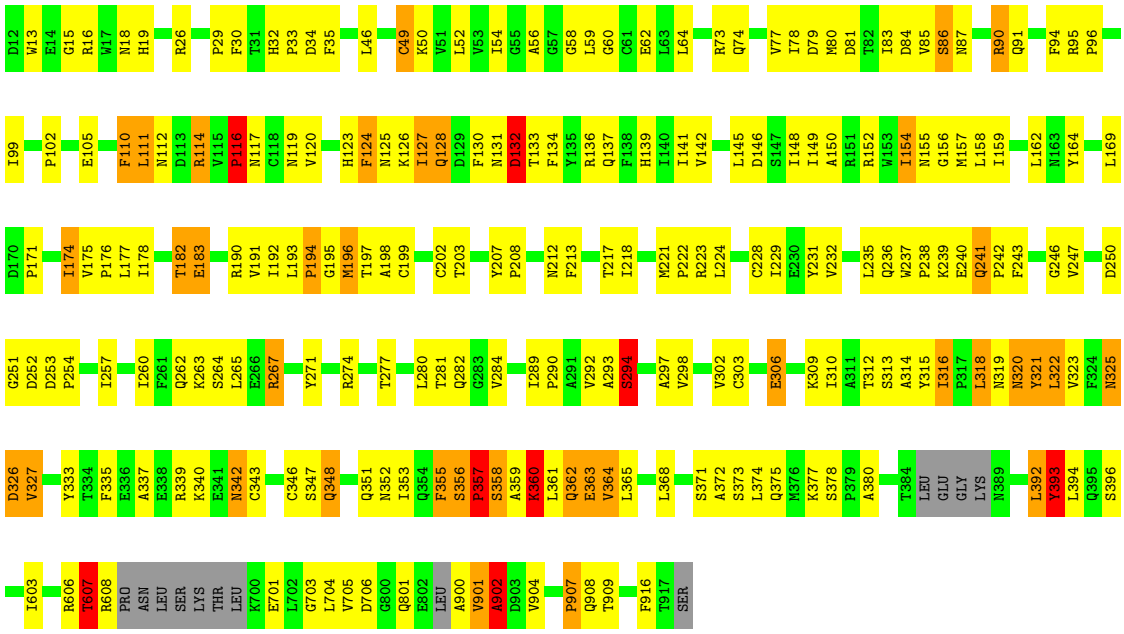
• Molecule 1: amyloid beta precursor protein-binding protein 1

Chain G:



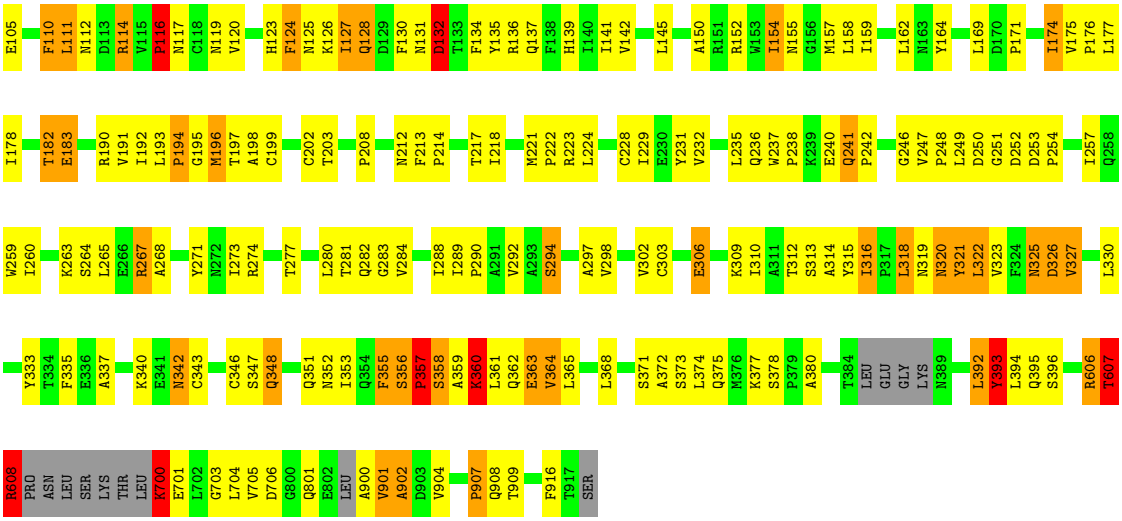
- Molecule 2: ubiquitin-activating enzyme E1C

Chain B:



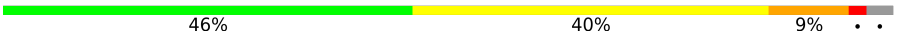
- Molecule 2: ubiquitin-activating enzyme E1C

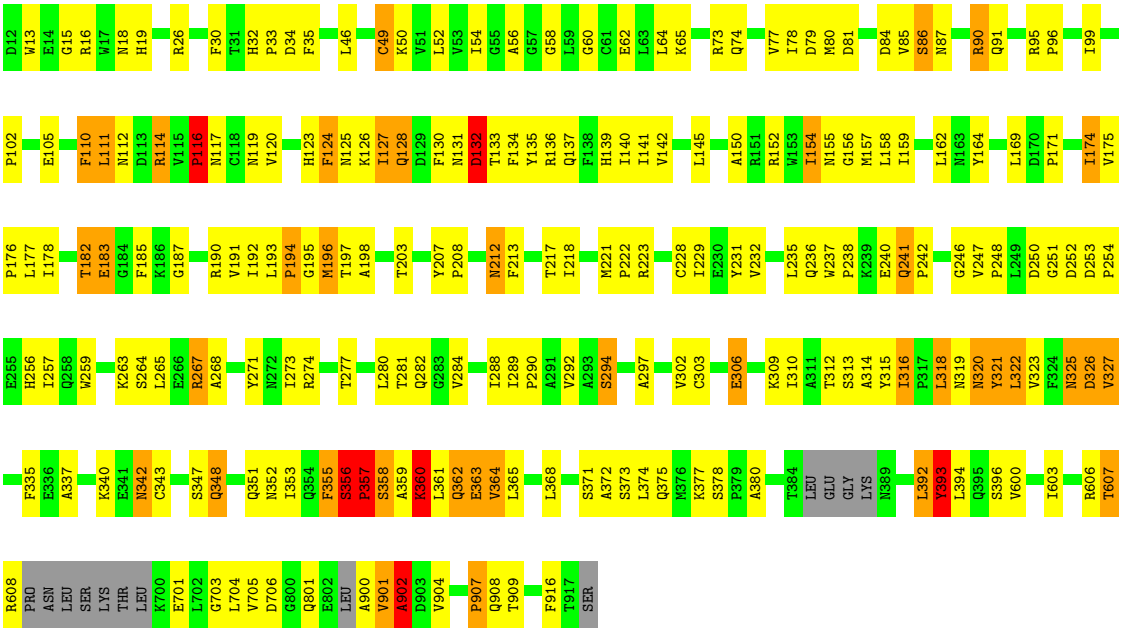
Chain D:



- Molecule 2: ubiquitin-activating enzyme E1C

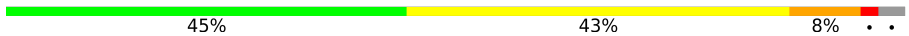
Chain F:

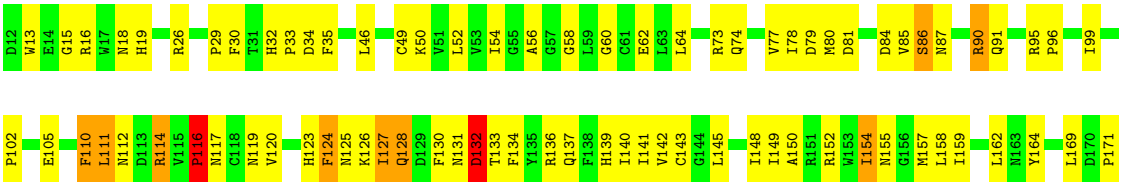




- Molecule 2: ubiquitin-activating enzyme E1C

Chain H:





I174 V175 P176 L177 I178 T182 E183 G187 R190 V191 I192 L193 P194 G195 M196 T197 A198 T203 Y207 P208 N212 F213 T217 I218 M221 P222 R223 L224 C228 I229 E230 Y231 V232 L235 Q236 W237 P238 K239 E240 Q241 P242 G246 L249 D250 G251 D252 D253

P254 E255 H256 I257 Q258 W259 I260 K263 S264 L265 E266 R267 A268 Y271 N272 I273 R274 T277 L280 T281 Q282 G283 V284 I288 I289 P290 A291 V292 A293 S294 A297 V298 V302 C303 E306 K309 I310 A311 T312 S313 A314 Y315 I316 P317 L318 N319 N320 Y321 L322 V323 F324

N325 D326 V327 Y333 T334 F335 E336 A337 E338 R339 K340 E341 N342 C343 C346 S347 Q348 Q351 N352 I353 Q354 F355 S356 P357 S358 A359 K360 L361 Q362 E363 V364 L365 L368 S371 A372 S373 L374 Q375 M376 K377 S378 P379 A380 T384 LEU GLU GLY LYS N389 L392 Y393 L394 Q395

S396 I603 R606 T607 R608 PRO ASN LEU SER LYS THR LEU K700 E701 L702 G703 L704 V705 D706 G800 Q801 E802 LEU A900 V901 A902 D903 V904 P907 Q908 T909 F916 T917 SER

- Molecule 3: Ubiquitin-like protein NEDD8

Chain I: 42% 54% •

M101 L102 I103 K104 V105 K106 T107 L108 T109 G110 K111 E112 I113 E114 I115 D116 I117 E118 P119 T120 D121 K122 V123 E124 R125 I126 V130 P138 Q141 R142 L143 I144 Y145 S146 Q149 M150 N151 D152 E153 K154 T155 A156 A157 D158 I161 L162 L167 H168 L169 V170 L171 G176

- Molecule 3: Ubiquitin-like protein NEDD8

Chain J: 39% 54% 7%

M101 L102 I103 K104 V105 K106 T107 L108 T109 G110 K111 E112 I113 E114 I115 D116 I117 E118 P119 T120 D121 K122 V123 E124 R125 I126 V130 G135 I136 P137 P138 Q141 R142 L143 I144 Y145 S146 Q149 M150 N151 D152 E153 K154 T155 A156 A157 D158 I161 L162 L167 H168 L169 V170 L171

G176

- Molecule 3: Ubiquitin-like protein NEDD8

Chain K: 39% 55% 5%

M101 L102 I103 K104 V105 K106 T107 L108 T109 G110 K111 E112 I113 E114 I115 D116 I117 E118 P119 T120 D121 K122 V123 E124 R125 I126 V130 P138 Q141 R142 L143 I144 Y145 S146 Q149 M150 N151 D152 E153 K154 T155 A156 A157 D158 I161 L162 L167 H168 L169 V170 L171 A172 L173

G176

- Molecule 3: Ubiquitin-like protein NEDD8

Chain L: 42% 53% 5%

M101 L102 I103 K104 V105 K106 T107 L108 T109 G110 K111 E112 I113 E114 I115 D116 I117 E118 P119 T120 D121 K122 V123 E124 R125 I126 V130 P138 Q141 R142 L143 I144 Y145 S146 Q149 M150 N151 D152 E153 K154 T155 A156 A157 D158 I161 L162 L167 H168 L169 V170 L171 A172 L173

G176

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.00Å 197.90Å 211.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.60)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31744	wwPDB-VP
Average B, all atoms ($Å^2$)	85.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.54	5/4185 (0.1%)	0.72	9/5661 (0.2%)
1	C	0.52	6/4185 (0.1%)	0.75	9/5661 (0.2%)
1	E	0.56	3/4185 (0.1%)	0.74	9/5661 (0.2%)
1	G	0.54	6/4185 (0.1%)	0.74	11/5661 (0.2%)
2	B	0.53	1/3268 (0.0%)	0.93	8/4447 (0.2%)
2	D	0.75	9/3269 (0.3%)	0.82	12/4450 (0.3%)
2	F	0.50	1/3268 (0.0%)	0.77	8/4447 (0.2%)
2	H	0.49	2/3268 (0.1%)	0.76	7/4447 (0.2%)
3	I	0.36	0/605	0.67	0/808
3	J	0.32	0/605	0.66	0/808
3	K	0.35	0/605	0.66	0/808
3	L	0.34	0/605	0.66	0/808
All	All	0.54	33/32233 (0.1%)	0.77	73/43667 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	G	0	1
2	B	0	1
2	D	0	2
2	F	0	1
2	H	0	1
All	All	0	8

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	700	LYS	N-CA	16.70	1.79	1.46
1	C	259	PRO	N-CA	14.05	1.71	1.47
1	A	259	PRO	N-CA	13.99	1.71	1.47
2	D	608	ARG	N-CA	13.42	1.73	1.46
2	B	392	LEU	CG-CD2	-13.03	1.03	1.51
1	E	259	PRO	N-CA	12.57	1.68	1.47
1	G	259	PRO	N-CA	12.22	1.68	1.47
2	D	700	LYS	C-N	11.95	1.61	1.34
2	D	608	ARG	C-N	11.85	1.61	1.34
2	D	608	ARG	CA-C	11.47	1.82	1.52
2	D	700	LYS	CA-C	10.56	1.80	1.52
1	A	253	LYS	C-N	9.71	1.52	1.34
1	E	253	LYS	CA-C	9.58	1.77	1.52
2	D	607	THR	C-N	9.56	1.56	1.34
1	E	253	LYS	C-N	9.23	1.51	1.34
1	C	253	LYS	CA-C	9.12	1.76	1.52
1	A	253	LYS	CA-C	8.87	1.76	1.52
1	G	253	LYS	CA-C	7.78	1.73	1.52
1	G	253	LYS	C-N	7.17	1.47	1.34
1	G	252	LEU	C-N	-6.97	1.18	1.34
1	A	252	LEU	C-N	-6.86	1.18	1.34
2	D	607	THR	CA-C	6.74	1.70	1.52
1	C	253	LYS	C-N	6.70	1.47	1.34
1	C	252	LEU	C-N	-6.55	1.19	1.34
2	F	392	LEU	CG-CD2	-5.56	1.31	1.51
2	D	392	LEU	CG-CD2	-5.56	1.31	1.51
1	A	253	LYS	CA-CB	5.53	1.66	1.53
1	G	253	LYS	CA-CB	5.51	1.66	1.53
1	C	259	PRO	C-N	-5.40	1.21	1.34
1	C	253	LYS	CA-CB	5.38	1.65	1.53
2	H	143	CYS	CB-SG	-5.35	1.73	1.81
2	H	392	LEU	CG-CD2	-5.22	1.32	1.51
1	G	259	PRO	C-N	-5.12	1.22	1.34

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	392	LEU	CB-CG-CD2	-32.12	56.40	111.00
2	B	392	LEU	CB-CG-CD1	14.82	136.20	111.00
1	C	259	PRO	CA-N-CD	-14.32	91.45	111.50
1	E	259	PRO	CA-N-CD	-12.19	94.43	111.50
2	D	700	LYS	N-CA-C	11.93	143.21	111.00
1	A	253	LYS	CB-CA-C	11.19	132.77	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	259	PRO	CA-N-CD	-10.24	97.17	111.50
2	D	608	ARG	N-CA-C	10.08	138.21	111.00
2	B	392	LEU	CA-CB-CG	9.88	138.01	115.30
1	E	253	LYS	CB-CA-C	9.79	129.97	110.40
1	A	259	PRO	CA-N-CD	-9.77	97.82	111.50
1	C	259	PRO	CA-CB-CG	-9.60	85.76	104.00
2	B	392	LEU	CD1-CG-CD2	-9.24	82.78	110.50
1	E	259	PRO	CA-CB-CG	-9.23	86.45	104.00
1	G	259	PRO	CA-CB-CG	-9.16	86.59	104.00
1	C	253	LYS	C-N-CD	-9.14	100.49	120.60
1	G	252	LEU	C-N-CA	-8.28	101.00	121.70
1	A	259	PRO	CA-CB-CG	-8.16	88.49	104.00
1	C	253	LYS	CB-CA-C	8.07	126.54	110.40
1	G	253	LYS	CB-CA-C	7.91	126.22	110.40
1	C	252	LEU	C-N-CA	-7.87	102.02	121.70
2	F	392	LEU	CB-CG-CD2	-7.81	97.73	111.00
2	D	392	LEU	CB-CG-CD2	-7.76	97.80	111.00
1	G	259	PRO	N-CA-C	7.52	131.65	112.10
1	G	253	LYS	C-N-CD	-7.43	104.26	120.60
2	D	392	LEU	CB-CG-CD1	7.40	123.58	111.00
2	F	392	LEU	CB-CG-CD1	7.39	123.56	111.00
2	F	607	THR	C-N-CA	7.36	140.10	121.70
1	C	259	PRO	N-CA-C	7.28	131.03	112.10
2	D	902	ALA	N-CA-C	-7.08	91.89	111.00
1	C	253	LYS	C-N-CA	6.85	150.77	122.00
1	G	253	LYS	C-N-CA	6.84	150.72	122.00
2	D	606	ARG	C-N-CA	-6.83	104.63	121.70
2	H	392	LEU	CB-CG-CD1	6.78	122.53	111.00
2	H	392	LEU	CB-CG-CD2	-6.59	99.79	111.00
2	F	902	ALA	N-CA-C	-6.54	93.35	111.00
1	A	259	PRO	N-CA-C	6.34	128.57	112.10
2	F	607	THR	CA-C-N	-6.31	103.32	117.20
1	A	252	LEU	C-N-CA	-6.28	106.00	121.70
2	D	607	THR	CA-C-N	6.26	130.98	117.20
1	A	253	LYS	C-N-CA	6.14	147.80	122.00
1	A	253	LYS	N-CA-CB	-6.07	99.67	110.60
1	E	252	LEU	C-N-CA	-6.01	106.68	121.70
1	C	253	LYS	CA-C-N	6.00	133.89	117.10
1	C	253	LYS	N-CA-CB	-6.00	99.81	110.60
2	H	356	SER	C-N-CD	-5.97	107.47	120.60
1	E	253	LYS	N-CA-CB	-5.95	99.89	110.60
2	H	907	PRO	N-CA-CB	5.92	110.41	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	907	PRO	N-CA-CB	5.79	110.25	103.30
2	D	907	PRO	N-CA-CB	5.78	110.23	103.30
2	H	607	THR	CA-C-N	-5.64	104.79	117.20
2	B	907	PRO	N-CA-CB	5.61	110.03	103.30
2	B	607	THR	CA-C-N	-5.56	104.97	117.20
2	H	360	LYS	N-CA-C	5.49	125.82	111.00
1	E	253	LYS	C-N-CA	5.48	145.03	122.00
2	H	902	ALA	N-CA-C	-5.42	96.36	111.00
1	G	253	LYS	N-CA-CB	-5.41	100.87	110.60
1	E	259	PRO	N-CA-C	5.38	126.09	112.10
2	B	902	ALA	N-CA-C	-5.32	96.65	111.00
2	D	360	LYS	N-CA-C	5.28	125.27	111.00
2	F	360	LYS	N-CA-C	5.25	125.19	111.00
2	B	360	LYS	N-CA-C	5.25	125.19	111.00
2	D	700	LYS	N-CA-CB	-5.24	101.16	110.60
2	D	608	ARG	C-N-CA	5.20	134.70	121.70
1	A	533	GLN	N-CA-C	5.20	125.03	111.00
2	F	356	SER	C-N-CD	-5.17	109.23	120.60
1	A	259	PRO	N-CA-CB	-5.16	96.92	102.60
1	E	533	GLN	N-CA-C	5.15	124.91	111.00
1	E	259	PRO	C-N-CA	-5.15	108.83	121.70
1	G	253	LYS	CA-C-N	5.13	131.45	117.10
1	G	237	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	G	533	GLN	N-CA-C	5.03	124.57	111.00
2	D	607	THR	O-C-N	-5.00	114.69	122.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	PRO	Peptide
2	B	355	PHE	Sidechain
1	C	259	PRO	Peptide
2	D	355	PHE	Sidechain
2	D	393	TYR	Sidechain
2	F	355	PHE	Sidechain
1	G	259	PRO	Peptide
2	H	355	PHE	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	4105	0	4063	272	0
1	C	4105	0	4063	266	0
1	E	4105	0	4063	278	0
1	G	4105	0	4063	264	0
2	B	3199	0	3066	265	0
2	D	3199	0	3067	263	0
2	F	3199	0	3062	255	0
2	H	3199	0	3062	261	0
3	I	600	0	635	59	0
3	J	600	0	635	60	0
3	K	600	0	635	64	0
3	L	600	0	635	61	0
4	B	31	0	12	3	0
4	D	31	0	12	4	0
4	F	31	0	11	6	0
4	H	31	0	12	10	0
5	F	1	0	0	0	0
5	H	2	0	0	0	0
5	J	1	0	0	0	0
All	All	31744	0	31096	2256	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (2256) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LYS:CA	1:A:253:LYS:C	1.76	1.54
1:C:253:LYS:CA	1:C:253:LYS:C	1.76	1.52
1:E:253:LYS:C	1:E:253:LYS:CA	1.77	1.50
2:D:700:LYS:CA	2:D:700:LYS:C	1.80	1.49
2:D:608:ARG:N	2:D:608:ARG:CA	1.73	1.47
2:D:608:ARG:CA	2:D:608:ARG:C	1.82	1.45
2:D:700:LYS:CA	2:D:700:LYS:N	1.79	1.43
1:C:259:PRO:N	1:C:259:PRO:CA	1.71	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:PRO:N	1:E:259:PRO:CA	1.68	1.30
1:G:259:PRO:N	1:G:259:PRO:CA	1.68	1.30
1:A:259:PRO:N	1:A:259:PRO:CA	1.71	1.28
2:B:361:LEU:HD11	2:B:704:LEU:HA	1.32	1.12
2:B:274:ARG:HH22	1:E:107:GLU:HA	0.99	1.11
2:F:361:LEU:HD11	2:F:704:LEU:HA	1.34	1.09
2:H:380:ALA:HB2	2:H:394:LEU:HD13	1.31	1.09
2:D:361:LEU:HD11	2:D:704:LEU:HA	1.31	1.09
2:H:361:LEU:HD11	2:H:704:LEU:HA	1.29	1.09
2:D:380:ALA:HB2	2:D:394:LEU:HD13	1.35	1.08
2:B:262:GLN:NE2	1:E:67:GLY:H	1.49	1.07
1:A:396:ARG:HG3	1:A:534:LEU:HD11	1.36	1.07
2:B:380:ALA:HB2	2:B:394:LEU:HD13	1.35	1.05
2:F:380:ALA:HB2	2:F:394:LEU:HD13	1.37	1.05
2:B:274:ARG:NH2	1:E:107:GLU:HA	1.73	1.04
1:A:344:ASN:ND2	1:E:111:ASN:HD22	1.57	1.02
1:G:396:ARG:HG3	1:G:534:LEU:HD11	1.39	1.02
2:B:262:GLN:HE22	1:E:67:GLY:N	1.59	1.01
1:E:396:ARG:HG3	1:E:534:LEU:HD11	1.39	1.01
1:E:518:ASN:ND2	1:E:533:GLN:HG3	1.77	1.00
1:G:336:SER:HG	2:H:271:TYR:HD2	1.07	0.99
1:A:252:LEU:O	1:A:253:LYS:C	2.00	0.99
1:G:518:ASN:ND2	1:G:533:GLN:HG3	1.78	0.98
2:B:128:GLN:H	2:B:128:GLN:NE2	1.59	0.98
2:H:128:GLN:H	2:H:128:GLN:NE2	1.61	0.97
2:B:128:GLN:HE21	2:B:128:GLN:N	1.59	0.97
2:F:58:GLY:H	2:F:91:GLN:HG2	1.29	0.97
2:F:229:ILE:HD13	2:F:281:THR:HA	1.45	0.97
1:C:396:ARG:HG3	1:C:534:LEU:HD11	1.41	0.97
2:F:128:GLN:H	2:F:128:GLN:NE2	1.63	0.97
2:H:128:GLN:HE21	2:H:128:GLN:N	1.61	0.96
2:B:606:ARG:C	2:B:608:ARG:H	1.68	0.96
2:D:58:GLY:H	2:D:91:GLN:HG2	1.31	0.96
2:D:128:GLN:H	2:D:128:GLN:NE2	1.63	0.95
2:F:128:GLN:HE21	2:F:128:GLN:N	1.64	0.95
2:D:229:ILE:HD13	2:D:281:THR:HA	1.48	0.95
2:D:128:GLN:HE21	2:D:128:GLN:N	1.65	0.94
1:A:344:ASN:ND2	1:E:111:ASN:ND2	2.15	0.94
1:E:253:LYS:O	1:E:260:GLU:CG	2.16	0.94
1:C:518:ASN:ND2	1:C:533:GLN:HG3	1.82	0.93
2:B:606:ARG:O	2:B:608:ARG:N	2.02	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:252:LEU:O	1:G:253:LYS:C	2.04	0.92
2:F:323:VAL:HG21	3:K:170:VAL:HG22	1.48	0.92
1:A:253:LYS:O	1:A:260:GLU:CG	2.18	0.92
2:H:229:ILE:HD13	2:H:281:THR:HA	1.50	0.91
2:D:208:PRO:HG3	3:J:171:LEU:HD11	1.53	0.90
1:A:285:ILE:HD11	1:A:388:ALA:HA	1.53	0.90
1:G:285:ILE:HD11	1:G:388:ALA:HA	1.54	0.90
2:B:229:ILE:HD13	2:B:281:THR:HA	1.50	0.90
2:B:267:ARG:HG2	2:B:267:ARG:HH11	1.37	0.90
1:A:518:ASN:ND2	1:A:533:GLN:HG3	1.87	0.89
2:H:58:GLY:H	2:H:91:GLN:HG2	1.37	0.89
3:I:138:PRO:HA	3:I:141:GLN:HE21	1.38	0.89
3:L:138:PRO:HA	3:L:141:GLN:HE21	1.38	0.89
2:B:274:ARG:HH22	1:E:107:GLU:CA	1.84	0.88
1:C:252:LEU:O	1:C:253:LYS:C	2.12	0.88
1:E:252:LEU:O	1:E:253:LYS:C	2.12	0.88
1:C:309:ARG:HG3	1:C:364:LEU:HD21	1.56	0.88
1:E:307:LEU:HB3	1:E:383:LEU:HD22	1.56	0.88
2:B:58:GLY:H	2:B:91:GLN:HG2	1.39	0.87
2:H:323:VAL:HG21	3:L:170:VAL:HG22	1.57	0.87
1:E:285:ILE:HD11	1:E:388:ALA:HA	1.57	0.86
2:D:267:ARG:HG2	2:D:267:ARG:HH11	1.39	0.86
2:D:361:LEU:CD1	2:D:704:LEU:HA	2.06	0.86
2:H:208:PRO:HG3	3:L:171:LEU:HD11	1.55	0.86
2:H:380:ALA:HB2	2:H:394:LEU:CD1	2.06	0.86
1:A:309:ARG:HG3	1:A:364:LEU:HD21	1.56	0.86
2:H:267:ARG:HG2	2:H:267:ARG:HH11	1.38	0.86
2:H:322:LEU:HD12	2:H:323:VAL:N	1.91	0.86
1:E:232:ARG:HB3	1:E:234:PRO:HD3	1.57	0.85
2:F:208:PRO:HG3	3:K:171:LEU:HD11	1.58	0.85
2:B:208:PRO:HG3	3:I:171:LEU:HD11	1.58	0.85
3:K:138:PRO:HA	3:K:141:GLN:HE21	1.41	0.85
1:G:232:ARG:HB3	1:G:234:PRO:HD3	1.56	0.85
1:A:232:ARG:HB3	1:A:234:PRO:HD3	1.56	0.85
1:E:61:ASP:HB3	1:E:86:ALA:HB2	1.56	0.85
1:E:307:LEU:HB3	1:E:383:LEU:CD2	2.07	0.85
2:F:316:ILE:HD12	2:F:316:ILE:H	1.41	0.85
1:A:344:ASN:HD21	1:E:111:ASN:HD22	1.22	0.84
1:C:285:ILE:HD11	1:C:388:ALA:HA	1.57	0.84
2:D:316:ILE:H	2:D:316:ILE:HD12	1.40	0.84
1:G:309:ARG:HG3	1:G:364:LEU:HD21	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:ARG:HB3	1:C:234:PRO:HD3	1.58	0.84
1:G:61:ASP:HB3	1:G:86:ALA:HB2	1.59	0.84
2:H:361:LEU:CD1	2:H:704:LEU:HA	2.07	0.84
1:C:236:THR:O	1:C:237:TYR:HB2	1.76	0.84
1:E:309:ARG:HG3	1:E:364:LEU:HD21	1.57	0.84
3:I:155:THR:HG22	3:I:158:ASP:OD2	1.78	0.84
2:F:267:ARG:HG2	2:F:267:ARG:HH11	1.41	0.83
3:J:138:PRO:HA	3:J:141:GLN:HE21	1.41	0.83
1:A:61:ASP:HB3	1:A:86:ALA:HB2	1.58	0.83
1:C:307:LEU:HB3	1:C:383:LEU:HD22	1.57	0.83
2:B:361:LEU:CD1	2:B:704:LEU:HA	2.07	0.83
2:H:606:ARG:O	2:H:608:ARG:N	2.09	0.83
2:B:316:ILE:H	2:B:316:ILE:HD12	1.43	0.82
1:C:61:ASP:HB3	1:C:86:ALA:HB2	1.60	0.82
1:A:307:LEU:HB3	1:A:383:LEU:HD22	1.60	0.82
2:F:361:LEU:CD1	2:F:704:LEU:HA	2.09	0.82
2:F:901:VAL:C	2:F:902:ALA:O	2.08	0.82
2:B:74:GLN:HE22	2:B:119:ASN:HD22	1.28	0.81
1:C:253:LYS:O	1:C:260:GLU:OE2	1.98	0.81
2:B:323:VAL:HG21	3:I:170:VAL:HG22	1.61	0.81
2:H:316:ILE:H	2:H:316:ILE:HD12	1.44	0.81
2:D:323:VAL:HG21	3:J:170:VAL:HG22	1.63	0.81
2:H:361:LEU:HD11	2:H:704:LEU:CA	2.11	0.81
2:B:368:LEU:HA	2:B:374:LEU:HD12	1.63	0.81
1:C:307:LEU:HB3	1:C:383:LEU:CD2	2.10	0.81
1:G:307:LEU:HB3	1:G:383:LEU:CD2	2.11	0.81
1:C:56:SER:HB3	1:C:101:SER:OG	1.80	0.80
1:E:236:THR:O	1:E:237:TYR:HB2	1.79	0.80
1:G:421:ASN:O	1:G:424:VAL:HG23	1.81	0.80
2:D:380:ALA:HB2	2:D:394:LEU:CD1	2.10	0.80
1:A:307:LEU:HB3	1:A:383:LEU:CD2	2.12	0.80
1:C:253:LYS:C	1:C:253:LYS:HA	2.00	0.80
2:D:325:ASN:ND2	2:D:327:VAL:HG22	1.97	0.80
2:D:322:LEU:HD12	2:D:323:VAL:N	1.97	0.80
1:A:236:THR:O	1:A:237:TYR:HB2	1.81	0.80
2:D:361:LEU:HD11	2:D:704:LEU:CA	2.12	0.79
1:A:533:GLN:O	1:A:534:LEU:HG	1.81	0.79
2:F:380:ALA:HB2	2:F:394:LEU:CD1	2.13	0.79
1:A:253:LYS:C	1:A:253:LYS:HA	2.01	0.79
2:H:325:ASN:ND2	2:H:327:VAL:HG22	1.97	0.79
2:B:380:ALA:HB2	2:B:394:LEU:CD1	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:533:GLN:O	1:G:534:LEU:HG	1.82	0.79
2:F:368:LEU:HA	2:F:374:LEU:HD12	1.64	0.79
1:A:344:ASN:HD22	1:E:111:ASN:ND2	1.79	0.79
1:E:533:GLN:O	1:E:534:LEU:HG	1.82	0.79
2:F:701:GLU:HA	2:F:704:LEU:CB	2.13	0.79
3:K:123:VAL:HB	3:K:152:ASP:HA	1.65	0.79
1:G:307:LEU:HB3	1:G:383:LEU:HD22	1.64	0.79
1:A:56:SER:HB3	1:A:101:SER:OG	1.83	0.78
2:H:368:LEU:HA	2:H:374:LEU:HD12	1.64	0.78
2:D:368:LEU:HA	2:D:374:LEU:HD12	1.64	0.78
2:F:322:LEU:HD12	2:F:323:VAL:N	1.98	0.78
3:J:123:VAL:HB	3:J:152:ASP:HA	1.66	0.78
3:J:155:THR:HG22	3:J:158:ASP:OD2	1.81	0.78
3:K:155:THR:HG22	3:K:158:ASP:OD2	1.83	0.78
2:H:325:ASN:HD21	2:H:327:VAL:HG22	1.49	0.77
3:L:155:THR:HG22	3:L:158:ASP:OD2	1.84	0.77
2:D:74:GLN:HE22	2:D:119:ASN:HD22	1.29	0.77
2:F:81:ASP:HB2	4:F:7:ATP:O2'	1.85	0.77
3:I:123:VAL:HB	3:I:152:ASP:HA	1.66	0.77
3:K:155:THR:HG23	3:K:158:ASP:H	1.50	0.77
3:I:124:GLU:HB2	3:I:152:ASP:O	1.84	0.77
3:J:124:GLU:HB2	3:J:152:ASP:O	1.85	0.76
1:E:421:ASN:O	1:E:424:VAL:HG23	1.85	0.76
1:G:56:SER:HB3	1:G:101:SER:OG	1.84	0.76
2:B:361:LEU:HD11	2:B:704:LEU:CA	2.13	0.76
3:I:155:THR:HG23	3:I:158:ASP:H	1.49	0.76
2:B:81:ASP:HB2	4:B:5:ATP:O2'	1.84	0.76
1:C:421:ASN:O	1:C:424:VAL:HG23	1.85	0.76
2:H:701:GLU:HA	2:H:704:LEU:CB	2.16	0.76
3:L:155:THR:HG23	3:L:158:ASP:H	1.50	0.76
1:G:307:LEU:HD13	1:G:383:LEU:HD22	1.68	0.76
1:G:393:VAL:HG13	1:G:517:ASN:HD22	1.50	0.76
2:B:262:GLN:HE22	1:E:67:GLY:H	0.79	0.76
3:L:123:VAL:HB	3:L:152:ASP:HA	1.68	0.76
1:A:233:ILE:N	1:A:234:PRO:CD	2.49	0.75
2:D:325:ASN:HD21	2:D:327:VAL:HG22	1.48	0.75
1:G:51:LEU:HB2	1:G:52:PRO:HD3	1.68	0.75
2:H:64:LEU:HB3	2:H:111:LEU:CD1	2.16	0.75
2:F:325:ASN:ND2	2:F:327:VAL:HG22	2.00	0.75
1:C:51:LEU:HB2	1:C:52:PRO:HD3	1.68	0.75
1:E:56:SER:HB3	1:E:101:SER:OG	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:ILE:N	1:E:234:PRO:CD	2.49	0.75
1:G:233:ILE:N	1:G:234:PRO:CD	2.50	0.75
2:F:74:GLN:HE22	2:F:119:ASN:HD22	1.32	0.75
2:D:64:LEU:HB3	2:D:111:LEU:CD1	2.17	0.75
2:H:380:ALA:CB	2:H:394:LEU:HD13	2.13	0.75
1:C:163:ARG:HG2	1:C:163:ARG:HH11	1.52	0.75
2:H:901:VAL:C	2:H:902:ALA:O	2.17	0.75
3:J:155:THR:HG23	3:J:158:ASP:H	1.51	0.74
2:F:64:LEU:HB3	2:F:111:LEU:CD1	2.17	0.74
1:E:253:LYS:O	1:E:260:GLU:HG2	1.87	0.74
1:A:396:ARG:CG	1:A:534:LEU:HD11	2.17	0.74
1:A:51:LEU:HB2	1:A:52:PRO:HD3	1.70	0.74
1:A:253:LYS:O	1:A:260:GLU:HG3	1.85	0.74
2:D:701:GLU:HA	2:D:704:LEU:CB	2.17	0.74
1:E:163:ARG:HH11	1:E:163:ARG:HG2	1.50	0.74
1:A:348:GLU:HG3	1:E:115:ASN:ND2	2.03	0.74
1:A:533:GLN:HG3	1:A:533:GLN:O	1.87	0.74
1:A:351:LYS:O	1:A:354:ALA:HB3	1.88	0.74
2:B:325:ASN:ND2	2:B:327:VAL:HG22	2.02	0.74
1:C:393:VAL:HG13	1:C:517:ASN:HD22	1.53	0.74
1:G:163:ARG:HG2	1:G:163:ARG:HH11	1.51	0.74
1:G:34:CYS:HB2	1:G:123:PHE:CD2	2.23	0.74
1:A:421:ASN:O	1:A:424:VAL:HG23	1.86	0.73
2:B:322:LEU:HD12	2:B:323:VAL:N	2.03	0.73
2:B:901:VAL:C	2:B:902:ALA:O	2.22	0.73
1:E:351:LYS:O	1:E:354:ALA:HB3	1.87	0.73
2:B:701:GLU:HA	2:B:704:LEU:CB	2.17	0.73
1:C:233:ILE:N	1:C:234:PRO:CD	2.50	0.73
2:F:325:ASN:HD21	2:F:327:VAL:HG22	1.54	0.73
2:H:74:GLN:HE22	2:H:119:ASN:HD22	1.34	0.73
2:H:318:LEU:HD21	2:H:321:TYR:H	1.54	0.73
2:D:84:ASP:H	2:D:87:ASN:ND2	1.86	0.73
3:K:124:GLU:HB2	3:K:152:ASP:O	1.86	0.73
2:B:237:TRP:HB3	2:B:238:PRO:HD3	1.71	0.73
1:G:45:ILE:HG12	1:G:498:GLY:HA2	1.70	0.73
3:L:124:GLU:HB2	3:L:152:ASP:O	1.87	0.73
1:E:143:LEU:CD1	1:E:150:LEU:HD13	2.19	0.72
1:E:396:ARG:CG	1:E:534:LEU:HD11	2.19	0.72
1:A:163:ARG:HG2	1:A:163:ARG:HH11	1.54	0.72
2:B:361:LEU:HA	2:B:364:VAL:HG22	1.71	0.72
2:F:361:LEU:HD11	2:F:704:LEU:CA	2.16	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:GLN:HG3	1:C:533:GLN:O	1.88	0.72
2:H:158:LEU:HD22	2:H:175:VAL:HB	1.70	0.72
1:E:34:CYS:HB2	1:E:123:PHE:CD2	2.24	0.72
2:F:84:ASP:H	2:F:87:ASN:ND2	1.87	0.72
1:G:396:ARG:CG	1:G:534:LEU:HD11	2.19	0.72
3:L:123:VAL:HG11	3:L:150:MET:HB3	1.72	0.72
1:C:351:LYS:O	1:C:354:ALA:HB3	1.90	0.72
2:H:32:HIS:ND1	2:H:33:PRO:HD2	2.05	0.72
1:C:533:GLN:O	1:C:534:LEU:HG	1.90	0.71
3:J:101:MET:HB3	3:J:117:ILE:O	1.90	0.71
1:G:351:LYS:O	1:G:354:ALA:HB3	1.89	0.71
2:B:606:ARG:C	2:B:608:ARG:N	2.39	0.71
2:H:84:ASP:H	2:H:87:ASN:ND2	1.88	0.71
1:E:481:GLU:HG2	1:E:525:MET:HE3	1.70	0.71
1:A:143:LEU:CD1	1:A:150:LEU:HD13	2.20	0.71
2:F:171:PRO:O	2:F:174:ILE:HG13	1.91	0.71
2:H:357:PRO:O	2:H:358:SER:HB3	1.89	0.71
2:D:237:TRP:HB3	2:D:238:PRO:HD3	1.72	0.71
2:D:608:ARG:N	2:D:608:ARG:CB	2.54	0.71
3:J:106:LYS:HA	3:J:112:GLU:HA	1.73	0.71
2:H:606:ARG:C	2:H:608:ARG:N	2.43	0.71
2:B:361:LEU:O	2:B:364:VAL:HG23	1.91	0.71
2:D:318:LEU:HD21	2:D:321:TYR:H	1.56	0.71
2:D:700:LYS:C	2:D:700:LYS:CB	2.58	0.71
2:F:901:VAL:O	2:F:902:ALA:O	2.07	0.71
2:D:700:LYS:C	2:D:700:LYS:HA	2.05	0.71
2:B:325:ASN:HD21	2:B:327:VAL:HG22	1.56	0.71
2:D:158:LEU:HD22	2:D:175:VAL:HB	1.73	0.71
1:G:533:GLN:HG3	1:G:533:GLN:O	1.89	0.71
2:H:361:LEU:O	2:H:364:VAL:HG23	1.90	0.71
1:C:34:CYS:HB2	1:C:123:PHE:CD2	2.26	0.70
1:C:264:ASN:HD22	1:C:264:ASN:N	1.89	0.70
1:G:236:THR:O	1:G:237:TYR:HB2	1.90	0.70
1:G:422:GLU:HG3	1:G:530:ALA:HB3	1.73	0.70
2:D:342:ASN:HD22	2:D:342:ASN:H	1.38	0.70
1:G:143:LEU:CD1	1:G:150:LEU:HD13	2.21	0.70
2:B:84:ASP:H	2:B:87:ASN:ND2	1.89	0.70
1:E:45:ILE:HG12	1:E:498:GLY:HA2	1.74	0.70
2:H:606:ARG:C	2:H:608:ARG:H	1.95	0.70
3:I:123:VAL:HG11	3:I:150:MET:HB3	1.72	0.70
1:E:51:LEU:HB2	1:E:52:PRO:HD3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:158:LEU:HD22	2:F:175:VAL:HB	1.72	0.70
2:F:606:ARG:O	2:F:608:ARG:N	2.22	0.70
2:H:237:TRP:HB3	2:H:238:PRO:HD3	1.74	0.70
1:A:348:GLU:HG3	1:E:115:ASN:CG	2.12	0.70
1:C:236:THR:O	1:C:237:TYR:CB	2.39	0.70
1:A:285:ILE:CD1	1:A:388:ALA:HA	2.22	0.70
2:B:318:LEU:HD21	2:B:321:TYR:H	1.56	0.70
2:D:361:LEU:HA	2:D:364:VAL:HG22	1.73	0.70
2:H:237:TRP:CE3	2:H:242:PRO:HG2	2.27	0.70
1:C:422:GLU:HG3	1:C:530:ALA:HB3	1.73	0.69
2:F:342:ASN:HD22	2:F:342:ASN:H	1.39	0.69
1:E:533:GLN:HG3	1:E:533:GLN:O	1.90	0.69
2:F:237:TRP:HB3	2:F:238:PRO:HD3	1.72	0.69
3:K:106:LYS:HA	3:K:112:GLU:HA	1.74	0.69
2:B:32:HIS:ND1	2:B:33:PRO:HD2	2.07	0.69
1:C:45:ILE:HG12	1:C:498:GLY:HA2	1.72	0.69
2:F:32:HIS:ND1	2:F:33:PRO:HD2	2.08	0.69
3:K:105:VAL:HG11	3:K:130:VAL:HG22	1.74	0.69
1:A:393:VAL:HG13	1:A:517:ASN:HD22	1.56	0.69
2:B:64:LEU:HB3	2:B:111:LEU:CD1	2.21	0.69
3:L:106:LYS:HA	3:L:112:GLU:HA	1.74	0.69
2:B:262:GLN:NE2	1:E:67:GLY:N	2.29	0.69
2:D:361:LEU:O	2:D:364:VAL:HG23	1.92	0.69
1:E:422:GLU:HG3	1:E:530:ALA:HB3	1.74	0.69
2:F:318:LEU:HD21	2:F:321:TYR:H	1.56	0.69
2:F:361:LEU:HA	2:F:364:VAL:HG22	1.73	0.69
1:A:45:ILE:HG12	1:A:498:GLY:HA2	1.75	0.69
2:B:158:LEU:HD22	2:B:175:VAL:HB	1.74	0.69
1:G:264:ASN:N	1:G:264:ASN:HD22	1.88	0.69
2:D:237:TRP:CE3	2:D:242:PRO:HG2	2.28	0.69
3:I:101:MET:HB3	3:I:117:ILE:O	1.93	0.68
1:E:393:VAL:HG13	1:E:517:ASN:HD22	1.58	0.68
1:A:264:ASN:HD22	1:A:264:ASN:N	1.88	0.68
3:L:101:MET:HB3	3:L:117:ILE:O	1.92	0.68
2:D:128:GLN:H	2:D:128:GLN:HE21	0.80	0.68
2:B:202:CYS:HG	2:B:343:CYS:HG	1.39	0.68
2:B:342:ASN:H	2:B:342:ASN:HD22	1.41	0.68
2:F:380:ALA:CB	2:F:394:LEU:HD13	2.21	0.68
3:K:123:VAL:HG11	3:K:150:MET:HB3	1.76	0.68
2:H:380:ALA:HB1	2:H:394:LEU:HB2	1.75	0.68
1:A:236:THR:O	1:A:237:TYR:CB	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:237:TRP:CE3	2:F:242:PRO:HG2	2.28	0.68
1:G:253:LYS:O	1:G:260:GLU:OE2	2.11	0.68
1:G:211:HIS:HB3	1:G:335:ASP:HB2	1.75	0.68
3:L:105:VAL:HG11	3:L:130:VAL:HG22	1.76	0.68
2:D:380:ALA:CB	2:D:394:LEU:HD13	2.19	0.68
2:D:700:LYS:N	2:D:700:LYS:CB	2.57	0.68
1:E:264:ASN:HD22	1:E:264:ASN:N	1.89	0.68
2:H:357:PRO:O	2:H:358:SER:CB	2.42	0.68
1:A:34:CYS:HB2	1:A:123:PHE:CD2	2.28	0.67
1:A:396:ARG:HG3	1:A:534:LEU:CD1	2.19	0.67
1:A:422:GLU:HG3	1:A:530:ALA:HB3	1.74	0.67
1:C:285:ILE:CD1	1:C:388:ALA:HA	2.24	0.67
1:E:211:HIS:HB3	1:E:335:ASP:HB2	1.77	0.67
1:E:253:LYS:C	1:E:253:LYS:HA	2.04	0.67
1:G:262:GLU:HB3	1:G:265:PHE:HB2	1.76	0.67
2:F:361:LEU:O	2:F:364:VAL:HG23	1.94	0.67
3:I:106:LYS:HA	3:I:112:GLU:HA	1.74	0.67
3:K:101:MET:HB3	3:K:117:ILE:O	1.93	0.67
1:A:264:ASN:HD22	1:A:264:ASN:H	1.43	0.67
1:C:211:HIS:HB3	1:C:335:ASP:HB2	1.75	0.67
1:C:213:PRO:HB3	1:C:332:MET:CE	2.24	0.67
2:D:164:TYR:HE2	2:D:169:LEU:HB2	1.59	0.67
2:F:154:ILE:HD13	2:F:154:ILE:O	1.95	0.67
2:F:192:ILE:HG22	2:F:194:PRO:HD3	1.75	0.67
1:G:75:PHE:CE2	1:G:96:LEU:HD11	2.30	0.67
2:H:251:GLY:O	2:H:257:ILE:HD11	1.95	0.67
2:H:361:LEU:HA	2:H:364:VAL:HG22	1.77	0.67
2:D:32:HIS:ND1	2:D:33:PRO:HD2	2.09	0.67
2:D:213:PHE:HB2	2:D:218:ILE:HD11	1.77	0.67
3:J:105:VAL:HG11	3:J:130:VAL:HG22	1.76	0.67
1:E:49:LEU:C	1:E:52:PRO:HD2	2.15	0.67
1:E:285:ILE:CD1	1:E:388:ALA:HA	2.23	0.66
2:H:64:LEU:HB3	2:H:111:LEU:HD13	1.76	0.66
1:A:376:SER:OG	1:A:379:GLU:HG3	1.95	0.66
2:D:192:ILE:HG22	2:D:194:PRO:HD3	1.78	0.66
1:E:376:SER:OG	1:E:379:GLU:HG3	1.95	0.66
2:H:164:TYR:HE2	2:H:169:LEU:HB2	1.58	0.66
2:H:342:ASN:H	2:H:342:ASN:HD22	1.42	0.66
1:A:36:ILE:HG22	1:A:37:ASN:N	2.11	0.66
1:C:390:LEU:O	1:C:391:ARG:HG2	1.96	0.66
2:F:64:LEU:HB3	2:F:111:LEU:HD13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:PRO:HB3	1:A:332:MET:CE	2.24	0.66
1:E:262:GLU:HB3	1:E:265:PHE:HB2	1.76	0.66
1:E:307:LEU:HD13	1:E:383:LEU:HD22	1.78	0.66
1:A:49:LEU:C	1:A:52:PRO:HD2	2.16	0.66
1:A:397:SER:OG	1:A:400:GLU:HG3	1.95	0.66
1:C:396:ARG:CG	1:C:534:LEU:HD11	2.22	0.65
1:E:397:SER:OG	1:E:400:GLU:HG3	1.96	0.65
2:H:359:ALA:HB1	2:H:363:GLU:OE1	1.97	0.65
1:A:213:PRO:HB3	1:A:332:MET:HE3	1.77	0.65
1:E:390:LEU:O	1:E:391:ARG:HG2	1.96	0.65
1:G:213:PRO:HB3	1:G:332:MET:CE	2.25	0.65
1:G:390:LEU:O	1:G:391:ARG:HG2	1.95	0.65
1:G:397:SER:OG	1:G:400:GLU:HG3	1.97	0.65
1:A:252:LEU:C	1:A:253:LYS:C	2.53	0.65
2:D:608:ARG:C	2:D:608:ARG:HA	2.08	0.65
2:H:213:PHE:HB2	2:H:218:ILE:HD11	1.77	0.65
2:H:217:THR:HA	2:H:221:MET:HG2	1.77	0.65
2:B:164:TYR:HE2	2:B:169:LEU:HB2	1.61	0.65
1:A:211:HIS:HB3	1:A:335:ASP:HB2	1.77	0.65
2:B:154:ILE:O	2:B:154:ILE:HD13	1.97	0.65
1:C:143:LEU:CD1	1:C:150:LEU:HD13	2.26	0.65
2:D:608:ARG:C	2:D:608:ARG:CB	2.64	0.65
1:E:262:GLU:OE1	1:E:262:GLU:HA	1.97	0.65
1:E:264:ASN:HD22	1:E:264:ASN:H	1.44	0.65
1:A:262:GLU:HB3	1:A:265:PHE:HB2	1.79	0.65
3:J:123:VAL:HG11	3:J:150:MET:HB3	1.77	0.65
2:H:171:PRO:O	2:H:174:ILE:HG13	1.97	0.65
2:B:217:THR:HG21	2:B:223:ARG:HH22	1.60	0.65
1:C:36:ILE:HG22	1:C:37:ASN:N	2.10	0.65
1:G:264:ASN:HD22	1:G:264:ASN:H	1.43	0.65
1:G:447:ASN:ND2	2:H:26:ARG:HE	1.95	0.65
2:B:213:PHE:HB2	2:B:218:ILE:HD11	1.78	0.65
2:B:251:GLY:O	2:B:257:ILE:HD11	1.97	0.65
2:D:154:ILE:O	2:D:154:ILE:HD13	1.96	0.65
2:D:171:PRO:O	2:D:174:ILE:HG13	1.97	0.65
1:E:36:ILE:HG22	1:E:37:ASN:N	2.10	0.65
1:A:266:GLU:HA	1:A:269:ILE:HD12	1.79	0.65
2:B:356:SER:HB2	2:B:359:ALA:HB3	1.79	0.65
2:F:703:GLY:HA2	2:F:706:ASP:CB	2.26	0.65
2:B:237:TRP:CE3	2:B:242:PRO:HG2	2.32	0.65
2:F:606:ARG:C	2:F:608:ARG:H	1.99	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ALA:O	1:A:490:PRO:HD3	1.97	0.64
2:F:213:PHE:HB2	2:F:218:ILE:HD11	1.79	0.64
1:G:49:LEU:C	1:G:52:PRO:HD2	2.17	0.64
2:D:356:SER:HB2	2:D:359:ALA:HB3	1.80	0.64
1:E:36:ILE:HB	1:E:128:ALA:HA	1.79	0.64
1:C:49:LEU:C	1:C:52:PRO:HD2	2.18	0.64
1:C:213:PRO:HB3	1:C:332:MET:HE3	1.79	0.64
1:C:262:GLU:HB3	1:C:265:PHE:HB2	1.78	0.64
1:C:307:LEU:HD13	1:C:383:LEU:HD22	1.80	0.64
1:E:213:PRO:HB3	1:E:332:MET:CE	2.27	0.64
2:F:159:ILE:HG23	2:F:162:LEU:HD12	1.78	0.64
1:A:261:ASP:O	1:A:262:GLU:CB	2.45	0.64
2:B:361:LEU:HA	2:B:364:VAL:CG2	2.27	0.64
2:B:380:ALA:HB1	2:B:394:LEU:HB2	1.79	0.64
2:D:608:ARG:N	2:D:608:ARG:HA	2.02	0.64
2:F:380:ALA:HB1	2:F:394:LEU:HB2	1.79	0.64
1:A:307:LEU:HD13	1:A:383:LEU:HD22	1.78	0.64
2:B:703:GLY:HA2	2:B:706:ASP:CB	2.28	0.64
1:C:75:PHE:CE2	1:C:96:LEU:HD11	2.32	0.64
2:D:217:THR:HA	2:D:221:MET:HG2	1.78	0.64
2:F:356:SER:HB2	2:F:359:ALA:HB3	1.79	0.64
1:A:366:GLN:C	1:A:368:ILE:H	2.01	0.64
1:G:396:ARG:HG3	1:G:534:LEU:CD1	2.22	0.64
2:B:171:PRO:O	2:B:174:ILE:HG13	1.97	0.64
3:I:105:VAL:HG11	3:I:130:VAL:HG22	1.78	0.64
1:C:33:VAL:HG23	1:C:54:ILE:HD11	1.80	0.64
2:D:54:ILE:HD13	2:D:127:ILE:HG21	1.80	0.64
2:H:154:ILE:O	2:H:154:ILE:HD13	1.98	0.64
2:H:703:GLY:HA2	2:H:706:ASP:CB	2.28	0.64
1:A:46:LEU:HD23	1:A:93:LEU:HD13	1.79	0.64
1:A:527:GLN:OE1	2:B:302:VAL:HG13	1.97	0.64
1:G:285:ILE:CD1	1:G:388:ALA:HA	2.24	0.64
1:G:533:GLN:O	1:G:534:LEU:CG	2.45	0.64
2:B:192:ILE:HG22	2:B:194:PRO:HD3	1.79	0.64
1:C:251:ILE:HG23	1:C:262:GLU:HG2	1.80	0.64
1:C:264:ASN:HD22	1:C:264:ASN:H	1.44	0.64
2:B:217:THR:HA	2:B:221:MET:HG2	1.80	0.63
1:E:229:THR:O	1:E:230:ASN:HB2	1.98	0.63
1:E:251:ILE:HG23	1:E:262:GLU:HG2	1.79	0.63
2:F:164:TYR:HE2	2:F:169:LEU:HB2	1.62	0.63
3:K:107:THR:CG2	3:K:111:LYS:H	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:LEU:HD13	2:B:150:ALA:HB1	1.80	0.63
1:C:488:ALA:O	1:C:490:PRO:HD3	1.97	0.63
2:D:267:ARG:HG2	2:D:267:ARG:NH1	2.13	0.63
2:D:361:LEU:HA	2:D:364:VAL:CG2	2.28	0.63
1:E:72:ASN:HD22	1:E:72:ASN:C	2.00	0.63
1:E:396:ARG:HG3	1:E:534:LEU:CD1	2.22	0.63
1:A:262:GLU:OE1	1:A:262:GLU:HA	1.98	0.63
1:C:446:SER:HB2	1:C:449:GLN:HG3	1.79	0.63
1:C:450:VAL:O	1:C:454:ILE:HG13	1.98	0.63
2:D:64:LEU:HB3	2:D:111:LEU:HD13	1.79	0.63
3:L:107:THR:CG2	3:L:111:LYS:H	2.12	0.63
3:K:150:MET:CE	3:K:167:LEU:HD22	2.28	0.63
1:G:262:GLU:OE1	1:G:262:GLU:HA	1.98	0.63
1:A:533:GLN:O	1:A:534:LEU:CG	2.46	0.63
2:B:351:GLN:HE21	2:B:351:GLN:HA	1.64	0.63
3:I:107:THR:CG2	3:I:111:LYS:H	2.12	0.63
1:C:447:ASN:HD22	2:D:26:ARG:HH21	1.45	0.63
1:E:253:LYS:O	1:E:260:GLU:OE2	2.16	0.63
2:F:360:LYS:C	2:F:361:LEU:HD23	2.18	0.63
1:G:376:SER:OG	1:G:379:GLU:HG3	1.98	0.63
1:G:450:VAL:O	1:G:454:ILE:HG13	1.97	0.63
1:C:72:ASN:C	1:C:72:ASN:HD22	2.02	0.63
1:C:261:ASP:O	1:C:262:GLU:HB2	1.98	0.63
2:D:74:GLN:NE2	2:D:119:ASN:HD22	1.96	0.63
2:D:360:LYS:C	2:D:361:LEU:HD23	2.18	0.63
1:E:366:GLN:C	1:E:368:ILE:H	2.01	0.63
1:G:260:GLU:C	1:G:261:ASP:OD1	2.37	0.63
2:H:318:LEU:HD21	2:H:321:TYR:N	2.12	0.63
3:L:138:PRO:HA	3:L:141:GLN:NE2	2.10	0.63
1:A:261:ASP:O	1:A:262:GLU:HB2	1.98	0.63
3:I:138:PRO:HA	3:I:141:GLN:NE2	2.10	0.63
1:E:253:LYS:O	1:E:260:GLU:HG3	1.97	0.63
1:E:488:ALA:O	1:E:490:PRO:HD3	1.99	0.63
2:F:217:THR:HA	2:F:221:MET:HG2	1.79	0.63
1:G:72:ASN:C	1:G:72:ASN:HD22	1.99	0.63
3:I:107:THR:HA	3:I:169:LEU:HD12	1.81	0.63
2:D:217:THR:HG21	2:D:223:ARG:HH22	1.64	0.63
1:E:75:PHE:CE2	1:E:96:LEU:HD11	2.34	0.63
1:A:229:THR:O	1:A:230:ASN:HB2	1.98	0.63
3:I:107:THR:HG22	3:I:111:LYS:H	1.64	0.63
1:C:261:ASP:O	1:C:262:GLU:CB	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:LEU:O	1:E:52:PRO:HD2	1.98	0.63
3:K:138:PRO:HA	3:K:141:GLN:NE2	2.12	0.63
1:G:488:ALA:O	1:G:490:PRO:HD3	1.99	0.63
1:C:229:THR:O	1:C:230:ASN:HB2	1.98	0.62
2:D:348:GLN:HE21	2:D:348:GLN:C	2.02	0.62
1:E:61:ASP:CB	1:E:86:ALA:HB2	2.26	0.62
2:F:251:GLY:O	2:F:257:ILE:HD11	1.99	0.62
2:F:359:ALA:HB1	2:F:363:GLU:OE1	1.99	0.62
2:B:74:GLN:NE2	2:B:119:ASN:HD22	1.96	0.62
1:C:448:TYR:HE2	2:H:240:GLU:OE2	1.82	0.62
2:D:703:GLY:HA2	2:D:706:ASP:CB	2.30	0.62
2:F:361:LEU:HA	2:F:364:VAL:CG2	2.29	0.62
1:G:229:THR:O	1:G:230:ASN:HB2	1.98	0.62
2:H:348:GLN:HE21	2:H:348:GLN:C	2.02	0.62
3:J:107:THR:CG2	3:J:111:LYS:H	2.12	0.62
2:H:351:GLN:HA	2:H:351:GLN:HE21	1.65	0.62
1:A:36:ILE:HB	1:A:128:ALA:HA	1.82	0.62
1:A:61:ASP:CB	1:A:86:ALA:HB2	2.29	0.62
1:E:447:ASN:ND2	2:F:26:ARG:HE	1.95	0.62
3:J:156:ALA:HA	3:J:161:ILE:HD12	1.80	0.62
1:E:518:ASN:HD22	1:E:533:GLN:HG3	1.63	0.62
2:F:606:ARG:C	2:F:608:ARG:N	2.51	0.62
1:G:72:ASN:C	1:G:72:ASN:ND2	2.53	0.62
1:A:260:GLU:C	1:A:261:ASP:OD1	2.38	0.62
3:I:156:ALA:HA	3:I:161:ILE:HD12	1.80	0.62
1:C:36:ILE:HB	1:C:128:ALA:HA	1.81	0.62
1:G:36:ILE:HB	1:G:128:ALA:HA	1.82	0.62
1:A:232:ARG:C	1:A:234:PRO:HD3	2.20	0.62
2:D:145:LEU:HD13	2:D:150:ALA:HB1	1.81	0.62
1:E:233:ILE:N	1:E:234:PRO:HD3	2.14	0.62
1:E:236:THR:O	1:E:237:TYR:CB	2.42	0.62
1:E:446:SER:HB2	1:E:449:GLN:HG3	1.80	0.62
2:D:80:MET:HG2	4:D:6:ATP:C2	2.34	0.62
1:G:36:ILE:HG22	1:G:37:ASN:N	2.15	0.62
1:G:260:GLU:CB	1:G:261:ASP:OD1	2.48	0.62
1:A:233:ILE:N	1:A:234:PRO:HD3	2.15	0.62
2:B:365:LEU:HD22	2:B:393:TYR:OH	1.99	0.62
1:C:266:GLU:HA	1:C:269:ILE:HD12	1.81	0.62
1:G:253:LYS:O	1:G:260:GLU:CG	2.48	0.62
2:H:102:PRO:HB2	2:H:105:GLU:HB2	1.82	0.62
1:A:253:LYS:O	1:A:260:GLU:HG2	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:GLU:CB	1:A:261:ASP:OD1	2.48	0.61
1:A:390:LEU:O	1:A:391:ARG:HG2	2.00	0.61
1:A:510:THR:HB	1:A:512:GLN:HG3	1.81	0.61
2:B:318:LEU:HD21	2:B:321:TYR:N	2.15	0.61
2:B:348:GLN:C	2:B:348:GLN:HE21	2.02	0.61
1:E:533:GLN:O	1:E:534:LEU:CG	2.47	0.61
2:H:360:LYS:C	2:H:361:LEU:HD23	2.20	0.61
1:C:376:SER:OG	1:C:379:GLU:HG3	1.99	0.61
2:D:318:LEU:HD21	2:D:321:TYR:N	2.15	0.61
2:D:380:ALA:HB1	2:D:394:LEU:HB2	1.81	0.61
3:K:156:ALA:HA	3:K:161:ILE:HD12	1.80	0.61
1:G:46:LEU:HD23	1:G:93:LEU:HD13	1.81	0.61
2:H:178:ILE:HD11	2:H:310:ILE:HD12	1.82	0.61
1:C:262:GLU:OE1	1:C:262:GLU:HA	1.98	0.61
1:C:347:ARG:HH22	2:D:274:ARG:HH11	1.46	0.61
2:D:252:ASP:O	2:D:254:PRO:HD3	2.01	0.61
1:E:213:PRO:HB3	1:E:332:MET:HE3	1.82	0.61
3:L:107:THR:HG22	3:L:111:LYS:H	1.65	0.61
3:K:107:THR:HG22	3:K:111:LYS:H	1.65	0.61
1:G:232:ARG:C	1:G:234:PRO:HD3	2.20	0.61
1:C:260:GLU:C	1:C:261:ASP:OD1	2.39	0.61
1:G:61:ASP:CB	1:G:86:ALA:HB2	2.29	0.61
1:G:266:GLU:HA	1:G:269:ILE:HD12	1.81	0.61
2:H:217:THR:HG21	2:H:223:ARG:HH22	1.64	0.61
3:L:150:MET:CE	3:L:167:LEU:HD22	2.29	0.61
2:B:380:ALA:CB	2:B:394:LEU:HD13	2.20	0.61
2:B:360:LYS:C	2:B:361:LEU:HD23	2.20	0.61
2:H:54:ILE:HD13	2:H:127:ILE:HG21	1.83	0.61
2:H:901:VAL:O	2:H:902:ALA:O	2.18	0.61
2:B:359:ALA:HB1	2:B:363:GLU:OE1	2.01	0.61
3:I:138:PRO:CA	3:I:141:GLN:HE21	2.13	0.61
1:C:366:GLN:C	1:C:368:ILE:H	2.02	0.61
3:J:150:MET:CE	3:J:167:LEU:HD22	2.30	0.61
2:F:351:GLN:HA	2:F:351:GLN:HE21	1.66	0.61
3:K:107:THR:HA	3:K:169:LEU:HD12	1.82	0.61
3:L:107:THR:HA	3:L:169:LEU:HD12	1.81	0.61
1:A:75:PHE:CE2	1:A:96:LEU:HD11	2.36	0.61
1:C:214:TRP:CD1	1:C:214:TRP:C	2.74	0.61
1:C:428:MET:O	1:C:431:ALA:HB3	2.01	0.61
2:F:102:PRO:HB2	2:F:105:GLU:HB2	1.83	0.61
2:F:318:LEU:HD21	2:F:321:TYR:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:394:LEU:CG	2:F:396:SER:HB3	2.31	0.61
1:G:38:ALA:O	1:G:85:ARG:HD3	2.00	0.61
1:G:49:LEU:O	1:G:52:PRO:HD2	2.00	0.61
1:C:309:ARG:CG	1:C:364:LEU:HD21	2.31	0.60
1:A:72:ASN:C	1:A:72:ASN:HD22	2.02	0.60
2:B:54:ILE:HD13	2:B:127:ILE:HG21	1.82	0.60
3:K:118:GLU:O	3:K:120:THR:N	2.29	0.60
2:H:145:LEU:HD13	2:H:150:ALA:HB1	1.81	0.60
3:L:156:ALA:HA	3:L:161:ILE:HD12	1.82	0.60
2:B:252:ASP:O	2:B:254:PRO:HD3	2.02	0.60
2:D:64:LEU:HD21	2:D:77:VAL:HG22	1.83	0.60
2:D:257:ILE:HD13	2:D:282:GLN:HG2	1.82	0.60
2:D:335:PHE:HE1	2:D:337:ALA:HB2	1.65	0.60
3:J:138:PRO:HA	3:J:141:GLN:NE2	2.13	0.60
1:E:72:ASN:C	1:E:72:ASN:ND2	2.54	0.60
3:K:141:GLN:O	3:K:142:ARG:HD3	2.02	0.60
1:G:446:SER:HB2	1:G:449:GLN:HG3	1.83	0.60
1:C:260:GLU:CB	1:C:261:ASP:OD1	2.50	0.60
1:C:397:SER:OG	1:C:400:GLU:HG3	2.01	0.60
1:E:232:ARG:C	1:E:234:PRO:HD3	2.21	0.60
2:B:110:PHE:HD2	2:B:110:PHE:C	2.04	0.60
1:C:49:LEU:O	1:C:52:PRO:HD2	2.01	0.60
1:E:347:ARG:HH22	2:F:274:ARG:HH11	1.48	0.60
1:G:213:PRO:HB3	1:G:332:MET:HE3	1.83	0.60
1:G:428:MET:O	1:G:431:ALA:HB3	2.01	0.60
2:H:394:LEU:CG	2:H:396:SER:HB3	2.31	0.60
1:C:232:ARG:C	1:C:234:PRO:HD3	2.21	0.60
2:D:102:PRO:HB2	2:D:105:GLU:HB2	1.83	0.60
2:D:359:ALA:HB1	2:D:363:GLU:OE1	2.02	0.60
2:F:217:THR:HG21	2:F:223:ARG:HH22	1.66	0.60
1:G:518:ASN:HD22	1:G:533:GLN:HG3	1.66	0.60
1:C:481:GLU:OE1	1:C:481:GLU:HA	2.02	0.60
3:J:107:THR:HA	3:J:169:LEU:HD12	1.83	0.60
1:G:214:TRP:CD1	1:G:214:TRP:C	2.75	0.60
1:G:366:GLN:C	1:G:368:ILE:H	2.03	0.60
2:B:267:ARG:HG2	2:B:267:ARG:NH1	2.12	0.60
2:F:74:GLN:NE2	2:F:119:ASN:HD22	1.99	0.60
2:H:192:ILE:HG22	2:H:194:PRO:HD3	1.82	0.60
2:B:64:LEU:HB3	2:B:111:LEU:HD13	1.82	0.60
1:G:8:LEU:HD12	1:G:11:GLN:OE1	2.01	0.60
2:H:54:ILE:CD1	2:H:154:ILE:HG13	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:394:LEU:HD21	2:F:396:SER:HB3	1.82	0.60
1:A:49:LEU:O	1:A:52:PRO:HD2	2.01	0.59
2:B:229:ILE:HA	2:B:264:SER:OG	2.02	0.59
3:I:118:GLU:O	3:I:120:THR:N	2.30	0.59
1:G:261:ASP:OD1	1:G:261:ASP:N	2.35	0.59
2:H:81:ASP:HB2	4:H:8:ATP:O2'	2.02	0.59
3:L:138:PRO:CA	3:L:141:GLN:HE21	2.13	0.59
1:A:16:GLN:NE2	1:A:20:TRP:HZ2	2.01	0.59
3:I:150:MET:CE	3:I:167:LEU:HD22	2.32	0.59
1:E:13:TYR:O	1:E:17:LEU:HG	2.01	0.59
1:G:422:GLU:HG3	1:G:530:ALA:CB	2.31	0.59
1:A:309:ARG:CG	1:A:364:LEU:HD21	2.30	0.59
2:B:394:LEU:CG	2:B:396:SER:HB3	2.32	0.59
1:C:233:ILE:N	1:C:234:PRO:HD3	2.16	0.59
1:E:260:GLU:C	1:E:261:ASP:OD1	2.39	0.59
1:E:450:VAL:O	1:E:454:ILE:HG13	2.01	0.59
2:F:348:GLN:HE21	2:F:348:GLN:C	2.05	0.59
1:C:46:LEU:HD23	1:C:93:LEU:HD13	1.84	0.59
2:D:251:GLY:O	2:D:257:ILE:HD11	2.02	0.59
3:J:107:THR:HG22	3:J:111:LYS:H	1.67	0.59
1:E:407:ILE:O	1:E:407:ILE:HG23	2.02	0.59
1:G:233:ILE:N	1:G:234:PRO:HD3	2.16	0.59
2:H:356:SER:HB2	2:H:359:ALA:HB3	1.84	0.59
1:C:34:CYS:HB2	1:C:123:PHE:CE2	2.38	0.59
1:C:61:ASP:CB	1:C:86:ALA:HB2	2.30	0.59
1:C:510:THR:HB	1:C:512:GLN:HG3	1.83	0.59
2:D:351:GLN:HE21	2:D:351:GLN:HA	1.67	0.59
2:D:394:LEU:CG	2:D:396:SER:HB3	2.33	0.59
1:G:518:ASN:ND2	1:G:533:GLN:CG	2.62	0.59
2:H:229:ILE:HA	2:H:264:SER:OG	2.01	0.59
2:B:178:ILE:HD11	2:B:310:ILE:HD12	1.84	0.59
3:I:170:VAL:HG13	3:I:171:LEU:N	2.16	0.59
1:G:261:ASP:O	1:G:262:GLU:CB	2.51	0.59
2:D:56:ALA:HA	2:D:60:GLY:HA3	1.83	0.59
2:F:277:THR:HG23	2:F:280:LEU:H	1.68	0.59
2:H:322:LEU:HD12	2:H:322:LEU:C	2.23	0.59
1:A:243:PHE:O	1:A:246:LEU:HB3	2.02	0.59
1:A:261:ASP:OD1	1:A:261:ASP:N	2.35	0.59
1:A:450:VAL:O	1:A:454:ILE:HG13	2.01	0.59
2:B:64:LEU:HD21	2:B:77:VAL:HG22	1.84	0.59
1:C:243:PHE:O	1:C:246:LEU:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:PRO:C	1:C:260:GLU:HG2	2.22	0.59
1:C:422:GLU:HG3	1:C:530:ALA:CB	2.32	0.59
1:E:214:TRP:CD1	1:E:214:TRP:C	2.76	0.59
2:F:335:PHE:HE1	2:F:337:ALA:HB2	1.67	0.59
2:H:159:ILE:HG23	2:H:162:LEU:HD12	1.83	0.59
2:B:357:PRO:O	2:B:358:SER:CB	2.51	0.59
1:C:396:ARG:HG3	1:C:534:LEU:CD1	2.24	0.59
1:E:447:ASN:HD22	2:F:26:ARG:HH21	1.50	0.59
2:F:54:ILE:HD13	2:F:127:ILE:HG21	1.85	0.59
2:H:110:PHE:HD2	2:H:110:PHE:C	2.06	0.59
3:L:117:ILE:CD1	3:L:126:ILE:HG23	2.32	0.59
1:E:366:GLN:O	1:E:368:ILE:N	2.36	0.59
1:G:236:THR:O	1:G:237:TYR:CB	2.49	0.59
1:G:347:ARG:HH22	2:H:274:ARG:HH11	1.50	0.59
1:A:72:ASN:C	1:A:72:ASN:ND2	2.56	0.58
2:B:152:ARG:O	2:B:155:ASN:HB3	2.04	0.58
1:C:8:LEU:HD12	1:C:11:GLN:OE1	2.03	0.58
2:F:357:PRO:O	2:F:358:SER:CB	2.51	0.58
2:H:64:LEU:HD21	2:H:77:VAL:HG22	1.86	0.58
3:L:141:GLN:O	3:L:142:ARG:HD3	2.03	0.58
2:F:357:PRO:O	2:F:358:SER:HB3	2.03	0.58
2:H:74:GLN:NE2	2:H:119:ASN:HD22	2.00	0.58
1:C:214:TRP:CE3	1:C:332:MET:HB3	2.39	0.58
2:D:700:LYS:N	2:D:700:LYS:HA	2.04	0.58
2:H:128:GLN:HE22	4:H:8:ATP:HN62	1.51	0.58
1:A:33:VAL:HG23	1:A:54:ILE:HD11	1.84	0.58
1:A:446:SER:HB2	1:A:449:GLN:HG3	1.84	0.58
1:G:307:LEU:HB3	1:G:383:LEU:HD21	1.85	0.58
1:A:214:TRP:C	1:A:214:TRP:CD1	2.76	0.58
2:B:102:PRO:HB2	2:B:105:GLU:HB2	1.85	0.58
1:G:332:MET:HG2	1:G:339:TYR:HE1	1.68	0.58
1:G:527:GLN:OE1	2:H:302:VAL:HG13	2.04	0.58
1:A:422:GLU:HG3	1:A:530:ALA:CB	2.34	0.58
3:I:141:GLN:O	3:I:142:ARG:HD3	2.04	0.58
2:D:178:ILE:HD11	2:D:310:ILE:HD12	1.85	0.58
1:E:199:TYR:CD2	1:E:216:VAL:HG11	2.39	0.58
2:B:56:ALA:HA	2:B:60:GLY:HA3	1.86	0.58
1:E:266:GLU:HA	1:E:269:ILE:HD12	1.84	0.58
1:E:341:LYS:O	1:E:345:VAL:HG23	2.04	0.58
2:F:54:ILE:CD1	2:F:154:ILE:HG13	2.33	0.58
3:K:138:PRO:CA	3:K:141:GLN:HE21	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:80:MET:HG2	4:H:8:ATP:C4	2.39	0.58
2:H:361:LEU:HA	2:H:364:VAL:CG2	2.32	0.58
2:B:277:THR:HG23	2:B:280:LEU:H	1.69	0.58
1:C:199:TYR:CD2	1:C:216:VAL:HG11	2.39	0.58
2:D:229:ILE:HA	2:D:264:SER:OG	2.03	0.58
1:E:422:GLU:HG3	1:E:530:ALA:CB	2.33	0.58
3:K:117:ILE:CD1	3:K:126:ILE:HG23	2.34	0.58
1:G:481:GLU:OE1	1:G:481:GLU:HA	2.04	0.57
2:D:110:PHE:HD2	2:D:110:PHE:C	2.07	0.57
3:J:118:GLU:O	3:J:120:THR:N	2.31	0.57
1:E:259:PRO:C	1:E:260:GLU:HG2	2.23	0.57
1:E:261:ASP:OD1	1:E:261:ASP:N	2.36	0.57
3:K:170:VAL:HG13	3:K:171:LEU:N	2.18	0.57
1:A:8:LEU:HD12	1:A:11:GLN:OE1	2.04	0.57
1:C:341:LYS:O	1:C:345:VAL:HG23	2.04	0.57
1:C:533:GLN:O	1:C:534:LEU:CG	2.52	0.57
2:F:56:ALA:N	2:F:79:ASP:OD1	2.38	0.57
1:A:199:TYR:CD2	1:A:216:VAL:HG11	2.40	0.57
1:E:16:GLN:NE2	1:E:20:TRP:HZ2	2.02	0.57
1:E:260:GLU:CB	1:E:261:ASP:OD1	2.52	0.57
2:F:64:LEU:HD21	2:F:77:VAL:HG22	1.86	0.57
1:A:297:ILE:HD11	1:A:309:ARG:HG2	1.87	0.57
2:B:13:TRP:HZ3	2:B:116:PRO:HG2	1.69	0.57
2:B:87:ASN:HB3	2:B:91:GLN:CD	2.25	0.57
1:E:46:LEU:HD23	1:E:93:LEU:HD13	1.85	0.57
1:G:16:GLN:NE2	1:G:20:TRP:HZ2	2.03	0.57
2:H:110:PHE:C	2:H:110:PHE:CD2	2.78	0.57
2:H:365:LEU:HD22	2:H:393:TYR:OH	2.05	0.57
3:L:118:GLU:O	3:L:120:THR:N	2.30	0.57
2:B:110:PHE:C	2:B:110:PHE:CD2	2.76	0.57
1:E:307:LEU:CB	1:E:383:LEU:HD22	2.33	0.57
2:F:229:ILE:HA	2:F:264:SER:OG	2.03	0.57
2:F:365:LEU:HD22	2:F:393:TYR:OH	2.04	0.57
2:H:152:ARG:O	2:H:155:ASN:HB3	2.04	0.57
1:C:72:ASN:C	1:C:72:ASN:ND2	2.56	0.57
1:E:8:LEU:HD12	1:E:11:GLN:OE1	2.03	0.57
2:F:145:LEU:HD13	2:F:150:ALA:HB1	1.85	0.57
2:H:277:THR:HG23	2:H:280:LEU:H	1.69	0.57
2:H:335:PHE:HE1	2:H:337:ALA:HB2	1.70	0.57
1:A:366:GLN:O	1:A:368:ILE:N	2.38	0.57
1:C:261:ASP:OD1	1:C:261:ASP:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:VAL:HG23	1:G:54:ILE:HD11	1.87	0.57
1:G:251:ILE:HG23	1:G:262:GLU:HG2	1.85	0.57
2:B:257:ILE:HD13	2:B:282:GLN:HG2	1.87	0.57
2:B:335:PHE:HE1	2:B:337:ALA:HB2	1.69	0.57
3:I:150:MET:HE1	3:I:167:LEU:HD22	1.87	0.57
1:E:307:LEU:HB3	1:E:383:LEU:HD21	1.86	0.57
1:A:251:ILE:HG23	1:A:262:GLU:HG2	1.85	0.57
1:C:84:ASN:OD1	1:C:106:GLU:HG2	2.05	0.57
2:D:46:LEU:O	2:D:73:ARG:HB2	2.05	0.57
2:D:54:ILE:CD1	2:D:154:ILE:HG13	2.35	0.57
2:D:58:GLY:N	2:D:91:GLN:HG2	2.12	0.57
1:E:481:GLU:OE1	1:E:481:GLU:HA	2.05	0.57
2:F:152:ARG:O	2:F:155:ASN:HB3	2.05	0.57
1:G:13:TYR:O	1:G:17:LEU:HG	2.04	0.57
1:G:199:TYR:CD2	1:G:216:VAL:HG11	2.40	0.57
1:A:347:ARG:HH22	2:B:274:ARG:HH11	1.52	0.56
1:E:407:ILE:HD12	1:E:409:LYS:HB3	1.86	0.56
1:E:510:THR:HB	1:E:512:GLN:HG3	1.87	0.56
1:G:84:ASN:OD1	1:G:106:GLU:HG2	2.04	0.56
1:A:332:MET:HG2	1:A:339:TYR:HE1	1.70	0.56
1:A:341:LYS:O	1:A:345:VAL:HG23	2.06	0.56
1:C:342:LEU:HD11	1:C:346:TYR:HE1	1.69	0.56
2:D:110:PHE:C	2:D:110:PHE:CD2	2.79	0.56
1:G:214:TRP:CE3	1:G:332:MET:HB3	2.40	0.56
2:H:56:ALA:HA	2:H:60:GLY:HA3	1.86	0.56
2:B:267:ARG:HH11	2:B:267:ARG:CG	2.16	0.56
3:J:141:GLN:O	3:J:142:ARG:HD3	2.05	0.56
1:E:243:PHE:O	1:E:246:LEU:HB3	2.04	0.56
1:E:407:ILE:O	1:E:409:LYS:N	2.38	0.56
2:F:110:PHE:HD2	2:F:110:PHE:C	2.08	0.56
2:H:335:PHE:CZ	3:L:144:ILE:HD13	2.40	0.56
1:A:13:TYR:O	1:A:17:LEU:HG	2.04	0.56
1:A:84:ASN:OD1	1:A:106:GLU:HG2	2.05	0.56
2:D:394:LEU:HG	2:D:396:SER:H	1.71	0.56
1:E:38:ALA:O	1:E:85:ARG:HD3	2.05	0.56
2:F:257:ILE:HD13	2:F:282:GLN:HG2	1.88	0.56
1:G:407:ILE:O	1:G:409:LYS:N	2.38	0.56
2:D:357:PRO:O	2:D:358:SER:HB3	2.05	0.56
1:E:34:CYS:HB2	1:E:123:PHE:CE2	2.40	0.56
1:E:261:ASP:O	1:E:262:GLU:HB2	2.05	0.56
1:G:185:LEU:O	1:G:188:PRO:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:252:ASP:O	2:H:254:PRO:HD3	2.05	0.56
2:D:394:LEU:HD21	2:D:396:SER:HB3	1.88	0.56
3:J:117:ILE:CD1	3:J:126:ILE:HG23	2.35	0.56
1:G:407:ILE:HD12	1:G:409:LYS:HB3	1.87	0.56
2:B:357:PRO:O	2:B:358:SER:HB3	2.05	0.56
2:D:277:THR:HG23	2:D:280:LEU:H	1.69	0.56
3:J:150:MET:HE1	3:J:167:LEU:HD22	1.87	0.56
1:E:214:TRP:CE3	1:E:332:MET:HB3	2.40	0.56
1:E:261:ASP:O	1:E:262:GLU:CB	2.54	0.56
2:F:394:LEU:HG	2:F:396:SER:H	1.71	0.56
1:G:510:THR:HB	1:G:512:GLN:HG3	1.88	0.56
2:H:267:ARG:HG2	2:H:267:ARG:NH1	2.13	0.56
1:C:39:THR:O	1:C:43:THR:HB	2.06	0.56
2:D:365:LEU:HD22	2:D:393:TYR:OH	2.06	0.56
1:E:50:VAL:HG13	1:E:100:VAL:HG21	1.88	0.56
1:G:407:ILE:O	1:G:407:ILE:HG23	2.06	0.56
1:A:235:LYS:HB2	1:A:239:GLU:OE1	2.06	0.56
2:B:54:ILE:CD1	2:B:154:ILE:HG13	2.36	0.56
2:B:64:LEU:HD11	2:B:77:VAL:HG21	1.88	0.56
1:E:342:LEU:HD11	1:E:346:TYR:HE1	1.71	0.56
1:G:243:PHE:O	1:G:246:LEU:HB3	2.04	0.56
2:D:343:CYS:SG	2:D:346:CYS:SG	3.04	0.56
2:F:335:PHE:CZ	3:K:144:ILE:HD13	2.41	0.56
2:D:322:LEU:HD12	2:D:322:LEU:C	2.27	0.55
2:D:357:PRO:O	2:D:358:SER:CB	2.54	0.55
1:E:33:VAL:HG23	1:E:54:ILE:HD11	1.88	0.55
1:E:309:ARG:CG	1:E:364:LEU:HD21	2.31	0.55
2:F:64:LEU:HD11	2:F:77:VAL:HG21	1.88	0.55
1:G:309:ARG:CG	1:G:364:LEU:HD21	2.33	0.55
2:H:394:LEU:HG	2:H:396:SER:H	1.71	0.55
2:B:16:ARG:NH2	2:B:116:PRO:HB2	2.21	0.55
2:D:335:PHE:HE2	3:J:170:VAL:HG21	1.71	0.55
3:J:170:VAL:HG13	3:J:171:LEU:N	2.20	0.55
1:A:407:ILE:HG23	1:A:407:ILE:O	2.07	0.55
1:A:481:GLU:HA	1:A:481:GLU:OE1	2.06	0.55
1:E:332:MET:HG2	1:E:339:TYR:HE1	1.71	0.55
2:F:178:ILE:N	2:F:178:ILE:HD12	2.21	0.55
1:G:261:ASP:O	1:G:262:GLU:HB2	2.06	0.55
1:G:533:GLN:O	1:G:534:LEU:CB	2.55	0.55
2:B:159:ILE:HG23	2:B:162:LEU:HD12	1.87	0.55
1:C:229:THR:HG22	1:C:231:GLY:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ILE:HD11	1:C:309:ARG:HG2	1.89	0.55
2:D:64:LEU:HD11	2:D:77:VAL:HG21	1.88	0.55
1:E:518:ASN:ND2	1:E:533:GLN:CG	2.61	0.55
1:G:341:LYS:O	1:G:345:VAL:HG23	2.06	0.55
2:H:351:GLN:HA	2:H:351:GLN:NE2	2.22	0.55
2:D:901:VAL:C	2:D:902:ALA:O	2.40	0.55
1:E:46:LEU:HD21	1:E:57:PHE:CD1	2.41	0.55
1:E:84:ASN:OD1	1:E:106:GLU:HG2	2.06	0.55
1:E:428:MET:O	1:E:431:ALA:HB3	2.07	0.55
3:K:117:ILE:HD13	3:K:126:ILE:HG12	1.89	0.55
1:A:229:THR:HG22	1:A:231:GLY:N	2.22	0.55
1:A:259:PRO:C	1:A:260:GLU:HG2	2.27	0.55
2:B:164:TYR:CE2	2:B:169:LEU:HD13	2.41	0.55
3:I:117:ILE:CD1	3:I:126:ILE:HG23	2.37	0.55
1:C:16:GLN:NE2	1:C:20:TRP:HZ2	2.05	0.55
2:D:240:GLU:O	2:D:241:GLN:C	2.45	0.55
3:J:138:PRO:CA	3:J:141:GLN:HE21	2.16	0.55
2:F:252:ASP:O	2:F:254:PRO:HD3	2.06	0.55
2:B:394:LEU:HG	2:B:396:SER:H	1.72	0.55
1:C:407:ILE:HG23	1:C:407:ILE:O	2.07	0.55
2:D:152:ARG:O	2:D:155:ASN:HB3	2.06	0.55
2:D:325:ASN:HD22	2:D:326:ASP:N	2.04	0.55
1:A:229:THR:O	1:A:230:ASN:CB	2.55	0.55
1:C:235:LYS:HB2	1:C:239:GLU:OE1	2.07	0.55
1:G:342:LEU:HD11	1:G:346:TYR:HE1	1.72	0.55
2:H:240:GLU:O	2:H:241:GLN:C	2.45	0.55
2:H:380:ALA:CB	2:H:394:LEU:HB2	2.37	0.55
2:B:351:GLN:HA	2:B:351:GLN:NE2	2.21	0.54
1:C:41:THR:O	1:C:45:ILE:HG13	2.07	0.54
1:C:353:ASP:O	1:C:357:VAL:HG23	2.07	0.54
2:D:237:TRP:CD2	2:D:242:PRO:HG2	2.41	0.54
2:F:237:TRP:CD2	2:F:242:PRO:HG2	2.42	0.54
1:G:229:THR:HG22	1:G:231:GLY:H	1.73	0.54
2:B:356:SER:CB	2:B:359:ALA:HB3	2.38	0.54
2:F:56:ALA:HA	2:F:60:GLY:HA3	1.88	0.54
2:F:110:PHE:C	2:F:110:PHE:CD2	2.80	0.54
2:F:178:ILE:HD11	2:F:310:ILE:HD12	1.89	0.54
2:F:325:ASN:HD22	2:F:326:ASP:N	2.05	0.54
2:B:85:VAL:HG13	2:B:86:SER:N	2.22	0.54
2:B:394:LEU:HD21	2:B:396:SER:HB3	1.89	0.54
3:K:103:ILE:CD1	3:K:115:ILE:HB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:ASN:HB3	2:H:91:GLN:CD	2.27	0.54
2:H:162:LEU:HD21	2:H:174:ILE:HG23	1.89	0.54
2:H:237:TRP:CD2	2:H:242:PRO:HG2	2.41	0.54
1:A:60:ILE:HD11	1:A:119:PHE:HE2	1.73	0.54
1:A:214:TRP:CE3	1:A:332:MET:HB3	2.42	0.54
1:A:229:THR:HG22	1:A:231:GLY:H	1.71	0.54
1:C:232:ARG:CB	1:C:234:PRO:HD3	2.35	0.54
1:C:366:GLN:O	1:C:368:ILE:N	2.40	0.54
2:D:13:TRP:HZ3	2:D:116:PRO:HG2	1.72	0.54
1:G:297:ILE:HD11	1:G:309:ARG:HG2	1.90	0.54
1:A:317:LYS:HB3	1:A:318:GLU:OE1	2.08	0.54
1:C:185:LEU:O	1:C:188:PRO:HD3	2.06	0.54
1:C:518:ASN:HD22	1:C:533:GLN:HG3	1.71	0.54
2:D:64:LEU:HD21	2:D:77:VAL:CG2	2.37	0.54
2:D:159:ILE:HG23	2:D:162:LEU:HD12	1.89	0.54
1:E:185:LEU:O	1:E:188:PRO:HD3	2.07	0.54
1:E:229:THR:HG22	1:E:231:GLY:H	1.72	0.54
3:K:150:MET:HE3	3:K:167:LEU:HD22	1.89	0.54
2:H:325:ASN:HD22	2:H:326:ASP:N	2.05	0.54
1:A:221:TYR:OH	1:A:250:GLY:HA3	2.07	0.54
1:C:221:TYR:OH	1:C:250:GLY:HA3	2.07	0.54
2:D:81:ASP:HB2	4:D:6:ATP:O2'	2.08	0.54
2:F:195:GLY:O	2:F:196:MET:HG3	2.08	0.54
2:F:232:VAL:HG11	2:F:263:LYS:HB2	1.88	0.54
1:A:248:ARG:C	1:A:250:GLY:H	2.11	0.54
1:A:447:ASN:ND2	2:B:26:ARG:HE	2.04	0.54
2:B:56:ALA:N	2:B:79:ASP:OD1	2.40	0.54
1:C:253:LYS:O	1:C:260:GLU:CG	2.55	0.54
2:F:164:TYR:CE2	2:F:169:LEU:HD13	2.43	0.54
1:G:426:TYR:CZ	1:G:430:ARG:HD3	2.43	0.54
1:C:332:MET:HG2	1:C:339:TYR:HE1	1.73	0.54
2:D:351:GLN:HA	2:D:351:GLN:NE2	2.23	0.54
1:E:235:LYS:HB2	1:E:239:GLU:OE1	2.08	0.54
2:F:58:GLY:N	2:F:91:GLN:HG2	2.11	0.54
2:F:351:GLN:HA	2:F:351:GLN:NE2	2.22	0.54
2:B:87:ASN:HB3	2:B:91:GLN:NE2	2.23	0.54
2:B:217:THR:CG2	2:B:223:ARG:HH22	2.21	0.54
2:B:240:GLU:O	2:B:241:GLN:C	2.46	0.54
2:D:178:ILE:HD12	2:D:178:ILE:N	2.23	0.54
1:E:16:GLN:CB	2:F:292:VAL:HG12	2.38	0.54
2:F:316:ILE:H	2:F:316:ILE:CD1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:CYS:HB2	1:G:123:PHE:CE2	2.42	0.54
1:G:366:GLN:O	1:G:368:ILE:N	2.41	0.54
1:A:232:ARG:CB	1:A:234:PRO:HD3	2.33	0.53
1:C:293:ARG:HG2	1:C:305:TRP:CD1	2.43	0.53
2:D:164:TYR:CE2	2:D:169:LEU:HD13	2.44	0.53
2:F:162:LEU:HD21	2:F:174:ILE:HG23	1.90	0.53
2:H:13:TRP:HZ3	2:H:116:PRO:HG2	1.73	0.53
1:A:533:GLN:O	1:A:534:LEU:CB	2.56	0.53
3:I:101:MET:SD	3:I:162:LEU:HA	2.48	0.53
3:I:103:ILE:HD11	3:I:115:ILE:HB	1.90	0.53
3:I:155:THR:O	3:I:158:ASP:HB2	2.09	0.53
1:C:13:TYR:O	1:C:17:LEU:HG	2.08	0.53
1:C:229:THR:HG22	1:C:231:GLY:N	2.23	0.53
2:F:87:ASN:HB3	2:F:91:GLN:CD	2.29	0.53
2:H:371:SER:O	2:H:373:SER:N	2.41	0.53
3:L:103:ILE:CD1	3:L:115:ILE:HB	2.38	0.53
1:A:407:ILE:O	1:A:409:LYS:N	2.40	0.53
2:B:178:ILE:HD12	2:B:178:ILE:N	2.23	0.53
2:B:380:ALA:CB	2:B:394:LEU:HB2	2.38	0.53
1:C:248:ARG:C	1:C:250:GLY:H	2.12	0.53
1:C:407:ILE:HD12	1:C:409:LYS:HB3	1.89	0.53
2:F:87:ASN:HB3	2:F:91:GLN:NE2	2.23	0.53
2:H:58:GLY:N	2:H:91:GLN:HG2	2.17	0.53
1:A:407:ILE:HD12	1:A:409:LYS:HB3	1.91	0.53
2:D:195:GLY:O	2:D:196:MET:HG3	2.09	0.53
2:F:13:TRP:HZ3	2:F:116:PRO:HG2	1.74	0.53
3:L:150:MET:HE1	3:L:167:LEU:HD22	1.90	0.53
1:C:307:LEU:HB3	1:C:383:LEU:HD21	1.90	0.53
2:D:356:SER:CB	2:D:359:ALA:HB3	2.39	0.53
2:F:128:GLN:H	2:F:128:GLN:HE21	0.79	0.53
2:F:240:GLU:O	2:F:241:GLN:C	2.46	0.53
2:H:158:LEU:CD1	2:H:177:LEU:HB2	2.38	0.53
2:H:320:ASN:O	2:H:321:TYR:HB2	2.09	0.53
1:A:34:CYS:HB2	1:A:123:PHE:CE2	2.43	0.53
1:E:181:GLU:OE1	1:E:181:GLU:HA	2.08	0.53
1:G:50:VAL:HG13	1:G:100:VAL:HG21	1.91	0.53
3:L:170:VAL:HG13	3:L:171:LEU:N	2.22	0.53
1:A:260:GLU:HB3	1:A:261:ASP:OD1	2.09	0.53
2:B:46:LEU:O	2:B:73:ARG:HB2	2.08	0.53
1:E:229:THR:HG22	1:E:231:GLY:N	2.24	0.53
2:H:111:LEU:O	2:H:111:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:THR:HG22	2:B:198:ALA:N	2.23	0.53
2:B:901:VAL:O	2:B:902:ALA:O	2.26	0.53
3:I:103:ILE:HD12	3:I:103:ILE:O	2.09	0.53
1:E:297:ILE:HD11	1:E:309:ARG:HG2	1.91	0.53
1:E:357:VAL:O	1:E:361:VAL:HG23	2.08	0.53
2:F:356:SER:CB	2:F:359:ALA:HB3	2.38	0.53
3:K:101:MET:SD	3:K:162:LEU:HA	2.49	0.53
1:A:496:PHE:CE1	2:B:298:VAL:HG13	2.43	0.53
2:B:90:ARG:NH2	4:B:5:ATP:O2G	2.42	0.53
2:B:213:PHE:CB	2:B:218:ILE:HD11	2.39	0.53
2:F:197:THR:HG22	2:F:198:ALA:N	2.24	0.53
3:K:103:ILE:HD11	3:K:115:ILE:HB	1.90	0.53
2:H:62:GLU:HG2	2:H:297:ALA:HA	1.90	0.53
2:H:394:LEU:HD21	2:H:396:SER:HB3	1.89	0.53
1:A:342:LEU:HD11	1:A:346:TYR:HE1	1.74	0.53
1:A:428:MET:O	1:A:431:ALA:HB3	2.08	0.53
1:C:229:THR:O	1:C:230:ASN:CB	2.57	0.53
2:D:199:CYS:HG	2:D:202:CYS:HG	1.53	0.53
2:H:164:TYR:CE2	2:H:169:LEU:HD13	2.44	0.53
2:H:164:TYR:CE2	2:H:169:LEU:HB2	2.42	0.53
2:H:257:ILE:HD13	2:H:282:GLN:HG2	1.91	0.53
2:H:360:LYS:N	2:H:363:GLU:OE1	2.42	0.53
3:I:117:ILE:HD13	3:I:126:ILE:HG12	1.91	0.52
1:C:177:ASP:O	1:C:178:ASN:HB2	2.09	0.52
1:C:251:ILE:HG23	1:C:262:GLU:CG	2.39	0.52
1:C:252:LEU:C	1:C:253:LYS:C	2.67	0.52
1:C:307:LEU:CB	1:C:383:LEU:HD22	2.34	0.52
3:J:108:LEU:HG	3:J:108:LEU:O	2.10	0.52
1:E:229:THR:O	1:E:230:ASN:CB	2.56	0.52
1:G:221:TYR:OH	1:G:250:GLY:HA3	2.08	0.52
3:L:103:ILE:HD11	3:L:115:ILE:HB	1.90	0.52
2:B:162:LEU:HD21	2:B:174:ILE:HG23	1.91	0.52
1:G:229:THR:O	1:G:230:ASN:CB	2.57	0.52
1:A:518:ASN:HD22	1:A:533:GLN:HG3	1.73	0.52
2:B:111:LEU:O	2:B:111:LEU:HD23	2.09	0.52
1:C:18:ARG:NH2	2:D:288:ILE:HD12	2.23	0.52
1:C:527:GLN:OE1	2:D:302:VAL:HG13	2.10	0.52
2:D:197:THR:HG22	2:D:198:ALA:N	2.24	0.52
3:L:155:THR:O	3:L:158:ASP:HB2	2.08	0.52
1:A:15:ARG:HG3	1:A:15:ARG:HH11	1.74	0.52
3:J:117:ILE:HD13	3:J:126:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:THR:O	1:E:43:THR:HB	2.09	0.52
1:E:248:ARG:C	1:E:250:GLY:H	2.11	0.52
1:G:19:LEU:HD21	2:H:290:PRO:HB2	1.92	0.52
1:G:34:CYS:HB2	1:G:123:PHE:CG	2.43	0.52
1:G:259:PRO:C	1:G:260:GLU:HG2	2.28	0.52
2:H:127:ILE:HG13	2:H:128:GLN:NE2	2.24	0.52
1:A:47:LYS:HD3	1:A:51:LEU:HD11	1.91	0.52
2:B:335:PHE:HE2	3:I:170:VAL:HG21	1.75	0.52
2:B:361:LEU:CG	2:B:704:LEU:HA	2.40	0.52
3:I:107:THR:HG23	3:I:109:THR:H	1.74	0.52
1:C:309:ARG:HD2	1:C:313:GLU:HG2	1.92	0.52
2:F:111:LEU:O	2:F:111:LEU:HD23	2.09	0.52
2:F:158:LEU:CD1	2:F:177:LEU:HB2	2.40	0.52
2:F:393:TYR:HB3	2:F:606:ARG:CB	2.39	0.52
1:G:47:LYS:HD3	1:G:51:LEU:HD11	1.91	0.52
3:L:108:LEU:HG	3:L:108:LEU:O	2.09	0.52
3:I:108:LEU:HG	3:I:108:LEU:O	2.08	0.52
1:C:60:ILE:HD11	1:C:119:PHE:HE2	1.75	0.52
1:G:229:THR:HG22	1:G:231:GLY:N	2.25	0.52
1:G:232:ARG:CB	1:G:234:PRO:HD3	2.33	0.52
2:H:127:ILE:HG12	4:H:8:ATP:HN62	1.73	0.52
4:H:8:ATP:O1A	4:H:8:ATP:O2B	2.28	0.52
1:A:185:LEU:O	1:A:188:PRO:HD3	2.09	0.52
2:B:195:GLY:O	2:B:196:MET:HG3	2.09	0.52
1:C:407:ILE:O	1:C:409:LYS:N	2.41	0.52
2:D:606:ARG:O	2:D:607:THR:C	2.46	0.52
1:E:489:GLU:O	1:E:489:GLU:HG2	2.10	0.52
2:F:136:ARG:HG2	2:F:136:ARG:HH11	1.75	0.52
3:K:108:LEU:O	3:K:108:LEU:HG	2.09	0.52
1:G:244:ARG:HD3	1:G:269:ILE:CG2	2.39	0.52
2:H:371:SER:C	2:H:373:SER:H	2.13	0.52
1:A:192:LEU:HG	1:A:196:PHE:CE1	2.45	0.52
1:E:533:GLN:O	1:E:534:LEU:CB	2.58	0.52
2:F:901:VAL:O	2:F:902:ALA:C	2.44	0.52
2:H:54:ILE:HD12	2:H:154:ILE:HG13	1.92	0.52
2:H:64:LEU:HD11	2:H:77:VAL:HG21	1.91	0.52
2:B:342:ASN:HD22	2:B:342:ASN:N	2.02	0.52
1:C:489:GLU:HG2	1:C:489:GLU:O	2.10	0.52
2:D:87:ASN:HB3	2:D:91:GLN:CD	2.30	0.52
2:D:606:ARG:O	2:D:608:ARG:N	2.43	0.52
2:H:197:THR:HG22	2:H:198:ALA:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:213:PHE:CB	2:H:218:ILE:HD11	2.40	0.52
2:H:394:LEU:HG	2:H:396:SER:HB3	1.92	0.52
2:B:239:LYS:HG2	1:E:448:TYR:CZ	2.45	0.52
1:C:47:LYS:HD3	1:C:51:LEU:HD11	1.91	0.52
1:C:50:VAL:HG13	1:C:100:VAL:HG21	1.92	0.52
1:E:309:ARG:HD2	1:E:313:GLU:HG2	1.93	0.52
2:H:603:ILE:O	2:H:607:THR:N	2.43	0.52
1:A:261:ASP:O	1:A:262:GLU:HG2	2.10	0.51
1:A:293:ARG:HG2	1:A:305:TRP:CD1	2.45	0.51
1:A:307:LEU:HB3	1:A:383:LEU:HD21	1.91	0.51
2:F:394:LEU:CD2	2:F:396:SER:HB3	2.40	0.51
4:F:7:ATP:H3'	4:F:7:ATP:O1B	2.10	0.51
2:H:80:MET:HG2	4:H:8:ATP:N3	2.25	0.51
2:B:158:LEU:CD1	2:B:177:LEU:HB2	2.40	0.51
2:D:361:LEU:CG	2:D:704:LEU:HA	2.39	0.51
2:D:371:SER:O	2:D:373:SER:N	2.43	0.51
2:F:900:ALA:O	2:F:901:VAL:CB	2.58	0.51
3:K:155:THR:O	3:K:158:ASP:HB2	2.10	0.51
2:H:46:LEU:O	2:H:73:ARG:HB2	2.10	0.51
2:H:393:TYR:HB3	2:H:606:ARG:CB	2.40	0.51
2:D:342:ASN:HD22	2:D:342:ASN:N	2.01	0.51
2:F:15:GLY:HA2	2:F:18:ASN:OD1	2.10	0.51
1:G:41:THR:O	1:G:45:ILE:HG13	2.11	0.51
1:A:236:THR:O	1:A:237:TYR:CD1	2.64	0.51
3:I:103:ILE:CD1	3:I:115:ILE:HB	2.40	0.51
2:D:342:ASN:H	2:D:342:ASN:ND2	2.07	0.51
3:J:103:ILE:CD1	3:J:115:ILE:HB	2.41	0.51
1:E:244:ARG:HD3	1:E:269:ILE:CG2	2.40	0.51
1:E:252:LEU:C	1:E:253:LYS:C	2.69	0.51
2:F:16:ARG:NH2	2:F:116:PRO:HB2	2.24	0.51
2:H:901:VAL:O	2:H:902:ALA:C	2.47	0.51
2:B:237:TRP:CD2	2:B:242:PRO:HG2	2.45	0.51
1:E:15:ARG:NH1	4:F:7:ATP:O1G	2.44	0.51
2:F:342:ASN:HD22	2:F:342:ASN:N	2.01	0.51
2:F:603:ILE:O	2:F:607:THR:N	2.43	0.51
1:G:317:LYS:HB3	1:G:318:GLU:OE1	2.10	0.51
1:A:309:ARG:HD2	1:A:313:GLU:HG2	1.93	0.51
2:B:393:TYR:HB3	2:B:606:ARG:CB	2.41	0.51
1:G:16:GLN:CB	2:H:292:VAL:HG12	2.41	0.51
2:H:56:ALA:N	2:H:79:ASP:OD1	2.43	0.51
2:H:87:ASN:HB3	2:H:91:GLN:NE2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:197:THR:HG21	2:H:320:ASN:HB3	1.93	0.51
1:A:236:THR:O	1:A:237:TYR:HD1	1.92	0.51
2:B:15:GLY:HA2	2:B:18:ASN:OD1	2.11	0.51
1:C:15:ARG:HH11	1:C:15:ARG:HG3	1.76	0.51
1:C:259:PRO:CA	1:C:260:GLU:HG2	2.40	0.51
3:K:117:ILE:HD11	3:K:126:ILE:HG23	1.92	0.51
3:K:150:MET:CE	3:K:167:LEU:HD13	2.41	0.51
1:G:248:ARG:C	1:G:250:GLY:H	2.13	0.51
2:B:316:ILE:H	2:B:316:ILE:CD1	2.10	0.51
2:D:16:ARG:NH2	2:D:116:PRO:HB2	2.25	0.51
1:E:84:ASN:C	1:E:84:ASN:ND2	2.64	0.51
2:F:46:LEU:O	2:F:73:ARG:HB2	2.11	0.51
2:H:90:ARG:HH11	2:H:90:ARG:HG2	1.74	0.51
2:H:96:PRO:O	2:H:99:ILE:HG13	2.11	0.51
2:H:178:ILE:N	2:H:178:ILE:HD12	2.25	0.51
2:B:59:LEU:HD12	3:I:176:GLY:CA	2.41	0.51
3:I:150:MET:CE	3:I:167:LEU:HD13	2.41	0.51
1:C:166:ILE:HD11	1:C:508:ILE:HD13	1.93	0.51
2:D:111:LEU:HD23	2:D:111:LEU:O	2.10	0.51
2:F:380:ALA:CB	2:F:394:LEU:HB2	2.40	0.51
1:G:260:GLU:HB3	1:G:261:ASP:OD1	2.10	0.51
2:H:232:VAL:HG11	2:H:263:LYS:HB2	1.93	0.51
3:L:107:THR:HG22	3:L:111:LYS:N	2.26	0.51
3:L:117:ILE:HD11	3:L:126:ILE:HG23	1.92	0.51
1:C:244:ARG:HD3	1:C:269:ILE:CG2	2.41	0.51
2:D:54:ILE:HD12	2:D:154:ILE:HG13	1.93	0.51
3:J:155:THR:O	3:J:158:ASP:HB2	2.11	0.51
1:E:232:ARG:CB	1:E:234:PRO:HD3	2.34	0.51
1:E:317:LYS:HB3	1:E:318:GLU:OE1	2.11	0.51
2:F:320:ASN:O	2:F:321:TYR:HB2	2.11	0.51
3:K:107:THR:HG22	3:K:111:LYS:N	2.26	0.51
1:C:140:ALA:HA	1:C:150:LEU:HD22	1.93	0.50
1:C:481:GLU:OE2	1:C:525:MET:HE3	2.10	0.50
2:F:360:LYS:N	2:F:363:GLU:OE1	2.44	0.50
1:A:19:LEU:HD21	2:B:290:PRO:HB2	1.93	0.50
2:D:178:ILE:HG21	2:D:303:CYS:HB3	1.93	0.50
1:E:163:ARG:HG2	1:E:163:ARG:NH1	2.24	0.50
1:G:163:ARG:HG2	1:G:163:ARG:NH1	2.24	0.50
1:A:181:GLU:OE1	1:A:181:GLU:HA	2.10	0.50
1:A:489:GLU:H	2:B:19:HIS:CD2	2.29	0.50
2:B:320:ASN:O	2:B:321:TYR:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:THR:O	1:C:237:TYR:CD1	2.65	0.50
1:C:317:LYS:HB3	1:C:318:GLU:OE1	2.11	0.50
1:C:447:ASN:ND2	2:D:26:ARG:HE	2.09	0.50
2:F:371:SER:O	2:F:373:SER:N	2.44	0.50
1:G:407:ILE:C	1:G:407:ILE:HD13	2.31	0.50
1:G:489:GLU:O	1:G:489:GLU:HG2	2.12	0.50
3:L:105:VAL:HG13	3:L:105:VAL:O	2.11	0.50
1:A:235:LYS:HB2	1:A:239:GLU:CD	2.31	0.50
2:B:136:ARG:HG2	2:B:136:ARG:HH11	1.76	0.50
2:D:15:GLY:HA2	2:D:18:ASN:OD1	2.10	0.50
2:D:213:PHE:CB	2:D:218:ILE:HD11	2.40	0.50
2:F:322:LEU:HD12	2:F:322:LEU:C	2.31	0.50
2:F:361:LEU:CG	2:F:704:LEU:HA	2.40	0.50
3:K:107:THR:HG23	3:K:109:THR:H	1.76	0.50
1:G:47:LYS:O	1:G:51:LEU:HD12	2.11	0.50
1:G:140:ALA:HA	1:G:150:LEU:HD22	1.94	0.50
1:G:309:ARG:HD2	1:G:313:GLU:HG2	1.94	0.50
2:H:49:CYS:HA	2:H:139:HIS:CD2	2.46	0.50
2:H:217:THR:CG2	2:H:223:ARG:HH22	2.24	0.50
1:A:396:ARG:HH11	1:A:533:GLN:NE2	2.10	0.50
1:C:163:ARG:HG2	1:C:163:ARG:NH1	2.25	0.50
1:C:422:GLU:CD	1:C:422:GLU:H	2.14	0.50
2:D:56:ALA:N	2:D:79:ASP:OD1	2.44	0.50
3:J:105:VAL:HG13	3:J:105:VAL:O	2.11	0.50
1:E:527:GLN:OE1	2:F:302:VAL:HG13	2.11	0.50
1:G:60:ILE:HD11	1:G:119:PHE:HE2	1.76	0.50
1:G:117:PRO:C	1:G:119:PHE:H	2.15	0.50
2:H:191:VAL:H	2:H:320:ASN:HA	1.77	0.50
2:B:62:GLU:HG2	2:B:297:ALA:HA	1.93	0.50
1:E:47:LYS:HD3	1:E:51:LEU:HD11	1.93	0.50
1:G:157:GLY:HA3	1:G:485:TYR:CG	2.46	0.50
1:G:353:ASP:O	1:G:357:VAL:HG23	2.11	0.50
1:A:407:ILE:C	1:A:407:ILE:HD13	2.31	0.50
2:B:157:MET:HA	2:B:157:MET:HE3	1.94	0.50
2:D:62:GLU:HG2	2:D:297:ALA:HA	1.94	0.50
2:D:335:PHE:CE2	3:J:170:VAL:HG21	2.47	0.50
1:E:133:GLU:O	1:E:134:SER:C	2.50	0.50
2:F:85:VAL:HG13	2:F:86:SER:N	2.27	0.50
2:H:235:LEU:O	2:H:238:PRO:HD2	2.12	0.50
2:H:342:ASN:HD22	2:H:342:ASN:N	2.03	0.50
2:B:64:LEU:HD21	2:B:77:VAL:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ALA:HB1	1:C:131:LEU:HD11	1.93	0.50
2:D:217:THR:CG2	2:D:223:ARG:HH22	2.25	0.50
1:E:244:ARG:HD3	1:E:269:ILE:HG23	1.93	0.50
1:E:407:ILE:HD13	1:E:407:ILE:C	2.31	0.50
2:F:126:LYS:HA	4:F:7:ATP:C2	2.47	0.50
2:F:342:ASN:H	2:F:342:ASN:ND2	2.07	0.50
1:G:244:ARG:HD3	1:G:269:ILE:HG23	1.93	0.50
1:A:140:ALA:HA	1:A:150:LEU:HD22	1.94	0.50
1:A:166:ILE:HD11	1:A:508:ILE:HD13	1.94	0.50
1:A:447:ASN:HD22	2:B:26:ARG:HH21	1.60	0.50
2:B:164:TYR:CE2	2:B:169:LEU:HB2	2.45	0.50
2:B:199:CYS:HG	2:B:343:CYS:HG	1.59	0.50
2:B:371:SER:C	2:B:373:SER:H	2.16	0.50
2:B:371:SER:O	2:B:373:SER:N	2.45	0.50
2:D:371:SER:C	2:D:373:SER:H	2.15	0.50
3:K:105:VAL:O	3:K:105:VAL:HG13	2.12	0.50
1:G:39:THR:O	1:G:43:THR:HB	2.12	0.50
1:G:46:LEU:HD21	1:G:57:PHE:CD1	2.47	0.50
1:A:37:ASN:HB2	1:A:129:THR:O	2.12	0.49
1:A:489:GLU:HG2	1:A:489:GLU:O	2.12	0.49
1:C:50:VAL:HA	1:C:54:ILE:HG22	1.94	0.49
3:J:103:ILE:HD11	3:J:115:ILE:HB	1.93	0.49
1:E:221:TYR:OH	1:E:250:GLY:HA3	2.11	0.49
2:H:15:GLY:HA2	2:H:18:ASN:OD1	2.11	0.49
2:B:131:ASN:O	2:B:132:ASP:C	2.50	0.49
3:I:107:THR:HG22	3:I:111:LYS:N	2.26	0.49
1:C:489:GLU:H	2:D:19:HIS:CD2	2.30	0.49
2:D:360:LYS:N	2:D:363:GLU:OE1	2.45	0.49
1:E:251:ILE:HG23	1:E:262:GLU:CG	2.42	0.49
1:E:416:MET:C	1:E:418:ASN:H	2.16	0.49
2:F:267:ARG:HG2	2:F:267:ARG:NH1	2.15	0.49
1:G:15:ARG:HH11	1:G:15:ARG:HG3	1.77	0.49
2:H:195:GLY:O	2:H:196:MET:HG3	2.12	0.49
2:B:380:ALA:O	2:B:904:VAL:HA	2.12	0.49
1:C:236:THR:O	1:C:237:TYR:HD1	1.95	0.49
2:D:85:VAL:HG13	2:D:86:SER:N	2.27	0.49
1:E:84:ASN:C	1:E:84:ASN:HD22	2.14	0.49
1:E:192:LEU:O	1:E:195:HIS:HB3	2.11	0.49
2:F:213:PHE:CB	2:F:218:ILE:HD11	2.42	0.49
3:K:161:ILE:O	3:K:162:LEU:HD23	2.12	0.49
1:G:37:ASN:HB2	1:G:129:THR:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:ARG:O	1:G:81:ILE:HG13	2.12	0.49
1:G:251:ILE:HG23	1:G:262:GLU:CG	2.42	0.49
1:G:261:ASP:O	1:G:262:GLU:HG2	2.12	0.49
2:H:131:ASN:O	2:H:132:ASP:C	2.50	0.49
1:A:39:THR:O	1:A:43:THR:HB	2.11	0.49
2:B:73:ARG:HD3	2:B:117:ASN:O	2.12	0.49
2:B:360:LYS:N	2:B:363:GLU:OE1	2.46	0.49
2:D:162:LEU:HD21	2:D:174:ILE:HG23	1.94	0.49
2:D:393:TYR:HB3	2:D:606:ARG:CB	2.42	0.49
1:E:353:ASP:O	1:E:357:VAL:HG23	2.12	0.49
1:E:503:GLN:OE1	1:E:503:GLN:HA	2.12	0.49
2:F:235:LEU:O	2:F:238:PRO:HD2	2.12	0.49
1:G:192:LEU:O	1:G:195:HIS:HB3	2.11	0.49
1:A:41:THR:O	1:A:45:ILE:HG13	2.12	0.49
1:A:481:GLU:OE2	1:A:525:MET:HE3	2.13	0.49
2:B:49:CYS:HA	2:B:139:HIS:CD2	2.47	0.49
1:C:38:ALA:O	1:C:85:ARG:HD3	2.11	0.49
1:C:192:LEU:O	1:C:195:HIS:HB3	2.12	0.49
1:C:253:LYS:CA	1:C:253:LYS:O	2.49	0.49
1:C:407:ILE:HD13	1:C:407:ILE:C	2.33	0.49
1:C:533:GLN:O	1:C:534:LEU:CB	2.60	0.49
2:D:123:HIS:O	2:D:125:ASN:N	2.46	0.49
2:D:164:TYR:CE2	2:D:169:LEU:HB2	2.44	0.49
2:D:232:VAL:HG11	2:D:263:LYS:HB2	1.95	0.49
2:F:80:MET:HG2	4:F:7:ATP:C4	2.47	0.49
2:H:139:HIS:O	2:H:176:PRO:HD2	2.13	0.49
2:H:178:ILE:HG21	2:H:303:CYS:HB3	1.94	0.49
1:A:133:GLU:O	1:A:134:SER:C	2.51	0.49
1:C:34:CYS:HB2	1:C:123:PHE:CG	2.47	0.49
1:C:181:GLU:OE1	1:C:181:GLU:HA	2.13	0.49
2:D:191:VAL:H	2:D:320:ASN:HA	1.77	0.49
3:J:106:LYS:HG3	3:J:112:GLU:HB2	1.94	0.49
1:E:34:CYS:HB2	1:E:123:PHE:CG	2.47	0.49
1:E:143:LEU:HD22	1:E:148:ILE:HG21	1.94	0.49
1:E:444:GLY:HA2	1:E:449:GLN:HB2	1.95	0.49
2:F:128:GLN:HE22	4:F:7:ATP:HN62	1.60	0.49
1:A:192:LEU:O	1:A:195:HIS:HB3	2.12	0.49
2:B:199:CYS:SG	2:B:346:CYS:SG	3.10	0.49
1:E:293:ARG:HG2	1:E:305:TRP:CD1	2.48	0.49
2:F:54:ILE:HD12	2:F:154:ILE:HG13	1.94	0.49
2:F:62:GLU:HG2	2:F:297:ALA:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:394:LEU:HD11	2:F:396:SER:CB	2.43	0.49
3:K:150:MET:HE1	3:K:167:LEU:HD22	1.93	0.49
2:H:112:ASN:HD21	2:H:120:VAL:HB	1.77	0.49
3:L:150:MET:CE	3:L:167:LEU:HD13	2.43	0.49
2:B:74:GLN:NE2	2:B:74:GLN:HA	2.28	0.49
2:B:190:ARG:NH2	2:B:203:THR:OG1	2.45	0.49
2:D:380:ALA:O	2:D:904:VAL:HA	2.13	0.49
1:E:60:ILE:HD11	1:E:119:PHE:HE2	1.76	0.49
2:F:380:ALA:O	2:F:904:VAL:HA	2.13	0.49
2:H:241:GLN:HE21	2:H:246:GLY:H	1.61	0.49
3:L:106:LYS:HG2	3:L:110:GLY:HA2	1.95	0.49
1:A:244:ARG:HD3	1:A:269:ILE:CG2	2.42	0.49
2:B:78:ILE:O	2:B:79:ASP:HB2	2.12	0.49
2:B:235:LEU:O	2:B:238:PRO:HD2	2.11	0.49
2:B:322:LEU:HD12	2:B:322:LEU:C	2.33	0.49
1:C:260:GLU:HB3	1:C:261:ASP:OD1	2.12	0.49
1:C:430:ARG:NH1	1:C:430:ARG:HB3	2.28	0.49
2:D:141:ILE:HD12	2:D:158:LEU:HD11	1.93	0.49
2:D:380:ALA:CB	2:D:394:LEU:HB2	2.42	0.49
1:E:50:VAL:HA	1:E:54:ILE:HG22	1.94	0.49
1:E:253:LYS:O	1:E:260:GLU:CD	2.51	0.49
2:F:190:ARG:NH2	2:F:203:THR:OG1	2.46	0.49
1:G:166:ILE:HD11	1:G:508:ILE:HD13	1.93	0.49
2:H:380:ALA:O	2:H:904:VAL:HA	2.12	0.49
2:H:900:ALA:O	2:H:901:VAL:CB	2.61	0.49
2:B:58:GLY:N	2:B:91:GLN:HG2	2.19	0.49
2:D:49:CYS:HA	2:D:139:HIS:CD2	2.48	0.49
2:F:49:CYS:HA	2:F:139:HIS:CD2	2.48	0.49
2:F:191:VAL:H	2:F:320:ASN:HA	1.78	0.49
1:G:133:GLU:O	1:G:134:SER:C	2.52	0.49
1:A:430:ARG:HB3	1:A:430:ARG:NH1	2.28	0.48
2:B:236:GLN:HE22	2:B:263:LYS:HB3	1.78	0.48
1:C:252:LEU:O	1:C:259:PRO:N	2.46	0.48
2:D:131:ASN:O	2:D:132:ASP:C	2.51	0.48
1:E:422:GLU:H	1:E:422:GLU:CD	2.16	0.48
1:G:481:GLU:HG2	1:G:525:MET:HE3	1.95	0.48
3:L:117:ILE:HD13	3:L:126:ILE:HG12	1.94	0.48
2:B:335:PHE:CE2	3:I:170:VAL:HG21	2.48	0.48
3:I:105:VAL:HG21	3:I:143:LEU:HD21	1.94	0.48
1:C:18:ARG:CZ	2:D:288:ILE:HD12	2.42	0.48
1:C:336:SER:OG	2:D:271:TYR:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:241:GLN:NE2	2:D:246:GLY:H	2.11	0.48
1:G:50:VAL:HA	1:G:54:ILE:HG22	1.94	0.48
1:G:181:GLU:OE1	1:G:181:GLU:HA	2.13	0.48
2:H:112:ASN:ND2	2:H:120:VAL:HB	2.28	0.48
1:A:78:ARG:O	1:A:81:ILE:HG13	2.13	0.48
1:C:133:GLU:O	1:C:134:SER:C	2.51	0.48
1:E:177:ASP:O	1:E:178:ASN:HB2	2.13	0.48
2:F:164:TYR:CE2	2:F:169:LEU:HB2	2.47	0.48
2:F:183:GLU:HG3	2:F:289:ILE:CG2	2.43	0.48
1:G:192:LEU:HG	1:G:196:PHE:CE1	2.48	0.48
1:G:252:LEU:O	1:G:259:PRO:N	2.44	0.48
2:H:355:PHE:O	2:H:356:SER:CB	2.61	0.48
1:A:244:ARG:HD3	1:A:269:ILE:HG23	1.95	0.48
3:I:123:VAL:HA	3:I:126:ILE:HD12	1.95	0.48
2:D:78:ILE:O	2:D:79:ASP:HB2	2.13	0.48
2:D:320:ASN:O	2:D:321:TYR:HB2	2.13	0.48
2:D:900:ALA:O	2:D:901:VAL:CB	2.61	0.48
3:J:117:ILE:HD11	3:J:126:ILE:HG23	1.94	0.48
1:E:15:ARG:HH11	1:E:15:ARG:HG3	1.79	0.48
2:F:217:THR:CG2	2:F:223:ARG:HH22	2.27	0.48
2:F:241:GLN:HE21	2:F:246:GLY:H	1.61	0.48
1:G:264:ASN:N	1:G:264:ASN:ND2	2.61	0.48
2:H:78:ILE:O	2:H:79:ASP:HB2	2.12	0.48
3:L:101:MET:SD	3:L:162:LEU:HA	2.53	0.48
1:A:50:VAL:HA	1:A:54:ILE:HG22	1.95	0.48
1:A:244:ARG:O	1:A:247:ILE:N	2.46	0.48
1:A:261:ASP:O	1:A:262:GLU:CG	2.62	0.48
1:A:307:LEU:CB	1:A:383:LEU:HD22	2.38	0.48
2:H:85:VAL:HG13	2:H:86:SER:N	2.28	0.48
2:H:232:VAL:O	2:H:232:VAL:HG12	2.12	0.48
1:A:474:VAL:O	1:A:475:LYS:C	2.51	0.48
2:D:335:PHE:CZ	3:J:144:ILE:HD13	2.48	0.48
3:J:107:THR:HG22	3:J:111:LYS:N	2.28	0.48
1:G:235:LYS:HB2	1:G:239:GLU:OE1	2.14	0.48
1:A:177:ASP:O	1:A:178:ASN:HB2	2.13	0.48
1:E:140:ALA:HA	1:E:150:LEU:HD22	1.96	0.48
2:H:355:PHE:O	2:H:356:SER:OG	2.24	0.48
2:H:908:GLN:O	2:H:909:THR:C	2.52	0.48
1:A:157:GLY:HA3	1:A:485:TYR:CG	2.49	0.48
2:B:30:PHE:N	2:B:30:PHE:CD1	2.82	0.48
2:B:197:THR:CG2	2:B:198:ALA:N	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:GLY:HA3	1:C:485:TYR:CG	2.49	0.48
3:K:106:LYS:HG2	3:K:110:GLY:HA2	1.95	0.48
2:H:32:HIS:CE1	2:H:33:PRO:HD2	2.48	0.48
1:A:251:ILE:HG23	1:A:262:GLU:CG	2.44	0.48
1:A:366:GLN:C	1:A:368:ILE:N	2.67	0.48
2:B:139:HIS:O	2:B:176:PRO:HD2	2.13	0.48
1:C:117:PRO:C	1:C:119:PHE:H	2.16	0.48
1:C:177:ASP:O	1:C:178:ASN:CB	2.61	0.48
1:C:235:LYS:HB2	1:C:239:GLU:CD	2.34	0.48
2:D:199:CYS:SG	2:D:346:CYS:SG	3.10	0.48
2:D:394:LEU:CD2	2:D:396:SER:HB3	2.44	0.48
1:E:335:ASP:HB3	1:E:338:LYS:HB2	1.96	0.48
1:G:84:ASN:ND2	1:G:84:ASN:C	2.67	0.48
1:G:236:THR:O	1:G:237:TYR:HD1	1.97	0.48
3:L:107:THR:HG23	3:L:109:THR:H	1.78	0.48
3:L:150:MET:HE3	3:L:167:LEU:HD22	1.95	0.48
1:A:426:TYR:CZ	1:A:430:ARG:HD3	2.49	0.48
2:B:191:VAL:H	2:B:320:ASN:HA	1.79	0.48
1:C:35:LEU:HD23	1:C:46:LEU:HD22	1.95	0.48
2:D:87:ASN:HB3	2:D:91:GLN:NE2	2.29	0.48
2:D:197:THR:HG21	2:D:320:ASN:HB3	1.96	0.48
2:F:371:SER:C	2:F:373:SER:H	2.16	0.48
1:G:124:THR:HG22	1:G:125:VAL:HG23	1.96	0.48
2:H:361:LEU:CG	2:H:704:LEU:HA	2.44	0.48
1:A:34:CYS:HB2	1:A:123:PHE:CG	2.48	0.47
1:A:221:TYR:CD2	1:A:247:ILE:HA	2.49	0.47
2:B:312:THR:O	2:B:313:SER:HB2	2.14	0.47
1:C:37:ASN:HB2	1:C:129:THR:O	2.13	0.47
3:J:106:LYS:HG2	3:J:110:GLY:HA2	1.96	0.47
1:E:489:GLU:H	2:F:19:HIS:CD2	2.32	0.47
2:F:64:LEU:HD21	2:F:77:VAL:CG2	2.43	0.47
3:K:103:ILE:HD12	3:K:103:ILE:O	2.14	0.47
1:G:307:LEU:CD1	1:G:383:LEU:HD22	2.42	0.47
2:B:13:TRP:CZ3	2:B:116:PRO:HG2	2.48	0.47
2:B:325:ASN:HD22	2:B:326:ASP:N	2.12	0.47
2:B:394:LEU:HG	2:B:396:SER:HB3	1.95	0.47
1:C:244:ARG:HD3	1:C:269:ILE:HG23	1.95	0.47
1:C:340:ILE:HD11	2:D:273:ILE:HG12	1.95	0.47
2:D:30:PHE:N	2:D:30:PHE:CD1	2.82	0.47
2:D:236:GLN:HE22	2:D:263:LYS:HB3	1.79	0.47
3:J:101:MET:SD	3:J:162:LEU:HA	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:LYS:HB2	1:E:239:GLU:CD	2.33	0.47
1:A:285:ILE:HD11	1:A:388:ALA:CA	2.36	0.47
2:B:356:SER:HA	2:B:357:PRO:HD3	1.55	0.47
3:I:117:ILE:HD11	3:I:126:ILE:HG23	1.96	0.47
1:C:16:GLN:CB	2:D:292:VAL:HG12	2.43	0.47
2:D:112:ASN:ND2	2:D:120:VAL:HB	2.29	0.47
2:D:136:ARG:HH11	2:D:136:ARG:HG2	1.79	0.47
2:D:190:ARG:NH2	2:D:203:THR:OG1	2.47	0.47
1:E:117:PRO:C	1:E:119:PHE:H	2.16	0.47
1:E:124:THR:HG22	1:E:125:VAL:HG23	1.96	0.47
2:F:112:ASN:ND2	2:F:120:VAL:HB	2.28	0.47
2:F:112:ASN:HD21	2:F:120:VAL:HB	1.79	0.47
2:F:394:LEU:HD11	2:F:396:SER:HB3	1.97	0.47
2:H:73:ARG:HD3	2:H:117:ASN:O	2.13	0.47
3:L:106:LYS:HG3	3:L:112:GLU:HB2	1.96	0.47
1:A:503:GLN:OE1	1:A:503:GLN:HA	2.14	0.47
2:B:901:VAL:O	2:B:902:ALA:C	2.51	0.47
1:C:78:ARG:O	1:C:81:ILE:HG13	2.14	0.47
1:C:496:PHE:CE1	2:D:298:VAL:HG13	2.50	0.47
2:F:73:ARG:HD3	2:F:117:ASN:O	2.14	0.47
1:G:236:THR:O	1:G:237:TYR:CD1	2.67	0.47
2:H:394:LEU:CD2	2:H:396:SER:HB3	2.44	0.47
2:B:351:GLN:HB3	2:B:916:PHE:CB	2.44	0.47
1:E:264:ASN:N	1:E:264:ASN:ND2	2.61	0.47
1:G:211:HIS:O	1:G:338:LYS:HD2	2.15	0.47
2:H:267:ARG:HH11	2:H:267:ARG:CG	2.17	0.47
2:B:162:LEU:HD22	2:B:169:LEU:HD11	1.97	0.47
1:C:264:ASN:N	1:C:264:ASN:ND2	2.61	0.47
2:D:162:LEU:HD22	2:D:169:LEU:HD11	1.96	0.47
1:E:78:ARG:O	1:E:81:ILE:HG13	2.14	0.47
1:E:157:GLY:HA3	1:E:485:TYR:CG	2.49	0.47
1:E:426:TYR:CZ	1:E:430:ARG:HD3	2.49	0.47
3:K:106:LYS:HG3	3:K:112:GLU:HB2	1.97	0.47
1:G:307:LEU:CB	1:G:383:LEU:HD22	2.39	0.47
1:A:128:ALA:HB1	1:A:131:LEU:HD11	1.96	0.47
1:A:262:GLU:OE1	1:A:262:GLU:CA	2.63	0.47
1:A:264:ASN:N	1:A:264:ASN:ND2	2.60	0.47
2:B:394:LEU:HD11	2:B:396:SER:HB3	1.96	0.47
3:I:106:LYS:HG3	3:I:112:GLU:HB2	1.97	0.47
2:D:241:GLN:HE21	2:D:246:GLY:H	1.61	0.47
1:E:45:ILE:CG1	1:E:498:GLY:HA2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:78:ILE:O	2:F:79:ASP:HB2	2.15	0.47
2:F:157:MET:HA	2:F:157:MET:HE3	1.96	0.47
2:F:241:GLN:NE2	2:F:246:GLY:H	2.12	0.47
2:F:312:THR:O	2:F:313:SER:HB2	2.14	0.47
2:F:392:LEU:HA	2:F:392:LEU:HD23	1.45	0.47
3:K:105:VAL:HG11	3:K:130:VAL:CG2	2.41	0.47
1:G:225:TRP:CE2	1:G:233:ILE:HG12	2.50	0.47
1:G:422:GLU:H	1:G:422:GLU:CD	2.17	0.47
1:G:489:GLU:H	2:H:19:HIS:CD2	2.33	0.47
2:H:241:GLN:NE2	2:H:246:GLY:H	2.12	0.47
1:A:143:LEU:HD22	1:A:148:ILE:HG21	1.96	0.47
2:B:394:LEU:HD11	2:B:396:SER:CB	2.45	0.47
2:D:139:HIS:O	2:D:176:PRO:HD2	2.14	0.47
2:D:361:LEU:HD23	2:D:361:LEU:N	2.29	0.47
2:D:908:GLN:O	2:D:909:THR:C	2.51	0.47
2:F:30:PHE:CD1	2:F:30:PHE:N	2.83	0.47
2:F:351:GLN:HB3	2:F:916:PHE:CB	2.45	0.47
1:G:331:ASP:HB2	2:H:224:LEU:HD11	1.96	0.47
1:G:447:ASN:HD22	2:H:26:ARG:HH21	1.61	0.47
2:H:52:LEU:HD11	2:H:78:ILE:HG13	1.96	0.47
2:H:314:ALA:O	2:H:315:TYR:CD1	2.67	0.47
1:A:265:PHE:O	1:A:269:ILE:HG13	2.15	0.47
2:B:146:ASP:HB3	4:B:5:ATP:H5'2	1.97	0.47
3:I:105:VAL:O	3:I:105:VAL:HG13	2.15	0.47
3:I:106:LYS:HG2	3:I:110:GLY:HA2	1.96	0.47
3:I:155:THR:HG22	3:I:158:ASP:CG	2.35	0.47
1:E:396:ARG:HH11	1:E:533:GLN:NE2	2.13	0.47
1:E:474:VAL:O	1:E:475:LYS:C	2.52	0.47
2:F:394:LEU:HG	2:F:396:SER:HB3	1.96	0.47
3:K:123:VAL:HA	3:K:126:ILE:HD12	1.97	0.47
1:G:415:SER:O	1:G:417:ASP:N	2.48	0.47
2:H:342:ASN:H	2:H:342:ASN:ND2	2.10	0.47
3:L:113:ILE:HD11	3:L:130:VAL:HG13	1.97	0.47
1:A:117:PRO:C	1:A:119:PHE:H	2.19	0.47
1:A:163:ARG:HG2	1:A:163:ARG:NH1	2.26	0.47
1:A:211:HIS:O	1:A:338:LYS:HD2	2.15	0.47
1:C:221:TYR:CD2	1:C:247:ILE:HA	2.50	0.47
1:C:225:TRP:CE2	1:C:233:ILE:HG12	2.50	0.47
1:C:357:VAL:O	1:C:361:VAL:HG23	2.14	0.47
2:F:197:THR:HG21	2:F:320:ASN:HB3	1.96	0.47
1:G:177:ASP:O	1:G:178:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:ILE:HD11	1:G:268:ALA:O	2.14	0.47
2:H:64:LEU:HD21	2:H:77:VAL:CG2	2.44	0.47
2:H:190:ARG:NH2	2:H:203:THR:OG1	2.48	0.47
2:H:356:SER:CB	2:H:359:ALA:HB3	2.45	0.47
2:B:394:LEU:CD2	2:B:396:SER:HB3	2.45	0.46
2:D:229:ILE:HG21	2:D:284:VAL:HB	1.96	0.46
3:J:105:VAL:HG21	3:J:143:LEU:HD21	1.97	0.46
1:G:235:LYS:HB2	1:G:239:GLU:CD	2.34	0.46
1:G:335:ASP:HB3	1:G:338:LYS:HB2	1.97	0.46
1:G:366:GLN:C	1:G:368:ILE:N	2.69	0.46
2:H:16:ARG:NH2	2:H:116:PRO:HB2	2.30	0.46
2:H:126:LYS:HA	4:H:8:ATP:C2	2.50	0.46
2:H:158:LEU:HD12	2:H:177:LEU:HB2	1.96	0.46
2:H:351:GLN:HB3	2:H:916:PHE:CB	2.45	0.46
3:L:103:ILE:HD12	3:L:103:ILE:O	2.15	0.46
1:A:124:THR:HG22	1:A:125:VAL:HG23	1.97	0.46
2:B:178:ILE:HG21	2:B:303:CYS:HB3	1.97	0.46
2:B:236:GLN:NE2	2:B:263:LYS:HB3	2.30	0.46
1:C:366:GLN:C	1:C:368:ILE:N	2.68	0.46
2:D:158:LEU:CD1	2:D:177:LEU:HB2	2.44	0.46
2:D:232:VAL:O	2:D:232:VAL:HG12	2.14	0.46
2:F:212:ASN:HD22	2:F:212:ASN:HA	1.59	0.46
2:F:236:GLN:HE22	2:F:263:LYS:HB3	1.79	0.46
3:L:105:VAL:HG21	3:L:143:LEU:HD21	1.96	0.46
1:A:33:VAL:CG2	1:A:54:ILE:HD11	2.46	0.46
1:A:421:ASN:O	1:A:423:ILE:N	2.48	0.46
2:B:54:ILE:HD12	2:B:154:ILE:HG13	1.98	0.46
2:B:112:ASN:ND2	2:B:120:VAL:HB	2.30	0.46
2:D:13:TRP:CZ3	2:D:116:PRO:HG2	2.49	0.46
2:D:80:MET:HG2	4:D:6:ATP:N3	2.29	0.46
2:D:335:PHE:CE1	2:D:337:ALA:HB2	2.49	0.46
3:K:105:VAL:HG21	3:K:143:LEU:HD21	1.97	0.46
1:G:84:ASN:C	1:G:84:ASN:HD22	2.17	0.46
1:G:221:TYR:CD2	1:G:247:ILE:HA	2.50	0.46
1:G:416:MET:C	1:G:418:ASN:H	2.19	0.46
1:G:444:GLY:HA2	1:G:449:GLN:HB2	1.98	0.46
1:A:416:MET:C	1:A:418:ASN:H	2.19	0.46
3:I:105:VAL:HG11	3:I:130:VAL:CG2	2.44	0.46
1:C:84:ASN:C	1:C:84:ASN:ND2	2.69	0.46
1:C:299:LYS:HA	1:C:368:ILE:CG2	2.46	0.46
1:C:396:ARG:HH11	1:C:533:GLN:NE2	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:ARG:HD3	2:D:117:ASN:O	2.15	0.46
2:D:197:THR:CG2	2:D:198:ALA:N	2.78	0.46
3:J:107:THR:HG23	3:J:109:THR:H	1.79	0.46
1:E:262:GLU:OE1	1:E:262:GLU:CA	2.64	0.46
1:G:112:LEU:C	1:G:114:ASP:N	2.68	0.46
1:A:143:LEU:HD13	1:A:150:LEU:HD13	1.96	0.46
1:A:355:ALA:O	1:A:358:GLY:N	2.48	0.46
1:A:357:VAL:O	1:A:361:VAL:HG23	2.16	0.46
2:B:158:LEU:HD12	2:B:177:LEU:HB2	1.98	0.46
1:C:175:HIS:HD2	1:C:512:GLN:O	1.99	0.46
2:D:112:ASN:HD21	2:D:120:VAL:HB	1.80	0.46
1:E:128:ALA:HB1	1:E:131:LEU:HD11	1.98	0.46
1:E:143:LEU:HD13	1:E:150:LEU:HD13	1.95	0.46
2:F:13:TRP:CD1	2:F:13:TRP:C	2.88	0.46
2:F:197:THR:CG2	2:F:198:ALA:N	2.78	0.46
2:F:340:LYS:HB3	2:F:342:ASN:ND2	2.30	0.46
2:F:908:GLN:O	2:F:909:THR:C	2.54	0.46
1:G:481:GLU:OE2	1:G:525:MET:HE3	2.16	0.46
1:A:422:GLU:CD	1:A:422:GLU:H	2.17	0.46
2:B:229:ILE:HD12	2:B:284:VAL:HG21	1.97	0.46
2:B:232:VAL:HG11	2:B:263:LYS:HB2	1.97	0.46
1:C:15:ARG:HD3	1:C:15:ARG:HA	1.82	0.46
1:C:47:LYS:O	1:C:51:LEU:HD12	2.16	0.46
2:D:157:MET:HA	2:D:157:MET:HE3	1.98	0.46
1:E:211:HIS:O	1:E:338:LYS:HD2	2.15	0.46
1:E:288:ILE:HG23	1:E:305:TRP:CZ3	2.51	0.46
2:F:182:THR:CG2	2:F:183:GLU:N	2.77	0.46
2:F:193:LEU:O	2:F:194:PRO:C	2.54	0.46
1:G:140:ALA:HA	1:G:150:LEU:CD2	2.45	0.46
2:H:30:PHE:N	2:H:30:PHE:CD1	2.83	0.46
2:H:340:LYS:HB3	2:H:342:ASN:ND2	2.30	0.46
1:A:335:ASP:HB3	1:A:338:LYS:HB2	1.98	0.46
2:B:127:ILE:HG13	2:B:128:GLN:NE2	2.30	0.46
2:B:900:ALA:O	2:B:901:VAL:CB	2.64	0.46
1:C:19:LEU:HD21	2:D:290:PRO:HB2	1.98	0.46
3:J:103:ILE:HD12	3:J:103:ILE:O	2.16	0.46
3:J:161:ILE:O	3:J:162:LEU:HD23	2.15	0.46
1:A:15:ARG:HA	1:A:15:ARG:HD3	1.84	0.46
1:C:33:VAL:CG2	1:C:54:ILE:HD11	2.44	0.46
2:D:236:GLN:NE2	2:D:263:LYS:HB3	2.31	0.46
2:D:394:LEU:HD11	2:D:396:SER:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:ILE:HD12	1:E:342:LEU:HD21	1.98	0.46
1:E:218:ILE:HD11	1:E:268:ALA:O	2.15	0.46
1:E:221:TYR:CD2	1:E:247:ILE:HA	2.51	0.46
1:E:244:ARG:O	1:E:247:ILE:N	2.48	0.46
1:E:336:SER:OG	2:F:271:TYR:HD2	1.99	0.46
1:E:430:ARG:NH1	1:E:430:ARG:HB3	2.30	0.46
2:H:222:PRO:HD2	2:H:271:TYR:CD2	2.50	0.46
3:L:123:VAL:HA	3:L:126:ILE:HD12	1.97	0.46
1:A:38:ALA:O	1:A:85:ARG:HD3	2.16	0.46
1:C:84:ASN:C	1:C:84:ASN:HD22	2.19	0.46
1:C:96:LEU:HD23	2:D:95:ARG:HH21	1.79	0.46
1:C:426:TYR:CZ	1:C:430:ARG:HD3	2.51	0.46
2:F:74:GLN:NE2	2:F:74:GLN:HA	2.31	0.46
2:F:123:HIS:O	2:F:125:ASN:N	2.47	0.46
2:F:267:ARG:HH11	2:F:267:ARG:CG	2.19	0.46
3:L:105:VAL:HG11	3:L:130:VAL:CG2	2.43	0.46
2:B:49:CYS:HA	2:B:139:HIS:HD2	1.80	0.46
2:B:262:GLN:NE2	1:E:66:SER:OG	2.49	0.46
3:J:107:THR:OG1	3:J:108:LEU:N	2.49	0.46
2:H:271:TYR:N	2:H:271:TYR:CD1	2.84	0.46
2:B:112:ASN:HD21	2:B:120:VAL:HB	1.81	0.45
2:B:335:PHE:CZ	3:I:144:ILE:HD13	2.51	0.45
1:C:218:ILE:HD11	1:C:268:ALA:O	2.15	0.45
1:C:265:PHE:O	1:C:269:ILE:HG13	2.16	0.45
2:D:33:PRO:C	2:D:35:PHE:H	2.18	0.45
2:F:32:HIS:CE1	2:F:33:PRO:HD2	2.51	0.45
2:F:182:THR:O	2:F:183:GLU:HB2	2.16	0.45
1:G:128:ALA:HB1	1:G:131:LEU:HD11	1.97	0.45
2:H:127:ILE:CG1	2:H:128:GLN:NE2	2.79	0.45
3:I:161:ILE:O	3:I:162:LEU:HD23	2.15	0.45
1:C:140:ALA:HA	1:C:150:LEU:CD2	2.46	0.45
2:D:74:GLN:NE2	2:D:74:GLN:HA	2.30	0.45
2:D:183:GLU:HG3	2:D:289:ILE:CG2	2.46	0.45
1:E:41:THR:O	1:E:45:ILE:HG13	2.16	0.45
1:E:84:ASN:HD22	1:E:85:ARG:N	2.13	0.45
1:E:192:LEU:HG	1:E:196:PHE:CE1	2.50	0.45
3:K:115:ILE:HG22	3:K:116:ASP:N	2.32	0.45
2:H:236:GLN:HE22	2:H:263:LYS:HB3	1.80	0.45
1:A:311:LEU:HD12	1:A:311:LEU:HA	1.82	0.45
1:C:61:ASP:OD2	1:C:85:ARG:HD2	2.17	0.45
1:C:518:ASN:ND2	1:C:533:GLN:CG	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:182:THR:CG2	2:D:183:GLU:N	2.79	0.45
2:D:377:LYS:O	2:D:378:SER:C	2.54	0.45
3:J:105:VAL:HG11	3:J:130:VAL:CG2	2.44	0.45
1:E:37:ASN:HB2	1:E:129:THR:O	2.16	0.45
1:E:299:LYS:HA	1:E:368:ILE:CG2	2.46	0.45
1:G:47:LYS:CD	1:G:51:LEU:HD11	2.46	0.45
1:G:47:LYS:C	1:G:47:LYS:HD2	2.37	0.45
1:G:215:ILE:HD12	1:G:342:LEU:HD21	1.99	0.45
1:G:233:ILE:HG22	1:G:233:ILE:O	2.16	0.45
1:G:262:GLU:OE1	1:G:262:GLU:CA	2.64	0.45
1:G:333:ILE:HA	2:H:223:ARG:HH21	1.81	0.45
2:H:74:GLN:NE2	2:H:74:GLN:HA	2.31	0.45
2:H:232:VAL:HA	2:H:236:GLN:HB3	1.99	0.45
1:A:46:LEU:HD21	1:A:57:PHE:CD1	2.52	0.45
1:A:404:LEU:HD21	1:A:467:GLU:O	2.16	0.45
1:C:42:GLY:HA2	1:C:129:THR:HG21	1.99	0.45
1:C:186:ASP:OD2	1:C:279:THR:HB	2.16	0.45
1:C:416:MET:C	1:C:418:ASN:H	2.18	0.45
1:C:444:GLY:HA2	1:C:449:GLN:HB2	1.98	0.45
1:C:481:GLU:O	1:C:484:ARG:HB3	2.16	0.45
2:D:312:THR:O	2:D:313:SER:HB2	2.16	0.45
3:J:150:MET:CE	3:J:167:LEU:HD13	2.46	0.45
2:F:136:ARG:HG2	2:F:136:ARG:NH1	2.31	0.45
2:F:314:ALA:O	2:F:315:TYR:CD1	2.69	0.45
2:F:361:LEU:HD23	2:F:361:LEU:N	2.29	0.45
1:G:488:ALA:C	1:G:490:PRO:HD3	2.36	0.45
1:A:227:SER:C	1:A:229:THR:H	2.20	0.45
1:A:415:SER:O	1:A:417:ASP:N	2.50	0.45
2:B:32:HIS:CE1	2:B:33:PRO:HD2	2.51	0.45
2:B:102:PRO:HB3	2:B:124:PHE:CD2	2.52	0.45
2:B:232:VAL:O	2:B:232:VAL:HG12	2.14	0.45
1:E:75:PHE:O	1:E:76:LEU:HD23	2.16	0.45
1:E:233:ILE:O	1:E:233:ILE:HG22	2.17	0.45
1:E:274:THR:O	1:E:276:LEU:N	2.50	0.45
1:G:15:ARG:HA	1:G:15:ARG:HD3	1.83	0.45
1:G:143:LEU:HD22	1:G:148:ILE:HG21	1.99	0.45
2:H:33:PRO:C	2:H:35:PHE:H	2.20	0.45
1:A:47:LYS:CD	1:A:51:LEU:HD11	2.46	0.45
1:A:143:LEU:HD22	1:A:148:ILE:CG2	2.47	0.45
1:A:253:LYS:HA	1:A:259:PRO:CD	2.47	0.45
2:B:136:ARG:HG2	2:B:136:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:CYS:HA	2:D:139:HIS:HD2	1.82	0.45
2:D:394:LEU:HG	2:D:396:SER:HB3	1.97	0.45
3:J:113:ILE:HD11	3:J:130:VAL:HG13	1.98	0.45
1:E:112:LEU:C	1:E:114:ASP:N	2.68	0.45
2:F:158:LEU:HD12	2:F:177:LEU:HB2	1.99	0.45
2:F:229:ILE:HD12	2:F:284:VAL:HG21	1.98	0.45
1:G:288:ILE:HG23	1:G:305:TRP:CZ3	2.52	0.45
2:H:228:CYS:O	2:H:231:TYR:HB3	2.17	0.45
2:H:377:LYS:O	2:H:378:SER:C	2.54	0.45
2:H:392:LEU:HD23	2:H:392:LEU:HA	1.50	0.45
1:A:37:ASN:HD22	1:A:37:ASN:HA	1.62	0.45
1:C:262:GLU:OE1	1:C:262:GLU:CA	2.65	0.45
1:C:474:VAL:O	1:C:475:LYS:C	2.55	0.45
2:D:342:ASN:N	2:D:342:ASN:ND2	2.63	0.45
1:E:143:LEU:HD22	1:E:148:ILE:CG2	2.46	0.45
1:E:177:ASP:O	1:E:178:ASN:CB	2.65	0.45
2:F:90:ARG:HG2	2:F:90:ARG:HH11	1.81	0.45
2:F:95:ARG:HD3	2:F:95:ARG:HA	1.67	0.45
2:F:232:VAL:HA	2:F:236:GLN:HB3	1.99	0.45
2:F:377:LYS:O	2:F:378:SER:C	2.55	0.45
1:G:474:VAL:O	1:G:475:LYS:C	2.54	0.45
2:H:162:LEU:HD22	2:H:169:LEU:HD11	1.98	0.45
2:H:236:GLN:NE2	2:H:263:LYS:HB3	2.32	0.45
2:H:335:PHE:CZ	3:L:144:ILE:CD1	2.99	0.45
1:A:177:ASP:O	1:A:178:ASN:CB	2.65	0.45
1:A:518:ASN:ND2	1:A:534:LEU:HD12	2.32	0.45
2:B:183:GLU:HG3	2:B:289:ILE:CG2	2.47	0.45
2:B:229:ILE:HG21	2:B:284:VAL:HB	1.99	0.45
2:B:342:ASN:H	2:B:342:ASN:ND2	2.09	0.45
1:C:259:PRO:N	1:C:260:GLU:HG2	2.32	0.45
1:C:274:THR:O	1:C:276:LEU:N	2.49	0.45
1:C:288:ILE:HG23	1:C:305:TRP:CZ3	2.52	0.45
1:C:518:ASN:ND2	1:C:534:LEU:HD12	2.32	0.45
2:D:90:ARG:HG2	2:D:90:ARG:HH11	1.80	0.45
3:J:155:THR:HG22	3:J:158:ASP:CG	2.37	0.45
1:E:18:ARG:NH2	2:F:288:ILE:HD12	2.31	0.45
1:E:285:ILE:HD11	1:E:387:SER:O	2.17	0.45
1:E:366:GLN:C	1:E:368:ILE:N	2.66	0.45
1:E:504:GLU:O	1:E:508:ILE:HG13	2.17	0.45
2:F:356:SER:HA	2:F:357:PRO:HD3	1.52	0.45
2:H:136:ARG:HG2	2:H:136:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:161:ILE:O	3:L:162:LEU:HD23	2.17	0.45
1:E:265:PHE:O	1:E:269:ILE:HG13	2.17	0.45
2:F:110:PHE:HE2	2:F:114:ARG:HB2	1.82	0.45
1:G:18:ARG:NH2	2:H:288:ILE:HD12	2.32	0.45
1:G:293:ARG:HG2	1:G:305:TRP:CD1	2.52	0.45
1:G:396:ARG:HH11	1:G:533:GLN:NE2	2.15	0.45
2:H:182:THR:O	2:H:183:GLU:HB2	2.16	0.45
2:H:229:ILE:HG21	2:H:284:VAL:HB	1.99	0.45
1:A:233:ILE:O	1:A:233:ILE:HG22	2.17	0.45
1:A:353:ASP:O	1:A:357:VAL:HG23	2.17	0.45
2:B:306:GLU:OE2	2:B:309:LYS:HD2	2.17	0.45
1:C:335:ASP:HB3	1:C:338:LYS:HB2	1.99	0.45
1:C:355:ALA:O	1:C:358:GLY:N	2.49	0.45
2:D:199:CYS:HG	2:D:346:CYS:HG	1.60	0.45
2:D:340:LYS:HB3	2:D:342:ASN:ND2	2.32	0.45
2:D:351:GLN:HB3	2:D:916:PHE:CB	2.47	0.45
3:J:107:THR:CG2	3:J:111:LYS:HB3	2.47	0.45
2:F:183:GLU:HG3	2:F:289:ILE:HG21	1.99	0.45
2:F:236:GLN:NE2	2:F:263:LYS:HB3	2.31	0.45
1:G:227:SER:C	1:G:229:THR:H	2.21	0.45
2:H:356:SER:HA	2:H:357:PRO:HD3	1.55	0.45
1:A:16:GLN:CB	2:B:292:VAL:HG12	2.47	0.44
1:A:225:TRP:CE2	1:A:233:ILE:HG12	2.52	0.44
2:B:908:GLN:O	2:B:909:THR:C	2.52	0.44
1:C:211:HIS:O	1:C:338:LYS:HD2	2.16	0.44
1:C:447:ASN:ND2	2:D:26:ARG:HH21	2.12	0.44
2:D:127:ILE:HG13	2:D:128:GLN:NE2	2.33	0.44
2:D:236:GLN:HE22	2:D:263:LYS:HD2	1.82	0.44
1:E:42:GLY:HA2	1:E:129:THR:HG21	1.99	0.44
1:E:112:LEU:C	1:E:114:ASP:H	2.20	0.44
2:F:80:MET:HB3	2:F:126:LYS:HB3	1.98	0.44
2:F:232:VAL:O	2:F:232:VAL:HG12	2.16	0.44
1:G:432:VAL:HG13	1:G:443:PRO:CD	2.46	0.44
1:A:218:ILE:HD11	1:A:268:ALA:O	2.17	0.44
1:A:288:ILE:HG23	1:A:305:TRP:CZ3	2.52	0.44
2:D:394:LEU:HD11	2:D:396:SER:HB3	1.98	0.44
2:D:607:THR:O	2:D:608:ARG:CB	2.65	0.44
1:E:146:SER:O	1:E:147:GLN:HB2	2.17	0.44
2:F:335:PHE:HE2	3:K:170:VAL:HG21	1.81	0.44
2:F:360:LYS:H	2:F:360:LYS:HG3	1.61	0.44
3:K:155:THR:HG22	3:K:158:ASP:CG	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:GLY:HA2	1:G:129:THR:HG21	2.00	0.44
1:G:112:LEU:C	1:G:114:ASP:H	2.19	0.44
1:G:421:ASN:O	1:G:423:ILE:N	2.50	0.44
2:H:197:THR:CG2	2:H:198:ALA:N	2.79	0.44
2:H:283:GLY:HA2	2:H:288:ILE:HG13	1.98	0.44
2:H:312:THR:O	2:H:313:SER:HB2	2.16	0.44
1:A:43:THR:HG22	1:A:44:GLU:N	2.33	0.44
1:A:112:LEU:C	1:A:114:ASP:N	2.70	0.44
1:A:432:VAL:HG13	1:A:443:PRO:CD	2.47	0.44
2:B:33:PRO:C	2:B:35:PHE:H	2.21	0.44
2:B:156:GLY:O	2:B:157:MET:C	2.55	0.44
2:B:361:LEU:HD23	2:B:361:LEU:N	2.31	0.44
1:C:143:LEU:HD22	1:C:148:ILE:HG21	1.99	0.44
1:C:331:ASP:HB2	2:D:224:LEU:HD11	1.99	0.44
2:D:314:ALA:O	2:D:315:TYR:CD1	2.70	0.44
1:E:133:GLU:HG3	1:E:433:ASP:HB3	1.99	0.44
2:F:187:GLY:CA	3:K:173:LEU:CD1	2.95	0.44
2:F:268:ALA:HB1	2:F:273:ILE:O	2.16	0.44
1:G:281:ILE:HA	1:G:282:PRO:HD3	1.84	0.44
1:G:357:VAL:O	1:G:361:VAL:HG23	2.16	0.44
1:A:488:ALA:C	1:A:490:PRO:HD3	2.38	0.44
2:B:124:PHE:O	2:B:124:PHE:CD1	2.70	0.44
2:B:197:THR:HG21	2:B:320:ASN:HB3	1.99	0.44
2:B:342:ASN:N	2:B:342:ASN:ND2	2.64	0.44
1:C:156:TYR:CE1	1:C:487:ALA:HA	2.53	0.44
1:C:233:ILE:O	1:C:233:ILE:HG22	2.17	0.44
2:D:335:PHE:C	2:D:335:PHE:CD1	2.91	0.44
3:J:123:VAL:HA	3:J:126:ILE:HD12	1.98	0.44
2:F:33:PRO:C	2:F:35:PHE:H	2.20	0.44
2:H:112:ASN:OD1	2:H:120:VAL:N	2.46	0.44
2:H:394:LEU:HD11	2:H:396:SER:HB3	2.00	0.44
2:B:132:ASP:O	2:B:133:THR:C	2.56	0.44
3:I:145:TYR:O	3:I:146:SER:C	2.55	0.44
1:C:488:ALA:C	1:C:490:PRO:HD3	2.38	0.44
2:D:192:ILE:HG22	2:D:194:PRO:CD	2.47	0.44
2:D:321:TYR:CD2	2:D:322:LEU:N	2.86	0.44
1:E:47:LYS:HD2	1:E:47:LYS:C	2.37	0.44
1:E:415:SER:O	1:E:417:ASP:N	2.50	0.44
2:F:13:TRP:CZ3	2:F:116:PRO:HG2	2.52	0.44
2:F:131:ASN:O	2:F:132:ASP:C	2.55	0.44
2:H:13:TRP:CZ3	2:H:116:PRO:HG2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:50:LYS:H	2:H:139:HIS:CD2	2.35	0.44
2:H:236:GLN:HE22	2:H:263:LYS:HD2	1.82	0.44
3:L:115:ILE:HG22	3:L:116:ASP:N	2.33	0.44
3:L:155:THR:HG22	3:L:158:ASP:CG	2.37	0.44
1:A:61:ASP:OD2	1:A:85:ARG:HD2	2.17	0.44
1:A:112:LEU:C	1:A:114:ASP:H	2.21	0.44
1:A:131:LEU:HA	1:A:132:PRO:HD3	1.86	0.44
2:B:314:ALA:O	2:B:315:TYR:CD1	2.71	0.44
1:C:43:THR:HG22	1:C:44:GLU:N	2.31	0.44
2:D:78:ILE:HD11	2:D:134:PHE:HE2	1.83	0.44
2:F:187:GLY:HA2	3:K:173:LEU:CD1	2.47	0.44
1:G:393:VAL:HG13	1:G:517:ASN:ND2	2.28	0.44
2:H:123:HIS:O	2:H:125:ASN:N	2.49	0.44
1:A:299:LYS:HA	1:A:368:ILE:CG2	2.47	0.44
1:A:444:GLY:HA2	1:A:449:GLN:HB2	1.98	0.44
1:A:481:GLU:O	1:A:484:ARG:HB3	2.18	0.44
2:B:131:ASN:HD22	2:D:131:ASN:HB3	1.83	0.44
1:C:227:SER:C	1:C:229:THR:H	2.22	0.44
2:D:80:MET:HB3	2:D:126:LYS:HB3	1.98	0.44
2:D:343:CYS:O	2:D:347:SER:HB3	2.18	0.44
2:F:343:CYS:O	2:F:347:SER:HB3	2.18	0.44
2:F:351:GLN:O	2:F:353:ILE:N	2.51	0.44
2:H:80:MET:HG2	4:H:8:ATP:C2	2.52	0.44
2:H:229:ILE:HD12	2:H:284:VAL:HG21	1.99	0.44
2:H:268:ALA:HB1	2:H:273:ILE:O	2.18	0.44
1:A:42:GLY:HA2	1:A:129:THR:HG21	1.99	0.44
1:A:480:HIS:HB2	2:B:29:PRO:HG2	1.99	0.44
2:B:335:PHE:CE1	2:B:337:ALA:HB2	2.51	0.44
1:C:39:THR:HB	1:C:489:GLU:OE1	2.17	0.44
1:C:112:LEU:C	1:C:114:ASP:H	2.20	0.44
1:C:532:PHE:HB3	1:C:533:GLN:H	1.37	0.44
1:E:266:GLU:HG3	1:E:270:LYS:HE3	2.00	0.44
2:F:50:LYS:H	2:F:139:HIS:CD2	2.36	0.44
2:F:192:ILE:HG22	2:F:194:PRO:CD	2.43	0.44
3:K:113:ILE:HD11	3:K:130:VAL:HG13	1.99	0.44
3:K:155:THR:O	3:K:158:ASP:N	2.51	0.44
2:H:141:ILE:HD12	2:H:158:LEU:HD11	2.00	0.44
2:H:250:ASP:H	2:H:256:HIS:CE1	2.36	0.44
2:B:123:HIS:O	2:B:125:ASN:N	2.49	0.44
2:B:250:ASP:OD2	2:B:253:ASP:HB2	2.17	0.44
1:C:131:LEU:HA	1:C:132:PRO:HD3	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:353:ILE:HG23	2:D:355:PHE:HE1	1.82	0.44
1:E:421:ASN:O	1:E:423:ILE:N	2.50	0.44
1:E:447:ASN:ND2	2:F:26:ARG:HH21	2.14	0.44
2:F:52:LEU:HD11	2:F:78:ILE:HG13	1.98	0.44
2:F:156:GLY:O	2:F:157:MET:C	2.54	0.44
1:G:35:LEU:HD23	1:G:46:LEU:HD22	2.00	0.44
1:G:261:ASP:O	1:G:262:GLU:CG	2.66	0.44
2:H:110:PHE:HE2	2:H:114:ARG:HB2	1.83	0.44
2:H:306:GLU:OE2	2:H:309:LYS:HD2	2.18	0.44
3:L:155:THR:O	3:L:158:ASP:N	2.51	0.44
1:A:504:GLU:O	1:A:508:ILE:HG13	2.18	0.43
3:J:115:ILE:HG22	3:J:116:ASP:N	2.33	0.43
1:E:47:LYS:HD2	1:E:51:LEU:HD12	2.00	0.43
1:E:481:GLU:O	1:E:484:ARG:N	2.51	0.43
3:K:107:THR:CG2	3:K:111:LYS:HB3	2.48	0.43
3:K:107:THR:OG1	3:K:108:LEU:N	2.51	0.43
1:G:497:LEU:HD12	1:G:497:LEU:HA	1.87	0.43
2:H:187:GLY:CA	3:L:173:LEU:CD1	2.96	0.43
1:A:518:ASN:ND2	1:A:533:GLN:CG	2.71	0.43
2:B:16:ARG:HH22	2:B:116:PRO:HB2	1.83	0.43
2:B:127:ILE:CG1	2:B:128:GLN:NE2	2.81	0.43
2:B:236:GLN:HE22	2:B:263:LYS:HD2	1.83	0.43
3:I:150:MET:HE3	3:I:167:LEU:HD13	1.99	0.43
1:E:35:LEU:HD12	1:E:36:ILE:N	2.33	0.43
2:F:228:CYS:O	2:F:231:TYR:HB3	2.19	0.43
2:F:236:GLN:HE22	2:F:263:LYS:HD2	1.83	0.43
1:G:47:LYS:HD2	1:G:51:LEU:HD12	2.00	0.43
1:G:146:SER:O	1:G:147:GLN:HB2	2.17	0.43
1:G:323:LEU:HB3	1:G:324:PRO:CD	2.48	0.43
1:G:323:LEU:HD22	1:G:387:SER:HB2	2.00	0.43
1:G:532:PHE:HB3	1:G:533:GLN:H	1.37	0.43
2:H:242:PRO:HG3	2:H:259:TRP:CH2	2.53	0.43
2:H:361:LEU:HD23	2:H:361:LEU:N	2.31	0.43
2:B:78:ILE:HD11	2:B:134:PHE:HE2	1.83	0.43
2:B:80:MET:HB3	2:B:126:LYS:HB3	2.00	0.43
2:B:134:PHE:O	2:B:137:GLN:HG3	2.17	0.43
1:C:47:LYS:CD	1:C:51:LEU:HD11	2.48	0.43
1:C:281:ILE:HA	1:C:282:PRO:HD3	1.85	0.43
1:C:432:VAL:HG13	1:C:443:PRO:CD	2.48	0.43
1:C:503:GLN:HA	1:C:503:GLN:OE1	2.18	0.43
1:E:19:LEU:HD13	2:F:185:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:335:PHE:CZ	3:K:144:ILE:CD1	3.01	0.43
1:G:340:ILE:HD11	2:H:273:ILE:HG12	2.00	0.43
2:H:49:CYS:HA	2:H:139:HIS:HD2	1.81	0.43
1:A:50:VAL:HG13	1:A:100:VAL:HG21	2.00	0.43
1:A:133:GLU:HG3	1:A:433:ASP:HB3	2.00	0.43
2:B:50:LYS:H	2:B:139:HIS:CD2	2.36	0.43
1:C:112:LEU:C	1:C:114:ASP:N	2.70	0.43
1:C:192:LEU:HG	1:C:196:PHE:CE1	2.52	0.43
1:C:415:SER:O	1:C:417:ASP:N	2.50	0.43
2:D:333:TYR:CZ	2:D:335:PHE:HB3	2.54	0.43
2:F:49:CYS:HA	2:F:139:HIS:HD2	1.81	0.43
2:F:178:ILE:HG21	2:F:303:CYS:HB3	1.99	0.43
1:G:221:TYR:O	1:G:243:PHE:HE1	2.01	0.43
1:G:333:ILE:HA	2:H:223:ARG:NH2	2.34	0.43
1:G:430:ARG:HB3	1:G:430:ARG:NH1	2.32	0.43
2:H:182:THR:CG2	2:H:183:GLU:N	2.81	0.43
2:H:335:PHE:HE2	3:L:170:VAL:HG21	1.83	0.43
2:H:335:PHE:CE1	2:H:337:ALA:HB2	2.52	0.43
1:A:340:ILE:O	1:A:343:GLN:N	2.51	0.43
2:B:333:TYR:CZ	2:B:335:PHE:HB3	2.54	0.43
1:C:236:THR:HG23	1:C:240:LYS:HE3	2.01	0.43
1:C:421:ASN:O	1:C:423:ILE:N	2.51	0.43
3:J:111:LYS:O	3:J:112:GLU:HB3	2.18	0.43
1:E:225:TRP:CE2	1:E:233:ILE:HG12	2.54	0.43
1:E:236:THR:O	1:E:237:TYR:HD1	2.02	0.43
1:E:285:ILE:HD11	1:E:388:ALA:CA	2.39	0.43
2:F:139:HIS:O	2:F:176:PRO:HD2	2.18	0.43
3:K:103:ILE:HD11	3:K:117:ILE:HD12	2.01	0.43
1:G:183:LEU:HD22	1:G:215:ILE:HD11	2.00	0.43
1:G:265:PHE:O	1:G:269:ILE:HG13	2.19	0.43
1:G:518:ASN:ND2	1:G:534:LEU:HD12	2.33	0.43
3:L:107:THR:CG2	3:L:111:LYS:HB3	2.48	0.43
1:A:113:LEU:HD22	1:A:142:VAL:HG21	2.01	0.43
1:A:253:LYS:O	1:A:260:GLU:OE2	2.36	0.43
2:B:377:LYS:O	2:B:378:SER:C	2.56	0.43
2:F:124:PHE:CD1	2:F:124:PHE:C	2.92	0.43
2:F:182:THR:HG23	2:F:183:GLU:N	2.33	0.43
2:F:267:ARG:NH1	2:F:267:ARG:CG	2.80	0.43
1:G:177:ASP:O	1:G:178:ASN:CB	2.67	0.43
1:G:244:ARG:O	1:G:247:ILE:N	2.51	0.43
2:H:395:GLN:H	2:H:395:GLN:HG3	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:GLN:HE21	2:B:351:GLN:CA	2.26	0.43
1:C:47:LYS:HD2	1:C:47:LYS:C	2.38	0.43
1:C:96:LEU:HD23	2:D:95:ARG:NH2	2.33	0.43
1:C:124:THR:HG22	1:C:125:VAL:HG23	2.01	0.43
1:C:266:GLU:HG3	1:C:270:LYS:HE3	2.00	0.43
2:D:32:HIS:CE1	2:D:33:PRO:HD2	2.54	0.43
2:D:271:TYR:CD1	2:D:271:TYR:N	2.85	0.43
2:F:335:PHE:CE1	2:F:337:ALA:HB2	2.51	0.43
1:G:75:PHE:CZ	1:G:96:LEU:HD11	2.53	0.43
1:G:504:GLU:O	1:G:508:ILE:HG13	2.19	0.43
1:A:84:ASN:C	1:A:84:ASN:ND2	2.71	0.43
3:I:115:ILE:HG22	3:I:116:ASP:N	2.33	0.43
1:C:107:GLU:OE2	1:G:351:LYS:NZ	2.51	0.43
1:C:133:GLU:HG3	1:C:433:ASP:HB3	2.01	0.43
1:C:139:LEU:HG	1:C:143:LEU:HD12	2.01	0.43
1:E:47:LYS:CD	1:E:51:LEU:HD11	2.48	0.43
1:E:53:GLY:O	1:E:54:ILE:C	2.57	0.43
1:E:166:ILE:HD11	1:E:508:ILE:HD13	2.00	0.43
1:E:175:HIS:HD2	1:E:512:GLN:O	2.02	0.43
1:E:186:ASP:OD2	1:E:279:THR:HB	2.19	0.43
1:E:264:ASN:ND2	1:E:265:PHE:H	2.16	0.43
1:G:266:GLU:HG3	1:G:270:LYS:HE3	2.01	0.43
1:G:285:ILE:HD11	1:G:388:ALA:CA	2.38	0.43
2:H:267:ARG:NH1	2:H:267:ARG:CG	2.78	0.43
1:A:47:LYS:HD2	1:A:51:LEU:HD12	2.00	0.43
1:A:84:ASN:C	1:A:84:ASN:HD22	2.22	0.43
1:C:128:ALA:HB1	1:C:131:LEU:CD1	2.49	0.43
1:C:261:ASP:O	1:C:262:GLU:HG2	2.18	0.43
2:D:178:ILE:CG2	2:D:303:CYS:HB3	2.49	0.43
1:E:227:SER:C	1:E:229:THR:H	2.23	0.43
1:E:518:ASN:ND2	1:E:534:LEU:HD12	2.34	0.43
1:G:496:PHE:CE1	2:H:298:VAL:HG13	2.53	0.43
2:H:178:ILE:CG2	2:H:303:CYS:HB3	2.49	0.43
1:A:172:ILE:HA	1:A:390:LEU:HD23	2.01	0.43
2:B:207:TYR:HA	2:B:208:PRO:HD3	1.90	0.43
3:I:113:ILE:HD11	3:I:130:VAL:HG13	2.01	0.43
1:C:163:ARG:HH11	1:C:163:ARG:CG	2.25	0.43
1:C:215:ILE:HD12	1:C:342:LEU:HD21	2.01	0.43
2:D:126:LYS:HA	4:D:6:ATP:C2	2.54	0.43
2:D:235:LEU:O	2:D:238:PRO:HD2	2.18	0.43
3:J:149:GLN:HG3	3:J:149:GLN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:118:GLU:O	3:K:121:ASP:OD1	2.37	0.43
3:K:145:TYR:O	3:K:146:SER:C	2.58	0.43
1:G:43:THR:HG22	1:G:44:GLU:N	2.33	0.43
1:G:84:ASN:O	1:G:85:ARG:C	2.56	0.43
2:H:164:TYR:HD2	2:H:169:LEU:HA	1.84	0.43
2:H:314:ALA:O	2:H:315:TYR:CG	2.72	0.43
2:H:320:ASN:O	2:H:321:TYR:CB	2.67	0.43
1:A:53:GLY:O	1:A:54:ILE:C	2.57	0.42
2:B:182:THR:O	2:B:183:GLU:HB2	2.18	0.42
1:C:35:LEU:HD12	1:C:36:ILE:N	2.34	0.42
1:C:56:SER:HB3	1:C:101:SER:HG	1.80	0.42
1:C:415:SER:C	1:C:417:ASP:H	2.22	0.42
1:C:497:LEU:HD12	1:C:497:LEU:HA	1.91	0.42
2:D:130:PHE:CG	2:D:134:PHE:CD2	3.07	0.42
2:D:228:CYS:O	2:D:231:TYR:HB3	2.19	0.42
2:D:229:ILE:HD12	2:D:284:VAL:HG21	2.00	0.42
2:D:306:GLU:OE2	2:D:309:LYS:HD2	2.19	0.42
2:D:395:GLN:H	2:D:395:GLN:HG3	1.69	0.42
3:J:150:MET:HE3	3:J:167:LEU:HD22	1.99	0.42
1:E:16:GLN:HB2	2:F:292:VAL:HG12	2.00	0.42
1:E:305:TRP:O	1:E:308:ALA:HB3	2.19	0.42
2:F:187:GLY:HA2	3:K:173:LEU:HD12	2.01	0.42
2:F:250:ASP:OD2	2:F:253:ASP:HB2	2.19	0.42
1:G:415:SER:C	1:G:417:ASP:H	2.22	0.42
1:G:462:THR:O	1:G:463:GLY:C	2.57	0.42
2:H:228:CYS:SG	2:H:268:ALA:HA	2.59	0.42
1:A:16:GLN:NE2	1:A:20:TRP:CZ2	2.85	0.42
1:A:401:GLU:HG3	1:A:533:GLN:HE22	1.85	0.42
1:A:517:ASN:OD1	1:A:534:LEU:HB2	2.18	0.42
2:B:124:PHE:HD1	2:B:124:PHE:C	2.22	0.42
2:B:182:THR:CG2	2:B:183:GLU:N	2.81	0.42
2:B:232:VAL:HA	2:B:236:GLN:HB3	2.00	0.42
2:B:241:GLN:NE2	2:B:246:GLY:H	2.17	0.42
2:B:271:TYR:N	2:B:271:TYR:CD1	2.87	0.42
1:C:46:LEU:HD21	1:C:57:PHE:CD1	2.54	0.42
1:C:84:ASN:O	1:C:85:ARG:C	2.57	0.42
1:C:244:ARG:O	1:C:247:ILE:N	2.50	0.42
1:C:520:TYR:CG	2:D:330:LEU:HD12	2.54	0.42
2:D:54:ILE:HG22	2:D:145:LEU:HD21	2.01	0.42
2:D:232:VAL:HA	2:D:236:GLN:HB3	2.01	0.42
2:D:242:PRO:HG3	2:D:259:TRP:CH2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:ASP:OD2	2:D:253:ASP:HB2	2.19	0.42
1:E:96:LEU:HD23	2:F:95:ARG:HH21	1.84	0.42
1:E:260:GLU:HB3	1:E:261:ASP:OD1	2.19	0.42
1:E:355:ALA:O	1:E:358:GLY:N	2.52	0.42
2:F:132:ASP:O	2:F:133:THR:C	2.58	0.42
2:F:207:TYR:HA	2:F:208:PRO:HD3	1.90	0.42
2:H:335:PHE:CD1	2:H:335:PHE:C	2.93	0.42
1:A:183:LEU:HD22	1:A:215:ILE:HD11	2.01	0.42
1:C:72:ASN:HD22	1:C:73:ASN:N	2.17	0.42
2:D:193:LEU:O	2:D:194:PRO:C	2.58	0.42
2:D:222:PRO:HD2	2:D:271:TYR:CD2	2.54	0.42
3:J:136:ILE:HG22	3:J:141:GLN:HG2	2.01	0.42
1:E:236:THR:O	1:E:237:TYR:CD1	2.71	0.42
2:F:141:ILE:HD12	2:F:158:LEU:HD11	2.02	0.42
1:G:47:LYS:HD2	1:G:51:LEU:CD1	2.49	0.42
1:G:299:LYS:HA	1:G:368:ILE:CG2	2.49	0.42
1:G:311:LEU:O	1:G:314:PHE:HB3	2.19	0.42
1:G:503:GLN:OE1	1:G:503:GLN:HA	2.19	0.42
2:H:353:ILE:HG23	2:H:355:PHE:HE1	1.84	0.42
2:H:360:LYS:H	2:H:360:LYS:HG3	1.65	0.42
2:B:222:PRO:HD2	2:B:271:TYR:CD2	2.54	0.42
2:B:293:ALA:O	2:B:294:SER:C	2.57	0.42
2:B:351:GLN:O	2:B:353:ILE:N	2.52	0.42
3:I:107:THR:OG1	3:I:108:LEU:N	2.52	0.42
2:D:136:ARG:HG2	2:D:136:ARG:NH1	2.34	0.42
2:D:182:THR:HG23	2:D:183:GLU:N	2.34	0.42
2:D:232:VAL:HG12	2:D:260:ILE:HG23	2.01	0.42
1:E:72:ASN:HD22	1:E:73:ASN:N	2.17	0.42
1:E:84:ASN:O	1:E:85:ARG:C	2.58	0.42
1:E:491:HIS:NE2	2:F:65:LYS:NZ	2.64	0.42
2:F:222:PRO:HD2	2:F:271:TYR:CD2	2.54	0.42
2:F:314:ALA:O	2:F:315:TYR:CG	2.73	0.42
2:F:335:PHE:CD1	2:F:335:PHE:C	2.93	0.42
1:G:72:ASN:HD22	1:G:73:ASN:N	2.18	0.42
1:A:47:LYS:O	1:A:51:LEU:HD12	2.19	0.42
1:A:266:GLU:HG3	1:A:270:LYS:HE3	2.00	0.42
1:A:274:THR:O	1:A:276:LEU:N	2.52	0.42
1:A:415:SER:C	1:A:417:ASP:H	2.23	0.42
2:B:228:CYS:O	2:B:231:TYR:HB3	2.19	0.42
3:I:107:THR:CG2	3:I:111:LYS:HB3	2.50	0.42
1:C:189:PHE:CE1	1:C:192:LEU:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:ALA:O	1:C:374:SER:N	2.48	0.42
2:D:52:LEU:HD11	2:D:78:ILE:HG13	2.01	0.42
2:D:355:PHE:O	2:D:356:SER:CB	2.68	0.42
2:D:356:SER:HA	2:D:357:PRO:HD3	1.53	0.42
1:E:61:ASP:OD2	1:E:85:ARG:HD2	2.19	0.42
2:F:124:PHE:CD1	2:F:124:PHE:O	2.72	0.42
2:F:353:ILE:HG23	2:F:355:PHE:HE1	1.84	0.42
1:G:259:PRO:CA	1:G:260:GLU:HG2	2.50	0.42
1:G:355:ALA:O	1:G:358:GLY:N	2.53	0.42
1:G:404:LEU:HD21	1:G:467:GLU:O	2.19	0.42
2:H:124:PHE:CD1	2:H:124:PHE:C	2.92	0.42
2:H:124:PHE:C	2:H:124:PHE:HD1	2.22	0.42
2:H:183:GLU:HG3	2:H:289:ILE:CG2	2.50	0.42
2:H:249:LEU:CD1	2:H:260:ILE:HD11	2.49	0.42
2:H:343:CYS:O	2:H:347:SER:HB3	2.19	0.42
4:H:8:ATP:H3'	4:H:8:ATP:O1B	2.18	0.42
1:A:195:HIS:O	1:A:198:SER:HB3	2.20	0.42
2:B:241:GLN:HE21	2:B:246:GLY:H	1.67	0.42
2:B:353:ILE:HG23	2:B:355:PHE:HE1	1.84	0.42
1:C:517:ASN:OD1	1:C:534:LEU:HB2	2.20	0.42
2:D:392:LEU:HA	2:D:392:LEU:HD23	1.46	0.42
1:E:111:ASN:OD1	1:E:111:ASN:O	2.37	0.42
1:E:317:LYS:HG2	1:E:318:GLU:N	2.35	0.42
1:G:39:THR:HB	1:G:489:GLU:OE1	2.19	0.42
2:H:102:PRO:HB3	2:H:124:PHE:CD2	2.55	0.42
2:H:351:GLN:HE21	2:H:351:GLN:CA	2.27	0.42
1:A:47:LYS:HD2	1:A:51:LEU:CD1	2.49	0.42
1:A:146:SER:O	1:A:147:GLN:HB2	2.19	0.42
1:A:261:ASP:HB2	1:A:262:GLU:H	1.66	0.42
1:A:331:ASP:OD1	2:B:223:ARG:HD2	2.19	0.42
2:B:74:GLN:HA	2:B:74:GLN:HE21	1.84	0.42
2:B:130:PHE:CG	2:B:134:PHE:CD2	3.08	0.42
2:B:148:ILE:O	2:B:149:ILE:C	2.58	0.42
2:B:183:GLU:HG3	2:B:289:ILE:HG21	2.02	0.42
2:B:243:PHE:O	2:B:247:VAL:HG21	2.19	0.42
1:C:47:LYS:HD2	1:C:51:LEU:HD12	2.02	0.42
1:C:504:GLU:HG3	1:C:516:PHE:CE2	2.55	0.42
2:D:351:GLN:O	2:D:353:ILE:N	2.53	0.42
1:E:47:LYS:HD2	1:E:51:LEU:CD1	2.50	0.42
1:E:281:ILE:HA	1:E:282:PRO:HD3	1.85	0.42
2:F:96:PRO:O	2:F:99:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:127:ILE:HG13	2:F:128:GLN:NE2	2.34	0.42
2:F:355:PHE:O	2:F:356:SER:CB	2.67	0.42
1:G:84:ASN:HD22	1:G:85:ARG:N	2.16	0.42
1:G:143:LEU:HD13	1:G:150:LEU:HD13	2.00	0.42
3:L:145:TYR:O	3:L:146:SER:C	2.58	0.42
1:A:47:LYS:HD2	1:A:47:LYS:C	2.40	0.42
1:A:175:HIS:HD2	1:A:512:GLN:O	2.02	0.42
1:A:323:LEU:HD22	1:A:387:SER:HB2	2.01	0.42
2:B:13:TRP:CD1	2:B:13:TRP:C	2.93	0.42
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.79	0.42
1:C:75:PHE:O	1:C:76:LEU:HD23	2.20	0.42
1:C:221:TYR:O	1:C:243:PHE:HE1	2.03	0.42
1:C:504:GLU:O	1:C:508:ILE:HG13	2.20	0.42
2:D:74:GLN:HA	2:D:74:GLN:HE21	1.85	0.42
2:D:164:TYR:HD2	2:D:169:LEU:HA	1.84	0.42
1:E:19:LEU:HD21	2:F:290:PRO:HB2	2.01	0.42
1:E:144:TRP:CZ3	1:E:397:SER:HA	2.55	0.42
2:F:130:PHE:CG	2:F:134:PHE:CD2	3.07	0.42
1:G:163:ARG:NH1	1:G:163:ARG:CG	2.82	0.42
1:G:274:THR:O	1:G:276:LEU:N	2.53	0.42
1:G:305:TRP:O	1:G:308:ALA:HB3	2.19	0.42
2:H:132:ASP:O	2:H:133:THR:C	2.58	0.42
1:A:35:LEU:HD23	1:A:46:LEU:HD22	2.01	0.42
1:A:39:THR:HB	1:A:489:GLU:OE1	2.19	0.42
1:A:84:ASN:O	1:A:85:ARG:C	2.58	0.42
2:B:131:ASN:HB3	2:D:131:ASN:HD22	1.85	0.42
2:B:193:LEU:O	2:B:194:PRO:C	2.57	0.42
2:B:703:GLY:C	2:B:705:VAL:H	2.23	0.42
3:J:122:LYS:HA	3:J:154:LYS:O	2.20	0.42
2:F:140:ILE:HG22	2:F:141:ILE:N	2.35	0.42
1:G:18:ARG:CZ	2:H:288:ILE:HD12	2.49	0.42
1:G:143:LEU:HD22	1:G:148:ILE:CG2	2.50	0.42
2:H:321:TYR:CD2	2:H:322:LEU:N	2.87	0.42
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.94	0.42
1:A:140:ALA:HA	1:A:150:LEU:CD2	2.49	0.42
1:A:323:LEU:HB3	1:A:324:PRO:CD	2.50	0.42
1:A:348:GLU:OE2	1:E:107:GLU:OE1	2.38	0.42
2:B:232:VAL:HG21	2:B:264:SER:N	2.35	0.42
2:B:274:ARG:NH1	1:E:106:GLU:O	2.53	0.42
1:C:404:LEU:HD21	1:C:467:GLU:O	2.20	0.42
2:D:50:LYS:H	2:D:139:HIS:CD2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:ILE:HG12	1:E:55:GLY:N	2.35	0.42
1:E:140:ALA:HA	1:E:150:LEU:CD2	2.49	0.42
1:E:441:ARG:HH21	1:E:453:ASP:CG	2.23	0.42
2:F:124:PHE:C	2:F:124:PHE:HD1	2.22	0.42
2:F:250:ASP:H	2:F:256:HIS:CE1	2.38	0.42
1:G:264:ASN:ND2	1:G:265:PHE:H	2.17	0.42
2:H:80:MET:HB3	2:H:126:LYS:HB3	2.02	0.42
2:H:157:MET:HE3	2:H:157:MET:HA	2.01	0.42
1:A:347:ARG:HH22	2:B:274:ARG:NH1	2.17	0.41
2:B:394:LEU:CD1	2:B:396:SER:HB3	2.50	0.41
1:C:113:LEU:HD11	1:C:139:LEU:HB2	2.02	0.41
2:D:110:PHE:HE2	2:D:114:ARG:HB2	1.85	0.41
1:E:432:VAL:HG13	1:E:443:PRO:CD	2.49	0.41
1:G:33:VAL:CG2	1:G:54:ILE:HD11	2.49	0.41
1:G:96:LEU:HD23	2:H:95:ARG:HH21	1.84	0.41
1:G:480:HIS:HB2	2:H:29:PRO:HG2	2.02	0.41
2:H:362:GLN:H	2:H:362:GLN:HG3	1.49	0.41
3:L:103:ILE:HD11	3:L:117:ILE:HD12	2.01	0.41
1:A:171:VAL:HG13	1:A:391:ARG:O	2.20	0.41
1:A:186:ASP:OD2	1:A:279:THR:HB	2.19	0.41
2:B:124:PHE:CD1	2:B:124:PHE:C	2.92	0.41
3:I:111:LYS:O	3:I:112:GLU:HB3	2.21	0.41
1:C:19:LEU:HD23	1:C:19:LEU:HA	1.90	0.41
1:C:239:GLU:O	1:C:240:LYS:C	2.59	0.41
1:E:47:LYS:O	1:E:51:LEU:HD12	2.20	0.41
1:E:260:GLU:HB2	1:E:261:ASP:OD1	2.20	0.41
3:K:150:MET:HE3	3:K:167:LEU:HD13	2.01	0.41
1:G:175:HIS:HD2	1:G:512:GLN:O	2.03	0.41
1:G:435:PHE:CD2	1:G:435:PHE:C	2.94	0.41
2:H:250:ASP:OD2	2:H:253:ASP:HB2	2.20	0.41
3:L:144:ILE:HD12	3:L:170:VAL:HG11	2.02	0.41
3:L:149:GLN:HG3	3:L:149:GLN:O	2.20	0.41
1:A:253:LYS:O	1:A:260:GLU:CD	2.59	0.41
2:B:340:LYS:HB3	2:B:342:ASN:ND2	2.34	0.41
2:B:343:CYS:O	2:B:347:SER:HB3	2.19	0.41
3:J:103:ILE:HD11	3:J:117:ILE:HD12	2.02	0.41
1:E:441:ARG:HH11	1:E:441:ARG:HG2	1.85	0.41
2:F:187:GLY:CA	3:K:173:LEU:HD12	2.51	0.41
3:K:122:LYS:HA	3:K:154:LYS:O	2.19	0.41
1:G:61:ASP:OD2	1:G:85:ARG:HD2	2.20	0.41
1:G:332:MET:HE1	1:G:342:LEU:CD2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:124:PHE:CD1	2:H:124:PHE:O	2.73	0.41
2:H:126:LYS:HA	4:H:8:ATP:N1	2.35	0.41
3:L:122:LYS:HA	3:L:154:LYS:O	2.20	0.41
1:A:317:LYS:HG2	1:A:318:GLU:N	2.36	0.41
1:A:333:ILE:HA	2:B:223:ARG:HH21	1.85	0.41
1:A:481:GLU:O	1:A:484:ARG:N	2.53	0.41
2:B:95:ARG:HD3	2:B:95:ARG:HA	1.66	0.41
2:B:96:PRO:O	2:B:99:ILE:HG13	2.20	0.41
2:B:355:PHE:O	2:B:356:SER:CB	2.68	0.41
2:D:158:LEU:HD12	2:D:177:LEU:HB2	2.01	0.41
1:E:36:ILE:HD13	1:E:36:ILE:HA	1.92	0.41
1:E:143:LEU:HD12	1:E:150:LEU:HD13	1.97	0.41
1:E:323:LEU:HB3	1:E:324:PRO:CD	2.50	0.41
1:E:488:ALA:C	1:E:490:PRO:HD3	2.40	0.41
2:F:130:PHE:HB2	2:F:135:TYR:CE1	2.56	0.41
2:F:174:ILE:HG23	2:F:194:PRO:O	2.20	0.41
2:F:316:ILE:HD12	2:F:316:ILE:N	2.23	0.41
2:H:333:TYR:CZ	2:H:335:PHE:HB3	2.56	0.41
2:H:351:GLN:O	2:H:353:ILE:N	2.53	0.41
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.87	0.41
1:A:462:THR:O	1:A:463:GLY:C	2.59	0.41
2:B:603:ILE:O	2:B:607:THR:N	2.53	0.41
3:I:122:LYS:HA	3:I:154:LYS:O	2.20	0.41
1:C:40:ALA:HB3	1:C:489:GLU:CD	2.41	0.41
1:C:84:ASN:HD22	1:C:85:ARG:N	2.18	0.41
1:C:220:LYS:HD2	1:C:220:LYS:HA	1.94	0.41
2:D:283:GLY:HA2	2:D:288:ILE:HG13	2.03	0.41
1:E:66:SER:O	1:E:69:ASP:HB2	2.20	0.41
1:E:311:LEU:HD12	1:E:311:LEU:HA	1.81	0.41
1:E:404:LEU:HD21	1:E:467:GLU:O	2.21	0.41
2:F:271:TYR:CD1	2:F:271:TYR:N	2.88	0.41
2:F:306:GLU:OE2	2:F:309:LYS:HD2	2.20	0.41
3:K:149:GLN:HG3	3:K:149:GLN:O	2.21	0.41
2:H:394:LEU:HD11	2:H:396:SER:CB	2.49	0.41
1:A:156:TYR:CE1	1:A:487:ALA:HA	2.56	0.41
1:C:307:LEU:CD1	1:C:383:LEU:HD22	2.50	0.41
2:F:102:PRO:HB3	2:F:124:PHE:CD2	2.56	0.41
2:F:134:PHE:O	2:F:137:GLN:HG3	2.20	0.41
2:F:320:ASN:O	2:F:321:TYR:CB	2.68	0.41
1:G:253:LYS:O	1:G:260:GLU:HG2	2.20	0.41
2:H:148:ILE:O	2:H:149:ILE:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:309:LYS:O	2:H:313:SER:N	2.39	0.41
1:A:139:LEU:HG	1:A:143:LEU:HD12	2.02	0.41
2:B:335:PHE:CD1	2:B:335:PHE:C	2.94	0.41
3:I:103:ILE:HD12	3:I:103:ILE:C	2.40	0.41
3:I:118:GLU:O	3:I:121:ASP:OD1	2.38	0.41
1:C:164:ILE:HD13	1:C:515:ILE:HD12	2.02	0.41
2:D:59:LEU:HD12	3:J:176:GLY:CA	2.50	0.41
2:D:82:THR:O	2:D:82:THR:HG23	2.20	0.41
2:D:130:PHE:HB2	2:D:135:TYR:CE1	2.56	0.41
2:D:182:THR:O	2:D:183:GLU:HB2	2.20	0.41
1:E:16:GLN:NE2	1:E:20:TRP:CZ2	2.86	0.41
1:E:158:LEU:HA	1:E:158:LEU:HD23	1.82	0.41
1:E:163:ARG:NH1	1:E:163:ARG:CG	2.83	0.41
1:E:323:LEU:HD22	1:E:387:SER:HB2	2.03	0.41
2:F:33:PRO:O	2:F:35:PHE:N	2.54	0.41
2:F:351:GLN:HE21	2:F:351:GLN:CA	2.28	0.41
2:F:703:GLY:C	2:F:705:VAL:H	2.23	0.41
1:G:75:PHE:O	1:G:76:LEU:HD23	2.21	0.41
2:H:187:GLY:CA	3:L:173:LEU:HD12	2.50	0.41
2:H:249:LEU:HD11	2:H:260:ILE:HD11	2.03	0.41
1:A:259:PRO:CA	1:A:260:GLU:HG2	2.51	0.41
2:B:124:PHE:O	2:B:124:PHE:HD1	2.04	0.41
1:C:253:LYS:O	1:C:260:GLU:CD	2.58	0.41
1:C:264:ASN:ND2	1:C:265:PHE:H	2.18	0.41
1:C:311:LEU:O	1:C:314:PHE:HB3	2.21	0.41
2:F:247:VAL:HA	2:F:248:PRO:HD3	1.81	0.41
3:K:150:MET:HE3	3:K:167:LEU:CD2	2.51	0.41
1:G:45:ILE:CG1	1:G:498:GLY:HA2	2.43	0.41
1:G:117:PRO:O	1:G:119:PHE:N	2.53	0.41
1:G:157:GLY:HA3	1:G:485:TYR:CD1	2.55	0.41
1:A:155:THR:HG23	1:A:493:ILE:CG2	2.51	0.41
1:A:236:THR:HG23	1:A:240:LYS:HE3	2.03	0.41
2:B:74:GLN:HE22	2:B:119:ASN:ND2	2.08	0.41
2:B:110:PHE:HE2	2:B:114:ARG:HB2	1.85	0.41
2:B:127:ILE:HG13	2:B:128:GLN:N	2.36	0.41
2:B:232:VAL:HG12	2:B:260:ILE:HG23	2.03	0.41
2:B:274:ARG:NH2	1:E:108:SER:N	2.69	0.41
2:B:320:ASN:O	2:B:321:TYR:CB	2.68	0.41
2:B:339:ARG:NH2	2:B:346:CYS:O	2.54	0.41
3:I:149:GLN:O	3:I:149:GLN:HG3	2.21	0.41
1:C:37:ASN:HD22	1:C:37:ASN:HA	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:SER:O	1:C:147:GLN:HB2	2.21	0.41
1:C:369:GLY:O	1:C:370:GLN:C	2.59	0.41
2:D:13:TRP:CD1	2:D:13:TRP:C	2.94	0.41
2:D:158:LEU:HA	2:D:158:LEU:HD23	1.85	0.41
2:D:202:CYS:SG	2:D:343:CYS:SG	3.02	0.41
2:D:268:ALA:HB1	2:D:273:ILE:O	2.20	0.41
2:D:361:LEU:CA	2:D:364:VAL:CG2	2.99	0.41
3:J:145:TYR:O	3:J:146:SER:C	2.59	0.41
1:E:225:TRP:CD1	1:E:225:TRP:O	2.74	0.41
1:E:261:ASP:HB2	1:E:262:GLU:H	1.64	0.41
1:E:371:ALA:O	1:E:374:SER:N	2.51	0.41
1:E:532:PHE:HB3	1:E:533:GLN:H	1.40	0.41
2:F:232:VAL:HG21	2:F:264:SER:N	2.35	0.41
2:F:392:LEU:O	2:F:393:TYR:O	2.39	0.41
2:F:394:LEU:CD1	2:F:396:SER:HB3	2.51	0.41
3:K:111:LYS:O	3:K:112:GLU:HB3	2.20	0.41
3:K:151:ASN:C	3:K:153:GLU:H	2.24	0.41
1:G:16:GLN:HB2	2:H:292:VAL:HG12	2.03	0.41
1:G:34:CYS:HB3	1:G:126:VAL:HG22	2.02	0.41
1:G:311:LEU:HD12	1:G:311:LEU:HA	1.87	0.41
1:G:435:PHE:CZ	1:G:439:GLN:HG3	2.56	0.41
1:G:481:GLU:O	1:G:484:ARG:N	2.54	0.41
1:A:232:ARG:C	1:A:233:ILE:HG13	2.42	0.41
1:C:462:THR:O	1:C:463:GLY:C	2.59	0.41
2:D:124:PHE:HD1	2:D:124:PHE:C	2.25	0.41
2:D:127:ILE:CG1	2:D:128:GLN:NE2	2.84	0.41
2:D:392:LEU:O	2:D:393:TYR:O	2.39	0.41
1:E:15:ARG:HA	1:E:15:ARG:HD3	1.81	0.41
1:E:232:ARG:C	1:E:233:ILE:HG13	2.41	0.41
1:E:369:GLY:O	1:E:370:GLN:C	2.59	0.41
1:E:512:GLN:C	1:E:513:PHE:CD1	2.95	0.41
2:F:164:TYR:HD2	2:F:169:LEU:HA	1.86	0.41
2:F:396:SER:O	2:F:600:VAL:N	2.54	0.41
1:G:172:ILE:HA	1:G:390:LEU:HD23	2.02	0.41
2:H:293:ALA:O	2:H:294:SER:C	2.59	0.41
3:L:111:LYS:O	3:L:112:GLU:HB3	2.21	0.41
1:A:36:ILE:HD13	1:A:36:ILE:HA	1.91	0.40
1:A:139:LEU:C	1:A:141:ASP:H	2.24	0.40
1:A:331:ASP:HB2	2:B:224:LEU:HD11	2.02	0.40
2:B:218:ILE:O	2:B:218:ILE:HG22	2.21	0.40
2:B:237:TRP:O	2:B:242:PRO:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:ARG:NH1	2:B:267:ARG:CG	2.77	0.40
2:B:335:PHE:CZ	3:I:144:ILE:CD1	3.04	0.40
1:C:111:ASN:OD1	1:C:111:ASN:O	2.39	0.40
1:C:143:LEU:HD13	1:C:150:LEU:HD13	1.99	0.40
1:C:457:LEU:HD23	1:C:479:VAL:HG12	2.02	0.40
2:D:102:PRO:HB3	2:D:124:PHE:CD2	2.56	0.40
2:D:134:PHE:O	2:D:137:GLN:HG3	2.21	0.40
2:D:249:LEU:CD1	2:D:260:ILE:HD11	2.51	0.40
1:E:117:PRO:O	1:E:119:PHE:N	2.54	0.40
1:E:221:TYR:O	1:E:243:PHE:HE1	2.04	0.40
1:G:53:GLY:O	1:G:54:ILE:C	2.59	0.40
1:G:113:LEU:HD23	1:G:113:LEU:HA	1.87	0.40
1:G:317:LYS:HG2	1:G:318:GLU:N	2.37	0.40
2:H:207:TYR:HA	2:H:208:PRO:HD3	1.90	0.40
2:H:392:LEU:O	2:H:393:TYR:O	2.39	0.40
1:A:148:ILE:HA	1:A:149:PRO:HD3	1.95	0.40
1:A:493:ILE:HD13	1:A:493:ILE:HA	1.91	0.40
2:B:164:TYR:HD2	2:B:169:LEU:HA	1.85	0.40
1:C:143:LEU:HD22	1:C:148:ILE:CG2	2.50	0.40
1:C:261:ASP:O	1:C:262:GLU:CG	2.69	0.40
2:D:703:GLY:C	2:D:705:VAL:H	2.23	0.40
3:J:155:THR:O	3:J:158:ASP:N	2.54	0.40
1:E:239:GLU:O	1:E:240:LYS:C	2.59	0.40
2:F:84:ASP:H	2:F:87:ASN:HD22	1.67	0.40
2:F:362:GLN:H	2:F:362:GLN:HG3	1.48	0.40
1:G:232:ARG:C	1:G:233:ILE:HG13	2.42	0.40
1:G:239:GLU:O	1:G:240:LYS:C	2.59	0.40
1:G:517:ASN:OD1	1:G:534:LEU:HB2	2.22	0.40
2:H:134:PHE:O	2:H:137:GLN:HG3	2.20	0.40
2:H:187:GLY:HA2	3:L:173:LEU:CD1	2.51	0.40
2:H:316:ILE:HA	2:H:317:PRO:HD3	1.95	0.40
1:A:45:ILE:CG1	1:A:498:GLY:HA2	2.49	0.40
1:A:215:ILE:HD12	1:A:342:LEU:HD21	2.03	0.40
2:B:83:ILE:HD13	2:B:94:PHE:CG	2.57	0.40
2:B:141:ILE:HD12	2:B:158:LEU:HD11	2.03	0.40
2:B:362:GLN:H	2:B:362:GLN:HG3	1.50	0.40
3:I:150:MET:HE3	3:I:167:LEU:HD22	2.03	0.40
2:D:247:VAL:HA	2:D:248:PRO:HD3	1.80	0.40
3:J:118:GLU:O	3:J:121:ASP:OD1	2.39	0.40
1:E:113:LEU:HD23	1:E:113:LEU:HA	1.90	0.40
1:E:507:LYS:HG2	1:E:513:PHE:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:517:ASN:OD1	1:E:534:LEU:HB2	2.21	0.40
1:G:481:GLU:O	1:G:484:ARG:HB3	2.21	0.40
2:H:95:ARG:HD3	2:H:95:ARG:HA	1.67	0.40
2:H:130:PHE:CG	2:H:134:PHE:CD2	3.08	0.40
2:H:140:ILE:HG22	2:H:141:ILE:N	2.36	0.40
3:L:107:THR:OG1	3:L:108:LEU:N	2.54	0.40
1:A:84:ASN:HD22	1:A:85:ARG:N	2.19	0.40
1:A:225:TRP:O	1:A:225:TRP:CD1	2.75	0.40
1:A:457:LEU:HD23	1:A:479:VAL:CG1	2.52	0.40
2:B:52:LEU:HD11	2:B:78:ILE:HG13	2.02	0.40
1:C:105:VAL:HG12	1:C:107:GLU:H	1.86	0.40
2:D:33:PRO:O	2:D:35:PHE:N	2.53	0.40
2:D:213:PHE:HA	2:D:214:PRO:HD3	1.98	0.40
2:D:357:PRO:O	2:D:357:PRO:CG	2.69	0.40
1:E:359:ASN:HD22	1:E:359:ASN:HA	1.69	0.40
2:F:229:ILE:HG21	2:F:284:VAL:HB	2.04	0.40
1:G:416:MET:SD	1:G:423:ILE:HG23	2.61	0.40
2:H:339:ARG:NH2	2:H:346:CYS:O	2.54	0.40
1:A:72:ASN:HD22	1:A:73:ASN:N	2.19	0.40
1:A:128:ALA:HB1	1:A:131:LEU:CD1	2.52	0.40
1:A:144:TRP:CZ3	1:A:397:SER:HA	2.56	0.40
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.87	0.40
1:A:252:LEU:O	1:A:259:PRO:N	2.54	0.40
1:C:45:ILE:CG1	1:C:498:GLY:HA2	2.48	0.40
1:C:180:LEU:HD23	3:J:135:GLY:CA	2.52	0.40
1:E:340:ILE:O	1:E:341:LYS:C	2.60	0.40
2:F:141:ILE:HD12	2:F:158:LEU:HD21	2.04	0.40
2:F:242:PRO:HG3	2:F:259:TRP:CH2	2.56	0.40
1:G:16:GLN:NE2	1:G:20:TRP:CZ2	2.86	0.40
1:G:171:VAL:HG13	1:G:391:ARG:O	2.21	0.40
1:G:264:ASN:H	1:G:264:ASN:ND2	2.14	0.40
2:H:136:ARG:HG2	2:H:136:ARG:NH1	2.37	0.40
2:H:316:ILE:H	2:H:316:ILE:CD1	2.12	0.40
3:L:118:GLU:O	3:L:121:ASP:OD1	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/529 (97%)	418 (82%)	66 (13%)	28 (6%)	2	19
1	C	512/529 (97%)	418 (82%)	67 (13%)	27 (5%)	2	19
1	E	512/529 (97%)	416 (81%)	70 (14%)	26 (5%)	2	20
1	G	512/529 (97%)	412 (80%)	72 (14%)	28 (6%)	2	19
2	B	408/431 (95%)	310 (76%)	73 (18%)	25 (6%)	1	17
2	D	410/431 (95%)	307 (75%)	76 (18%)	27 (7%)	1	16
2	F	408/431 (95%)	309 (76%)	75 (18%)	24 (6%)	1	18
2	H	408/431 (95%)	308 (76%)	77 (19%)	23 (6%)	2	19
3	I	74/76 (97%)	65 (88%)	7 (10%)	2 (3%)	5	35
3	J	74/76 (97%)	65 (88%)	6 (8%)	3 (4%)	3	26
3	K	74/76 (97%)	66 (89%)	6 (8%)	2 (3%)	5	35
3	L	74/76 (97%)	66 (89%)	6 (8%)	2 (3%)	5	35
All	All	3978/4144 (96%)	3160 (79%)	601 (15%)	217 (6%)	2	19

All (217) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	ILE
1	A	259	PRO
1	A	262	GLU
1	A	275	ALA
1	A	533	GLN
2	B	116	PRO
2	B	356	SER
2	B	357	PRO
2	B	393	TYR
2	B	901	VAL
1	C	36	ILE
1	C	233	ILE

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Mol	Chain	Res	Type
1	C	259	PRO
1	C	262	GLU
1	C	275	ALA
1	C	533	GLN
2	D	116	PRO
2	D	356	SER
2	D	357	PRO
2	D	393	TYR
2	D	607	THR
2	D	608	ARG
2	D	700	LYS
2	D	901	VAL
1	E	233	ILE
1	E	259	PRO
1	E	262	GLU
1	E	275	ALA
1	E	533	GLN
2	F	116	PRO
2	F	356	SER
2	F	357	PRO
2	F	393	TYR
2	F	901	VAL
2	F	902	ALA
1	G	233	ILE
1	G	259	PRO
1	G	262	GLU
1	G	275	ALA
1	G	533	GLN
2	H	116	PRO
2	H	356	SER
2	H	357	PRO
2	H	393	TYR
2	H	901	VAL
2	H	902	ALA
1	A	21	GLY
1	A	36	ILE
1	A	237	TYR
1	A	317	LYS
1	A	367	SER
1	A	408	ASN
1	A	416	MET
1	A	422	GLU

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Mol	Chain	Res	Type
2	B	34	ASP
2	B	127	ILE
2	B	132	ASP
2	B	183	GLU
2	B	294	SER
2	B	320	ASN
2	B	352	ASN
2	B	358	SER
2	B	372	ALA
2	B	902	ALA
3	I	152	ASP
1	C	21	GLY
1	C	237	TYR
1	C	317	LYS
1	C	367	SER
1	C	408	ASN
1	C	416	MET
1	C	422	GLU
2	D	34	ASP
2	D	127	ILE
2	D	132	ASP
2	D	183	GLU
2	D	294	SER
2	D	320	ASN
2	D	352	ASN
2	D	358	SER
2	D	372	ALA
3	J	152	ASP
1	E	21	GLY
1	E	36	ILE
1	E	237	TYR
1	E	276	LEU
1	E	367	SER
1	E	408	ASN
1	E	416	MET
1	E	422	GLU
2	F	34	ASP
2	F	127	ILE
2	F	132	ASP
2	F	183	GLU
2	F	294	SER
2	F	320	ASN

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Mol	Chain	Res	Type
2	F	352	ASN
2	F	358	SER
2	F	372	ALA
3	K	152	ASP
1	G	21	GLY
1	G	36	ILE
1	G	237	TYR
1	G	276	LEU
1	G	367	SER
1	G	408	ASN
1	G	416	MET
1	G	422	GLU
2	H	34	ASP
2	H	127	ILE
2	H	183	GLU
2	H	294	SER
2	H	320	ASN
2	H	352	ASN
2	H	358	SER
2	H	372	ALA
3	L	152	ASP
1	A	118	SER
1	A	228	GLU
1	A	249	GLN
1	A	276	LEU
1	A	318	GLU
2	B	86	SER
2	B	360	LYS
2	B	607	THR
1	C	118	SER
1	C	190	PRO
1	C	228	GLU
1	C	249	GLN
1	C	276	LEU
1	C	318	GLU
2	D	86	SER
2	D	360	LYS
2	D	375	GLN
1	E	118	SER
1	E	190	PRO
1	E	228	GLU
1	E	249	GLN

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Mol	Chain	Res	Type
1	E	317	LYS
1	E	318	GLU
2	F	86	SER
2	F	360	LYS
2	F	801	GLN
1	G	118	SER
1	G	190	PRO
1	G	228	GLU
1	G	249	GLN
1	G	317	LYS
1	G	318	GLU
2	H	86	SER
2	H	132	ASP
2	H	360	LYS
2	H	801	GLN
1	A	106	GLU
1	A	190	PRO
1	A	230	ASN
1	A	450	VAL
2	B	90	ARG
2	B	241	GLN
2	B	801	GLN
2	B	907	PRO
3	I	119	PRO
1	C	106	GLU
1	C	450	VAL
2	D	801	GLN
2	D	907	PRO
3	J	119	PRO
1	E	106	GLU
1	E	450	VAL
2	F	375	GLN
2	F	907	PRO
3	K	119	PRO
2	H	375	GLN
2	H	907	PRO
3	L	119	PRO
1	A	280	GLN
1	C	230	ASN
1	C	280	GLN
1	C	519	THR
2	D	88	LEU

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Mol	Chain	Res	Type
2	D	90	ARG
2	D	241	GLN
1	E	230	ASN
1	E	280	GLN
2	F	90	ARG
2	F	241	GLN
1	G	106	GLU
1	G	280	GLN
1	G	519	THR
2	H	90	ARG
2	H	241	GLN
1	A	443	PRO
1	A	519	THR
2	B	196	MET
2	B	375	GLN
2	D	194	PRO
2	D	196	MET
3	J	146	SER
1	E	419	PRO
2	F	194	PRO
2	F	196	MET
1	G	230	ASN
1	G	419	PRO
1	G	450	VAL
1	A	419	PRO
2	B	194	PRO
1	C	419	PRO
1	C	443	PRO
1	G	54	ILE
2	H	194	PRO
1	A	54	ILE
1	A	333	ILE
1	E	54	ILE
1	E	443	PRO
1	G	443	PRO
1	C	372	PRO
1	G	333	ILE

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	450/461 (98%)	428 (95%)	22 (5%)	25	59
1	C	450/461 (98%)	428 (95%)	22 (5%)	25	59
1	E	450/461 (98%)	428 (95%)	22 (5%)	25	59
1	G	450/461 (98%)	427 (95%)	23 (5%)	24	58
2	B	334/379 (88%)	301 (90%)	33 (10%)	8	35
2	D	334/379 (88%)	302 (90%)	32 (10%)	8	37
2	F	334/379 (88%)	302 (90%)	32 (10%)	8	37
2	H	334/379 (88%)	304 (91%)	30 (9%)	9	39
3	I	66/66 (100%)	64 (97%)	2 (3%)	41	71
3	J	66/66 (100%)	63 (96%)	3 (4%)	27	62
3	K	66/66 (100%)	63 (96%)	3 (4%)	27	62
3	L	66/66 (100%)	63 (96%)	3 (4%)	27	62
All	All	3400/3624 (94%)	3173 (93%)	227 (7%)	16	50

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	43	THR
1	A	56	SER
1	A	72	ASN
1	A	84	ASN
1	A	171	VAL
1	A	214	TRP
1	A	234	PRO
1	A	237	TYR
1	A	259	PRO
1	A	261	ASP
1	A	262	GLU
1	A	264	ASN
1	A	293	ARG
1	A	311	LEU
1	A	332	MET
1	A	353	ASP
1	A	406	THR

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Mol	Chain	Res	Type
1	A	407	ILE
1	A	410	ASP
1	A	418	ASN
1	A	525	MET
2	B	49	CYS
2	B	110	PHE
2	B	111	LEU
2	B	114	ARG
2	B	116	PRO
2	B	124	PHE
2	B	128	GLN
2	B	132	ASP
2	B	142	VAL
2	B	154	ILE
2	B	174	ILE
2	B	182	THR
2	B	212	ASN
2	B	265	LEU
2	B	267	ARG
2	B	294	SER
2	B	306	GLU
2	B	316	ILE
2	B	318	LEU
2	B	319	ASN
2	B	321	TYR
2	B	322	LEU
2	B	325	ASN
2	B	326	ASP
2	B	327	VAL
2	B	342	ASN
2	B	348	GLN
2	B	357	PRO
2	B	362	GLN
2	B	363	GLU
2	B	364	VAL
2	B	392	LEU
2	B	393	TYR
3	I	121	ASP
3	I	170	VAL
1	C	22	ASP
1	C	43	THR
1	C	56	SER

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Mol	Chain	Res	Type
1	C	72	ASN
1	C	84	ASN
1	C	171	VAL
1	C	214	TRP
1	C	234	PRO
1	C	237	TYR
1	C	259	PRO
1	C	261	ASP
1	C	262	GLU
1	C	264	ASN
1	C	293	ARG
1	C	311	LEU
1	C	332	MET
1	C	353	ASP
1	C	406	THR
1	C	407	ILE
1	C	410	ASP
1	C	418	ASN
1	C	525	MET
2	D	49	CYS
2	D	110	PHE
2	D	111	LEU
2	D	114	ARG
2	D	116	PRO
2	D	124	PHE
2	D	128	GLN
2	D	132	ASP
2	D	142	VAL
2	D	154	ILE
2	D	174	ILE
2	D	182	THR
2	D	212	ASN
2	D	265	LEU
2	D	267	ARG
2	D	294	SER
2	D	306	GLU
2	D	316	ILE
2	D	318	LEU
2	D	319	ASN
2	D	321	TYR
2	D	322	LEU
2	D	325	ASN

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Mol	Chain	Res	Type
2	D	326	ASP
2	D	327	VAL
2	D	342	ASN
2	D	348	GLN
2	D	357	PRO
2	D	362	GLN
2	D	363	GLU
2	D	364	VAL
2	D	393	TYR
3	J	121	ASP
3	J	150	MET
3	J	170	VAL
1	E	22	ASP
1	E	43	THR
1	E	56	SER
1	E	72	ASN
1	E	84	ASN
1	E	171	VAL
1	E	214	TRP
1	E	234	PRO
1	E	237	TYR
1	E	259	PRO
1	E	261	ASP
1	E	262	GLU
1	E	264	ASN
1	E	293	ARG
1	E	311	LEU
1	E	332	MET
1	E	353	ASP
1	E	406	THR
1	E	407	ILE
1	E	410	ASP
1	E	418	ASN
1	E	525	MET
2	F	49	CYS
2	F	110	PHE
2	F	111	LEU
2	F	114	ARG
2	F	116	PRO
2	F	124	PHE
2	F	128	GLN
2	F	132	ASP

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Mol	Chain	Res	Type
2	F	142	VAL
2	F	154	ILE
2	F	174	ILE
2	F	182	THR
2	F	212	ASN
2	F	265	LEU
2	F	267	ARG
2	F	294	SER
2	F	306	GLU
2	F	316	ILE
2	F	318	LEU
2	F	319	ASN
2	F	321	TYR
2	F	322	LEU
2	F	325	ASN
2	F	326	ASP
2	F	327	VAL
2	F	342	ASN
2	F	348	GLN
2	F	357	PRO
2	F	362	GLN
2	F	363	GLU
2	F	364	VAL
2	F	393	TYR
3	K	121	ASP
3	K	150	MET
3	K	170	VAL
1	G	22	ASP
1	G	43	THR
1	G	56	SER
1	G	72	ASN
1	G	84	ASN
1	G	171	VAL
1	G	214	TRP
1	G	234	PRO
1	G	237	TYR
1	G	259	PRO
1	G	261	ASP
1	G	262	GLU
1	G	264	ASN
1	G	293	ARG
1	G	311	LEU

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Mol	Chain	Res	Type
1	G	318	GLU
1	G	332	MET
1	G	353	ASP
1	G	406	THR
1	G	407	ILE
1	G	410	ASP
1	G	418	ASN
1	G	525	MET
2	H	110	PHE
2	H	111	LEU
2	H	114	ARG
2	H	116	PRO
2	H	124	PHE
2	H	128	GLN
2	H	132	ASP
2	H	142	VAL
2	H	154	ILE
2	H	174	ILE
2	H	182	THR
2	H	212	ASN
2	H	265	LEU
2	H	267	ARG
2	H	294	SER
2	H	306	GLU
2	H	316	ILE
2	H	318	LEU
2	H	319	ASN
2	H	321	TYR
2	H	322	LEU
2	H	325	ASN
2	H	326	ASP
2	H	327	VAL
2	H	342	ASN
2	H	348	GLN
2	H	357	PRO
2	H	363	GLU
2	H	364	VAL
2	H	393	TYR
3	L	121	ASP
3	L	150	MET
3	L	170	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	72	ASN
1	A	77	GLN
1	A	197	GLN
1	A	264	ASN
1	A	271	ASN
1	A	277	ASN
1	A	320	GLN
1	A	344	ASN
1	A	359	ASN
1	A	418	ASN
1	A	439	GLN
1	A	447	ASN
1	A	533	GLN
2	B	19	HIS
2	B	74	GLN
2	B	87	ASN
2	B	125	ASN
2	B	128	GLN
2	B	139	HIS
2	B	212	ASN
2	B	236	GLN
2	B	262	GLN
2	B	325	ASN
2	B	342	ASN
2	B	348	GLN
2	B	351	GLN
3	I	141	GLN
1	C	37	ASN
1	C	72	ASN
1	C	77	GLN
1	C	197	GLN
1	C	264	ASN
1	C	271	ASN
1	C	277	ASN
1	C	320	GLN
1	C	359	ASN
1	C	418	ASN
1	C	439	GLN
1	C	447	ASN
1	C	533	GLN
2	D	19	HIS

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Mol	Chain	Res	Type
2	D	74	GLN
2	D	87	ASN
2	D	125	ASN
2	D	128	GLN
2	D	139	HIS
2	D	212	ASN
2	D	236	GLN
2	D	325	ASN
2	D	342	ASN
2	D	348	GLN
2	D	351	GLN
3	J	141	GLN
1	E	37	ASN
1	E	72	ASN
1	E	77	GLN
1	E	115	ASN
1	E	178	ASN
1	E	197	GLN
1	E	264	ASN
1	E	271	ASN
1	E	277	ASN
1	E	320	GLN
1	E	359	ASN
1	E	418	ASN
1	E	439	GLN
1	E	447	ASN
1	E	533	GLN
2	F	19	HIS
2	F	74	GLN
2	F	87	ASN
2	F	125	ASN
2	F	128	GLN
2	F	139	HIS
2	F	212	ASN
2	F	236	GLN
2	F	325	ASN
2	F	342	ASN
2	F	348	GLN
2	F	351	GLN
3	K	141	GLN
1	G	37	ASN
1	G	72	ASN

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Mol	Chain	Res	Type
1	G	77	GLN
1	G	197	GLN
1	G	264	ASN
1	G	271	ASN
1	G	277	ASN
1	G	320	GLN
1	G	359	ASN
1	G	418	ASN
1	G	439	GLN
1	G	447	ASN
1	G	533	GLN
2	H	19	HIS
2	H	74	GLN
2	H	87	ASN
2	H	125	ASN
2	H	128	GLN
2	H	139	HIS
2	H	212	ASN
2	H	236	GLN
2	H	325	ASN
2	H	342	ASN
2	H	348	GLN
2	H	351	GLN
3	L	141	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
4	ATP	H	8	-	26,33,33	1.42	4 (15%)	31,52,52	1.93	8 (25%)
4	ATP	B	5	-	26,33,33	1.60	5 (19%)	31,52,52	1.92	10 (32%)
4	ATP	F	7	-	26,33,33	1.46	5 (19%)	31,52,52	1.94	7 (22%)
4	ATP	D	6	-	26,33,33	1.31	4 (15%)	31,52,52	1.88	9 (29%)

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
4	ATP	H	8	-	-	10/18/38/38	0/3/3/3
4	ATP	B	5	-	-	9/18/38/38	0/3/3/3
4	ATP	F	7	-	-	7/18/38/38	0/3/3/3
4	ATP	D	6	-	-	9/18/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5	ATP	C2-N3	5.00	1.40	1.32
4	F	7	ATP	C2-N3	3.98	1.38	1.32
4	D	6	ATP	C2-N3	3.80	1.38	1.32
4	H	8	ATP	C2-N3	3.42	1.37	1.32
4	H	8	ATP	O4'-C1'	3.33	1.45	1.41
4	B	5	ATP	O4'-C1'	2.93	1.45	1.41
4	D	6	ATP	C2'-C1'	-2.72	1.49	1.53
4	F	7	ATP	C2'-C1'	-2.71	1.49	1.53
4	F	7	ATP	O2'-C2'	-2.61	1.36	1.43
4	H	8	ATP	C2'-C1'	-2.47	1.50	1.53
4	H	8	ATP	O2'-C2'	-2.45	1.37	1.43
4	B	5	ATP	C2'-C1'	-2.44	1.50	1.53
4	B	5	ATP	C2-N1	2.30	1.38	1.33
4	D	6	ATP	O4'-C1'	2.30	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	6	ATP	O2'-C2'	-2.29	1.37	1.43
4	F	7	ATP	O4'-C1'	2.23	1.44	1.41
4	B	5	ATP	O2'-C2'	-2.11	1.38	1.43
4	F	7	ATP	C8-N7	-2.02	1.31	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	7	ATP	N3-C2-N1	-5.89	119.48	128.68
4	B	5	ATP	N3-C2-N1	-5.40	120.23	128.68
4	H	8	ATP	N3-C2-N1	-5.38	120.26	128.68
4	D	6	ATP	N3-C2-N1	-5.08	120.74	128.68
4	H	8	ATP	C5-C6-N6	4.51	127.20	120.35
4	F	7	ATP	PB-O3B-PG	-4.41	117.71	132.83
4	D	6	ATP	C5-C6-N6	4.00	126.43	120.35
4	F	7	ATP	C5-C6-N6	3.91	126.30	120.35
4	B	5	ATP	PB-O3B-PG	-3.89	119.49	132.83
4	F	7	ATP	C4-C5-N7	-3.61	105.64	109.40
4	D	6	ATP	PB-O3B-PG	-3.60	120.49	132.83
4	D	6	ATP	C4-C5-N7	-3.46	105.79	109.40
4	B	5	ATP	C4-C5-N7	-3.41	105.84	109.40
4	B	5	ATP	O2B-PB-O1B	3.36	128.84	112.24
4	H	8	ATP	O2B-PB-O1B	3.22	128.17	112.24
4	H	8	ATP	PB-O3B-PG	-3.13	122.10	132.83
4	D	6	ATP	O2B-PB-O1B	3.06	127.36	112.24
4	H	8	ATP	C4-C5-N7	-3.02	106.25	109.40
4	B	5	ATP	C5-C6-N6	2.96	124.85	120.35
4	H	8	ATP	O4'-C1'-C2'	-2.73	102.94	106.93
4	B	5	ATP	O2'-C2'-C3'	2.68	120.49	111.82
4	F	7	ATP	O2B-PB-O1B	2.65	125.35	112.24
4	H	8	ATP	N6-C6-N1	-2.56	113.27	118.57
4	B	5	ATP	O4'-C1'-C2'	-2.54	103.21	106.93
4	D	6	ATP	O4'-C1'-C2'	-2.53	103.23	106.93
4	D	6	ATP	O2G-PG-O3B	2.34	112.49	104.64
4	H	8	ATP	O2G-PG-O3B	2.32	112.42	104.64
4	F	7	ATP	N6-C6-N1	-2.26	113.88	118.57
4	B	5	ATP	O3'-C3'-C4'	-2.24	104.57	111.05
4	B	5	ATP	C1'-N9-C4	2.21	130.52	126.64
4	D	6	ATP	O2'-C2'-C3'	2.19	118.92	111.82
4	D	6	ATP	N6-C6-N1	-2.02	114.38	118.57
4	B	5	ATP	O2G-PG-O3B	2.02	111.41	104.64
4	F	7	ATP	O2G-PG-O3B	2.01	111.37	104.64

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	5	ATP	C5'-O5'-PA-O3A
4	B	5	ATP	O4'-C4'-C5'-O5'
4	D	6	ATP	C5'-O5'-PA-O1A
4	D	6	ATP	C5'-O5'-PA-O2A
4	D	6	ATP	C5'-O5'-PA-O3A
4	F	7	ATP	C5'-O5'-PA-O3A
4	H	8	ATP	PB-O3B-PG-O2G
4	H	8	ATP	C5'-O5'-PA-O3A
4	D	6	ATP	O4'-C4'-C5'-O5'
4	F	7	ATP	O4'-C4'-C5'-O5'
4	B	5	ATP	C3'-C4'-C5'-O5'
4	F	7	ATP	C3'-C4'-C5'-O5'
4	H	8	ATP	O4'-C4'-C5'-O5'
4	B	5	ATP	PA-O3A-PB-O2B
4	D	6	ATP	PA-O3A-PB-O2B
4	F	7	ATP	PA-O3A-PB-O2B
4	H	8	ATP	PA-O3A-PB-O2B
4	H	8	ATP	PB-O3A-PA-O1A
4	B	5	ATP	C5'-O5'-PA-O1A
4	B	5	ATP	C5'-O5'-PA-O2A
4	F	7	ATP	C5'-O5'-PA-O2A
4	H	8	ATP	C5'-O5'-PA-O1A
4	H	8	ATP	C5'-O5'-PA-O2A
4	D	6	ATP	C3'-C4'-C5'-O5'
4	B	5	ATP	C4'-C5'-O5'-PA
4	H	8	ATP	C3'-C4'-C5'-O5'
4	D	6	ATP	PB-O3A-PA-O1A
4	H	8	ATP	PB-O3B-PG-O3G
4	B	5	ATP	PA-O3A-PB-O1B
4	B	5	ATP	PB-O3A-PA-O1A
4	D	6	ATP	PG-O3B-PB-O2B
4	D	6	ATP	PA-O3A-PB-O1B
4	F	7	ATP	PA-O3A-PB-O1B
4	H	8	ATP	PA-O3A-PB-O1B
4	F	7	ATP	C5'-O5'-PA-O1A

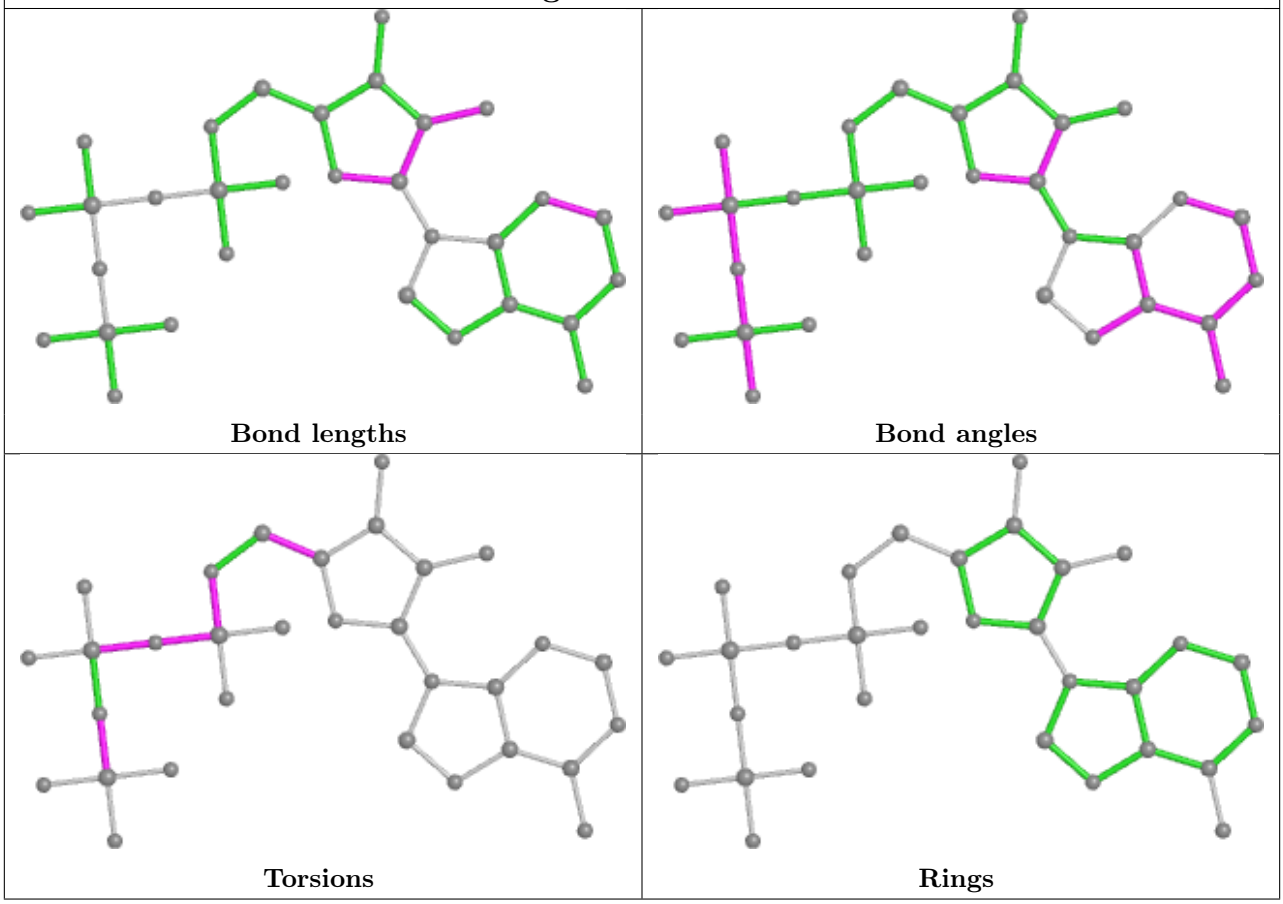
There are no ring outliers.

4 monomers are involved in 23 short contacts:

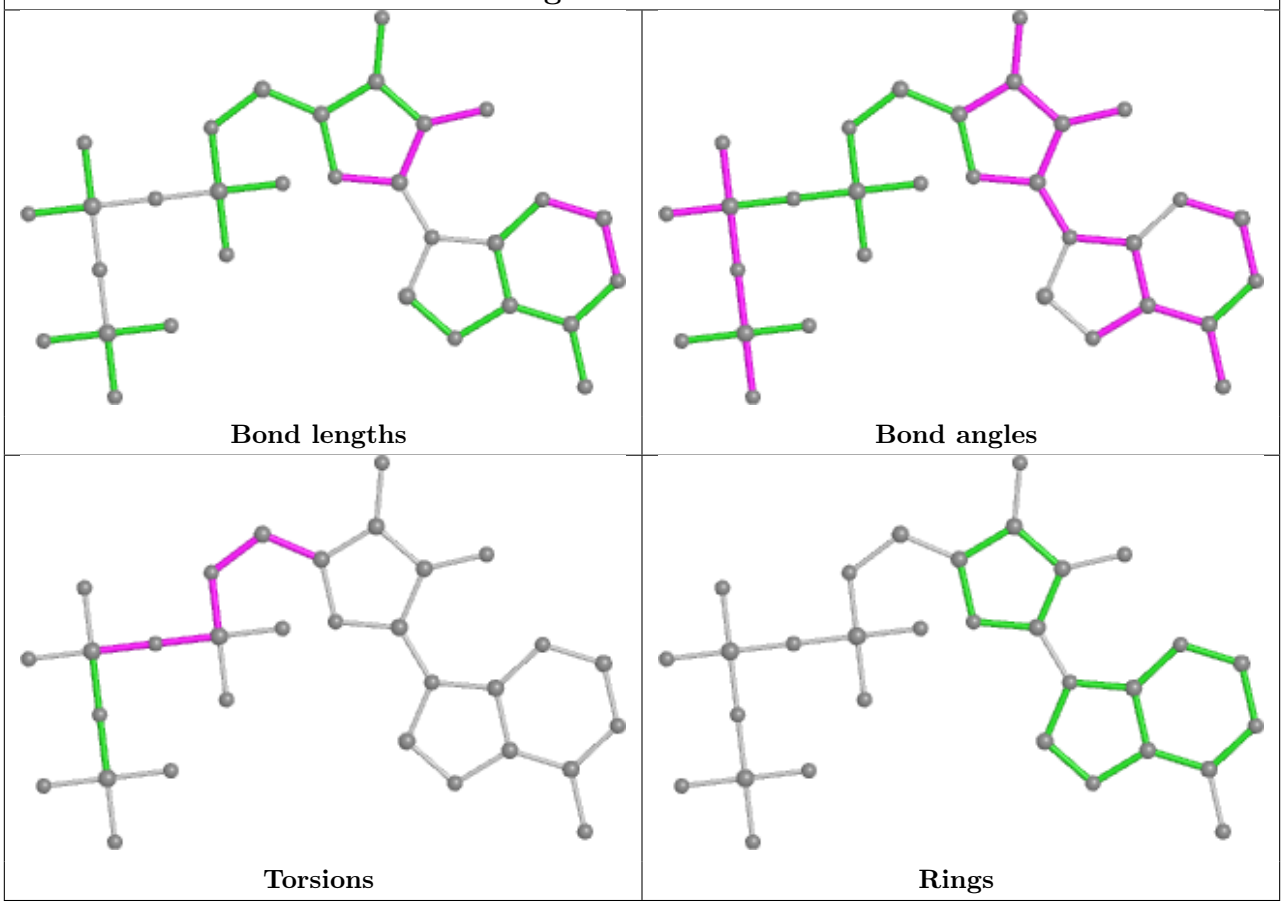
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	8	ATP	10	0
4	B	5	ATP	3	0
4	F	7	ATP	6	0
4	D	6	ATP	4	0

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.

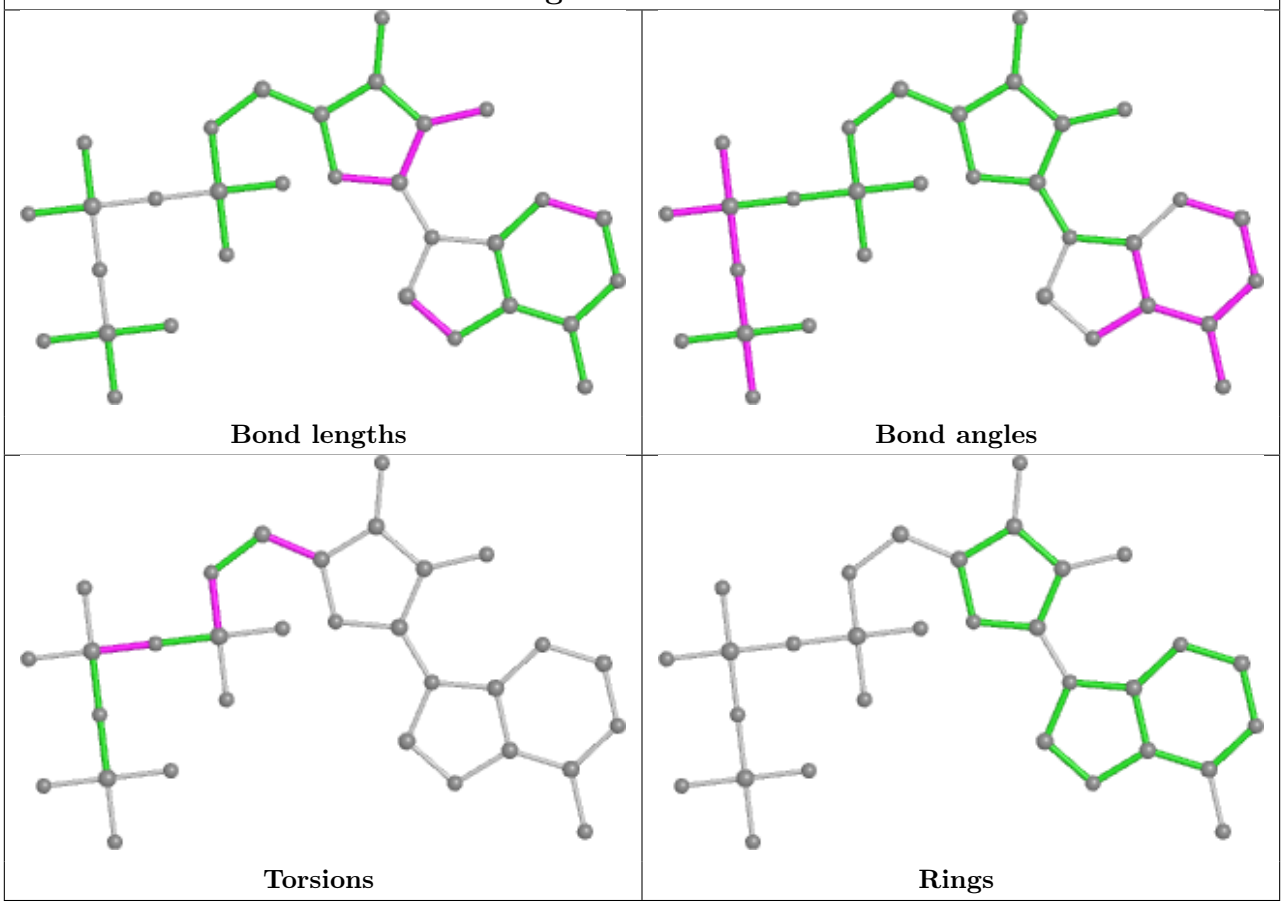
Ligand ATP H 8



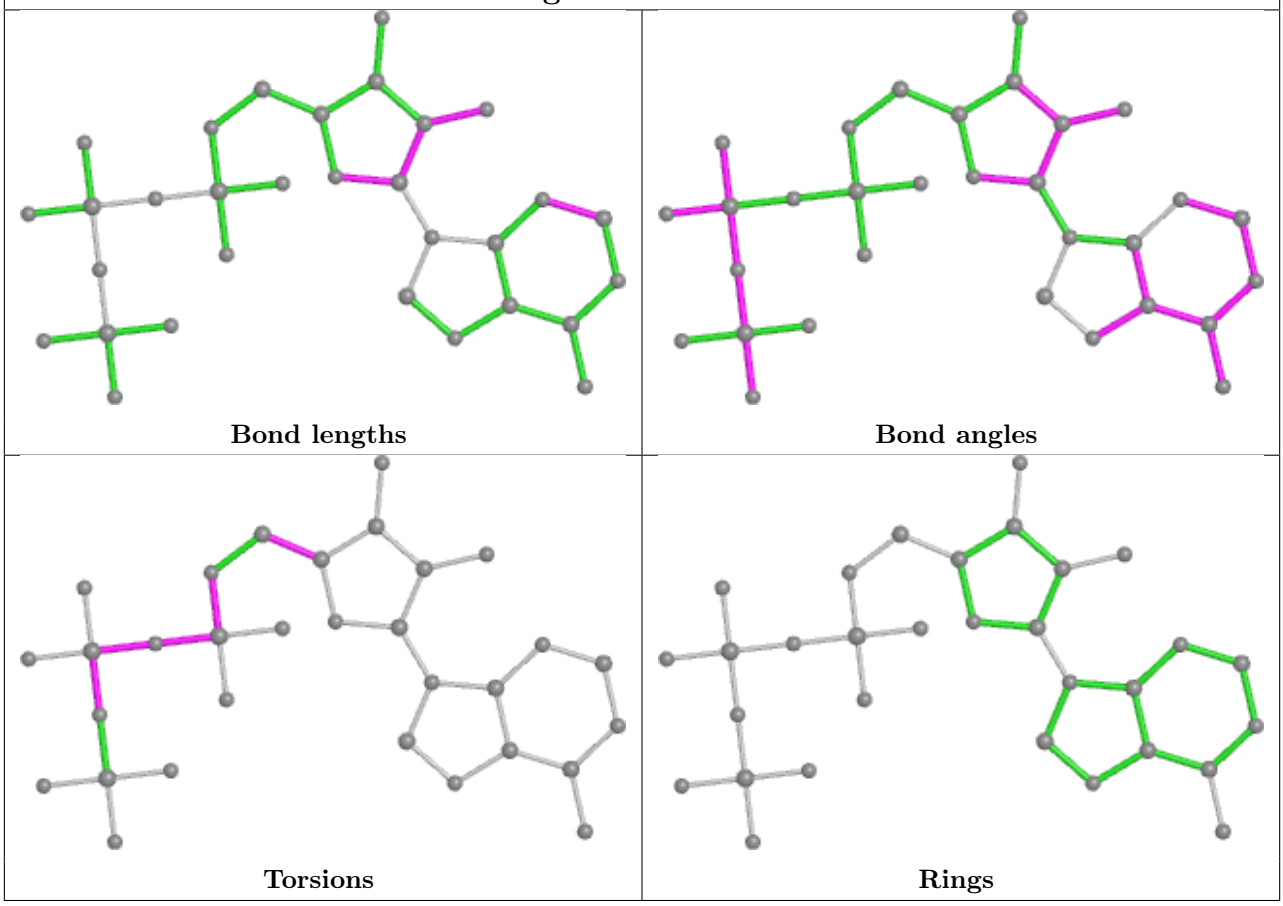
Ligand ATP B 5



Ligand ATP F 7



Ligand ATP D 6



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	2
2	B	1
2	H	1
2	F	1
1	C	1
1	A	1
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	396:SER	C	600:VAL	N	2.96
1	D	396:SER	C	600:VAL	N	2.96
1	H	396:SER	C	600:VAL	N	2.96
1	F	396:SER	C	600:VAL	N	2.95
1	D	700:LYS	C	701:GLU	N	1.61
1	C	252:LEU	C	253:LYS	N	1.19
1	A	252:LEU	C	253:LYS	N	1.18
1	G	252:LEU	C	253:LYS	N	1.18

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.