Full wwPDB EM Validation Report (i)

Aug 17, 2026 – 05:08 PM JST

PDB ID	:	9WIF / pdb_00009wif
EMDB ID	:	EMD-65992
Title	:	AMP-PNP bound E.coli CnoX-GroEL/ES complex, state III
Authors	:	Kim, J.; Roh, S.H.
Deposited on	:	2025-08-27
Resolution	:	2.83 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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 (i)) were used in the production of this report:

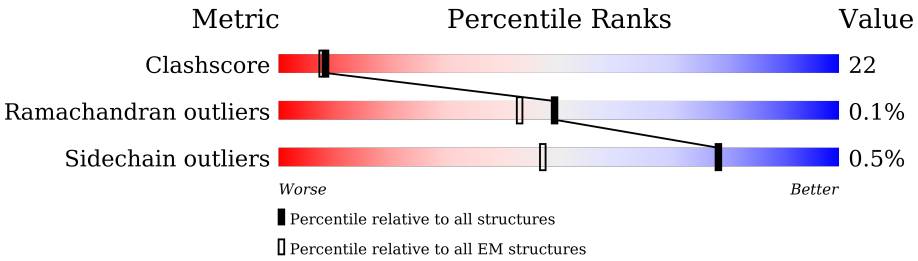
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

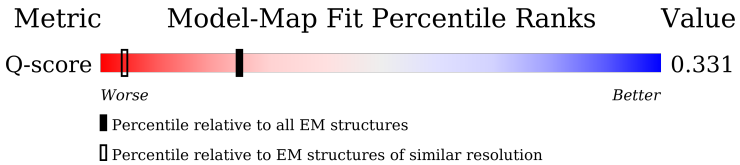
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11847 (2.33 - 3.33)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	97	5% 39% 59% ·
1	1	97	· 42% 55% ·
1	2	97	· 39% 57% ·
1	3	97	6% 35% 61% ·

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Mol	Chain	Length	Quality of chain
1	4	97	7% 36% 61%
1	5	97	5% 36% 61%
1	6	97	6% 39% 59%
2	A	548	73% 23%
2	C	548	74% 22%
2	E	548	74% 23%
2	G	548	73% 23%
2	I	548	72% 24%
2	K	548	74% 22%
2	M	548	74% 22%
2	a	548	68% 28%
2	c	548	69% 27%
2	e	548	70% 27%
2	g	548	70% 26%
2	i	548	70% 27%
2	k	548	71% 26%
2	m	548	68% 28%
3	B	284	15% 15% 69%
3	D	284	17% 13% 69%
3	F	284	15% 15% 69%
3	H	284	15% 15% 69%
3	J	284	14% 16% 69%
3	L	284	17% 14% 69%
3	N	284	17% 14% 69%
3	b	284	13% 18% 69%

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Mol	Chain	Length	Quality of chain
3	d	284	16% 15% 69%
3	f	284	14% 16% • 69%
3	h	284	13% 17% • 69%
3	j	284	13% 18% 69%
3	l	284	15% 15% • 69%
3	n	284	13% 17% • 69%

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
5	ANP	k	603	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 69580 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Co-chaperonin GroES.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	97	728	454	127	145	2	0	0
1	1	97	728	454	127	145	2	0	0
1	2	97	728	454	127	145	2	0	0
1	3	97	728	454	127	145	2	0	0
1	4	97	728	454	127	145	2	0	0
1	5	97	728	454	127	145	2	0	0
1	6	97	728	454	127	145	2	0	0

- Molecule 2 is a protein called Chaperonin GroEL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	527	3880	2412	670	777	21	0	0
2	C	527	3880	2412	670	777	21	0	0
2	E	527	3880	2412	670	777	21	0	0
2	G	527	3880	2412	670	777	21	0	0
2	I	527	3880	2412	670	777	21	0	0
2	K	527	3880	2412	670	777	21	0	0
2	M	527	3880	2412	670	777	21	0	0
2	a	527	3880	2412	670	777	21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	c	527	3880	2412	670	777	21	0	0
2	e	527	3880	2412	670	777	21	0	0
2	g	527	3880	2412	670	777	21	0	0
2	i	527	3880	2412	670	777	21	0	0
2	k	527	3880	2412	670	777	21	0	0
2	m	527	3880	2412	670	777	21	0	0

- Molecule 3 is a protein called Chaperedoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	B	88	698	435	125	138	1	0
3	D	88	698	435	125	138	1	0
3	F	88	698	435	125	138	1	0
3	H	88	698	435	125	138	1	0
3	J	88	698	435	125	138	1	0
3	L	88	698	435	125	138	1	0
3	N	88	698	435	125	138	1	0
3	b	88	689	430	123	136	0	0
3	d	88	689	430	123	136	0	0
3	f	88	689	430	123	136	0	0
3	h	88	689	430	123	136	0	0
3	j	88	689	430	123	136	0	0
3	l	88	689	430	123	136	0	0

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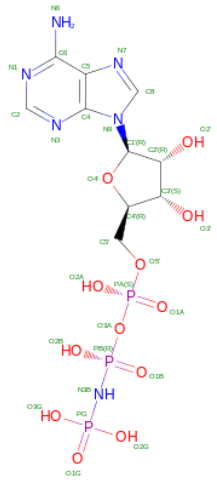
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	n	88	689	430	123	136	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0
4	C	1	1	1	0
4	E	1	1	1	0
4	G	1	1	1	0
4	I	1	1	1	0
4	K	1	1	1	0
4	M	1	1	1	0
4	a	1	1	1	0
4	c	1	1	1	0
4	e	1	1	1	0
4	g	1	1	1	0
4	i	1	1	1	0
4	k	1	1	1	0
4	m	1	1	1	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).

ANP



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	C	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	E	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	G	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	I	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	K	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	M	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	a	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	c	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	e	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	g	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	i	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	k	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	m	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

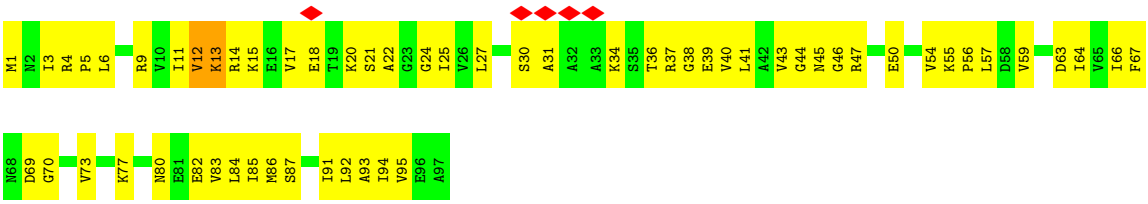
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
6	a	1	1	1	0
6	c	1	1	1	0
6	e	1	1	1	0
6	g	1	1	1	0
6	i	1	1	1	0
6	k	1	1	1	0
6	m	1	1	1	0

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

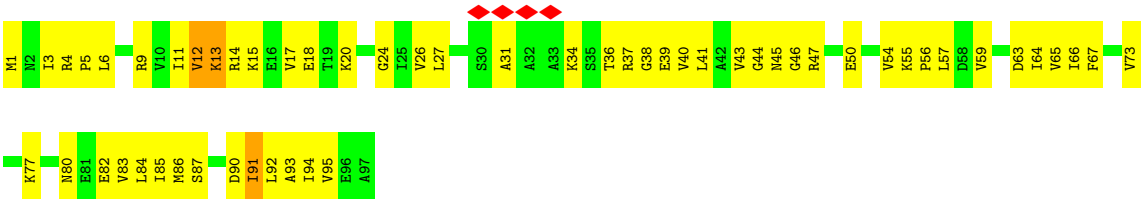
• Molecule 1: Co-chaperonin GroES

Chain 0:



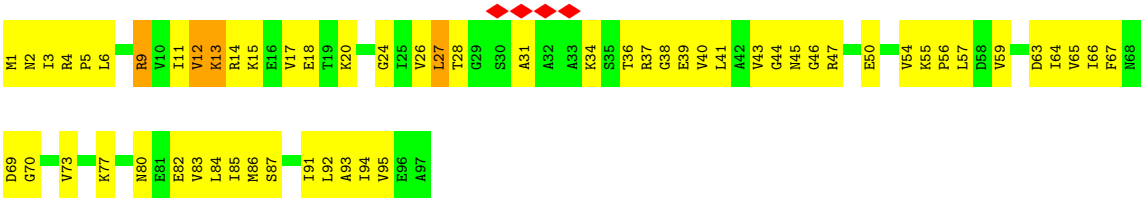
• Molecule 1: Co-chaperonin GroES

Chain 1:



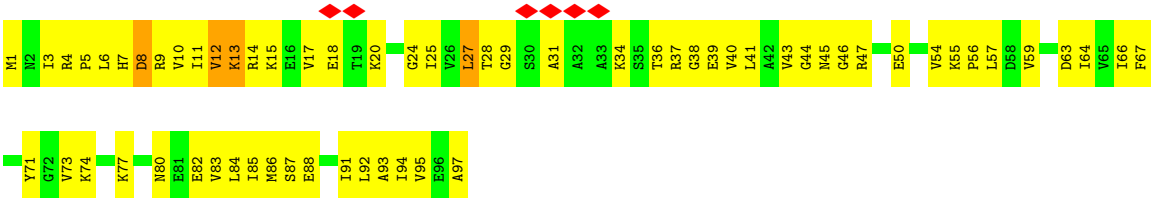
• Molecule 1: Co-chaperonin GroES

Chain 2:



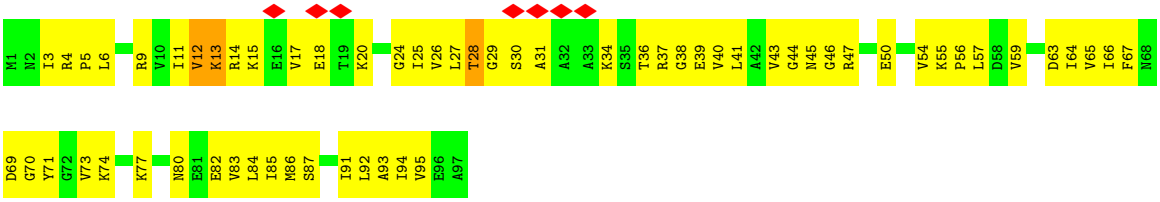
• Molecule 1: Co-chaperonin GroES

Chain 3:



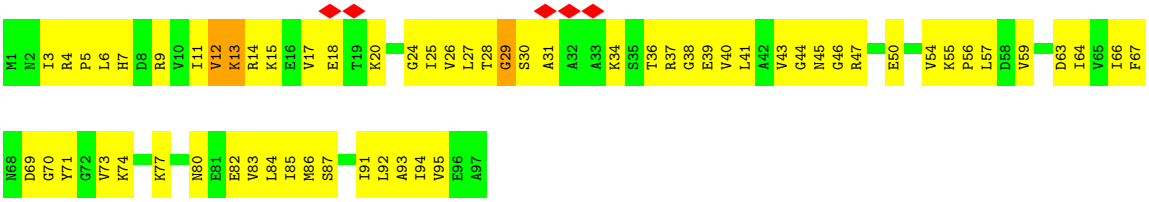
• Molecule 1: Co-chaperonin GroES

Chain 4:



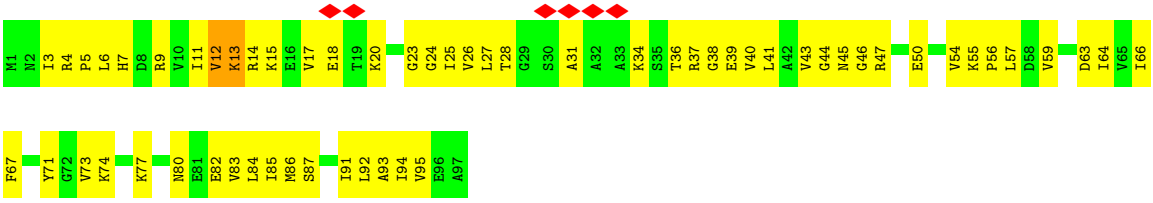
• Molecule 1: Co-chaperonin GroES

Chain 5:



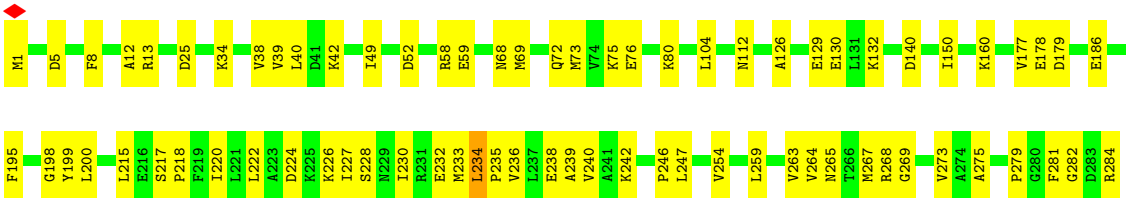
• Molecule 1: Co-chaperonin GroES

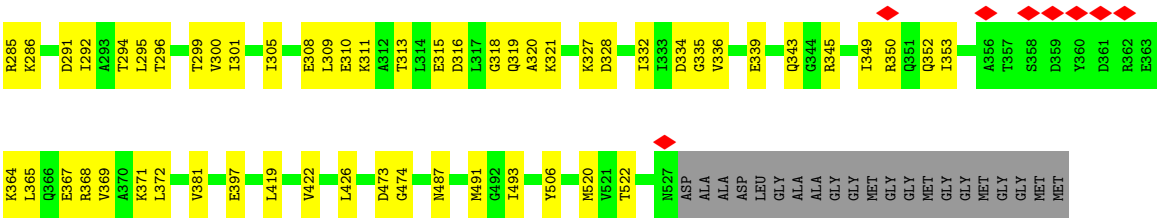
Chain 6:



• Molecule 2: Chaperonin GroEL

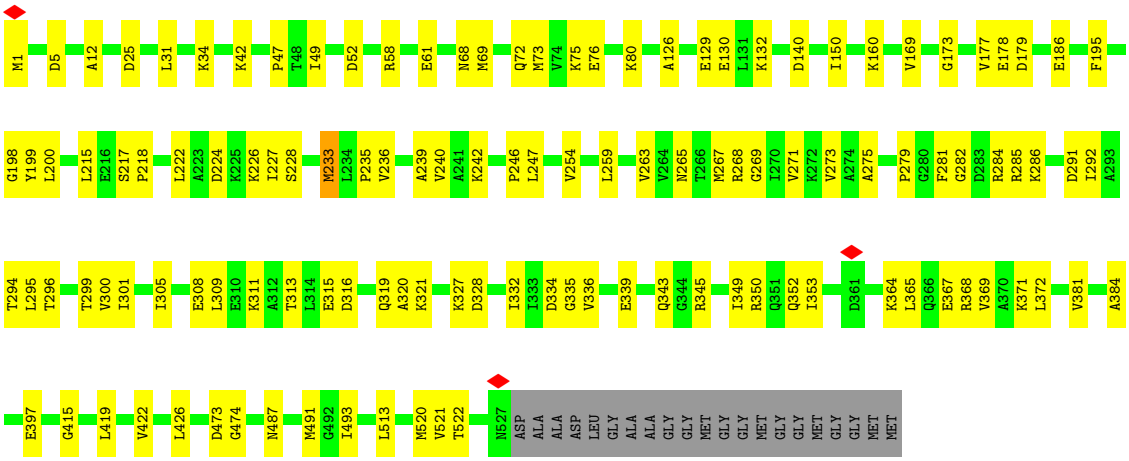
Chain A:





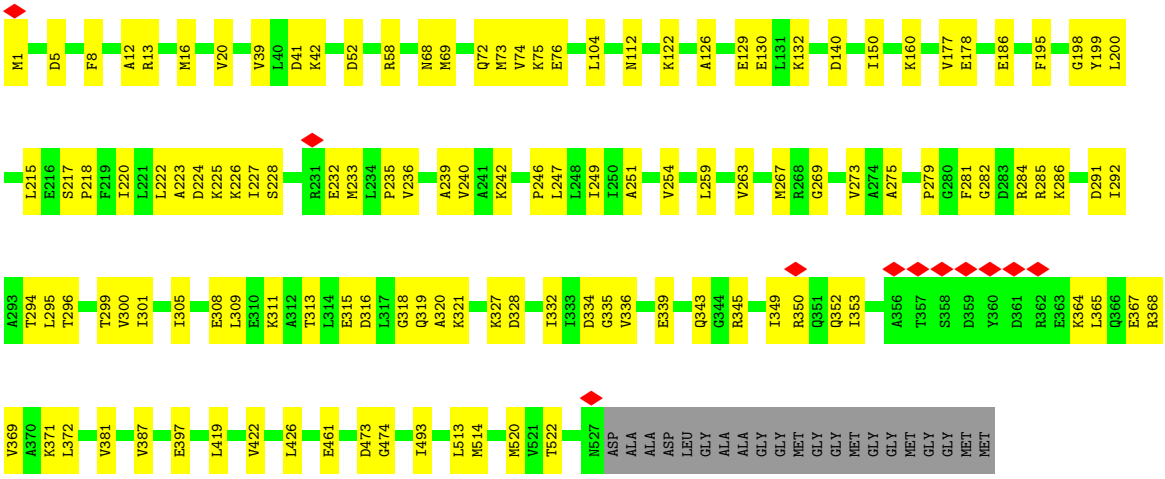
• Molecule 2: Chaperonin GroEL

Chain C:



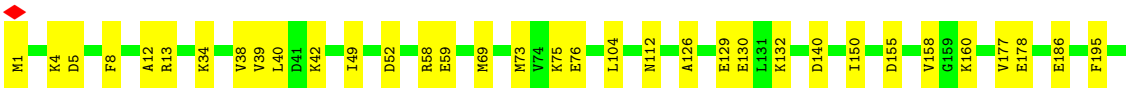
• Molecule 2: Chaperonin GroEL

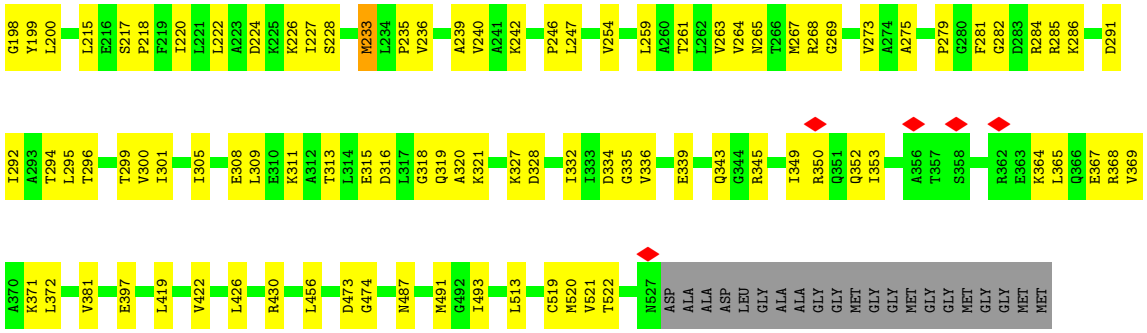
Chain E:



• Molecule 2: Chaperonin GroEL

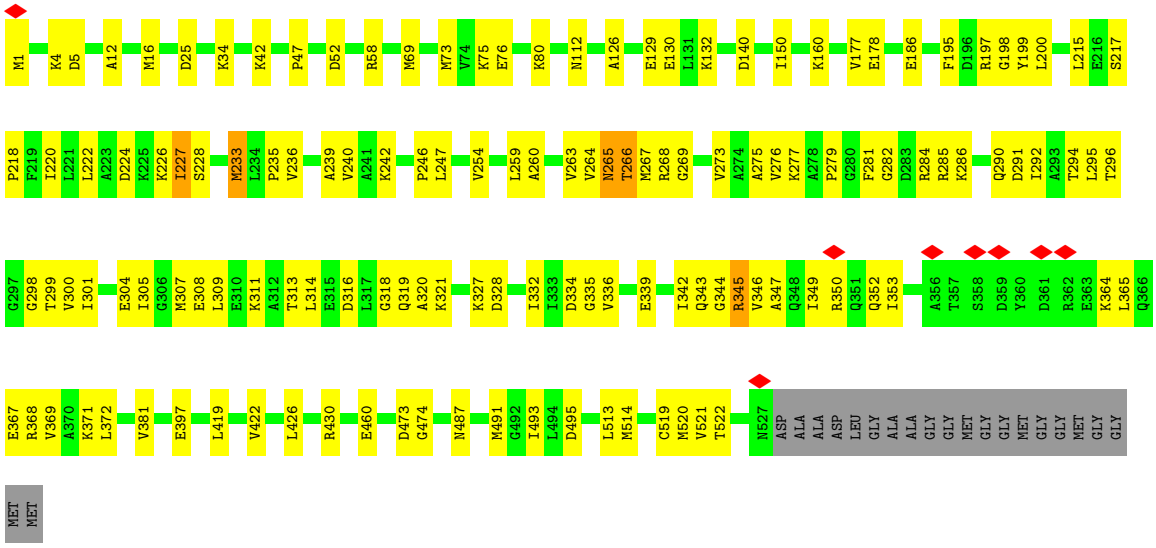
Chain G:





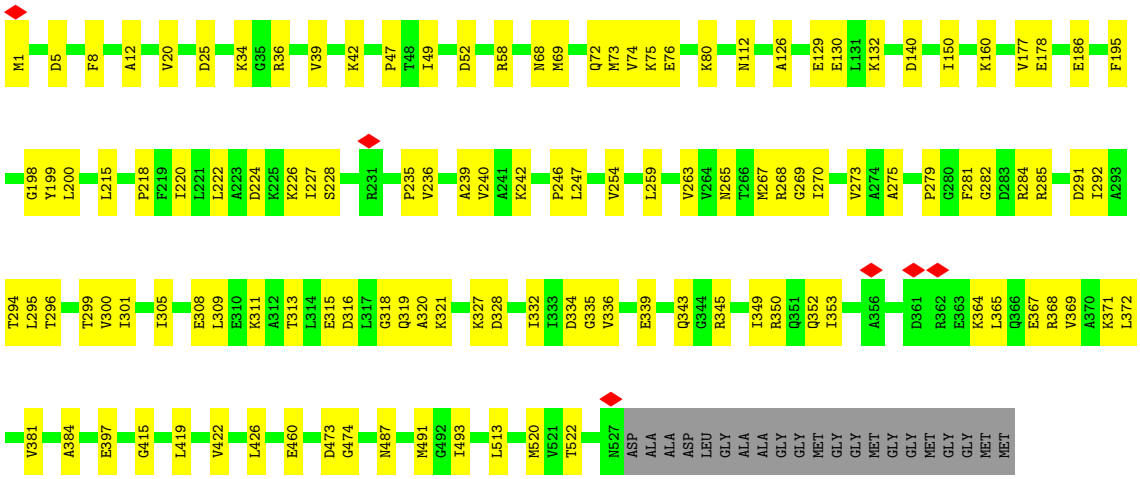
• Molecule 2: Chaperonin GroEL

Chain I:



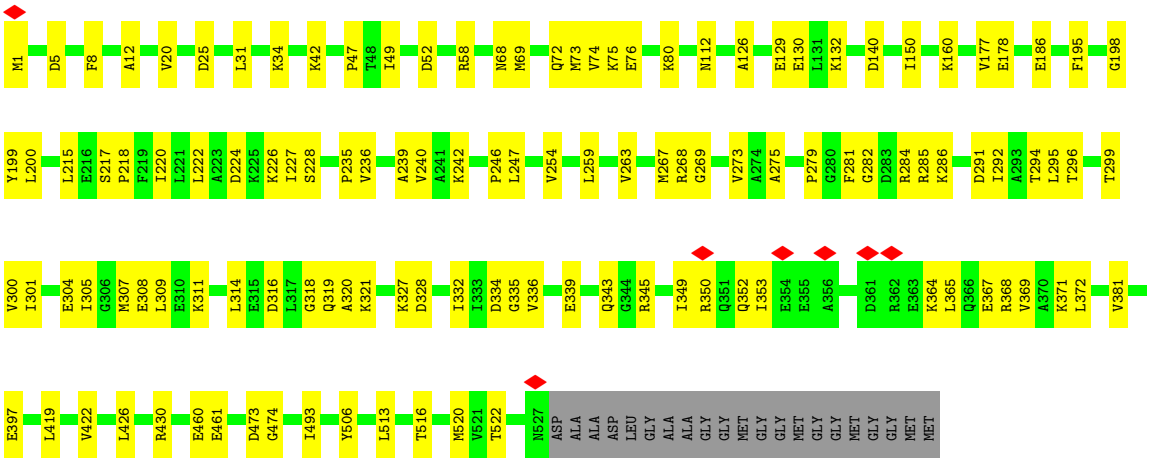
• Molecule 2: Chaperonin GroEL

Chain K:



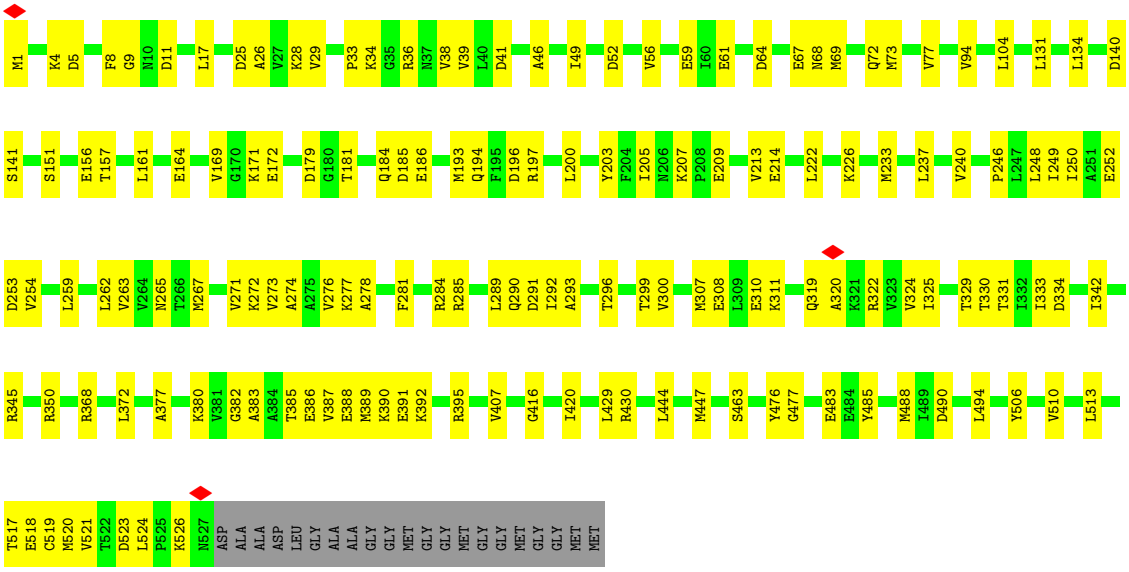
• Molecule 2: Chaperonin GroEL

Chain M:



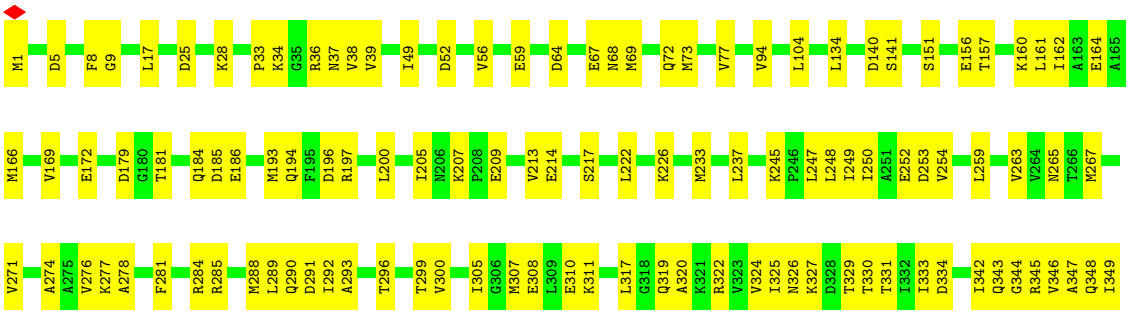
• Molecule 2: Chaperonin GroEL

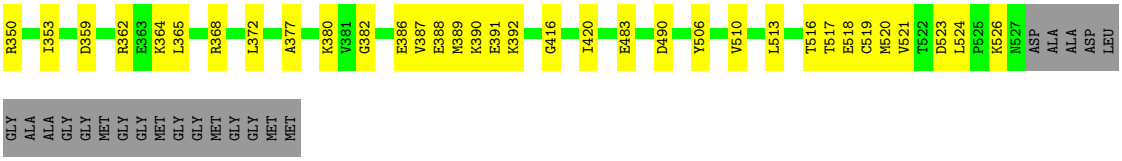
Chain a:



• Molecule 2: Chaperonin GroEL

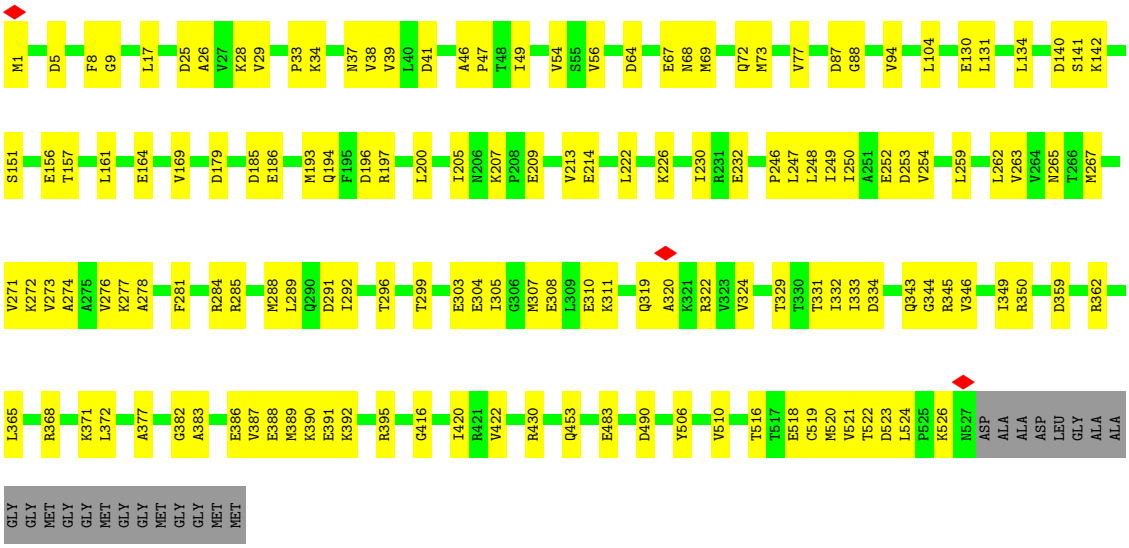
Chain c:





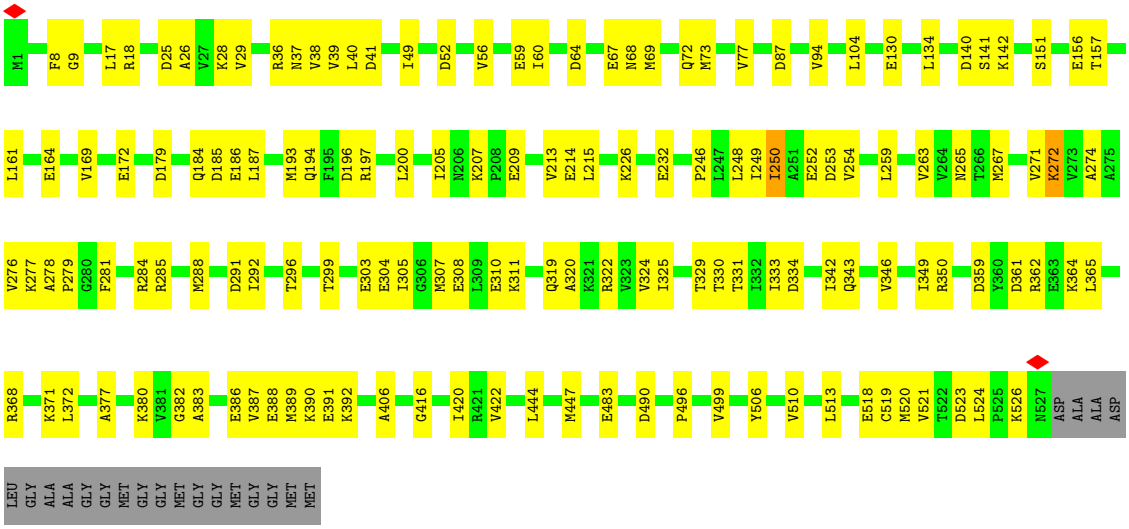
• Molecule 2: Chaperonin GroEL

Chain e:



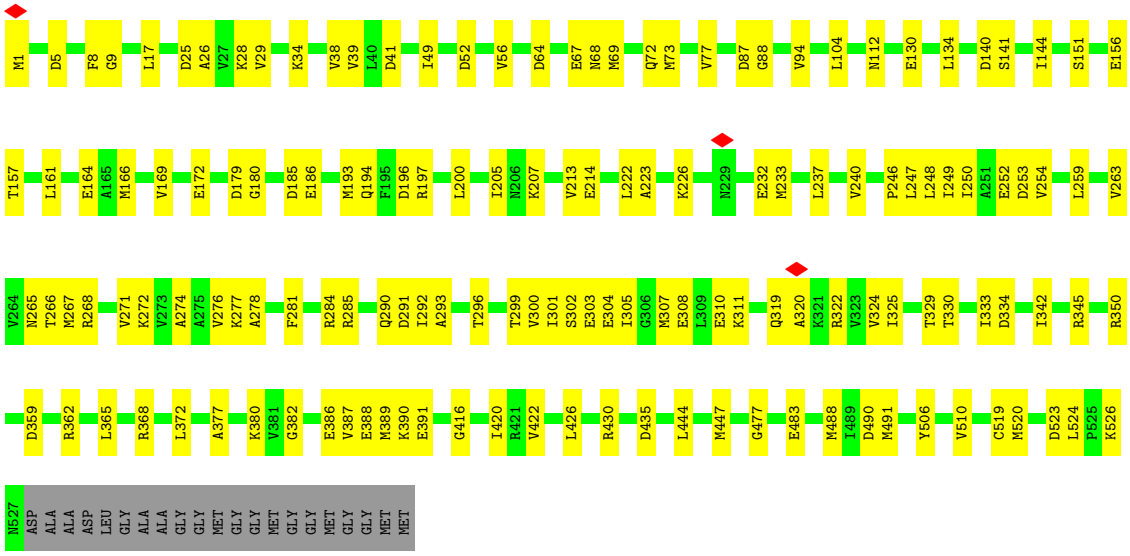
• Molecule 2: Chaperonin GroEL

Chain g:



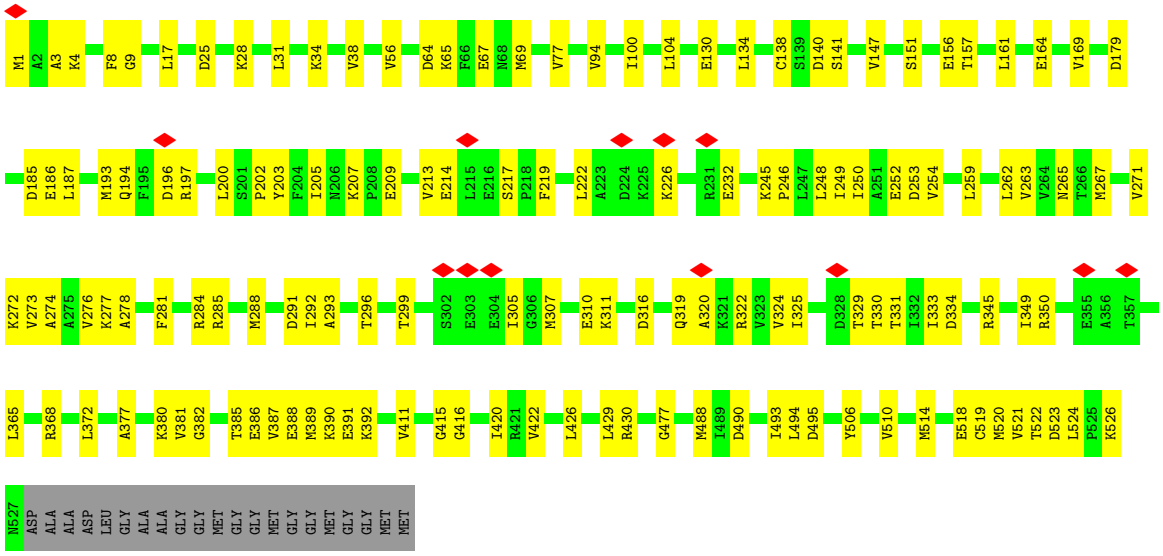
• Molecule 2: Chaperonin GroEL

Chain i:



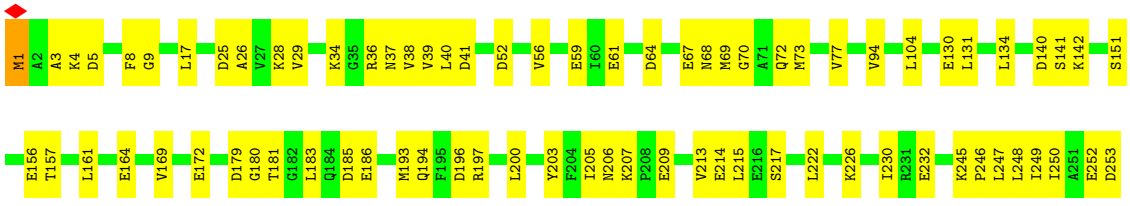
- Molecule 2: Chaperonin GroEL

Chain k:



- Molecule 2: Chaperonin GroEL

Chain m:



V254 L259 L262 V263 V264 N265 T266 M267 V271 K272 V273 A274 A275 V276 K277 A278 F281 R284 R285 L289 Q290 D291 I292 A293 T296 T299 V300 E303 M307 E310 K311 Q319 A320 K321 R322 V323 V324 I325 N326 K327 D328 T329 T330 T331 I332 I333 D334

I342 R345 I349 R350 E355 R368 K371 L372 A377 K380 V381 G382 A383 A384 T385 E386 V387 E388 M389 K390 E391 K392 G415 G416 I420 R421 V422 K425 L444 M447 Q453 S463 E483 D490 I493 L494 Y506 V510 L513 M514

E518 G519 M520 V521 K526 N527 ASP ALA ALA ASP LEU GLY ALA ALA GLY GLY MET GLY GLY MET GLY GLY GLY MET GLY GLY MET MET

- Molecule 3: Chaperedoxin

Chain B: 15% 15% • 69%

MET SER VAL GLU ASN ILE VAL ASN ILE ASN GLU SER ASN LEU GLN GLN SER MET THR THR PRO VAL LEU PHE TYR PHE TRP SER GLU ARG SER GLN HIS CYS LEU GLN LEU THR PRO ILE LEU GLU SER LEU ALA ALA GLN TYR ASN GLY GLN PHE ILE LEU ALA LYS

LEU ASP CYS ASP ALA GLU GLN MET ILE ALA ALA GLN PHE GLY LEU ARG ALA ILE PRO THR VAL TYR LEU PHE GLN ASN GLY GLN PRO VAL ASP GLY PHE GLN GLY PRO GLN PRO GLU GLU ALA ILE ARG ALA LEU LEU ASP LYS VAL LEU PRO ARG GLU GLU GLU LEU LYS ALA GLN GLN

ALA MET GLN LEU MET GLN GLU SER ASN TYR THR ASP ALA LEU PRO LEU LEU LYS ASP ALA TRP GLN LEU SER ASN GLN ASN GLY GLU ILE GLY LEU LEU LEU ALA GLU THR LEU ILE ALA LEU ASN ARG SER GLU ASP ALA GLU ALA VAL LEU LYS THR ILE PRO LEU GLN ASP GLN ASP

THR ARG TYR GLN GLY LEU VAL ALA GLN ILE GLU LEU LEU LYS GLN ALA A197 V209 D215 A216 A217 L218 A219 T220 Q221 L222 A223 L224 Q225 Q228 E234 A235 L236 E237 L238 L239 F240 G241 H242 L243 R244 D251 G252 Q253 T254 R255 K256 T257 F258 Q259 E260 I261 L262 L265

G266 T267 G268 D269 A270 S273 K274 Y275 R276 R277 Q278 L279 Y280 A281 L282 L283 Y284

- Molecule 3: Chaperedoxin

Chain D: 17% 13% 69%

MET SER VAL GLU ASN ILE VAL ASN ILE ASN GLU SER ASN LEU GLN GLN SER MET THR THR PRO VAL LEU PHE TYR PHE TRP SER GLU ARG SER GLN HIS CYS LEU GLN LEU THR PRO ILE LEU GLU SER LEU ALA ALA GLN TYR ASN GLY GLN PHE ILE LEU ALA LYS

LEU ASP CYS ASP ALA GLU GLN MET ILE ALA ALA GLN PHE GLY LEU ARG ALA ILE PRO THR VAL TYR LEU PHE GLN ASN GLY GLN PRO VAL ASP GLY PHE GLN GLY PRO GLN PRO GLU GLU ALA ILE ARG ALA LEU LEU ASP LYS VAL LEU PRO ARG GLU GLU GLU LEU LYS ALA GLN GLN

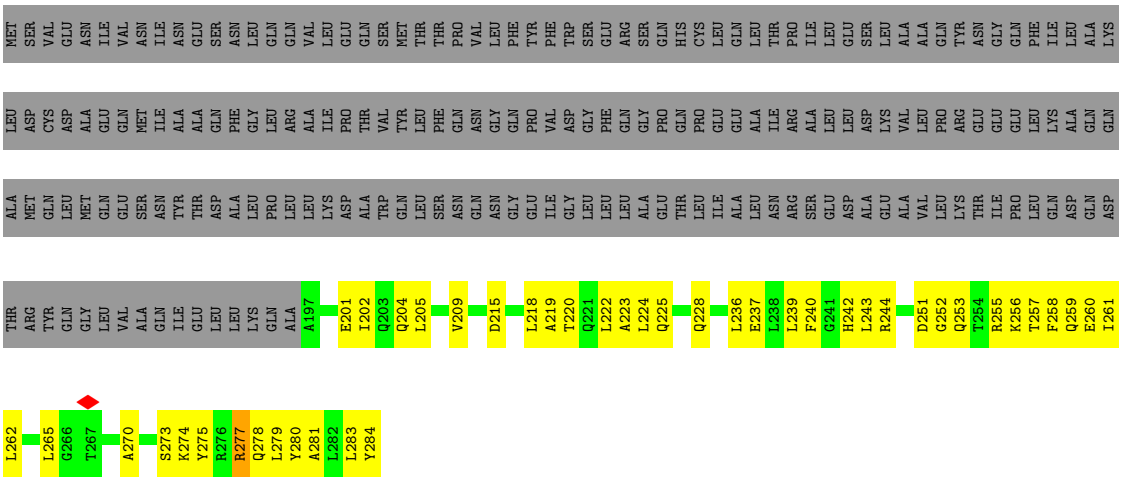
ALA MET GLN LEU MET GLN GLU SER ASN TYR THR ASP ALA LEU PRO LEU LEU LYS ASP ALA TRP GLN LEU SER ASN GLN ASN GLY GLU ILE GLY LEU LEU LEU ALA GLU THR LEU ILE ALA LEU ASN ARG SER GLU ASP ALA GLU ALA VAL LEU LYS THR ILE PRO LEU GLN ASP GLN ASP

THR ARG TYR GLN GLY LEU VAL ALA GLN ILE GLU LEU LEU LYS GLN ALA A197 E201 Q204 D215 A216 A217 L218 A219 T220 Q225 Q228 L236 E237 L238 L239 F240 G241 H242 L243 R244 D251 G252 Q253 T254 R255 K256 T257 F258 Q259 E260 I261 L262 L265 G266 T267

A270 S273 K274 Y275 R276 R277 Q278 L279 Y280 A281 L282 L283 Y284

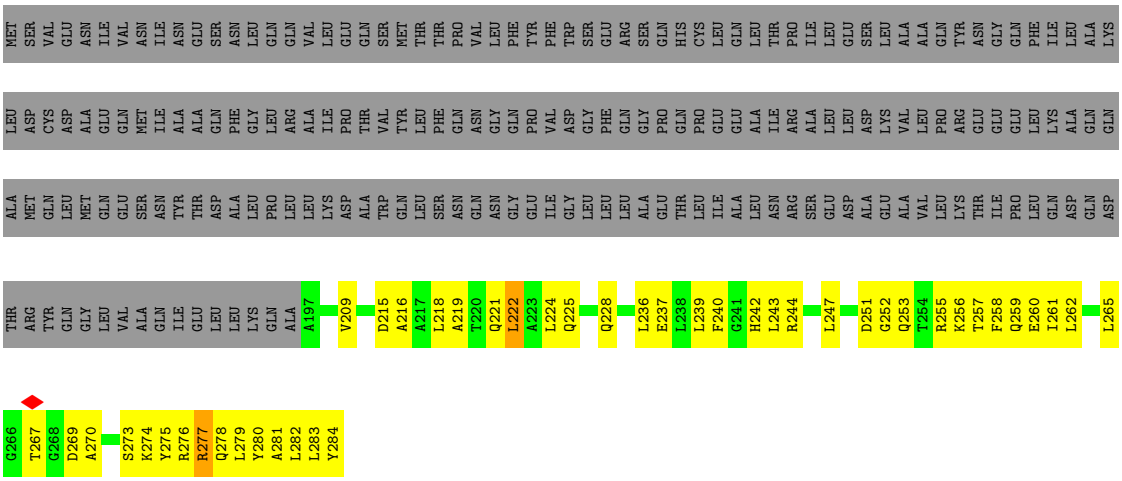
- Molecule 3: Chaperedoxin

Chain F: 15% 15% 69%



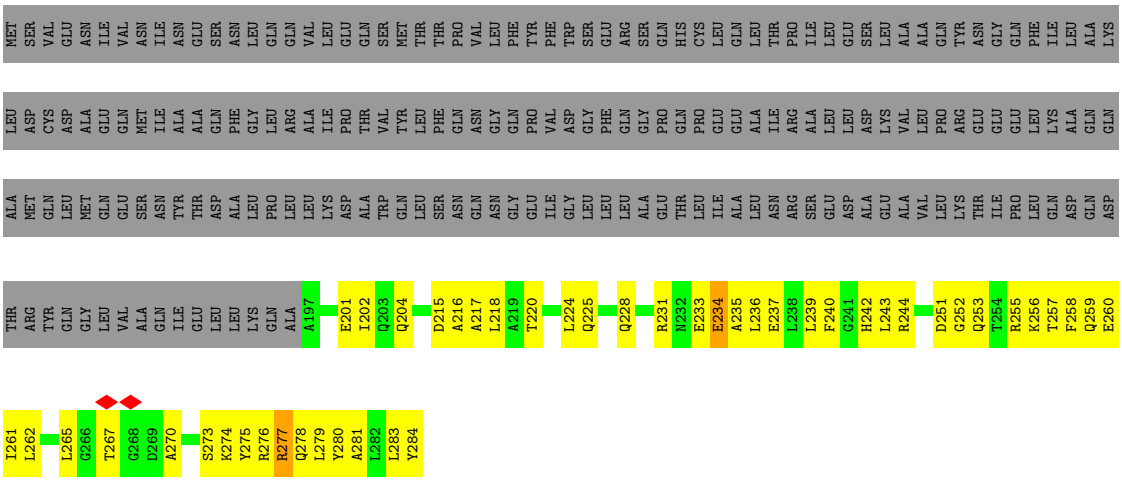
- Molecule 3: Chaperedoxin

Chain H: 15% 15% • 69%



- Molecule 3: Chaperedoxin

Chain J: 14% 16% • 69%



- Molecule 3: Chaperedoxin

Chain L: 17% 14% 69%

MET SER VAL GLU ASN ILE VAL ASN ILE ASN GLU SER ASN LEU GLN GLN VAL LEU GLU GLN SER MET THR THR PRO VAL LEU PHE TYR PHE TRP SER GLU ARG SER GLN HIS CYS LEU GLN LEU THR PRO ILE LEU GLU SER LEU ALA ALA GLN TYR ASN GLY GLN PHE ILE LEU ALA LYS

LEU ASP CYS ASP ALA GLU GLN MET ILE ALA ALA GLN PHE GLY LEU ARG ALA ILE PRO THR VAL TYR LEU PHE GLN ASN GLY GLN PRO VAL ASP GLY PHE GLN GLY PRO GLN PRO GLU GLU ALA ILE ARG ALA LEU LEU ASP LYS VAL LEU PRO ARG GLU GLU GLU LEU LYS ALA GLN GLN

ALA MET GLN LEU MET GLN GLU SER ASN TYR THR ASP ALA LEU PRO LEU LEU LYS ASP ALA TRP GLN LEU SER ASN GLN ASN GLY GLU ILE GLY LEU LEU LEU ALA GLU THR LEU ILE ALA LEU ASN ARG SER GLU ASP ALA GLU ALA VAL LEU LYS THR ILE PRO LEU GLN ASP GLN ASP

THR ARG TYR GLN GLY LEU VAL ALA GLN ILE GLU LEU LEU LYS GLN ALA A197 E201 Q204 D215 A216 A217 L218 A219 T220 Q221 L222 A223 L224 Q225 Q228 L236 E237 L238 L239 F240 G241 H242 L243 R244 D251 G252 Q253 T254 R255 K256 T257 F258 Q259 E260 I261 L262 L265

G266 T267 G268 D269 A270 S273 K274 Y275 R276 R277 Q278 L279 Y280 A281 L282 L283 Y284

- Molecule 3: Chaperedoxin

Chain N: 17% 14% 69%

MET SER VAL GLU ASN ILE VAL ASN ILE ASN GLU SER ASN LEU GLN GLN VAL LEU GLU GLN SER MET THR THR PRO VAL LEU PHE TYR PHE TRP SER GLU ARG SER GLN HIS CYS LEU GLN LEU THR PRO ILE LEU GLU SER LEU ALA ALA GLN TYR ASN GLY GLN PHE ILE LEU ALA LYS

LEU ASP CYS ASP ALA GLU GLN MET ILE ALA ALA GLN PHE GLY LEU ARG ALA ILE PRO THR VAL TYR LEU PHE GLN ASN GLY GLN PRO VAL ASP GLY PHE GLN GLY PRO GLN PRO GLU GLU ALA ILE ARG ALA LEU LEU ASP LYS VAL LEU PRO ARG GLU GLU GLU LEU LYS ALA GLN GLN

ALA MET GLN LEU MET GLN GLU SER ASN TYR THR ASP ALA LEU PRO LEU LEU LYS ASP ALA TRP GLN LEU SER ASN GLN ASN GLY GLU ILE GLY LEU LEU LEU ALA GLU THR LEU ILE ALA LEU ASN ARG SER GLU ASP ALA GLU ALA VAL LEU LYS THR ILE PRO LEU GLN ASP GLN ASP

THR ARG TYR GLN GLY LEU VAL ALA GLN ILE GLU LEU LEU LYS GLN ALA A197 E201 Q204 D215 A216 A217 L218 A219 T220 L224 Q225 Q228 L236 E237 L238 L239 F240 G241 H242 L243 R244 D251 G252 Q253 T254 R255 K256 T257 F258 Q259 E260 I261 L262 L265 G266 T267

A270 S273 K274 Y275 R276 R277 Q278 L279 Y280 A281 L282 L283 Y284

- Molecule 3: Chaperedoxin

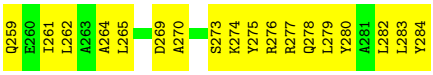
Chain b: 13% 18% 69%

MET SER VAL GLU ASN ILE VAL ASN ILE ASN GLU SER ASN LEU GLN GLN VAL LEU GLU GLN SER MET THR THR PRO VAL LEU PHE TYR PHE TRP SER GLU ARG SER GLN HIS CYS LEU GLN LEU THR PRO ILE LEU GLU SER LEU ALA ALA GLN TYR ASN GLY GLN PHE ILE LEU ALA LYS

LEU ASP CYS ASP ALA GLU GLN MET ILE ALA ALA GLN PHE GLY LEU ARG ALA ILE PRO THR VAL TYR LEU PHE GLN ASN GLY GLN PRO VAL ASP GLY PHE GLN GLY PRO GLN PRO GLU GLU ALA ILE ARG ALA LEU LEU ASP LYS VAL LEU PRO ARG GLU GLU GLU LEU LYS ALA GLN GLN

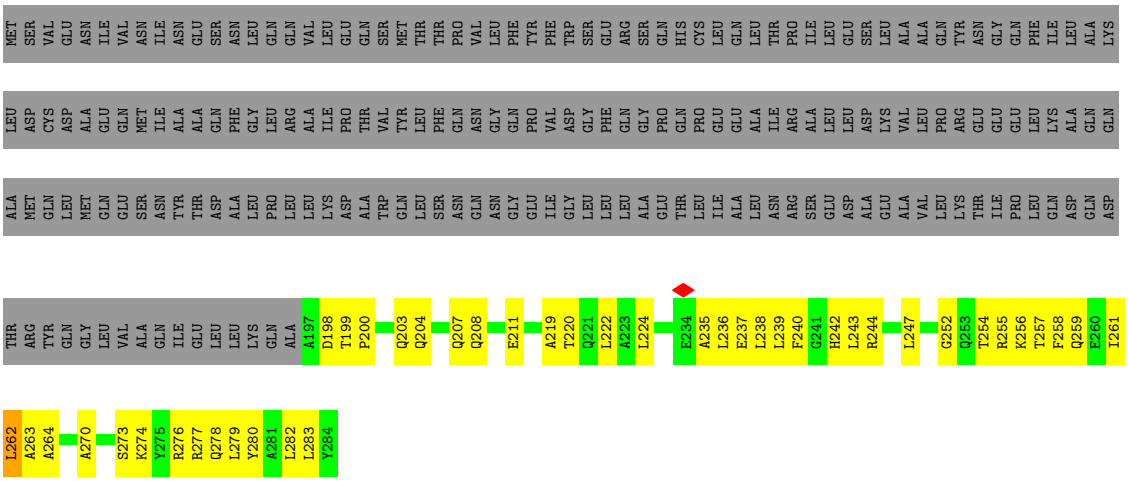
ALA MET GLN LEU MET GLN GLU SER ASN TYR THR ASP ALA LEU PRO LEU LEU LYS ASP ALA TRP GLN LEU SER ASN GLN ASN GLY GLU ILE GLY LEU LEU LEU ALA GLU THR LEU ILE ALA LEU ASN ARG SER GLU ASP ALA GLU ALA VAL LEU LYS THR ILE PRO LEU GLN ASP GLN ASP

THR ARG TYR GLN GLY LEU VAL ALA GLN ILE GLU LEU LEU LYS GLN ALA A197 D198 T199 P200 E201 I202 Q203 Q204 Q207 Q208 E211 N212 A219 T220 Q221 L222 A223 L224 Q225 E234 A235 L236 E237 L238 L239 F240 G241 H242 L243 R244 L247 G252 Q253 T254 R255 K256 T257 F258



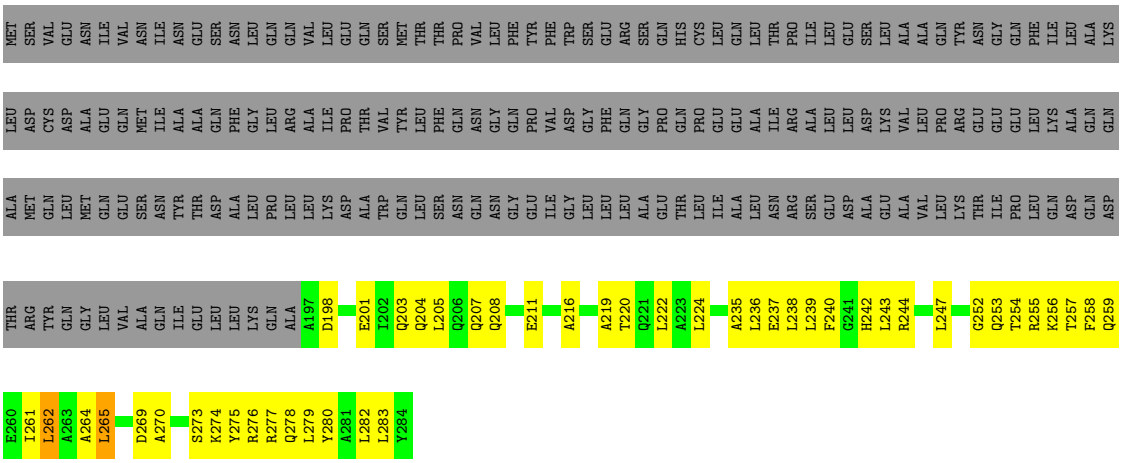
- Molecule 3: Chaperedoxin

Chain d:



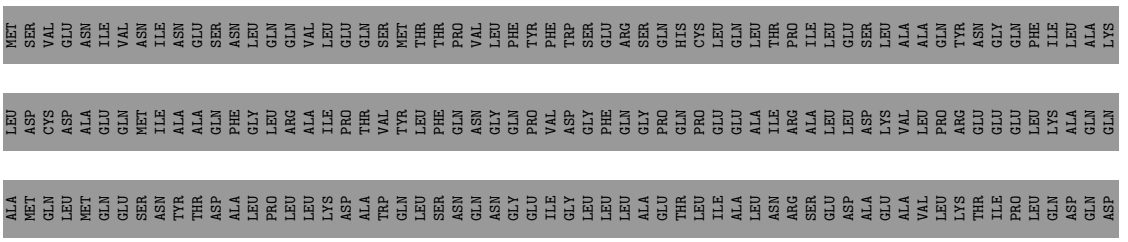
- Molecule 3: Chaperedoxin

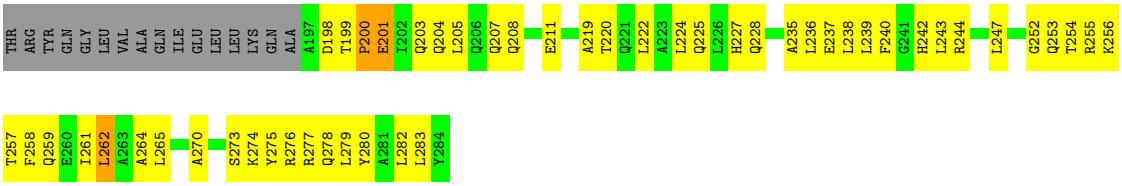
Chain f:



- Molecule 3: Chaperedoxin

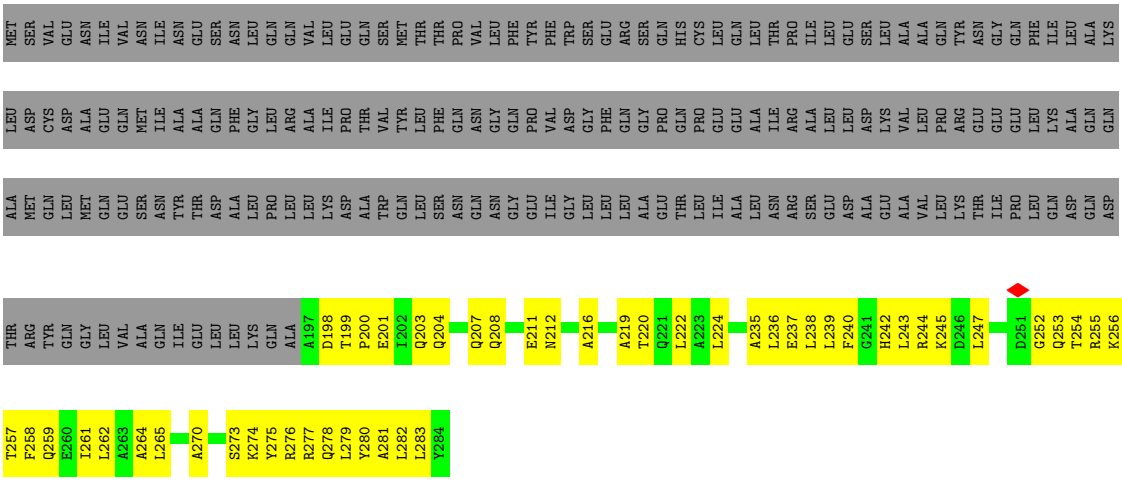
Chain h:





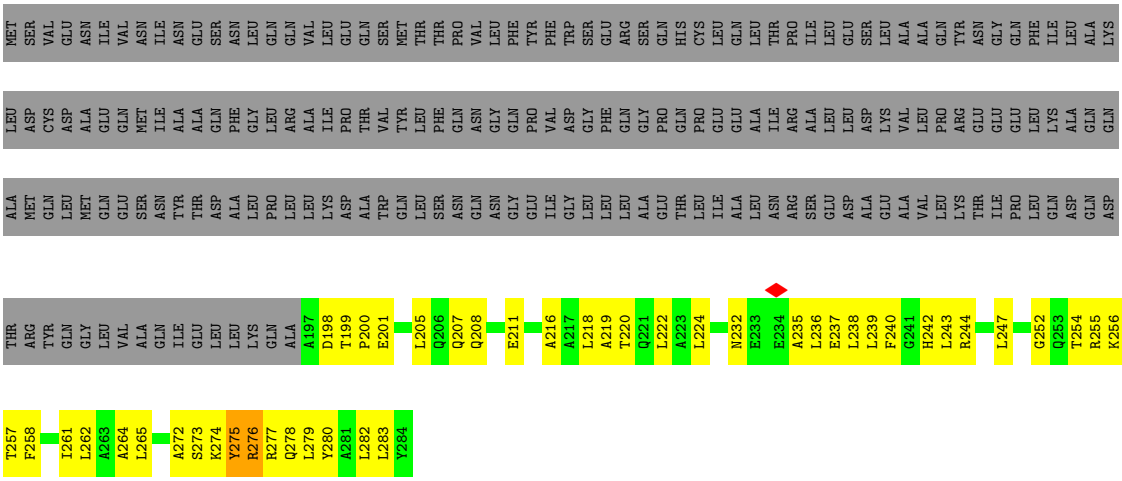
- Molecule 3: Chaperedoxin

Chain j:



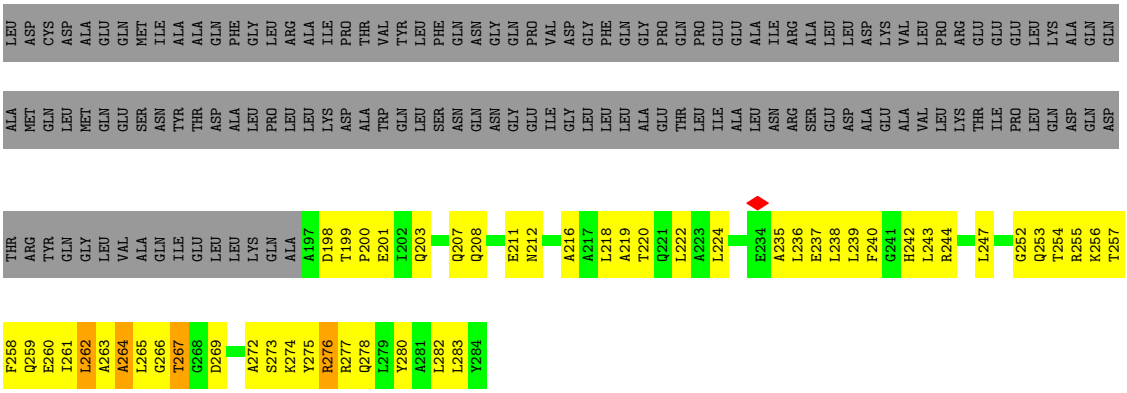
- Molecule 3: Chaperedoxin

Chain l:



- Molecule 3: Chaperedoxin

Chain n:


LEU ASP CYS ASP ALA GLU GLN MET ILE ALA ALA GLN PHE GLY LEU ARG ALA ILE PRO THR VAL TYR LEU PHE GLN ASN GLY GLN PRO VAL ASP GLY PHE GLN GLY PRO GLN PRO GLU GLU ALA ILE ARG ALA LEU LEU ASP LYS VAL LEU PRO ARG GLU GLU GLU LEU LYS ALA GLN GLN
ALA MET GLN LEU MET GLN GLU SER ASN TYR THR ASP ALA LEU PRO LEU LEU LYS ASP ALA TRP GLN LEU SER ASN GLN ASN GLY GLU ILE GLY LEU LEU LEU ALA GLU THR LEU ILE ALA LEU ASN ARG SER GLU ASP ALA GLU ALA VAL LEU LYS THR ILE PRO LEU GLN ASP GLN ASP
THR ARG TYR GLN GLY LEU VAL ALA GLN ILE GLU LEU LEU LYS GLN ALA A197 D198 T199 P200 E201 I202 Q203 Q207 Q208 E211 N212 A216 A217 L218 A219 T220 Q221 L222 A223 L224 E234 A235 L236 E237 L238 L239 F240 G241 H242 L243 R244 L247 G252 Q253 T254 R255 K256 T257
F258 Q259 E260 I261 L262 A263 A264 L265 G266 T267 G268 D269 A272 S273 K274 Y275 R276 R277 Q278 L279 Y280 A281 L282 L283 Y284

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.999	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	528.0, 528.0, 528.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

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: ANP, K, MG

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	0	0.62	2/732 (0.3%)	0.77	0/983
1	1	0.68	3/732 (0.4%)	0.83	0/983
1	2	0.62	2/732 (0.3%)	0.81	0/983
1	3	0.62	2/732 (0.3%)	0.81	0/983
1	4	0.60	2/732 (0.3%)	0.78	0/983
1	5	0.59	2/732 (0.3%)	0.77	0/983
1	6	0.60	2/732 (0.3%)	0.78	0/983
2	A	0.16	0/3908	0.42	0/5275
2	C	0.17	0/3908	0.43	0/5275
2	E	0.18	0/3908	0.44	0/5275
2	G	0.17	0/3908	0.43	0/5275
2	I	0.22	0/3908	0.47	0/5275
2	K	0.18	0/3908	0.45	0/5275
2	M	0.20	1/3908 (0.0%)	0.43	0/5275
2	a	0.24	1/3908 (0.0%)	0.53	0/5275
2	c	0.20	0/3908	0.51	0/5275
2	e	0.20	0/3908	0.52	0/5275
2	g	0.20	0/3908	0.50	0/5275
2	i	0.26	1/3908 (0.0%)	0.53	0/5275
2	k	0.20	0/3908	0.48	0/5275
2	m	0.19	0/3908	0.48	0/5275
3	B	0.38	0/706	0.76	0/954
3	D	0.28	0/706	0.67	0/954
3	F	0.33	0/706	0.73	0/954
3	H	0.38	0/706	0.82	0/954
3	J	0.34	0/706	0.70	0/954
3	L	0.31	0/706	0.69	0/954
3	N	0.28	0/706	0.66	0/954
3	b	0.26	0/697	0.79	0/942
3	d	0.27	0/697	0.80	0/942
3	f	0.32	0/697	0.82	0/942
3	h	0.39	2/697 (0.3%)	0.84	0/942

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	j	0.26	0/697	0.77	0/942
3	l	0.30	0/697	0.82	0/942
3	n	0.49	1/697 (0.1%)	0.92	0/942
All	All	0.27	21/69657 (0.0%)	0.55	0/94003

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	13	LYS	C-N	7.14	1.43	1.33
1	6	13	LYS	C-N	7.08	1.43	1.33
1	1	13	LYS	C-N	7.05	1.43	1.33
1	3	13	LYS	C-N	7.01	1.43	1.33
1	2	13	LYS	C-N	6.99	1.43	1.33
1	0	13	LYS	C-N	6.98	1.43	1.33
2	i	87	ASP	C-N	-6.98	1.23	1.33
1	5	13	LYS	C-N	6.97	1.43	1.33
1	4	12	VAL	C-N	6.61	1.42	1.33
1	0	12	VAL	C-N	6.59	1.42	1.33
1	6	12	VAL	C-N	6.58	1.42	1.33
1	2	12	VAL	C-N	6.54	1.42	1.33
1	5	12	VAL	C-N	6.54	1.42	1.33
1	3	12	VAL	C-N	6.53	1.42	1.33
1	1	12	VAL	C-N	6.53	1.42	1.33
3	n	276	ARG	C-N	-5.92	1.26	1.33
1	1	91	ILE	C-N	-5.41	1.25	1.33
2	a	11	ASP	C-N	-5.17	1.27	1.33
3	h	200	PRO	C-N	5.07	1.41	1.33
3	h	201	GLU	C-N	-5.07	1.28	1.33
2	M	314	LEU	C-N	5.06	1.41	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	728	0	762	86	0
1	1	728	0	762	84	0
1	2	728	0	762	107	0
1	3	728	0	762	117	0
1	4	728	0	762	97	0
1	5	728	0	762	90	0
1	6	728	0	762	88	0
2	A	3880	0	4007	126	0
2	C	3880	0	4007	117	0
2	E	3880	0	4007	113	0
2	G	3880	0	4007	124	0
2	I	3880	0	4007	162	0
2	K	3880	0	4007	113	0
2	M	3880	0	4007	127	0
2	a	3880	0	4007	158	0
2	c	3880	0	4007	178	0
2	e	3880	0	4007	171	0
2	g	3880	0	4007	141	0
2	i	3880	0	4007	140	0
2	k	3880	0	4007	180	0
2	m	3880	0	4007	184	0
3	B	698	0	693	58	0
3	D	698	0	693	39	0
3	F	698	0	693	56	0
3	H	698	0	693	69	0
3	J	698	0	693	72	0
3	L	698	0	693	39	0
3	N	698	0	693	59	0
3	b	689	0	686	56	0
3	d	689	0	686	52	0
3	f	689	0	686	61	0
3	h	689	0	686	61	0
3	j	689	0	686	65	0
3	l	689	0	686	66	0
3	n	689	0	686	64	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	c	1	0	0	0	0
4	e	1	0	0	0	0
4	g	1	0	0	0	0
4	i	1	0	0	0	0
4	k	1	0	0	0	0
4	m	1	0	0	0	0
5	A	31	0	13	0	0
5	C	31	0	13	2	0
5	E	31	0	13	0	0
5	G	31	0	13	0	0
5	I	31	0	13	1	0
5	K	31	0	13	3	0
5	M	31	0	13	1	0
5	a	31	0	13	1	0
5	c	31	0	13	2	0
5	e	31	0	13	4	0
5	g	31	0	13	0	0
5	i	31	0	13	0	0
5	k	31	0	13	9	0
5	m	31	0	13	5	0
6	a	1	0	0	0	0
6	c	1	0	0	0	0
6	e	1	0	0	0	0
6	g	1	0	0	0	0
6	i	1	0	0	0	0
6	k	1	0	0	0	0
6	m	1	0	0	0	0
All	All	69580	0	71267	3043	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 22.

All (3043) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:4:LYS:CE	2:m:59:GLU:HG3	1.53	1.37
2:k:4:LYS:HE2	2:m:59:GLU:CG	1.62	1.28
2:k:1:MET:HE2	2:m:59:GLU:OE2	1.30	1.28
2:k:521:VAL:CG2	2:m:39:VAL:HB	1.67	1.24
1:5:27:LEU:HA	2:K:269:GLY:CA	1.70	1.21
1:5:27:LEU:HA	2:K:269:GLY:HA2	1.25	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:305:ILE:HD13	3:j:276:ARG:NH1	1.60	1.16
1:2:6:LEU:HD21	1:3:91:ILE:HB	1.13	1.13
2:a:520:MET:HE1	2:c:38:VAL:HG22	1.28	1.12
1:3:13:LYS:HB2	1:3:15:LYS:HZ2	1.16	1.10
1:3:6:LEU:HD21	1:4:91:ILE:HB	1.34	1.10
2:k:520:MET:HE1	2:m:38:VAL:HG22	1.33	1.10
1:1:13:LYS:HB2	1:1:15:LYS:HZ2	1.16	1.09
2:c:513:LEU:HD21	2:e:49:ILE:HD13	1.14	1.09
1:2:13:LYS:HB2	1:2:15:LYS:HZ2	1.16	1.08
2:k:522:THR:HB	2:m:40:LEU:HD23	1.32	1.08
1:2:6:LEU:HD11	1:3:91:ILE:HG22	1.23	1.07
1:5:13:LYS:HB2	1:5:15:LYS:HZ2	1.17	1.06
1:4:13:LYS:HB2	1:4:15:LYS:HZ2	1.16	1.06
2:e:520:MET:HE1	2:g:38:VAL:HG22	1.36	1.05
1:0:13:LYS:HB2	1:0:15:LYS:HZ2	1.16	1.05
2:k:521:VAL:HG23	2:m:39:VAL:CB	1.86	1.04
2:c:520:MET:HE1	2:e:38:VAL:HG22	1.32	1.04
1:6:13:LYS:HB2	1:6:15:LYS:HZ2	1.16	1.03
2:k:518:GLU:HB3	2:m:36:ARG:HB3	1.39	1.03
2:c:513:LEU:CD2	2:e:49:ILE:HD13	1.90	1.02
2:c:69:MET:CE	2:e:41:ASP:HB2	1.90	1.02
3:f:276:ARG:CZ	3:f:279:LEU:HG	1.90	1.01
3:f:276:ARG:NH2	3:f:279:LEU:HG	1.74	1.00
2:k:69:MET:HE3	2:m:39:VAL:HG12	1.42	1.00
2:g:305:ILE:HD13	3:h:276:ARG:NH1	1.76	0.99
1:1:27:LEU:HD23	2:C:269:GLY:HA3	1.41	0.98
1:2:6:LEU:HD21	1:3:91:ILE:CB	1.92	0.98
2:a:38:VAL:HG22	2:m:520:MET:HE1	1.45	0.98
2:c:69:MET:HE2	2:e:41:ASP:HB2	0.98	0.98
1:3:6:LEU:HD11	1:4:91:ILE:HG22	1.46	0.97
2:k:521:VAL:HG23	2:m:39:VAL:HB	0.97	0.97
3:N:283:LEU:HG	3:N:284:TYR:CD2	2.00	0.97
1:4:27:LEU:HG	2:I:269:GLY:CA	1.95	0.96
1:6:25:ILE:HB	1:6:27:LEU:HD13	1.46	0.96
2:K:49:ILE:HD11	2:M:73:MET:HE1	1.44	0.96
2:E:223:ALA:HB2	2:E:249:ILE:HD11	1.48	0.95
1:2:27:LEU:HD23	2:A:269:GLY:HA3	1.49	0.95
2:k:493:ILE:HG12	5:k:603:ANP:C6	1.96	0.95
3:n:262:LEU:HA	3:n:276:ARG:NH2	1.82	0.95
2:c:69:MET:HE2	2:e:41:ASP:CB	1.94	0.94
2:M:300:VAL:HB	3:N:280:TYR:HE2	1.33	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:518:GLU:HB3	2:m:36:ARG:CB	1.98	0.93
1:0:25:ILE:HB	1:0:27:LEU:HG	1.47	0.93
3:F:283:LEU:HG	3:F:284:TYR:CD2	2.04	0.93
3:B:283:LEU:HG	3:B:284:TYR:CD2	2.04	0.92
3:J:283:LEU:HG	3:J:284:TYR:CD2	2.04	0.92
3:L:283:LEU:HG	3:L:284:TYR:CD2	2.05	0.91
2:c:299:THR:HG22	3:d:277:ARG:HH12	1.35	0.91
2:k:518:GLU:HG2	2:m:36:ARG:HG3	1.49	0.91
1:2:6:LEU:CD2	1:3:91:ILE:HB	2.01	0.90
2:k:299:THR:HA	3:l:280:TYR:CE2	2.06	0.90
1:4:25:ILE:HB	1:4:27:LEU:HD13	1.51	0.90
2:e:69:MET:HE2	2:g:41:ASP:HB2	1.54	0.89
3:H:215:ASP:HB3	3:H:218:LEU:HD23	1.53	0.89
1:4:27:LEU:HG	2:I:269:GLY:HA3	1.52	0.89
2:c:521:VAL:HG23	2:e:39:VAL:O	1.74	0.88
2:I:286:LYS:NZ	3:J:284:TYR:HB2	1.88	0.88
2:a:387:VAL:HA	2:a:390:LYS:NZ	1.89	0.86
3:D:283:LEU:HG	3:D:284:TYR:CD2	2.09	0.86
2:k:522:THR:HB	2:m:40:LEU:CD2	2.06	0.86
1:4:27:LEU:O	2:I:268:ARG:HB2	1.76	0.86
2:k:1:MET:CE	2:m:59:GLU:OE2	2.21	0.85
2:A:230:ILE:HG22	2:A:234:LEU:HD23	1.59	0.85
3:n:265:LEU:HD12	3:n:265:LEU:H	1.41	0.85
2:g:299:THR:HG22	3:h:277:ARG:HH12	1.41	0.85
2:k:169:VAL:HG11	2:k:377:ALA:HB2	1.59	0.85
2:i:169:VAL:HG11	2:i:377:ALA:HB2	1.58	0.85
2:k:522:THR:CB	2:m:40:LEU:HD23	2.07	0.84
2:c:169:VAL:HG11	2:c:377:ALA:HB2	1.59	0.84
2:m:169:VAL:HG11	2:m:377:ALA:HB2	1.59	0.84
2:a:169:VAL:HG11	2:a:377:ALA:HB2	1.58	0.84
2:e:169:VAL:HG11	2:e:377:ALA:HB2	1.58	0.84
3:n:262:LEU:HA	3:n:276:ARG:CZ	2.07	0.84
2:k:3:ALA:HA	2:m:61:GLU:HB3	1.60	0.84
2:k:200:LEU:HD21	2:k:277:LYS:HD3	1.60	0.84
3:n:265:LEU:HD13	3:n:276:ARG:HH21	1.41	0.83
2:k:69:MET:HE3	2:m:39:VAL:CG1	2.07	0.83
1:0:20:LYS:HB2	1:0:24:GLY:HA2	1.59	0.83
2:c:350:ARG:NH1	2:c:350:ARG:HA	1.94	0.83
2:m:200:LEU:HD21	2:m:277:LYS:HD3	1.61	0.83
2:m:326:ASN:OD1	2:m:327:LYS:N	2.11	0.83
2:a:387:VAL:HA	2:a:390:LYS:HZ2	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:169:VAL:HG11	2:g:377:ALA:HB2	1.59	0.83
2:c:326:ASN:OD1	2:c:327:LYS:N	2.11	0.83
2:c:520:MET:HE1	2:e:38:VAL:CG2	2.09	0.82
1:3:27:LEU:O	2:G:265:ASN:HA	1.79	0.82
2:I:339:GLU:HB2	2:I:343:GLN:HE22	1.41	0.82
2:a:200:LEU:HD21	2:a:277:LYS:HD3	1.61	0.82
1:3:6:LEU:HD13	1:3:9:ARG:HH12	1.43	0.82
1:4:27:LEU:H	1:4:27:LEU:HD12	1.42	0.82
2:e:200:LEU:HD21	2:e:277:LYS:HD3	1.60	0.82
2:i:200:LEU:HD21	2:i:277:LYS:HD3	1.61	0.82
2:g:246:PRO:HB3	2:g:272:LYS:HB2	1.62	0.81
3:l:240:PHE:HA	3:l:243:LEU:HD12	1.61	0.81
2:c:200:LEU:HD21	2:c:277:LYS:HD3	1.60	0.81
2:A:73:MET:HE1	2:C:49:ILE:HD11	1.60	0.81
2:g:200:LEU:HD21	2:g:277:LYS:HD3	1.61	0.80
2:I:233:MET:HE1	2:I:236:VAL:HG23	1.60	0.80
2:k:200:LEU:O	2:m:183:LEU:HD23	1.80	0.80
2:A:39:VAL:HB	2:G:520:MET:HG2	1.62	0.80
1:5:28:THR:HB	2:K:265:ASN:OD1	1.82	0.80
2:c:299:THR:HG22	3:d:277:ARG:NH1	1.96	0.80
2:I:300:VAL:HB	3:J:280:TYR:HE2	1.46	0.80
2:i:299:THR:HB	3:j:277:ARG:HH12	1.48	0.79
1:2:4:ARG:HB3	1:3:94:ILE:CG2	2.12	0.79
3:d:240:PHE:HA	3:d:243:LEU:HD12	1.64	0.79
2:c:520:MET:SD	2:e:38:VAL:HG13	2.22	0.79
2:k:518:GLU:CG	2:m:36:ARG:HG3	2.13	0.79
2:E:233:MET:HE1	2:E:236:VAL:HG23	1.62	0.79
2:e:284:ARG:HB2	2:e:368:ARG:HH12	1.48	0.79
2:A:320:ALA:HA	2:A:334:ASP:HB3	1.65	0.79
2:C:320:ALA:HA	2:C:334:ASP:HB3	1.65	0.79
2:G:320:ALA:HA	2:G:334:ASP:HB3	1.65	0.79
1:6:47:ARG:NH1	1:6:47:ARG:O	2.16	0.79
3:H:224:LEU:HG	3:H:228:GLN:HE21	1.48	0.79
3:f:279:LEU:HA	3:f:282:LEU:HG	1.65	0.78
2:g:305:ILE:HD13	3:h:276:ARG:HH12	1.46	0.78
1:0:47:ARG:NH1	1:0:47:ARG:O	2.16	0.78
1:1:47:ARG:NH1	1:1:47:ARG:O	2.16	0.78
1:5:47:ARG:NH1	1:5:47:ARG:O	2.16	0.78
2:E:320:ALA:HA	2:E:334:ASP:HB3	1.65	0.78
2:i:284:ARG:HB2	2:i:368:ARG:HH12	1.48	0.78
1:4:77:LYS:HZ3	1:4:80:ASN:H	1.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:218:LEU:HD12	3:B:219:ALA:N	1.99	0.78
2:i:305:ILE:CD1	3:j:276:ARG:NH1	2.43	0.78
3:f:240:PHE:HA	3:f:243:LEU:HD12	1.65	0.78
1:2:47:ARG:NH1	1:2:47:ARG:O	2.16	0.78
2:I:320:ALA:HA	2:I:334:ASP:HB3	1.65	0.78
3:l:258:PHE:HA	3:l:261:ILE:HG22	1.65	0.78
2:M:320:ALA:HA	2:M:334:ASP:HB3	1.65	0.78
1:3:47:ARG:NH1	1:3:47:ARG:O	2.16	0.78
2:i:246:PRO:HB3	2:i:272:LYS:HB2	1.66	0.78
2:e:518:GLU:HG2	2:g:36:ARG:HG3	1.66	0.78
1:0:5:PRO:HG2	1:0:44:GLY:HA2	1.66	0.77
1:1:86:MET:HE3	1:1:90:ASP:HB2	1.65	0.77
2:a:181:THR:HG23	2:m:203:TYR:HE2	1.50	0.77
3:b:240:PHE:HA	3:b:243:LEU:HD12	1.66	0.77
3:d:258:PHE:HA	3:d:261:ILE:HG22	1.66	0.77
3:j:240:PHE:HA	3:j:243:LEU:HD12	1.65	0.77
1:1:77:LYS:HZ3	1:1:80:ASN:H	1.32	0.77
3:J:224:LEU:HG	3:J:228:GLN:HE21	1.48	0.77
1:0:91:ILE:HB	1:6:6:LEU:HD21	1.67	0.77
1:1:5:PRO:HG2	1:1:44:GLY:HA2	1.66	0.77
1:2:27:LEU:HB3	2:A:265:ASN:ND2	1.99	0.77
3:f:273:SER:O	3:f:277:ARG:HG2	1.83	0.77
2:k:8:PHE:CE1	2:m:25:ASP:OD1	2.37	0.77
1:6:77:LYS:HZ3	1:6:80:ASN:H	1.32	0.77
3:H:256:LYS:HB3	3:H:259:GLN:HE21	1.49	0.77
2:a:520:MET:SD	2:c:38:VAL:HG13	2.25	0.77
1:5:77:LYS:HZ3	1:5:80:ASN:H	1.32	0.77
3:D:256:LYS:HB3	3:D:259:GLN:HE21	1.49	0.77
3:J:256:LYS:HB3	3:J:259:GLN:HE21	1.50	0.77
1:6:5:PRO:HG2	1:6:44:GLY:HA2	1.66	0.77
2:K:34:LYS:HE3	2:M:112:ASN:ND2	2.00	0.77
2:i:299:THR:HB	3:j:277:ARG:NH1	2.00	0.77
1:1:6:LEU:HD21	1:2:91:ILE:HB	1.67	0.77
1:4:27:LEU:HG	2:I:269:GLY:HA2	1.66	0.77
2:A:49:ILE:HD11	2:G:73:MET:HE1	1.65	0.77
3:B:256:LYS:HB3	3:B:259:GLN:HE21	1.49	0.77
2:K:320:ALA:HA	2:K:334:ASP:HB3	1.65	0.77
2:k:523:ASP:OD1	2:k:524:LEU:N	2.18	0.77
1:4:47:ARG:NH1	1:4:47:ARG:O	2.16	0.77
3:N:256:LYS:HB3	3:N:259:GLN:HE21	1.49	0.77
2:m:493:ILE:HG12	5:m:603:ANP:C6	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:233:MET:HE1	2:C:236:VAL:HG23	1.67	0.76
2:g:520:MET:HE1	2:i:38:VAL:HG22	1.67	0.76
3:L:256:LYS:HB3	3:L:259:GLN:HE21	1.49	0.76
3:H:218:LEU:HD12	3:H:219:ALA:N	1.99	0.76
2:c:300:VAL:HG23	3:d:280:TYR:HD2	1.49	0.76
1:3:66:ILE:O	1:3:92:LEU:HB2	1.85	0.76
1:3:77:LYS:HZ3	1:3:80:ASN:H	1.32	0.76
1:2:5:PRO:HG2	1:2:44:GLY:HA2	1.66	0.76
1:4:5:PRO:HG2	1:4:44:GLY:HA2	1.66	0.76
1:5:5:PRO:HG2	1:5:44:GLY:HA2	1.66	0.76
3:B:256:LYS:HA	3:B:259:GLN:HG3	1.66	0.76
3:N:224:LEU:HG	3:N:228:GLN:HE21	1.51	0.76
3:n:265:LEU:HG	3:n:269:ASP:HB3	1.65	0.76
3:n:240:PHE:HA	3:n:243:LEU:HD12	1.68	0.76
1:0:77:LYS:HZ3	1:0:80:ASN:H	1.32	0.76
3:h:256:LYS:HA	3:h:259:GLN:HB3	1.68	0.76
2:m:284:ARG:HB2	2:m:368:ARG:HH12	1.50	0.76
2:k:69:MET:CE	2:m:39:VAL:HG12	2.15	0.76
3:l:275:TYR:O	3:l:278:GLN:HG2	1.86	0.76
1:2:27:LEU:O	2:A:268:ARG:HB2	1.87	0.75
1:3:5:PRO:HG2	1:3:44:GLY:HA2	1.66	0.75
2:C:31:LEU:HD12	5:C:602:ANP:O1A	1.86	0.75
3:H:256:LYS:HA	3:H:259:GLN:HG3	1.66	0.75
3:F:205:LEU:HG	3:F:222:LEU:HD23	1.69	0.75
3:J:256:LYS:HA	3:J:259:GLN:HG3	1.66	0.75
2:g:365:LEU:HG	2:g:368:ARG:HH21	1.50	0.75
3:N:256:LYS:HA	3:N:259:GLN:HG3	1.66	0.75
1:3:28:THR:HA	2:G:264:VAL:HG12	1.69	0.75
1:0:6:LEU:HD21	1:1:91:ILE:HB	1.67	0.75
2:I:260:ALA:O	2:I:264:VAL:HG23	1.87	0.75
3:D:256:LYS:HA	3:D:259:GLN:HG3	1.66	0.75
3:F:256:LYS:HA	3:F:259:GLN:HG3	1.66	0.75
2:I:197:ARG:HB3	2:I:277:LYS:HG3	1.67	0.75
2:e:520:MET:SD	2:g:38:VAL:HG13	2.27	0.75
2:c:516:THR:CG2	2:e:37:ASN:OD1	2.34	0.75
3:F:256:LYS:HB3	3:F:259:GLN:HE21	1.49	0.74
2:I:286:LYS:HZ1	3:J:284:TYR:HB2	1.52	0.74
3:L:256:LYS:HA	3:L:259:GLN:HG3	1.66	0.74
2:a:284:ARG:HB2	2:a:368:ARG:HH12	1.49	0.74
3:n:274:LYS:H	3:n:274:LYS:HD2	1.52	0.74
2:A:198:GLY:HA2	2:A:328:ASP:HA	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:13:LYS:HB2	1:5:15:LYS:NZ	2.01	0.74
2:e:523:ASP:OD1	2:e:524:LEU:N	2.21	0.74
1:2:77:LYS:HZ3	1:2:80:ASN:H	1.32	0.74
1:3:13:LYS:HB2	1:3:15:LYS:NZ	2.01	0.74
2:G:198:GLY:HA2	2:G:328:ASP:HA	1.70	0.74
3:b:258:PHE:HA	3:b:261:ILE:HG22	1.70	0.74
3:n:220:THR:HG21	3:n:253:GLN:HG3	1.68	0.74
1:4:13:LYS:HB2	1:4:15:LYS:NZ	2.01	0.74
2:i:325:ILE:HG22	2:i:330:THR:HB	1.69	0.74
1:2:13:LYS:HB2	1:2:15:LYS:NZ	2.01	0.74
2:c:513:LEU:HD21	2:e:49:ILE:CD1	2.08	0.74
3:f:258:PHE:HA	3:f:261:ILE:HG22	1.70	0.74
3:h:258:PHE:HA	3:h:261:ILE:HG22	1.70	0.74
2:a:49:ILE:HD13	2:m:513:LEU:HD21	1.69	0.74
2:G:49:ILE:HD11	2:I:73:MET:HE1	1.70	0.73
2:I:198:GLY:HA2	2:I:328:ASP:HA	1.70	0.73
2:K:198:GLY:HA2	2:K:328:ASP:HA	1.70	0.73
2:c:523:ASP:OD1	2:c:524:LEU:N	2.21	0.73
2:k:520:MET:CE	2:m:38:VAL:HG22	2.16	0.73
2:C:198:GLY:HA2	2:C:328:ASP:HA	1.70	0.73
2:K:296:THR:HG22	2:K:335:GLY:HA2	1.70	0.73
2:k:1:MET:HE2	2:m:59:GLU:CD	2.11	0.73
2:C:296:THR:HG22	2:C:335:GLY:HA2	1.70	0.73
3:H:280:TYR:O	3:H:283:LEU:HG	1.88	0.73
2:I:296:THR:HG22	2:I:335:GLY:HA2	1.70	0.73
2:K:49:ILE:CD1	2:M:73:MET:HE1	2.16	0.73
2:M:198:GLY:HA2	2:M:328:ASP:HA	1.70	0.73
1:6:13:LYS:HB2	1:6:15:LYS:NZ	2.01	0.73
2:E:296:THR:HG22	2:E:335:GLY:HA2	1.70	0.73
2:e:232:GLU:OE1	2:e:232:GLU:N	2.21	0.73
2:E:198:GLY:HA2	2:E:328:ASP:HA	1.70	0.73
2:G:233:MET:HE1	2:G:236:VAL:HG23	1.70	0.73
2:a:520:MET:HE1	2:c:38:VAL:CG2	2.13	0.73
2:i:523:ASP:OD1	2:i:524:LEU:N	2.21	0.73
2:M:349:ILE:HA	2:M:352:GLN:NE2	2.04	0.73
2:k:518:GLU:CB	2:m:36:ARG:HG3	2.19	0.73
1:4:66:ILE:O	1:4:92:LEU:HB2	1.88	0.73
3:j:258:PHE:HA	3:j:261:ILE:HG22	1.71	0.73
1:3:4:ARG:HB3	1:4:94:ILE:CG2	2.19	0.73
3:j:254:THR:OG1	3:j:255:ARG:NH2	2.21	0.73
2:E:349:ILE:HA	2:E:352:GLN:NE2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:280:TYR:HA	3:H:283:LEU:CD2	2.19	0.72
3:n:258:PHE:HA	3:n:261:ILE:HG22	1.71	0.72
3:n:265:LEU:H	3:n:265:LEU:CD1	2.01	0.72
2:A:349:ILE:HA	2:A:352:GLN:NE2	2.04	0.72
2:C:349:ILE:HA	2:C:352:GLN:NE2	2.04	0.72
2:G:296:THR:HG22	2:G:335:GLY:HA2	1.70	0.72
2:K:281:PHE:HA	2:K:285:ARG:HE	1.55	0.72
3:L:224:LEU:HG	3:L:228:GLN:HE21	1.53	0.72
2:a:299:THR:HG22	3:b:277:ARG:HH12	1.53	0.72
3:b:256:LYS:HA	3:b:259:GLN:HB3	1.71	0.72
2:g:523:ASP:OD1	2:g:524:LEU:N	2.22	0.72
2:G:349:ILE:HA	2:G:352:GLN:NE2	2.04	0.72
2:I:281:PHE:HA	2:I:285:ARG:HE	1.54	0.72
3:j:256:LYS:HA	3:j:259:GLN:HB3	1.70	0.72
2:K:349:ILE:HA	2:K:352:GLN:NE2	2.04	0.72
2:M:296:THR:HG22	2:M:335:GLY:HA2	1.70	0.72
2:A:296:THR:HG22	2:A:335:GLY:HA2	1.70	0.72
2:I:345:ARG:HD2	2:I:372:LEU:HD22	1.70	0.72
2:i:305:ILE:CG1	3:j:276:ARG:HH12	2.03	0.72
3:H:215:ASP:HB3	3:H:218:LEU:CD2	2.19	0.72
2:a:203:TYR:HE2	2:c:181:THR:HG23	1.54	0.72
2:a:513:LEU:HD21	2:c:49:ILE:HD13	1.72	0.72
2:G:281:PHE:HA	2:G:285:ARG:HE	1.54	0.72
2:K:327:LYS:HA	2:K:327:LYS:HE2	1.72	0.72
3:h:220:THR:HG21	3:h:253:GLN:HG3	1.71	0.72
1:1:66:ILE:O	1:1:92:LEU:HB2	1.89	0.72
1:5:34:LYS:NZ	1:5:67:PHE:O	2.21	0.72
2:C:281:PHE:HA	2:C:285:ARG:HE	1.54	0.71
2:M:327:LYS:HE2	2:M:327:LYS:HA	1.72	0.71
2:I:349:ILE:HA	2:I:352:GLN:NE2	2.04	0.71
3:B:224:LEU:HG	3:B:228:GLN:HE21	1.55	0.71
3:b:279:LEU:HA	3:b:282:LEU:HG	1.71	0.71
2:m:193:MET:HE2	2:m:193:MET:HA	1.71	0.71
1:5:27:LEU:CA	2:K:269:GLY:CA	2.62	0.71
2:E:327:LYS:HE2	2:E:327:LYS:HA	1.72	0.71
2:M:281:PHE:HA	2:M:285:ARG:HE	1.54	0.71
2:e:520:MET:HE1	2:g:38:VAL:CG2	2.16	0.71
3:l:240:PHE:CE1	3:l:282:LEU:HD21	2.25	0.71
2:c:513:LEU:HD11	2:e:49:ILE:HG21	1.72	0.71
2:c:520:MET:CE	2:e:38:VAL:HG22	2.18	0.71
3:h:240:PHE:HA	3:h:243:LEU:HD12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:516:THR:HG23	2:e:37:ASN:OD1	1.90	0.71
3:d:256:LYS:HA	3:d:259:GLN:HB3	1.72	0.71
1:3:27:LEU:O	2:G:268:ARG:HB2	1.89	0.71
3:d:243:LEU:HD23	3:d:255:ARG:HH21	1.55	0.71
1:0:13:LYS:HB2	1:0:15:LYS:NZ	2.01	0.71
2:I:327:LYS:HE2	2:I:327:LYS:HA	1.72	0.71
3:j:273:SER:O	3:j:277:ARG:HG2	1.91	0.71
2:m:310:GLU:OE1	2:m:310:GLU:N	2.23	0.71
1:3:34:LYS:NZ	1:3:67:PHE:O	2.21	0.71
1:6:34:LYS:NZ	1:6:67:PHE:O	2.21	0.71
3:j:236:LEU:HB3	3:j:275:TYR:CE2	2.26	0.71
2:k:8:PHE:CZ	2:m:25:ASP:OD1	2.43	0.71
2:A:281:PHE:HA	2:A:285:ARG:HE	1.54	0.70
2:a:521:VAL:HG23	2:c:39:VAL:HB	1.73	0.70
1:5:73:VAL:HG13	1:5:86:MET:HB2	1.73	0.70
2:I:265:ASN:C	2:I:267:MET:H	1.98	0.70
2:c:73:MET:HG2	2:e:47:PRO:HD2	1.73	0.70
1:2:91:ILE:HG22	1:2:92:LEU:O	1.91	0.70
2:E:281:PHE:HA	2:E:285:ARG:HE	1.54	0.70
2:k:415:GLY:N	5:k:603:ANP:O2'	2.21	0.70
2:C:327:LYS:HE2	2:C:327:LYS:HA	1.72	0.70
1:3:9:ARG:HB2	1:3:87:SER:HA	1.72	0.70
1:4:34:LYS:NZ	1:4:67:PHE:O	2.21	0.70
2:G:327:LYS:HE2	2:G:327:LYS:HA	1.72	0.70
3:n:261:ILE:C	3:n:276:ARG:HH22	1.99	0.70
1:2:66:ILE:HB	1:2:92:LEU:CB	2.22	0.70
1:4:66:ILE:HB	1:4:92:LEU:CB	2.21	0.70
3:l:254:THR:OG1	3:l:255:ARG:NH2	2.25	0.70
2:E:223:ALA:CB	2:E:249:ILE:HD11	2.22	0.69
3:H:280:TYR:CE1	3:H:283:LEU:HD11	2.27	0.69
1:2:28:THR:OG1	2:A:264:VAL:HG11	1.92	0.69
3:n:236:LEU:HA	3:n:239:LEU:HD13	1.74	0.69
1:5:27:LEU:CA	2:K:269:GLY:HA2	2.14	0.69
3:b:201:GLU:O	3:b:204:GLN:NE2	2.24	0.69
2:c:73:MET:SD	2:e:49:ILE:HD11	2.32	0.69
1:4:73:VAL:HG13	1:4:86:MET:HB2	1.74	0.69
2:A:327:LYS:HE2	2:A:327:LYS:HA	1.72	0.69
3:H:283:LEU:HD12	3:H:284:TYR:N	2.08	0.69
2:a:181:THR:HG23	2:m:203:TYR:CE2	2.27	0.69
3:h:239:LEU:HA	3:h:242:HIS:CE1	2.26	0.69
1:3:66:ILE:C	1:3:92:LEU:HB2	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:66:ILE:HB	1:5:92:LEU:CB	2.22	0.69
2:g:73:MET:HE2	2:i:49:ILE:HD11	1.74	0.69
3:f:201:GLU:OE1	3:f:201:GLU:N	2.24	0.69
2:k:288:MET:HE1	2:k:368:ARG:HH11	1.57	0.69
3:l:239:LEU:HA	3:l:242:HIS:CE1	2.28	0.69
2:M:286:LYS:NZ	3:N:284:TYR:HB2	2.07	0.69
2:c:365:LEU:HG	2:c:368:ARG:HH21	1.56	0.69
2:e:299:THR:HG22	3:f:277:ARG:HH12	1.55	0.69
1:0:73:VAL:HG13	1:0:86:MET:HB2	1.73	0.69
1:0:91:ILE:HG22	1:0:92:LEU:O	1.92	0.69
1:6:73:VAL:HG13	1:6:86:MET:HB2	1.74	0.69
2:a:307:MET:HA	2:a:307:MET:HE2	1.75	0.69
3:n:239:LEU:HA	3:n:242:HIS:CE1	2.27	0.69
1:0:34:LYS:NZ	1:0:67:PHE:O	2.21	0.69
1:6:37:ARG:HH21	1:6:66:ILE:HG12	1.58	0.69
2:e:307:MET:HE2	2:e:307:MET:HA	1.75	0.69
1:6:66:ILE:HB	1:6:92:LEU:CB	2.23	0.69
2:C:69:MET:O	2:C:73:MET:HG3	1.93	0.69
2:c:64:ASP:HB3	2:c:67:GLU:HB2	1.74	0.69
2:c:307:MET:HE2	2:c:307:MET:HA	1.75	0.69
2:i:386:GLU:OE1	2:i:386:GLU:N	2.26	0.69
2:k:4:LYS:HD2	2:m:59:GLU:O	1.91	0.69
1:1:73:VAL:HG13	1:1:86:MET:HB2	1.74	0.68
2:a:385:THR:O	2:a:389:MET:HG2	1.94	0.68
1:1:13:LYS:HB2	1:1:15:LYS:NZ	2.01	0.68
1:3:37:ARG:HH21	1:3:66:ILE:HG12	1.59	0.68
2:A:69:MET:O	2:A:73:MET:HG3	1.93	0.68
2:A:234:LEU:H	2:A:235:PRO:HD3	1.58	0.68
2:E:69:MET:O	2:E:73:MET:HG3	1.93	0.68
1:1:37:ARG:HH21	1:1:66:ILE:HG12	1.58	0.68
1:2:73:VAL:HG13	1:2:86:MET:HB2	1.74	0.68
3:H:280:TYR:CD1	3:H:283:LEU:HD11	2.28	0.68
2:M:69:MET:O	2:M:73:MET:HG3	1.93	0.68
2:m:64:ASP:HB3	2:m:67:GLU:HB2	1.75	0.68
1:2:37:ARG:HH21	1:2:66:ILE:HG12	1.59	0.68
2:K:69:MET:O	2:K:73:MET:HG3	1.93	0.68
1:6:66:ILE:O	1:6:92:LEU:HB2	1.93	0.68
3:d:239:LEU:HA	3:d:242:HIS:CE1	2.27	0.68
3:d:247:LEU:O	3:d:255:ARG:NH1	2.27	0.68
1:3:9:ARG:HA	1:3:88:GLU:N	2.09	0.68
2:G:315:GLU:OE1	3:H:270:ALA:HA	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:77:VAL:HG21	2:c:510:VAL:HB	1.76	0.68
2:e:193:MET:HE2	2:e:193:MET:HA	1.75	0.68
2:m:307:MET:HE2	2:m:307:MET:HA	1.75	0.68
2:G:69:MET:O	2:G:73:MET:HG3	1.93	0.68
3:d:276:ARG:NH2	3:d:279:LEU:HG	2.09	0.68
2:e:64:ASP:HB3	2:e:67:GLU:HB2	1.74	0.68
2:e:299:THR:HG22	3:f:277:ARG:NH1	2.09	0.68
3:h:243:LEU:HD23	3:h:255:ARG:HH21	1.59	0.68
3:j:247:LEU:O	3:j:255:ARG:NH1	2.27	0.68
1:3:73:VAL:HG13	1:3:86:MET:HB2	1.73	0.68
2:G:39:VAL:HB	2:I:520:MET:HG2	1.76	0.68
2:M:305:ILE:O	3:N:255:ARG:NE	2.27	0.68
1:0:66:ILE:HB	1:0:92:LEU:CB	2.24	0.67
1:4:37:ARG:HH21	1:4:66:ILE:HG12	1.58	0.67
1:5:37:ARG:HH21	1:5:66:ILE:HG12	1.58	0.67
2:I:69:MET:O	2:I:73:MET:HG3	1.93	0.67
3:f:276:ARG:HH21	3:f:280:TYR:N	1.91	0.67
2:k:284:ARG:HB2	2:k:368:ARG:HH12	1.59	0.67
1:1:34:LYS:NZ	1:1:67:PHE:O	2.21	0.67
2:i:307:MET:HA	2:i:307:MET:HE2	1.75	0.67
2:k:193:MET:HA	2:k:193:MET:HE2	1.77	0.67
2:g:386:GLU:OE1	2:g:386:GLU:N	2.26	0.67
2:i:186:GLU:OE1	2:i:186:GLU:N	2.28	0.67
1:0:37:ARG:HH21	1:0:66:ILE:HG12	1.58	0.67
3:H:247:LEU:HD21	3:H:282:LEU:HG	1.77	0.67
1:4:12:VAL:HG11	1:4:67:PHE:CZ	2.29	0.67
1:5:91:ILE:HG22	1:5:92:LEU:O	1.94	0.67
2:E:224:ASP:HB2	2:E:300:VAL:HG12	1.77	0.67
2:I:199:TYR:HD2	2:I:327:LYS:HZ1	1.43	0.67
2:i:193:MET:HE2	2:i:193:MET:HA	1.77	0.67
2:i:214:GLU:HG2	2:i:324:VAL:HG22	1.74	0.67
3:l:201:GLU:OE1	3:l:201:GLU:N	2.26	0.67
1:1:12:VAL:HG11	1:1:67:PHE:CZ	2.29	0.67
1:3:73:VAL:HG12	1:3:84:LEU:HD21	1.77	0.67
2:I:266:THR:HB	2:I:267:MET:HE1	1.75	0.67
2:a:325:ILE:HG22	2:a:330:THR:HB	1.75	0.67
2:g:64:ASP:HB3	2:g:67:GLU:HG3	1.77	0.67
2:g:307:MET:HE2	2:g:307:MET:HA	1.75	0.67
1:2:34:LYS:NZ	1:2:67:PHE:O	2.21	0.67
1:4:73:VAL:HG12	1:4:84:LEU:HD21	1.77	0.67
1:0:12:VAL:HG11	1:0:67:PHE:CZ	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:12:VAL:HG11	1:2:67:PHE:CZ	2.29	0.67
3:h:276:ARG:NH2	3:h:279:LEU:HG	2.09	0.67
1:0:73:VAL:HG12	1:0:84:LEU:HD21	1.77	0.67
1:2:73:VAL:HG12	1:2:84:LEU:HD21	1.77	0.67
1:3:12:VAL:HG11	1:3:67:PHE:CZ	2.30	0.67
1:5:12:VAL:HG11	1:5:67:PHE:CZ	2.30	0.67
1:6:73:VAL:HG12	1:6:84:LEU:HD21	1.77	0.67
3:N:273:SER:HB2	3:N:277:ARG:NH1	2.10	0.67
2:k:64:ASP:HB3	2:k:67:GLU:HB2	1.77	0.67
3:n:274:LYS:O	3:n:277:ARG:HB2	1.94	0.67
1:1:73:VAL:HG12	1:1:84:LEU:HD21	1.77	0.66
2:E:199:TYR:HD2	2:E:327:LYS:HZ1	1.42	0.66
2:G:319:GLN:HE22	2:G:336:VAL:HA	1.60	0.66
3:f:236:LEU:HD12	3:f:275:TYR:CD2	2.30	0.66
2:k:307:MET:HE2	2:k:307:MET:HA	1.75	0.66
1:2:9:ARG:HB3	1:2:87:SER:HA	1.77	0.66
1:5:73:VAL:HG12	1:5:84:LEU:HD21	1.77	0.66
1:6:12:VAL:HG11	1:6:67:PHE:CZ	2.29	0.66
2:g:299:THR:HG22	3:h:277:ARG:NH1	2.07	0.66
2:M:281:PHE:O	2:M:284:ARG:HD3	1.96	0.66
3:b:276:ARG:NH2	3:b:279:LEU:HG	2.10	0.66
2:e:343:GLN:O	2:e:346:VAL:HG12	1.95	0.66
2:K:25:ASP:OD1	2:M:8:PHE:HZ	1.78	0.66
2:g:193:MET:HE2	2:g:193:MET:HA	1.77	0.66
3:j:220:THR:HG21	3:j:253:GLN:HG3	1.77	0.66
3:l:254:THR:HA	3:l:257:THR:HG23	1.78	0.66
1:4:91:ILE:HG22	1:4:92:LEU:O	1.95	0.66
1:6:27:LEU:O	2:M:268:ARG:HB2	1.95	0.66
2:I:319:GLN:HE22	2:I:336:VAL:HA	1.61	0.66
2:a:193:MET:HE2	2:a:193:MET:HA	1.77	0.66
2:a:383:ALA:H	2:a:389:MET:HE1	1.60	0.66
2:a:386:GLU:O	2:a:389:MET:HB2	1.95	0.66
3:h:205:LEU:HD22	3:h:222:LEU:HB2	1.75	0.66
2:k:147:VAL:HG23	2:k:494:LEU:HD23	1.77	0.66
2:G:199:TYR:HD2	2:G:327:LYS:HZ1	1.43	0.66
2:a:64:ASP:HB3	2:a:67:GLU:HB2	1.76	0.66
3:h:274:LYS:O	3:h:277:ARG:HB2	1.96	0.66
2:A:199:TYR:HD2	2:A:327:LYS:HZ1	1.43	0.66
3:b:236:LEU:HD12	3:b:275:TYR:CD2	2.30	0.66
2:i:305:ILE:HD13	3:j:276:ARG:HH11	1.58	0.66
3:j:201:GLU:O	3:j:204:GLN:NE2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:186:GLU:N	2:e:186:GLU:OE1	2.28	0.66
3:l:236:LEU:HA	3:l:239:LEU:HD13	1.77	0.66
2:I:265:ASN:O	2:I:267:MET:N	2.30	0.66
2:c:186:GLU:OE1	2:c:186:GLU:N	2.28	0.66
2:c:386:GLU:OE1	2:c:386:GLU:N	2.25	0.66
2:m:186:GLU:N	2:m:186:GLU:OE1	2.28	0.66
1:0:66:ILE:O	1:0:92:LEU:HB2	1.96	0.65
2:I:281:PHE:O	2:I:284:ARG:HD3	1.96	0.65
2:K:281:PHE:O	2:K:284:ARG:HD3	1.96	0.65
3:N:237:GLU:HA	3:N:240:PHE:CE2	2.32	0.65
3:D:237:GLU:HA	3:D:240:PHE:CE2	2.32	0.65
3:b:247:LEU:O	3:b:255:ARG:NH1	2.29	0.65
3:h:247:LEU:O	3:h:255:ARG:NH1	2.29	0.65
2:i:130:GLU:HG2	2:i:422:VAL:HG22	1.78	0.65
3:n:261:ILE:HG23	3:n:276:ARG:HH12	1.60	0.65
2:C:281:PHE:O	2:C:284:ARG:HD3	1.96	0.65
2:c:345:ARG:HA	2:c:348:GLN:CD	2.22	0.65
2:i:64:ASP:HB3	2:i:67:GLU:HB2	1.79	0.65
2:A:319:GLN:HE22	2:A:336:VAL:HA	1.61	0.65
3:L:237:GLU:HA	3:L:240:PHE:CE2	2.32	0.65
2:A:8:PHE:HZ	2:C:25:ASP:OD1	1.78	0.65
2:C:286:LYS:NZ	3:D:280:TYR:HE1	1.93	0.65
3:F:237:GLU:HA	3:F:240:PHE:CE2	2.32	0.65
2:G:281:PHE:O	2:G:284:ARG:HD3	1.96	0.65
3:H:237:GLU:HA	3:H:240:PHE:CE2	2.32	0.65
2:c:193:MET:HA	2:c:193:MET:HE2	1.77	0.65
2:c:284:ARG:HD3	2:c:364:LYS:HG2	1.78	0.65
3:h:236:LEU:HA	3:h:239:LEU:HD23	1.78	0.65
2:i:232:GLU:OE1	2:i:232:GLU:N	2.23	0.65
3:n:265:LEU:HG	3:n:269:ASP:CB	2.26	0.65
2:a:186:GLU:OE1	2:a:186:GLU:N	2.30	0.65
2:k:214:GLU:OE1	2:k:322:ARG:NH1	2.30	0.65
3:n:262:LEU:CA	3:n:276:ARG:NH2	2.59	0.65
1:2:66:ILE:O	1:2:92:LEU:HB2	1.96	0.65
2:I:316:ASP:HA	3:J:277:ARG:HH22	1.62	0.65
3:J:237:GLU:HA	3:J:240:PHE:CE2	2.32	0.65
2:K:319:GLN:HE22	2:K:336:VAL:HA	1.61	0.65
2:E:281:PHE:O	2:E:284:ARG:HD3	1.96	0.65
2:M:319:GLN:HE22	2:M:336:VAL:HA	1.61	0.65
3:f:220:THR:HG21	3:f:253:GLN:HG3	1.79	0.65
3:h:236:LEU:HD12	3:h:275:TYR:CD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:247:LEU:HD22	2:i:248:LEU:H	1.62	0.65
1:3:1:MET:HE1	1:4:95:VAL:HG13	1.79	0.65
1:5:27:LEU:HA	2:K:269:GLY:N	2.11	0.65
2:A:281:PHE:O	2:A:284:ARG:HD3	1.96	0.65
3:H:283:LEU:HD12	3:H:284:TYR:H	1.61	0.65
3:b:239:LEU:HA	3:b:242:HIS:CE1	2.31	0.65
1:5:66:ILE:HB	1:5:92:LEU:HB2	1.79	0.64
3:B:237:GLU:HA	3:B:240:PHE:CE2	2.32	0.64
2:i:520:MET:HE1	2:k:38:VAL:HG22	1.80	0.64
1:6:5:PRO:O	1:6:45:ASN:ND2	2.30	0.64
2:e:9:GLY:N	2:e:519:CYS:SG	2.70	0.64
2:e:386:GLU:N	2:e:386:GLU:OE1	2.26	0.64
2:g:130:GLU:HG2	2:g:422:VAL:HG22	1.79	0.64
2:E:319:GLN:HE22	2:E:336:VAL:HA	1.61	0.64
2:I:34:LYS:HE3	2:K:112:ASN:ND2	2.12	0.64
1:3:66:ILE:HB	1:3:92:LEU:CB	2.28	0.64
2:C:319:GLN:HE22	2:C:336:VAL:HA	1.61	0.64
2:E:316:ASP:HA	3:F:277:ARG:HH12	1.61	0.64
1:6:91:ILE:HG22	1:6:92:LEU:O	1.98	0.64
3:n:247:LEU:O	3:n:255:ARG:NH1	2.31	0.64
3:n:265:LEU:HD12	3:n:265:LEU:N	2.12	0.64
3:n:265:LEU:CD1	3:n:276:ARG:HH21	2.11	0.64
3:B:215:ASP:HB3	3:B:218:LEU:CD2	2.28	0.64
2:E:282:GLY:H	2:E:285:ARG:NH2	1.96	0.64
1:0:5:PRO:O	1:0:45:ASN:ND2	2.30	0.64
2:a:39:VAL:O	2:m:521:VAL:HG23	1.97	0.64
2:c:284:ARG:HB2	2:c:368:ARG:HH12	1.62	0.64
3:l:247:LEU:O	3:l:255:ARG:NH1	2.31	0.64
2:A:282:GLY:H	2:A:285:ARG:NH2	1.95	0.64
2:g:513:LEU:HD21	2:i:49:ILE:HG21	1.79	0.64
2:A:59:GLU:O	2:G:4:LYS:HG3	1.99	0.64
2:I:300:VAL:HB	3:J:280:TYR:CE2	2.32	0.64
2:K:415:GLY:HA2	5:K:600:ANP:H1'	1.79	0.64
2:e:1:MET:N	2:e:1:MET:SD	2.70	0.64
3:f:239:LEU:HA	3:f:242:HIS:CE1	2.33	0.64
2:m:386:GLU:O	2:m:389:MET:HB2	1.97	0.64
3:B:283:LEU:HG	3:B:284:TYR:HD2	1.60	0.63
2:M:282:GLY:H	2:M:285:ARG:NH2	1.96	0.63
2:k:386:GLU:OE1	2:k:386:GLU:N	2.25	0.63
2:k:518:GLU:HB3	2:m:36:ARG:CG	2.27	0.63
2:C:267:MET:HE2	2:C:267:MET:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:267:MET:H	2:G:267:MET:HE2	1.64	0.63
2:k:186:GLU:OE1	2:k:186:GLU:N	2.31	0.63
1:2:4:ARG:C	1:3:93:ALA:HB1	2.22	0.63
2:A:308:GLU:HG3	2:A:311:LYS:H	1.64	0.63
2:C:186:GLU:OE1	2:C:186:GLU:N	2.32	0.63
2:C:259:LEU:O	2:C:263:VAL:HG23	1.99	0.63
2:C:308:GLU:HG3	2:C:311:LYS:H	1.64	0.63
2:E:73:MET:HE1	2:M:49:ILE:HD11	1.80	0.63
2:E:225:LYS:HD3	2:E:309:LEU:HD21	1.80	0.63
2:G:286:LYS:NZ	3:H:284:TYR:HB2	2.14	0.63
2:c:305:ILE:HD13	3:d:276:ARG:HH12	1.64	0.63
3:l:261:ILE:HD12	3:l:264:ALA:HB3	1.81	0.63
1:2:6:LEU:HD11	1:3:91:ILE:CG2	2.15	0.63
2:C:282:GLY:H	2:C:285:ARG:NH2	1.96	0.63
2:E:186:GLU:N	2:E:186:GLU:OE1	2.32	0.63
2:G:186:GLU:OE1	2:G:186:GLU:N	2.32	0.63
2:g:388:GLU:HA	2:g:391:GLU:OE2	1.98	0.63
2:m:130:GLU:HG2	2:m:422:VAL:HG22	1.81	0.63
2:A:267:MET:HE2	2:A:267:MET:H	1.64	0.63
2:E:308:GLU:HG3	2:E:311:LYS:H	1.64	0.63
3:L:236:LEU:HA	3:L:239:LEU:HD12	1.81	0.63
2:M:259:LEU:O	2:M:263:VAL:HG23	1.99	0.63
2:a:214:GLU:OE1	2:a:322:ARG:NH1	2.29	0.63
3:l:240:PHE:CE1	3:l:282:LEU:CD2	2.81	0.63
1:1:5:PRO:O	1:1:45:ASN:ND2	2.30	0.63
1:3:5:PRO:O	1:3:45:ASN:ND2	2.30	0.63
2:A:186:GLU:OE1	2:A:186:GLU:N	2.32	0.63
3:F:224:LEU:HG	3:F:228:GLN:HE21	1.64	0.63
2:e:130:GLU:HG2	2:e:422:VAL:HG22	1.80	0.63
3:h:273:SER:O	3:h:277:ARG:HG2	1.98	0.63
2:i:305:ILE:CB	3:j:276:ARG:HH12	2.12	0.63
1:4:27:LEU:H	1:4:27:LEU:CD1	2.11	0.63
3:B:236:LEU:HA	3:B:239:LEU:HD12	1.81	0.63
2:E:223:ALA:O	2:E:251:ALA:HA	1.98	0.63
2:E:267:MET:H	2:E:267:MET:HE2	1.64	0.63
2:G:282:GLY:H	2:G:285:ARG:NH2	1.95	0.63
3:H:236:LEU:HA	3:H:239:LEU:HD12	1.81	0.63
2:I:259:LEU:O	2:I:263:VAL:HG23	1.99	0.63
2:a:25:ASP:OD1	2:m:8:PHE:CE1	2.51	0.63
2:e:345:ARG:O	2:e:349:ILE:HG12	1.99	0.63
3:n:265:LEU:CG	3:n:269:ASP:HB3	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1:MET:HE3	2:A:1:MET:HA	1.80	0.63
2:G:301:ILE:HG21	2:G:309:LEU:HA	1.81	0.63
2:I:282:GLY:H	2:I:285:ARG:NH2	1.96	0.63
2:I:301:ILE:HG21	2:I:309:LEU:HA	1.81	0.63
3:N:236:LEU:HA	3:N:239:LEU:HD12	1.81	0.63
2:i:185:ASP:OD1	2:i:382:GLY:N	2.32	0.63
3:j:239:LEU:HA	3:j:242:HIS:CE1	2.34	0.63
2:k:365:LEU:HG	2:k:368:ARG:HH21	1.64	0.63
2:C:1:MET:HA	2:C:1:MET:HE3	1.81	0.62
2:E:259:LEU:O	2:E:263:VAL:HG23	1.99	0.62
2:c:299:THR:HA	3:d:280:TYR:HE2	1.63	0.62
2:k:185:ASP:OD1	2:k:382:GLY:N	2.30	0.62
2:m:250:ILE:HD13	2:m:276:VAL:HG13	1.81	0.62
1:2:4:ARG:HB3	1:3:94:ILE:HG23	1.80	0.62
2:A:301:ILE:HG21	2:A:309:LEU:HA	1.81	0.62
2:I:186:GLU:OE1	2:I:186:GLU:N	2.32	0.62
3:J:236:LEU:HA	3:J:239:LEU:HD12	1.81	0.62
2:K:1:MET:HA	2:K:1:MET:HE3	1.81	0.62
3:N:283:LEU:HG	3:N:284:TYR:HD2	1.62	0.62
2:c:350:ARG:HA	2:c:350:ARG:HH11	1.64	0.62
3:f:247:LEU:O	3:f:255:ARG:NH1	2.32	0.62
2:m:185:ASP:OD1	2:m:382:GLY:N	2.32	0.62
2:E:1:MET:HA	2:E:1:MET:HE3	1.80	0.62
3:b:243:LEU:HD23	3:b:255:ARG:HH21	1.62	0.62
3:D:236:LEU:HA	3:D:239:LEU:HD12	1.81	0.62
3:F:236:LEU:HA	3:F:239:LEU:HD12	1.81	0.62
2:G:1:MET:HA	2:G:1:MET:HE3	1.81	0.62
2:I:1:MET:HE3	2:I:1:MET:HA	1.81	0.62
2:K:199:TYR:HD2	2:K:327:LYS:HZ1	1.48	0.62
2:K:282:GLY:H	2:K:285:ARG:NH2	1.96	0.62
2:I:308:GLU:HG3	2:I:311:LYS:H	1.64	0.62
2:M:186:GLU:N	2:M:186:GLU:OE1	2.32	0.62
2:M:300:VAL:HB	3:N:280:TYR:CE2	2.25	0.62
2:M:308:GLU:HG3	2:M:311:LYS:H	1.64	0.62
3:B:273:SER:HB2	3:B:277:ARG:NH1	2.14	0.62
2:K:364:LYS:O	2:K:368:ARG:HG3	2.00	0.62
2:c:172:GLU:OE1	2:c:172:GLU:N	2.33	0.62
3:j:244:ARG:NH1	3:j:244:ARG:HA	2.14	0.62
3:j:274:LYS:HA	3:j:277:ARG:CG	2.28	0.62
2:C:309:LEU:H	2:C:309:LEU:HD12	1.65	0.62
2:I:364:LYS:O	2:I:368:ARG:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:186:GLU:OE1	2:K:186:GLU:N	2.32	0.62
2:M:267:MET:H	2:M:267:MET:HE2	1.64	0.62
3:b:220:THR:HG21	3:b:253:GLN:HG3	1.80	0.62
2:g:69:MET:HE1	2:g:523:ASP:HB2	1.82	0.62
2:G:259:LEU:O	2:G:263:VAL:HG23	1.99	0.62
2:K:267:MET:H	2:K:267:MET:HE2	1.64	0.62
2:K:308:GLU:HG3	2:K:311:LYS:H	1.64	0.62
2:M:364:LYS:O	2:M:368:ARG:HG3	2.00	0.62
3:b:208:GLN:HA	3:b:211:GLU:HB2	1.81	0.62
2:A:49:ILE:CD1	2:G:73:MET:HE1	2.29	0.62
2:C:364:LYS:O	2:C:368:ARG:HG3	2.00	0.62
2:G:309:LEU:H	2:G:309:LEU:HD12	1.65	0.62
2:K:259:LEU:O	2:K:263:VAL:HG23	1.99	0.62
3:f:207:GLN:OE1	3:f:207:GLN:N	2.33	0.62
3:j:274:LYS:O	3:j:277:ARG:HB2	2.00	0.62
2:k:4:LYS:CE	2:m:59:GLU:CG	2.44	0.62
2:k:493:ILE:HG12	5:k:603:ANP:N1	2.14	0.62
2:k:518:GLU:CB	2:m:36:ARG:CG	2.78	0.62
2:G:308:GLU:HG3	2:G:311:LYS:H	1.64	0.61
3:b:273:SER:O	3:b:277:ARG:HG2	1.99	0.61
3:d:198:ASP:OD2	3:d:203:GLN:NE2	2.33	0.61
3:f:243:LEU:HD23	3:f:255:ARG:HH21	1.65	0.61
2:A:259:LEU:O	2:A:263:VAL:HG23	1.99	0.61
2:C:301:ILE:HG21	2:C:309:LEU:HA	1.81	0.61
2:E:301:ILE:HG21	2:E:309:LEU:HA	1.81	0.61
2:I:265:ASN:C	2:I:267:MET:N	2.53	0.61
2:I:345:ARG:CD	2:I:372:LEU:HD22	2.29	0.61
2:K:301:ILE:HG21	2:K:309:LEU:HA	1.81	0.61
3:h:274:LYS:HA	3:h:277:ARG:CG	2.30	0.61
1:0:55:LYS:HD2	1:0:56:PRO:HD2	1.82	0.61
1:0:66:ILE:HB	1:0:92:LEU:HB2	1.82	0.61
1:3:17:VAL:HG21	1:3:36:THR:H	1.65	0.61
2:G:364:LYS:O	2:G:368:ARG:HG3	2.00	0.61
2:M:316:ASP:HA	3:N:277:ARG:HH12	1.64	0.61
3:d:274:LYS:O	3:d:277:ARG:HB2	1.99	0.61
1:2:1:MET:HE1	1:3:95:VAL:HG13	1.82	0.61
1:4:66:ILE:C	1:4:92:LEU:HB2	2.24	0.61
1:5:66:ILE:O	1:5:92:LEU:HB2	2.00	0.61
2:M:286:LYS:HZ1	3:N:284:TYR:HB2	1.65	0.61
2:e:140:ASP:OD1	2:e:141:SER:N	2.33	0.61
2:e:522:THR:HG21	2:g:59:GLU:OE2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:55:LYS:HD2	1:1:56:PRO:HD2	1.82	0.61
2:A:364:LYS:O	2:A:368:ARG:HG3	2.00	0.61
2:M:1:MET:HA	2:M:1:MET:HE3	1.81	0.61
2:M:301:ILE:HG21	2:M:309:LEU:HA	1.81	0.61
2:M:309:LEU:HD12	2:M:309:LEU:H	1.65	0.61
2:a:299:THR:HG22	3:b:277:ARG:HH22	1.66	0.61
2:c:365:LEU:HA	2:c:368:ARG:HE	1.65	0.61
1:6:55:LYS:HD2	1:6:56:PRO:HD2	1.82	0.61
2:E:309:LEU:HD12	2:E:309:LEU:H	1.65	0.61
2:K:34:LYS:HG2	2:M:112:ASN:HD21	1.66	0.61
2:c:140:ASP:OD1	2:c:141:SER:N	2.33	0.61
3:H:273:SER:HB2	3:H:277:ARG:NH1	2.15	0.61
2:I:313:THR:HB	3:J:267:THR:HA	1.82	0.61
2:m:140:ASP:OD1	2:m:141:SER:N	2.34	0.61
3:n:237:GLU:OE1	3:n:237:GLU:N	2.22	0.61
1:1:17:VAL:HG21	1:1:36:THR:H	1.65	0.61
2:A:38:VAL:HG22	2:G:519:CYS:HB3	1.83	0.61
2:c:346:VAL:HA	2:c:349:ILE:HG12	1.83	0.61
2:g:172:GLU:N	2:g:172:GLU:OE1	2.33	0.61
2:g:252:GLU:HG3	2:g:285:ARG:HH12	1.66	0.61
1:2:5:PRO:O	1:2:45:ASN:ND2	2.30	0.61
1:2:17:VAL:HG21	1:2:36:THR:H	1.65	0.61
1:2:66:ILE:HB	1:2:92:LEU:HB2	1.81	0.61
1:4:17:VAL:HG21	1:4:36:THR:H	1.66	0.61
1:6:17:VAL:HG21	1:6:36:THR:H	1.66	0.61
3:F:283:LEU:HG	3:F:284:TYR:HD2	1.60	0.61
2:g:69:MET:HE2	2:i:41:ASP:HB2	1.83	0.61
3:l:208:GLN:HA	3:l:211:GLU:HB2	1.82	0.61
1:5:5:PRO:O	1:5:45:ASN:ND2	2.30	0.61
2:A:73:MET:HG2	2:C:47:PRO:HG2	1.83	0.61
2:a:203:TYR:CE2	2:c:181:THR:HG23	2.35	0.61
2:c:214:GLU:OE1	2:c:322:ARG:NH1	2.31	0.61
1:5:17:VAL:HG21	1:5:36:THR:H	1.66	0.60
2:i:305:ILE:HD13	3:j:276:ARG:HH12	1.57	0.60
2:E:364:LYS:O	2:E:368:ARG:HG3	2.00	0.60
2:I:309:LEU:H	2:I:309:LEU:HD12	1.65	0.60
2:k:387:VAL:O	2:k:391:GLU:HG3	2.01	0.60
3:n:243:LEU:HD23	3:n:255:ARG:HH21	1.64	0.60
1:4:55:LYS:HD2	1:4:56:PRO:HD2	1.82	0.60
3:D:273:SER:O	3:D:277:ARG:HG2	2.02	0.60
2:K:309:LEU:H	2:K:309:LEU:HD12	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:254:THR:OG1	3:h:255:ARG:NH2	2.34	0.60
2:k:164:GLU:HG3	2:k:187:LEU:HD21	1.83	0.60
1:5:9:ARG:HH22	1:6:93:ALA:N	2.00	0.60
1:6:66:ILE:HB	1:6:92:LEU:HB2	1.82	0.60
2:m:415:GLY:N	5:m:603:ANP:O2'	2.32	0.60
2:K:25:ASP:OD1	2:M:8:PHE:CZ	2.53	0.60
2:g:140:ASP:OD1	2:g:141:SER:N	2.35	0.60
1:2:13:LYS:HG3	1:2:41:LEU:HD22	1.83	0.60
1:4:66:ILE:HB	1:4:92:LEU:HB2	1.83	0.60
1:5:55:LYS:HD2	1:5:56:PRO:HD2	1.82	0.60
2:A:8:PHE:CZ	2:C:25:ASP:OD1	2.55	0.60
2:A:309:LEU:H	2:A:309:LEU:HD12	1.65	0.60
3:h:208:GLN:HA	3:h:211:GLU:HB2	1.83	0.60
2:k:299:THR:HA	3:l:280:TYR:HE2	1.61	0.60
1:2:46:GLY:H	1:2:57:LEU:HD22	1.67	0.60
1:2:55:LYS:HD2	1:2:56:PRO:HD2	1.82	0.60
1:3:46:GLY:H	1:3:57:LEU:HD22	1.67	0.60
1:5:13:LYS:HG3	1:5:41:LEU:HD22	1.83	0.60
1:5:46:GLY:H	1:5:57:LEU:HD22	1.67	0.60
1:6:13:LYS:HG3	1:6:41:LEU:HD22	1.83	0.60
2:k:140:ASP:OD1	2:k:141:SER:N	2.34	0.60
3:l:240:PHE:CZ	3:l:282:LEU:HD21	2.35	0.60
1:0:17:VAL:HG21	1:0:36:THR:H	1.65	0.60
1:1:13:LYS:HG3	1:1:41:LEU:HD22	1.83	0.60
2:M:199:TYR:HD2	2:M:327:LYS:HZ1	1.50	0.60
2:e:77:VAL:HG21	2:e:510:VAL:HB	1.82	0.60
3:f:198:ASP:OD2	3:f:203:GLN:NE2	2.35	0.60
2:i:77:VAL:HG21	2:i:510:VAL:HB	1.83	0.60
2:i:140:ASP:OD1	2:i:141:SER:N	2.34	0.60
1:0:46:GLY:H	1:0:57:LEU:HD22	1.67	0.60
2:I:266:THR:HB	2:I:267:MET:CE	2.31	0.60
2:a:140:ASP:OD1	2:a:141:SER:N	2.34	0.60
2:e:388:GLU:HA	2:e:391:GLU:OE1	2.02	0.60
2:i:250:ILE:HD13	2:i:276:VAL:HG13	1.84	0.60
2:i:388:GLU:HA	2:i:391:GLU:OE1	2.02	0.60
2:m:387:VAL:HA	2:m:390:LYS:NZ	2.17	0.60
1:0:27:LEU:HA	2:E:269:GLY:CA	2.32	0.59
1:3:55:LYS:HD2	1:3:56:PRO:HD2	1.82	0.59
2:E:300:VAL:HB	3:F:280:TYR:HE2	1.67	0.59
2:a:59:GLU:O	2:m:4:LYS:HD2	2.02	0.59
2:a:520:MET:CE	2:c:38:VAL:HG22	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:198:ASP:OD2	3:b:203:GLN:NE2	2.35	0.59
3:d:208:GLN:HA	3:d:211:GLU:HB2	1.82	0.59
3:f:276:ARG:HH21	3:f:279:LEU:C	2.10	0.59
2:k:250:ILE:HD13	2:k:276:VAL:HG13	1.83	0.59
1:0:27:LEU:HD23	2:E:269:GLY:HA2	1.84	0.59
1:1:46:GLY:H	1:1:57:LEU:HD22	1.67	0.59
2:A:40:LEU:HD23	2:G:521:VAL:HB	1.84	0.59
3:n:201:GLU:OE1	3:n:201:GLU:N	2.30	0.59
2:c:252:GLU:HG3	2:c:285:ARG:HH12	1.67	0.59
2:e:54:VAL:HG23	5:e:603:ANP:O2G	2.02	0.59
2:k:365:LEU:HA	2:k:368:ARG:HE	1.67	0.59
1:3:13:LYS:HG3	1:3:41:LEU:HD22	1.83	0.59
1:4:46:GLY:H	1:4:57:LEU:HD22	1.67	0.59
2:a:28:LYS:HG2	2:a:94:VAL:HG22	1.84	0.59
3:f:208:GLN:HA	3:f:211:GLU:HB2	1.83	0.59
1:4:5:PRO:O	1:4:45:ASN:ND2	2.30	0.59
2:G:315:GLU:OE1	3:H:270:ALA:CA	2.50	0.59
2:I:294:THR:HG21	2:I:345:ARG:HB2	1.85	0.59
3:J:240:PHE:HA	3:J:243:LEU:HD23	1.85	0.59
3:L:283:LEU:HG	3:L:284:TYR:HD2	1.64	0.59
3:h:244:ARG:HA	3:h:244:ARG:NH1	2.17	0.59
1:4:13:LYS:HG3	1:4:41:LEU:HD22	1.83	0.59
3:L:240:PHE:HA	3:L:243:LEU:HD23	1.85	0.59
2:c:325:ILE:HD13	2:c:330:THR:HG22	1.83	0.59
1:0:91:ILE:HG22	1:6:6:LEU:HD11	1.85	0.59
1:3:4:ARG:HB3	1:4:94:ILE:HG22	1.84	0.59
2:I:266:THR:C	2:I:267:MET:SD	2.85	0.59
2:I:307:MET:HE1	3:J:262:LEU:CD1	2.33	0.59
2:a:299:THR:HA	3:b:280:TYR:HE2	1.68	0.59
2:g:77:VAL:HG21	2:g:510:VAL:HB	1.83	0.59
3:l:244:ARG:HH11	3:l:244:ARG:HA	1.68	0.59
3:N:240:PHE:HA	3:N:243:LEU:HD23	1.85	0.59
2:c:28:LYS:HG2	2:c:94:VAL:HG22	1.84	0.59
3:H:240:PHE:HA	3:H:243:LEU:HD23	1.85	0.59
3:h:201:GLU:O	3:h:204:GLN:NE2	2.36	0.59
2:m:325:ILE:HD13	2:m:330:THR:HG22	1.85	0.59
1:0:9:ARG:HH22	1:1:92:LEU:HA	1.68	0.58
1:0:13:LYS:HG3	1:0:41:LEU:HD22	1.83	0.58
2:K:215:LEU:HD23	2:K:246:PRO:HG2	1.85	0.58
2:i:28:LYS:HG2	2:i:94:VAL:HG22	1.85	0.58
2:k:28:LYS:HG2	2:k:94:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:203:TYR:CE1	2:m:181:THR:HG23	2.38	0.58
3:n:272:ALA:O	3:n:276:ARG:HG2	2.03	0.58
2:c:353:ILE:HD11	2:c:362:ARG:HD3	1.85	0.58
3:n:220:THR:O	3:n:224:LEU:HG	2.03	0.58
2:E:223:ALA:HB3	2:E:251:ALA:HB2	1.85	0.58
3:d:244:ARG:NH1	3:d:244:ARG:HA	2.17	0.58
2:g:250:ILE:HD13	2:g:276:VAL:HG13	1.86	0.58
1:3:6:LEU:HD21	1:4:91:ILE:CB	2.22	0.58
1:3:8:ASP:OD1	1:3:47:ARG:HA	2.03	0.58
2:A:34:LYS:HG2	2:G:112:ASN:HD21	1.68	0.58
3:B:240:PHE:HA	3:B:243:LEU:HD23	1.85	0.58
2:a:4:LYS:HE2	2:c:59:GLU:HG3	1.86	0.58
2:c:387:VAL:HA	2:c:390:LYS:NZ	2.18	0.58
2:k:202:PRO:HB3	2:m:384:ALA:O	2.03	0.58
1:6:46:GLY:H	1:6:57:LEU:HD22	1.67	0.58
2:c:305:ILE:HD13	3:d:276:ARG:NH1	2.18	0.58
2:g:365:LEU:HA	2:g:368:ARG:HE	1.68	0.58
1:6:66:ILE:C	1:6:92:LEU:HB2	2.28	0.58
2:I:197:ARG:HD3	2:I:277:LYS:HE2	1.86	0.58
3:f:252:GLY:O	3:f:256:LYS:NZ	2.34	0.58
2:i:304:GLU:HB2	3:j:283:LEU:CD2	2.33	0.58
2:k:4:LYS:HE2	2:m:59:GLU:HG3	0.70	0.58
2:k:316:ASP:C	3:l:277:ARG:HH22	2.11	0.58
2:a:387:VAL:HG12	2:a:390:LYS:NZ	2.19	0.58
2:a:388:GLU:HA	2:a:391:GLU:OE2	2.03	0.58
2:k:305:ILE:HG12	3:l:283:LEU:HD21	1.84	0.58
3:l:244:ARG:HA	3:l:244:ARG:NH1	2.18	0.58
2:m:28:LYS:HG2	2:m:94:VAL:HG22	1.86	0.58
1:0:40:VAL:HG21	1:0:59:VAL:HG12	1.86	0.58
1:5:6:LEU:HD21	1:6:91:ILE:HB	1.86	0.58
3:f:261:ILE:HD12	3:f:264:ALA:HB3	1.85	0.58
2:g:28:LYS:HG2	2:g:94:VAL:HG22	1.86	0.58
2:g:387:VAL:O	2:g:391:GLU:HG3	2.04	0.58
3:j:236:LEU:HA	3:j:239:LEU:HD13	1.86	0.58
3:j:277:ARG:O	3:j:280:TYR:HB2	2.03	0.58
3:L:278:GLN:O	3:L:281:ALA:N	2.37	0.58
2:a:41:ASP:HB2	2:m:69:MET:SD	2.44	0.58
3:b:244:ARG:NH1	3:b:244:ARG:HA	2.19	0.58
2:I:346:VAL:O	2:I:349:ILE:N	2.37	0.58
2:m:493:ILE:CG1	5:m:603:ANP:C6	2.82	0.58
3:n:244:ARG:NE	3:n:244:ARG:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:n:273:SER:O	3:n:276:ARG:HB2	2.04	0.58
1:1:40:VAL:HG21	1:1:59:VAL:HG12	1.86	0.57
2:A:233:MET:HA	2:A:310:GLU:CD	2.29	0.57
3:J:273:SER:HB2	3:J:277:ARG:NH1	2.19	0.57
3:N:283:LEU:CG	3:N:284:TYR:CD2	2.84	0.57
3:d:273:SER:O	3:d:277:ARG:HG2	2.04	0.57
2:m:387:VAL:O	2:m:391:GLU:HG3	2.04	0.57
3:F:240:PHE:HA	3:F:243:LEU:HD23	1.85	0.57
2:I:305:ILE:HD11	3:J:280:TYR:CD1	2.40	0.57
2:I:307:MET:HE1	3:J:262:LEU:HD13	1.86	0.57
2:c:345:ARG:O	2:c:348:GLN:HB2	2.05	0.57
2:g:296:THR:OG1	2:g:319:GLN:O	2.21	0.57
3:j:277:ARG:HA	3:j:280:TYR:HD2	1.68	0.57
3:l:207:GLN:N	3:l:207:GLN:OE1	2.36	0.57
1:3:66:ILE:HD12	1:3:93:ALA:O	2.04	0.57
2:C:226:LYS:NZ	2:C:228:SER:HB3	2.20	0.57
2:K:226:LYS:NZ	2:K:228:SER:HB3	2.20	0.57
2:k:387:VAL:HA	2:k:390:LYS:NZ	2.20	0.57
1:2:6:LEU:HD21	1:3:91:ILE:CG2	2.34	0.57
1:3:8:ASP:HA	1:3:46:GLY:O	2.05	0.57
2:G:226:LYS:NZ	2:G:228:SER:HB3	2.20	0.57
2:e:28:LYS:HG2	2:e:94:VAL:HG22	1.87	0.57
2:E:226:LYS:NZ	2:E:228:SER:HB3	2.20	0.57
3:F:273:SER:HB2	3:F:277:ARG:NH1	2.20	0.57
3:j:244:ARG:HA	3:j:244:ARG:HH11	1.69	0.57
3:D:240:PHE:HA	3:D:243:LEU:HD23	1.85	0.57
2:a:387:VAL:HG23	2:a:388:GLU:N	2.20	0.57
3:b:254:THR:OG1	3:b:255:ARG:NH2	2.38	0.57
2:c:162:ILE:O	2:c:166:MET:HG2	2.04	0.57
2:e:387:VAL:HA	2:e:390:LYS:NZ	2.20	0.57
1:2:9:ARG:O	1:2:44:GLY:HA3	2.04	0.57
3:B:218:LEU:HD12	3:B:219:ALA:H	1.68	0.57
3:D:244:ARG:O	3:D:244:ARG:NH1	2.35	0.57
2:G:349:ILE:O	2:G:353:ILE:HG13	2.05	0.57
3:J:244:ARG:O	3:J:244:ARG:NH1	2.35	0.57
2:M:226:LYS:NZ	2:M:228:SER:HB3	2.20	0.57
3:b:220:THR:O	3:b:224:LEU:HG	2.04	0.57
2:c:250:ILE:HD13	2:c:276:VAL:HG13	1.86	0.57
1:6:40:VAL:HG21	1:6:59:VAL:HG12	1.86	0.57
2:A:349:ILE:O	2:A:353:ILE:HG13	2.05	0.57
3:J:273:SER:HB2	3:J:277:ARG:CZ	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:274:LYS:O	3:f:277:ARG:HB2	2.04	0.57
2:k:493:ILE:CG1	5:k:603:ANP:C6	2.77	0.57
3:l:252:GLY:O	3:l:256:LYS:NZ	2.33	0.57
1:2:40:VAL:HG21	1:2:59:VAL:HG12	1.86	0.57
2:k:520:MET:HE1	2:m:38:VAL:CG2	2.19	0.57
2:C:349:ILE:O	2:C:353:ILE:HG13	2.05	0.57
3:F:244:ARG:O	3:F:244:ARG:NH1	2.35	0.57
2:a:172:GLU:H	2:a:172:GLU:CD	2.12	0.57
3:b:277:ARG:NH1	3:b:280:TYR:OH	2.36	0.57
3:l:220:THR:O	3:l:224:LEU:HG	2.04	0.57
2:A:226:LYS:NZ	2:A:228:SER:HB3	2.20	0.56
2:A:300:VAL:HB	3:B:280:TYR:HE2	1.70	0.56
3:D:283:LEU:HG	3:D:284:TYR:HD2	1.69	0.56
2:M:349:ILE:O	2:M:353:ILE:HG13	2.05	0.56
3:d:252:GLY:O	3:d:256:LYS:NZ	2.33	0.56
2:e:305:ILE:HG21	3:f:276:ARG:HH12	1.70	0.56
3:f:259:GLN:HA	3:f:262:LEU:HD21	1.87	0.56
2:m:9:GLY:N	2:m:519:CYS:SG	2.77	0.56
1:4:66:ILE:HB	1:4:92:LEU:HB3	1.87	0.56
2:K:349:ILE:O	2:K:353:ILE:HG13	2.05	0.56
2:k:217:SER:O	2:k:245:LYS:NZ	2.37	0.56
2:m:333:ILE:HD12	2:m:334:ASP:HB2	1.87	0.56
1:0:27:LEU:HA	2:E:269:GLY:HA2	1.87	0.56
1:3:4:ARG:C	1:4:93:ALA:HB1	2.31	0.56
1:4:27:LEU:O	2:I:265:ASN:HA	2.04	0.56
3:B:244:ARG:O	3:B:244:ARG:NH1	2.35	0.56
3:D:277:ARG:O	3:D:280:TYR:N	2.38	0.56
3:H:244:ARG:O	3:H:244:ARG:NH1	2.35	0.56
2:I:226:LYS:NZ	2:I:228:SER:HB3	2.20	0.56
2:I:344:GLY:C	2:I:346:VAL:N	2.59	0.56
2:a:523:ASP:OD1	2:a:524:LEU:N	2.38	0.56
2:c:333:ILE:HD12	2:c:334:ASP:HB2	1.88	0.56
3:d:220:THR:O	3:d:224:LEU:HG	2.04	0.56
2:e:185:ASP:OD1	2:e:382:GLY:N	2.38	0.56
2:e:333:ILE:HD12	2:e:334:ASP:HB2	1.87	0.56
2:g:214:GLU:OE1	2:g:322:ARG:NH1	2.35	0.56
2:g:346:VAL:HA	2:g:349:ILE:HG12	1.87	0.56
2:g:521:VAL:HG23	2:i:39:VAL:HB	1.86	0.56
3:h:274:LYS:HA	3:h:277:ARG:HG2	1.88	0.56
2:i:387:VAL:HA	2:i:390:LYS:NZ	2.19	0.56
2:k:385:THR:OG1	2:k:388:GLU:OE1	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:345:ARG:NH1	2:m:349:ILE:HD11	2.21	0.56
1:3:40:VAL:HG21	1:3:59:VAL:HG12	1.86	0.56
1:4:27:LEU:HA	2:I:268:ARG:HB3	1.87	0.56
2:a:196:ASP:O	2:a:197:ARG:NH1	2.36	0.56
3:b:237:GLU:CD	3:b:237:GLU:H	2.13	0.56
2:e:252:GLU:HG3	2:e:285:ARG:HH12	1.71	0.56
3:f:220:THR:O	3:f:224:LEU:HG	2.05	0.56
2:g:9:GLY:N	2:g:519:CYS:SG	2.78	0.56
2:i:304:GLU:HB2	3:j:283:LEU:HD23	1.87	0.56
2:k:156:GLU:OE1	2:k:156:GLU:N	2.36	0.56
2:k:252:GLU:HG3	2:k:285:ARG:HH12	1.70	0.56
2:k:333:ILE:HD12	2:k:334:ASP:HB2	1.88	0.56
2:C:292:ILE:O	2:C:296:THR:OG1	2.21	0.56
3:J:278:GLN:O	3:J:281:ALA:N	2.39	0.56
3:b:235:ALA:O	3:b:238:LEU:HG	2.06	0.56
1:2:27:LEU:CD2	2:A:269:GLY:HA3	2.29	0.56
2:E:349:ILE:O	2:E:353:ILE:HG13	2.05	0.56
2:a:77:VAL:HG21	2:a:510:VAL:HB	1.87	0.56
3:f:274:LYS:HA	3:f:277:ARG:CG	2.34	0.56
2:g:387:VAL:HA	2:g:390:LYS:NZ	2.20	0.56
2:A:112:ASN:ND2	2:C:34:LYS:HE3	2.20	0.56
2:G:315:GLU:OE1	3:H:270:ALA:N	2.39	0.56
2:a:252:GLU:HG3	2:a:285:ARG:HH12	1.71	0.56
1:3:66:ILE:HB	1:3:92:LEU:HB3	1.86	0.56
1:4:28:THR:HA	2:I:264:VAL:HG12	1.88	0.56
2:I:349:ILE:O	2:I:353:ILE:HG13	2.05	0.56
3:f:244:ARG:NE	3:f:244:ARG:O	2.38	0.56
1:2:5:PRO:HA	1:3:93:ALA:HB2	1.88	0.56
3:F:278:GLN:O	3:F:281:ALA:N	2.39	0.56
2:c:9:GLY:N	2:c:519:CYS:SG	2.79	0.56
2:e:299:THR:HG22	3:f:277:ARG:HH22	1.71	0.56
2:i:223:ALA:HA	2:i:301:ILE:HB	1.87	0.56
2:k:520:MET:HE3	2:m:37:ASN:O	2.06	0.56
2:k:522:THR:CB	2:m:40:LEU:CD2	2.76	0.56
1:6:27:LEU:HG	2:M:269:GLY:HA3	1.88	0.56
2:C:313:THR:HG1	2:C:315:GLU:HG3	1.71	0.56
2:I:286:LYS:HE2	3:J:284:TYR:CD2	2.41	0.56
2:a:333:ILE:HD12	2:a:334:ASP:HB2	1.88	0.56
1:5:38:GLY:HA3	1:5:67:PHE:HZ	1.71	0.55
1:5:40:VAL:HG21	1:5:59:VAL:HG12	1.86	0.55
2:A:195:PHE:HB3	2:A:279:PRO:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:236:LEU:HD11	3:F:275:TYR:HD2	1.70	0.55
2:G:195:PHE:HB3	2:G:279:PRO:HG3	1.88	0.55
3:L:273:SER:O	3:L:277:ARG:HG2	2.06	0.55
2:e:518:GLU:HB3	2:g:36:ARG:HB3	1.87	0.55
3:j:252:GLY:O	3:j:256:LYS:NZ	2.34	0.55
2:k:4:LYS:CD	2:m:59:GLU:HG3	2.31	0.55
3:l:243:LEU:HD23	3:l:255:ARG:HH21	1.71	0.55
1:2:4:ARG:HB3	1:3:94:ILE:HG22	1.88	0.55
1:3:6:LEU:HD13	1:3:9:ARG:NH1	2.16	0.55
2:I:34:LYS:HG2	2:K:112:ASN:HD21	1.70	0.55
3:d:243:LEU:HD13	3:d:282:LEU:HD22	1.87	0.55
3:f:254:THR:OG1	3:f:255:ARG:NH2	2.40	0.55
3:j:220:THR:O	3:j:224:LEU:HG	2.05	0.55
1:4:40:VAL:HG21	1:4:59:VAL:HG12	1.86	0.55
2:E:222:LEU:HB2	2:E:299:THR:O	2.07	0.55
2:a:386:GLU:HG3	2:a:387:VAL:N	2.22	0.55
2:c:300:VAL:HG23	3:d:280:TYR:CD2	2.37	0.55
3:h:235:ALA:O	3:h:238:LEU:HG	2.07	0.55
2:I:195:PHE:HB3	2:I:279:PRO:HG3	1.88	0.55
3:d:254:THR:OG1	3:d:255:ARG:NH2	2.40	0.55
2:i:9:GLY:N	2:i:519:CYS:SG	2.79	0.55
3:j:243:LEU:HD23	3:j:255:ARG:HH21	1.69	0.55
1:2:27:LEU:HA	2:A:269:GLY:CA	2.37	0.55
1:3:6:LEU:CD1	1:3:9:ARG:HH22	2.20	0.55
2:c:387:VAL:O	2:c:391:GLU:HG3	2.06	0.55
3:d:243:LEU:HD11	3:d:258:PHE:CE2	2.42	0.55
2:e:296:THR:OG1	2:e:319:GLN:O	2.23	0.55
2:i:214:GLU:OE1	2:i:322:ARG:NH1	2.33	0.55
2:i:333:ILE:HD12	2:i:334:ASP:HB2	1.88	0.55
1:1:38:GLY:HA3	1:1:67:PHE:HZ	1.71	0.55
1:5:28:THR:OG1	1:5:29:GLY:N	2.31	0.55
2:A:73:MET:HE1	2:C:49:ILE:CD1	2.33	0.55
2:E:369:VAL:HA	2:E:372:LEU:HD12	1.89	0.55
3:F:257:THR:O	3:F:261:ILE:HG12	2.07	0.55
2:I:344:GLY:O	2:I:345:ARG:C	2.50	0.55
3:N:257:THR:O	3:N:261:ILE:HG12	2.07	0.55
2:i:252:GLU:HG3	2:i:285:ARG:HH12	1.70	0.55
2:i:305:ILE:CD1	3:j:276:ARG:HH12	2.12	0.55
3:D:257:THR:O	3:D:261:ILE:HG12	2.07	0.55
3:H:244:ARG:HA	3:H:282:LEU:HD21	1.88	0.55
3:H:257:THR:O	3:H:261:ILE:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:520:MET:CE	2:e:38:VAL:HG13	2.37	0.55
2:e:38:VAL:HG11	2:e:56:VAL:HG22	1.89	0.55
2:e:156:GLU:OE1	2:e:156:GLU:N	2.35	0.55
2:g:185:ASP:OD1	2:g:382:GLY:N	2.36	0.55
2:k:38:VAL:HG11	2:k:56:VAL:HG22	1.89	0.55
1:3:9:ARG:HA	1:3:88:GLU:HB2	1.89	0.55
1:3:67:PHE:CA	1:3:92:LEU:HD23	2.37	0.55
2:I:369:VAL:HA	2:I:372:LEU:HD12	1.89	0.55
3:J:257:THR:O	3:J:261:ILE:HG12	2.07	0.55
2:K:224:ASP:HB2	2:K:300:VAL:HG12	1.89	0.55
2:M:195:PHE:HB3	2:M:279:PRO:HG3	1.88	0.55
3:N:253:GLN:O	3:N:257:THR:HG23	2.07	0.55
2:a:26:ALA:HA	2:m:520:MET:HG2	1.89	0.55
2:a:250:ILE:HD13	2:a:276:VAL:HG13	1.89	0.55
3:h:252:GLY:O	3:h:256:LYS:NZ	2.30	0.55
3:H:253:GLN:O	3:H:257:THR:HG23	2.07	0.55
2:I:350:ARG:HA	2:I:353:ILE:HD12	1.89	0.55
3:b:252:GLY:O	3:b:256:LYS:NZ	2.34	0.55
2:k:521:VAL:HG21	2:m:39:VAL:HB	1.79	0.55
3:l:275:TYR:HA	3:l:278:GLN:HG2	1.88	0.55
1:1:63:ASP:HB3	1:1:94:ILE:HD13	1.89	0.55
1:2:38:GLY:HA3	1:2:67:PHE:HZ	1.71	0.55
3:B:257:THR:O	3:B:261:ILE:HG12	2.07	0.55
3:D:253:GLN:O	3:D:257:THR:HG23	2.07	0.55
3:F:202:ILE:HG12	3:F:225:GLN:HG3	1.88	0.55
2:K:369:VAL:HA	2:K:372:LEU:HD12	1.89	0.55
3:L:244:ARG:O	3:L:244:ARG:NH1	2.35	0.55
2:M:224:ASP:HB2	2:M:300:VAL:HG12	1.89	0.55
2:c:324:VAL:HB	2:c:331:THR:OG1	2.07	0.55
2:e:299:THR:HG22	3:f:277:ARG:NH2	2.21	0.55
2:g:284:ARG:HB2	2:g:368:ARG:HH12	1.71	0.55
1:0:25:ILE:HD12	1:0:27:LEU:HD12	1.89	0.54
1:3:38:GLY:HA3	1:3:67:PHE:HZ	1.71	0.54
1:4:6:LEU:HD21	1:5:91:ILE:HB	1.89	0.54
2:A:254:VAL:HG21	2:A:275:ALA:HB1	1.90	0.54
3:B:253:GLN:O	3:B:257:THR:HG23	2.07	0.54
2:C:195:PHE:HB3	2:C:279:PRO:HG3	1.88	0.54
2:E:350:ARG:HA	2:E:353:ILE:HD12	1.89	0.54
2:G:350:ARG:HA	2:G:353:ILE:HD12	1.89	0.54
3:N:244:ARG:O	3:N:244:ARG:NH1	2.35	0.54
3:j:274:LYS:HA	3:j:277:ARG:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:388:GLU:HA	2:m:391:GLU:OE2	2.07	0.54
1:3:15:LYS:NZ	1:3:39:GLU:H	2.05	0.54
2:E:195:PHE:HB3	2:E:279:PRO:HG3	1.88	0.54
2:I:224:ASP:HB2	2:I:300:VAL:HG12	1.89	0.54
2:a:185:ASP:OD1	2:a:382:GLY:N	2.40	0.54
2:a:518:GLU:HB3	2:c:36:ARG:HB3	1.90	0.54
2:c:38:VAL:HG11	2:c:56:VAL:HG22	1.88	0.54
2:k:1:MET:HE3	2:k:4:LYS:HZ1	1.73	0.54
2:k:324:VAL:HB	2:k:331:THR:OG1	2.08	0.54
2:C:199:TYR:HD2	2:C:327:LYS:HZ1	1.54	0.54
2:G:254:VAL:HG21	2:G:275:ALA:HB1	1.90	0.54
2:K:254:VAL:HG21	2:K:275:ALA:HB1	1.90	0.54
2:M:254:VAL:HG21	2:M:275:ALA:HB1	1.90	0.54
2:g:305:ILE:CD1	3:h:276:ARG:HH12	2.18	0.54
2:m:77:VAL:HG21	2:m:510:VAL:HB	1.89	0.54
1:0:18:GLU:HA	1:0:31:ALA:HB1	1.90	0.54
1:4:15:LYS:NZ	1:4:39:GLU:H	2.05	0.54
1:4:38:GLY:HA3	1:4:67:PHE:HZ	1.71	0.54
3:L:257:THR:O	3:L:261:ILE:HG12	2.07	0.54
2:e:520:MET:CE	2:g:38:VAL:HG22	2.24	0.54
2:g:333:ILE:HD12	2:g:334:ASP:HB2	1.88	0.54
2:k:9:GLY:N	2:k:519:CYS:SG	2.80	0.54
3:n:258:PHE:HE1	3:n:275:TYR:HE1	1.56	0.54
3:n:259:GLN:HA	3:n:262:LEU:HD21	1.90	0.54
1:0:38:GLY:HA3	1:0:67:PHE:HZ	1.71	0.54
1:1:15:LYS:NZ	1:1:39:GLU:H	2.05	0.54
1:3:18:GLU:HA	1:3:31:ALA:HB1	1.90	0.54
2:C:350:ARG:HA	2:C:353:ILE:HD12	1.89	0.54
2:E:8:PHE:HZ	2:M:25:ASP:OD1	1.89	0.54
2:I:254:VAL:HG21	2:I:275:ALA:HB1	1.90	0.54
2:K:316:ASP:HA	3:L:277:ARG:HH12	1.72	0.54
2:c:185:ASP:OD1	2:c:382:GLY:N	2.40	0.54
3:f:235:ALA:O	3:f:238:LEU:HG	2.08	0.54
1:2:15:LYS:NZ	1:2:39:GLU:H	2.05	0.54
1:4:18:GLU:HA	1:4:31:ALA:HB1	1.90	0.54
1:4:66:ILE:HD12	1:4:93:ALA:O	2.07	0.54
1:5:15:LYS:NZ	1:5:39:GLU:H	2.05	0.54
2:A:350:ARG:HA	2:A:353:ILE:HD12	1.89	0.54
2:G:224:ASP:HB2	2:G:300:VAL:HG12	1.89	0.54
2:K:350:ARG:HA	2:K:353:ILE:HD12	1.89	0.54
2:M:369:VAL:HA	2:M:372:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:73:MET:SD	2:c:49:ILE:HD11	2.47	0.54
2:e:69:MET:HE1	2:e:523:ASP:HB2	1.89	0.54
2:g:386:GLU:O	2:g:389:MET:HB2	2.07	0.54
2:i:386:GLU:O	2:i:389:MET:HB2	2.08	0.54
2:k:477:GLY:HA3	2:k:488:MET:HE2	1.90	0.54
2:m:156:GLU:OE1	2:m:156:GLU:N	2.36	0.54
2:m:493:ILE:HG12	5:m:603:ANP:N1	2.22	0.54
1:1:18:GLU:HA	1:1:31:ALA:HB1	1.90	0.54
1:3:29:GLY:H	2:G:264:VAL:HG11	1.72	0.54
2:G:369:VAL:HA	2:G:372:LEU:HD12	1.89	0.54
3:J:253:GLN:O	3:J:257:THR:HG23	2.07	0.54
3:L:253:GLN:O	3:L:257:THR:HG23	2.07	0.54
2:c:520:MET:HE1	2:e:38:VAL:HG13	1.89	0.54
3:l:237:GLU:CD	3:l:237:GLU:H	2.14	0.54
1:6:18:GLU:HA	1:6:31:ALA:HB1	1.90	0.54
2:C:254:VAL:HG21	2:C:275:ALA:HB1	1.90	0.54
2:C:369:VAL:HA	2:C:372:LEU:HD12	1.89	0.54
2:K:140:ASP:OD1	2:K:140:ASP:N	2.40	0.54
2:c:483:GLU:OE1	2:c:483:GLU:N	2.40	0.54
2:e:386:GLU:O	2:e:389:MET:HB2	2.08	0.54
3:f:201:GLU:O	3:f:204:GLN:NE2	2.41	0.54
1:0:66:ILE:C	1:0:92:LEU:HB2	2.33	0.54
1:6:27:LEU:HA	2:M:269:GLY:N	2.23	0.54
3:B:253:GLN:HA	3:B:256:LYS:HZ1	1.72	0.54
2:E:254:VAL:HG21	2:E:275:ALA:HB1	1.90	0.54
3:F:253:GLN:HA	3:F:256:LYS:HZ1	1.72	0.54
2:I:343:GLN:O	2:I:346:VAL:HB	2.08	0.54
2:I:345:ARG:O	2:I:349:ILE:HG12	2.08	0.54
2:K:195:PHE:HB3	2:K:279:PRO:HG3	1.88	0.54
3:j:261:ILE:HD12	3:j:264:ALA:HB3	1.90	0.54
2:m:217:SER:O	2:m:245:LYS:NZ	2.41	0.54
1:2:18:GLU:HA	1:2:31:ALA:HB1	1.90	0.54
1:6:15:LYS:NZ	1:6:39:GLU:H	2.05	0.54
1:6:38:GLY:HA3	1:6:67:PHE:HZ	1.71	0.54
2:A:286:LYS:NZ	3:B:284:TYR:HB2	2.23	0.54
2:I:346:VAL:O	2:I:347:ALA:C	2.51	0.54
2:a:9:GLY:N	2:a:519:CYS:SG	2.81	0.54
2:a:156:GLU:OE1	2:a:156:GLU:N	2.36	0.54
2:a:300:VAL:HG23	3:b:280:TYR:HD2	1.73	0.54
2:c:233:MET:HE1	2:c:237:LEU:HD23	1.89	0.54
2:i:156:GLU:OE1	2:i:156:GLU:N	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:100:ILE:HD13	2:k:514:MET:HE3	1.91	0.54
2:I:286:LYS:HZ1	3:J:284:TYR:HD2	1.55	0.53
2:M:350:ARG:HA	2:M:353:ILE:HD12	1.89	0.53
3:d:237:GLU:OE1	3:d:237:GLU:N	2.34	0.53
2:g:288:MET:N	2:g:288:MET:SD	2.81	0.53
2:i:259:LEU:O	2:i:263:VAL:HG12	2.08	0.53
3:j:240:PHE:HB2	3:j:275:TYR:OH	2.09	0.53
2:m:296:THR:OG1	2:m:319:GLN:O	2.24	0.53
2:A:224:ASP:HB2	2:A:300:VAL:HG12	1.89	0.53
2:E:292:ILE:O	2:E:296:THR:OG1	2.21	0.53
3:H:273:SER:HB2	3:H:277:ARG:CZ	2.37	0.53
2:a:8:PHE:HD1	2:a:519:CYS:HB3	1.73	0.53
2:a:291:ASP:HB2	2:a:372:LEU:HD11	1.90	0.53
3:h:261:ILE:HD12	3:h:264:ALA:HB3	1.89	0.53
2:k:520:MET:HE2	2:m:29:VAL:HG23	1.89	0.53
1:1:3:ILE:HD11	1:1:11:ILE:HG21	1.90	0.53
1:2:6:LEU:HD13	1:2:9:ARG:HH21	1.72	0.53
1:3:11:ILE:HD11	1:3:83:VAL:HG22	1.91	0.53
1:4:27:LEU:HD12	1:4:27:LEU:N	2.18	0.53
3:B:253:GLN:HA	3:B:256:LYS:NZ	2.24	0.53
2:C:286:LYS:NZ	3:D:280:TYR:CE1	2.76	0.53
2:C:319:GLN:NE2	2:C:334:ASP:OD2	2.42	0.53
2:G:319:GLN:NE2	2:G:334:ASP:OD2	2.41	0.53
2:I:319:GLN:NE2	2:I:334:ASP:OD2	2.42	0.53
2:i:157:THR:O	2:i:161:LEU:HD13	2.08	0.53
1:0:15:LYS:NZ	1:0:39:GLU:H	2.05	0.53
1:4:11:ILE:HD11	1:4:83:VAL:HG22	1.91	0.53
1:5:27:LEU:HD22	2:K:270:ILE:H	1.74	0.53
2:C:224:ASP:HB2	2:C:300:VAL:HG12	1.89	0.53
3:D:253:GLN:HA	3:D:256:LYS:NZ	2.24	0.53
2:E:130:GLU:HB2	2:E:422:VAL:HG23	1.91	0.53
2:c:156:GLU:OE1	2:c:156:GLU:N	2.36	0.53
3:d:261:ILE:HD12	3:d:264:ALA:HB3	1.89	0.53
2:e:350:ARG:CZ	2:e:350:ARG:HA	2.39	0.53
3:j:208:GLN:H	3:j:208:GLN:CD	2.17	0.53
1:0:3:ILE:HD11	1:0:11:ILE:HG21	1.90	0.53
2:A:315:GLU:OE1	3:B:270:ALA:HA	2.08	0.53
2:C:140:ASP:OD1	2:C:140:ASP:N	2.40	0.53
3:F:253:GLN:HA	3:F:256:LYS:NZ	2.24	0.53
3:N:253:GLN:HA	3:N:256:LYS:NZ	2.24	0.53
2:a:213:VAL:HB	2:a:325:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:157:THR:O	2:e:161:LEU:HD13	2.08	0.53
2:g:38:VAL:HG11	2:g:56:VAL:HG22	1.91	0.53
2:g:157:THR:O	2:g:161:LEU:HD13	2.08	0.53
2:k:202:PRO:HD2	2:k:203:TYR:HD1	1.73	0.53
1:2:66:ILE:C	1:2:92:LEU:HB2	2.33	0.53
1:5:3:ILE:HD11	1:5:11:ILE:HG21	1.90	0.53
1:6:3:ILE:HD11	1:6:11:ILE:HG21	1.90	0.53
2:A:369:VAL:HA	2:A:372:LEU:HD12	1.89	0.53
3:F:236:LEU:HD11	3:F:275:TYR:CD2	2.43	0.53
2:G:49:ILE:CD1	2:I:73:MET:HE1	2.37	0.53
2:I:304:GLU:O	3:J:255:ARG:NH1	2.42	0.53
2:e:343:GLN:OE1	2:e:343:GLN:N	2.29	0.53
2:e:518:GLU:CB	2:g:36:ARG:HB3	2.39	0.53
2:i:350:ARG:HA	2:i:350:ARG:CZ	2.39	0.53
3:l:235:ALA:O	3:l:238:LEU:HG	2.08	0.53
2:m:252:GLU:HG3	2:m:285:ARG:HH12	1.72	0.53
2:m:276:VAL:HG21	2:m:330:THR:HG21	1.89	0.53
2:C:130:GLU:HB2	2:C:422:VAL:HG23	1.91	0.53
3:F:253:GLN:O	3:F:257:THR:HG23	2.07	0.53
2:M:130:GLU:HB2	2:M:422:VAL:HG23	1.91	0.53
2:a:38:VAL:HG11	2:a:56:VAL:HG22	1.90	0.53
2:c:259:LEU:O	2:c:263:VAL:HG22	2.09	0.53
2:c:386:GLU:O	2:c:389:MET:HB2	2.08	0.53
2:g:196:ASP:O	2:g:197:ARG:NH1	2.37	0.53
2:g:305:ILE:HB	3:h:276:ARG:HH12	1.74	0.53
2:k:31:LEU:HD12	5:k:603:ANP:O1A	2.08	0.53
2:k:345:ARG:HH12	2:k:349:ILE:HD11	1.74	0.53
3:l:275:TYR:N	3:l:275:TYR:CD1	2.74	0.53
2:m:8:PHE:HD1	2:m:519:CYS:HB3	1.73	0.53
1:4:26:VAL:O	2:I:268:ARG:HD3	2.09	0.53
1:5:11:ILE:HD11	1:5:83:VAL:HG22	1.91	0.53
1:6:11:ILE:HD11	1:6:83:VAL:HG22	1.91	0.53
1:6:66:ILE:HB	1:6:92:LEU:HB3	1.90	0.53
2:E:319:GLN:NE2	2:E:334:ASP:OD2	2.42	0.53
2:a:296:THR:OG1	2:a:319:GLN:O	2.25	0.53
2:k:157:THR:O	2:k:161:LEU:HD13	2.09	0.53
2:m:196:ASP:O	2:m:197:ARG:NH1	2.37	0.53
2:m:350:ARG:CZ	2:m:350:ARG:HA	2.39	0.53
1:2:3:ILE:HD11	1:2:11:ILE:HG21	1.90	0.53
2:A:319:GLN:NE2	2:A:334:ASP:OD2	2.41	0.53
3:L:253:GLN:HA	3:L:256:LYS:NZ	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:157:THR:O	2:a:161:LEU:HD13	2.08	0.53
2:c:73:MET:HG2	2:e:47:PRO:CD	2.39	0.53
3:f:237:GLU:H	3:f:237:GLU:CD	2.16	0.53
3:f:276:ARG:CZ	3:f:279:LEU:CG	2.77	0.53
2:k:350:ARG:CZ	2:k:350:ARG:HA	2.39	0.53
1:2:11:ILE:HD11	1:2:83:VAL:HG22	1.91	0.53
3:D:277:ARG:O	3:D:278:GLN:C	2.52	0.53
2:K:130:GLU:HB2	2:K:422:VAL:HG23	1.91	0.53
3:N:278:GLN:O	3:N:281:ALA:N	2.42	0.53
2:e:291:ASP:HB2	2:e:372:LEU:HD11	1.91	0.53
2:e:518:GLU:HG3	2:g:29:VAL:HG11	1.90	0.53
1:5:18:GLU:HA	1:5:31:ALA:HB1	1.90	0.52
3:B:278:GLN:O	3:B:281:ALA:N	2.42	0.52
3:J:253:GLN:HA	3:J:256:LYS:NZ	2.24	0.52
2:K:319:GLN:NE2	2:K:334:ASP:OD2	2.41	0.52
2:M:319:GLN:NE2	2:M:334:ASP:OD2	2.42	0.52
2:c:157:THR:O	2:c:161:LEU:HD13	2.09	0.52
3:l:236:LEU:HD13	3:l:275:TYR:HD2	1.75	0.52
2:A:130:GLU:HB2	2:A:422:VAL:HG23	1.91	0.52
2:E:222:LEU:HD12	2:E:300:VAL:HG22	1.92	0.52
2:I:265:ASN:HB3	2:I:268:ARG:O	2.09	0.52
2:M:5:ASP:N	2:M:522:THR:O	2.32	0.52
2:i:296:THR:OG1	2:i:319:GLN:O	2.23	0.52
2:k:521:VAL:HG23	2:m:39:VAL:O	2.09	0.52
3:l:254:THR:HG1	3:l:255:ARG:NH2	2.07	0.52
3:H:253:GLN:HA	3:H:256:LYS:NZ	2.24	0.52
2:I:130:GLU:HB2	2:I:422:VAL:HG23	1.91	0.52
2:I:290:GLN:OE1	2:I:345:ARG:NH2	2.42	0.52
2:K:292:ILE:O	2:K:296:THR:OG1	2.21	0.52
2:c:72:GLN:HB3	2:e:46:ALA:HA	1.92	0.52
2:e:521:VAL:HG23	2:g:39:VAL:O	2.08	0.52
3:f:243:LEU:HD11	3:f:258:PHE:CZ	2.44	0.52
2:m:157:THR:O	2:m:161:LEU:HD13	2.08	0.52
2:m:387:VAL:HA	2:m:390:LYS:HZ3	1.73	0.52
1:0:11:ILE:HD11	1:0:83:VAL:HG22	1.91	0.52
1:1:11:ILE:HD11	1:1:83:VAL:HG22	1.91	0.52
1:1:86:MET:SD	1:1:87:SER:N	2.83	0.52
1:3:3:ILE:HD11	1:3:11:ILE:HG21	1.90	0.52
1:3:27:LEU:HD12	1:3:27:LEU:H	1.73	0.52
2:A:140:ASP:OD1	2:A:140:ASP:N	2.40	0.52
2:a:69:MET:HE3	2:c:39:VAL:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:236:LEU:HA	3:f:239:LEU:HD13	1.91	0.52
2:i:291:ASP:HB2	2:i:372:LEU:HD11	1.92	0.52
3:n:235:ALA:O	3:n:238:LEU:HG	2.08	0.52
1:0:86:MET:SD	1:0:87:SER:N	2.83	0.52
1:3:6:LEU:HD11	1:4:91:ILE:CG2	2.29	0.52
1:3:67:PHE:HA	1:3:92:LEU:HD23	1.90	0.52
1:6:20:LYS:HB3	1:6:24:GLY:HA2	1.91	0.52
3:B:277:ARG:O	3:B:280:TYR:N	2.43	0.52
3:D:275:TYR:O	3:D:278:GLN:HB3	2.09	0.52
2:a:350:ARG:HA	2:a:350:ARG:CZ	2.39	0.52
2:e:250:ILE:HD13	2:e:276:VAL:HG12	1.91	0.52
3:j:243:LEU:HD11	3:j:258:PHE:CZ	2.45	0.52
3:l:275:TYR:HA	3:l:278:GLN:CD	2.34	0.52
1:5:86:MET:SD	1:5:87:SER:N	2.83	0.52
2:I:345:ARG:O	2:I:345:ARG:HD3	2.09	0.52
2:c:8:PHE:HD1	2:c:519:CYS:HB3	1.75	0.52
2:c:33:PRO:HG3	5:c:603:ANP:C5	2.40	0.52
2:c:513:LEU:HD11	2:e:49:ILE:CG2	2.39	0.52
2:g:8:PHE:HD1	2:g:519:CYS:HB3	1.75	0.52
2:g:284:ARG:HD3	2:g:364:LYS:HG2	1.91	0.52
1:2:86:MET:SD	1:2:87:SER:N	2.83	0.52
1:3:66:ILE:HB	1:3:92:LEU:HB2	1.89	0.52
1:4:3:ILE:HD11	1:4:11:ILE:HG21	1.90	0.52
2:G:292:ILE:O	2:G:296:THR:OG1	2.21	0.52
3:J:252:GLY:C	3:J:256:LYS:HZ3	2.18	0.52
3:h:243:LEU:HD11	3:h:258:PHE:CZ	2.45	0.52
2:k:276:VAL:HG21	2:k:330:THR:HG21	1.91	0.52
3:n:252:GLY:O	3:n:256:LYS:NZ	2.33	0.52
3:n:259:GLN:NE2	3:n:260:GLU:OE2	2.42	0.52
1:5:6:LEU:HD11	1:6:92:LEU:O	2.10	0.52
3:l:275:TYR:N	3:l:275:TYR:HD1	2.07	0.52
2:G:130:GLU:HB2	2:G:422:VAL:HG23	1.91	0.52
2:c:247:LEU:HD22	2:c:248:LEU:H	1.75	0.52
3:l:276:ARG:HD2	3:l:280:TYR:CE1	2.45	0.52
2:m:324:VAL:HB	2:m:331:THR:OG1	2.10	0.52
1:2:36:THR:O	1:2:37:ARG:NE	2.43	0.52
1:3:5:PRO:HG3	1:3:11:ILE:HG22	1.92	0.52
1:4:86:MET:SD	1:4:87:SER:N	2.83	0.52
2:G:265:ASN:O	2:G:268:ARG:O	2.28	0.52
2:I:305:ILE:HG22	3:J:276:ARG:CZ	2.41	0.52
2:a:383:ALA:HB3	2:a:389:MET:SD	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:236:LEU:HA	3:b:239:LEU:HD13	1.92	0.52
2:c:8:PHE:CE1	2:e:25:ASP:OD1	2.63	0.52
2:c:25:ASP:HA	2:c:28:LYS:HE2	1.92	0.52
2:c:359:ASP:HA	2:c:362:ARG:HB3	1.92	0.52
2:g:325:ILE:HG13	2:g:330:THR:HG22	1.91	0.52
2:i:38:VAL:HG11	2:i:56:VAL:HG22	1.92	0.52
3:j:208:GLN:HA	3:j:211:GLU:HB2	1.91	0.52
2:m:291:ASP:HB2	2:m:372:LEU:HD11	1.91	0.52
1:1:36:THR:O	1:1:37:ARG:NE	2.44	0.51
1:3:86:MET:SD	1:3:87:SER:N	2.83	0.51
1:4:5:PRO:HG3	1:4:11:ILE:HG22	1.92	0.51
3:L:262:LEU:HA	3:L:265:LEU:HD12	1.93	0.51
3:d:276:ARG:NH2	3:d:280:TYR:HD1	2.08	0.51
2:g:259:LEU:O	2:g:263:VAL:HG12	2.10	0.51
2:k:310:GLU:N	2:k:310:GLU:OE1	2.44	0.51
3:n:264:ALA:O	3:n:265:LEU:C	2.53	0.51
1:0:36:THR:O	1:0:37:ARG:NE	2.44	0.51
1:6:66:ILE:HD12	1:6:93:ALA:O	2.10	0.51
3:B:275:TYR:O	3:B:278:GLN:HB3	2.11	0.51
2:M:305:ILE:HG12	3:N:283:LEU:HD22	1.92	0.51
3:N:262:LEU:HA	3:N:265:LEU:HD12	1.93	0.51
3:d:243:LEU:HD11	3:d:258:PHE:CZ	2.45	0.51
2:e:324:VAL:HB	2:e:331:THR:OG1	2.10	0.51
2:g:281:PHE:O	2:g:284:ARG:HG2	2.10	0.51
3:h:237:GLU:H	3:h:237:GLU:CD	2.17	0.51
2:i:213:VAL:HB	2:i:325:ILE:HD11	1.92	0.51
1:6:86:MET:SD	1:6:87:SER:N	2.83	0.51
3:L:217:ALA:O	3:L:221:GLN:HG3	2.09	0.51
3:L:252:GLY:C	3:L:256:LYS:HZ3	2.18	0.51
2:e:8:PHE:HD1	2:e:519:CYS:HB3	1.76	0.51
2:e:259:LEU:O	2:e:263:VAL:HG12	2.10	0.51
2:k:259:LEU:O	2:k:263:VAL:HG12	2.11	0.51
2:G:300:VAL:HB	3:H:280:TYR:HE2	1.76	0.51
3:J:262:LEU:HA	3:J:265:LEU:HD12	1.93	0.51
3:J:283:LEU:HG	3:J:284:TYR:HD2	1.68	0.51
2:M:292:ILE:O	2:M:296:THR:OG1	2.21	0.51
2:e:345:ARG:HH12	2:e:349:ILE:HD11	1.75	0.51
3:h:220:THR:O	3:h:224:LEU:HG	2.10	0.51
1:0:1:MET:HE1	1:1:95:VAL:HG13	1.92	0.51
1:2:5:PRO:HG3	1:2:11:ILE:HG22	1.93	0.51
1:3:36:THR:O	1:3:37:ARG:NE	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:219:ALA:HA	3:B:222:LEU:HB3	1.92	0.51
3:B:277:ARG:O	3:B:278:GLN:C	2.53	0.51
3:F:277:ARG:O	3:F:278:GLN:C	2.53	0.51
3:H:270:ALA:O	3:H:274:LYS:HG2	2.11	0.51
3:J:202:ILE:HG21	3:J:231:ARG:NH1	2.24	0.51
3:J:234:GLU:O	3:J:237:GLU:N	2.43	0.51
2:M:126:ALA:HB3	2:M:426:LEU:HD21	1.93	0.51
2:M:473:ASP:OD1	2:M:474:GLY:N	2.44	0.51
2:a:39:VAL:HB	2:m:521:VAL:HG23	1.91	0.51
3:b:261:ILE:HD12	3:b:264:ALA:HB3	1.91	0.51
3:f:276:ARG:NH2	3:f:279:LEU:C	2.68	0.51
1:6:5:PRO:HG3	1:6:11:ILE:HG22	1.92	0.51
1:6:36:THR:O	1:6:37:ARG:NE	2.44	0.51
3:B:270:ALA:O	3:B:274:LYS:HG2	2.11	0.51
2:C:160:LYS:HB2	2:C:160:LYS:NZ	2.26	0.51
3:H:262:LEU:HA	3:H:265:LEU:HD12	1.92	0.51
2:a:25:ASP:HA	2:a:28:LYS:HE2	1.93	0.51
2:g:25:ASP:HA	2:g:28:LYS:HE2	1.93	0.51
2:k:386:GLU:O	2:k:389:MET:HB2	2.11	0.51
3:l:243:LEU:HD11	3:l:258:PHE:CZ	2.46	0.51
1:2:2:ASN:OD1	1:3:97:ALA:O	2.29	0.51
1:5:5:PRO:HG3	1:5:11:ILE:HG22	1.92	0.51
1:5:36:THR:O	1:5:37:ARG:NE	2.44	0.51
1:6:27:LEU:HA	2:M:269:GLY:CA	2.40	0.51
2:A:160:LYS:HB2	2:A:160:LYS:NZ	2.26	0.51
2:C:126:ALA:HB3	2:C:426:LEU:HD21	1.93	0.51
2:E:126:ALA:HB3	2:E:426:LEU:HD21	1.93	0.51
2:E:160:LYS:HB2	2:E:160:LYS:NZ	2.26	0.51
2:K:415:GLY:N	5:K:600:ANP:O2'	2.34	0.51
2:e:226:LYS:HG2	2:e:253:ASP:HB2	1.93	0.51
2:e:246:PRO:HG3	2:e:272:LYS:HD3	1.92	0.51
1:1:87:SER:O	1:1:91:ILE:HD11	2.11	0.51
1:4:47:ARG:H	1:4:54:VAL:HG13	1.76	0.51
2:c:276:VAL:HG21	2:c:330:THR:HG21	1.92	0.51
3:j:262:LEU:HA	3:j:265:LEU:HD23	1.93	0.51
2:m:259:LEU:O	2:m:263:VAL:HG12	2.10	0.51
1:1:27:LEU:HA	2:C:269:GLY:CA	2.41	0.51
2:G:126:ALA:HB3	2:G:426:LEU:HD21	1.93	0.51
2:a:38:VAL:HG13	2:m:520:MET:SD	2.51	0.51
2:a:233:MET:HE1	2:a:237:LEU:HB3	1.93	0.51
3:b:243:LEU:HD11	3:b:258:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:261:ILE:O	3:h:262:LEU:C	2.54	0.51
2:i:8:PHE:HD1	2:i:519:CYS:HB3	1.75	0.51
1:0:5:PRO:HG3	1:0:11:ILE:HG22	1.92	0.51
1:1:5:PRO:HG3	1:1:11:ILE:HG22	1.92	0.51
1:1:6:LEU:HD11	1:2:91:ILE:HG22	1.91	0.51
1:2:27:LEU:HB3	2:A:265:ASN:CG	2.35	0.51
1:4:36:THR:O	1:4:37:ARG:NE	2.43	0.51
2:A:126:ALA:HB3	2:A:426:LEU:HD21	1.93	0.51
2:A:339:GLU:HB2	2:A:343:GLN:HE22	1.76	0.51
2:E:132:LYS:HB2	2:E:132:LYS:NZ	2.26	0.51
2:E:473:ASP:OD1	2:E:474:GLY:N	2.44	0.51
3:F:262:LEU:HA	3:F:265:LEU:HD12	1.93	0.51
2:I:132:LYS:HB2	2:I:132:LYS:NZ	2.26	0.51
2:K:126:ALA:HB3	2:K:426:LEU:HD21	1.93	0.51
2:a:299:THR:HG22	3:b:277:ARG:NH1	2.23	0.51
2:g:350:ARG:HA	2:g:350:ARG:CZ	2.40	0.51
2:m:38:VAL:HG11	2:m:56:VAL:HG22	1.92	0.51
1:1:27:LEU:O	2:C:265:ASN:HA	2.11	0.50
3:B:262:LEU:HA	3:B:265:LEU:HD12	1.93	0.50
2:C:339:GLU:HB2	2:C:343:GLN:HE22	1.76	0.50
2:C:473:ASP:OD1	2:C:474:GLY:N	2.44	0.50
2:G:339:GLU:HB2	2:G:343:GLN:HE22	1.76	0.50
2:G:473:ASP:OD1	2:G:474:GLY:N	2.44	0.50
2:I:126:ALA:HB3	2:I:426:LEU:HD21	1.93	0.50
3:J:270:ALA:O	3:J:274:LYS:HG2	2.11	0.50
2:K:384:ALA:O	2:M:506:TYR:HE1	1.94	0.50
2:a:387:VAL:O	2:a:390:LYS:HD3	2.11	0.50
2:e:299:THR:HG22	3:f:277:ARG:CZ	2.41	0.50
2:k:429:LEU:C	2:k:430:ARG:HD2	2.36	0.50
2:A:239:ALA:O	2:A:242:LYS:HG3	2.12	0.50
2:A:473:ASP:OD1	2:A:474:GLY:N	2.44	0.50
3:D:262:LEU:HA	3:D:265:LEU:HD12	1.93	0.50
3:D:270:ALA:O	3:D:274:LYS:HG2	2.11	0.50
2:K:339:GLU:HB2	2:K:343:GLN:HE22	1.76	0.50
2:a:226:LYS:HG2	2:a:253:ASP:HB2	1.92	0.50
2:c:299:THR:HG22	3:d:277:ARG:CZ	2.40	0.50
3:n:254:THR:OG1	3:n:255:ARG:NH2	2.43	0.50
1:1:27:LEU:HB3	2:C:265:ASN:ND2	2.26	0.50
1:2:6:LEU:CD1	1:3:91:ILE:HG22	2.16	0.50
1:3:47:ARG:H	1:3:54:VAL:HG13	1.76	0.50
1:5:38:GLY:HA3	1:5:67:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:47:ARG:H	1:5:54:VAL:HG13	1.76	0.50
2:G:34:LYS:HG2	2:I:112:ASN:HD21	1.75	0.50
2:K:160:LYS:HB2	2:K:160:LYS:NZ	2.26	0.50
2:K:473:ASP:OD1	2:K:474:GLY:N	2.44	0.50
2:c:226:LYS:HG2	2:c:253:ASP:HB2	1.93	0.50
2:e:196:ASP:O	2:e:197:ARG:NH1	2.36	0.50
2:i:299:THR:CB	3:j:277:ARG:NH1	2.72	0.50
3:j:276:ARG:HH21	3:j:280:TYR:N	2.09	0.50
2:k:288:MET:HE1	2:k:368:ARG:HD3	1.94	0.50
2:k:388:GLU:OE1	2:k:388:GLU:N	2.37	0.50
2:m:345:ARG:HH12	2:m:349:ILE:HD11	1.75	0.50
1:0:27:LEU:CD2	2:E:269:GLY:HA2	2.41	0.50
1:4:38:GLY:HA3	1:4:67:PHE:CZ	2.47	0.50
2:E:339:GLU:HB2	2:E:343:GLN:HE22	1.76	0.50
3:H:209:VAL:HG22	3:H:218:LEU:HD13	1.94	0.50
2:K:239:ALA:O	2:K:242:LYS:HG3	2.11	0.50
2:M:160:LYS:HB2	2:M:160:LYS:NZ	2.26	0.50
2:a:248:LEU:HD23	2:a:274:ALA:HB3	1.93	0.50
2:a:259:LEU:O	2:a:263:VAL:HG12	2.10	0.50
3:b:278:GLN:O	3:b:282:LEU:HG	2.12	0.50
2:k:226:LYS:HG2	2:k:253:ASP:HB2	1.93	0.50
2:I:473:ASP:OD1	2:I:474:GLY:N	2.44	0.50
2:K:49:ILE:CG1	2:M:73:MET:HE1	2.41	0.50
2:M:339:GLU:HB2	2:M:343:GLN:HE22	1.76	0.50
3:f:253:GLN:O	3:f:257:THR:HG23	2.11	0.50
3:f:274:LYS:HA	3:f:277:ARG:HG2	1.93	0.50
3:j:277:ARG:HA	3:j:280:TYR:CD2	2.47	0.50
2:k:415:GLY:HA2	5:k:603:ANP:H1'	1.94	0.50
3:l:240:PHE:HE1	3:l:282:LEU:HD22	1.77	0.50
2:m:226:LYS:HG2	2:m:253:ASP:HB2	1.93	0.50
1:2:20:LYS:HB3	1:2:24:GLY:HA2	1.94	0.50
2:A:132:LYS:HB2	2:A:132:LYS:NZ	2.26	0.50
2:A:316:ASP:HA	3:B:277:ARG:HH12	1.75	0.50
2:E:8:PHE:CZ	2:M:25:ASP:OD1	2.64	0.50
2:G:160:LYS:NZ	2:G:160:LYS:HB2	2.26	0.50
2:I:286:LYS:CE	3:J:284:TYR:HB2	2.41	0.50
2:M:239:ALA:O	2:M:242:LYS:HG3	2.12	0.50
2:a:36:ARG:HB3	2:m:518:GLU:HB3	1.94	0.50
2:c:73:MET:SD	2:e:47:PRO:HG2	2.51	0.50
2:g:184:GLN:O	2:g:380:LYS:NZ	2.44	0.50
2:i:302:SER:HB3	3:j:280:TYR:HD1	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:246:PRO:HG3	2:k:272:LYS:HB2	1.93	0.50
1:1:13:LYS:O	1:1:15:LYS:HD3	2.12	0.50
1:2:27:LEU:O	2:A:265:ASN:HA	2.11	0.50
1:2:66:ILE:HB	1:2:92:LEU:HB3	1.93	0.50
1:3:9:ARG:HG3	1:3:10:VAL:N	2.27	0.50
1:3:9:ARG:CB	1:3:87:SER:HA	2.39	0.50
1:4:41:LEU:HD23	1:4:41:LEU:H	1.77	0.50
1:6:47:ARG:H	1:6:54:VAL:HG13	1.76	0.50
2:C:239:ALA:O	2:C:242:LYS:HG3	2.11	0.50
2:E:239:ALA:O	2:E:242:LYS:HG3	2.12	0.50
3:F:270:ALA:O	3:F:274:LYS:HG2	2.11	0.50
2:G:239:ALA:O	2:G:242:LYS:HG3	2.12	0.50
2:I:25:ASP:OD1	2:K:8:PHE:HZ	1.95	0.50
2:K:132:LYS:NZ	2:K:132:LYS:HB2	2.27	0.50
2:a:151:SER:O	2:a:151:SER:OG	2.29	0.50
3:d:237:GLU:H	3:d:237:GLU:CD	2.17	0.50
2:g:156:GLU:OE1	2:g:156:GLU:N	2.36	0.50
2:g:214:GLU:HG2	2:g:324:VAL:HG22	1.94	0.50
3:j:276:ARG:HE	3:j:276:ARG:C	2.18	0.50
3:n:198:ASP:OD2	3:n:203:GLN:NE2	2.44	0.50
1:2:13:LYS:O	1:2:15:LYS:HD3	2.12	0.50
2:A:112:ASN:HD21	2:C:34:LYS:HG2	1.75	0.50
2:A:220:ILE:O	2:A:318:GLY:N	2.37	0.50
3:L:270:ALA:O	3:L:274:LYS:HG2	2.11	0.50
2:a:300:VAL:HG23	3:b:280:TYR:CD2	2.47	0.50
2:c:388:GLU:O	2:c:389:MET:C	2.55	0.50
2:i:207:LYS:O	2:i:207:LYS:HD3	2.12	0.50
2:k:4:LYS:CD	2:m:59:GLU:O	2.59	0.50
2:k:248:LEU:HD23	2:k:274:ALA:HB3	1.94	0.50
2:m:380:LYS:C	2:m:380:LYS:HD3	2.36	0.50
1:0:47:ARG:H	1:0:54:VAL:HG13	1.76	0.50
1:1:4:ARG:C	1:2:93:ALA:HB1	2.37	0.50
1:6:38:GLY:HA3	1:6:67:PHE:CZ	2.47	0.50
2:I:160:LYS:HB2	2:I:160:LYS:NZ	2.26	0.50
3:L:220:THR:O	3:L:223:ALA:HB3	2.12	0.50
3:N:270:ALA:O	3:N:274:LYS:HG2	2.11	0.50
3:b:208:GLN:H	3:b:208:GLN:CD	2.20	0.50
2:g:18:ARG:HB3	2:g:67:GLU:OE1	2.12	0.50
2:i:325:ILE:HD12	2:i:325:ILE:O	2.12	0.50
2:k:17:LEU:HB2	2:k:104:LEU:HD12	1.94	0.50
2:k:196:ASP:O	2:k:197:ARG:NH1	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:322:ARG:HB2	2:k:333:ILE:HD11	1.94	0.50
1:0:13:LYS:O	1:0:15:LYS:HD3	2.12	0.49
1:3:38:GLY:HA3	1:3:67:PHE:CZ	2.47	0.49
1:6:23:GLY:O	1:6:24:GLY:C	2.54	0.49
2:a:61:GLU:O	2:m:4:LYS:N	2.41	0.49
2:a:521:VAL:HG23	2:c:39:VAL:O	2.11	0.49
1:0:64:ILE:HG13	1:0:95:VAL:HB	1.95	0.49
1:2:6:LEU:H	1:2:9:ARG:NE	2.11	0.49
1:3:6:LEU:HD13	1:3:9:ARG:HH22	1.77	0.49
1:3:8:ASP:CG	1:3:47:ARG:HA	2.37	0.49
1:5:41:LEU:H	1:5:41:LEU:HD23	1.77	0.49
3:H:280:TYR:HA	3:H:283:LEU:HD21	1.90	0.49
2:I:5:ASP:N	2:I:522:THR:O	2.32	0.49
2:I:367:GLU:OE1	2:I:371:LYS:HE3	2.12	0.49
2:K:365:LEU:HD13	2:K:368:ARG:HD3	1.94	0.49
2:M:365:LEU:HD13	2:M:368:ARG:HD3	1.94	0.49
2:a:29:VAL:HG11	2:m:518:GLU:HG3	1.94	0.49
2:c:196:ASP:O	2:c:197:ARG:NH1	2.37	0.49
3:d:261:ILE:O	3:d:262:LEU:C	2.55	0.49
2:e:25:ASP:HA	2:e:28:LYS:HE2	1.94	0.49
2:g:226:LYS:HG2	2:g:253:ASP:HB2	1.94	0.49
2:k:8:PHE:HD1	2:k:519:CYS:HB3	1.75	0.49
3:n:208:GLN:HA	3:n:211:GLU:HB2	1.94	0.49
1:5:9:ARG:HH22	1:6:92:LEU:C	2.20	0.49
1:6:64:ILE:HG13	1:6:95:VAL:HB	1.94	0.49
2:G:367:GLU:OE1	2:G:371:LYS:HE3	2.12	0.49
2:K:5:ASP:N	2:K:522:THR:O	2.32	0.49
3:h:243:LEU:HD22	3:h:282:LEU:HD21	1.94	0.49
3:h:244:ARG:HA	3:h:244:ARG:HH11	1.76	0.49
1:1:41:LEU:HD23	1:1:41:LEU:H	1.77	0.49
1:1:64:ILE:O	1:1:94:ILE:HD12	2.12	0.49
1:3:13:LYS:O	1:3:15:LYS:HD3	2.12	0.49
1:4:9:ARG:O	1:4:44:GLY:HA3	2.13	0.49
1:5:9:ARG:O	1:5:44:GLY:HA3	2.12	0.49
1:5:66:ILE:C	1:5:92:LEU:HB2	2.36	0.49
2:C:132:LYS:NZ	2:C:132:LYS:HB2	2.27	0.49
2:E:365:LEU:HD13	2:E:368:ARG:HD3	1.95	0.49
3:F:277:ARG:O	3:F:280:TYR:N	2.45	0.49
2:G:132:LYS:HB2	2:G:132:LYS:NZ	2.27	0.49
2:G:220:ILE:O	2:G:318:GLY:N	2.37	0.49
3:N:239:LEU:HA	3:N:242:HIS:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:483:GLU:OE1	2:i:483:GLU:N	2.46	0.49
3:l:208:GLN:H	3:l:208:GLN:CD	2.20	0.49
3:l:258:PHE:HA	3:l:261:ILE:CG2	2.40	0.49
1:1:47:ARG:H	1:1:54:VAL:HG13	1.76	0.49
1:2:41:LEU:HD23	1:2:41:LEU:H	1.77	0.49
1:2:47:ARG:H	1:2:54:VAL:HG13	1.76	0.49
3:B:234:GLU:O	3:B:237:GLU:N	2.45	0.49
3:B:276:ARG:O	3:B:279:LEU:HB3	2.13	0.49
3:F:239:LEU:HA	3:F:242:HIS:NE2	2.27	0.49
2:G:5:ASP:N	2:G:522:THR:O	2.32	0.49
3:L:225:GLN:HA	3:L:228:GLN:NE2	2.28	0.49
2:c:281:PHE:O	2:c:284:ARG:HG2	2.13	0.49
2:g:483:GLU:N	2:g:483:GLU:OE1	2.45	0.49
3:h:239:LEU:HD13	3:h:242:HIS:HE1	1.77	0.49
3:h:253:GLN:O	3:h:257:THR:HG23	2.12	0.49
2:i:520:MET:HE1	2:k:38:VAL:HA	1.93	0.49
2:k:291:ASP:HA	2:k:345:ARG:HE	1.77	0.49
2:k:296:THR:OG1	2:k:319:GLN:O	2.23	0.49
2:k:388:GLU:HA	2:k:391:GLU:OE2	2.13	0.49
1:1:27:LEU:HD23	2:C:269:GLY:CA	2.27	0.49
1:1:64:ILE:HG13	1:1:95:VAL:HB	1.95	0.49
1:2:63:ASP:HB3	1:2:94:ILE:HD13	1.94	0.49
1:5:13:LYS:O	1:5:15:LYS:HD3	2.12	0.49
1:5:28:THR:C	2:K:268:ARG:HD3	2.37	0.49
1:6:41:LEU:HD23	1:6:41:LEU:H	1.77	0.49
3:B:239:LEU:HA	3:B:242:HIS:NE2	2.27	0.49
2:C:313:THR:HB	3:D:267:THR:HA	1.95	0.49
2:G:305:ILE:HD11	3:H:280:TYR:CD1	2.47	0.49
2:M:132:LYS:HB2	2:M:132:LYS:NZ	2.26	0.49
3:N:225:GLN:HA	3:N:228:GLN:NE2	2.28	0.49
2:c:299:THR:CG2	3:d:277:ARG:HH12	2.18	0.49
2:c:359:ASP:OD1	2:c:362:ARG:NH2	2.36	0.49
2:g:215:LEU:HB3	2:g:246:PRO:CG	2.42	0.49
2:g:252:GLU:HA	2:g:285:ARG:HH22	1.75	0.49
2:m:252:GLU:HG3	2:m:285:ARG:HH22	1.78	0.49
1:3:9:ARG:CA	1:3:88:GLU:HB2	2.42	0.49
1:4:13:LYS:O	1:4:15:LYS:HD3	2.12	0.49
1:4:67:PHE:CA	1:4:92:LEU:HD23	2.43	0.49
1:5:64:ILE:HG13	1:5:95:VAL:HB	1.95	0.49
1:6:26:VAL:O	2:M:268:ARG:HB3	2.12	0.49
2:C:365:LEU:HD13	2:C:368:ARG:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:368:ARG:O	2:G:372:LEU:HD12	2.13	0.49
2:K:367:GLU:OE1	2:K:371:LYS:HE3	2.13	0.49
3:L:239:LEU:HA	3:L:242:HIS:NE2	2.27	0.49
3:b:270:ALA:O	3:b:273:SER:OG	2.30	0.49
3:d:235:ALA:O	3:d:236:LEU:C	2.56	0.49
1:0:4:ARG:C	1:1:93:ALA:HB1	2.37	0.49
1:0:91:ILE:O	1:6:9:ARG:NH1	2.34	0.49
1:1:38:GLY:HA3	1:1:67:PHE:CZ	2.47	0.49
1:6:67:PHE:CA	1:6:92:LEU:HD23	2.43	0.49
2:C:368:ARG:O	2:C:372:LEU:HD12	2.13	0.49
3:D:239:LEU:HA	3:D:242:HIS:NE2	2.27	0.49
2:a:33:PRO:HG3	5:a:600:ANP:C5	2.43	0.49
2:c:345:ARG:NH1	2:c:348:GLN:OE1	2.44	0.49
2:e:151:SER:O	2:e:151:SER:OG	2.29	0.49
1:3:64:ILE:HG13	1:3:95:VAL:HB	1.95	0.49
2:A:367:GLU:OE1	2:A:371:LYS:HE3	2.13	0.49
2:C:299:THR:HB	3:D:277:ARG:HH12	1.76	0.49
2:K:39:VAL:HB	2:M:520:MET:HG2	1.95	0.49
2:K:368:ARG:O	2:K:372:LEU:HD12	2.13	0.49
3:f:208:GLN:H	3:f:208:GLN:CD	2.21	0.49
2:m:506:TYR:O	2:m:510:VAL:HG12	2.12	0.49
1:1:67:PHE:HA	1:1:92:LEU:HD23	1.94	0.49
1:3:63:ASP:HB3	1:3:94:ILE:HD13	1.94	0.49
1:4:64:ILE:HG13	1:4:95:VAL:HB	1.94	0.49
1:6:63:ASP:HB3	1:6:94:ILE:HD13	1.95	0.49
2:E:226:LYS:HD2	2:E:227:ILE:N	2.28	0.49
2:E:367:GLU:OE1	2:E:371:LYS:HE3	2.12	0.49
3:H:239:LEU:HA	3:H:242:HIS:NE2	2.27	0.49
2:I:365:LEU:HD13	2:I:368:ARG:HD3	1.95	0.49
2:M:368:ARG:O	2:M:372:LEU:HD12	2.13	0.49
2:a:184:GLN:O	2:a:380:LYS:NZ	2.46	0.49
2:c:217:SER:O	2:c:245:LYS:NZ	2.42	0.49
3:n:243:LEU:HD11	3:n:258:PHE:CZ	2.48	0.49
1:2:38:GLY:HA3	1:2:67:PHE:CZ	2.47	0.48
1:2:64:ILE:HG13	1:2:95:VAL:HB	1.95	0.48
1:6:9:ARG:O	1:6:44:GLY:HA3	2.12	0.48
2:A:368:ARG:O	2:A:372:LEU:HD12	2.13	0.48
2:C:226:LYS:HD2	2:C:227:ILE:N	2.28	0.48
3:D:252:GLY:C	3:D:256:LYS:HZ3	2.21	0.48
2:E:58:ARG:HA	2:E:75:LYS:HD3	1.95	0.48
3:F:222:LEU:C	3:F:222:LEU:HD13	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:273:SER:O	3:F:277:ARG:HG2	2.13	0.48
2:I:25:ASP:OD1	2:K:8:PHE:CZ	2.66	0.48
2:I:239:ALA:O	2:I:242:LYS:HG3	2.11	0.48
2:I:368:ARG:O	2:I:372:LEU:HD12	2.13	0.48
2:a:319:GLN:HG3	2:a:320:ALA:N	2.28	0.48
2:c:391:GLU:OE1	2:c:392:LYS:N	2.45	0.48
2:e:483:GLU:OE1	2:e:483:GLU:N	2.46	0.48
2:i:226:LYS:HG2	2:i:253:ASP:HB2	1.93	0.48
3:l:240:PHE:HE1	3:l:282:LEU:CD2	2.26	0.48
2:A:25:ASP:OD1	2:G:8:PHE:CZ	2.65	0.48
2:A:313:THR:OG1	2:A:315:GLU:HG3	2.13	0.48
2:C:69:MET:CE	2:E:41:ASP:HB2	2.44	0.48
2:M:367:GLU:OE1	2:M:371:LYS:HE3	2.13	0.48
3:b:253:GLN:O	3:b:257:THR:HG23	2.13	0.48
2:e:252:GLU:HG3	2:e:285:ARG:HH22	1.78	0.48
2:g:40:LEU:HD22	2:g:59:GLU:HG2	1.95	0.48
2:g:520:MET:HG2	2:i:26:ALA:HA	1.95	0.48
2:m:483:GLU:OE1	2:m:483:GLU:N	2.45	0.48
1:0:41:LEU:HD23	1:0:41:LEU:H	1.77	0.48
1:1:9:ARG:HB2	1:1:86:MET:O	2.13	0.48
1:4:29:GLY:H	2:I:264:VAL:CG1	2.27	0.48
1:4:63:ASP:HB3	1:4:94:ILE:HD13	1.94	0.48
2:A:365:LEU:HD13	2:A:368:ARG:HD3	1.94	0.48
2:C:313:THR:OG1	3:D:267:THR:HB	2.12	0.48
3:H:278:GLN:O	3:H:282:LEU:N	2.42	0.48
3:J:234:GLU:O	3:J:237:GLU:HB2	2.13	0.48
3:J:239:LEU:HA	3:J:242:HIS:NE2	2.27	0.48
2:K:177:VAL:HG11	2:K:397:GLU:HG2	1.96	0.48
2:g:17:LEU:HB2	2:g:104:LEU:HD12	1.96	0.48
3:h:207:GLN:OE1	3:h:207:GLN:N	2.45	0.48
3:j:198:ASP:OD2	3:j:203:GLN:NE2	2.45	0.48
2:k:25:ASP:HA	2:k:28:LYS:HE2	1.95	0.48
2:k:521:VAL:CG2	2:m:39:VAL:CB	2.62	0.48
2:m:151:SER:O	2:m:151:SER:OG	2.29	0.48
1:0:66:ILE:HB	1:0:92:LEU:HB3	1.95	0.48
2:A:226:LYS:HD2	2:A:227:ILE:N	2.28	0.48
2:C:5:ASP:N	2:C:522:THR:O	2.32	0.48
2:E:368:ARG:O	2:E:372:LEU:HD12	2.13	0.48
2:G:365:LEU:HD13	2:G:368:ARG:HD3	1.95	0.48
2:I:220:ILE:O	2:I:318:GLY:N	2.36	0.48
2:K:76:GLU:OE1	2:K:76:GLU:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:58:ARG:HA	2:M:75:LYS:HD3	1.95	0.48
2:a:252:GLU:HG3	2:a:285:ARG:HH22	1.78	0.48
2:a:521:VAL:CG2	2:c:39:VAL:HB	2.41	0.48
2:e:305:ILE:CG2	3:f:276:ARG:HH12	2.25	0.48
2:i:252:GLU:HG3	2:i:285:ARG:HH22	1.77	0.48
2:m:193:MET:HE1	2:m:371:LYS:HG3	1.95	0.48
3:n:265:LEU:CD2	3:n:269:ASP:HB3	2.43	0.48
1:0:9:ARG:HB2	1:0:86:MET:O	2.13	0.48
1:6:13:LYS:O	1:6:15:LYS:HD3	2.12	0.48
2:C:367:GLU:OE1	2:C:371:LYS:HE3	2.12	0.48
2:K:313:THR:OG1	2:K:315:GLU:HG3	2.13	0.48
2:a:387:VAL:HG23	2:a:388:GLU:H	1.77	0.48
3:b:244:ARG:HA	3:b:244:ARG:HH11	1.78	0.48
2:c:291:ASP:HB2	2:c:372:LEU:HD11	1.95	0.48
3:d:244:ARG:HA	3:d:244:ARG:HH11	1.78	0.48
2:g:194:GLN:NE2	2:g:331:THR:HG22	2.27	0.48
1:0:9:ARG:O	1:0:44:GLY:HA3	2.12	0.48
1:0:63:ASP:HB3	1:0:94:ILE:HD13	1.95	0.48
1:1:9:ARG:O	1:1:44:GLY:HA3	2.13	0.48
1:4:67:PHE:HA	1:4:92:LEU:HD23	1.95	0.48
1:5:9:ARG:HB2	1:5:86:MET:O	2.14	0.48
2:C:58:ARG:HA	2:C:75:LYS:HD3	1.95	0.48
2:G:177:VAL:HG11	2:G:397:GLU:HG2	1.96	0.48
2:I:177:VAL:HG11	2:I:397:GLU:HG2	1.96	0.48
2:a:477:GLY:HA3	2:a:488:MET:HE2	1.95	0.48
2:c:299:THR:HG22	3:d:277:ARG:NH2	2.28	0.48
3:h:276:ARG:NH2	3:h:280:TYR:HD1	2.12	0.48
2:k:4:LYS:N	2:m:61:GLU:O	2.31	0.48
2:m:319:GLN:HG3	2:m:320:ALA:N	2.29	0.48
1:0:38:GLY:HA3	1:0:67:PHE:CZ	2.47	0.48
1:5:63:ASP:HB3	1:5:94:ILE:HD13	1.95	0.48
1:6:27:LEU:HG	2:M:269:GLY:CA	2.43	0.48
2:A:177:VAL:HG11	2:A:397:GLU:HG2	1.96	0.48
2:E:313:THR:OG1	2:E:315:GLU:HG3	2.13	0.48
2:I:47:PRO:HG2	2:K:73:MET:HG2	1.94	0.48
3:J:225:GLN:HA	3:J:228:GLN:NE2	2.28	0.48
2:a:292:ILE:O	2:a:296:THR:HG22	2.14	0.48
2:a:483:GLU:OE1	2:a:483:GLU:N	2.47	0.48
2:c:345:ARG:HA	2:c:348:GLN:OE1	2.12	0.48
3:d:254:THR:HA	3:d:257:THR:HG23	1.94	0.48
2:e:522:THR:OG1	2:g:59:GLU:OE1	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:252:GLU:HA	2:i:285:ARG:HH22	1.78	0.48
3:l:276:ARG:HD3	3:l:279:LEU:HD23	1.96	0.48
2:A:5:ASP:N	2:A:522:THR:O	2.32	0.48
2:C:177:VAL:HG11	2:C:397:GLU:HG2	1.96	0.48
3:J:276:ARG:O	3:J:279:LEU:HB3	2.14	0.48
3:b:236:LEU:HD23	3:b:236:LEU:H	1.78	0.48
2:e:343:GLN:H	2:e:343:GLN:CD	2.14	0.48
2:g:288:MET:HE1	2:g:368:ARG:HG2	1.95	0.48
2:g:322:ARG:HB2	2:g:333:ILE:HD11	1.94	0.48
2:k:284:ARG:O	2:k:288:MET:HE2	2.14	0.48
2:k:325:ILE:HD13	2:k:330:THR:HG22	1.95	0.48
2:m:70:GLY:HA2	2:m:73:MET:HE3	1.95	0.48
1:0:15:LYS:HE2	1:0:38:GLY:HA2	1.96	0.48
1:3:41:LEU:HD23	1:3:41:LEU:H	1.77	0.48
2:I:197:ARG:CD	2:I:277:LYS:HE2	2.44	0.48
2:M:177:VAL:HG11	2:M:397:GLU:HG2	1.96	0.48
2:a:214:GLU:HG2	2:a:324:VAL:HG22	1.95	0.48
2:e:247:LEU:HD22	2:e:248:LEU:H	1.77	0.48
3:f:265:LEU:HB3	3:f:269:ASP:HB3	1.95	0.48
2:i:299:THR:OG1	2:i:300:VAL:N	2.47	0.48
2:k:305:ILE:HG21	3:l:283:LEU:CD2	2.44	0.48
3:l:258:PHE:O	3:l:262:LEU:HG	2.14	0.48
3:n:273:SER:O	3:n:277:ARG:HG2	2.13	0.48
1:4:9:ARG:HB2	1:4:86:MET:O	2.13	0.48
2:A:506:TYR:HE1	2:C:384:ALA:O	1.97	0.48
3:B:225:GLN:HA	3:B:228:GLN:NE2	2.28	0.48
2:E:177:VAL:HG11	2:E:397:GLU:HG2	1.96	0.48
2:G:226:LYS:HD2	2:G:227:ILE:N	2.28	0.48
2:M:226:LYS:HD2	2:M:227:ILE:N	2.28	0.48
2:a:322:ARG:HB2	2:a:333:ILE:HD11	1.95	0.48
2:c:1:MET:SD	2:c:1:MET:N	2.80	0.48
2:c:322:ARG:HB2	2:c:333:ILE:HD11	1.95	0.48
2:g:186:GLU:OE1	2:g:186:GLU:N	2.47	0.48
3:j:276:ARG:NH2	3:j:279:LEU:HG	2.28	0.48
3:l:274:LYS:O	3:l:277:ARG:HB2	2.13	0.48
2:m:307:MET:SD	2:m:311:LYS:HD3	2.53	0.48
2:m:493:ILE:HG12	5:m:603:ANP:C5	2.44	0.48
1:0:92:LEU:O	1:6:6:LEU:HD11	2.14	0.47
1:3:3:ILE:HD13	1:4:93:ALA:CB	2.44	0.47
2:C:415:GLY:HA2	5:C:602:ANP:H1'	1.96	0.47
2:G:261:THR:O	2:G:265:ASN:CG	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:315:GLU:OE1	3:H:269:ASP:C	2.56	0.47
2:I:226:LYS:HD2	2:I:227:ILE:N	2.28	0.47
3:d:235:ALA:O	3:d:238:LEU:HG	2.14	0.47
2:e:252:GLU:HA	2:e:285:ARG:HH22	1.79	0.47
2:m:25:ASP:HA	2:m:28:LYS:HE2	1.95	0.47
3:B:234:GLU:O	3:B:237:GLU:HB2	2.14	0.47
2:C:305:ILE:HG22	3:D:276:ARG:NH2	2.28	0.47
2:a:252:GLU:HA	2:a:285:ARG:HH22	1.79	0.47
2:a:386:GLU:HG3	2:a:387:VAL:H	1.78	0.47
3:b:236:LEU:O	3:b:275:TYR:OH	2.30	0.47
2:c:388:GLU:HA	2:c:391:GLU:OE2	2.13	0.47
2:e:345:ARG:NH1	2:e:349:ILE:HD11	2.29	0.47
2:i:248:LEU:HD23	2:i:274:ALA:HB3	1.96	0.47
2:i:387:VAL:HA	2:i:390:LYS:HZ3	1.77	0.47
3:l:275:TYR:O	3:l:279:LEU:N	2.31	0.47
3:H:225:GLN:HA	3:H:228:GLN:NE2	2.28	0.47
2:K:226:LYS:HD2	2:K:227:ILE:N	2.28	0.47
3:L:277:ARG:O	3:L:280:TYR:HB3	2.14	0.47
2:c:156:GLU:O	2:c:160:LYS:HG3	2.14	0.47
2:g:506:TYR:O	2:g:510:VAL:HG12	2.14	0.47
2:k:495:ASP:OD2	5:k:603:ANP:O2'	2.29	0.47
2:k:520:MET:HE2	2:m:29:VAL:CG2	2.44	0.47
1:3:20:LYS:HB3	1:3:24:GLY:HA2	1.97	0.47
1:4:6:LEU:HD11	1:5:92:LEU:O	2.14	0.47
2:A:58:ARG:HA	2:A:75:LYS:HD3	1.95	0.47
3:F:283:LEU:CG	3:F:284:TYR:CD2	2.90	0.47
2:G:76:GLU:OE1	2:G:76:GLU:HA	2.14	0.47
2:G:313:THR:OG1	2:G:315:GLU:HG3	2.13	0.47
2:I:58:ARG:HA	2:I:75:LYS:HD3	1.95	0.47
2:I:76:GLU:OE1	2:I:76:GLU:HA	2.14	0.47
2:I:286:LYS:HZ2	3:J:284:TYR:HB2	1.78	0.47
2:c:252:GLU:HA	2:c:285:ARG:HH22	1.78	0.47
2:c:513:LEU:HD21	2:e:49:ILE:HG21	1.96	0.47
2:e:322:ARG:HB3	2:e:333:ILE:HD11	1.96	0.47
2:e:388:GLU:O	2:e:389:MET:C	2.56	0.47
2:g:292:ILE:O	2:g:296:THR:HG22	2.15	0.47
3:j:204:GLN:O	3:j:207:GLN:NE2	2.47	0.47
3:j:235:ALA:O	3:j:238:LEU:HG	2.14	0.47
2:k:202:PRO:HD2	2:k:203:TYR:CD1	2.49	0.47
3:l:236:LEU:HD23	3:l:239:LEU:HD22	1.96	0.47
3:l:279:LEU:O	3:l:280:TYR:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:76:GLU:OE1	2:A:76:GLU:HA	2.13	0.47
2:A:299:THR:HB	3:B:277:ARG:NH2	2.30	0.47
2:E:291:ASP:OD2	2:E:368:ARG:NH2	2.48	0.47
2:G:58:ARG:HA	2:G:75:LYS:HD3	1.95	0.47
2:c:319:GLN:HG3	2:c:320:ALA:N	2.30	0.47
2:g:299:THR:HG22	3:h:277:ARG:HH22	1.79	0.47
2:i:25:ASP:HA	2:i:28:LYS:HE2	1.97	0.47
1:2:15:LYS:HE2	1:2:38:GLY:HA2	1.96	0.47
1:2:67:PHE:CA	1:2:92:LEU:HD23	2.45	0.47
1:2:77:LYS:HE2	1:2:80:ASN:HA	1.96	0.47
1:4:27:LEU:HA	2:I:268:ARG:CB	2.44	0.47
1:5:77:LYS:HE2	1:5:80:ASN:HA	1.96	0.47
1:6:15:LYS:HE2	1:6:38:GLY:HA2	1.96	0.47
2:E:76:GLU:OE1	2:E:76:GLU:HA	2.14	0.47
2:G:240:VAL:HG11	2:G:247:LEU:HB2	1.97	0.47
2:I:240:VAL:HG11	2:I:247:LEU:HB2	1.97	0.47
2:I:305:ILE:HG22	3:J:276:ARG:NH2	2.29	0.47
2:M:76:GLU:OE1	2:M:76:GLU:HA	2.14	0.47
2:M:286:LYS:HZ1	3:N:284:TYR:CB	2.28	0.47
2:a:299:THR:HA	3:b:280:TYR:CE2	2.50	0.47
2:c:292:ILE:O	2:c:296:THR:HG22	2.15	0.47
2:c:296:THR:OG1	2:c:319:GLN:O	2.23	0.47
2:e:292:ILE:O	2:e:296:THR:HG22	2.15	0.47
2:i:151:SER:O	2:i:151:SER:OG	2.29	0.47
2:i:387:VAL:O	2:i:391:GLU:HG3	2.15	0.47
2:m:281:PHE:C	2:m:281:PHE:CD1	2.93	0.47
1:1:15:LYS:HE2	1:1:38:GLY:HA2	1.97	0.47
1:1:20:LYS:HB3	1:1:24:GLY:HA2	1.97	0.47
1:1:77:LYS:HE2	1:1:80:ASN:HA	1.96	0.47
1:6:9:ARG:HB2	1:6:86:MET:O	2.13	0.47
2:A:240:VAL:HG11	2:A:247:LEU:HB2	1.97	0.47
2:C:76:GLU:OE1	2:C:76:GLU:HA	2.14	0.47
2:C:313:THR:OG1	2:C:315:GLU:HG3	2.13	0.47
2:E:233:MET:CE	2:E:236:VAL:HG23	2.38	0.47
2:G:345:ARG:CZ	2:G:349:ILE:HD11	2.45	0.47
3:H:279:LEU:HA	3:H:282:LEU:HB3	1.97	0.47
2:K:58:ARG:HA	2:K:75:LYS:HD3	1.95	0.47
2:K:240:VAL:HG11	2:K:247:LEU:HB2	1.97	0.47
2:M:140:ASP:OD1	2:M:140:ASP:N	2.40	0.47
2:M:305:ILE:O	3:N:255:ARG:CZ	2.63	0.47
3:b:265:LEU:H	3:b:265:LEU:HD12	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:305:ILE:HG23	3:f:283:LEU:HD21	1.96	0.47
3:h:270:ALA:O	3:h:273:SER:OG	2.29	0.47
2:i:266:THR:O	2:i:268:ARG:N	2.47	0.47
2:i:281:PHE:CD1	2:i:281:PHE:C	2.93	0.47
2:k:138:CYS:HB2	2:k:411:VAL:HG11	1.96	0.47
2:k:138:CYS:HB2	2:k:411:VAL:CG1	2.44	0.47
2:k:307:MET:SD	2:k:311:LYS:HD3	2.55	0.47
2:m:213:VAL:HB	2:m:325:ILE:HG23	1.96	0.47
2:m:248:LEU:HD23	2:m:274:ALA:HB3	1.97	0.47
2:m:386:GLU:HG3	2:m:387:VAL:N	2.30	0.47
1:3:4:ARG:NH2	1:3:43:VAL:O	2.48	0.47
2:C:345:ARG:CZ	2:C:349:ILE:HD11	2.45	0.47
2:I:178:GLU:O	2:I:381:VAL:HG12	2.15	0.47
2:I:286:LYS:HE2	3:J:284:TYR:CG	2.49	0.47
2:c:344:GLY:O	2:c:348:GLN:HG3	2.14	0.47
2:e:88:GLY:N	5:e:603:ANP:O1B	2.43	0.47
2:i:196:ASP:O	2:i:197:ARG:NH1	2.36	0.47
2:i:292:ILE:O	2:i:296:THR:HG22	2.15	0.47
1:4:20:LYS:HB3	1:4:24:GLY:HA2	1.96	0.47
1:5:4:ARG:NH2	1:5:43:VAL:O	2.48	0.47
1:5:14:ARG:HB3	1:5:82:GLU:O	2.15	0.47
1:5:27:LEU:HA	2:K:269:GLY:HA3	1.80	0.47
1:5:66:ILE:HB	1:5:92:LEU:HB3	1.97	0.47
2:A:291:ASP:OD2	2:A:368:ARG:NH2	2.48	0.47
2:C:240:VAL:HG11	2:C:247:LEU:HB2	1.97	0.47
2:G:178:GLU:O	2:G:381:VAL:HG12	2.15	0.47
2:G:305:ILE:HG22	3:H:276:ARG:CZ	2.45	0.47
2:a:281:PHE:CD1	2:a:281:PHE:C	2.92	0.47
2:a:325:ILE:HD12	2:a:325:ILE:O	2.15	0.47
2:c:17:LEU:HB2	2:c:104:LEU:HD12	1.96	0.47
2:c:265:ASN:O	2:c:271:VAL:HG11	2.15	0.47
2:e:391:GLU:OE1	2:e:392:LYS:HG3	2.14	0.47
2:g:215:LEU:HB3	2:g:246:PRO:HG3	1.96	0.47
2:g:518:GLU:HG3	2:i:29:VAL:HG11	1.97	0.47
2:i:233:MET:HE1	2:i:237:LEU:HB3	1.95	0.47
3:j:207:GLN:OE1	3:j:208:GLN:N	2.47	0.47
2:k:305:ILE:HD13	3:l:276:ARG:HH22	1.79	0.47
3:l:236:LEU:HD13	3:l:275:TYR:CD2	2.49	0.47
2:m:292:ILE:O	2:m:296:THR:HG22	2.15	0.47
1:3:15:LYS:HE2	1:3:38:GLY:HA2	1.96	0.47
1:4:27:LEU:CG	2:I:269:GLY:HA3	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:283:LEU:CG	3:B:284:TYR:CD2	2.90	0.47
2:E:299:THR:HB	3:F:277:ARG:HH22	1.80	0.47
2:G:291:ASP:OD2	2:G:368:ARG:NH2	2.48	0.47
2:I:286:LYS:CE	3:J:284:TYR:CG	2.98	0.47
2:e:281:PHE:O	2:e:284:ARG:HG2	2.15	0.47
3:f:236:LEU:O	3:f:275:TYR:OH	2.29	0.47
2:i:17:LEU:HB2	2:i:104:LEU:HD12	1.97	0.47
2:i:322:ARG:HB2	2:i:333:ILE:HD11	1.96	0.47
2:k:252:GLU:HA	2:k:285:ARG:HH22	1.79	0.47
2:k:345:ARG:NH1	2:k:349:ILE:HD11	2.30	0.47
1:4:4:ARG:NH2	1:4:43:VAL:O	2.48	0.46
1:6:4:ARG:NH2	1:6:43:VAL:O	2.48	0.46
2:A:69:MET:HE2	2:A:522:THR:HB	1.97	0.46
2:A:345:ARG:CZ	2:A:349:ILE:HD11	2.45	0.46
2:C:178:GLU:O	2:C:381:VAL:HG12	2.15	0.46
2:E:178:GLU:O	2:E:381:VAL:HG12	2.15	0.46
3:F:218:LEU:O	3:F:222:LEU:CB	2.63	0.46
2:G:305:ILE:HG22	3:H:276:ARG:NH2	2.30	0.46
2:I:345:ARG:C	2:I:345:ARG:HD3	2.39	0.46
2:M:345:ARG:CZ	2:M:349:ILE:HD11	2.44	0.46
2:a:265:ASN:O	2:a:271:VAL:HG11	2.15	0.46
2:a:307:MET:SD	2:a:311:LYS:HD3	2.55	0.46
2:c:290:GLN:OE1	2:c:345:ARG:NH2	2.48	0.46
2:c:520:MET:HG2	2:e:26:ALA:HA	1.96	0.46
2:e:205:ILE:HD13	2:e:213:VAL:HG23	1.97	0.46
2:g:151:SER:O	2:g:151:SER:OG	2.29	0.46
2:k:232:GLU:HA	2:k:310:GLU:OE2	2.15	0.46
2:m:252:GLU:HA	2:m:285:ARG:HH22	1.79	0.46
3:n:208:GLN:O	3:n:212:ASN:N	2.35	0.46
1:3:27:LEU:HA	2:G:269:GLY:N	2.30	0.46
1:3:77:LYS:HE2	1:3:80:ASN:HA	1.96	0.46
1:4:14:ARG:HB3	1:4:82:GLU:O	2.15	0.46
1:5:20:LYS:HB3	1:5:24:GLY:HA2	1.96	0.46
2:A:178:GLU:O	2:A:381:VAL:HG12	2.15	0.46
2:E:5:ASP:N	2:E:522:THR:O	2.32	0.46
2:E:215:LEU:HD23	2:E:246:PRO:HG2	1.97	0.46
2:a:383:ALA:N	2:a:389:MET:HE1	2.30	0.46
2:c:73:MET:HG2	2:e:47:PRO:CG	2.45	0.46
2:c:248:LEU:HD23	2:c:274:ALA:HB3	1.96	0.46
2:c:518:GLU:HG3	2:e:29:VAL:HG11	1.97	0.46
2:g:383:ALA:HB2	2:g:392:LYS:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:17:LEU:HB2	2:m:104:LEU:HD12	1.97	0.46
1:1:26:VAL:O	1:1:27:LEU:C	2.58	0.46
1:1:46:GLY:CA	1:1:56:PRO:HA	2.46	0.46
2:C:215:LEU:HD23	2:C:246:PRO:HG2	1.97	0.46
2:C:299:THR:CG2	2:C:316:ASP:HB3	2.46	0.46
2:G:69:MET:HE2	2:G:522:THR:HB	1.97	0.46
2:I:286:LYS:CE	3:J:284:TYR:CB	2.94	0.46
2:K:47:PRO:HG2	2:M:73:MET:HG2	1.95	0.46
2:M:291:ASP:OD2	2:M:368:ARG:NH2	2.48	0.46
2:c:288:MET:HE1	2:c:368:ARG:HH11	1.81	0.46
2:e:319:GLN:HG3	2:e:320:ALA:N	2.29	0.46
3:h:236:LEU:H	3:h:236:LEU:HD23	1.80	0.46
2:k:252:GLU:HG3	2:k:285:ARG:HH22	1.80	0.46
1:0:46:GLY:CA	1:0:56:PRO:HA	2.46	0.46
1:1:46:GLY:HA2	1:1:56:PRO:HA	1.98	0.46
1:4:77:LYS:HE2	1:4:80:ASN:HA	1.97	0.46
1:6:14:ARG:HB3	1:6:82:GLU:O	2.16	0.46
1:6:55:LYS:HE3	1:6:56:PRO:O	2.15	0.46
1:6:77:LYS:HE2	1:6:80:ASN:HA	1.96	0.46
2:C:69:MET:HE2	2:C:522:THR:HB	1.97	0.46
2:C:291:ASP:OD2	2:C:368:ARG:NH2	2.48	0.46
2:E:345:ARG:CZ	2:E:349:ILE:HD11	2.45	0.46
3:H:277:ARG:O	3:H:278:GLN:C	2.58	0.46
3:H:283:LEU:CD1	3:H:284:TYR:HD2	2.29	0.46
3:f:236:LEU:HD23	3:f:236:LEU:H	1.81	0.46
2:g:265:ASN:O	2:g:271:VAL:HG11	2.15	0.46
2:g:281:PHE:CD1	2:g:281:PHE:C	2.93	0.46
2:i:305:ILE:HB	3:j:276:ARG:HH12	1.80	0.46
2:m:281:PHE:O	2:m:284:ARG:HG2	2.15	0.46
3:n:216:ALA:O	3:n:220:THR:OG1	2.31	0.46
1:0:77:LYS:HE2	1:0:80:ASN:HA	1.96	0.46
1:1:4:ARG:NH2	1:1:43:VAL:O	2.48	0.46
1:2:4:ARG:NH2	1:2:43:VAL:O	2.48	0.46
1:4:15:LYS:HE2	1:4:38:GLY:HA2	1.96	0.46
1:5:15:LYS:HE2	1:5:38:GLY:HA2	1.96	0.46
2:C:217:SER:O	2:C:217:SER:OG	2.33	0.46
2:E:240:VAL:HG11	2:E:247:LEU:HB2	1.97	0.46
2:E:299:THR:HB	3:F:277:ARG:NH2	2.31	0.46
2:G:313:THR:HB	3:H:267:THR:HA	1.97	0.46
2:K:345:ARG:CZ	2:K:349:ILE:HD11	2.45	0.46
2:M:240:VAL:HG11	2:M:247:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:194:GLN:NE2	2:a:331:THR:HG22	2.29	0.46
2:c:325:ILE:HD12	2:c:326:ASN:H	1.81	0.46
3:f:216:ALA:O	3:f:220:THR:OG1	2.32	0.46
2:i:365:LEU:HA	2:i:368:ARG:HE	1.81	0.46
1:0:4:ARG:NH2	1:0:43:VAL:O	2.48	0.46
1:0:67:PHE:CA	1:0:92:LEU:HD23	2.46	0.46
1:0:93:ALA:HB2	1:6:5:PRO:HA	1.98	0.46
1:1:14:ARG:HB3	1:1:82:GLU:O	2.15	0.46
1:3:14:ARG:HB3	1:3:82:GLU:O	2.15	0.46
1:4:27:LEU:HB3	2:I:265:ASN:CG	2.40	0.46
1:5:26:VAL:C	1:5:28:THR:H	2.23	0.46
1:5:46:GLY:CA	1:5:56:PRO:HA	2.46	0.46
3:F:209:VAL:HG21	3:F:222:LEU:HB2	1.96	0.46
3:F:275:TYR:HA	3:F:278:GLN:HB3	1.97	0.46
2:G:419:LEU:HA	2:G:422:VAL:HG12	1.98	0.46
3:H:252:GLY:C	3:H:256:LYS:HZ3	2.23	0.46
2:I:69:MET:HE2	2:I:522:THR:HB	1.97	0.46
2:I:291:ASP:OD2	2:I:368:ARG:NH2	2.48	0.46
2:I:299:THR:CG2	2:I:316:ASP:HB3	2.46	0.46
2:I:339:GLU:HB2	2:I:343:GLN:NE2	2.21	0.46
2:a:387:VAL:HA	2:a:390:LYS:HZ3	1.77	0.46
2:e:193:MET:HE1	2:e:371:LYS:HG3	1.98	0.46
2:e:281:PHE:C	2:e:281:PHE:CD1	2.93	0.46
3:h:198:ASP:OD2	3:h:203:GLN:NE2	2.48	0.46
1:0:14:ARG:HB3	1:0:82:GLU:O	2.15	0.46
1:2:14:ARG:HB3	1:2:82:GLU:O	2.15	0.46
1:2:46:GLY:CA	1:2:56:PRO:HA	2.46	0.46
1:3:46:GLY:CA	1:3:56:PRO:HA	2.46	0.46
2:A:299:THR:CG2	2:A:316:ASP:HB3	2.46	0.46
2:A:419:LEU:HA	2:A:422:VAL:HG12	1.98	0.46
2:E:69:MET:HE2	2:E:522:THR:HB	1.97	0.46
2:I:419:LEU:HA	2:I:422:VAL:HG12	1.98	0.46
2:K:291:ASP:OD2	2:K:368:ARG:NH2	2.48	0.46
2:a:246:PRO:HG3	2:a:272:LYS:HD2	1.98	0.46
2:c:299:THR:HG22	3:d:277:ARG:HH22	1.79	0.46
2:e:265:ASN:O	2:e:271:VAL:HG11	2.15	0.46
2:e:387:VAL:O	2:e:391:GLU:HG3	2.15	0.46
2:i:319:GLN:HG3	2:i:320:ALA:N	2.30	0.46
2:k:281:PHE:CD1	2:k:281:PHE:C	2.93	0.46
1:0:55:LYS:HE3	1:0:56:PRO:O	2.16	0.46
1:2:5:PRO:HA	1:3:93:ALA:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:46:GLY:HA2	1:2:56:PRO:HA	1.98	0.46
1:5:5:PRO:HA	1:6:93:ALA:HB2	1.96	0.46
1:6:67:PHE:HA	1:6:92:LEU:HD23	1.98	0.46
2:A:215:LEU:HD23	2:A:246:PRO:HG2	1.97	0.46
3:F:256:LYS:O	3:F:260:GLU:HG3	2.16	0.46
2:K:34:LYS:HE3	2:M:112:ASN:HD21	1.79	0.46
2:K:220:ILE:O	2:K:318:GLY:N	2.37	0.46
2:K:299:THR:CG2	2:K:316:ASP:HB3	2.46	0.46
2:M:178:GLU:O	2:M:381:VAL:HG12	2.15	0.46
3:N:277:ARG:O	3:N:278:GLN:C	2.58	0.46
2:a:17:LEU:HB2	2:a:104:LEU:HD12	1.97	0.46
3:f:219:ALA:O	3:f:222:LEU:HG	2.16	0.46
3:f:280:TYR:O	3:f:283:LEU:HD12	2.16	0.46
2:g:252:GLU:HG3	2:g:285:ARG:HH22	1.79	0.46
2:g:319:GLN:HG3	2:g:320:ALA:N	2.30	0.46
2:k:205:ILE:HD13	2:k:213:VAL:HG23	1.98	0.46
2:k:265:ASN:O	2:k:271:VAL:HG11	2.16	0.46
2:k:299:THR:HA	3:l:280:TYR:CD2	2.47	0.46
1:2:26:VAL:O	1:2:27:LEU:C	2.59	0.46
1:3:27:LEU:HD23	2:G:269:GLY:HA3	1.97	0.46
1:5:28:THR:O	2:K:268:ARG:HD3	2.16	0.46
2:A:292:ILE:O	2:A:296:THR:OG1	2.21	0.46
2:E:235:PRO:HD2	2:E:236:VAL:H	1.81	0.46
2:E:299:THR:CG2	2:E:316:ASP:HB3	2.46	0.46
3:J:277:ARG:O	3:J:280:TYR:HB3	2.14	0.46
2:K:493:ILE:HD13	5:K:600:ANP:N1	2.31	0.46
2:M:69:MET:HE2	2:M:522:THR:HB	1.97	0.46
2:M:215:LEU:HD23	2:M:246:PRO:HG2	1.97	0.46
2:M:305:ILE:HG22	3:N:276:ARG:NH2	2.31	0.46
2:M:461:GLU:HG2	2:m:463:SER:HB3	1.97	0.46
2:c:205:ILE:HA	2:c:213:VAL:HG22	1.98	0.46
2:e:194:GLN:NE2	2:e:331:THR:HG22	2.31	0.46
2:e:248:LEU:HD22	2:e:249:ILE:H	1.81	0.46
2:g:25:ASP:C	2:g:25:ASP:OD1	2.59	0.46
2:g:416:GLY:O	2:g:420:ILE:HG12	2.16	0.46
2:i:194:GLN:HE22	2:i:329:THR:HB	1.80	0.46
2:k:368:ARG:O	2:k:372:LEU:HD23	2.16	0.46
2:m:34:LYS:HB2	2:m:34:LYS:HE3	1.73	0.46
3:n:244:ARG:HE	3:n:244:ARG:C	2.24	0.46
1:2:34:LYS:NZ	1:2:36:THR:HG22	2.31	0.46
1:5:55:LYS:HE3	1:5:56:PRO:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:67:PHE:CA	1:5:92:LEU:HD23	2.45	0.46
2:I:215:LEU:HD23	2:I:246:PRO:HG2	1.97	0.46
2:I:342:ILE:O	2:I:343:GLN:C	2.59	0.46
2:K:36:ARG:HB3	2:M:516:THR:O	2.16	0.46
2:a:429:LEU:C	2:a:430:ARG:HD2	2.41	0.46
2:e:214:GLU:HG2	2:e:324:VAL:HG22	1.97	0.46
2:g:304:GLU:HB2	3:h:283:LEU:HD23	1.98	0.46
2:i:365:LEU:HG	2:i:368:ARG:HH21	1.81	0.46
3:j:237:GLU:OE1	3:j:237:GLU:N	2.42	0.46
3:n:274:LYS:HD2	3:n:274:LYS:N	2.26	0.46
1:0:46:GLY:HA2	1:0:56:PRO:HA	1.98	0.45
1:4:55:LYS:HE3	1:4:56:PRO:O	2.16	0.45
1:6:46:GLY:CA	1:6:56:PRO:HA	2.46	0.45
2:A:234:LEU:O	2:A:238:GLU:HG2	2.17	0.45
2:A:299:THR:HB	3:B:277:ARG:HH22	1.81	0.45
3:B:256:LYS:O	3:B:260:GLU:HG3	2.16	0.45
2:C:235:PRO:HD2	2:C:236:VAL:H	1.81	0.45
2:C:316:ASP:OD1	3:D:277:ARG:NH1	2.49	0.45
2:G:217:SER:O	2:G:217:SER:OG	2.33	0.45
2:G:235:PRO:HD2	2:G:236:VAL:H	1.81	0.45
3:H:247:LEU:HD21	3:H:282:LEU:CG	2.45	0.45
3:N:256:LYS:O	3:N:260:GLU:HG3	2.16	0.45
2:a:1:MET:SD	2:a:1:MET:N	2.89	0.45
2:a:391:GLU:O	2:a:395:ARG:HG2	2.15	0.45
2:k:248:LEU:HD22	2:k:249:ILE:H	1.82	0.45
2:k:319:GLN:HG3	2:k:320:ALA:N	2.29	0.45
2:m:196:ASP:OD1	2:m:196:ASP:N	2.49	0.45
2:m:247:LEU:HD22	2:m:248:LEU:H	1.81	0.45
2:m:265:ASN:O	2:m:271:VAL:HG11	2.16	0.45
1:3:55:LYS:HE3	1:3:56:PRO:O	2.16	0.45
3:B:236:LEU:HD11	3:B:275:TYR:HD2	1.82	0.45
3:D:256:LYS:O	3:D:260:GLU:HG3	2.16	0.45
2:G:299:THR:CG2	2:G:316:ASP:HB3	2.45	0.45
3:H:218:LEU:HD12	3:H:218:LEU:C	2.41	0.45
3:H:256:LYS:O	3:H:260:GLU:HG3	2.16	0.45
2:I:266:THR:HB	2:I:267:MET:SD	2.57	0.45
2:K:178:GLU:O	2:K:381:VAL:HG12	2.15	0.45
2:K:296:THR:HA	2:K:335:GLY:C	2.42	0.45
3:L:236:LEU:HD11	3:L:275:TYR:HD2	1.82	0.45
2:M:299:THR:CG2	2:M:316:ASP:HB3	2.46	0.45
3:N:252:GLY:C	3:N:256:LYS:HZ3	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:17:LEU:HB2	2:e:104:LEU:HD12	1.97	0.45
3:j:216:ALA:O	3:j:220:THR:OG1	2.31	0.45
2:k:25:ASP:C	2:k:25:ASP:OD1	2.58	0.45
2:k:194:GLN:NE2	2:k:331:THR:HG22	2.32	0.45
2:k:292:ILE:O	2:k:296:THR:HG22	2.16	0.45
2:k:520:MET:CB	2:m:26:ALA:HA	2.46	0.45
1:1:1:MET:HE1	1:2:95:VAL:HG13	1.98	0.45
1:2:28:THR:OG1	2:A:264:VAL:CG1	2.61	0.45
1:5:46:GLY:HA2	1:5:56:PRO:HA	1.98	0.45
2:A:296:THR:HA	2:A:335:GLY:C	2.42	0.45
2:K:69:MET:HE2	2:K:522:THR:HB	1.97	0.45
2:K:299:THR:HB	3:L:277:ARG:HH22	1.81	0.45
2:e:506:TYR:O	2:e:510:VAL:HG12	2.17	0.45
3:f:201:GLU:O	3:f:205:LEU:HD23	2.17	0.45
2:g:8:PHE:CE1	2:i:25:ASP:OD1	2.69	0.45
2:g:307:MET:SD	2:g:311:LYS:HD3	2.57	0.45
2:k:151:SER:O	2:k:151:SER:OG	2.29	0.45
3:n:219:ALA:O	3:n:222:LEU:HG	2.16	0.45
1:1:6:LEU:HD11	1:2:92:LEU:O	2.16	0.45
1:1:34:LYS:NZ	1:1:36:THR:HG22	2.32	0.45
1:1:55:LYS:HE3	1:1:56:PRO:O	2.16	0.45
1:1:91:ILE:C	1:1:92:LEU:HD22	2.40	0.45
1:2:55:LYS:HE3	1:2:56:PRO:O	2.16	0.45
2:A:233:MET:HA	2:A:310:GLU:OE2	2.16	0.45
3:F:224:LEU:HG	3:F:228:GLN:NE2	2.31	0.45
2:G:296:THR:HA	2:G:335:GLY:C	2.42	0.45
2:I:296:THR:HA	2:I:335:GLY:C	2.42	0.45
3:J:256:LYS:O	3:J:260:GLU:HG3	2.16	0.45
2:M:316:ASP:HA	3:N:277:ARG:HH22	1.80	0.45
2:c:278:ALA:HB3	2:c:285:ARG:NH2	2.31	0.45
2:c:343:GLN:HA	2:c:346:VAL:HG12	1.98	0.45
2:c:350:ARG:HA	2:c:350:ARG:CZ	2.46	0.45
2:e:196:ASP:OD1	2:e:196:ASP:N	2.49	0.45
2:g:87:ASP:O	2:g:499:VAL:HG13	2.16	0.45
2:g:444:LEU:HD23	2:g:447:MET:HE3	1.98	0.45
3:j:253:GLN:O	3:j:257:THR:HG23	2.16	0.45
2:m:391:GLU:OE1	2:m:392:LYS:N	2.50	0.45
1:3:92:LEU:HD22	1:3:92:LEU:N	2.32	0.45
1:4:46:GLY:CA	1:4:56:PRO:HA	2.46	0.45
2:E:140:ASP:OD1	2:E:140:ASP:N	2.40	0.45
2:a:254:VAL:H	2:a:277:LYS:HZ2	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:281:PHE:O	2:a:284:ARG:HG2	2.15	0.45
2:c:205:ILE:HD13	2:c:213:VAL:HG23	1.99	0.45
2:c:248:LEU:HD22	2:c:249:ILE:H	1.82	0.45
2:c:281:PHE:CD1	2:c:281:PHE:C	2.94	0.45
2:c:387:VAL:HA	2:c:390:LYS:HZ3	1.80	0.45
3:f:256:LYS:HA	3:f:259:GLN:HB3	1.98	0.45
2:m:205:ILE:HD13	2:m:213:VAL:HG23	1.98	0.45
2:m:299:THR:HA	3:n:277:ARG:NH1	2.31	0.45
3:n:278:GLN:OE1	3:n:278:GLN:N	2.48	0.45
1:4:85:ILE:HD12	1:4:85:ILE:O	2.17	0.45
1:5:66:ILE:HD12	1:5:93:ALA:O	2.16	0.45
1:5:85:ILE:HD12	1:5:85:ILE:O	2.17	0.45
1:6:46:GLY:HA2	1:6:56:PRO:HA	1.98	0.45
2:C:419:LEU:HA	2:C:422:VAL:HG12	1.98	0.45
3:D:216:ALA:O	3:D:220:THR:HG23	2.17	0.45
3:D:278:GLN:O	3:D:281:ALA:N	2.49	0.45
2:I:129:GLU:OE1	2:I:129:GLU:HA	2.17	0.45
3:N:224:LEU:HG	3:N:228:GLN:NE2	2.26	0.45
2:a:250:ILE:HD11	2:a:278:ALA:HA	1.98	0.45
2:a:299:THR:HG22	3:b:277:ARG:NH2	2.31	0.45
2:e:25:ASP:OD1	2:e:25:ASP:C	2.60	0.45
2:e:303:GLU:O	3:f:283:LEU:CD2	2.64	0.45
3:j:201:GLU:OE1	3:j:201:GLU:N	2.38	0.45
1:2:5:PRO:CA	1:3:93:ALA:HB2	2.47	0.45
1:3:85:ILE:HD12	1:3:85:ILE:O	2.17	0.45
1:5:34:LYS:NZ	1:5:36:THR:HG22	2.32	0.45
2:E:296:THR:HA	2:E:335:GLY:C	2.42	0.45
2:E:419:LEU:HA	2:E:422:VAL:HG12	1.98	0.45
2:I:235:PRO:HD2	2:I:236:VAL:H	1.81	0.45
3:J:216:ALA:O	3:J:220:THR:HG23	2.17	0.45
3:J:236:LEU:HD11	3:J:275:TYR:HD2	1.82	0.45
3:J:283:LEU:CG	3:J:284:TYR:CD2	2.89	0.45
2:M:296:THR:HA	2:M:335:GLY:C	2.42	0.45
2:M:305:ILE:CG1	3:N:283:LEU:HD22	2.47	0.45
2:M:419:LEU:HA	2:M:422:VAL:HG12	1.98	0.45
3:b:262:LEU:HA	3:b:265:LEU:HD13	1.98	0.45
2:i:307:MET:SD	2:i:311:LYS:HD3	2.57	0.45
3:l:277:ARG:HD3	3:l:277:ARG:HA	1.59	0.45
1:0:92:LEU:C	1:6:9:ARG:HH22	2.25	0.45
1:1:66:ILE:HB	1:1:92:LEU:CB	2.46	0.45
1:3:46:GLY:HA2	1:3:56:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:112:ASN:ND2	2:M:34:LYS:HE3	2.32	0.45
2:G:129:GLU:OE1	2:G:129:GLU:HA	2.17	0.45
3:H:236:LEU:HD11	3:H:275:TYR:HD2	1.81	0.45
2:K:419:LEU:HA	2:K:422:VAL:HG12	1.98	0.45
3:L:218:LEU:HA	3:L:221:GLN:CD	2.42	0.45
2:a:34:LYS:HE3	2:a:34:LYS:HB2	1.74	0.45
2:c:307:MET:SD	2:c:311:LYS:HD3	2.57	0.45
2:i:205:ILE:HA	2:i:213:VAL:HG22	1.99	0.45
2:i:265:ASN:O	2:i:271:VAL:HG11	2.17	0.45
3:l:272:ALA:O	3:l:275:TYR:HB2	2.16	0.45
2:m:300:VAL:HG23	3:n:280:TYR:HD2	1.81	0.45
1:1:11:ILE:HD11	1:1:83:VAL:CG2	2.47	0.45
1:1:85:ILE:O	1:1:85:ILE:HD12	2.17	0.45
1:2:85:ILE:HD12	1:2:85:ILE:O	2.17	0.45
1:6:85:ILE:HD12	1:6:85:ILE:O	2.17	0.45
2:A:129:GLU:OE1	2:A:129:GLU:HA	2.17	0.45
2:C:296:THR:HA	2:C:335:GLY:C	2.42	0.45
2:G:215:LEU:HD23	2:G:246:PRO:HG2	1.97	0.45
2:G:286:LYS:NZ	3:H:280:TYR:HE1	2.14	0.45
2:K:235:PRO:HD2	2:K:236:VAL:H	1.81	0.45
2:M:129:GLU:OE1	2:M:129:GLU:HA	2.17	0.45
2:M:217:SER:O	2:M:217:SER:OG	2.33	0.45
3:N:277:ARG:O	3:N:280:TYR:HB3	2.17	0.45
2:a:494:LEU:HD23	2:a:494:LEU:HA	1.78	0.45
3:b:276:ARG:NH2	3:b:280:TYR:HD1	2.14	0.45
2:c:520:MET:HE1	2:e:38:VAL:CG1	2.47	0.45
2:i:1:MET:SD	2:i:1:MET:N	2.89	0.45
2:i:112:ASN:N	2:i:435:ASP:OD2	2.48	0.45
2:k:34:LYS:HE3	2:k:34:LYS:HB2	1.73	0.45
2:k:316:ASP:C	3:l:277:ARG:NH2	2.75	0.45
3:l:274:LYS:H	3:l:274:LYS:HD2	1.82	0.45
2:m:206:ASN:HD21	2:m:272:LYS:HG2	1.82	0.45
1:0:9:ARG:NH2	1:1:93:ALA:H	2.15	0.45
1:1:27:LEU:CD2	2:C:271:VAL:HG12	2.47	0.45
1:3:34:LYS:NZ	1:3:36:THR:HG22	2.32	0.45
2:C:513:LEU:HD12	2:E:387:VAL:HG23	1.99	0.45
2:E:129:GLU:OE1	2:E:129:GLU:HA	2.17	0.45
2:K:321:LYS:HE2	2:K:334:ASP:HB2	1.99	0.45
3:N:277:ARG:O	3:N:280:TYR:N	2.50	0.45
2:a:171:LYS:HG3	2:a:407:VAL:HG21	1.98	0.45
2:c:194:GLN:HE22	2:c:329:THR:HB	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:222:LEU:HD23	2:c:289:LEU:HD23	1.99	0.45
2:g:248:LEU:HD23	2:g:274:ALA:HB3	1.98	0.45
3:h:274:LYS:O	3:h:278:GLN:OE1	2.35	0.45
2:i:416:GLY:O	2:i:420:ILE:HG12	2.17	0.45
2:m:194:GLN:NE2	2:m:331:THR:HG22	2.31	0.45
2:m:248:LEU:HD22	2:m:249:ILE:H	1.81	0.45
2:m:299:THR:HA	3:n:280:TYR:HE2	1.82	0.45
2:m:416:GLY:O	2:m:420:ILE:HG12	2.17	0.45
2:m:494:LEU:HD23	2:m:494:LEU:HA	1.85	0.45
3:n:265:LEU:O	3:n:267:THR:N	2.44	0.45
1:0:85:ILE:HD12	1:0:85:ILE:O	2.17	0.44
1:2:11:ILE:HD11	1:2:83:VAL:CG2	2.47	0.44
2:A:305:ILE:HG22	3:B:276:ARG:NH2	2.32	0.44
2:A:321:LYS:HE2	2:A:334:ASP:HB2	2.00	0.44
3:D:252:GLY:O	3:D:255:ARG:HB3	2.17	0.44
2:E:461:GLU:HG2	2:a:463:SER:HB3	1.98	0.44
2:I:140:ASP:OD1	2:I:140:ASP:N	2.40	0.44
3:J:252:GLY:O	3:J:255:ARG:HB3	2.17	0.44
3:L:256:LYS:O	3:L:260:GLU:HG3	2.16	0.44
2:a:49:ILE:HG21	2:m:513:LEU:HD21	2.00	0.44
2:a:262:LEU:HD22	2:a:273:VAL:HG21	1.99	0.44
2:c:196:ASP:OD1	2:c:196:ASP:N	2.50	0.44
2:c:517:THR:HA	2:e:37:ASN:HB2	2.00	0.44
2:e:391:GLU:OE2	2:e:395:ARG:NH1	2.50	0.44
2:g:52:ASP:C	2:g:52:ASP:OD1	2.60	0.44
2:k:194:GLN:HE22	2:k:329:THR:HB	1.81	0.44
3:l:216:ALA:O	3:l:220:THR:OG1	2.33	0.44
3:l:262:LEU:HA	3:l:265:LEU:HD23	1.99	0.44
2:m:388:GLU:O	2:m:389:MET:C	2.60	0.44
1:0:11:ILE:HD11	1:0:83:VAL:CG2	2.47	0.44
1:0:34:LYS:NZ	1:0:36:THR:HG22	2.31	0.44
3:B:252:GLY:O	3:B:255:ARG:HB3	2.17	0.44
2:G:321:LYS:HE2	2:G:334:ASP:HB2	1.99	0.44
2:I:292:ILE:O	2:I:296:THR:OG1	2.21	0.44
2:K:129:GLU:OE1	2:K:129:GLU:HA	2.17	0.44
3:L:252:GLY:O	3:L:255:ARG:HB3	2.17	0.44
3:N:253:GLN:HA	3:N:256:LYS:HZ1	1.81	0.44
2:a:325:ILE:HD12	2:a:325:ILE:C	2.43	0.44
2:c:34:LYS:HE3	2:c:34:LYS:HB2	1.73	0.44
2:c:184:GLN:O	2:c:380:LYS:NZ	2.49	0.44
2:e:222:LEU:HD23	2:e:289:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:359:ASP:OD1	2:e:362:ARG:NH2	2.42	0.44
2:g:164:GLU:HG3	2:g:187:LEU:HD21	1.99	0.44
2:g:194:GLN:HE22	2:g:329:THR:HB	1.83	0.44
2:g:254:VAL:H	2:g:277:LYS:HZ2	1.65	0.44
2:k:391:GLU:OE1	2:k:392:LYS:N	2.50	0.44
3:l:275:TYR:HA	3:l:278:GLN:CG	2.47	0.44
1:1:5:PRO:HA	1:2:93:ALA:HB2	1.98	0.44
1:4:46:GLY:HA2	1:4:56:PRO:HA	1.98	0.44
2:C:265:ASN:O	2:C:268:ARG:O	2.35	0.44
2:C:321:LYS:HE2	2:C:334:ASP:HB2	2.00	0.44
2:E:305:ILE:O	3:F:255:ARG:NE	2.51	0.44
3:H:253:GLN:HA	3:H:256:LYS:HZ1	1.81	0.44
2:I:227:ILE:HD13	2:I:227:ILE:HA	1.90	0.44
2:I:321:LYS:HE2	2:I:334:ASP:HB2	2.00	0.44
3:N:216:ALA:O	3:N:220:THR:HG23	2.17	0.44
3:N:236:LEU:HD11	3:N:275:TYR:HD2	1.82	0.44
3:N:252:GLY:O	3:N:255:ARG:HB3	2.17	0.44
2:a:278:ALA:HB3	2:a:285:ARG:NH2	2.33	0.44
3:d:262:LEU:HD12	3:d:263:ALA:N	2.32	0.44
3:d:274:LYS:HA	3:d:277:ARG:CG	2.48	0.44
1:3:8:ASP:CG	1:3:47:ARG:HB2	2.42	0.44
1:4:34:LYS:NZ	1:4:36:THR:HG22	2.31	0.44
1:6:34:LYS:NZ	1:6:36:THR:HG22	2.32	0.44
3:F:277:ARG:O	3:F:280:TYR:HB3	2.18	0.44
2:G:200:LEU:HD21	2:G:254:VAL:HB	2.00	0.44
2:a:222:LEU:HD23	2:a:289:LEU:HD23	2.00	0.44
2:a:416:GLY:O	2:a:420:ILE:HG12	2.18	0.44
2:c:73:MET:CG	2:e:47:PRO:HG2	2.47	0.44
2:e:416:GLY:O	2:e:420:ILE:HG12	2.17	0.44
2:e:526:LYS:HA	2:e:526:LYS:HE3	1.99	0.44
2:k:506:TYR:O	2:k:510:VAL:HG12	2.16	0.44
1:0:66:ILE:HD12	1:0:93:ALA:O	2.16	0.44
1:0:67:PHE:HA	1:0:92:LEU:HD23	2.00	0.44
2:A:69:MET:CE	2:A:522:THR:HB	2.48	0.44
2:C:69:MET:CE	2:C:522:THR:HB	2.48	0.44
2:C:129:GLU:OE1	2:C:129:GLU:HA	2.17	0.44
3:F:220:THR:O	3:F:223:ALA:N	2.51	0.44
3:J:224:LEU:HG	3:J:228:GLN:NE2	2.24	0.44
2:K:200:LEU:HD21	2:K:254:VAL:HB	2.00	0.44
2:M:200:LEU:HD21	2:M:254:VAL:HB	2.00	0.44
2:a:517:THR:HA	2:c:37:ASN:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:52:ASP:C	2:c:52:ASP:OD1	2.60	0.44
2:g:193:MET:HE1	2:g:371:LYS:HG3	1.99	0.44
3:h:278:GLN:OE1	3:h:278:GLN:N	2.48	0.44
2:i:388:GLU:O	2:i:389:MET:C	2.59	0.44
2:k:520:MET:CE	2:m:37:ASN:O	2.66	0.44
2:m:254:VAL:H	2:m:277:LYS:HZ2	1.64	0.44
1:3:9:ARG:HA	1:3:87:SER:C	2.42	0.44
1:3:9:ARG:HD2	1:3:86:MET:O	2.18	0.44
1:6:11:ILE:HD11	1:6:83:VAL:CG2	2.47	0.44
2:E:222:LEU:CD1	2:E:300:VAL:HG22	2.47	0.44
2:G:233:MET:C	2:G:233:MET:SD	3.01	0.44
3:b:201:GLU:OE1	3:b:201:GLU:N	2.49	0.44
2:c:252:GLU:HG3	2:c:285:ARG:HH22	1.83	0.44
3:d:278:GLN:OE1	3:d:278:GLN:N	2.50	0.44
2:e:248:LEU:HD23	2:e:274:ALA:HB3	1.99	0.44
2:g:388:GLU:O	2:g:389:MET:C	2.60	0.44
3:h:219:ALA:O	3:h:222:LEU:HG	2.17	0.44
2:m:25:ASP:OD1	2:m:25:ASP:C	2.60	0.44
2:A:235:PRO:HD2	2:A:236:VAL:H	1.81	0.44
3:B:217:ALA:O	3:B:220:THR:HB	2.18	0.44
2:C:200:LEU:HD21	2:C:254:VAL:HB	2.00	0.44
3:D:236:LEU:HD11	3:D:275:TYR:HD2	1.81	0.44
2:G:38:VAL:HG22	2:I:519:CYS:HB3	2.00	0.44
3:H:277:ARG:O	3:H:280:TYR:N	2.51	0.44
2:M:69:MET:CE	2:M:522:THR:HB	2.48	0.44
2:M:227:ILE:HD13	2:M:227:ILE:HA	1.90	0.44
2:M:321:LYS:HE2	2:M:334:ASP:HB2	1.99	0.44
3:b:274:LYS:O	3:b:278:GLN:OE1	2.35	0.44
2:c:194:GLN:NE2	2:c:331:THR:HG22	2.32	0.44
2:e:307:MET:SD	2:e:311:LYS:HD3	2.57	0.44
2:e:430:ARG:HD3	2:e:430:ARG:HA	1.74	0.44
2:e:521:VAL:HG23	2:g:39:VAL:HB	1.99	0.44
3:h:236:LEU:O	3:h:275:TYR:OH	2.30	0.44
2:i:281:PHE:O	2:i:284:ARG:HG2	2.18	0.44
2:k:77:VAL:HG11	2:k:510:VAL:HB	1.99	0.44
2:m:1:MET:SD	2:m:1:MET:N	2.89	0.44
1:3:11:ILE:HD11	1:3:83:VAL:CG2	2.47	0.44
1:4:11:ILE:HD11	1:4:83:VAL:CG2	2.47	0.44
1:5:11:ILE:HD11	1:5:83:VAL:CG2	2.47	0.44
3:H:252:GLY:O	3:H:255:ARG:HB3	2.17	0.44
3:L:283:LEU:CG	3:L:284:TYR:CD2	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:80:LYS:HE2	2:M:80:LYS:HB3	1.78	0.44
2:M:235:PRO:HD2	2:M:236:VAL:H	1.81	0.44
2:M:316:ASP:OD1	3:N:277:ARG:NH2	2.51	0.44
2:a:506:TYR:O	2:a:510:VAL:HG12	2.18	0.44
2:c:33:PRO:HG3	5:c:603:ANP:C6	2.47	0.44
2:c:368:ARG:O	2:c:372:LEU:HD22	2.18	0.44
2:e:387:VAL:HA	2:e:390:LYS:HZ2	1.81	0.44
2:k:77:VAL:HG21	2:k:510:VAL:HG11	2.00	0.44
3:n:259:GLN:O	3:n:262:LEU:HG	2.18	0.44
1:5:9:ARG:HH21	1:6:93:ALA:HB2	1.83	0.44
2:E:69:MET:CE	2:E:522:THR:HB	2.48	0.44
2:E:200:LEU:HD21	2:E:254:VAL:HB	2.00	0.44
2:E:321:LYS:HE2	2:E:334:ASP:HB2	1.99	0.44
2:I:313:THR:OG1	2:I:314:LEU:N	2.50	0.44
3:b:282:LEU:O	3:b:283:LEU:C	2.61	0.44
2:c:526:LYS:HE3	2:c:526:LYS:HA	2.00	0.44
2:g:278:ALA:HB3	2:g:285:ARG:NH2	2.33	0.44
3:n:208:GLN:HG3	3:n:218:LEU:HD11	1.99	0.44
1:2:27:LEU:HA	2:A:269:GLY:N	2.33	0.43
3:F:252:GLY:O	3:F:255:ARG:HB3	2.17	0.43
3:F:278:GLN:HG3	3:F:279:LEU:N	2.30	0.43
2:G:261:THR:O	2:G:265:ASN:OD1	2.36	0.43
3:H:275:TYR:O	3:H:278:GLN:HB3	2.18	0.43
2:K:69:MET:CE	2:K:522:THR:HB	2.48	0.43
2:a:134:LEU:O	2:a:134:LEU:HD23	2.18	0.43
2:e:490:ASP:C	2:e:490:ASP:OD1	2.61	0.43
2:g:288:MET:HE1	2:g:368:ARG:HD3	2.00	0.43
2:i:526:LYS:HA	2:i:526:LYS:HE3	1.99	0.43
2:k:281:PHE:O	2:k:284:ARG:HG2	2.18	0.43
2:k:526:LYS:HA	2:k:526:LYS:HE3	2.00	0.43
1:0:3:ILE:HD13	1:1:93:ALA:CB	2.47	0.43
1:1:38:GLY:O	1:1:64:ILE:HA	2.19	0.43
1:6:38:GLY:O	1:6:64:ILE:HA	2.18	0.43
3:B:219:ALA:HB1	3:B:238:LEU:HD11	2.00	0.43
2:G:69:MET:CE	2:G:522:THR:HB	2.48	0.43
3:H:278:GLN:HG3	3:H:279:LEU:N	2.33	0.43
2:I:345:ARG:HD2	2:I:372:LEU:CD2	2.45	0.43
2:a:194:GLN:HE22	2:a:329:THR:HB	1.83	0.43
3:b:219:ALA:O	3:b:222:LEU:HG	2.18	0.43
2:c:416:GLY:O	2:c:420:ILE:HG12	2.18	0.43
2:g:490:ASP:C	2:g:490:ASP:OD1	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j:208:GLN:O	3:j:212:ASN:N	2.37	0.43
3:j:245:LYS:H	3:j:245:LYS:HG2	1.64	0.43
2:k:305:ILE:HG21	3:l:283:LEU:HD21	1.98	0.43
2:m:222:LEU:HD13	2:m:293:ALA:HB2	2.01	0.43
1:4:11:ILE:HG13	1:4:41:LEU:HD21	2.01	0.43
1:5:11:ILE:HG13	1:5:41:LEU:HD21	2.01	0.43
2:A:332:ILE:HD12	2:A:332:ILE:N	2.33	0.43
3:H:239:LEU:HD23	3:H:242:HIS:NE2	2.34	0.43
2:a:25:ASP:OD1	2:a:25:ASP:C	2.61	0.43
3:d:283:LEU:H	3:d:283:LEU:HD12	1.83	0.43
2:e:278:ALA:HB3	2:e:285:ARG:NH2	2.33	0.43
2:i:444:LEU:HD23	2:i:447:MET:HE3	1.99	0.43
2:i:477:GLY:HA3	2:i:488:MET:HE2	2.01	0.43
3:j:274:LYS:O	3:j:278:GLN:OE1	2.37	0.43
2:k:387:VAL:HA	2:k:390:LYS:HZ2	1.82	0.43
1:3:71:TYR:O	1:3:74:LYS:NZ	2.49	0.43
2:C:332:ILE:N	2:C:332:ILE:HD12	2.33	0.43
2:K:332:ILE:N	2:K:332:ILE:HD12	2.34	0.43
2:M:332:ILE:HD12	2:M:332:ILE:N	2.33	0.43
3:N:258:PHE:O	3:N:261:ILE:HG13	2.19	0.43
2:g:179:ASP:OD1	2:g:179:ASP:C	2.62	0.43
2:g:232:GLU:OE1	2:g:232:GLU:N	2.50	0.43
2:m:179:ASP:C	2:m:179:ASP:OD1	2.62	0.43
1:0:11:ILE:HG13	1:0:41:LEU:HD21	2.01	0.43
1:1:27:LEU:HA	2:C:269:GLY:HA3	2.00	0.43
1:4:38:GLY:O	1:4:64:ILE:HA	2.19	0.43
1:5:38:GLY:O	1:5:64:ILE:HA	2.19	0.43
1:5:47:ARG:HH22	1:5:50:GLU:CD	2.26	0.43
1:6:27:LEU:O	2:M:268:ARG:CB	2.65	0.43
3:B:215:ASP:HB3	3:B:218:LEU:HD21	1.99	0.43
3:B:218:LEU:O	3:B:222:LEU:N	2.31	0.43
3:b:275:TYR:HA	3:b:278:GLN:OE1	2.19	0.43
2:e:214:GLU:OE1	2:e:322:ARG:HD3	2.18	0.43
2:g:284:ARG:NH1	2:g:361:ASP:OD1	2.37	0.43
2:g:303:GLU:O	3:h:283:LEU:HD21	2.18	0.43
2:i:380:LYS:HD3	2:i:380:LYS:C	2.44	0.43
2:k:416:GLY:O	2:k:420:ILE:HG12	2.17	0.43
1:2:26:VAL:O	1:2:28:THR:N	2.51	0.43
1:6:11:ILE:HG13	1:6:41:LEU:HD21	2.01	0.43
3:H:277:ARG:O	3:H:280:TYR:HB3	2.18	0.43
2:I:286:LYS:NZ	3:J:284:TYR:CD2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:239:LEU:HD23	3:J:242:HIS:NE2	2.34	0.43
3:L:239:LEU:HD23	3:L:242:HIS:NE2	2.34	0.43
2:a:205:ILE:HD13	2:a:213:VAL:HG23	2.01	0.43
2:a:254:VAL:H	2:a:277:LYS:NZ	2.17	0.43
2:a:444:LEU:HD23	2:a:447:MET:HE3	2.01	0.43
3:b:282:LEU:O	3:b:284:TYR:N	2.51	0.43
2:c:161:LEU:O	2:c:164:GLU:HG2	2.18	0.43
3:d:270:ALA:O	3:d:273:SER:OG	2.30	0.43
3:h:240:PHE:HB2	3:h:275:TYR:OH	2.18	0.43
3:l:254:THR:HA	3:l:257:THR:CG2	2.48	0.43
1:2:38:GLY:O	1:2:64:ILE:HA	2.19	0.43
2:A:200:LEU:HD21	2:A:254:VAL:HB	2.00	0.43
2:G:332:ILE:HD12	2:G:332:ILE:N	2.34	0.43
3:H:276:ARG:O	3:H:279:LEU:HB3	2.19	0.43
2:I:298:GLY:O	3:J:277:ARG:HD2	2.19	0.43
2:I:495:ASP:OD2	5:I:602:ANP:O3'	2.34	0.43
2:M:42:LYS:NZ	2:M:42:LYS:HB3	2.34	0.43
2:M:220:ILE:O	2:M:318:GLY:N	2.36	0.43
2:e:304:GLU:HB2	3:f:283:LEU:CD2	2.49	0.43
2:g:279:PRO:HG2	2:g:288:MET:HG2	2.01	0.43
2:g:526:LYS:HA	2:g:526:LYS:HE3	1.99	0.43
2:i:52:ASP:OD1	2:i:52:ASP:C	2.61	0.43
3:j:219:ALA:O	3:j:222:LEU:HG	2.19	0.43
2:k:291:ASP:HB2	2:k:372:LEU:HD11	2.01	0.43
2:k:291:ASP:N	2:k:345:ARG:HH21	2.17	0.43
2:m:134:LEU:HD23	2:m:134:LEU:O	2.19	0.43
2:m:186:GLU:OE1	2:m:380:LYS:HD2	2.18	0.43
2:m:526:LYS:HA	2:m:526:LYS:HE3	2.00	0.43
3:n:208:GLN:H	3:n:208:GLN:CD	2.17	0.43
3:n:283:LEU:H	3:n:283:LEU:HD12	1.84	0.43
1:0:3:ILE:C	1:0:3:ILE:HD12	2.44	0.43
1:2:3:ILE:C	1:2:3:ILE:HD12	2.44	0.43
1:2:3:ILE:HD13	1:3:93:ALA:CB	2.49	0.43
1:5:6:LEU:HD11	1:6:91:ILE:HG22	2.00	0.43
3:B:273:SER:O	3:B:277:ARG:HG2	2.18	0.43
2:I:69:MET:CE	2:I:522:THR:HB	2.48	0.43
2:I:200:LEU:HD21	2:I:254:VAL:HB	2.00	0.43
2:M:305:ILE:HD11	3:N:283:LEU:CD2	2.48	0.43
2:a:490:ASP:OD1	2:a:490:ASP:C	2.62	0.43
2:a:526:LYS:HA	2:a:526:LYS:HE3	2.00	0.43
2:c:68:ASN:O	2:c:72:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:197:ARG:HD2	2:c:277:LYS:HB2	2.01	0.43
2:c:250:ILE:HD11	2:c:278:ALA:HA	2.00	0.43
2:c:342:ILE:O	2:c:346:VAL:HG12	2.19	0.43
2:c:520:MET:HE1	2:e:38:VAL:CB	2.49	0.43
2:e:73:MET:SD	2:g:49:ILE:HD11	2.59	0.43
2:e:194:GLN:HE22	2:e:329:THR:HB	1.83	0.43
3:f:274:LYS:O	3:f:278:GLN:OE1	2.37	0.43
2:g:267:MET:HE2	2:g:267:MET:C	2.44	0.43
2:i:248:LEU:HD22	2:i:249:ILE:H	1.83	0.43
3:j:204:GLN:HB2	3:j:207:GLN:HE21	1.84	0.43
2:m:161:LEU:O	2:m:164:GLU:HG2	2.19	0.43
2:m:172:GLU:O	2:m:172:GLU:HG3	2.19	0.43
2:m:194:GLN:HE22	2:m:329:THR:HB	1.84	0.43
2:m:254:VAL:H	2:m:277:LYS:NZ	2.17	0.43
1:3:11:ILE:HG13	1:3:41:LEU:HD21	2.01	0.43
1:4:47:ARG:HH22	1:4:50:GLU:CD	2.27	0.43
1:6:47:ARG:HH22	1:6:50:GLU:CD	2.27	0.43
3:L:258:PHE:O	3:L:261:ILE:HG13	2.19	0.43
2:a:61:GLU:OE1	2:m:3:ALA:HA	2.18	0.43
2:a:161:LEU:O	2:a:164:GLU:HG2	2.19	0.43
2:c:73:MET:HG2	2:e:47:PRO:HG2	2.01	0.43
2:c:490:ASP:C	2:c:490:ASP:OD1	2.61	0.43
2:c:506:TYR:O	2:c:510:VAL:HG12	2.19	0.43
3:h:208:GLN:H	3:h:208:GLN:CD	2.25	0.43
2:i:197:ARG:HD3	2:i:197:ARG:HA	1.89	0.43
3:j:278:GLN:OE1	3:j:278:GLN:N	2.44	0.43
2:k:130:GLU:HG2	2:k:422:VAL:HG22	2.00	0.43
2:k:278:ALA:HB3	2:k:285:ARG:NH2	2.33	0.43
3:l:273:SER:C	3:l:275:TYR:N	2.77	0.43
2:m:197:ARG:HD2	2:m:277:LYS:HB2	2.01	0.43
3:n:199:THR:HA	3:n:200:PRO:HD3	1.84	0.43
1:0:38:GLY:O	1:0:64:ILE:HA	2.19	0.43
1:0:47:ARG:HH22	1:0:50:GLU:CD	2.26	0.43
1:4:25:ILE:HB	1:4:27:LEU:CD1	2.34	0.43
3:B:221:GLN:O	3:B:222:LEU:C	2.62	0.43
2:C:233:MET:C	2:C:233:MET:SD	3.02	0.43
2:C:521:VAL:O	2:E:41:ASP:CB	2.67	0.43
2:E:42:LYS:NZ	2:E:42:LYS:HB3	2.34	0.43
2:E:332:ILE:HD12	2:E:332:ILE:N	2.33	0.43
3:F:239:LEU:HD23	3:F:242:HIS:NE2	2.34	0.43
2:a:179:ASP:OD1	2:a:179:ASP:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:197:ARG:HD2	2:a:277:LYS:HB2	2.01	0.43
3:b:222:LEU:HA	3:b:225:GLN:HG3	2.01	0.43
2:e:5:ASP:OD1	2:e:5:ASP:C	2.62	0.43
2:g:250:ILE:HD11	2:g:278:ALA:HA	2.00	0.43
2:i:247:LEU:HD22	2:i:248:LEU:N	2.30	0.43
3:n:207:GLN:OE1	3:n:208:GLN:N	2.51	0.43
1:2:47:ARG:HH22	1:2:50:GLU:CD	2.26	0.42
1:2:67:PHE:HA	1:2:92:LEU:HD23	2.01	0.42
1:6:3:ILE:C	1:6:3:ILE:HD12	2.44	0.42
3:B:239:LEU:HD23	3:B:242:HIS:NE2	2.34	0.42
2:C:150:ILE:HG13	2:C:493:ILE:HA	2.01	0.42
2:M:430:ARG:HD3	2:M:430:ARG:HA	1.92	0.42
2:g:359:ASP:OD1	2:g:362:ARG:NH2	2.43	0.42
2:i:134:LEU:O	2:i:134:LEU:HD23	2.19	0.42
2:i:266:THR:C	2:i:268:ARG:H	2.27	0.42
2:i:359:ASP:OD1	2:i:362:ARG:NH2	2.41	0.42
2:k:380:LYS:HD3	2:k:381:VAL:N	2.34	0.42
3:n:237:GLU:H	3:n:237:GLU:CD	2.20	0.42
3:n:253:GLN:O	3:n:257:THR:HG23	2.19	0.42
1:2:47:ARG:HD3	1:2:47:ARG:N	2.35	0.42
1:3:47:ARG:N	1:3:47:ARG:HD3	2.35	0.42
1:3:91:ILE:CG2	1:3:92:LEU:N	2.82	0.42
3:D:239:LEU:HD23	3:D:242:HIS:NE2	2.34	0.42
2:E:12:ALA:HB1	2:E:520:MET:HE2	2.01	0.42
2:E:150:ILE:HG13	2:E:493:ILE:HA	2.01	0.42
2:I:150:ILE:HG13	2:I:493:ILE:HA	2.01	0.42
2:I:197:ARG:CB	2:I:277:LYS:HG3	2.43	0.42
2:K:150:ILE:HG13	2:K:493:ILE:HA	2.01	0.42
2:M:284:ARG:CD	2:M:284:ARG:H	2.32	0.42
2:M:294:THR:HG21	2:M:345:ARG:HB2	2.01	0.42
2:a:383:ALA:HB1	2:a:388:GLU:CD	2.44	0.42
2:c:134:LEU:O	2:c:134:LEU:HD23	2.19	0.42
2:g:248:LEU:HD22	2:g:249:ILE:H	1.84	0.42
2:g:291:ASP:HB2	2:g:372:LEU:HD11	2.00	0.42
2:i:520:MET:SD	2:k:38:VAL:HG13	2.59	0.42
2:k:250:ILE:HD11	2:k:278:ALA:HA	2.00	0.42
2:k:254:VAL:H	2:k:277:LYS:NZ	2.18	0.42
3:l:236:LEU:HD21	3:l:261:ILE:HG12	2.01	0.42
2:m:230:ILE:HD12	2:m:230:ILE:HA	1.91	0.42
1:1:3:ILE:C	1:1:3:ILE:HD12	2.44	0.42
1:1:11:ILE:HG13	1:1:41:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:47:ARG:HH22	1:1:50:GLU:CD	2.27	0.42
1:3:3:ILE:C	1:3:3:ILE:HD12	2.44	0.42
1:3:38:GLY:O	1:3:64:ILE:HA	2.19	0.42
1:4:47:ARG:HD3	1:4:47:ARG:N	2.35	0.42
2:C:12:ALA:HB1	2:C:520:MET:HE2	2.02	0.42
2:C:247:LEU:HB3	2:C:273:VAL:HG12	2.02	0.42
2:E:284:ARG:CD	2:E:284:ARG:H	2.32	0.42
2:G:286:LYS:HZ3	3:H:284:TYR:HB2	1.82	0.42
2:G:430:ARG:HD3	2:G:430:ARG:HA	1.92	0.42
2:I:42:LYS:NZ	2:I:42:LYS:HB3	2.34	0.42
2:I:286:LYS:CE	3:J:284:TYR:CD2	3.02	0.42
2:I:332:ILE:HD12	2:I:332:ILE:N	2.33	0.42
2:K:12:ALA:HB1	2:K:520:MET:HE2	2.01	0.42
2:K:42:LYS:NZ	2:K:42:LYS:HB3	2.34	0.42
2:M:12:ALA:HB1	2:M:520:MET:HE2	2.02	0.42
2:M:304:GLU:O	3:N:255:ARG:NH1	2.52	0.42
3:N:239:LEU:HD23	3:N:242:HIS:NE2	2.33	0.42
3:b:240:PHE:HB2	3:b:275:TYR:OH	2.18	0.42
2:c:166:MET:HE3	2:c:166:MET:HB3	1.77	0.42
2:c:518:GLU:CG	2:e:29:VAL:HG11	2.49	0.42
2:e:250:ILE:HD11	2:e:278:ALA:HA	2.00	0.42
2:g:303:GLU:O	3:h:283:LEU:CD2	2.68	0.42
2:i:196:ASP:OD1	2:i:196:ASP:N	2.49	0.42
2:i:197:ARG:HD2	2:i:277:LYS:HB2	2.01	0.42
2:i:278:ALA:HB3	2:i:285:ARG:NH2	2.34	0.42
2:m:68:ASN:O	2:m:72:GLN:HG2	2.18	0.42
1:0:47:ARG:HD3	1:0:47:ARG:N	2.35	0.42
1:0:91:ILE:CG2	1:0:92:LEU:N	2.83	0.42
1:1:15:LYS:HG3	1:1:38:GLY:HA2	2.02	0.42
1:1:66:ILE:C	1:1:92:LEU:HB2	2.44	0.42
1:4:71:TYR:O	1:4:74:LYS:NZ	2.49	0.42
2:A:12:ALA:HB1	2:A:520:MET:HE2	2.02	0.42
2:E:294:THR:HG21	2:E:345:ARG:HB2	2.01	0.42
3:F:258:PHE:O	3:F:261:ILE:HG13	2.19	0.42
2:G:286:LYS:HZ2	3:H:280:TYR:HE1	1.66	0.42
2:G:513:LEU:HD23	2:G:513:LEU:HA	1.85	0.42
3:H:258:PHE:O	3:H:261:ILE:HG13	2.19	0.42
2:K:227:ILE:HD13	2:K:227:ILE:HA	1.90	0.42
2:M:295:LEU:O	2:M:336:VAL:HG12	2.20	0.42
3:N:275:TYR:O	3:N:278:GLN:HB3	2.19	0.42
3:b:262:LEU:HA	3:b:265:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:254:VAL:H	2:c:277:LYS:NZ	2.17	0.42
3:d:199:THR:HA	3:d:200:PRO:HD3	1.92	0.42
3:d:274:LYS:HA	3:d:277:ARG:HG2	2.01	0.42
2:e:8:PHE:CE1	2:g:25:ASP:OD1	2.73	0.42
2:e:288:MET:N	2:e:288:MET:SD	2.92	0.42
2:e:332:ILE:HD12	2:e:332:ILE:N	2.35	0.42
2:e:365:LEU:HA	2:e:368:ARG:HE	1.84	0.42
2:g:68:ASN:O	2:g:72:GLN:HG2	2.19	0.42
3:h:283:LEU:H	3:h:283:LEU:HD12	1.84	0.42
2:m:222:LEU:HD23	2:m:289:LEU:HD23	2.01	0.42
2:m:247:LEU:HD22	2:m:248:LEU:N	2.34	0.42
1:2:64:ILE:O	1:2:94:ILE:HD12	2.20	0.42
1:5:47:ARG:HD3	1:5:47:ARG:N	2.35	0.42
1:6:64:ILE:O	1:6:94:ILE:HD12	2.20	0.42
2:E:220:ILE:O	2:E:318:GLY:N	2.37	0.42
2:G:247:LEU:HB3	2:G:273:VAL:HG12	2.02	0.42
2:K:52:ASP:C	2:K:52:ASP:OD1	2.63	0.42
2:K:284:ARG:H	2:K:284:ARG:CD	2.32	0.42
2:M:150:ILE:HG13	2:M:493:ILE:HA	2.01	0.42
2:M:305:ILE:HD11	3:N:283:LEU:HD22	2.02	0.42
2:M:513:LEU:HD23	2:M:513:LEU:HA	1.85	0.42
2:c:5:ASP:C	2:c:5:ASP:OD1	2.62	0.42
2:i:161:LEU:O	2:i:164:GLU:HG2	2.19	0.42
2:i:490:ASP:OD1	2:i:490:ASP:C	2.62	0.42
2:m:262:LEU:HD22	2:m:273:VAL:HG21	2.01	0.42
1:1:27:LEU:HD21	2:C:271:VAL:H	1.85	0.42
1:1:47:ARG:HD3	1:1:47:ARG:N	2.35	0.42
1:2:11:ILE:HG13	1:2:41:LEU:HD21	2.01	0.42
1:2:26:VAL:O	2:A:268:ARG:HB3	2.19	0.42
1:5:3:ILE:HD12	1:5:3:ILE:C	2.44	0.42
1:6:47:ARG:N	1:6:47:ARG:HD3	2.35	0.42
2:A:150:ILE:HG13	2:A:493:ILE:HA	2.01	0.42
2:C:294:THR:HG21	2:C:345:ARG:HB2	2.01	0.42
2:I:247:LEU:HB3	2:I:273:VAL:HG12	2.02	0.42
2:I:295:LEU:O	2:I:336:VAL:HG12	2.20	0.42
2:M:150:ILE:HD13	2:M:150:ILE:HA	1.91	0.42
2:a:205:ILE:HD13	2:a:205:ILE:HA	1.91	0.42
2:c:179:ASP:C	2:c:179:ASP:OD1	2.63	0.42
2:e:68:ASN:O	2:e:72:GLN:HG2	2.19	0.42
2:e:161:LEU:O	2:e:164:GLU:HG2	2.19	0.42
2:i:205:ILE:HA	2:i:205:ILE:HD13	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:308:GLU:HG2	2:i:310:GLU:H	1.85	0.42
3:j:270:ALA:O	3:j:273:SER:OG	2.32	0.42
3:n:282:LEU:HD13	3:n:282:LEU:O	2.20	0.42
1:0:15:LYS:HG3	1:0:38:GLY:HA2	2.02	0.42
1:0:39:GLU:OE2	1:0:40:VAL:N	2.51	0.42
1:0:64:ILE:O	1:0:94:ILE:HD12	2.20	0.42
1:3:64:ILE:O	1:3:94:ILE:HD12	2.20	0.42
2:A:1:MET:O	2:C:61:GLU:OE2	2.38	0.42
2:A:150:ILE:HD13	2:A:150:ILE:HA	1.91	0.42
3:B:277:ARG:O	3:B:280:TYR:HB3	2.19	0.42
2:C:284:ARG:H	2:C:284:ARG:CD	2.32	0.42
3:D:242:HIS:CE1	3:D:243:LEU:HD22	2.55	0.42
3:D:258:PHE:O	3:D:261:ILE:HG13	2.19	0.42
2:E:247:LEU:HB3	2:E:273:VAL:HG12	2.02	0.42
2:G:294:THR:HG21	2:G:345:ARG:HB2	2.01	0.42
3:H:278:GLN:O	3:H:281:ALA:N	2.52	0.42
2:I:52:ASP:C	2:I:52:ASP:OD1	2.63	0.42
2:I:80:LYS:HB3	2:I:80:LYS:HE2	1.78	0.42
3:J:215:ASP:HB3	3:J:218:LEU:HG	2.02	0.42
3:J:242:HIS:CE1	3:J:243:LEU:HD22	2.55	0.42
3:L:215:ASP:HB3	3:L:218:LEU:HG	2.02	0.42
2:M:52:ASP:OD1	2:M:52:ASP:C	2.63	0.42
2:a:248:LEU:HD22	2:a:249:ILE:H	1.84	0.42
2:a:391:GLU:OE1	2:a:392:LYS:N	2.52	0.42
2:c:247:LEU:HD22	2:c:248:LEU:N	2.34	0.42
2:e:134:LEU:HD23	2:e:134:LEU:O	2.19	0.42
2:e:230:ILE:HD12	2:e:230:ILE:HA	1.92	0.42
3:f:278:GLN:OE1	3:f:278:GLN:N	2.52	0.42
2:g:197:ARG:HD2	2:g:277:LYS:HB2	2.01	0.42
2:g:254:VAL:H	2:g:277:LYS:NZ	2.17	0.42
3:h:243:LEU:HD11	3:h:258:PHE:CE2	2.54	0.42
2:i:25:ASP:OD1	2:i:25:ASP:C	2.62	0.42
2:i:254:VAL:H	2:i:277:LYS:HZ2	1.67	0.42
2:i:506:TYR:O	2:i:510:VAL:HG12	2.20	0.42
2:k:134:LEU:O	2:k:134:LEU:HD23	2.19	0.42
2:k:196:ASP:N	2:k:196:ASP:OD1	2.50	0.42
2:k:520:MET:HB2	2:m:26:ALA:HA	2.01	0.42
3:l:198:ASP:C	3:l:198:ASP:OD1	2.63	0.42
3:l:219:ALA:O	3:l:222:LEU:HG	2.19	0.42
2:m:215:LEU:HB3	2:m:246:PRO:HG2	2.02	0.42
1:2:15:LYS:HG3	1:2:38:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:47:ARG:HH22	1:3:50:GLU:CD	2.26	0.42
1:5:39:GLU:OE2	1:5:40:VAL:N	2.51	0.42
1:6:92:LEU:HD22	1:6:92:LEU:N	2.35	0.42
2:A:218:PRO:HD2	2:A:320:ALA:O	2.20	0.42
2:E:218:PRO:HD2	2:E:320:ALA:O	2.20	0.42
2:E:286:LYS:NZ	3:F:284:TYR:HB2	2.34	0.42
2:G:40:LEU:HD23	2:I:521:VAL:HB	2.02	0.42
2:G:59:GLU:O	2:I:4:LYS:HG3	2.20	0.42
2:G:284:ARG:H	2:G:284:ARG:CD	2.32	0.42
3:H:242:HIS:CE1	3:H:243:LEU:HD22	2.55	0.42
2:I:217:SER:O	2:I:217:SER:OG	2.33	0.42
2:I:284:ARG:H	2:I:284:ARG:CD	2.32	0.42
3:J:202:ILE:HG21	3:J:231:ARG:CZ	2.50	0.42
2:g:197:ARG:HD3	2:g:197:ARG:HA	1.89	0.42
2:i:233:MET:HE1	2:i:237:LEU:HD23	2.01	0.42
2:k:205:ILE:HA	2:k:213:VAL:CG2	2.49	0.42
2:m:278:ALA:HB3	2:m:285:ARG:NH2	2.34	0.42
1:0:92:LEU:N	1:0:92:LEU:HD22	2.35	0.42
1:2:85:ILE:HG12	1:3:92:LEU:HD12	2.00	0.42
1:4:3:ILE:C	1:4:3:ILE:HD12	2.44	0.42
2:A:247:LEU:HB3	2:A:273:VAL:HG12	2.02	0.42
3:B:242:HIS:CE1	3:B:243:LEU:HD22	2.55	0.42
2:G:12:ALA:HB1	2:G:520:MET:HE2	2.02	0.42
2:I:218:PRO:HD2	2:I:320:ALA:O	2.20	0.42
3:J:258:PHE:O	3:J:261:ILE:HG13	2.19	0.42
2:K:294:THR:HG21	2:K:345:ARG:HB2	2.01	0.42
2:M:247:LEU:HB3	2:M:273:VAL:HG12	2.02	0.42
2:e:516:THR:CG2	2:g:37:ASN:OD1	2.68	0.42
3:h:275:TYR:HA	3:h:278:GLN:OE1	2.19	0.42
2:i:144:ILE:HG21	2:i:166:MET:HG3	2.01	0.42
2:i:179:ASP:OD1	2:i:179:ASP:C	2.62	0.42
2:i:281:PHE:HA	2:i:285:ARG:HD2	2.02	0.42
2:k:179:ASP:OD1	2:k:179:ASP:C	2.62	0.42
2:k:262:LEU:HD22	2:k:273:VAL:HG21	2.01	0.42
2:m:205:ILE:HD13	2:m:205:ILE:HA	1.89	0.42
2:m:232:GLU:OE1	2:m:232:GLU:N	2.50	0.42
1:0:11:ILE:HD12	1:0:12:VAL:H	1.84	0.42
1:0:21:SER:O	1:0:22:ALA:HB3	2.20	0.42
1:3:25:ILE:HB	1:3:27:LEU:CD1	2.50	0.42
1:5:26:VAL:C	1:5:28:THR:N	2.78	0.42
3:B:252:GLY:C	3:B:256:LYS:HZ3	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:42:LYS:NZ	2:C:42:LYS:HB3	2.34	0.42
2:G:150:ILE:HG13	2:G:493:ILE:HA	2.02	0.42
2:I:307:MET:HE1	3:J:262:LEU:HD11	2.02	0.42
2:I:344:GLY:O	2:I:346:VAL:N	2.53	0.42
3:J:243:LEU:HA	3:J:251:ASP:OD2	2.20	0.42
2:K:247:LEU:HB3	2:K:273:VAL:HG12	2.02	0.42
2:a:222:LEU:HD13	2:a:293:ALA:HB2	2.02	0.42
2:a:518:GLU:HG2	2:c:36:ARG:HG3	2.01	0.42
2:c:308:GLU:HG2	2:c:310:GLU:H	1.85	0.42
2:e:179:ASP:OD1	2:e:179:ASP:C	2.63	0.42
3:f:239:LEU:HB3	3:f:258:PHE:CE1	2.55	0.42
2:i:254:VAL:H	2:i:277:LYS:NZ	2.17	0.42
2:k:490:ASP:OD1	2:k:490:ASP:C	2.62	0.42
2:m:214:GLU:HG2	2:m:324:VAL:HG22	2.02	0.42
1:5:9:ARG:NH1	1:6:91:ILE:O	2.50	0.41
2:A:42:LYS:NZ	2:A:42:LYS:HB3	2.34	0.41
2:A:315:GLU:OE1	3:B:269:ASP:C	2.63	0.41
3:B:258:PHE:O	3:B:261:ILE:HG13	2.19	0.41
2:C:68:ASN:O	2:C:72:GLN:HG2	2.20	0.41
2:E:52:ASP:C	2:E:52:ASP:OD1	2.63	0.41
2:E:315:GLU:OE1	3:F:270:ALA:HA	2.20	0.41
2:E:513:LEU:HD23	2:E:513:LEU:HA	1.85	0.41
2:G:218:PRO:HD2	2:G:320:ALA:O	2.20	0.41
2:a:387:VAL:CG2	2:a:388:GLU:N	2.82	0.41
3:b:208:GLN:O	3:b:212:ASN:N	2.40	0.41
3:d:239:LEU:HB3	3:d:258:PHE:CE2	2.54	0.41
2:e:262:LEU:HD22	2:e:273:VAL:HG21	2.02	0.41
3:f:239:LEU:HB3	3:f:258:PHE:CZ	2.55	0.41
2:i:172:GLU:HG3	2:i:172:GLU:O	2.20	0.41
3:l:208:GLN:HG3	3:l:218:LEU:HD11	2.01	0.41
2:m:131:LEU:HD12	2:m:131:LEU:HA	1.90	0.41
1:3:11:ILE:HD12	1:3:12:VAL:H	1.84	0.41
1:5:11:ILE:HD12	1:5:12:VAL:H	1.84	0.41
2:C:126:ALA:HB1	2:C:426:LEU:HD11	2.02	0.41
3:D:243:LEU:HA	3:D:251:ASP:OD2	2.20	0.41
2:E:217:SER:O	2:E:217:SER:OG	2.33	0.41
3:F:219:ALA:O	3:F:223:ALA:N	2.53	0.41
3:F:242:HIS:CE1	3:F:243:LEU:HD22	2.55	0.41
3:H:243:LEU:HA	3:H:251:ASP:OD2	2.20	0.41
2:I:12:ALA:HB1	2:I:520:MET:HE2	2.02	0.41
2:K:126:ALA:HB1	2:K:426:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:513:LEU:HD23	2:K:513:LEU:HA	1.85	0.41
3:L:243:LEU:HA	3:L:251:ASP:OD2	2.20	0.41
2:M:31:LEU:HD12	5:M:600:ANP:O1A	2.19	0.41
2:M:68:ASN:O	2:M:72:GLN:HG2	2.21	0.41
3:b:204:GLN:HA	3:b:207:GLN:HE22	1.84	0.41
2:c:347:ALA:O	2:c:350:ARG:N	2.43	0.41
3:d:204:GLN:HA	3:d:207:GLN:HE22	1.84	0.41
2:e:87:ASP:HB2	5:e:603:ANP:O1B	2.19	0.41
3:f:243:LEU:HD21	3:f:258:PHE:CE1	2.56	0.41
2:g:134:LEU:HD23	2:g:134:LEU:O	2.20	0.41
3:h:224:LEU:O	3:h:225:GLN:C	2.63	0.41
2:i:34:LYS:HE3	2:i:34:LYS:HB2	1.73	0.41
2:i:68:ASN:O	2:i:72:GLN:HG2	2.20	0.41
2:i:290:GLN:HE21	3:j:281:ALA:CB	2.33	0.41
2:i:325:ILE:HD12	2:i:325:ILE:C	2.44	0.41
2:k:495:ASP:OD2	5:k:603:ANP:C3'	2.68	0.41
3:n:262:LEU:HD12	3:n:263:ALA:N	2.35	0.41
1:4:91:ILE:CG2	1:4:92:LEU:N	2.82	0.41
2:A:294:THR:HG21	2:A:345:ARG:HB2	2.01	0.41
2:A:295:LEU:O	2:A:336:VAL:HG12	2.20	0.41
2:A:487:ASN:O	2:A:491:MET:HG3	2.21	0.41
2:C:69:MET:HE1	2:E:41:ASP:HB2	2.02	0.41
2:G:222:LEU:HB2	2:G:299:THR:O	2.21	0.41
2:I:126:ALA:HB1	2:I:426:LEU:HD11	2.02	0.41
3:J:234:GLU:O	3:J:235:ALA:C	2.64	0.41
2:K:218:PRO:HD2	2:K:320:ALA:O	2.20	0.41
2:K:295:LEU:O	2:K:336:VAL:HG12	2.20	0.41
3:L:242:HIS:CE1	3:L:243:LEU:HD22	2.55	0.41
3:N:276:ARG:O	3:N:279:LEU:HB3	2.19	0.41
3:N:277:ARG:O	3:N:281:ALA:N	2.52	0.41
3:d:239:LEU:HD22	3:d:239:LEU:H	1.85	0.41
3:d:274:LYS:O	3:d:278:GLN:OE1	2.37	0.41
2:i:222:LEU:HD13	2:i:293:ALA:HB2	2.02	0.41
2:k:3:ALA:HA	2:m:61:GLU:OE1	2.20	0.41
2:k:104:LEU:HD23	2:k:104:LEU:HA	1.88	0.41
2:m:444:LEU:HD23	2:m:447:MET:HE3	2.02	0.41
3:n:236:LEU:HD23	3:n:236:LEU:H	1.85	0.41
1:2:27:LEU:O	2:A:268:ARG:CB	2.61	0.41
1:2:91:ILE:CG2	1:2:92:LEU:N	2.83	0.41
1:3:7:HIS:ND1	1:3:7:HIS:N	2.67	0.41
1:4:92:LEU:N	1:4:92:LEU:HD22	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:6:LEU:HB3	1:5:7:HIS:H	1.70	0.41
2:A:217:SER:O	2:A:217:SER:OG	2.33	0.41
3:L:201:GLU:O	3:L:204[B]:GLN:HG3	2.21	0.41
3:N:215:ASP:HB3	3:N:218:LEU:HG	2.02	0.41
3:N:242:HIS:CE1	3:N:243:LEU:HD22	2.55	0.41
2:a:5:ASP:C	2:a:5:ASP:OD1	2.63	0.41
2:a:46:ALA:HA	2:m:72:GLN:HB3	2.02	0.41
2:a:290:GLN:OE1	2:a:345:ARG:NH2	2.53	0.41
2:a:324:VAL:HB	2:a:331:THR:OG1	2.20	0.41
3:b:199:THR:HA	3:b:200:PRO:HD3	1.91	0.41
2:e:254:VAL:H	2:e:277:LYS:HZ2	1.68	0.41
2:e:344:GLY:O	2:e:345:ARG:C	2.63	0.41
2:g:333:ILE:HD12	2:g:334:ASP:N	2.36	0.41
2:g:342:ILE:H	2:g:342:ILE:HG13	1.60	0.41
2:i:5:ASP:OD1	2:i:5:ASP:C	2.63	0.41
2:i:180:GLY:HA3	2:i:380:LYS:HG2	2.02	0.41
2:i:491:MET:HE3	2:i:491:MET:HB2	1.88	0.41
2:k:254:VAL:H	2:k:277:LYS:HZ2	1.67	0.41
2:k:523:ASP:HA	2:m:41:ASP:HB3	2.03	0.41
2:m:5:ASP:OD1	2:m:5:ASP:C	2.63	0.41
2:m:52:ASP:OD1	2:m:52:ASP:C	2.64	0.41
2:m:130:GLU:OE1	2:m:425:LYS:HD2	2.21	0.41
2:m:180:GLY:HA3	2:m:380:LYS:HG2	2.02	0.41
2:m:490:ASP:OD1	2:m:490:ASP:C	2.62	0.41
1:3:85:ILE:HG12	1:4:92:LEU:CD1	2.50	0.41
1:6:15:LYS:HG3	1:6:38:GLY:HA2	2.02	0.41
2:A:52:ASP:OD1	2:A:52:ASP:C	2.63	0.41
3:B:209:VAL:HG22	3:B:218:LEU:HD13	2.03	0.41
3:B:243:LEU:HA	3:B:251:ASP:OD2	2.20	0.41
2:C:52:ASP:OD1	2:C:52:ASP:C	2.63	0.41
2:E:73:MET:HG2	2:M:47:PRO:HG2	2.01	0.41
2:G:42:LYS:HB3	2:G:42:LYS:NZ	2.34	0.41
2:G:295:LEU:O	2:G:336:VAL:HG12	2.20	0.41
2:I:307:MET:CE	3:J:262:LEU:HD11	2.51	0.41
2:M:218:PRO:HD2	2:M:320:ALA:O	2.20	0.41
3:N:201:GLU:O	3:N:204[A]:GLN:HG3	2.21	0.41
3:N:201:GLU:O	3:N:204[B]:GLN:HG3	2.21	0.41
3:N:243:LEU:HA	3:N:251:ASP:OD2	2.21	0.41
3:b:278:GLN:OE1	3:b:278:GLN:N	2.48	0.41
3:f:244:ARG:HE	3:f:244:ARG:C	2.28	0.41
2:g:161:LEU:O	2:g:164:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:262:LEU:HA	3:h:265:LEU:HD23	2.03	0.41
2:k:161:LEU:O	2:k:164:GLU:HG2	2.20	0.41
2:k:197:ARG:HD2	2:k:277:LYS:HB2	2.01	0.41
3:l:199:THR:HA	3:l:200:PRO:HD3	1.87	0.41
1:1:27:LEU:HD22	2:C:271:VAL:HG12	2.01	0.41
3:B:244:ARG:HA	3:B:244:ARG:HD2	1.94	0.41
2:C:218:PRO:HD2	2:C:320:ALA:O	2.20	0.41
3:F:243:LEU:HA	3:F:251:ASP:OD2	2.21	0.41
2:G:487:ASN:O	2:G:491:MET:HG3	2.21	0.41
3:H:221:GLN:O	3:H:222:LEU:C	2.64	0.41
2:I:345:ARG:NH1	2:I:349:ILE:HD11	2.35	0.41
2:I:430:ARG:HD3	2:I:430:ARG:HA	1.92	0.41
2:M:126:ALA:HB1	2:M:426:LEU:HD11	2.02	0.41
3:N:244:ARG:HA	3:N:244:ARG:HD2	1.94	0.41
2:a:333:ILE:HD12	2:a:334:ASP:N	2.35	0.41
2:c:222:LEU:HD13	2:c:293:ALA:HB2	2.01	0.41
2:e:267:MET:HE2	2:e:267:MET:C	2.46	0.41
2:e:383:ALA:HB2	2:e:392:LYS:HD3	2.03	0.41
2:i:250:ILE:HD11	2:i:278:ALA:HA	2.02	0.41
2:i:430:ARG:HA	2:i:430:ARG:HD2	1.80	0.41
2:k:222:LEU:HD13	2:k:293:ALA:HB2	2.03	0.41
1:5:64:ILE:O	1:5:94:ILE:HD12	2.20	0.41
1:6:6:LEU:HB3	1:6:7:HIS:H	1.70	0.41
1:6:11:ILE:HD12	1:6:12:VAL:H	1.84	0.41
2:A:25:ASP:OD1	2:G:8:PHE:HZ	2.03	0.41
2:A:49:ILE:CG1	2:G:73:MET:HE1	2.49	0.41
3:B:209:VAL:HG21	3:B:222:LEU:HD22	2.03	0.41
2:C:295:LEU:O	2:C:336:VAL:HG12	2.20	0.41
2:E:295:LEU:O	2:E:336:VAL:HG12	2.20	0.41
3:F:252:GLY:C	3:F:256:LYS:HZ3	2.28	0.41
2:I:222:LEU:HB2	2:I:299:THR:O	2.21	0.41
2:I:487:ASN:O	2:I:491:MET:HG3	2.20	0.41
3:J:233:GLU:O	3:J:236:LEU:HB3	2.21	0.41
2:K:80:LYS:HE2	2:K:80:LYS:HB3	1.78	0.41
2:M:222:LEU:HB2	2:M:299:THR:O	2.21	0.41
2:c:207:LYS:HB2	2:c:209:GLU:CD	2.46	0.41
2:c:213:VAL:HB	2:c:325:ILE:CG2	2.50	0.41
2:c:254:VAL:H	2:c:277:LYS:HZ2	1.67	0.41
2:c:333:ILE:HD12	2:c:334:ASP:N	2.36	0.41
3:d:243:LEU:HD13	3:d:282:LEU:CD2	2.51	0.41
2:e:322:ARG:O	2:e:333:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:205:ILE:HA	2:g:213:VAL:HG22	2.02	0.41
2:g:205:ILE:HD13	2:g:213:VAL:HG23	2.03	0.41
3:h:224:LEU:O	3:h:227:HIS:N	2.52	0.41
3:l:276:ARG:CD	3:l:280:TYR:CE1	3.04	0.41
1:0:69:ASP:OD1	1:0:70:GLY:N	2.54	0.41
1:1:11:ILE:HD12	1:1:12:VAL:H	1.85	0.41
1:3:9:ARG:HB2	1:3:86:MET:O	2.21	0.41
1:5:15:LYS:HG3	1:5:38:GLY:HA2	2.02	0.41
1:5:25:ILE:HB	1:5:27:LEU:HG	2.02	0.41
3:D:225:GLN:HA	3:D:228:GLN:OE1	2.21	0.41
2:E:126:ALA:HB1	2:E:426:LEU:HD11	2.02	0.41
2:G:52:ASP:OD1	2:G:52:ASP:C	2.63	0.41
2:I:286:LYS:NZ	3:J:284:TYR:CB	2.74	0.41
3:J:215:ASP:OD1	3:J:217:ALA:N	2.53	0.41
3:L:201:GLU:O	3:L:204[A]:GLN:HG3	2.21	0.41
2:a:386:GLU:C	2:a:389:MET:H	2.29	0.41
3:b:265:LEU:HB3	3:b:269:ASP:HB3	2.03	0.41
2:c:205:ILE:HA	2:c:205:ILE:HD13	1.93	0.41
3:d:219:ALA:O	3:d:222:LEU:HG	2.21	0.41
2:e:247:LEU:HD22	2:e:248:LEU:N	2.35	0.41
2:e:333:ILE:HD12	2:e:334:ASP:N	2.36	0.41
2:g:207:LYS:HB2	2:g:209:GLU:CD	2.46	0.41
2:g:308:GLU:HG2	2:g:310:GLU:H	1.85	0.41
2:i:214:GLU:CG	2:i:324:VAL:HG22	2.48	0.41
2:k:207:LYS:HB2	2:k:209:GLU:CD	2.46	0.41
1:0:34:LYS:O	1:0:36:THR:HG23	2.21	0.41
1:2:11:ILE:HD12	1:2:12:VAL:H	1.84	0.41
1:2:66:ILE:HD12	1:2:93:ALA:O	2.20	0.41
1:4:15:LYS:HG3	1:4:38:GLY:HA2	2.02	0.41
1:4:34:LYS:O	1:4:36:THR:HG23	2.21	0.41
1:5:15:LYS:HZ1	1:5:39:GLU:H	1.68	0.41
2:A:126:ALA:HB1	2:A:426:LEU:HD11	2.02	0.41
2:C:80:LYS:HB3	2:C:80:LYS:HE2	1.78	0.41
2:C:343:GLN:H	2:C:343:GLN:CD	2.29	0.41
2:C:520:MET:HG2	2:E:39:VAL:HB	2.03	0.41
3:D:215:ASP:HB3	3:D:218:LEU:HG	2.02	0.41
3:F:201:GLU:O	3:F:204[A]:GLN:HG3	2.21	0.41
3:F:201:GLU:O	3:F:204[B]:GLN:HG3	2.21	0.41
2:G:140:ASP:OD1	2:G:140:ASP:N	2.40	0.41
3:H:216:ALA:C	3:H:218:LEU:N	2.77	0.41
3:J:234:GLU:H	3:J:234:GLU:HG3	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:68:ASN:O	2:K:72:GLN:HG2	2.20	0.41
3:L:215:ASP:OD1	3:L:217:ALA:N	2.53	0.41
3:L:275:TYR:O	3:L:278:GLN:HB3	2.21	0.41
2:M:20:VAL:HG22	2:M:74:VAL:HG21	2.03	0.41
2:a:25:ASP:OD1	2:m:8:PHE:HE1	1.99	0.41
2:a:52:ASP:C	2:a:52:ASP:OD1	2.63	0.41
2:a:237:LEU:HA	2:a:240:VAL:HB	2.03	0.41
2:a:308:GLU:HG2	2:a:310:GLU:H	1.86	0.41
2:a:342:ILE:H	2:a:342:ILE:HG13	1.60	0.41
2:c:267:MET:C	2:c:267:MET:HE2	2.46	0.41
2:c:281:PHE:HA	2:c:285:ARG:HD2	2.03	0.41
2:e:131:LEU:HD12	2:e:131:LEU:HA	1.87	0.41
2:e:197:ARG:HD2	2:e:277:LYS:HB2	2.01	0.41
2:e:308:GLU:HG2	2:e:310:GLU:H	1.84	0.41
2:e:365:LEU:HG	2:e:368:ARG:HH21	1.85	0.41
3:f:270:ALA:O	3:f:273:SER:OG	2.31	0.41
2:g:142:LYS:HE3	2:g:142:LYS:HB3	1.89	0.41
2:g:406:ALA:HB2	2:g:496:PRO:HB3	2.03	0.41
3:j:283:LEU:HD12	3:j:283:LEU:H	1.85	0.41
2:k:333:ILE:HD12	2:k:334:ASP:N	2.35	0.41
2:k:422:VAL:O	2:k:426:LEU:HG	2.21	0.41
3:l:232:ASN:OD1	3:l:236:LEU:HG	2.21	0.41
2:m:207:LYS:HB2	2:m:209:GLU:CD	2.46	0.41
2:m:214:GLU:OE1	2:m:322:ARG:HD3	2.20	0.41
2:m:291:ASP:N	2:m:345:ARG:HH21	2.19	0.41
2:m:384:ALA:HB3	2:m:388:GLU:OE2	2.20	0.41
3:n:262:LEU:CA	3:n:276:ARG:HH22	2.32	0.41
3:n:267:THR:O	3:n:267:THR:OG1	2.37	0.41
1:0:30:SER:O	1:0:31:ALA:C	2.64	0.41
1:1:34:LYS:O	1:1:36:THR:HG23	2.21	0.41
1:3:37:ARG:HD3	1:3:64:ILE:HD11	2.03	0.41
1:4:37:ARG:HD3	1:4:64:ILE:HD11	2.03	0.41
2:A:68:ASN:O	2:A:72:GLN:HG2	2.21	0.41
2:A:73:MET:HE1	2:C:49:ILE:CG1	2.51	0.41
2:A:80:LYS:HB3	2:A:80:LYS:HE2	1.78	0.41
2:A:234:LEU:N	2:A:235:PRO:HD3	2.29	0.41
2:A:281:PHE:C	2:A:285:ARG:HB2	2.46	0.41
2:C:222:LEU:HB2	2:C:299:THR:O	2.21	0.41
3:D:253:GLN:HA	3:D:256:LYS:HZ1	1.86	0.41
3:F:277:ARG:HG2	3:F:277:ARG:H	1.59	0.41
2:G:126:ALA:HB1	2:G:426:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:305:ILE:HD11	3:H:283:LEU:HD21	2.03	0.41
2:M:281:PHE:C	2:M:285:ARG:HB2	2.46	0.41
2:a:267:MET:C	2:a:267:MET:HE2	2.46	0.41
3:d:276:ARG:HH21	3:d:280:TYR:N	2.19	0.41
2:e:520:MET:HG2	2:g:26:ALA:HA	2.03	0.41
2:g:343:GLN:HA	2:g:346:VAL:HG12	2.03	0.41
3:h:236:LEU:HB2	3:h:275:TYR:CE2	2.56	0.41
2:i:422:VAL:O	2:i:426:LEU:HG	2.20	0.41
3:j:282:LEU:O	3:j:282:LEU:HD13	2.21	0.41
2:m:514:MET:HE3	2:m:514:MET:HB2	1.85	0.41
1:3:34:LYS:O	1:3:36:THR:HG23	2.21	0.40
1:5:30:SER:O	1:5:31:ALA:C	2.64	0.40
2:A:284:ARG:H	2:A:284:ARG:CD	2.32	0.40
2:E:343:GLN:H	2:E:343:GLN:CD	2.29	0.40
3:F:215:ASP:HB3	3:F:218:LEU:HG	2.02	0.40
2:I:286:LYS:HZ1	3:J:284:TYR:CB	2.27	0.40
2:I:305:ILE:CG1	3:J:283:LEU:HD22	2.51	0.40
2:I:513:LEU:HD23	2:I:513:LEU:HA	1.85	0.40
2:K:20:VAL:HG22	2:K:74:VAL:HG21	2.03	0.40
2:K:460:GLU:OE1	2:K:460:GLU:HA	2.22	0.40
2:e:33:PRO:HG3	5:e:603:ANP:N6	2.36	0.40
2:e:207:LYS:HB2	2:e:209:GLU:CD	2.46	0.40
3:f:201:GLU:HB2	3:f:204:GLN:NE2	2.35	0.40
2:g:299:THR:HG22	3:h:277:ARG:NH2	2.35	0.40
2:i:290:GLN:OE1	2:i:345:ARG:NH2	2.53	0.40
2:i:333:ILE:HD12	2:i:334:ASP:N	2.36	0.40
2:k:65:LYS:O	2:k:69:MET:HG2	2.22	0.40
2:k:322:ARG:O	2:k:333:ILE:HG13	2.21	0.40
2:m:267:MET:C	2:m:267:MET:HE2	2.46	0.40
2:m:333:ILE:HD12	2:m:334:ASP:N	2.36	0.40
1:2:69:ASP:OD1	1:2:70:GLY:N	2.54	0.40
1:2:85:ILE:HG12	1:3:92:LEU:CD1	2.51	0.40
1:4:27:LEU:C	2:I:268:ARG:HB2	2.44	0.40
1:4:64:ILE:O	1:4:94:ILE:HD12	2.20	0.40
1:5:34:LYS:O	1:5:36:THR:HG23	2.21	0.40
1:6:34:LYS:O	1:6:36:THR:HG23	2.21	0.40
2:A:222:LEU:HB2	2:A:299:THR:O	2.21	0.40
3:B:234:GLU:O	3:B:235:ALA:C	2.64	0.40
3:B:277:ARG:HG2	3:B:277:ARG:H	1.60	0.40
2:C:281:PHE:C	2:C:285:ARG:HB2	2.46	0.40
2:E:20:VAL:HG22	2:E:74:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:281:PHE:C	2:E:285:ARG:HB2	2.46	0.40
2:E:461:GLU:HG2	2:a:463:SER:CB	2.51	0.40
3:F:277:ARG:O	3:F:280:TYR:CB	2.69	0.40
2:G:281:PHE:C	2:G:285:ARG:HB2	2.46	0.40
2:I:16:MET:SD	2:I:514:MET:HG2	2.62	0.40
3:J:201:GLU:O	3:J:204[B]:GLN:HG3	2.21	0.40
2:M:286:LYS:HZ1	3:N:284:TYR:HD2	1.61	0.40
2:M:307:MET:SD	3:N:276:ARG:NH2	2.94	0.40
2:a:29:VAL:HG11	2:m:518:GLU:CG	2.51	0.40
2:a:131:LEU:HD12	2:a:131:LEU:HA	1.88	0.40
2:a:207:LYS:HB2	2:a:209:GLU:CD	2.46	0.40
2:a:387:VAL:CG2	2:a:388:GLU:H	2.34	0.40
2:e:254:VAL:H	2:e:277:LYS:NZ	2.18	0.40
2:i:237:LEU:HA	2:i:240:VAL:HB	2.03	0.40
2:i:276:VAL:HG21	2:i:330:THR:HG21	2.03	0.40
2:i:342:ILE:H	2:i:342:ILE:HG13	1.60	0.40
2:k:219:PHE:HE1	2:k:245:LYS:HB2	1.86	0.40
2:k:415:GLY:HA2	5:k:603:ANP:N3	2.36	0.40
1:2:92:LEU:N	1:2:92:LEU:HD22	2.36	0.40
1:4:65:VAL:HG12	1:4:67:PHE:CE1	2.57	0.40
1:5:71:TYR:O	1:5:74:LYS:NZ	2.49	0.40
1:6:91:ILE:CG2	1:6:92:LEU:N	2.84	0.40
2:A:179:ASP:OD1	2:A:179:ASP:N	2.55	0.40
2:C:179:ASP:OD1	2:C:179:ASP:N	2.55	0.40
2:C:487:ASN:O	2:C:491:MET:HG3	2.21	0.40
3:D:201:GLU:O	3:D:204[B]:GLN:HG3	2.21	0.40
2:G:155:ASP:HB3	2:G:158:VAL:HG22	2.03	0.40
2:G:286:LYS:CE	3:H:284:TYR:HB2	2.51	0.40
2:M:316:ASP:HA	3:N:277:ARG:NH1	2.35	0.40
2:e:104:LEU:HD23	2:e:104:LEU:HA	1.90	0.40
3:h:227:HIS:ND1	3:h:228:GLN:OE1	2.55	0.40
2:k:267:MET:C	2:k:267:MET:HE2	2.46	0.40
3:l:205:LEU:HA	3:l:208:GLN:NE2	2.36	0.40
1:0:5:PRO:HA	1:1:93:ALA:HB2	2.04	0.40
1:1:4:ARG:O	1:2:93:ALA:HB1	2.21	0.40
1:2:65:VAL:HG12	1:2:67:PHE:CE1	2.57	0.40
1:3:8:ASP:OD2	1:3:47:ARG:HB2	2.21	0.40
1:4:30:SER:O	1:4:31:ALA:C	2.64	0.40
1:4:69:ASP:OD1	1:4:70:GLY:N	2.54	0.40
1:5:69:ASP:OD1	1:5:70:GLY:N	2.54	0.40
1:6:71:TYR:O	1:6:74:LYS:NZ	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:311:LYS:HE2	2:C:311:LYS:HB3	1.91	0.40
2:E:13:ARG:HD2	2:E:104:LEU:HD22	2.04	0.40
2:E:16:MET:SD	2:E:514:MET:HG2	2.62	0.40
3:F:202:ILE:CG1	3:F:225:GLN:HG3	2.52	0.40
3:F:218:LEU:O	3:F:222:LEU:HB2	2.20	0.40
2:G:13:ARG:HD2	2:G:104:LEU:HD22	2.04	0.40
2:G:305:ILE:CD1	3:H:283:LEU:HD21	2.51	0.40
2:I:316:ASP:OD1	3:J:277:ARG:NH2	2.55	0.40
3:J:201:GLU:O	3:J:204[A]:GLN:HG3	2.21	0.40
2:K:487:ASN:O	2:K:491:MET:HG3	2.21	0.40
2:M:460:GLU:OE1	2:M:460:GLU:HA	2.21	0.40
2:a:68:ASN:O	2:a:72:GLN:HG2	2.22	0.40
2:a:476:TYR:CE1	2:a:485:TYR:HB3	2.56	0.40
2:c:151:SER:O	2:c:151:SER:OG	2.29	0.40
2:c:322:ARG:O	2:c:333:ILE:HG13	2.22	0.40
2:e:34:LYS:HE3	2:e:34:LYS:HB2	1.73	0.40
2:e:197:ARG:HD3	2:e:197:ARG:HA	1.89	0.40
2:g:60:ILE:HD13	2:g:60:ILE:HA	1.98	0.40
3:j:275:TYR:HA	3:j:278:GLN:OE1	2.21	0.40
2:k:197:ARG:HD3	2:k:197:ARG:HA	1.89	0.40
2:m:342:ILE:H	2:m:342:ILE:HG13	1.60	0.40
1:1:65:VAL:HG12	1:1:67:PHE:CE1	2.57	0.40
1:2:37:ARG:HD3	1:2:64:ILE:HD11	2.04	0.40
2:A:13:ARG:HD2	2:A:104:LEU:HD22	2.04	0.40
2:C:169:VAL:CG1	2:C:173:GLY:HA3	2.52	0.40
2:E:68:ASN:O	2:E:72:GLN:HG2	2.21	0.40
2:E:122:LYS:HB3	2:E:122:LYS:HE3	1.94	0.40
2:G:456:LEU:HD12	2:G:456:LEU:HA	1.89	0.40
3:H:242:HIS:HD1	3:H:243:LEU:N	2.20	0.40
2:I:460:GLU:OE1	2:I:460:GLU:HA	2.22	0.40
3:J:278:GLN:HG3	3:J:279:LEU:N	2.37	0.40
2:K:222:LEU:HB2	2:K:299:THR:O	2.21	0.40
2:K:281:PHE:C	2:K:285:ARG:HB2	2.46	0.40
2:K:305:ILE:HD11	3:L:280:TYR:CE1	2.57	0.40
2:M:343:GLN:H	2:M:343:GLN:CD	2.29	0.40
2:e:142:LYS:NZ	2:e:142:LYS:HB3	2.37	0.40
2:g:73:MET:HE1	2:i:39:VAL:HG22	2.03	0.40
3:h:199:THR:HA	3:h:200:PRO:HD3	1.96	0.40
2:i:69:MET:O	2:i:73:MET:HG3	2.21	0.40
2:i:303:GLU:HG3	2:i:304:GLU:H	1.86	0.40
3:j:199:THR:HA	3:j:200:PRO:HD3	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:203:TYR:CD1	2:k:203:TYR:N	2.89	0.40
2:m:142:LYS:NZ	2:m:142:LYS:HB3	2.37	0.40
3:n:239:LEU:HB3	3:n:258:PHE:CE2	2.57	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 PDB entries followed by that with respect to all EM entries.

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	0	95/97 (98%)	80 (84%)	15 (16%)	0	100	100
1	1	95/97 (98%)	83 (87%)	12 (13%)	0	100	100
1	2	95/97 (98%)	81 (85%)	13 (14%)	1 (1%)	11	23
1	3	95/97 (98%)	80 (84%)	15 (16%)	0	100	100
1	4	95/97 (98%)	84 (88%)	11 (12%)	0	100	100
1	5	95/97 (98%)	80 (84%)	14 (15%)	1 (1%)	11	23
1	6	95/97 (98%)	82 (86%)	13 (14%)	0	100	100
2	A	525/548 (96%)	507 (97%)	16 (3%)	2 (0%)	30	48
2	C	525/548 (96%)	509 (97%)	16 (3%)	0	100	100
2	E	525/548 (96%)	507 (97%)	18 (3%)	0	100	100
2	G	525/548 (96%)	509 (97%)	16 (3%)	0	100	100
2	I	525/548 (96%)	503 (96%)	21 (4%)	1 (0%)	43	62
2	K	525/548 (96%)	508 (97%)	17 (3%)	0	100	100
2	M	525/548 (96%)	508 (97%)	17 (3%)	0	100	100
2	a	525/548 (96%)	494 (94%)	31 (6%)	0	100	100
2	c	525/548 (96%)	498 (95%)	27 (5%)	0	100	100
2	e	525/548 (96%)	496 (94%)	29 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	g	525/548 (96%)	499 (95%)	26 (5%)	0	100	100
2	i	525/548 (96%)	496 (94%)	27 (5%)	2 (0%)	30	48
2	k	525/548 (96%)	498 (95%)	27 (5%)	0	100	100
2	m	525/548 (96%)	496 (94%)	29 (6%)	0	100	100
3	B	87/284 (31%)	85 (98%)	2 (2%)	0	100	100
3	D	87/284 (31%)	86 (99%)	1 (1%)	0	100	100
3	F	87/284 (31%)	84 (97%)	3 (3%)	0	100	100
3	H	87/284 (31%)	84 (97%)	3 (3%)	0	100	100
3	J	87/284 (31%)	83 (95%)	4 (5%)	0	100	100
3	L	87/284 (31%)	84 (97%)	3 (3%)	0	100	100
3	N	87/284 (31%)	85 (98%)	2 (2%)	0	100	100
3	b	86/284 (30%)	81 (94%)	5 (6%)	0	100	100
3	d	86/284 (30%)	81 (94%)	5 (6%)	0	100	100
3	f	86/284 (30%)	80 (93%)	6 (7%)	0	100	100
3	h	86/284 (30%)	79 (92%)	7 (8%)	0	100	100
3	j	86/284 (30%)	81 (94%)	5 (6%)	0	100	100
3	l	86/284 (30%)	79 (92%)	7 (8%)	0	100	100
3	n	86/284 (30%)	78 (91%)	5 (6%)	3 (4%)	3	5
All	All	9226/12327 (75%)	8748 (95%)	468 (5%)	10 (0%)	49	69

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	n	267	THR
2	I	266	THR
1	2	27	LEU
2	A	232	GLU
2	i	267	MET
1	5	29	GLY
3	n	264	ALA
2	A	234	LEU
3	n	266	GLY
2	i	88	GLY

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 PDB entries followed by that with respect to all EM entries.

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	0	80/80 (100%)	80 (100%)	0	100	100
1	1	80/80 (100%)	80 (100%)	0	100	100
1	2	80/80 (100%)	79 (99%)	1 (1%)	61	79
1	3	80/80 (100%)	78 (98%)	2 (2%)	42	66
1	4	80/80 (100%)	79 (99%)	1 (1%)	61	79
1	5	80/80 (100%)	80 (100%)	0	100	100
1	6	80/80 (100%)	79 (99%)	1 (1%)	61	79
2	A	407/415 (98%)	407 (100%)	0	100	100
2	C	407/415 (98%)	406 (100%)	1 (0%)	87	95
2	E	407/415 (98%)	406 (100%)	1 (0%)	87	95
2	G	407/415 (98%)	406 (100%)	1 (0%)	87	95
2	I	407/415 (98%)	402 (99%)	5 (1%)	63	80
2	K	407/415 (98%)	407 (100%)	0	100	100
2	M	407/415 (98%)	407 (100%)	0	100	100
2	a	407/415 (98%)	407 (100%)	0	100	100
2	c	407/415 (98%)	406 (100%)	1 (0%)	87	95
2	e	407/415 (98%)	406 (100%)	1 (0%)	87	95
2	g	407/415 (98%)	405 (100%)	2 (0%)	81	90
2	i	407/415 (98%)	407 (100%)	0	100	100
2	k	407/415 (98%)	407 (100%)	0	100	100
2	m	407/415 (98%)	405 (100%)	2 (0%)	81	90
3	B	70/238 (29%)	68 (97%)	2 (3%)	37	61
3	D	70/238 (29%)	69 (99%)	1 (1%)	59	78
3	F	70/238 (29%)	69 (99%)	1 (1%)	59	78
3	H	70/238 (29%)	68 (97%)	2 (3%)	37	61
3	J	70/238 (29%)	68 (97%)	2 (3%)	37	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	70/238 (29%)	70 (100%)	0	100	100
3	N	70/238 (29%)	69 (99%)	1 (1%)	59	78
3	b	69/238 (29%)	69 (100%)	0	100	100
3	d	69/238 (29%)	68 (99%)	1 (1%)	59	78
3	f	69/238 (29%)	67 (97%)	2 (3%)	37	61
3	h	69/238 (29%)	68 (99%)	1 (1%)	59	78
3	j	69/238 (29%)	69 (100%)	0	100	100
3	l	69/238 (29%)	67 (97%)	2 (3%)	37	61
3	n	69/238 (29%)	68 (99%)	1 (1%)	59	78
All	All	7231/9702 (74%)	7196 (100%)	35 (0%)	78	90

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	9	ARG
1	3	8	ASP
1	3	27	LEU
1	4	28	THR
1	6	28	THR
3	B	234	GLU
3	B	277	ARG
2	C	233	MET
3	D	228	GLN
2	E	232	GLU
3	F	277	ARG
2	G	233	MET
3	H	222	LEU
3	H	277	ARG
2	I	227	ILE
2	I	233	MET
2	I	265	ASN
2	I	276	VAL
2	I	345	ARG
3	J	234	GLU
3	J	277	ARG
3	N	277	ARG
2	c	317	LEU
3	d	262	LEU
2	e	453	GLN

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Mol	Chain	Res	Type
3	f	262	LEU
3	f	265	LEU
2	g	250	ILE
2	g	272	LYS
3	h	262	LEU
3	l	275	TYR
3	l	276	ARG
2	m	1	MET
2	m	453	GLN
3	n	262	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	319	GLN
3	B	206	GLN
3	B	207	GLN
3	B	208	GLN
3	B	221	GLN
3	B	225	GLN
3	B	228	GLN
3	B	259	GLN
2	C	319	GLN
3	D	206	GLN
3	D	207	GLN
3	D	208	GLN
3	D	225	GLN
3	D	259	GLN
2	E	319	GLN
3	F	206	GLN
3	F	207	GLN
3	F	208	GLN
3	F	228	GLN
3	F	259	GLN
2	G	319	GLN
3	H	206	GLN
3	H	207	GLN
3	H	208	GLN
3	H	221	GLN
3	H	225	GLN
3	H	228	GLN
3	H	259	GLN

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Mol	Chain	Res	Type
2	I	112	ASN
2	I	319	GLN
2	I	343	GLN
3	J	206	GLN
3	J	207	GLN
3	J	208	GLN
3	J	225	GLN
3	J	228	GLN
3	J	259	GLN
2	K	319	GLN
3	L	206	GLN
3	L	207	GLN
3	L	225	GLN
3	L	228	GLN
3	L	259	GLN
2	M	112	ASN
2	M	319	GLN
3	N	206	GLN
3	N	207	GLN
3	N	208	GLN
3	N	225	GLN
3	N	228	GLN
3	N	259	GLN
2	a	68	ASN
2	a	72	GLN
2	a	194	GLN
2	a	352	GLN
2	a	453	GLN
2	c	10	ASN
2	c	68	ASN
2	c	72	GLN
2	c	194	GLN
2	c	352	GLN
2	e	10	ASN
2	e	68	ASN
2	e	72	GLN
2	e	194	GLN
2	e	352	GLN
2	g	10	ASN
2	g	68	ASN
2	g	72	GLN
2	g	194	GLN

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Mol	Chain	Res	Type
2	g	352	GLN
3	h	204	GLN
3	h	242	HIS
2	i	10	ASN
2	i	194	GLN
2	i	352	GLN
2	i	487	ASN
2	k	10	ASN
2	k	68	ASN
2	k	72	GLN
2	k	194	GLN
2	k	206	ASN
2	k	352	GLN
2	m	10	ASN
2	m	68	ASN
2	m	72	GLN
2	m	146	GLN
2	m	194	GLN
2	m	206	ASN
2	m	352	GLN
2	m	467	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 21 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
5	ANP	M	600	4	32,33,33	0.90	4 (12%)	44,52,52	0.84	1 (2%)
5	ANP	e	603	4,6	32,33,33	0.93	4 (12%)	44,52,52	0.84	1 (2%)
5	ANP	G	602	4	32,33,33	0.90	4 (12%)	44,52,52	0.84	1 (2%)
5	ANP	C	602	4	32,33,33	0.89	4 (12%)	44,52,52	0.83	1 (2%)
5	ANP	i	603	4,6	32,33,33	1.03	5 (15%)	44,52,52	1.07	3 (6%)
5	ANP	g	603	4,6	32,33,33	1.05	5 (15%)	44,52,52	1.04	3 (6%)
5	ANP	c	603	4,6	32,33,33	0.93	4 (12%)	44,52,52	0.84	1 (2%)
5	ANP	A	602	4	32,33,33	0.91	4 (12%)	44,52,52	0.83	1 (2%)
5	ANP	k	603	4,6	32,33,33	0.93	4 (12%)	44,52,52	0.85	1 (2%)
5	ANP	I	602	4	32,33,33	0.92	4 (12%)	44,52,52	0.84	1 (2%)
5	ANP	E	602	4	32,33,33	0.90	4 (12%)	44,52,52	0.83	1 (2%)
5	ANP	a	600	4,6	32,33,33	0.92	4 (12%)	44,52,52	0.84	1 (2%)
5	ANP	K	600	4	32,33,33	0.91	4 (12%)	44,52,52	0.83	1 (2%)
5	ANP	m	603	4,6	32,33,33	0.94	4 (12%)	44,52,52	0.84	1 (2%)

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
5	ANP	M	600	4	-	2/18/38/38	0/3/3/3
5	ANP	e	603	4,6	-	7/18/38/38	0/3/3/3
5	ANP	G	602	4	-	2/18/38/38	0/3/3/3
5	ANP	C	602	4	-	2/18/38/38	0/3/3/3
5	ANP	i	603	4,6	-	4/18/38/38	0/3/3/3
5	ANP	g	603	4,6	-	4/18/38/38	0/3/3/3
5	ANP	c	603	4,6	-	7/18/38/38	0/3/3/3
5	ANP	A	602	4	-	2/18/38/38	0/3/3/3
5	ANP	k	603	4,6	-	7/18/38/38	0/3/3/3
5	ANP	I	602	4	-	2/18/38/38	0/3/3/3
5	ANP	E	602	4	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	a	600	4,6	-	7/18/38/38	0/3/3/3
5	ANP	K	600	4	-	2/18/38/38	0/3/3/3
5	ANP	m	603	4,6	-	7/18/38/38	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	g	603	ANP	PG-O1G	2.94	1.50	1.46
5	i	603	ANP	PB-O1B	2.86	1.50	1.46
5	g	603	ANP	PB-O1B	2.85	1.50	1.46
5	i	603	ANP	PG-O1G	2.77	1.50	1.46
5	m	603	ANP	PB-O3A	-2.58	1.55	1.59
5	e	603	ANP	PB-O3A	-2.54	1.55	1.59
5	c	603	ANP	PB-O3A	-2.52	1.55	1.59
5	a	600	ANP	PB-O3A	-2.49	1.55	1.59
5	k	603	ANP	PG-O1G	2.48	1.50	1.46
5	c	603	ANP	PG-O1G	2.46	1.50	1.46
5	k	603	ANP	PB-O3A	-2.46	1.56	1.59
5	e	603	ANP	PG-O1G	2.43	1.50	1.46
5	I	602	ANP	PG-O1G	2.41	1.50	1.46
5	c	603	ANP	PG-N3B	2.41	1.69	1.63
5	G	602	ANP	PG-O1G	2.41	1.50	1.46
5	K	600	ANP	PB-O3A	-2.40	1.56	1.59
5	A	602	ANP	PB-O3A	-2.39	1.56	1.59
5	K	600	ANP	PG-N3B	2.39	1.69	1.63
5	M	600	ANP	PG-N3B	2.39	1.69	1.63
5	M	600	ANP	PG-O1G	2.38	1.49	1.46
5	I	602	ANP	PB-O3A	-2.38	1.56	1.59
5	e	603	ANP	PG-N3B	2.37	1.69	1.63
5	a	600	ANP	PG-N3B	2.36	1.69	1.63
5	C	602	ANP	PG-O1G	2.36	1.49	1.46
5	E	602	ANP	PB-O3A	-2.36	1.56	1.59
5	m	603	ANP	PG-N3B	2.36	1.69	1.63
5	m	603	ANP	PG-O1G	2.36	1.49	1.46
5	k	603	ANP	PG-N3B	2.36	1.69	1.63
5	a	600	ANP	PG-O1G	2.35	1.49	1.46
5	C	602	ANP	PG-N3B	2.35	1.69	1.63
5	E	602	ANP	PG-O1G	2.35	1.49	1.46
5	A	602	ANP	PG-N3B	2.35	1.69	1.63
5	K	600	ANP	PG-O1G	2.34	1.49	1.46
5	A	602	ANP	PG-O1G	2.34	1.49	1.46
5	m	603	ANP	PB-O1B	2.34	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	602	ANP	PG-N3B	2.34	1.69	1.63
5	e	603	ANP	PB-O1B	2.33	1.49	1.46
5	I	602	ANP	PG-N3B	2.32	1.69	1.63
5	G	602	ANP	PG-N3B	2.30	1.69	1.63
5	M	600	ANP	PB-O3A	-2.30	1.56	1.59
5	G	602	ANP	PB-O3A	-2.29	1.56	1.59
5	k	603	ANP	PB-O1B	2.29	1.49	1.46
5	I	602	ANP	PB-O1B	2.27	1.49	1.46
5	i	603	ANP	PB-O2B	-2.26	1.50	1.56
5	a	600	ANP	PB-O1B	2.25	1.49	1.46
5	g	603	ANP	PG-O3G	-2.24	1.50	1.56
5	C	602	ANP	PB-O3A	-2.24	1.56	1.59
5	g	603	ANP	PB-O2B	-2.23	1.50	1.56
5	c	603	ANP	PB-O1B	2.22	1.49	1.46
5	i	603	ANP	PG-O2G	-2.21	1.50	1.56
5	g	603	ANP	PG-O2G	-2.20	1.50	1.56
5	A	602	ANP	PB-O1B	2.19	1.49	1.46
5	G	602	ANP	PB-O1B	2.19	1.49	1.46
5	E	602	ANP	PB-O1B	2.19	1.49	1.46
5	K	600	ANP	PB-O1B	2.18	1.49	1.46
5	C	602	ANP	PB-O1B	2.17	1.49	1.46
5	M	600	ANP	PB-O1B	2.14	1.49	1.46
5	i	603	ANP	PG-O3G	-2.11	1.51	1.56

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	i	603	ANP	O2B-PB-O1B	4.39	119.12	109.92
5	g	603	ANP	O2B-PB-O1B	4.31	118.95	109.92
5	k	603	ANP	PB-O3A-PA	-3.99	118.56	132.62
5	a	600	ANP	PB-O3A-PA	-3.98	118.61	132.62
5	e	603	ANP	PB-O3A-PA	-3.97	118.62	132.62
5	c	603	ANP	PB-O3A-PA	-3.97	118.64	132.62
5	m	603	ANP	PB-O3A-PA	-3.97	118.65	132.62
5	K	600	ANP	PB-O3A-PA	-3.60	119.93	132.62
5	A	602	ANP	PB-O3A-PA	-3.60	119.93	132.62
5	M	600	ANP	PB-O3A-PA	-3.60	119.94	132.62
5	C	602	ANP	PB-O3A-PA	-3.60	119.95	132.62
5	E	602	ANP	PB-O3A-PA	-3.60	119.95	132.62
5	G	602	ANP	PB-O3A-PA	-3.59	119.97	132.62
5	I	602	ANP	PB-O3A-PA	-3.58	119.99	132.62
5	i	603	ANP	O3A-PB-N3B	-3.33	97.34	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	g	603	ANP	O3A-PB-N3B	-2.87	98.64	106.59
5	i	603	ANP	O2G-PG-O1G	-2.34	107.58	113.45
5	g	603	ANP	O3G-PG-O1G	-2.15	108.06	113.45

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	ANP	PB-N3B-PG-O1G
5	A	602	ANP	PG-N3B-PB-O1B
5	C	602	ANP	PB-N3B-PG-O1G
5	C	602	ANP	PG-N3B-PB-O1B
5	E	602	ANP	PB-N3B-PG-O1G
5	E	602	ANP	PG-N3B-PB-O1B
5	G	602	ANP	PB-N3B-PG-O1G
5	G	602	ANP	PG-N3B-PB-O1B
5	I	602	ANP	PB-N3B-PG-O1G
5	I	602	ANP	PG-N3B-PB-O1B
5	K	600	ANP	PB-N3B-PG-O1G
5	K	600	ANP	PG-N3B-PB-O1B
5	M	600	ANP	PB-N3B-PG-O1G
5	M	600	ANP	PG-N3B-PB-O1B
5	a	600	ANP	PB-N3B-PG-O1G
5	a	600	ANP	PG-N3B-PB-O1B
5	a	600	ANP	C5'-O5'-PA-O1A
5	a	600	ANP	C5'-O5'-PA-O2A
5	a	600	ANP	C5'-O5'-PA-O3A
5	c	603	ANP	PB-N3B-PG-O1G
5	c	603	ANP	PG-N3B-PB-O1B
5	c	603	ANP	C5'-O5'-PA-O2A
5	c	603	ANP	C5'-O5'-PA-O3A
5	e	603	ANP	PB-N3B-PG-O1G
5	e	603	ANP	PG-N3B-PB-O1B
5	e	603	ANP	C5'-O5'-PA-O1A
5	e	603	ANP	C5'-O5'-PA-O2A
5	e	603	ANP	C5'-O5'-PA-O3A
5	g	603	ANP	PB-N3B-PG-O1G
5	g	603	ANP	PG-N3B-PB-O1B
5	g	603	ANP	C5'-O5'-PA-O3A
5	i	603	ANP	PG-N3B-PB-O1B
5	i	603	ANP	C5'-O5'-PA-O3A
5	k	603	ANP	PB-N3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
5	k	603	ANP	PG-N3B-PB-O1B
5	k	603	ANP	C5'-O5'-PA-O1A
5	k	603	ANP	C5'-O5'-PA-O2A
5	k	603	ANP	C5'-O5'-PA-O3A
5	m	603	ANP	PB-N3B-PG-O1G
5	m	603	ANP	PG-N3B-PB-O1B
5	m	603	ANP	C5'-O5'-PA-O1A
5	m	603	ANP	C5'-O5'-PA-O2A
5	m	603	ANP	C5'-O5'-PA-O3A
5	a	600	ANP	PB-O3A-PA-O1A
5	c	603	ANP	PB-O3A-PA-O1A
5	e	603	ANP	PB-O3A-PA-O1A
5	k	603	ANP	PB-O3A-PA-O1A
5	m	603	ANP	PB-O3A-PA-O1A
5	c	603	ANP	C5'-O5'-PA-O1A
5	i	603	ANP	C5'-O5'-PA-O1A
5	i	603	ANP	C5'-O5'-PA-O2A
5	a	600	ANP	PB-O3A-PA-O2A
5	c	603	ANP	PB-O3A-PA-O2A
5	e	603	ANP	PB-O3A-PA-O2A
5	k	603	ANP	PB-O3A-PA-O2A
5	m	603	ANP	PB-O3A-PA-O2A
5	g	603	ANP	C5'-O5'-PA-O1A

There are no ring outliers.

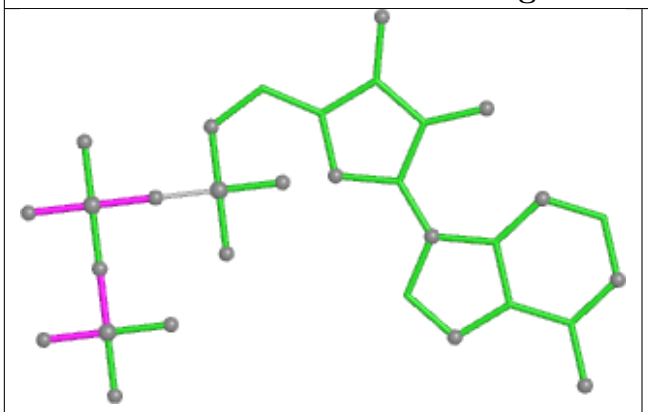
9 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	600	ANP	1	0
5	e	603	ANP	4	0
5	C	602	ANP	2	0
5	c	603	ANP	2	0
5	k	603	ANP	9	0
5	I	602	ANP	1	0
5	a	600	ANP	1	0
5	K	600	ANP	3	0
5	m	603	ANP	5	0

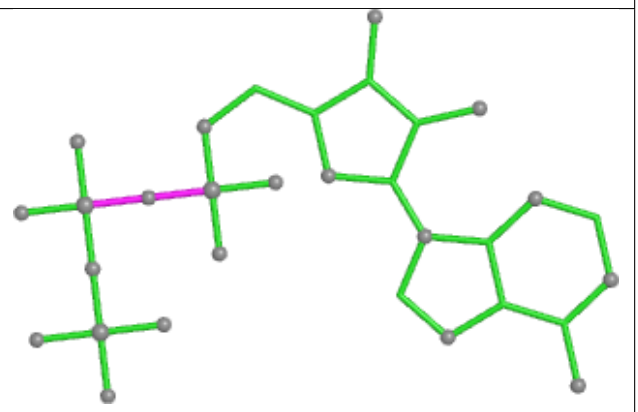
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

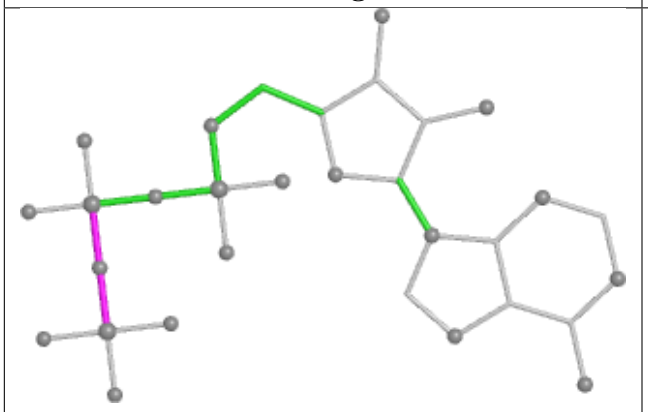
Ligand ANP M 600



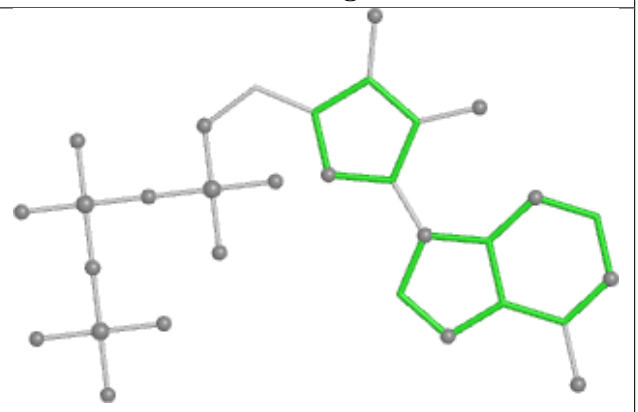
Bond lengths



Bond angles

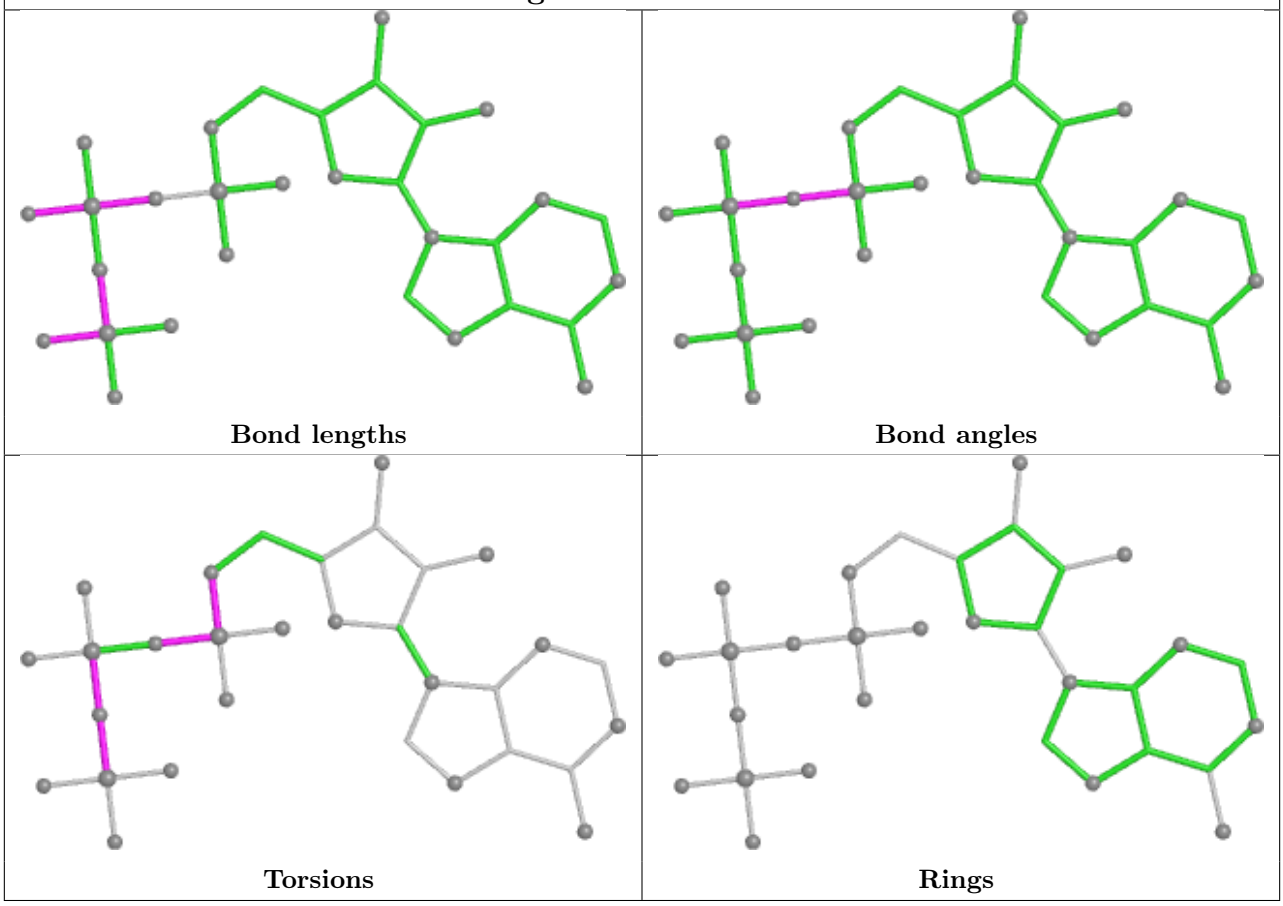


Torsions

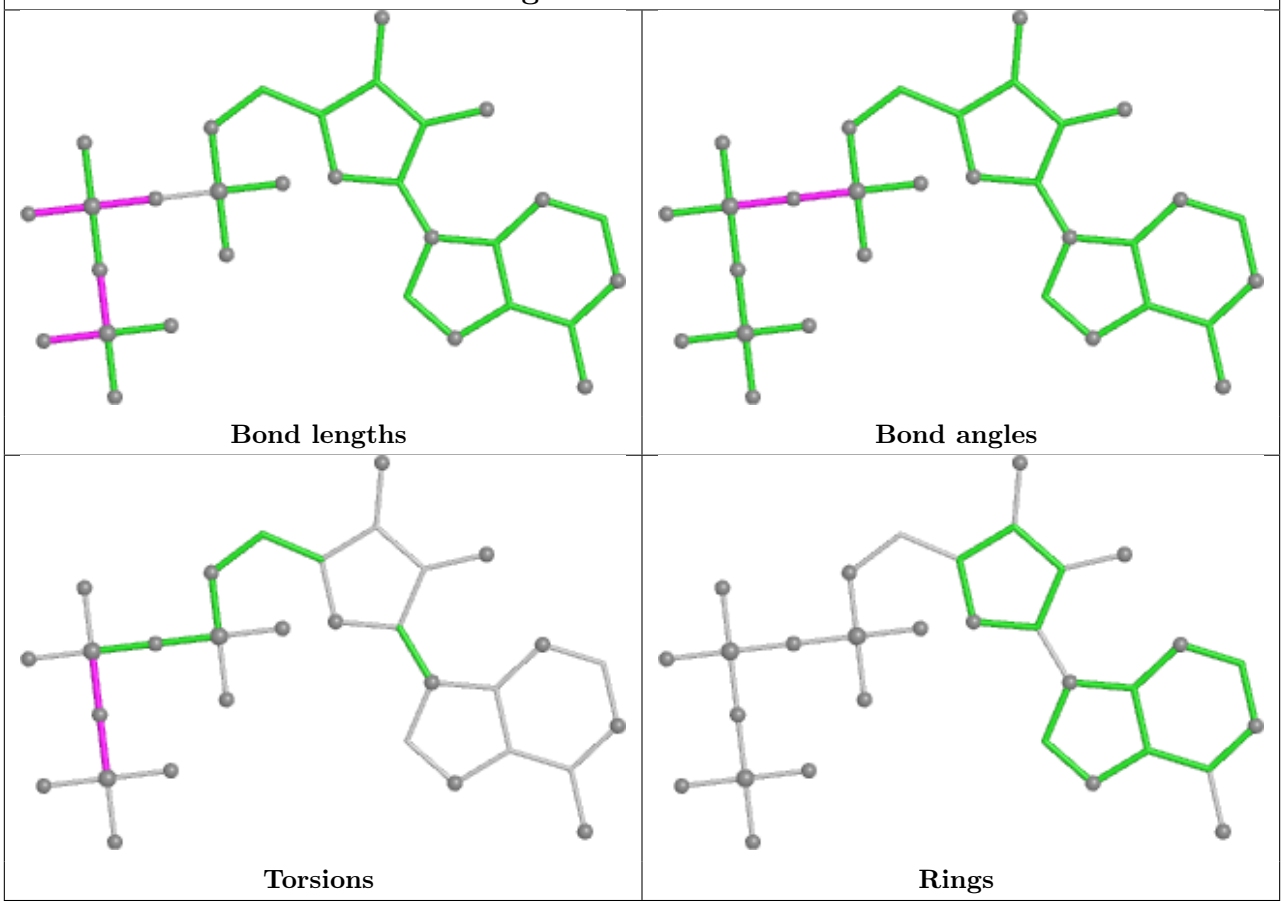


Rings

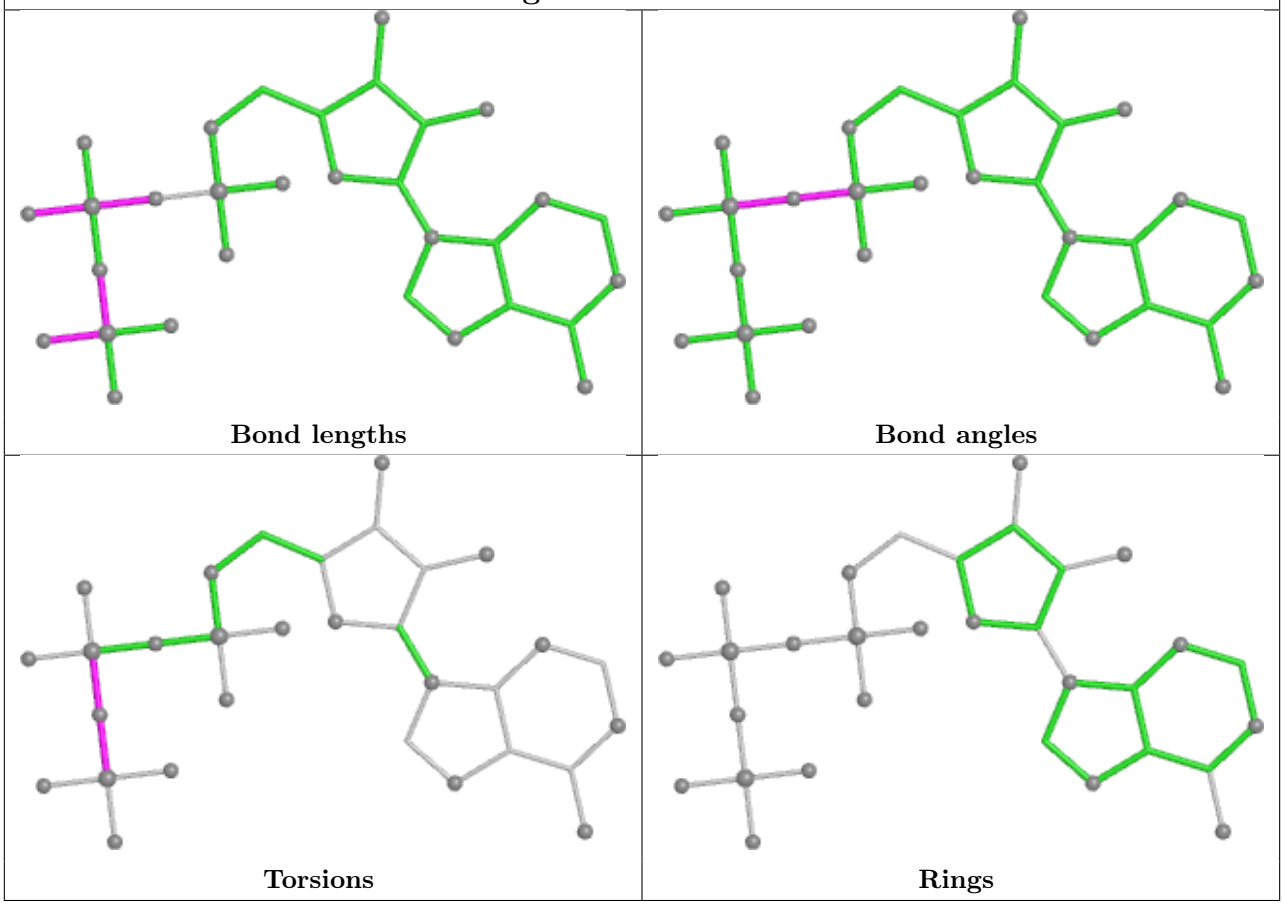
Ligand ANP e 603



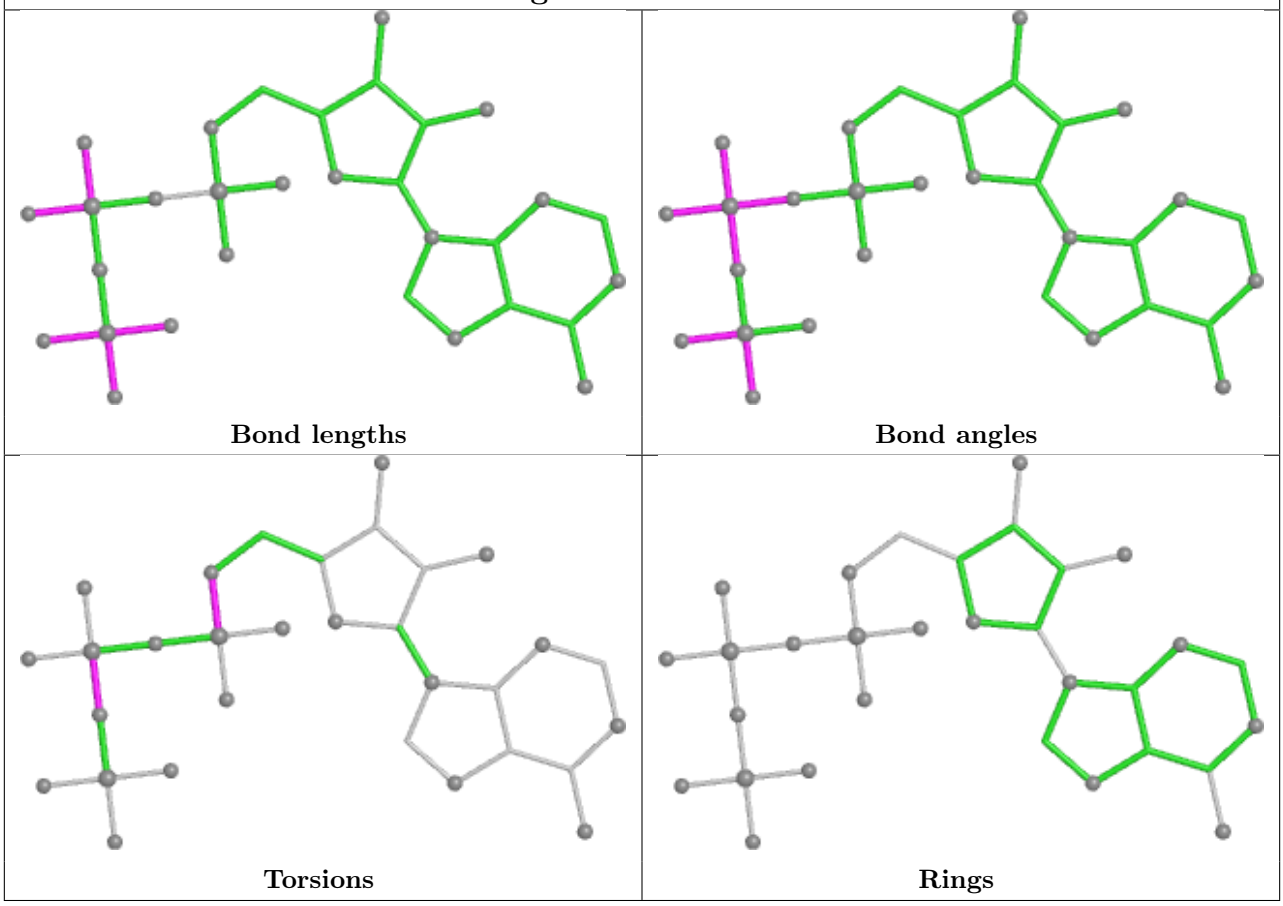
Ligand ANP G 602



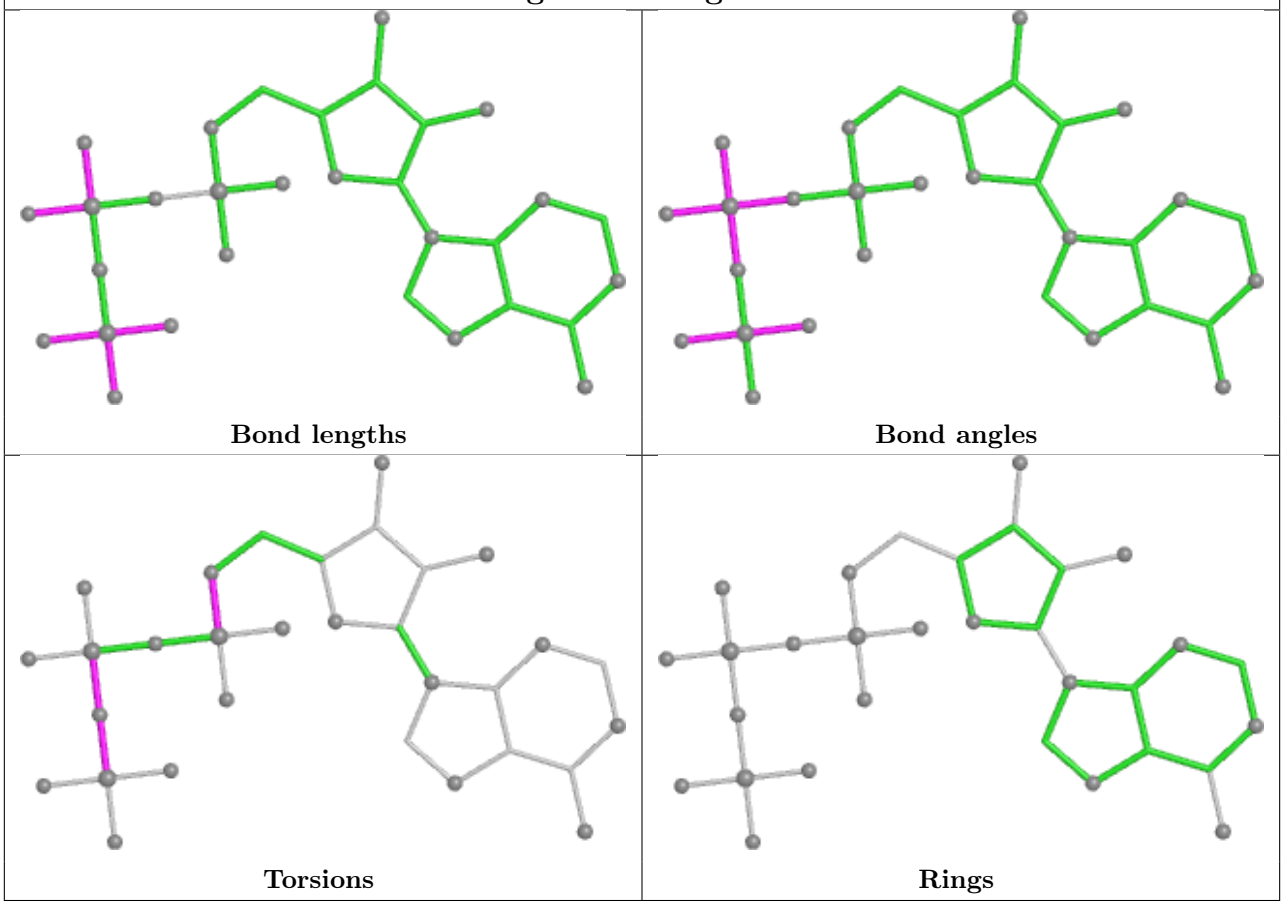
Ligand ANP C 602



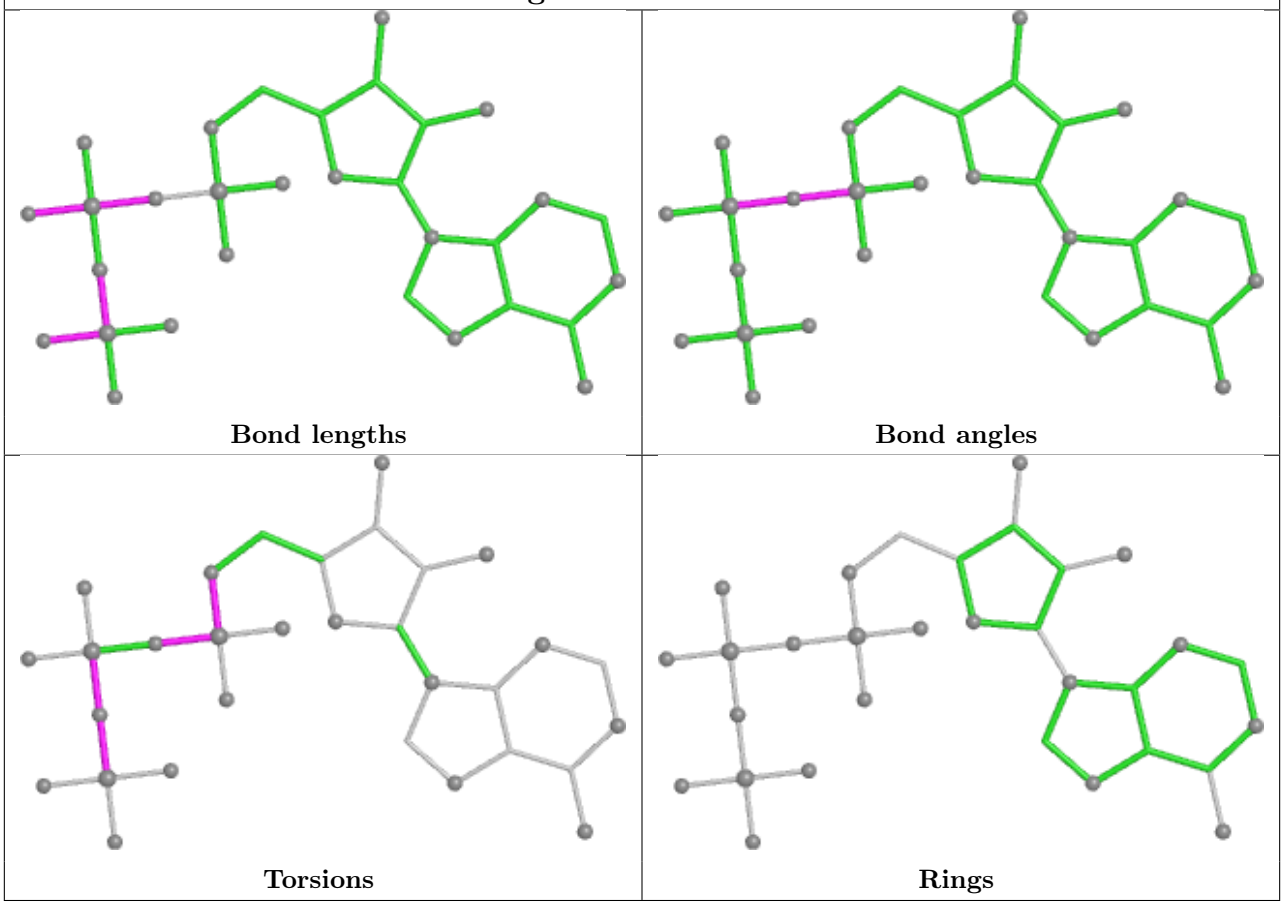
Ligand ANP i 603



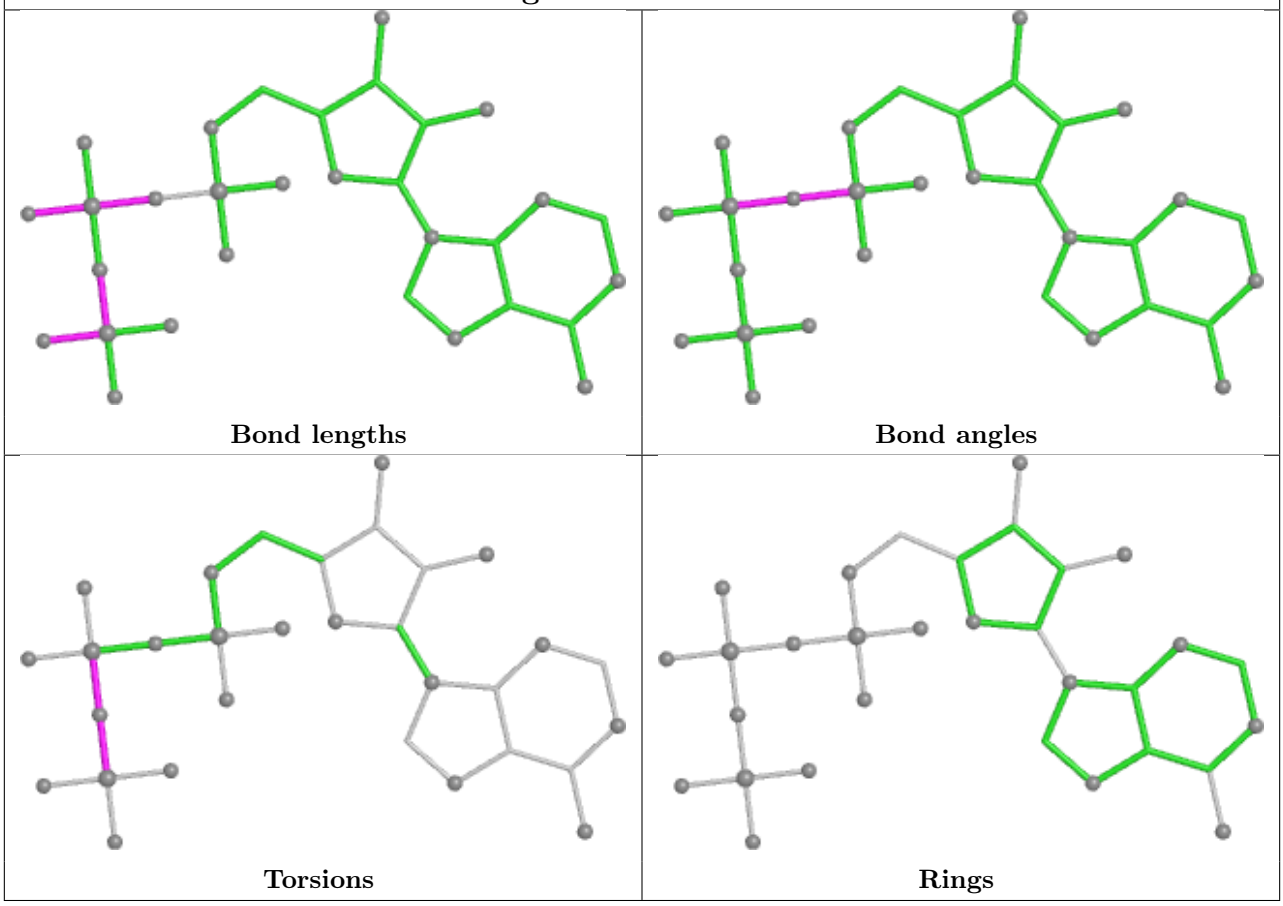
Ligand ANP g 603



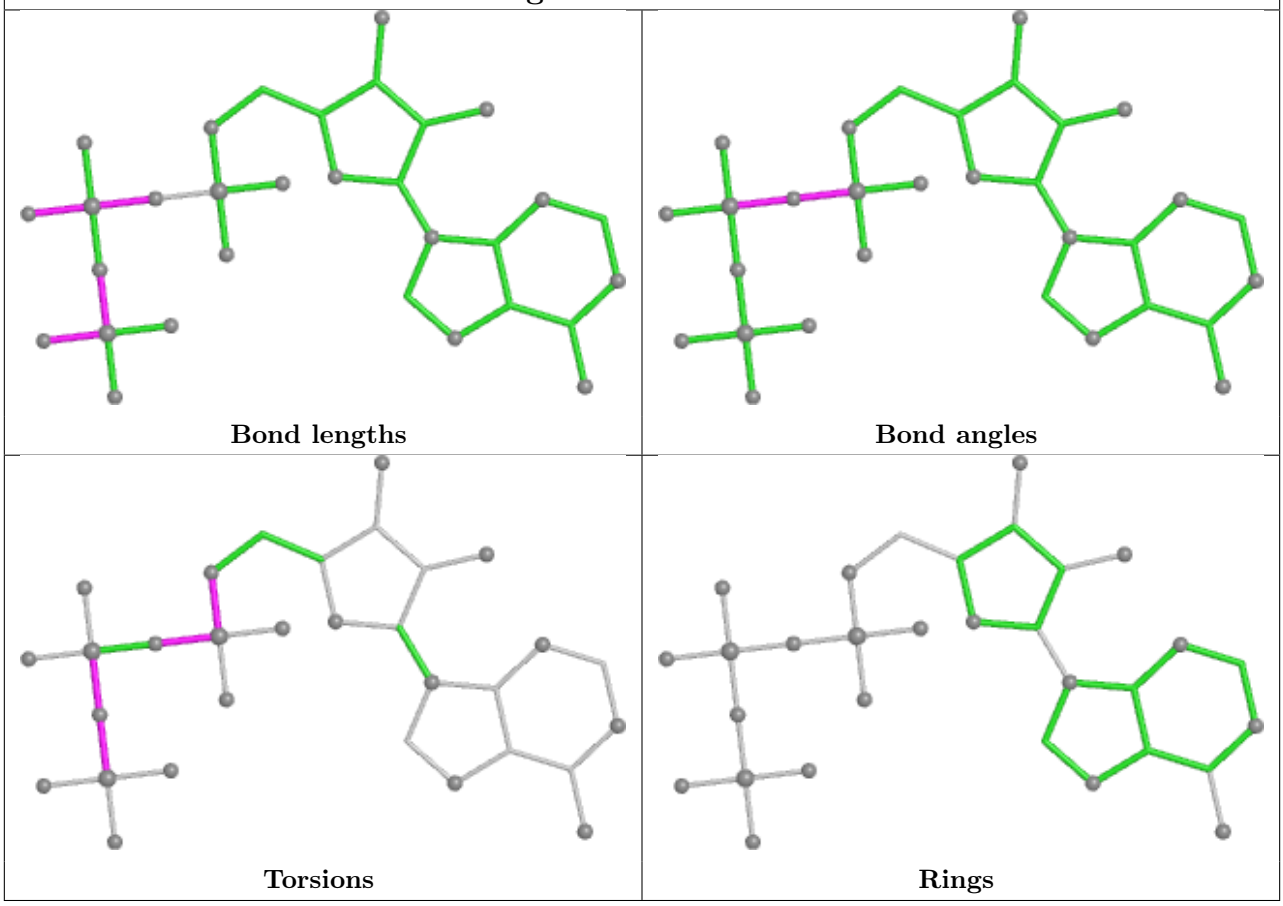
Ligand ANP c 603



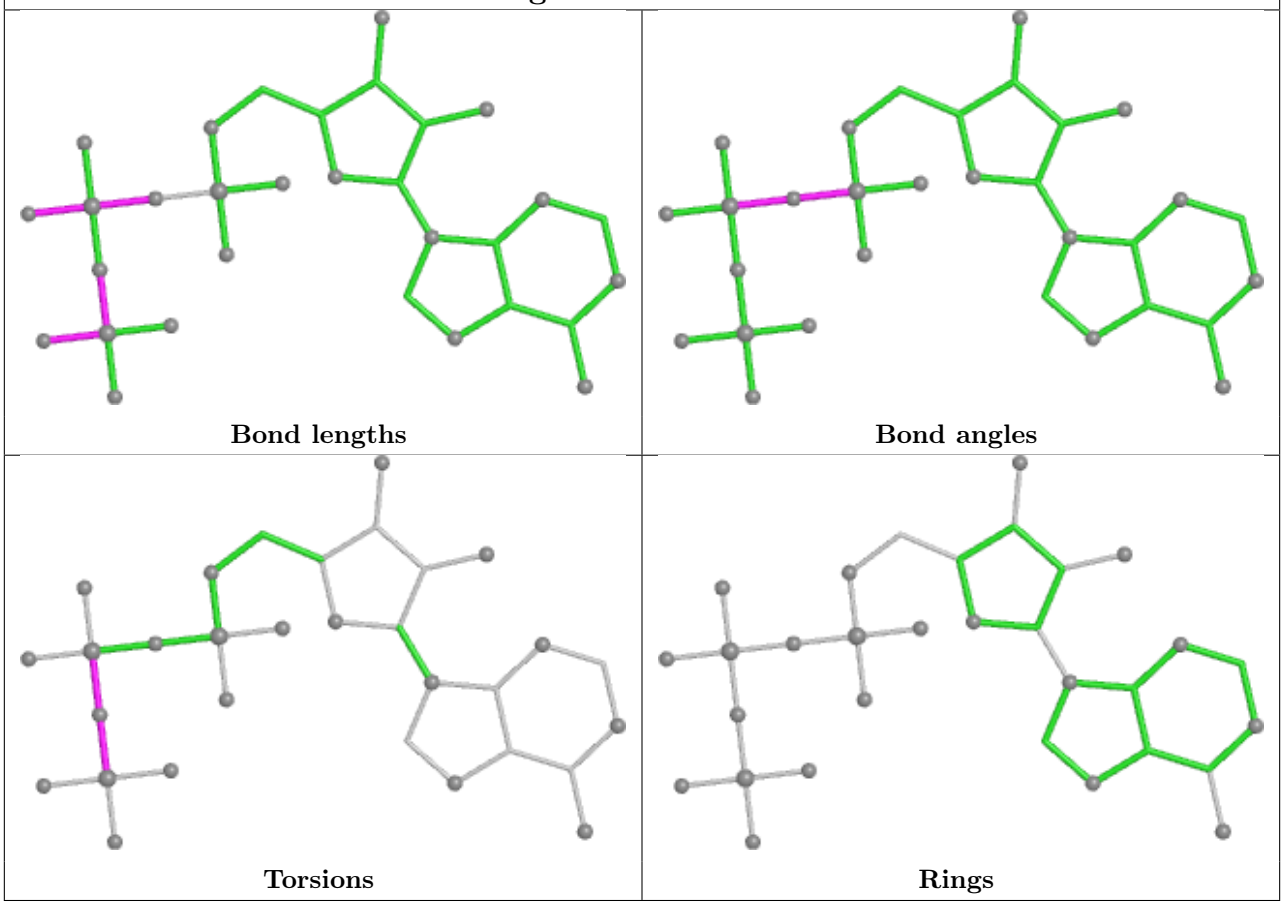
Ligand ANP A 602



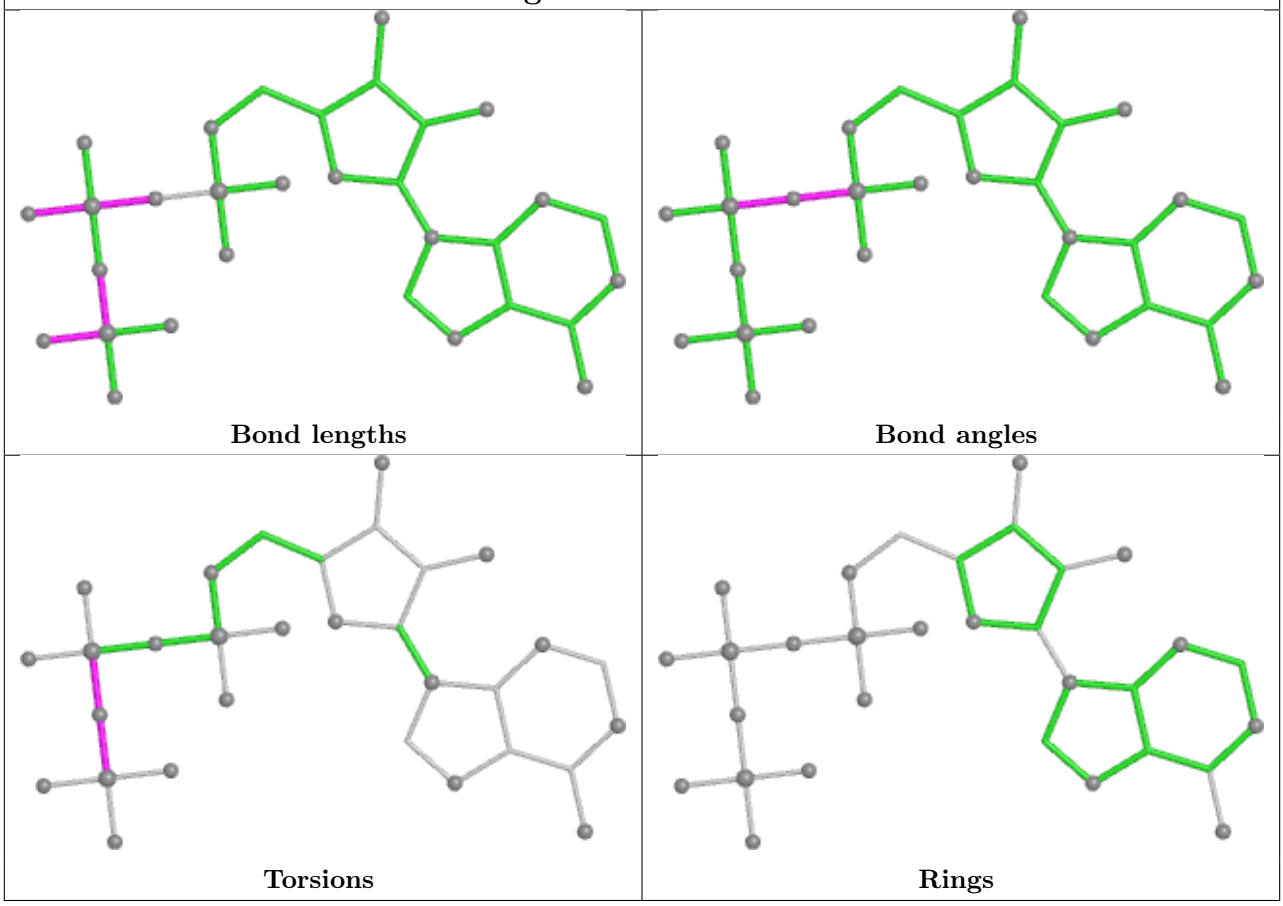
Ligand ANP k 603



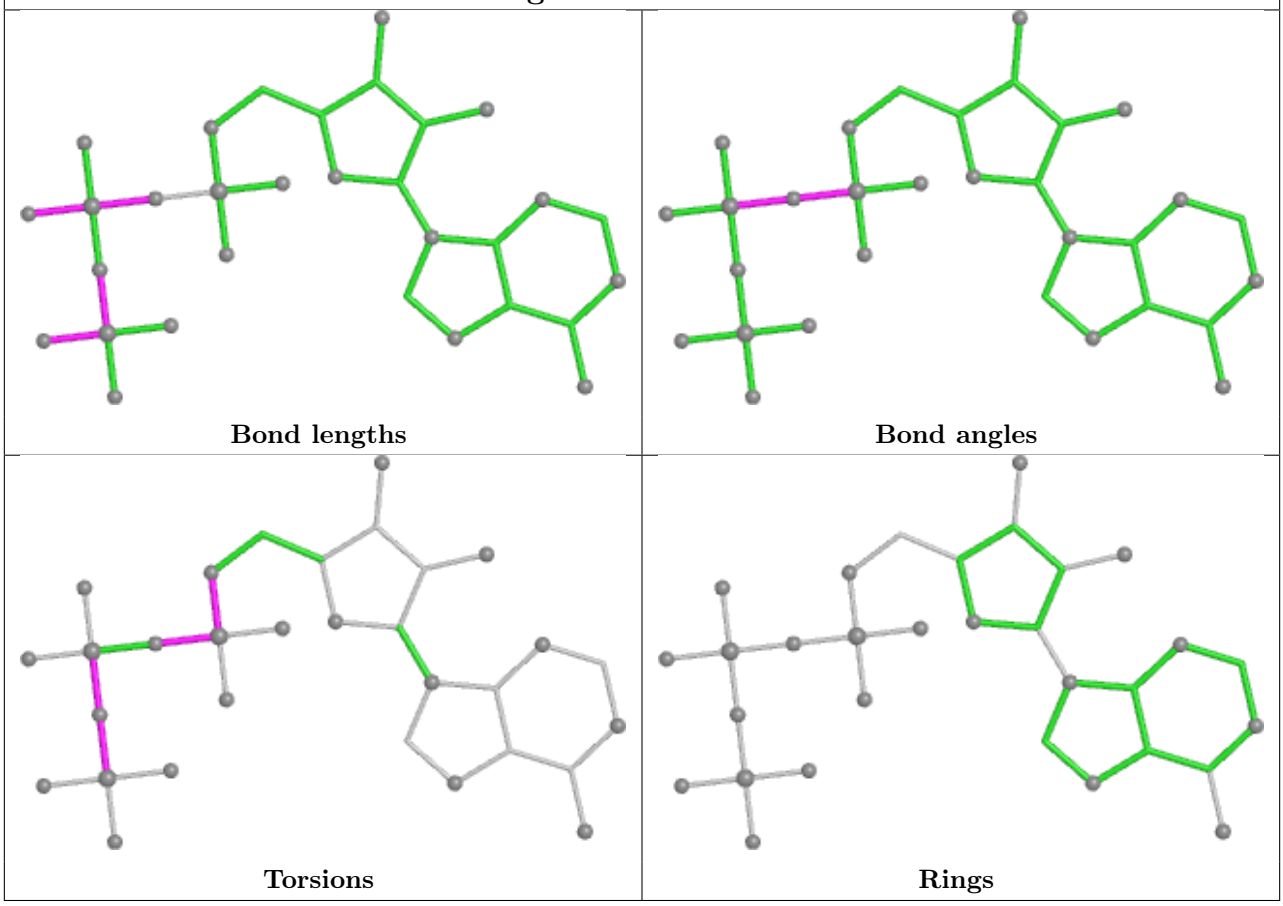
Ligand ANP I 602



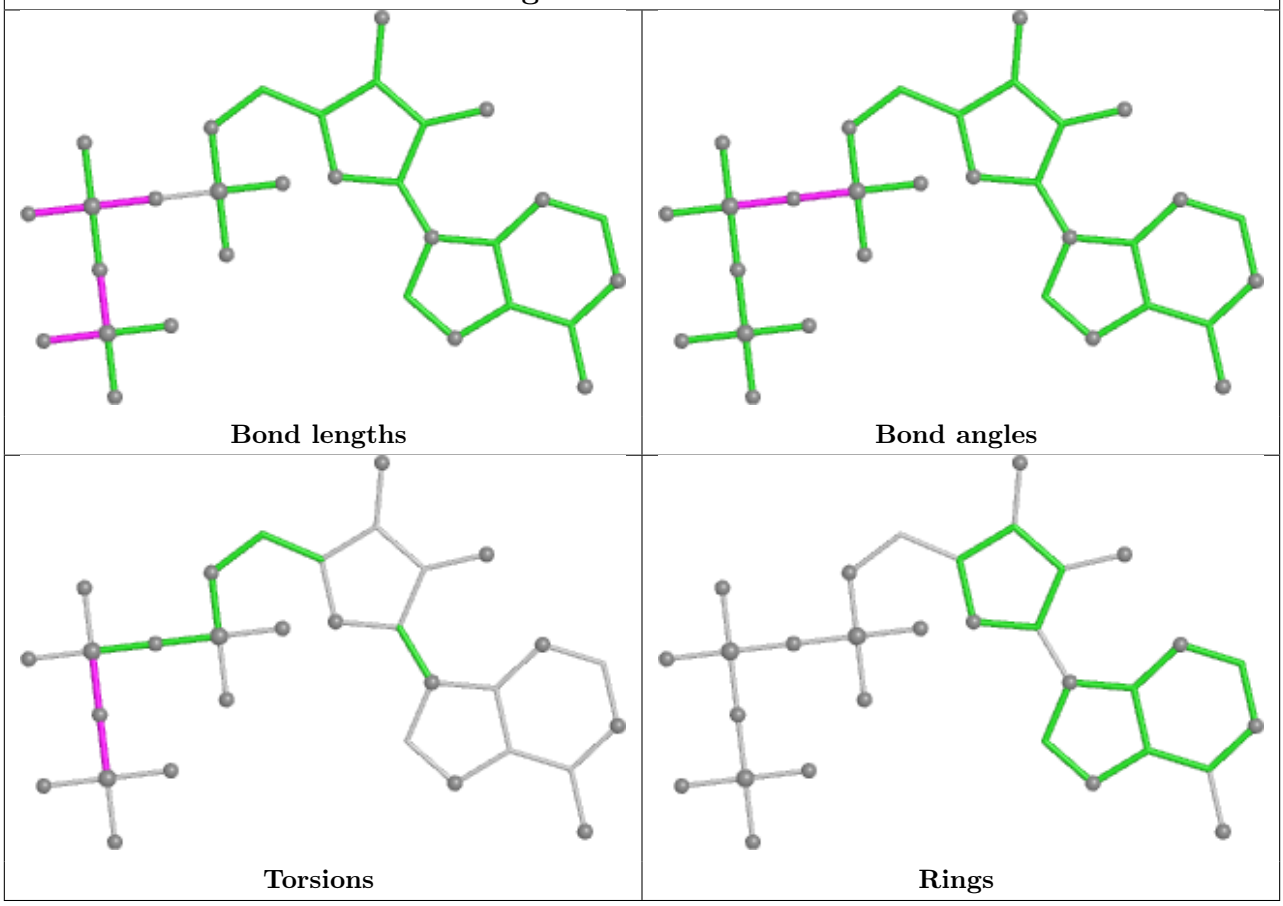
Ligand ANP E 602



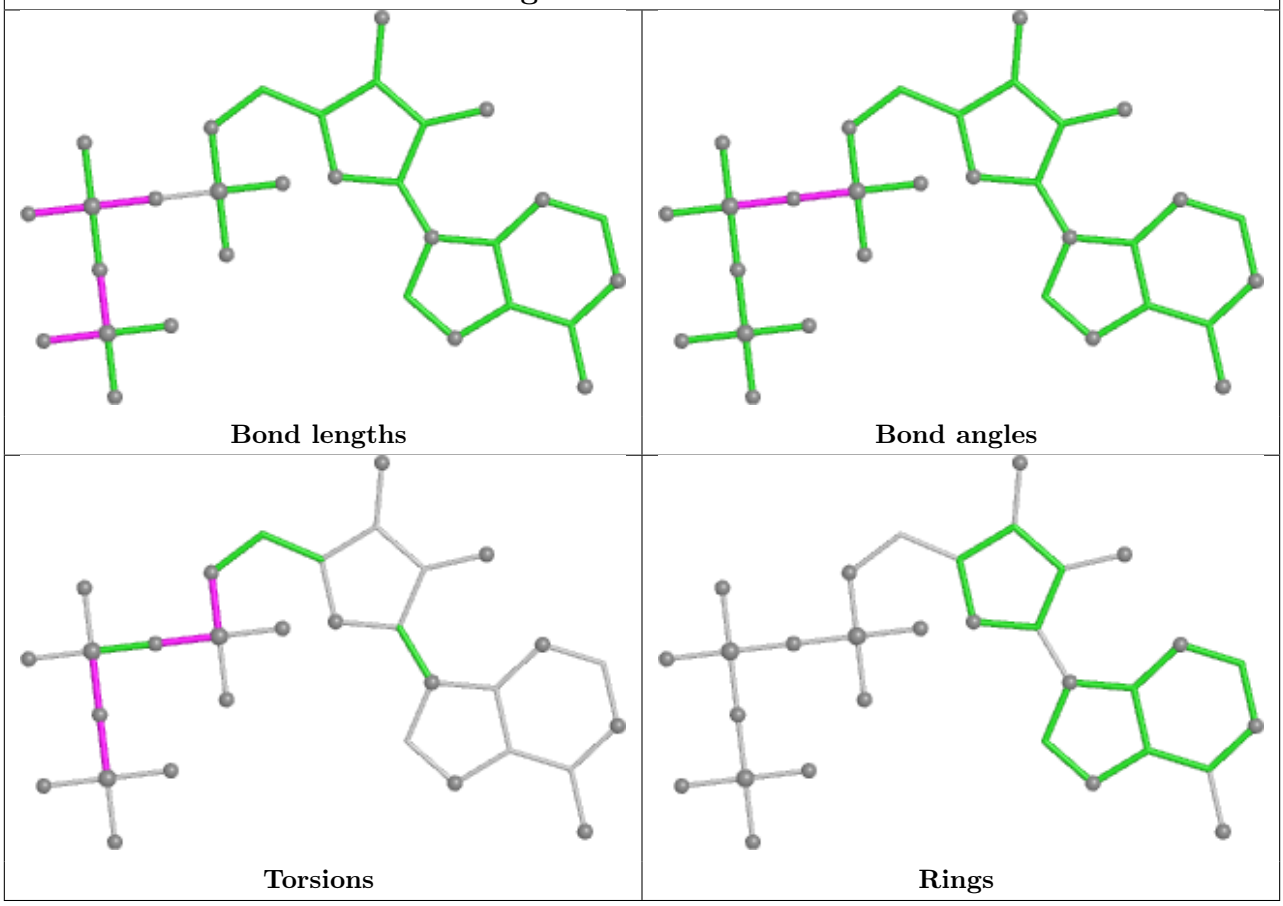
Ligand ANP a 600



Ligand ANP K 600



Ligand ANP m 603



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

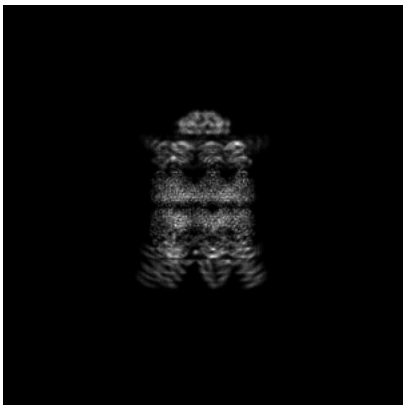
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-65992. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

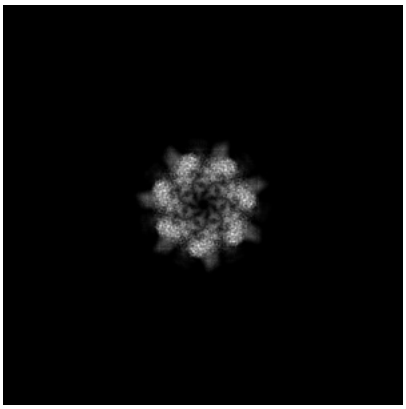
6.1 Orthogonal projections (i)

6.1.1 Primary map



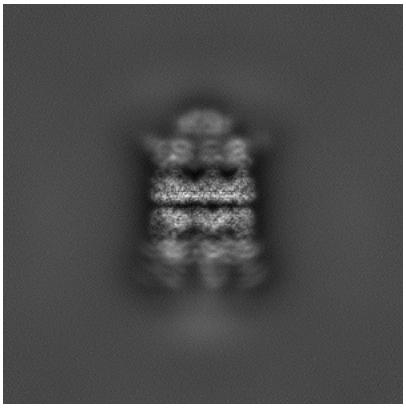
X

Y

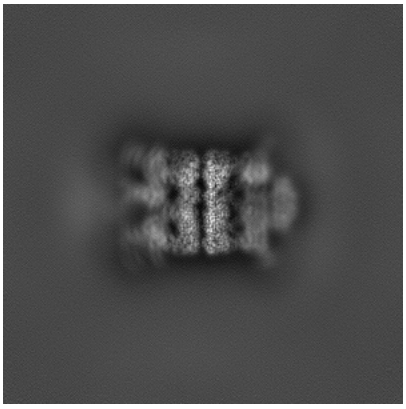


Z

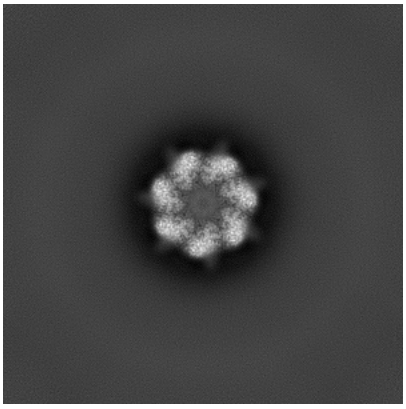
6.1.2 Raw map



X



Y



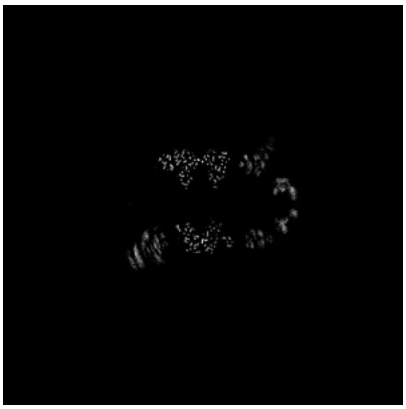
Z

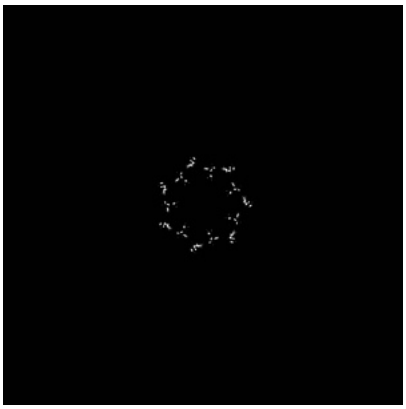
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

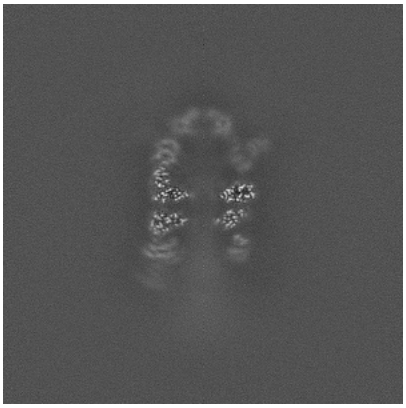
6.2.1 Primary map

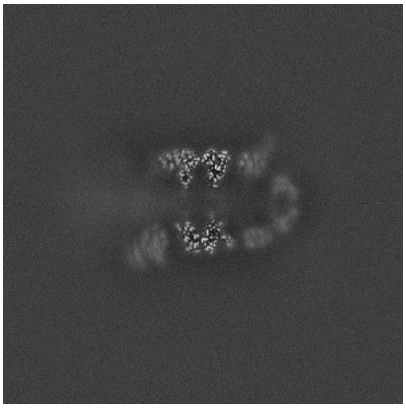
X Index: 240

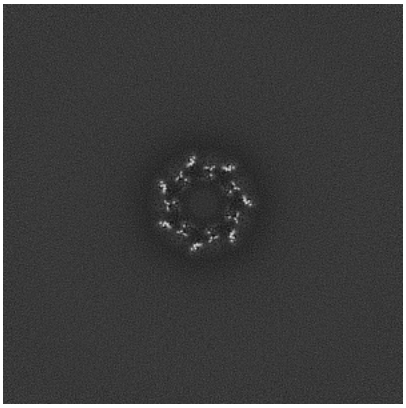

Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240

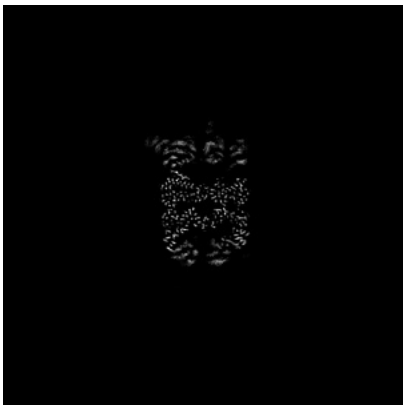

Y Index: 240


Z Index: 240

The images above show central slices of the map in three orthogonal directions.

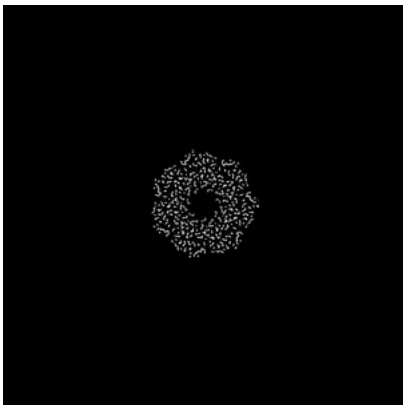
6.3 Largest variance slices (i)

6.3.1 Primary map



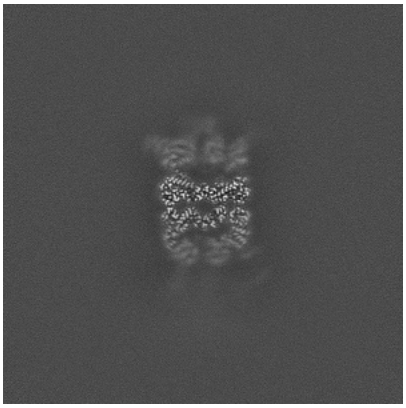
X Index: 275

Y Index: 206

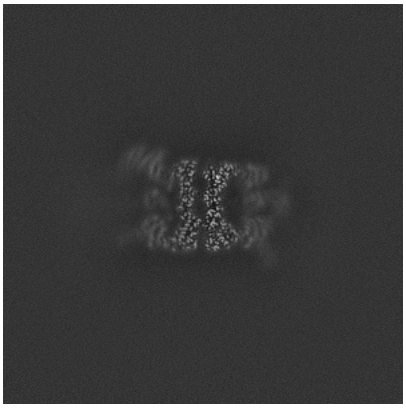


Z Index: 249

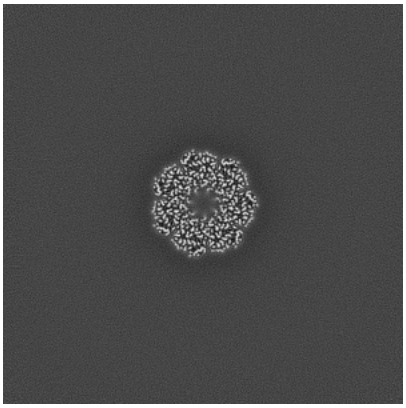
6.3.2 Raw map



X Index: 274



Y Index: 208

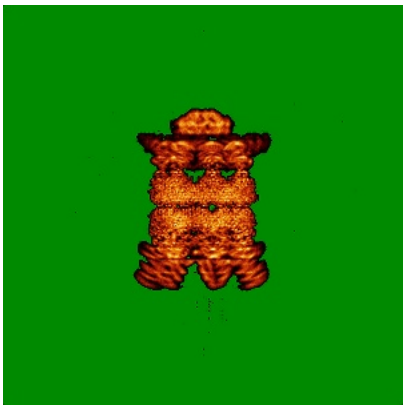


Z Index: 249

The images above show the largest variance slices of the map in three orthogonal directions.

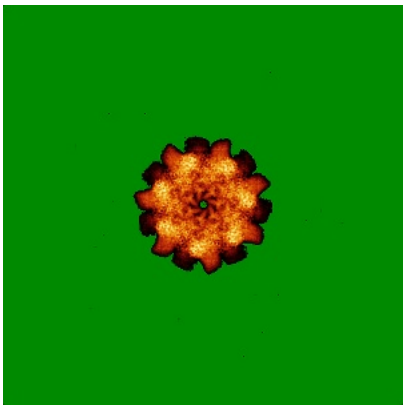
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



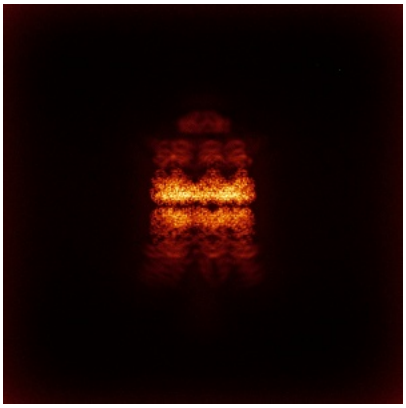
X

Y

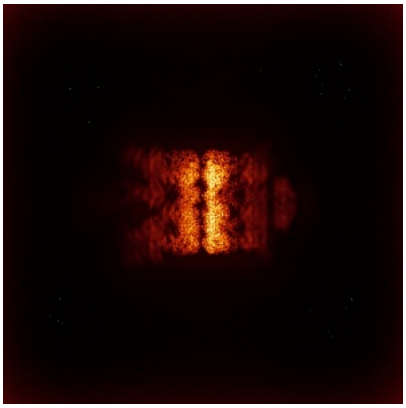


Z

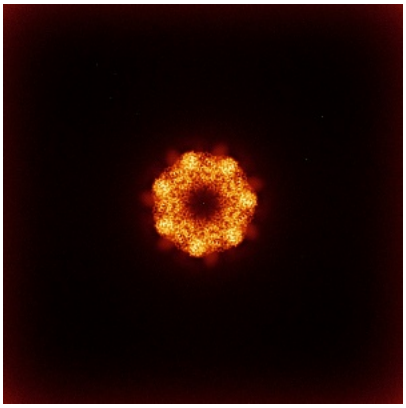
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

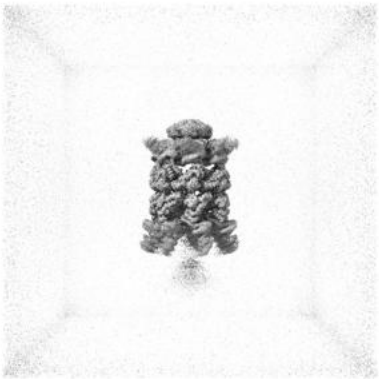
X

Y

Z

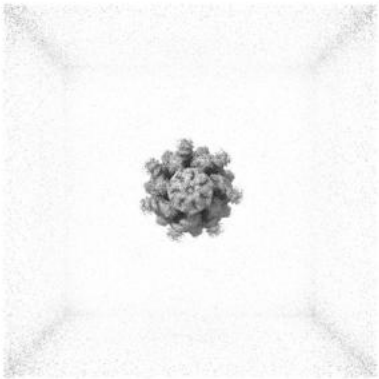
The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X

Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

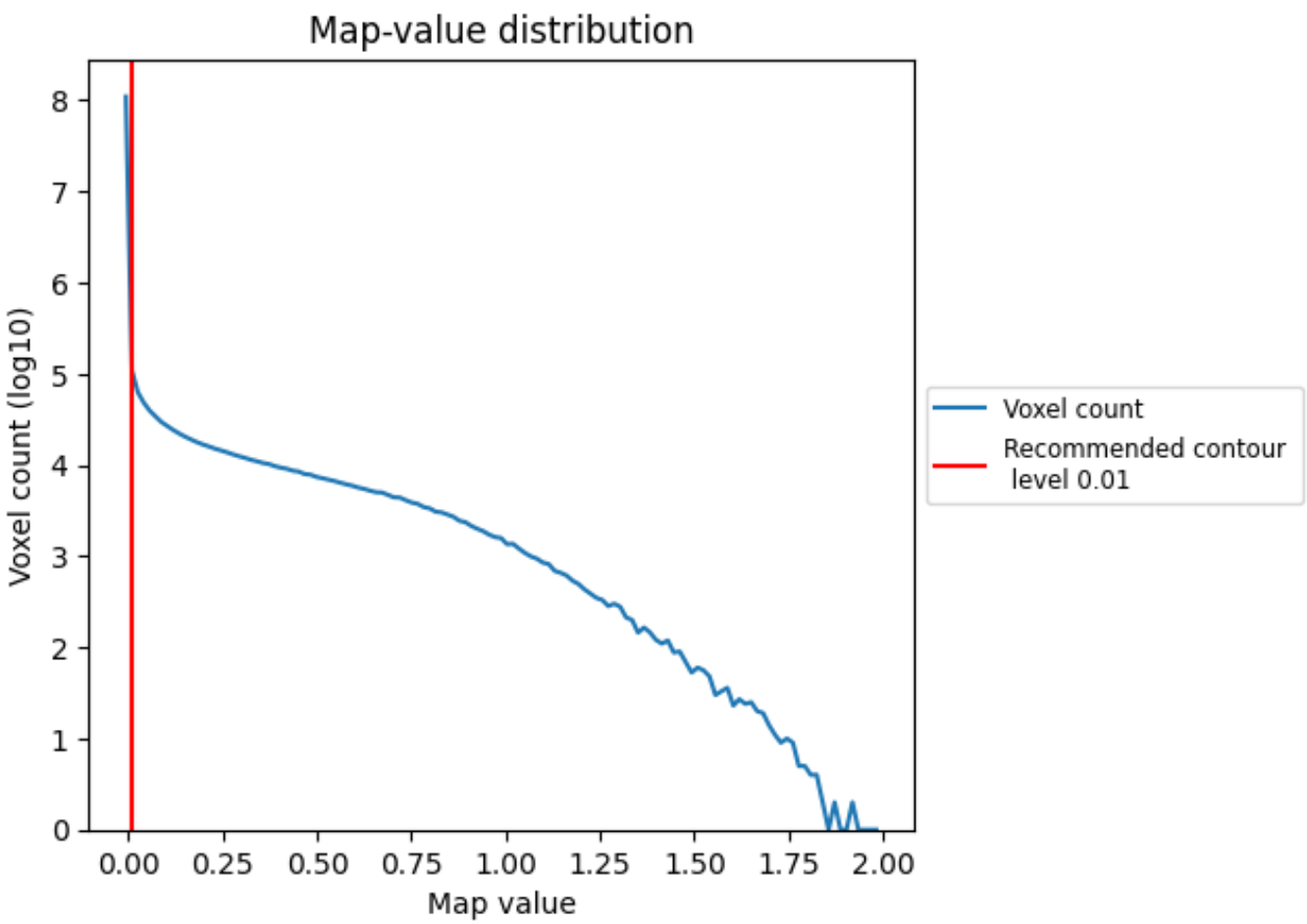
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

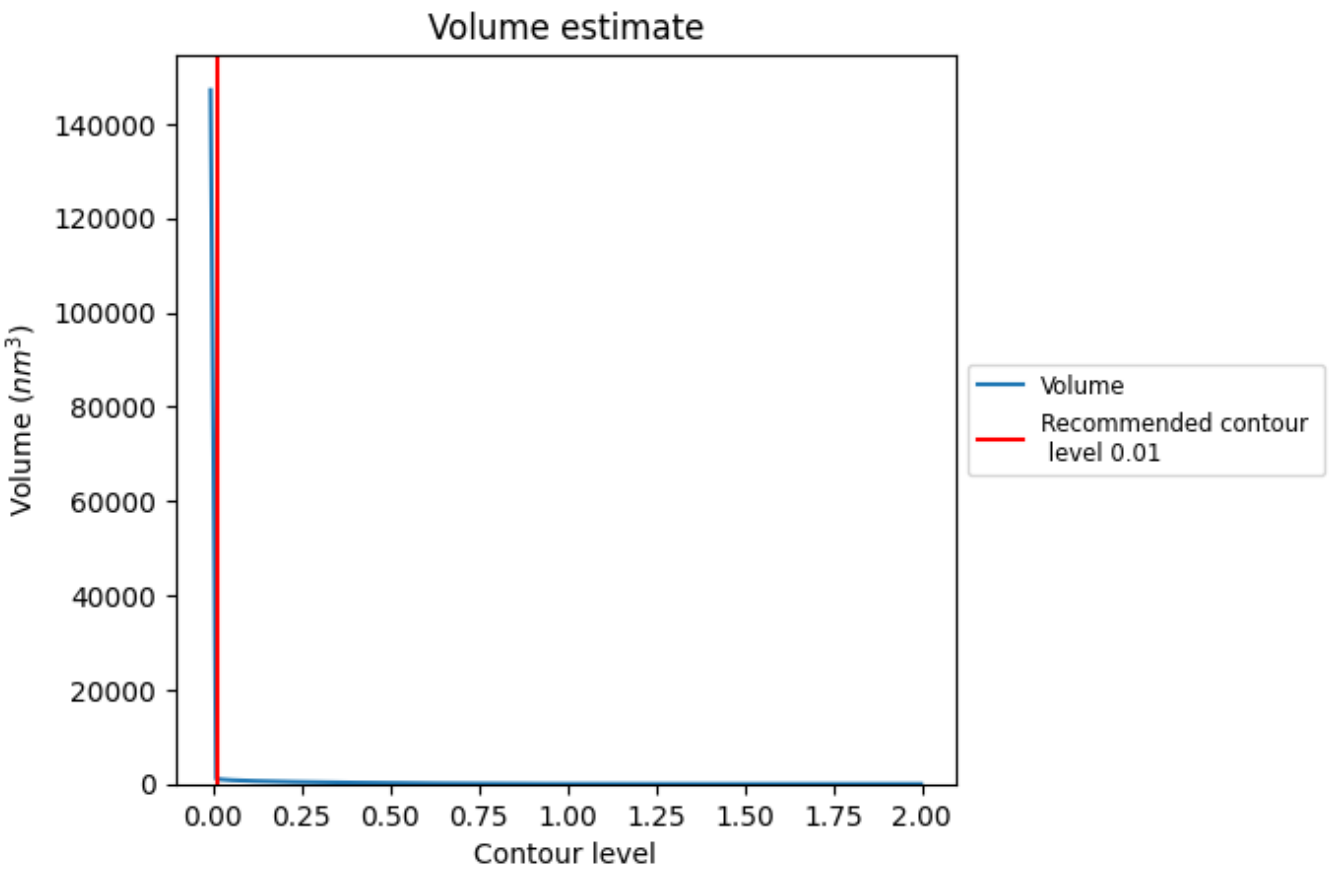
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

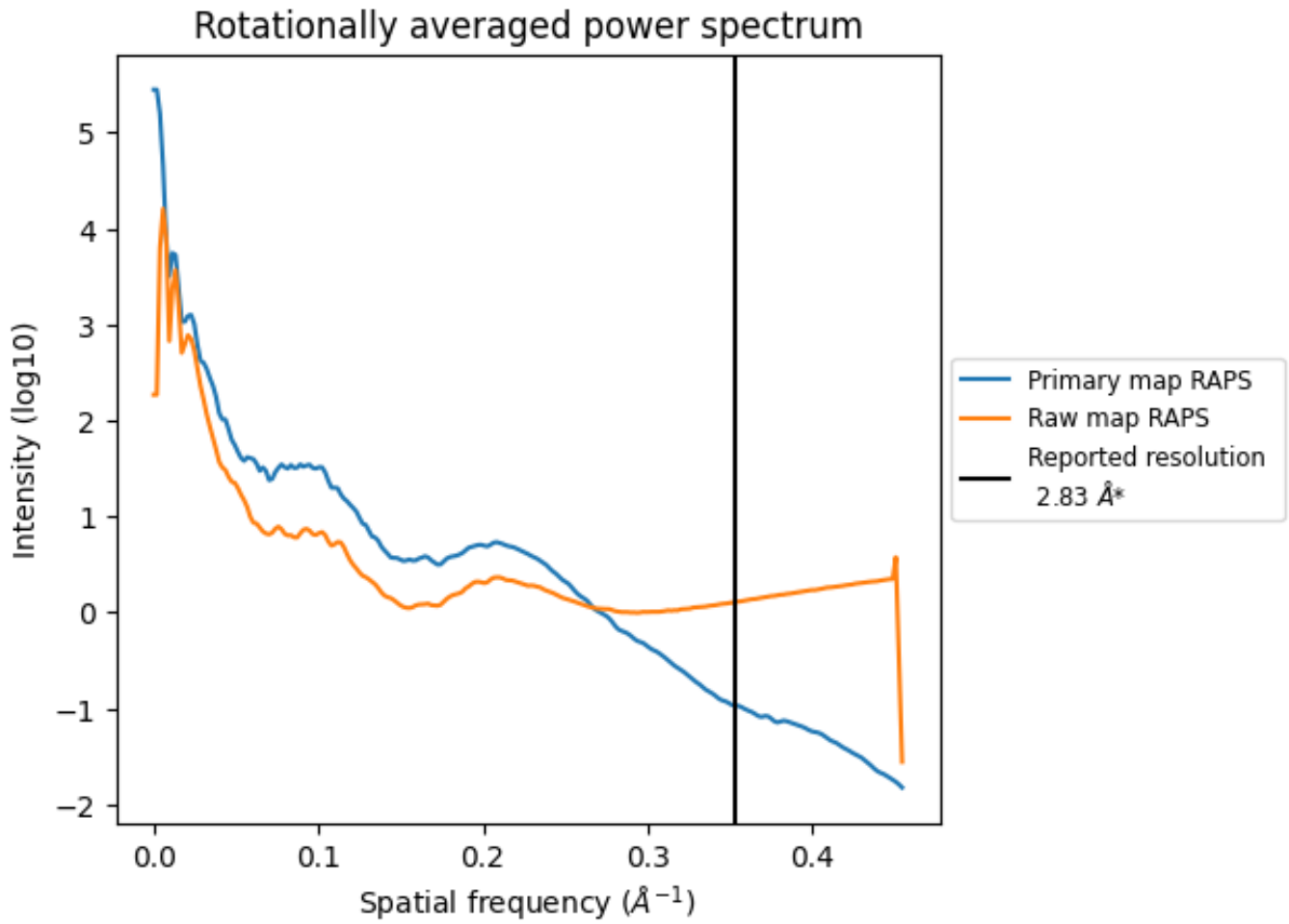
7.2 Volume estimate (i)



The volume at the recommended contour level is 1081 nm^3; this corresponds to an approximate mass of 976 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

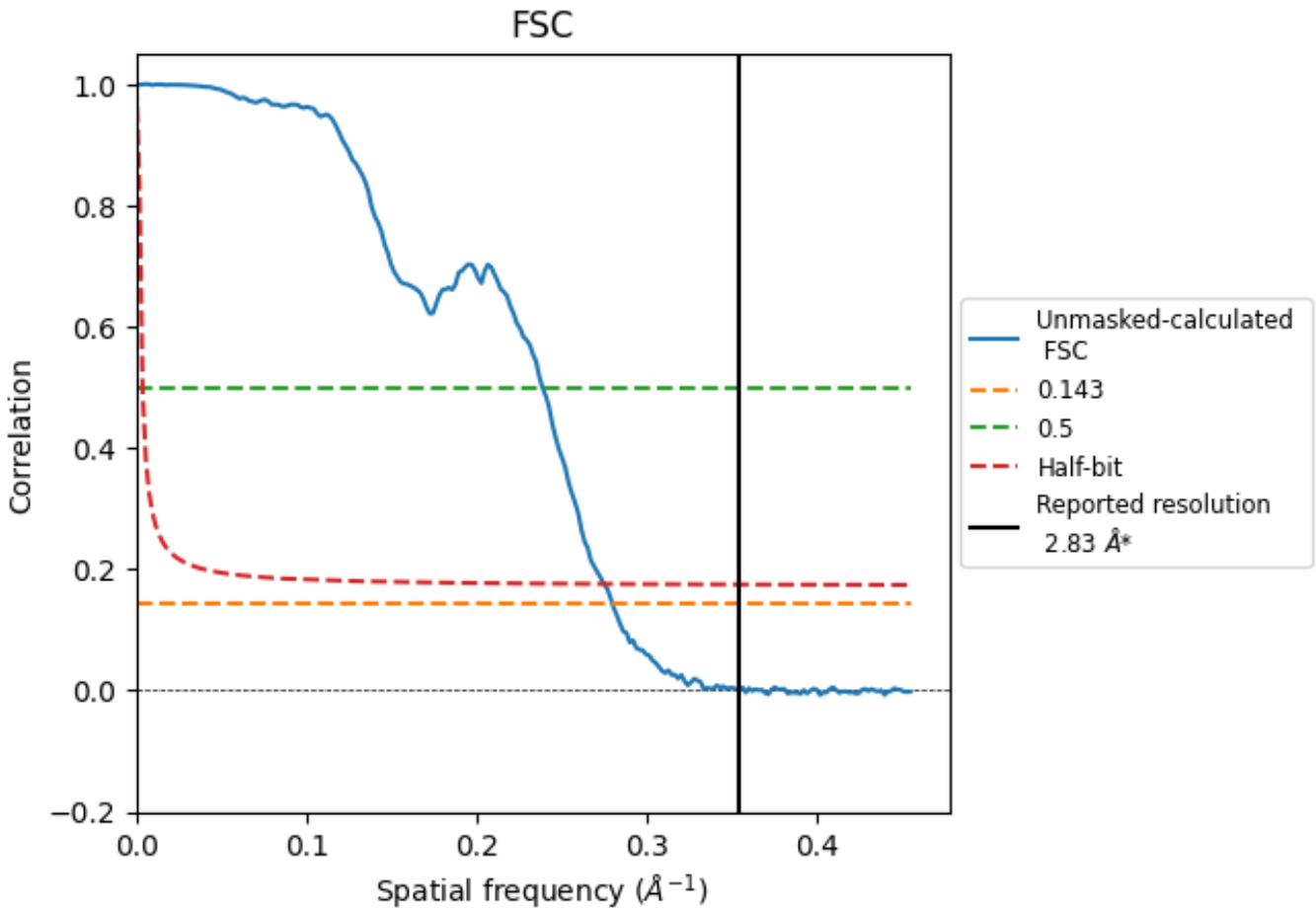


*Reported resolution corresponds to spatial frequency of 0.353 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.353 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	4.19	3.64

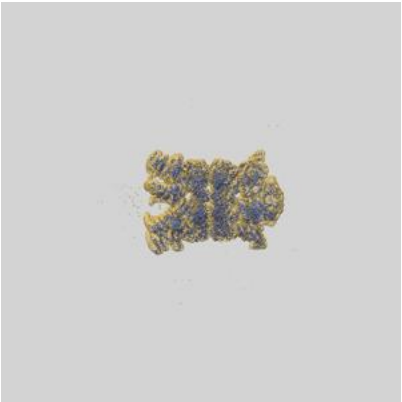
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.58 differs from the reported value 2.83 by more than 10 %

9 Map-model fit (i)

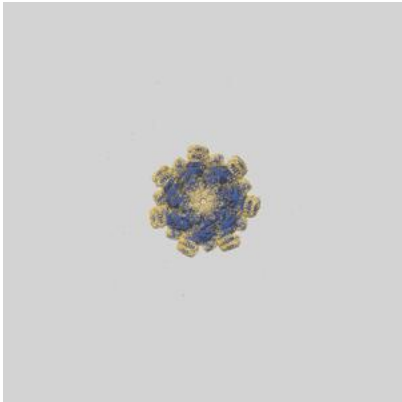
This section contains information regarding the fit between EMDB map EMD-65992 and PDB model 9WIF. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay (i)

X



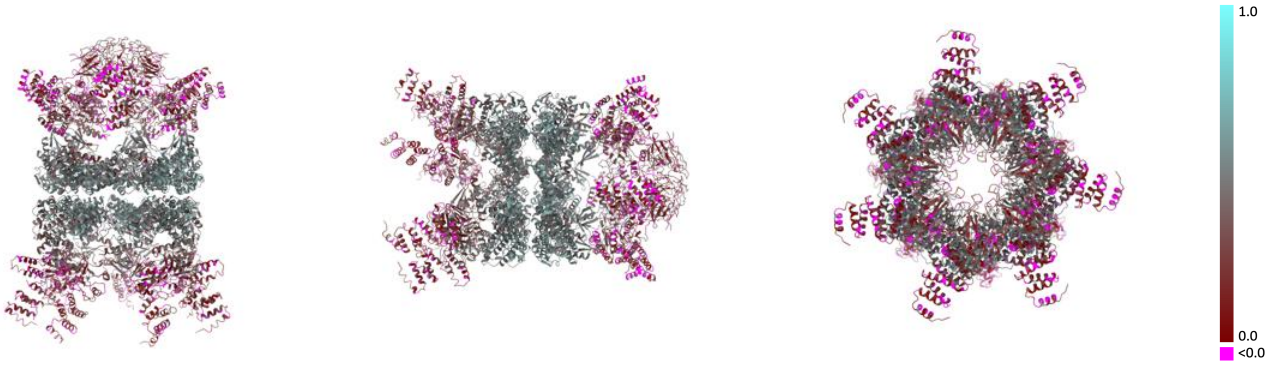
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

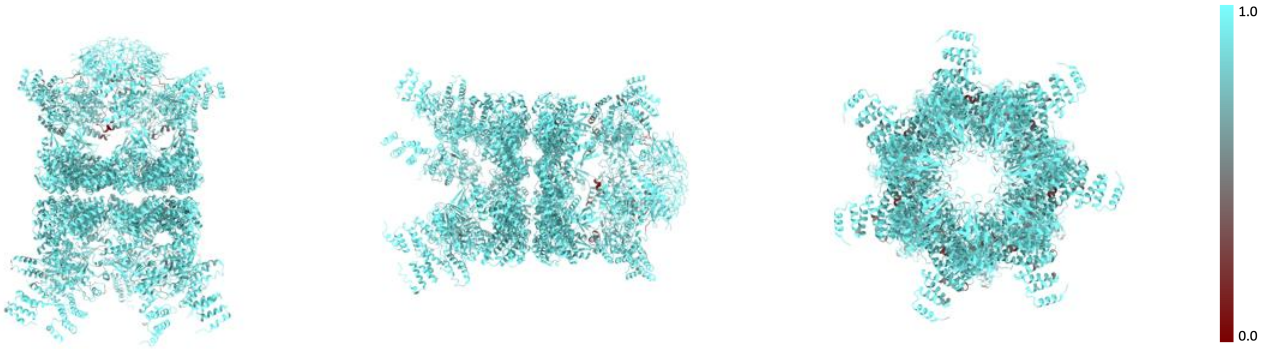
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

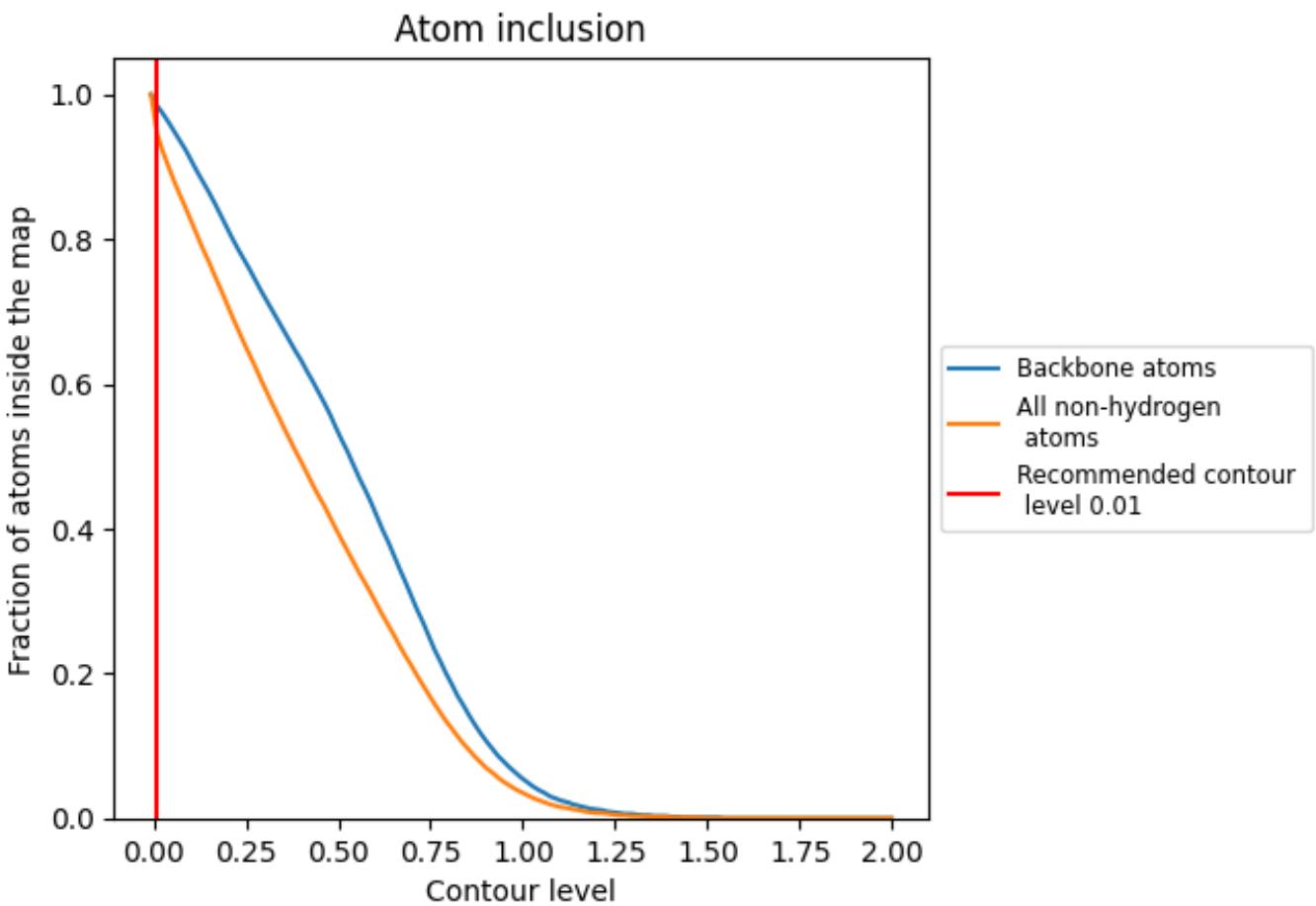
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9450	0.3310
0	0.9390	0.2060
1	0.9370	0.2030
2	0.9440	0.2090
3	0.9260	0.1960
4	0.9230	0.1940
5	0.9320	0.1980
6	0.9320	0.2090
A	0.9510	0.4120
B	0.9050	0.1190
C	0.9550	0.4190
D	0.9130	0.1070
E	0.9440	0.3770
F	0.8890	0.1010
G	0.9530	0.4010
H	0.8770	0.1120
I	0.9460	0.3790
J	0.8860	0.1120
K	0.9460	0.4070
L	0.8790	0.1080
M	0.9410	0.3630
N	0.8760	0.1100
a	0.9580	0.3700
b	0.9630	0.1550
c	0.9560	0.3600
d	0.9630	0.1440
e	0.9570	0.3660
f	0.9590	0.1400
g	0.9590	0.3930
h	0.9330	0.1270
i	0.9580	0.3900
j	0.9290	0.1280
k	0.9300	0.2870
l	0.9390	0.1480
m	0.9570	0.3900
n	0.9470	0.1560