Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 02:37 pm GMT

PDB ID	:	2C9G
EMDB ID	:	EMD-1178
Title	:	THE QUASI-ATOMIC MODEL OF THE ADENOVIRUS TYPE 3 PENTON BASE DODECAHEDRON
Authors	:	Fuschiotti, P.; Schoehn, G.; Fender, P.; Fabry, C.M.S.; Hewat, E.A.; Chroboczek, J.; Ruigrok, R.W.H.; Conway, J.F.
Deposited on	:	2005-12-12
Resolution	:	9.30 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:

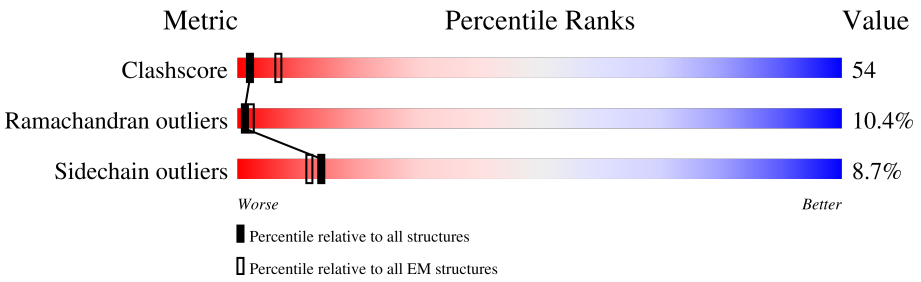
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 9.30 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	523	17% 30% 44% 11% • 14%
1	B	523	18% 29% 45% 11% • 14%
1	C	523	18% 30% 45% 11% • 14%
1	D	523	17% 29% 45% 11% • 14%
1	E	523	18% 29% 46% 11% • 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 17840 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 PENTON PROTEIN.

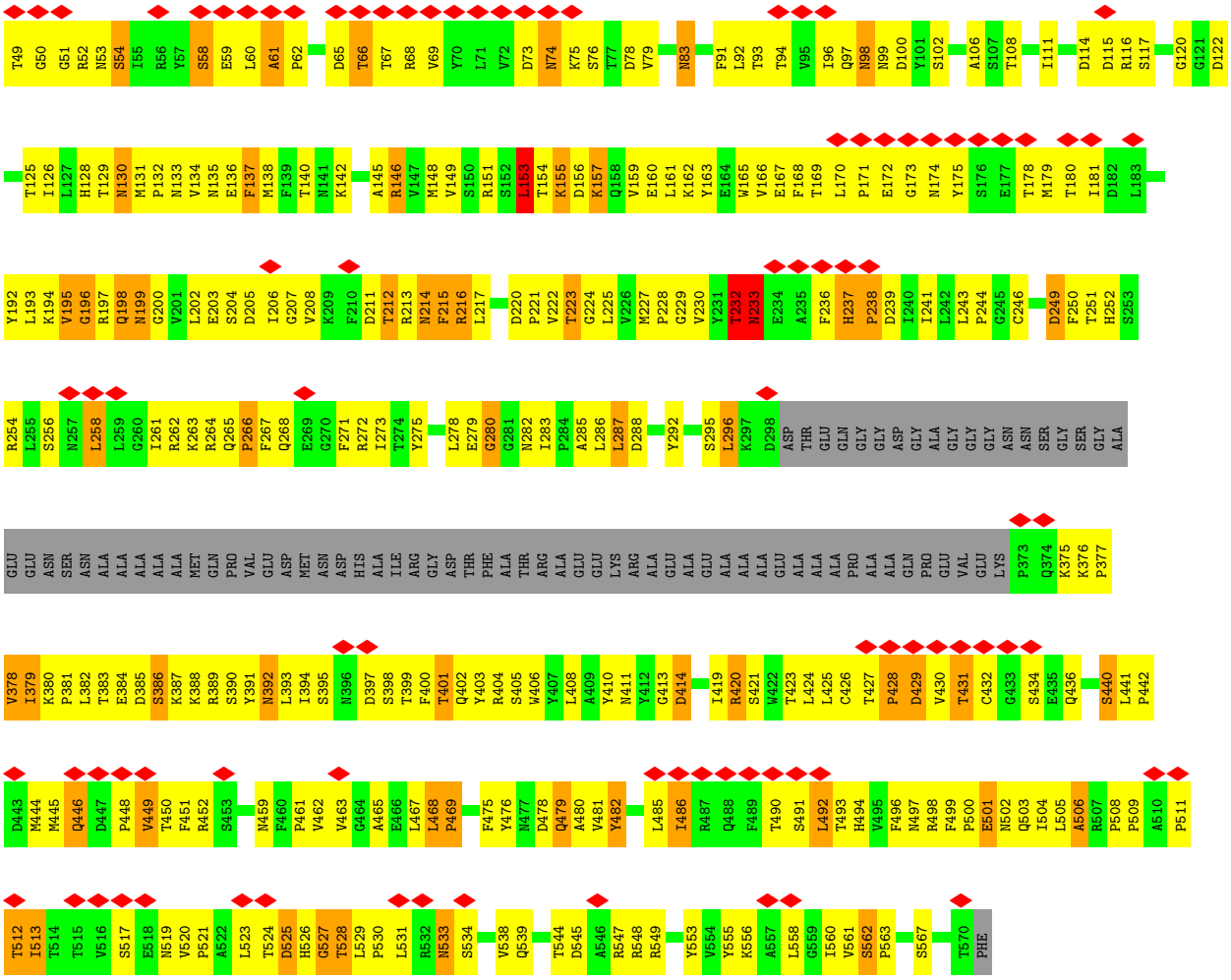
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	448	3568	2255	618	683	12	0	1
1	B	448	3568	2255	618	683	12	0	1
1	C	448	3568	2255	618	683	12	0	1
1	D	448	3568	2255	618	683	12	0	1
1	E	448	3568	2255	618	683	12	0	1

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.

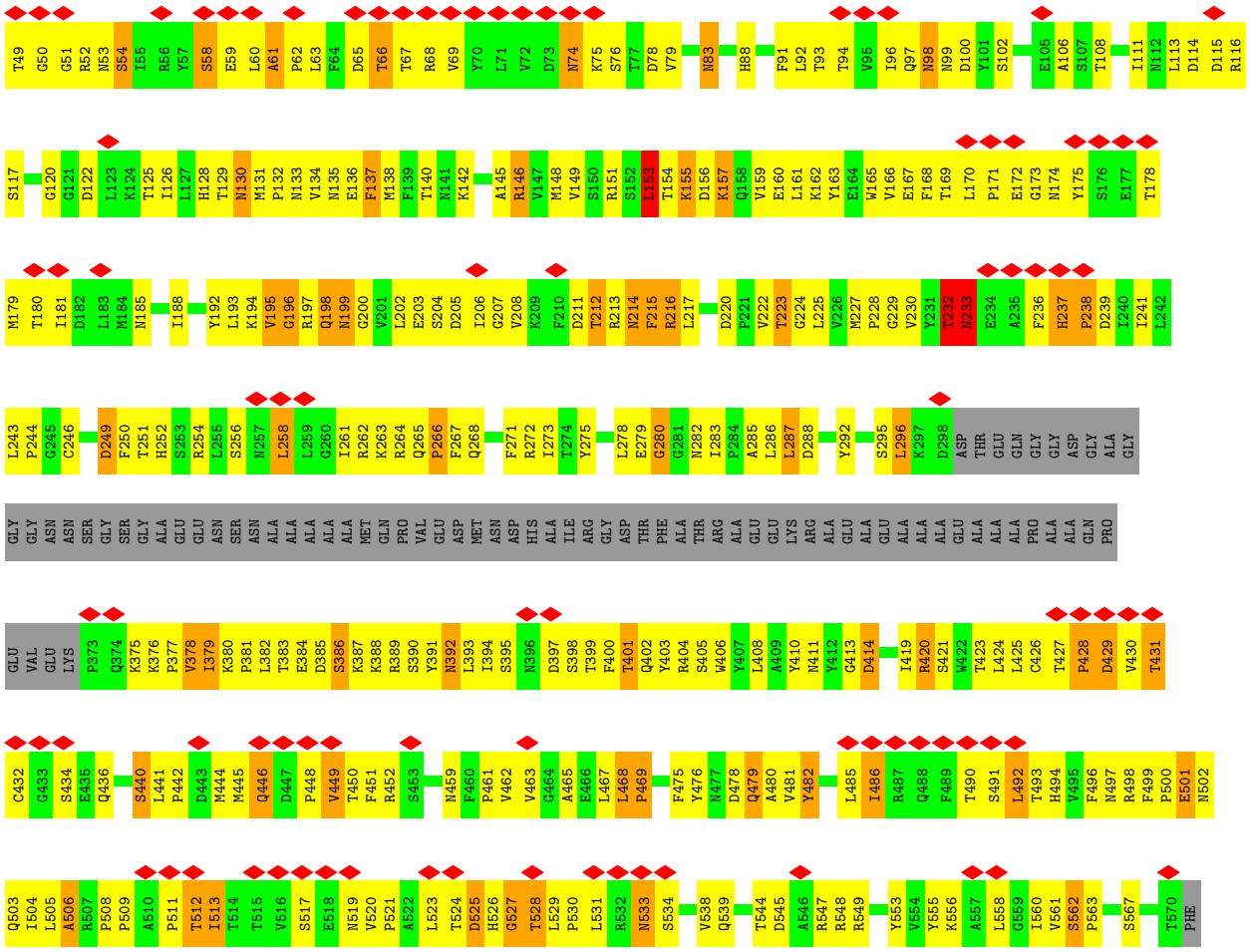
• Molecule 1: PENTON PROTEIN

Chain A: 17% 30% 44% 11% • 14%



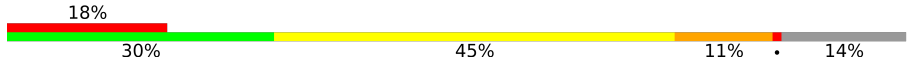
• Molecule 1: PENTON PROTEIN

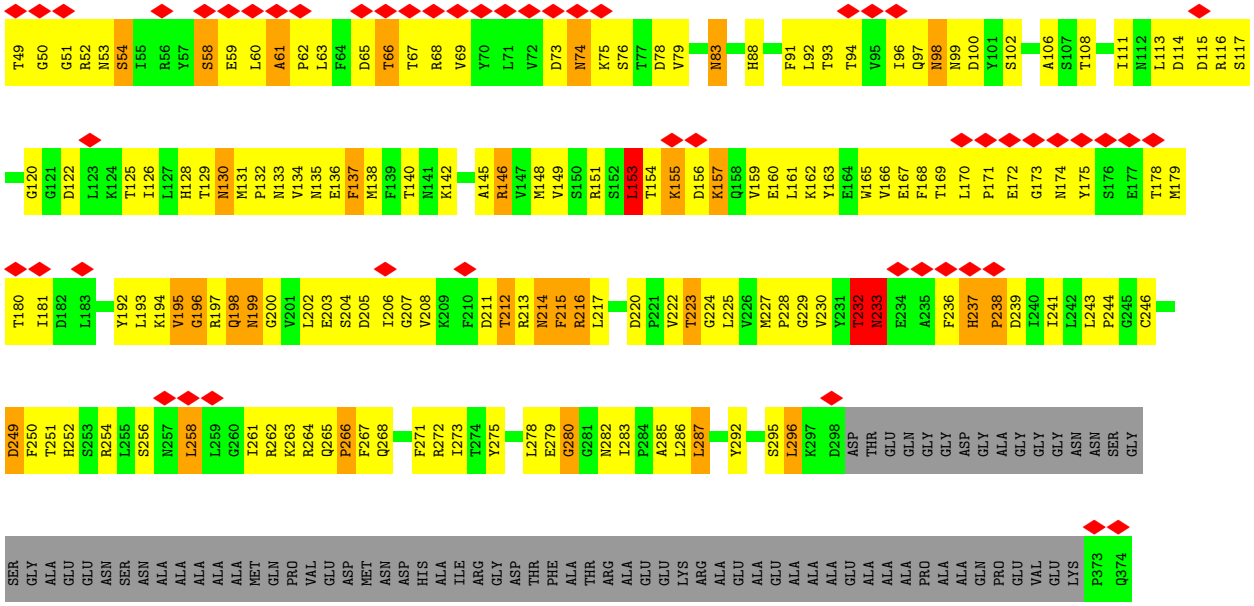
Chain B: 18% 29% 45% 11% • 14%

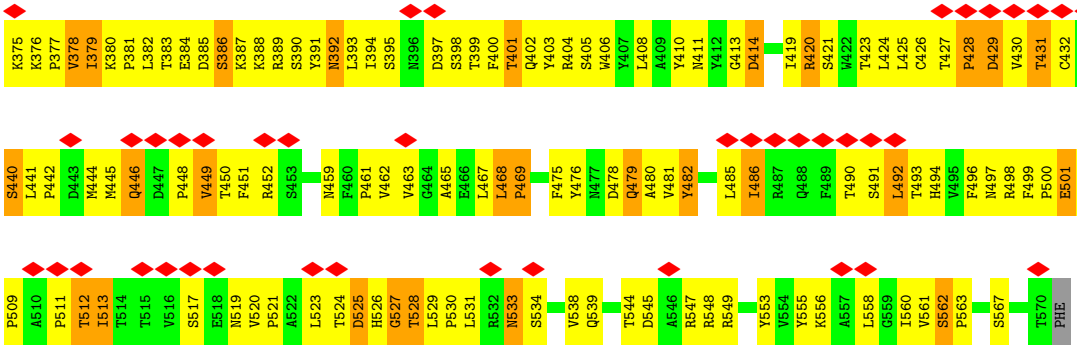


• Molecule 1: PENTON PROTEIN

Chain C:

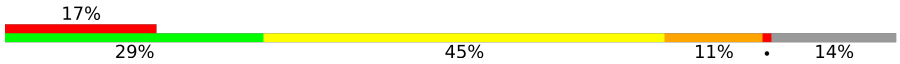


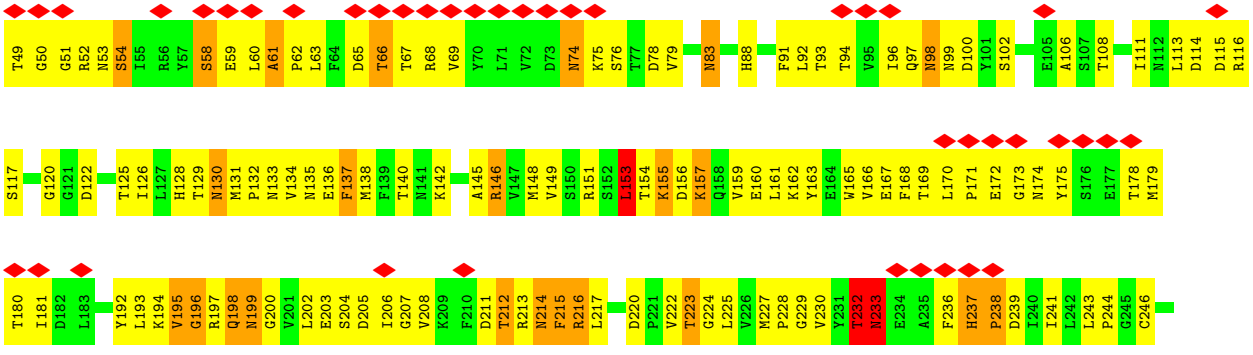




- Molecule 1: PENTON PROTEIN

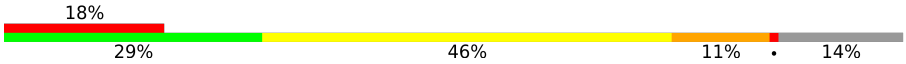
Chain D:

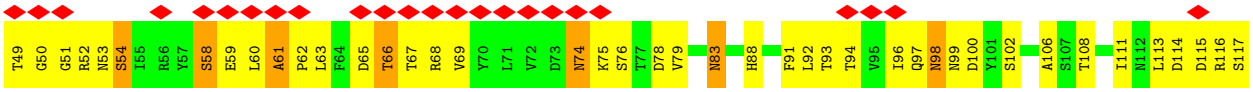


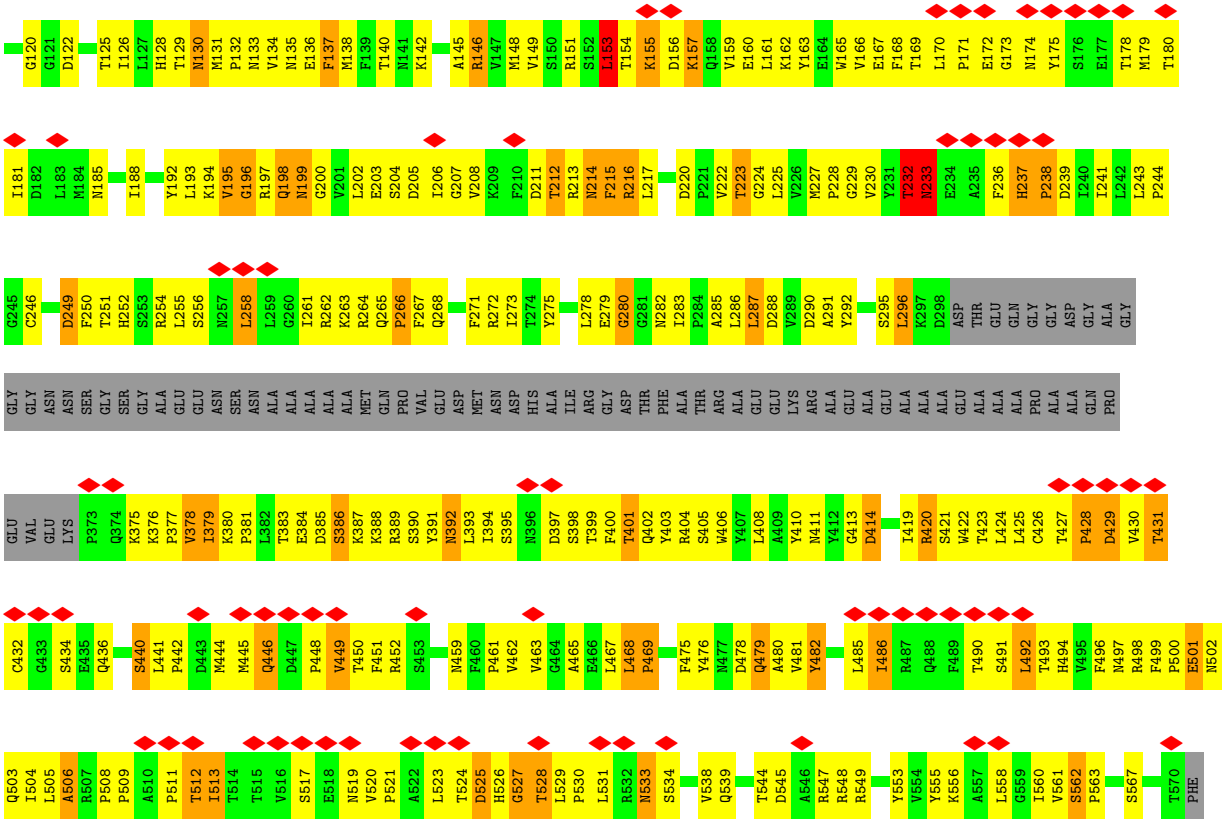


- Molecule 1: PENTON PROTEIN

Chain E:






G120 G121 D122 T125 I126 L127 H128 T129 N130 M131 P132 N133 V134 N135 E136 F137 M138 F139 T140 N141 K142 A145 R146 V147 M148 V149 S150 R151 S152 L153 T154 K155 D156 K157 Q158 V159 E160 L161 K162 Y163 E164 W165 V166 E167 F168 T169 L170 P171 E172 G173 N174 Y175 S176 E177 T178 M179 T180
I181 D182 L183 M184 N185 T188 Y192 L193 K194 V195 G196 R197 Q198 N199 G200 W201 L202 E203 S204 D205 I206 G207 V208 K209 F210 D211 T212 R213 N214 F215 R216 L217 D220 P221 V222 T223 G224 L225 V226 M227 P228 G229 V230 Y231 T232 N233 E234 A235 F236 H237 P238 D239 I240 I241 L242 L243 P244
G245 C246 D249 F250 T251 H252 S253 R254 L255 S256 N257 L258 L259 G260 I261 R262 K263 R264 Q265 P266 F267 Q268 F271 R272 I273 T274 Y275 L278 E279 G280 G281 N282 I283 P284 A285 L286 L287 D288 V289 D290 A291 Y292 S295 L296 K297 D298 ASP THR GLU GLN GLY GLY ASP GLY ALA GLY
GLY GLY ASN ASN SER GLY SER GLY ALA GLU GLU ASN SER ASN ALA ALA ALA ALA ALA MET GLN PRO VAL GLU ASP MET ASN ASP HIS ALA ILE ARG GLY ASP THR PHE ALA THR ARG ALA GLU GLU LYS ARG ALA GLU ALA GLU ALA ALA ALA GLU ALA ALA ALA PRO ALA ALA GLN PRO
GLU VAL GLU LYS P373 Q374 K375 K376 P377 V378 I379 K380 P381 L382 T383 E384 D385 S386 K387 K388 R389 S390 Y391 N392 L393 I394 S395 N396 D397 S398 T399 F400 T401 Q402 Y403 R404 S405 W406 Y407 L408 A409 Y410 N411 Y412 G413 D414 I419 R420 S421 W422 T423 L424 L425 C426 T427 P428 D429 V430 T431
C432 G433 S434 E435 Q436 S440 L441 P442 D443 M444 M445 Q446 D447 P448 V449 T450 F451 R452 S453 N459 F460 P461 V462 V463 G464 A465 E466 L467 L468 P469 F475 Y476 N477 D478 Q479 A480 V481 Y482 L485 I486 R487 Q488 F489 T490 S491 L492 T493 H494 V495 F496 N497 R498 F499 P500 E501 N502
Q503 I504 L505 A506 R507 P508 P509 A510 P511 T512 I513 T514 T515 V516 S517 E518 N519 V520 P521 A522 L523 T524 D525 H526 G527 T528 L529 P530 L531 R532 N533 S534 V538 Q539 T544 D545 A546 R547 R548 R549 Y553 Y554 Y555 K556 A557 L558 G559 I560 V561 S562 P563 S567 T570 PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1849	Depositor
Resolution determination method	Not provided	
CTF correction method	AMPLITUDE, PHASE	Depositor
Microscope	JEOL 2010F	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	51020	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	509.000	Depositor
Minimum map value	-335.000	Depositor
Average map value	3.055	Depositor
Map value standard deviation	52.415	Depositor
Recommended contour level	91.9	Depositor
Map size (Å)	382.23, 382.23, 382.23	wwPDB
Map dimensions	279, 279, 279	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.57	0/3652	0.81	2/4971 (0.0%)
1	B	0.57	0/3652	0.81	2/4971 (0.0%)
1	C	0.57	0/3652	0.81	2/4971 (0.0%)
1	D	0.57	0/3652	0.81	2/4971 (0.0%)
1	E	0.57	0/3652	0.81	2/4971 (0.0%)
All	All	0.57	0/18260	0.81	10/24855 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	207	GLY	N-CA-C	5.62	127.14	113.10
1	D	207	GLY	N-CA-C	5.60	127.10	113.10
1	A	207	GLY	N-CA-C	5.58	127.06	113.10
1	C	207	GLY	N-CA-C	5.58	127.06	113.10
1	B	207	GLY	N-CA-C	5.58	127.06	113.10
1	C	153	LEU	CB-CG-CD2	5.37	120.13	111.00
1	D	153	LEU	CB-CG-CD2	5.36	120.12	111.00
1	A	153	LEU	CB-CG-CD2	5.36	120.11	111.00
1	B	153	LEU	CB-CG-CD2	5.33	120.06	111.00
1	E	153	LEU	CB-CG-CD2	5.33	120.05	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3568	0	3498	414	0
1	B	3568	0	3498	421	0
1	C	3568	0	3498	421	0
1	D	3568	0	3498	424	0
1	E	3568	0	3498	422	0
All	All	17840	0	17490	1895	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 54.

All (1895) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ARG:HH21	1:C:99:ASN:HB3	1.14	1.13
1:C:452:ARG:HH21	1:D:99:ASN:HB3	1.14	1.11
1:D:452:ARG:HH21	1:E:99:ASN:HB3	1.14	1.10
1:A:99:ASN:HB3	1:E:452:ARG:HH21	1.14	1.07
1:A:452:ARG:HH21	1:B:99:ASN:HB3	1.14	1.06
1:D:68:ARG:HG2	1:D:68:ARG:HH11	1.25	1.02
1:A:68:ARG:HG2	1:A:68:ARG:HH11	1.25	1.01
1:E:68:ARG:HH11	1:E:68:ARG:HG2	1.25	0.99
1:B:68:ARG:HG2	1:B:68:ARG:HH11	1.25	0.98
1:C:68:ARG:HG2	1:C:68:ARG:HH11	1.25	0.97
1:C:452:ARG:NH2	1:D:99:ASN:HB3	1.86	0.91
1:B:278:LEU:HD23	1:B:419:ILE:HD12	1.53	0.91
1:A:99:ASN:HB3	1:E:452:ARG:NH2	1.86	0.91
1:A:278:LEU:HD23	1:A:419:ILE:HD12	1.53	0.91
1:B:292:TYR:HA	1:B:377:PRO:CG	2.01	0.90
1:C:292:TYR:HA	1:C:377:PRO:CG	2.01	0.90
1:A:452:ARG:NH2	1:B:99:ASN:HB3	1.86	0.90
1:E:278:LEU:HD23	1:E:419:ILE:HD12	1.53	0.90
1:D:292:TYR:HA	1:D:377:PRO:CG	2.02	0.90
1:E:292:TYR:HA	1:E:377:PRO:CG	2.01	0.90
1:B:452:ARG:NH2	1:C:99:ASN:HB3	1.86	0.90
1:B:295:SER:HB3	1:B:377:PRO:HG3	1.51	0.90
1:C:376:LYS:HB3	1:C:377:PRO:HD2	1.55	0.89
1:D:451:PHE:HD2	1:D:461:PRO:HA	1.38	0.89
1:B:68:ARG:HH12	1:B:562:SER:HB3	1.38	0.89
1:C:295:SER:HB3	1:C:377:PRO:HG3	1.51	0.89
1:D:452:ARG:NH2	1:E:99:ASN:HB3	1.86	0.89
1:B:376:LYS:HB3	1:B:377:PRO:HD2	1.55	0.89
1:D:68:ARG:HH12	1:D:562:SER:HB3	1.38	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:SER:HB3	1:D:377:PRO:HG3	1.51	0.89
1:D:376:LYS:HB3	1:D:377:PRO:HD2	1.54	0.89
1:C:451:PHE:HD2	1:C:461:PRO:HA	1.38	0.89
1:D:278:LEU:HD23	1:D:419:ILE:HD12	1.53	0.89
1:A:295:SER:HB3	1:A:377:PRO:HG3	1.51	0.89
1:E:295:SER:HB3	1:E:377:PRO:HG3	1.50	0.88
1:A:451:PHE:HD2	1:A:461:PRO:HA	1.38	0.88
1:C:278:LEU:HD23	1:C:419:ILE:HD12	1.53	0.88
1:A:292:TYR:HA	1:A:377:PRO:CG	2.02	0.88
1:A:68:ARG:HH12	1:A:562:SER:HB3	1.38	0.88
1:E:376:LYS:HB3	1:E:377:PRO:HD2	1.55	0.88
1:E:451:PHE:HD2	1:E:461:PRO:HA	1.38	0.88
1:A:376:LYS:HB3	1:A:377:PRO:HD2	1.54	0.87
1:C:68:ARG:HH12	1:C:562:SER:HB3	1.38	0.87
1:E:68:ARG:HH12	1:E:562:SER:HB3	1.38	0.87
1:B:211:ASP:HA	1:B:508:PRO:CG	2.05	0.87
1:B:262:ARG:NH1	1:C:130:ASN:HD22	1.73	0.87
1:A:52:ARG:HB3	1:A:117:SER:OG	1.75	0.86
1:A:130:ASN:HD22	1:E:262:ARG:NH1	1.73	0.86
1:D:83:ASN:HD22	1:D:91:PHE:HB2	1.40	0.86
1:D:504:ILE:HG22	1:D:505:LEU:HD23	1.57	0.86
1:E:52:ARG:HB3	1:E:117:SER:OG	1.75	0.86
1:B:504:ILE:HG22	1:B:505:LEU:HD23	1.57	0.86
1:C:211:ASP:HA	1:C:508:PRO:CG	2.05	0.86
1:E:211:ASP:HA	1:E:508:PRO:CG	2.05	0.86
1:E:504:ILE:HG22	1:E:505:LEU:HD23	1.57	0.86
1:D:262:ARG:NH1	1:E:130:ASN:HD22	1.73	0.86
1:B:451:PHE:HD2	1:B:461:PRO:HA	1.38	0.85
1:A:83:ASN:HD22	1:A:91:PHE:HB2	1.40	0.85
1:A:211:ASP:HA	1:A:508:PRO:CG	2.05	0.85
1:A:262:ARG:NH1	1:B:130:ASN:HD22	1.74	0.85
1:C:52:ARG:HB3	1:C:117:SER:OG	1.75	0.85
1:D:211:ASP:HA	1:D:508:PRO:CG	2.05	0.85
1:B:193:LEU:HD11	1:B:498:ARG:HH12	1.41	0.85
1:C:58:SER:O	1:C:60:LEU:N	2.09	0.85
1:B:52:ARG:HB3	1:B:117:SER:OG	1.75	0.85
1:C:262:ARG:NH1	1:D:130:ASN:HD22	1.73	0.85
1:B:58:SER:O	1:B:60:LEU:N	2.09	0.85
1:B:83:ASN:HD22	1:B:91:PHE:HB2	1.40	0.85
1:C:504:ILE:HG22	1:C:505:LEU:HD23	1.57	0.85
1:E:83:ASN:HD22	1:E:91:PHE:HB2	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ILE:HG22	1:A:505:LEU:HD23	1.58	0.84
1:C:83:ASN:HD22	1:C:91:PHE:HB2	1.40	0.84
1:D:52:ARG:HB3	1:D:117:SER:OG	1.75	0.84
1:E:58:SER:O	1:E:60:LEU:N	2.09	0.84
1:D:178:THR:HG21	1:D:511:PRO:HD2	1.60	0.84
1:D:58:SER:O	1:D:60:LEU:N	2.09	0.84
1:E:156:ASP:O	1:E:157:LYS:HG3	1.78	0.84
1:D:193:LEU:HD11	1:D:498:ARG:HH12	1.41	0.84
1:C:178:THR:HG21	1:C:511:PRO:HD2	1.60	0.84
1:A:58:SER:O	1:A:60:LEU:N	2.09	0.84
1:A:193:LEU:HD11	1:A:498:ARG:HH12	1.41	0.83
1:C:193:LEU:HD11	1:C:498:ARG:HH12	1.41	0.83
1:A:156:ASP:O	1:A:157:LYS:HG3	1.78	0.83
1:C:156:ASP:O	1:C:157:LYS:HG3	1.78	0.83
1:D:468:LEU:HD12	1:D:469:PRO:HD2	1.59	0.83
1:C:49:THR:HG23	1:C:53:ASN:OD1	1.79	0.83
1:B:178:THR:HG21	1:B:511:PRO:HD2	1.59	0.83
1:D:156:ASP:O	1:D:157:LYS:HG3	1.78	0.83
1:E:193:LEU:HD11	1:E:498:ARG:HH12	1.41	0.83
1:E:49:THR:HG23	1:E:53:ASN:OD1	1.79	0.83
1:E:178:THR:HG21	1:E:511:PRO:HD2	1.60	0.82
1:B:156:ASP:O	1:B:157:LYS:HG3	1.78	0.82
1:E:468:LEU:HD12	1:E:469:PRO:HD2	1.59	0.82
1:D:49:THR:HG23	1:D:53:ASN:OD1	1.79	0.82
1:B:49:THR:HG23	1:B:53:ASN:OD1	1.79	0.82
1:A:49:THR:HG23	1:A:53:ASN:OD1	1.79	0.82
1:C:468:LEU:HD12	1:C:469:PRO:HD2	1.60	0.82
1:D:544:THR:CG2	1:D:548:ARG:HA	2.10	0.82
1:B:468:LEU:HD12	1:B:469:PRO:HD2	1.60	0.82
1:A:178:THR:HG21	1:A:511:PRO:HD2	1.60	0.81
1:A:384:GLU:HG2	1:A:390:SER:HA	1.62	0.81
1:A:468:LEU:HD12	1:A:469:PRO:HD2	1.59	0.81
1:B:544:THR:CG2	1:B:548:ARG:HA	2.10	0.81
1:C:544:THR:CG2	1:C:548:ARG:HA	2.10	0.81
1:C:68:ARG:HG2	1:C:68:ARG:NH1	1.92	0.81
1:A:544:THR:CG2	1:A:548:ARG:HA	2.10	0.81
1:B:384:GLU:HG2	1:B:390:SER:HA	1.62	0.80
1:E:544:THR:CG2	1:E:548:ARG:HA	2.10	0.80
1:C:384:GLU:HG2	1:C:390:SER:HA	1.62	0.80
1:B:68:ARG:HG2	1:B:68:ARG:NH1	1.92	0.80
1:E:384:GLU:HG2	1:E:390:SER:HA	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:HIS:CD2	1:C:425:LEU:HD11	2.18	0.79
1:D:389:ARG:HD3	1:D:502:ASN:HD22	1.47	0.79
1:A:68:ARG:HG2	1:A:68:ARG:NH1	1.92	0.79
1:D:214:ASN:C	1:D:214:ASN:HD22	1.86	0.79
1:D:237:HIS:CD2	1:D:425:LEU:HD11	2.18	0.79
1:E:237:HIS:CD2	1:E:425:LEU:HD11	2.18	0.79
1:B:237:HIS:CD2	1:B:425:LEU:HD11	2.17	0.79
1:D:384:GLU:HG2	1:D:390:SER:HA	1.62	0.79
1:A:214:ASN:C	1:A:214:ASN:HD22	1.86	0.79
1:A:237:HIS:CD2	1:A:425:LEU:HD11	2.18	0.78
1:E:214:ASN:C	1:E:214:ASN:HD22	1.86	0.78
1:B:214:ASN:C	1:B:214:ASN:HD22	1.86	0.78
1:B:389:ARG:HD3	1:B:502:ASN:HD22	1.47	0.78
1:A:154:THR:OG1	1:A:160:GLU:HB2	1.84	0.77
1:E:154:THR:OG1	1:E:160:GLU:HB2	1.84	0.77
1:B:154:THR:OG1	1:B:160:GLU:HB2	1.84	0.77
1:C:214:ASN:HD22	1:C:214:ASN:C	1.86	0.77
1:C:379:ILE:O	1:C:381:PRO:HD3	1.85	0.77
1:E:389:ARG:HD3	1:E:502:ASN:HD22	1.47	0.77
1:A:379:ILE:O	1:A:381:PRO:HD3	1.85	0.77
1:D:154:THR:OG1	1:D:160:GLU:HB2	1.84	0.77
1:A:389:ARG:HD3	1:A:502:ASN:HD22	1.48	0.77
1:C:389:ARG:HD3	1:C:502:ASN:HD22	1.47	0.77
1:B:211:ASP:HA	1:B:508:PRO:HG3	1.67	0.77
1:C:154:THR:OG1	1:C:160:GLU:HB2	1.84	0.77
1:C:211:ASP:HA	1:C:508:PRO:HG3	1.67	0.77
1:A:403:TYR:CE1	1:A:504:ILE:HG21	2.21	0.76
1:C:403:TYR:CE1	1:C:504:ILE:HG21	2.21	0.76
1:D:292:TYR:HA	1:D:377:PRO:HG2	1.67	0.76
1:D:403:TYR:CE1	1:D:504:ILE:HG21	2.21	0.76
1:E:379:ILE:O	1:E:381:PRO:HD3	1.85	0.76
1:A:211:ASP:HA	1:A:508:PRO:HG3	1.67	0.76
1:B:403:TYR:CE1	1:B:504:ILE:HG21	2.21	0.76
1:B:379:ILE:O	1:B:381:PRO:HD3	1.85	0.76
1:C:292:TYR:HA	1:C:377:PRO:HG2	1.67	0.76
1:E:292:TYR:HA	1:E:377:PRO:HG2	1.67	0.76
1:C:475:PHE:O	1:C:513:ILE:HA	1.87	0.76
1:B:292:TYR:HA	1:B:377:PRO:HG2	1.67	0.75
1:D:379:ILE:O	1:D:381:PRO:HD3	1.85	0.75
1:E:403:TYR:CE1	1:E:504:ILE:HG21	2.21	0.75
1:C:68:ARG:NH1	1:C:562:SER:HB3	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:PHE:O	1:B:513:ILE:HA	1.87	0.75
1:D:452:ARG:HE	1:E:98:ASN:HD21	1.34	0.75
1:B:451:PHE:CD2	1:B:461:PRO:HA	2.22	0.75
1:D:211:ASP:HA	1:D:508:PRO:HG3	1.67	0.75
1:E:475:PHE:O	1:E:513:ILE:HA	1.87	0.75
1:A:68:ARG:NH1	1:A:562:SER:HB3	2.01	0.75
1:E:211:ASP:HA	1:E:508:PRO:HG3	1.67	0.75
1:D:68:ARG:NH1	1:D:562:SER:HB3	2.01	0.74
1:D:451:PHE:CD2	1:D:461:PRO:HA	2.22	0.74
1:E:68:ARG:NH1	1:E:562:SER:HB3	2.01	0.74
1:A:292:TYR:HA	1:A:377:PRO:HG2	1.67	0.74
1:B:68:ARG:NH1	1:B:562:SER:HB3	2.01	0.74
1:B:145:ALA:HB3	1:B:168:PHE:HE1	1.53	0.74
1:C:295:SER:O	1:C:296:LEU:HB2	1.88	0.74
1:C:451:PHE:CD2	1:C:461:PRO:HA	2.22	0.74
1:E:68:ARG:HG2	1:E:68:ARG:NH1	1.92	0.74
1:E:403:TYR:HD1	1:E:504:ILE:HD13	1.52	0.74
1:A:403:TYR:HD1	1:A:504:ILE:HD13	1.52	0.74
1:A:475:PHE:O	1:A:513:ILE:HA	1.87	0.74
1:C:142:LYS:HG2	1:C:169:THR:HG22	1.70	0.74
1:D:475:PHE:O	1:D:513:ILE:HA	1.86	0.74
1:B:295:SER:O	1:B:296:LEU:HB2	1.88	0.74
1:E:295:SER:O	1:E:296:LEU:HB2	1.88	0.74
1:C:145:ALA:HB3	1:C:168:PHE:HE1	1.53	0.74
1:C:249:ASP:C	1:C:249:ASP:OD1	2.26	0.74
1:D:142:LYS:HG2	1:D:169:THR:HG22	1.70	0.74
1:B:452:ARG:HE	1:C:98:ASN:HD21	1.34	0.73
1:B:243:LEU:HD21	1:B:403:TYR:CE2	2.23	0.73
1:D:68:ARG:HG2	1:D:68:ARG:NH1	1.92	0.73
1:D:249:ASP:C	1:D:249:ASP:OD1	2.26	0.73
1:E:451:PHE:CD2	1:E:461:PRO:HA	2.22	0.73
1:A:145:ALA:HB3	1:A:168:PHE:HE1	1.53	0.73
1:B:403:TYR:HD1	1:B:504:ILE:HD13	1.52	0.73
1:D:243:LEU:HD21	1:D:403:TYR:CE2	2.24	0.73
1:A:249:ASP:C	1:A:249:ASP:OD1	2.26	0.73
1:A:452:ARG:HE	1:B:98:ASN:HD21	1.34	0.73
1:C:403:TYR:HD1	1:C:504:ILE:HD13	1.52	0.73
1:C:452:ARG:HE	1:D:98:ASN:HD21	1.34	0.73
1:D:468:LEU:CD1	1:D:469:PRO:HD2	2.19	0.73
1:A:142:LYS:HG2	1:A:169:THR:HG22	1.70	0.73
1:A:295:SER:O	1:A:296:LEU:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:LEU:HD21	1:C:403:TYR:CE2	2.23	0.73
1:A:244:PRO:HA	1:A:275:TYR:CD2	2.24	0.73
1:D:295:SER:O	1:D:296:LEU:HB2	1.88	0.73
1:D:403:TYR:HD1	1:D:504:ILE:HD13	1.52	0.73
1:E:148:MET:HA	1:E:163:TYR:HD2	1.54	0.73
1:A:98:ASN:HD21	1:E:452:ARG:HE	1.34	0.72
1:D:244:PRO:HA	1:D:275:TYR:CD2	2.24	0.72
1:D:544:THR:HG22	1:D:548:ARG:HA	1.71	0.72
1:A:468:LEU:CD1	1:A:469:PRO:HD2	2.19	0.72
1:B:249:ASP:C	1:B:249:ASP:OD1	2.27	0.72
1:E:145:ALA:HB3	1:E:168:PHE:HE1	1.53	0.72
1:A:197:ARG:HG3	1:A:198:GLN:N	2.05	0.72
1:A:243:LEU:HD21	1:A:403:TYR:CE2	2.23	0.72
1:B:142:LYS:HG2	1:B:169:THR:HG22	1.70	0.72
1:B:148:MET:HA	1:B:163:TYR:HD2	1.54	0.72
1:B:544:THR:HG22	1:B:548:ARG:HA	1.71	0.72
1:D:145:ALA:HB3	1:D:168:PHE:HE1	1.53	0.72
1:E:142:LYS:HG2	1:E:169:THR:HG22	1.70	0.72
1:A:451:PHE:CD2	1:A:461:PRO:HA	2.22	0.72
1:E:197:ARG:HG3	1:E:198:GLN:N	2.05	0.72
1:E:249:ASP:C	1:E:249:ASP:OD1	2.26	0.72
1:B:244:PRO:HA	1:B:275:TYR:CD2	2.24	0.72
1:E:243:LEU:HD21	1:E:403:TYR:CE2	2.23	0.72
1:E:244:PRO:HA	1:E:275:TYR:CD2	2.24	0.72
1:B:468:LEU:CD1	1:B:469:PRO:HD2	2.19	0.72
1:D:148:MET:HA	1:D:163:TYR:HD2	1.54	0.72
1:E:468:LEU:CD1	1:E:469:PRO:HD2	2.19	0.72
1:C:148:MET:HA	1:C:163:TYR:HD2	1.54	0.71
1:C:244:PRO:HA	1:C:275:TYR:CD2	2.24	0.71
1:A:544:THR:HG22	1:A:548:ARG:HA	1.70	0.71
1:C:544:THR:HG22	1:C:548:ARG:HA	1.70	0.71
1:E:544:THR:HG22	1:E:548:ARG:HA	1.71	0.71
1:A:436:GLN:HE22	1:B:74:ASN:ND2	1.88	0.71
1:C:468:LEU:CD1	1:C:469:PRO:HD2	2.19	0.71
1:D:197:ARG:HG3	1:D:198:GLN:N	2.05	0.71
1:A:419:ILE:HG22	1:A:423:THR:CG2	2.21	0.71
1:B:419:ILE:HG22	1:B:423:THR:CG2	2.21	0.71
1:C:197:ARG:HG3	1:C:198:GLN:N	2.05	0.71
1:D:436:GLN:HE22	1:E:74:ASN:ND2	1.88	0.71
1:A:74:ASN:ND2	1:E:436:GLN:HE22	1.89	0.71
1:A:243:LEU:HD21	1:A:403:TYR:CD2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:MET:HA	1:A:163:TYR:HD2	1.54	0.71
1:B:197:ARG:HG3	1:B:198:GLN:N	2.05	0.71
1:C:419:ILE:HG22	1:C:423:THR:CG2	2.21	0.71
1:E:419:ILE:HG22	1:E:423:THR:CG2	2.21	0.71
1:C:436:GLN:HE22	1:D:74:ASN:ND2	1.89	0.71
1:C:243:LEU:HD21	1:C:403:TYR:CD2	2.26	0.70
1:E:249:ASP:HB2	1:E:272:ARG:HG2	1.73	0.70
1:D:419:ILE:HG22	1:D:423:THR:CG2	2.21	0.70
1:B:436:GLN:HE22	1:C:74:ASN:ND2	1.89	0.70
1:C:122:ASP:OD1	1:C:528:THR:HB	1.91	0.70
1:C:217:LEU:HB2	1:C:232:THR:HG21	1.73	0.70
1:E:243:LEU:HD21	1:E:403:TYR:CD2	2.26	0.70
1:A:122:ASP:OD1	1:A:528:THR:HB	1.91	0.70
1:B:160:GLU:OE2	1:B:162:LYS:HE3	1.91	0.70
1:D:249:ASP:HB2	1:D:272:ARG:HG2	1.73	0.70
1:B:122:ASP:OD1	1:B:528:THR:HB	1.91	0.70
1:A:160:GLU:OE2	1:A:162:LYS:HE3	1.91	0.70
1:B:215:PHE:CE1	1:B:241:ILE:HD11	2.27	0.70
1:D:217:LEU:HB2	1:D:232:THR:HG21	1.73	0.70
1:D:243:LEU:HD21	1:D:403:TYR:CD2	2.26	0.70
1:E:160:GLU:OE2	1:E:162:LYS:HE3	1.91	0.70
1:C:160:GLU:OE2	1:C:162:LYS:HE3	1.91	0.70
1:D:122:ASP:OD1	1:D:528:THR:HB	1.91	0.70
1:E:217:LEU:HB2	1:E:232:THR:HG21	1.73	0.70
1:A:419:ILE:HG22	1:A:423:THR:HG21	1.75	0.69
1:B:243:LEU:HD21	1:B:403:TYR:CD2	2.26	0.69
1:B:249:ASP:HB2	1:B:272:ARG:HG2	1.73	0.69
1:A:249:ASP:HB2	1:A:272:ARG:HG2	1.73	0.69
1:C:444:MET:HG2	1:C:444:MET:O	1.92	0.69
1:D:215:PHE:CE1	1:D:241:ILE:HD11	2.27	0.69
1:C:215:PHE:CE1	1:C:241:ILE:HD11	2.27	0.69
1:C:249:ASP:HB2	1:C:272:ARG:HG2	1.73	0.69
1:E:122:ASP:OD1	1:E:528:THR:HB	1.91	0.69
1:B:419:ILE:HG22	1:B:423:THR:HG21	1.75	0.69
1:B:444:MET:O	1:B:444:MET:HG2	1.92	0.69
1:D:419:ILE:HG22	1:D:423:THR:HG21	1.75	0.69
1:A:215:PHE:CE1	1:A:241:ILE:HD11	2.27	0.69
1:C:441:LEU:HD12	1:C:445:MET:HE1	1.75	0.69
1:D:160:GLU:OE2	1:D:162:LYS:HE3	1.91	0.69
1:E:512:THR:O	1:E:513:ILE:HB	1.93	0.69
1:A:217:LEU:HB2	1:A:232:THR:HG21	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LEU:HB2	1:B:232:THR:HG21	1.73	0.68
1:D:444:MET:O	1:D:444:MET:HG2	1.92	0.68
1:A:142:LYS:HD3	1:A:167:GLU:OE2	1.93	0.68
1:E:215:PHE:CE1	1:E:241:ILE:HD11	2.27	0.68
1:E:444:MET:HG2	1:E:444:MET:O	1.92	0.68
1:D:142:LYS:HD3	1:D:167:GLU:OE2	1.93	0.68
1:D:512:THR:O	1:D:513:ILE:HB	1.93	0.68
1:E:142:LYS:HD3	1:E:167:GLU:OE2	1.93	0.68
1:A:512:THR:O	1:A:513:ILE:HB	1.93	0.68
1:E:278:LEU:HD22	1:E:406:TRP:HA	1.76	0.68
1:C:419:ILE:HG22	1:C:423:THR:HG21	1.75	0.68
1:A:444:MET:O	1:A:444:MET:HG2	1.92	0.68
1:B:142:LYS:HD3	1:B:167:GLU:OE2	1.94	0.68
1:E:419:ILE:HG22	1:E:423:THR:HG21	1.75	0.68
1:A:146:ARG:O	1:A:246:CYS:HB2	1.94	0.68
1:B:149:VAL:HG23	1:B:195:VAL:HG11	1.76	0.68
1:B:512:THR:O	1:B:513:ILE:HB	1.93	0.68
1:A:386:SER:O	1:A:387:LYS:HB2	1.94	0.67
1:D:217:LEU:HB2	1:D:232:THR:CG2	2.25	0.67
1:E:149:VAL:HG23	1:E:195:VAL:HG11	1.76	0.67
1:C:217:LEU:HB2	1:C:232:THR:CG2	2.25	0.67
1:D:149:VAL:HG23	1:D:195:VAL:HG11	1.76	0.67
1:E:217:LEU:HB2	1:E:232:THR:CG2	2.25	0.67
1:A:278:LEU:HD22	1:A:406:TRP:HA	1.76	0.67
1:D:278:LEU:HD22	1:D:406:TRP:HA	1.76	0.67
1:A:149:VAL:HG23	1:A:195:VAL:HG11	1.76	0.67
1:C:83:ASN:OD1	1:C:83:ASN:N	2.27	0.67
1:C:142:LYS:HD3	1:C:167:GLU:OE2	1.94	0.67
1:C:227:MET:HB2	1:C:228:PRO:HD3	1.76	0.67
1:C:512:THR:O	1:C:513:ILE:HB	1.93	0.67
1:D:386:SER:O	1:D:387:LYS:HB2	1.94	0.67
1:E:386:SER:O	1:E:387:LYS:HB2	1.94	0.67
1:B:217:LEU:HB2	1:B:232:THR:CG2	2.25	0.67
1:A:227:MET:HB2	1:A:228:PRO:HD3	1.76	0.67
1:B:227:MET:HB2	1:B:228:PRO:HD3	1.76	0.67
1:D:227:MET:HB2	1:D:228:PRO:HD3	1.76	0.67
1:C:452:ARG:HH22	1:D:99:ASN:HD22	1.43	0.67
1:D:146:ARG:O	1:D:246:CYS:HB2	1.94	0.67
1:C:146:ARG:O	1:C:246:CYS:HB2	1.94	0.66
1:D:468:LEU:HD12	1:D:469:PRO:CD	2.25	0.66
1:E:146:ARG:O	1:E:246:CYS:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:CYS:HA	1:B:132:PRO:HG3	1.77	0.66
1:B:468:LEU:HD12	1:B:469:PRO:CD	2.26	0.66
1:C:426:CYS:HA	1:D:132:PRO:HG3	1.77	0.66
1:C:430:VAL:HG21	1:C:517:SER:N	2.10	0.66
1:D:452:ARG:HH22	1:E:99:ASN:HD22	1.43	0.66
1:B:278:LEU:HD22	1:B:406:TRP:HA	1.76	0.66
1:C:149:VAL:HG23	1:C:195:VAL:HG11	1.76	0.66
1:B:146:ARG:O	1:B:246:CYS:HB2	1.94	0.66
1:B:386:SER:O	1:B:387:LYS:HB2	1.94	0.66
1:D:441:LEU:HD12	1:D:445:MET:HE1	1.77	0.66
1:A:217:LEU:HB2	1:A:232:THR:CG2	2.25	0.66
1:A:468:LEU:HD12	1:A:469:PRO:CD	2.26	0.66
1:C:278:LEU:HD22	1:C:406:TRP:HA	1.76	0.66
1:C:386:SER:O	1:C:387:LYS:HB2	1.94	0.66
1:D:430:VAL:HG21	1:D:517:SER:N	2.11	0.66
1:A:452:ARG:HH22	1:B:99:ASN:HD22	1.43	0.66
1:B:426:CYS:HA	1:C:132:PRO:HG3	1.77	0.66
1:C:468:LEU:HD12	1:C:469:PRO:CD	2.26	0.66
1:E:227:MET:HB2	1:E:228:PRO:HD3	1.76	0.66
1:A:99:ASN:HD22	1:E:452:ARG:HH22	1.43	0.65
1:A:132:PRO:HG3	1:E:426:CYS:HA	1.77	0.65
1:B:430:VAL:HG21	1:B:517:SER:N	2.10	0.65
1:B:393:LEU:N	1:B:393:LEU:HD12	2.12	0.65
1:D:60:LEU:O	1:D:61:ALA:HB3	1.97	0.65
1:E:430:VAL:HG21	1:E:517:SER:N	2.11	0.65
1:D:193:LEU:HD11	1:D:498:ARG:NH1	2.12	0.65
1:D:426:CYS:HA	1:E:132:PRO:HG3	1.77	0.65
1:A:393:LEU:HD12	1:A:393:LEU:N	2.12	0.65
1:A:430:VAL:HG21	1:A:517:SER:N	2.10	0.65
1:B:60:LEU:O	1:B:61:ALA:HB3	1.97	0.65
1:C:60:LEU:O	1:C:61:ALA:HB3	1.97	0.65
1:A:436:GLN:HE22	1:B:74:ASN:HD21	1.45	0.65
1:B:452:ARG:HH22	1:C:99:ASN:HD22	1.43	0.65
1:D:393:LEU:HD12	1:D:393:LEU:N	2.12	0.65
1:D:436:GLN:NE2	1:E:74:ASN:HD21	1.95	0.65
1:E:133:ASN:HB2	1:E:174:ASN:OD1	1.97	0.65
1:A:211:ASP:O	1:A:212:THR:HG22	1.97	0.64
1:C:193:LEU:HD11	1:C:498:ARG:NH1	2.12	0.64
1:C:211:ASP:O	1:C:212:THR:HG22	1.97	0.64
1:D:436:GLN:HE22	1:E:74:ASN:HD21	1.45	0.64
1:C:513:ILE:O	1:C:513:ILE:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:468:LEU:HD12	1:E:469:PRO:CD	2.26	0.64
1:C:393:LEU:HD12	1:C:393:LEU:N	2.12	0.64
1:E:60:LEU:O	1:E:61:ALA:HB3	1.97	0.64
1:B:436:GLN:NE2	1:C:74:ASN:HD21	1.95	0.64
1:E:393:LEU:N	1:E:393:LEU:HD12	2.12	0.64
1:B:278:LEU:O	1:B:404:ARG:HD3	1.98	0.64
1:B:436:GLN:HE22	1:C:74:ASN:HD21	1.46	0.64
1:E:513:ILE:HG22	1:E:513:ILE:O	1.97	0.64
1:C:436:GLN:NE2	1:D:74:ASN:HD21	1.96	0.64
1:D:513:ILE:O	1:D:513:ILE:HG22	1.97	0.64
1:A:133:ASN:HB2	1:A:174:ASN:OD1	1.97	0.64
1:E:278:LEU:O	1:E:404:ARG:HD3	1.98	0.64
1:E:493:THR:HG21	1:E:497:ASN:O	1.99	0.64
1:E:499:PHE:N	1:E:500:PRO:HD3	2.13	0.64
1:A:74:ASN:HD21	1:E:436:GLN:NE2	1.95	0.63
1:B:133:ASN:HB2	1:B:174:ASN:OD1	1.97	0.63
1:C:133:ASN:HB2	1:C:174:ASN:OD1	1.97	0.63
1:A:436:GLN:NE2	1:B:74:ASN:HD21	1.95	0.63
1:B:493:THR:HG21	1:B:497:ASN:O	1.99	0.63
1:B:513:ILE:HG22	1:B:513:ILE:O	1.97	0.63
1:C:436:GLN:HE22	1:D:74:ASN:HD21	1.45	0.63
1:C:499:PHE:N	1:C:500:PRO:HD3	2.13	0.63
1:B:211:ASP:O	1:B:212:THR:HG22	1.97	0.63
1:B:499:PHE:N	1:B:500:PRO:HD3	2.13	0.63
1:D:211:ASP:O	1:D:212:THR:HG22	1.97	0.63
1:D:278:LEU:O	1:D:404:ARG:HD3	1.98	0.63
1:D:499:PHE:N	1:D:500:PRO:HD3	2.13	0.63
1:E:441:LEU:HD12	1:E:445:MET:HE1	1.81	0.63
1:A:60:LEU:O	1:A:61:ALA:HB3	1.97	0.63
1:E:211:ASP:O	1:E:212:THR:HG22	1.97	0.63
1:C:493:THR:HG21	1:C:497:ASN:O	1.98	0.63
1:A:493:THR:HG21	1:A:497:ASN:O	1.98	0.63
1:C:278:LEU:O	1:C:404:ARG:HD3	1.98	0.63
1:D:133:ASN:HB2	1:D:174:ASN:OD1	1.97	0.63
1:A:134:VAL:HA	1:A:140:THR:OG1	1.99	0.63
1:E:134:VAL:HA	1:E:140:THR:OG1	1.99	0.63
1:E:83:ASN:OD1	1:E:83:ASN:N	2.26	0.63
1:E:148:MET:HA	1:E:163:TYR:CD2	2.34	0.63
1:A:499:PHE:N	1:A:500:PRO:HD3	2.13	0.62
1:B:193:LEU:HD11	1:B:498:ARG:NH1	2.12	0.62
1:D:134:VAL:HA	1:D:140:THR:OG1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ILE:O	1:A:513:ILE:HG22	1.97	0.62
1:B:134:VAL:HA	1:B:140:THR:OG1	1.99	0.62
1:B:441:LEU:HD12	1:B:445:MET:HE1	1.79	0.62
1:D:148:MET:HA	1:D:163:TYR:CD2	2.34	0.62
1:D:544:THR:HG21	1:D:548:ARG:HD2	1.81	0.62
1:A:278:LEU:O	1:A:404:ARG:HD3	1.98	0.62
1:C:378:VAL:HG12	1:C:379:ILE:N	2.14	0.62
1:D:125:THR:HG23	1:D:524:THR:CG2	2.29	0.62
1:A:378:VAL:HG12	1:A:379:ILE:N	2.15	0.62
1:B:125:THR:HG23	1:B:524:THR:CG2	2.29	0.62
1:A:544:THR:HG21	1:A:548:ARG:HD2	1.81	0.62
1:D:258:LEU:HD12	1:D:258:LEU:O	2.00	0.62
1:E:544:THR:HG21	1:E:548:ARG:HD2	1.81	0.62
1:A:125:THR:HG23	1:A:524:THR:CG2	2.29	0.62
1:A:258:LEU:HD12	1:A:258:LEU:O	2.00	0.62
1:B:178:THR:CG2	1:B:511:PRO:HD2	2.29	0.62
1:B:544:THR:HG21	1:B:548:ARG:HD2	1.81	0.62
1:A:148:MET:HA	1:A:163:TYR:CD2	2.34	0.62
1:B:148:MET:HA	1:B:163:TYR:CD2	2.34	0.62
1:D:493:THR:HG21	1:D:497:ASN:O	1.99	0.62
1:B:125:THR:CG2	1:B:526:HIS:NE2	2.63	0.62
1:C:125:THR:HG23	1:C:524:THR:CG2	2.29	0.62
1:C:134:VAL:HA	1:C:140:THR:OG1	1.99	0.62
1:C:148:MET:HA	1:C:163:TYR:CD2	2.34	0.62
1:E:125:THR:HG23	1:E:524:THR:CG2	2.29	0.62
1:A:125:THR:CG2	1:A:526:HIS:NE2	2.63	0.62
1:B:60:LEU:O	1:B:60:LEU:HG	2.00	0.62
1:D:125:THR:CG2	1:D:526:HIS:NE2	2.63	0.61
1:E:378:VAL:HG12	1:E:379:ILE:N	2.15	0.61
1:B:394:ILE:HG23	1:B:398:SER:HB2	1.82	0.61
1:D:60:LEU:O	1:D:60:LEU:HG	2.00	0.61
1:E:125:THR:CG2	1:E:526:HIS:NE2	2.63	0.61
1:A:193:LEU:HD11	1:A:498:ARG:NH1	2.12	0.61
1:A:394:ILE:HG23	1:A:398:SER:HB2	1.82	0.61
1:E:220:ASP:OD1	1:E:222:VAL:HG12	2.00	0.61
1:B:220:ASP:OD1	1:B:222:VAL:HG12	2.00	0.61
1:D:394:ILE:HG23	1:D:398:SER:HB2	1.82	0.61
1:E:60:LEU:O	1:E:60:LEU:HG	2.00	0.61
1:B:378:VAL:HG12	1:B:379:ILE:N	2.15	0.61
1:C:220:ASP:OD1	1:C:222:VAL:HG12	2.00	0.61
1:E:444:MET:HB2	1:E:539:GLN:OE1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ASN:HD21	1:E:436:GLN:HE22	1.46	0.61
1:D:220:ASP:OD1	1:D:222:VAL:HG12	2.00	0.61
1:B:258:LEU:HD12	1:B:258:LEU:O	2.00	0.61
1:C:258:LEU:HD12	1:C:258:LEU:O	2.00	0.61
1:C:444:MET:HB2	1:C:539:GLN:OE1	2.00	0.61
1:C:74:ASN:ND2	1:C:556:LYS:HZ1	1.98	0.61
1:C:394:ILE:HG23	1:C:398:SER:HB2	1.82	0.61
1:D:178:THR:CG2	1:D:511:PRO:HD2	2.30	0.61
1:E:193:LEU:HD11	1:E:498:ARG:NH1	2.12	0.61
1:A:220:ASP:OD1	1:A:222:VAL:HG12	2.00	0.61
1:B:444:MET:HB2	1:B:539:GLN:OE1	2.01	0.61
1:C:125:THR:CG2	1:C:526:HIS:NE2	2.63	0.61
1:C:544:THR:HG21	1:C:548:ARG:HD2	1.81	0.61
1:D:378:VAL:HG12	1:D:379:ILE:N	2.15	0.61
1:C:178:THR:CG2	1:C:511:PRO:HD2	2.30	0.60
1:D:444:MET:HB2	1:D:539:GLN:OE1	2.01	0.60
1:E:258:LEU:HD12	1:E:258:LEU:O	2.00	0.60
1:C:440:SER:HB3	1:C:461:PRO:O	2.02	0.60
1:D:440:SER:HB3	1:D:461:PRO:O	2.01	0.60
1:A:263:LYS:NZ	1:A:268:GLN:HB2	2.16	0.60
1:A:383:THR:HG22	1:A:384:GLU:HG3	1.84	0.60
1:B:125:THR:HG21	1:B:526:HIS:NE2	2.17	0.60
1:B:394:ILE:HG23	1:B:395:SER:H	1.67	0.60
1:C:60:LEU:O	1:C:60:LEU:HG	2.00	0.60
1:E:263:LYS:NZ	1:E:268:GLN:HB2	2.16	0.60
1:B:425:LEU:HD23	1:C:172:GLU:HB3	1.83	0.60
1:D:125:THR:HG21	1:D:526:HIS:NE2	2.16	0.60
1:E:383:THR:HG22	1:E:384:GLU:HG3	1.83	0.60
1:A:125:THR:HG21	1:A:526:HIS:NE2	2.17	0.60
1:A:394:ILE:HG23	1:A:395:SER:H	1.67	0.60
1:B:220:ASP:HB2	1:B:227:MET:HG2	1.84	0.60
1:C:383:THR:HG22	1:C:384:GLU:HG3	1.84	0.60
1:E:394:ILE:HG23	1:E:395:SER:H	1.66	0.60
1:A:60:LEU:O	1:A:60:LEU:HG	2.00	0.60
1:A:440:SER:HB3	1:A:461:PRO:O	2.02	0.60
1:D:383:THR:HG22	1:D:384:GLU:HG3	1.84	0.60
1:A:444:MET:HB2	1:A:539:GLN:OE1	2.01	0.60
1:B:278:LEU:CD2	1:B:406:TRP:HA	2.32	0.60
1:D:449:VAL:CG2	1:E:67:THR:HG21	2.32	0.60
1:E:125:THR:HG21	1:E:526:HIS:NE2	2.17	0.60
1:A:172:GLU:HB3	1:E:425:LEU:HD23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASP:HB2	1:A:227:MET:HG2	1.84	0.60
1:A:449:VAL:CG2	1:B:67:THR:HG21	2.32	0.60
1:C:410:TYR:CD1	1:C:420:ARG:HA	2.37	0.60
1:A:436:GLN:NE2	1:B:556:LYS:HZ3	2.00	0.60
1:B:214:ASN:C	1:B:214:ASN:ND2	2.55	0.60
1:C:243:LEU:HD11	1:C:403:TYR:HE2	1.67	0.60
1:C:394:ILE:HG23	1:C:395:SER:H	1.67	0.60
1:C:449:VAL:CG2	1:D:67:THR:HG21	2.32	0.60
1:E:278:LEU:CD2	1:E:406:TRP:HA	2.32	0.60
1:A:425:LEU:HD23	1:B:172:GLU:HB3	1.84	0.59
1:C:389:ARG:NH1	1:C:389:ARG:HG2	2.17	0.59
1:D:278:LEU:CD2	1:D:406:TRP:HA	2.32	0.59
1:D:389:ARG:HG2	1:D:389:ARG:NH1	2.17	0.59
1:D:410:TYR:CD1	1:D:420:ARG:HA	2.37	0.59
1:D:425:LEU:HD23	1:E:172:GLU:HB3	1.84	0.59
1:A:67:THR:HG21	1:E:449:VAL:CG2	2.32	0.59
1:C:220:ASP:HB2	1:C:227:MET:HG2	1.84	0.59
1:E:282:ASN:HD21	1:E:404:ARG:HE	1.51	0.59
1:E:389:ARG:HG2	1:E:389:ARG:NH1	2.17	0.59
1:A:389:ARG:NH1	1:A:389:ARG:HG2	2.17	0.59
1:B:263:LYS:NZ	1:B:268:GLN:HB2	2.16	0.59
1:B:410:TYR:CD1	1:B:420:ARG:HA	2.37	0.59
1:D:214:ASN:C	1:D:214:ASN:ND2	2.55	0.59
1:D:220:ASP:HB2	1:D:227:MET:HG2	1.84	0.59
1:E:278:LEU:HD23	1:E:419:ILE:CD1	2.30	0.59
1:E:394:ILE:HG23	1:E:398:SER:HB2	1.82	0.59
1:E:440:SER:HB3	1:E:461:PRO:O	2.01	0.59
1:A:410:TYR:CD1	1:A:420:ARG:HA	2.37	0.59
1:B:449:VAL:CG2	1:C:67:THR:HG21	2.32	0.59
1:D:243:LEU:HD11	1:D:403:TYR:HE2	1.67	0.59
1:E:243:LEU:HD11	1:E:403:TYR:HE2	1.67	0.59
1:A:378:VAL:O	1:A:380:LYS:N	2.35	0.59
1:B:383:THR:HG22	1:B:384:GLU:HG3	1.83	0.59
1:E:378:VAL:O	1:E:380:LYS:N	2.36	0.59
1:E:410:TYR:CD1	1:E:420:ARG:HA	2.37	0.59
1:B:282:ASN:HD21	1:B:404:ARG:HE	1.50	0.59
1:C:378:VAL:O	1:C:380:LYS:N	2.36	0.59
1:D:243:LEU:CD2	1:D:403:TYR:CD2	2.86	0.59
1:B:243:LEU:CD2	1:B:403:TYR:CD2	2.86	0.59
1:C:263:LYS:NZ	1:C:268:GLN:HB2	2.16	0.59
1:C:425:LEU:HD23	1:D:172:GLU:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:GLY:O	1:B:399:THR:HB	2.03	0.59
1:C:125:THR:HG21	1:C:526:HIS:NE2	2.17	0.59
1:C:520:VAL:CG2	1:C:521:PRO:HD2	2.33	0.59
1:A:178:THR:CG2	1:A:511:PRO:HD2	2.30	0.59
1:A:278:LEU:CD2	1:A:406:TRP:HA	2.32	0.59
1:C:214:ASN:C	1:C:214:ASN:ND2	2.55	0.59
1:E:520:VAL:CG2	1:E:521:PRO:HD2	2.33	0.59
1:C:278:LEU:CD2	1:C:406:TRP:HA	2.32	0.59
1:D:287:LEU:HD23	1:D:287:LEU:C	2.24	0.59
1:A:197:ARG:HG3	1:A:198:GLN:CG	2.33	0.58
1:B:197:ARG:HG3	1:B:198:GLN:CG	2.33	0.58
1:B:243:LEU:HD11	1:B:403:TYR:HE2	1.67	0.58
1:C:243:LEU:CD2	1:C:403:TYR:CD2	2.86	0.58
1:C:282:ASN:HD21	1:C:404:ARG:HE	1.50	0.58
1:B:378:VAL:O	1:B:380:LYS:N	2.35	0.58
1:B:389:ARG:HG2	1:B:389:ARG:NH1	2.17	0.58
1:C:224:GLY:O	1:C:399:THR:HB	2.03	0.58
1:E:220:ASP:HB2	1:E:227:MET:HG2	1.84	0.58
1:E:224:GLY:O	1:E:399:THR:HB	2.03	0.58
1:B:278:LEU:HD23	1:B:419:ILE:CD1	2.30	0.58
1:C:197:ARG:HG3	1:C:198:GLN:CG	2.33	0.58
1:D:154:THR:HG22	1:D:155:LYS:N	2.19	0.58
1:D:263:LYS:NZ	1:D:268:GLN:HB2	2.16	0.58
1:D:394:ILE:HG23	1:D:395:SER:H	1.67	0.58
1:E:243:LEU:CD2	1:E:403:TYR:CD2	2.86	0.58
1:A:224:GLY:O	1:A:399:THR:HB	2.03	0.58
1:A:282:ASN:HD21	1:A:404:ARG:HE	1.50	0.58
1:B:154:THR:HG22	1:B:155:LYS:N	2.19	0.58
1:D:282:ASN:HD21	1:D:404:ARG:HE	1.50	0.58
1:E:154:THR:HG22	1:E:155:LYS:N	2.18	0.58
1:A:243:LEU:CD2	1:A:403:TYR:CD2	2.86	0.58
1:B:440:SER:HB3	1:B:461:PRO:O	2.02	0.58
1:C:278:LEU:HD23	1:C:419:ILE:CD1	2.30	0.58
1:C:287:LEU:HD23	1:C:287:LEU:C	2.24	0.58
1:E:178:THR:CG2	1:E:511:PRO:HD2	2.30	0.58
1:A:520:VAL:CG2	1:A:521:PRO:HD2	2.33	0.58
1:B:211:ASP:O	1:B:212:THR:CG2	2.52	0.58
1:C:410:TYR:HE2	1:D:172:GLU:OE1	1.87	0.58
1:D:211:ASP:O	1:D:212:THR:CG2	2.52	0.58
1:A:172:GLU:OE1	1:E:410:TYR:HE2	1.87	0.58
1:C:211:ASP:O	1:C:212:THR:CG2	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:ASN:C	1:E:214:ASN:ND2	2.55	0.58
1:A:278:LEU:HD23	1:A:419:ILE:CD1	2.30	0.58
1:C:494:HIS:C	1:C:496:PHE:H	2.07	0.58
1:E:211:ASP:O	1:E:212:THR:CG2	2.52	0.58
1:A:154:THR:HG22	1:A:155:LYS:N	2.19	0.58
1:A:211:ASP:O	1:A:212:THR:CG2	2.52	0.58
1:B:287:LEU:C	1:B:287:LEU:HD23	2.24	0.58
1:D:378:VAL:O	1:D:380:LYS:N	2.35	0.58
1:A:287:LEU:HD23	1:A:287:LEU:C	2.24	0.57
1:C:154:THR:HG22	1:C:155:LYS:N	2.18	0.57
1:A:243:LEU:HD11	1:A:403:TYR:HE2	1.67	0.57
1:A:282:ASN:ND2	1:A:404:ARG:HE	2.03	0.57
1:A:410:TYR:HE2	1:B:172:GLU:OE1	1.87	0.57
1:B:410:TYR:HE2	1:C:172:GLU:OE1	1.87	0.57
1:E:287:LEU:HD23	1:E:287:LEU:C	2.24	0.57
1:B:282:ASN:ND2	1:B:404:ARG:HE	2.03	0.57
1:C:479:GLN:HG2	1:C:479:GLN:O	2.05	0.57
1:D:197:ARG:HG3	1:D:198:GLN:CG	2.33	0.57
1:D:224:GLY:O	1:D:399:THR:HB	2.03	0.57
1:D:410:TYR:HE2	1:E:172:GLU:OE1	1.87	0.57
1:E:197:ARG:HG3	1:E:198:GLN:CG	2.33	0.57
1:B:520:VAL:CG2	1:B:521:PRO:HD2	2.33	0.57
1:D:403:TYR:CD1	1:D:504:ILE:HD13	2.39	0.57
1:A:233:ASN:CG	1:A:233:ASN:O	2.43	0.57
1:D:282:ASN:ND2	1:D:404:ARG:HE	2.03	0.57
1:D:482:TYR:CE1	1:D:486:ILE:HD12	2.40	0.57
1:D:520:VAL:CG2	1:D:521:PRO:HD2	2.33	0.57
1:A:441:LEU:HD12	1:A:445:MET:HE1	1.87	0.57
1:B:479:GLN:O	1:B:479:GLN:HG2	2.05	0.57
1:C:567:SER:HB2	1:D:49:THR:HG21	1.87	0.57
1:B:482:TYR:CE1	1:B:486:ILE:HD12	2.40	0.57
1:E:444:MET:HE3	1:E:561:VAL:HG21	1.87	0.57
1:E:233:ASN:CG	1:E:233:ASN:O	2.43	0.57
1:A:134:VAL:HG22	1:A:173:GLY:O	2.05	0.56
1:C:436:GLN:NE2	1:D:556:LYS:HZ3	2.03	0.56
1:E:134:VAL:HG22	1:E:173:GLY:O	2.05	0.56
1:E:282:ASN:ND2	1:E:404:ARG:HE	2.03	0.56
1:A:482:TYR:CE1	1:A:486:ILE:HD12	2.40	0.56
1:B:233:ASN:CG	1:B:233:ASN:O	2.43	0.56
1:A:567:SER:HB2	1:B:49:THR:HG21	1.87	0.56
1:B:134:VAL:HG22	1:B:173:GLY:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ASN:HB3	1:B:402:GLN:NE2	2.21	0.56
1:B:434:SER:N	1:C:555:TYR:HE2	2.04	0.56
1:B:494:HIS:C	1:B:496:PHE:H	2.08	0.56
1:C:282:ASN:ND2	1:C:404:ARG:HE	2.02	0.56
1:D:479:GLN:O	1:D:479:GLN:HG2	2.05	0.56
1:E:273:ILE:O	1:E:273:ILE:HG23	2.05	0.56
1:E:479:GLN:O	1:E:479:GLN:HG2	2.05	0.56
1:C:125:THR:CG2	1:C:524:THR:HG23	2.36	0.56
1:A:434:SER:N	1:B:555:TYR:HE2	2.04	0.56
1:C:233:ASN:O	1:C:233:ASN:CG	2.43	0.56
1:C:392:ASN:HB3	1:C:402:GLN:NE2	2.21	0.56
1:D:392:ASN:HB3	1:D:402:GLN:NE2	2.21	0.56
1:D:567:SER:HB2	1:E:49:THR:HG21	1.87	0.56
1:E:392:ASN:HB3	1:E:402:GLN:NE2	2.21	0.56
1:A:125:THR:CG2	1:A:524:THR:HG23	2.35	0.56
1:B:403:TYR:CD1	1:B:504:ILE:HD13	2.39	0.56
1:C:482:TYR:CE1	1:C:486:ILE:HD12	2.40	0.56
1:D:273:ILE:HG23	1:D:273:ILE:O	2.05	0.56
1:E:74:ASN:ND2	1:E:556:LYS:HZ1	2.04	0.56
1:E:493:THR:HG22	1:E:494:HIS:N	2.21	0.56
1:A:392:ASN:HB3	1:A:402:GLN:NE2	2.21	0.56
1:A:67:THR:O	1:A:68:ARG:HG2	2.06	0.56
1:B:273:ILE:O	1:B:273:ILE:HG23	2.05	0.56
1:B:419:ILE:O	1:B:423:THR:HG22	2.06	0.56
1:B:567:SER:HB2	1:C:49:THR:HG21	1.87	0.56
1:C:428:PRO:O	1:C:429:ASP:HB3	2.06	0.56
1:D:134:VAL:HG22	1:D:173:GLY:O	2.05	0.56
1:D:494:HIS:C	1:D:496:PHE:H	2.07	0.56
1:E:482:TYR:CE1	1:E:486:ILE:HD12	2.40	0.56
1:A:273:ILE:HG23	1:A:273:ILE:O	2.05	0.56
1:E:125:THR:CG2	1:E:524:THR:HG23	2.35	0.56
1:A:68:ARG:NH1	1:A:68:ARG:CG	2.66	0.56
1:A:493:THR:HG22	1:A:494:HIS:N	2.21	0.56
1:C:403:TYR:CD1	1:C:504:ILE:HD13	2.39	0.56
1:A:555:TYR:HE2	1:E:434:SER:N	2.04	0.55
1:C:283:ILE:O	1:C:401:THR:HG23	2.07	0.55
1:C:434:SER:N	1:D:555:TYR:HE2	2.04	0.55
1:D:67:THR:O	1:D:68:ARG:HG2	2.06	0.55
1:A:49:THR:HG21	1:E:567:SER:HB2	1.87	0.55
1:A:479:GLN:O	1:A:479:GLN:HG2	2.05	0.55
1:A:494:HIS:C	1:A:496:PHE:H	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:THR:CG2	1:B:524:THR:HG23	2.36	0.55
1:B:403:TYR:HD1	1:B:504:ILE:CD1	2.20	0.55
1:B:501:GLU:H	1:B:501:GLU:CD	2.10	0.55
1:D:233:ASN:CG	1:D:233:ASN:O	2.42	0.55
1:A:283:ILE:O	1:A:401:THR:HG23	2.07	0.55
1:A:440:SER:C	1:A:442:PRO:HD3	2.27	0.55
1:B:283:ILE:O	1:B:401:THR:HG23	2.07	0.55
1:C:197:ARG:HG3	1:C:198:GLN:H	1.71	0.55
1:C:440:SER:C	1:C:442:PRO:HD3	2.27	0.55
1:D:68:ARG:HH11	1:D:68:ARG:CG	2.07	0.55
1:D:403:TYR:HD1	1:D:504:ILE:CD1	2.19	0.55
1:D:419:ILE:O	1:D:423:THR:HG22	2.06	0.55
1:E:283:ILE:O	1:E:401:THR:HG23	2.06	0.55
1:A:428:PRO:O	1:A:429:ASP:HB3	2.06	0.55
1:B:493:THR:HG22	1:B:494:HIS:N	2.21	0.55
1:A:419:ILE:O	1:A:423:THR:HG22	2.06	0.55
1:C:449:VAL:HG22	1:D:67:THR:HG21	1.89	0.55
1:A:214:ASN:C	1:A:214:ASN:ND2	2.55	0.55
1:A:501:GLU:CD	1:A:501:GLU:H	2.10	0.55
1:B:428:PRO:O	1:B:429:ASP:HB3	2.06	0.55
1:C:67:THR:O	1:C:68:ARG:HG2	2.06	0.55
1:D:125:THR:CG2	1:D:524:THR:HG23	2.35	0.55
1:D:440:SER:C	1:D:442:PRO:HD3	2.27	0.55
1:E:67:THR:O	1:E:68:ARG:HG2	2.06	0.55
1:E:494:HIS:C	1:E:496:PHE:H	2.08	0.55
1:E:501:GLU:H	1:E:501:GLU:CD	2.10	0.55
1:A:444:MET:HE3	1:A:561:VAL:HG21	1.88	0.55
1:B:449:VAL:HG22	1:C:67:THR:HG21	1.88	0.55
1:C:134:VAL:HG22	1:C:173:GLY:O	2.05	0.55
1:D:449:VAL:HG22	1:E:67:THR:HG21	1.89	0.55
1:A:449:VAL:HG22	1:B:67:THR:HG21	1.89	0.55
1:B:67:THR:O	1:B:68:ARG:HG2	2.06	0.55
1:C:136:GLU:O	1:C:137:PHE:HB2	2.07	0.55
1:D:493:THR:HG22	1:D:494:HIS:N	2.21	0.55
1:E:197:ARG:HG3	1:E:198:GLN:H	1.71	0.55
1:A:197:ARG:HG3	1:A:198:GLN:H	1.71	0.55
1:C:273:ILE:HG23	1:C:273:ILE:O	2.05	0.55
1:D:215:PHE:HE1	1:D:241:ILE:HD11	1.71	0.55
1:A:529:LEU:HD21	1:B:68:ARG:NE	2.22	0.55
1:B:136:GLU:O	1:B:137:PHE:HB2	2.07	0.55
1:D:434:SER:N	1:E:555:TYR:HE2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:419:ILE:O	1:E:423:THR:HG22	2.06	0.55
1:A:74:ASN:ND2	1:A:556:LYS:HZ1	2.05	0.54
1:A:403:TYR:CD1	1:A:504:ILE:HD13	2.39	0.54
1:B:440:SER:C	1:B:442:PRO:HD3	2.27	0.54
1:B:525:ASP:C	1:B:525:ASP:OD1	2.45	0.54
1:C:419:ILE:O	1:C:423:THR:HG22	2.06	0.54
1:D:83:ASN:OD1	1:D:83:ASN:N	2.26	0.54
1:C:544:THR:HG21	1:C:548:ARG:HA	1.89	0.54
1:D:278:LEU:HD23	1:D:419:ILE:CD1	2.30	0.54
1:D:283:ILE:O	1:D:401:THR:HG23	2.07	0.54
1:A:505:LEU:O	1:A:506:ALA:O	2.26	0.54
1:B:263:LYS:HZ3	1:B:268:GLN:HB2	1.73	0.54
1:D:136:GLU:O	1:D:137:PHE:HB2	2.07	0.54
1:E:428:PRO:O	1:E:429:ASP:HB3	2.07	0.54
1:A:263:LYS:HZ3	1:A:268:GLN:HB2	1.73	0.54
1:B:529:LEU:HD21	1:C:68:ARG:NE	2.23	0.54
1:C:501:GLU:CD	1:C:501:GLU:H	2.10	0.54
1:D:428:PRO:O	1:D:429:ASP:HB3	2.06	0.54
1:C:211:ASP:CG	1:C:212:THR:H	2.10	0.54
1:C:525:ASP:C	1:C:525:ASP:OD1	2.45	0.54
1:D:385:ASP:O	1:D:386:SER:C	2.45	0.54
1:D:463:VAL:HB	1:D:529:LEU:CD1	2.38	0.54
1:D:501:GLU:CD	1:D:501:GLU:H	2.10	0.54
1:E:211:ASP:CG	1:E:212:THR:H	2.10	0.54
1:E:440:SER:C	1:E:442:PRO:HD3	2.27	0.54
1:D:525:ASP:C	1:D:525:ASP:OD1	2.45	0.54
1:E:215:PHE:HE1	1:E:241:ILE:HD11	1.71	0.54
1:A:525:ASP:C	1:A:525:ASP:OD1	2.45	0.54
1:B:203:GLU:C	1:B:205:ASP:H	2.11	0.54
1:E:192:TYR:CZ	1:E:197:ARG:HB3	2.43	0.54
1:E:208:VAL:HG23	1:E:208:VAL:O	2.08	0.54
1:E:389:ARG:HG2	1:E:389:ARG:HH11	1.73	0.54
1:E:505:LEU:O	1:E:506:ALA:O	2.26	0.54
1:A:68:ARG:NE	1:E:529:LEU:HD21	2.23	0.54
1:A:136:GLU:O	1:A:137:PHE:HB2	2.07	0.54
1:B:192:TYR:CZ	1:B:197:ARG:HB3	2.43	0.54
1:C:505:LEU:O	1:C:506:ALA:O	2.26	0.54
1:D:197:ARG:HG3	1:D:198:GLN:H	1.71	0.54
1:D:505:LEU:O	1:D:506:ALA:O	2.26	0.54
1:E:463:VAL:HB	1:E:529:LEU:CD1	2.38	0.54
1:E:525:ASP:C	1:E:525:ASP:OD1	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:TYR:CZ	1:A:197:ARG:HB3	2.43	0.54
1:A:239:ASP:C	1:A:239:ASP:OD1	2.46	0.54
1:B:208:VAL:HG23	1:B:208:VAL:O	2.08	0.54
1:B:385:ASP:O	1:B:386:SER:C	2.45	0.54
1:C:192:TYR:CZ	1:C:197:ARG:HB3	2.43	0.54
1:C:385:ASP:O	1:C:386:SER:C	2.45	0.54
1:C:493:THR:HG22	1:C:494:HIS:N	2.21	0.54
1:D:192:TYR:CZ	1:D:197:ARG:HB3	2.43	0.54
1:A:67:THR:HG21	1:E:449:VAL:HG22	1.89	0.54
1:A:203:GLU:C	1:A:205:ASP:H	2.11	0.54
1:E:136:GLU:O	1:E:137:PHE:HB2	2.07	0.54
1:A:385:ASP:O	1:A:386:SER:C	2.45	0.53
1:B:197:ARG:HG3	1:B:198:GLN:H	1.71	0.53
1:C:239:ASP:C	1:C:239:ASP:OD1	2.45	0.53
1:D:211:ASP:CG	1:D:212:THR:H	2.10	0.53
1:E:239:ASP:OD1	1:E:239:ASP:C	2.46	0.53
1:E:385:ASP:O	1:E:386:SER:C	2.46	0.53
1:E:544:THR:HG21	1:E:548:ARG:HA	1.89	0.53
1:A:478:ASP:C	1:A:480:ALA:H	2.12	0.53
1:B:544:THR:HG21	1:B:548:ARG:HA	1.89	0.53
1:C:203:GLU:C	1:C:205:ASP:H	2.11	0.53
1:D:449:VAL:HG12	1:D:450:THR:N	2.23	0.53
1:D:478:ASP:C	1:D:480:ALA:H	2.12	0.53
1:E:403:TYR:HD1	1:E:504:ILE:CD1	2.19	0.53
1:B:215:PHE:HE1	1:B:241:ILE:HD11	1.71	0.53
1:B:478:ASP:C	1:B:480:ALA:H	2.12	0.53
1:B:154:THR:CG2	1:B:155:LYS:N	2.72	0.53
1:B:389:ARG:HG2	1:B:389:ARG:HH11	1.73	0.53
1:C:478:ASP:C	1:C:480:ALA:H	2.12	0.53
1:D:151:ARG:HG3	1:D:161:LEU:CD2	2.39	0.53
1:A:93:THR:HG22	1:A:94:THR:N	2.23	0.53
1:A:295:SER:HB3	1:A:377:PRO:CG	2.33	0.53
1:A:389:ARG:HG2	1:A:389:ARG:HH11	1.73	0.53
1:A:463:VAL:HB	1:A:529:LEU:CD1	2.38	0.53
1:B:452:ARG:NH2	1:C:99:ASN:HD22	2.07	0.53
1:C:93:THR:HG22	1:C:94:THR:N	2.23	0.53
1:D:208:VAL:HG23	1:D:208:VAL:O	2.08	0.53
1:D:529:LEU:HD21	1:E:68:ARG:NE	2.23	0.53
1:C:69:VAL:CG2	1:C:561:VAL:HB	2.39	0.53
1:C:403:TYR:HD1	1:C:504:ILE:CD1	2.19	0.53
1:C:529:LEU:HD21	1:D:68:ARG:NE	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:THR:CG2	1:D:155:LYS:N	2.72	0.53
1:E:203:GLU:C	1:E:205:ASP:H	2.11	0.53
1:A:236:PHE:O	1:A:237:HIS:HB3	2.09	0.53
1:B:211:ASP:CG	1:B:212:THR:H	2.10	0.53
1:C:386:SER:O	1:C:387:LYS:CB	2.57	0.53
1:D:69:VAL:CG2	1:D:561:VAL:HB	2.39	0.53
1:D:93:THR:HG22	1:D:94:THR:N	2.23	0.53
1:D:151:ARG:HG3	1:D:161:LEU:HD21	1.91	0.53
1:D:389:ARG:HG2	1:D:389:ARG:HH11	1.73	0.53
1:B:449:VAL:HG12	1:B:450:THR:N	2.23	0.53
1:B:505:LEU:O	1:B:506:ALA:O	2.26	0.53
1:C:151:ARG:HG3	1:C:161:LEU:HD21	1.91	0.53
1:C:154:THR:CG2	1:C:155:LYS:N	2.72	0.53
1:C:236:PHE:O	1:C:237:HIS:HB3	2.09	0.53
1:E:69:VAL:CG2	1:E:561:VAL:HB	2.39	0.53
1:E:292:TYR:HA	1:E:377:PRO:HG3	1.91	0.53
1:B:222:VAL:HG13	1:B:223:THR:N	2.24	0.53
1:E:151:ARG:HG3	1:E:161:LEU:HD21	1.91	0.53
1:A:544:THR:HG21	1:A:548:ARG:HA	1.89	0.52
1:C:197:ARG:CG	1:C:198:GLN:N	2.72	0.52
1:C:208:VAL:O	1:C:208:VAL:HG23	2.08	0.52
1:C:222:VAL:HG13	1:C:223:THR:N	2.24	0.52
1:C:295:SER:HB3	1:C:377:PRO:CG	2.33	0.52
1:E:120:GLY:O	1:E:563:PRO:HA	2.10	0.52
1:E:151:ARG:HG3	1:E:161:LEU:CD2	2.39	0.52
1:A:215:PHE:HE1	1:A:241:ILE:HD11	1.71	0.52
1:A:449:VAL:HG12	1:A:450:THR:N	2.23	0.52
1:B:69:VAL:CG2	1:B:561:VAL:HB	2.39	0.52
1:B:239:ASP:C	1:B:239:ASP:OD1	2.45	0.52
1:C:180:THR:HG21	1:C:258:LEU:CD2	2.40	0.52
1:D:236:PHE:O	1:D:237:HIS:HB3	2.09	0.52
1:D:266:PRO:O	1:D:268:GLN:N	2.43	0.52
1:E:93:THR:HG22	1:E:94:THR:N	2.23	0.52
1:A:69:VAL:CG2	1:A:561:VAL:HB	2.39	0.52
1:A:151:ARG:HG3	1:A:161:LEU:CD2	2.39	0.52
1:A:154:THR:CG2	1:A:155:LYS:N	2.72	0.52
1:A:211:ASP:CG	1:A:212:THR:H	2.10	0.52
1:A:386:SER:O	1:A:387:LYS:CB	2.57	0.52
1:B:120:GLY:O	1:B:563:PRO:HA	2.10	0.52
1:B:151:ARG:HG3	1:B:161:LEU:HD21	1.91	0.52
1:D:53:ASN:O	1:D:54:SER:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:THR:HG21	1:D:258:LEU:CD2	2.40	0.52
1:A:452:ARG:NH2	1:B:99:ASN:HD22	2.06	0.52
1:B:180:THR:HG21	1:B:258:LEU:CD2	2.40	0.52
1:B:266:PRO:O	1:B:268:GLN:N	2.43	0.52
1:B:463:VAL:HB	1:B:529:LEU:CD1	2.38	0.52
1:C:151:ARG:HG3	1:C:161:LEU:CD2	2.39	0.52
1:C:389:ARG:HG2	1:C:389:ARG:HH11	1.73	0.52
1:C:449:VAL:HG12	1:C:450:THR:N	2.23	0.52
1:E:171:PRO:O	1:E:175:TYR:OH	2.25	0.52
1:E:180:THR:HG21	1:E:258:LEU:CD2	2.40	0.52
1:E:236:PHE:O	1:E:237:HIS:HB3	2.09	0.52
1:B:197:ARG:CG	1:B:198:GLN:N	2.72	0.52
1:D:197:ARG:CG	1:D:198:GLN:N	2.72	0.52
1:D:441:LEU:N	1:D:442:PRO:HD3	2.24	0.52
1:E:154:THR:CG2	1:E:155:LYS:N	2.71	0.52
1:E:449:VAL:HG12	1:E:450:THR:N	2.23	0.52
1:A:208:VAL:HG23	1:A:208:VAL:O	2.08	0.52
1:A:211:ASP:HA	1:A:508:PRO:HG2	1.89	0.52
1:C:403:TYR:CD1	1:C:504:ILE:HG21	2.45	0.52
1:C:520:VAL:HG23	1:C:521:PRO:HD2	1.92	0.52
1:D:386:SER:O	1:D:387:LYS:CB	2.57	0.52
1:E:197:ARG:CG	1:E:198:GLN:N	2.72	0.52
1:E:478:ASP:C	1:E:480:ALA:H	2.12	0.52
1:E:520:VAL:HG23	1:E:521:PRO:HD2	1.92	0.52
1:A:171:PRO:O	1:A:175:TYR:OH	2.25	0.52
1:A:266:PRO:O	1:A:268:GLN:N	2.43	0.52
1:A:403:TYR:HD1	1:A:504:ILE:CD1	2.20	0.52
1:B:93:THR:HG22	1:B:94:THR:N	2.23	0.52
1:C:74:ASN:HD22	1:C:556:LYS:HZ1	1.58	0.52
1:C:211:ASP:HA	1:C:508:PRO:HG2	1.89	0.52
1:C:262:ARG:HH11	1:D:130:ASN:HD22	1.55	0.52
1:C:463:VAL:HB	1:C:529:LEU:CD1	2.38	0.52
1:E:222:VAL:HG13	1:E:223:THR:N	2.24	0.52
1:E:386:SER:O	1:E:387:LYS:CB	2.57	0.52
1:A:99:ASN:HD22	1:E:452:ARG:NH2	2.07	0.52
1:A:197:ARG:CG	1:A:198:GLN:N	2.72	0.52
1:A:222:VAL:HG13	1:A:223:THR:N	2.24	0.52
1:B:125:THR:HG22	1:B:524:THR:HG23	1.92	0.52
1:B:151:ARG:HG3	1:B:161:LEU:CD2	2.39	0.52
1:B:403:TYR:CD1	1:B:504:ILE:HG21	2.45	0.52
1:D:120:GLY:O	1:D:563:PRO:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:VAL:HG13	1:D:223:THR:N	2.24	0.52
1:A:180:THR:HG21	1:A:258:LEU:CD2	2.40	0.52
1:D:125:THR:CG2	1:D:524:THR:CG2	2.88	0.52
1:D:151:ARG:HB3	1:D:200:GLY:O	2.10	0.52
1:C:263:LYS:HZ3	1:C:268:GLN:HB2	1.74	0.52
1:E:295:SER:HB3	1:E:377:PRO:CG	2.33	0.52
1:E:403:TYR:CD1	1:E:504:ILE:HG21	2.45	0.52
1:A:441:LEU:N	1:A:442:PRO:HD3	2.24	0.51
1:C:125:THR:CG2	1:C:524:THR:CG2	2.88	0.51
1:D:452:ARG:NH2	1:E:99:ASN:HD22	2.06	0.51
1:A:53:ASN:O	1:A:54:SER:C	2.48	0.51
1:C:151:ARG:HB3	1:C:200:GLY:O	2.10	0.51
1:C:215:PHE:HE1	1:C:241:ILE:HD11	1.71	0.51
1:C:295:SER:OG	1:C:377:PRO:HD3	2.10	0.51
1:E:151:ARG:HB3	1:E:200:GLY:O	2.10	0.51
1:A:125:THR:CG2	1:A:524:THR:CG2	2.88	0.51
1:B:441:LEU:N	1:B:442:PRO:HD3	2.24	0.51
1:C:436:GLN:CD	1:D:556:LYS:HZ3	2.14	0.51
1:D:138:MET:HB3	1:D:254:ARG:NH1	2.26	0.51
1:D:239:ASP:C	1:D:239:ASP:OD1	2.45	0.51
1:D:295:SER:OG	1:D:377:PRO:HD3	2.10	0.51
1:E:125:THR:CG2	1:E:524:THR:CG2	2.88	0.51
1:A:151:ARG:HG3	1:A:161:LEU:HD21	1.91	0.51
1:A:151:ARG:HB3	1:A:200:GLY:O	2.10	0.51
1:B:53:ASN:O	1:B:54:SER:C	2.48	0.51
1:C:125:THR:HG22	1:C:524:THR:HG23	1.92	0.51
1:C:132:PRO:HD3	1:C:553:TYR:CE2	2.46	0.51
1:C:171:PRO:O	1:C:175:TYR:OH	2.25	0.51
1:D:425:LEU:HD12	1:D:426:CYS:N	2.26	0.51
1:E:53:ASN:O	1:E:54:SER:C	2.48	0.51
1:E:132:PRO:HD3	1:E:553:TYR:CE2	2.46	0.51
1:E:494:HIS:C	1:E:496:PHE:N	2.64	0.51
1:A:120:GLY:O	1:A:563:PRO:HA	2.10	0.51
1:A:295:SER:OG	1:A:377:PRO:HD3	2.10	0.51
1:B:125:THR:CG2	1:B:524:THR:CG2	2.88	0.51
1:B:211:ASP:HA	1:B:508:PRO:HG2	1.89	0.51
1:B:444:MET:HE3	1:B:561:VAL:HG21	1.93	0.51
1:D:125:THR:HG22	1:D:524:THR:HG23	1.92	0.51
1:D:203:GLU:C	1:D:205:ASP:H	2.11	0.51
1:E:264:ARG:NH1	1:E:424:LEU:HD13	2.26	0.51
1:A:520:VAL:HG23	1:A:521:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:PRO:HD3	1:B:553:TYR:CE2	2.46	0.51
1:B:138:MET:HB3	1:B:254:ARG:NH1	2.26	0.51
1:B:151:ARG:HB3	1:B:200:GLY:O	2.10	0.51
1:B:264:ARG:NH1	1:B:424:LEU:HD13	2.26	0.51
1:B:295:SER:OG	1:B:377:PRO:HD3	2.10	0.51
1:C:120:GLY:O	1:C:563:PRO:HA	2.10	0.51
1:C:451:PHE:CE1	1:D:97:GLN:HB2	2.46	0.51
1:D:132:PRO:HD3	1:D:553:TYR:CE2	2.46	0.51
1:D:547:ARG:O	1:D:548:ARG:HB2	2.11	0.51
1:E:425:LEU:HD12	1:E:426:CYS:N	2.25	0.51
1:A:60:LEU:O	1:A:61:ALA:CB	2.59	0.51
1:A:556:LYS:HZ3	1:E:436:GLN:NE2	2.08	0.51
1:B:295:SER:HB3	1:B:377:PRO:CG	2.33	0.51
1:C:60:LEU:O	1:C:61:ALA:CB	2.59	0.51
1:C:138:MET:HB3	1:C:254:ARG:NH1	2.26	0.51
1:C:395:SER:C	1:C:397:ASP:H	2.14	0.51
1:C:441:LEU:N	1:C:442:PRO:HD3	2.24	0.51
1:C:494:HIS:C	1:C:496:PHE:N	2.64	0.51
1:D:295:SER:HB3	1:D:377:PRO:CG	2.33	0.51
1:D:494:HIS:C	1:D:496:PHE:N	2.64	0.51
1:D:544:THR:HG21	1:D:548:ARG:HA	1.89	0.51
1:E:125:THR:HG22	1:E:524:THR:HG23	1.92	0.51
1:E:263:LYS:HZ3	1:E:268:GLN:HB2	1.75	0.51
1:E:403:TYR:CD1	1:E:504:ILE:HD13	2.39	0.51
1:A:97:GLN:HB2	1:E:451:PHE:CE1	2.46	0.51
1:A:264:ARG:NH1	1:A:424:LEU:HD13	2.26	0.51
1:A:403:TYR:CD1	1:A:504:ILE:HG21	2.45	0.51
1:B:451:PHE:CE1	1:C:97:GLN:HB2	2.46	0.51
1:B:520:VAL:HG23	1:B:521:PRO:HD2	1.92	0.51
1:C:53:ASN:O	1:C:54:SER:C	2.48	0.51
1:C:491:SER:O	1:C:492:LEU:O	2.29	0.51
1:D:403:TYR:CD1	1:D:504:ILE:HG21	2.45	0.51
1:D:430:VAL:HG23	1:D:517:SER:HB2	1.93	0.51
1:E:197:ARG:HG3	1:E:198:GLN:HG2	1.93	0.51
1:C:425:LEU:HD12	1:C:426:CYS:N	2.25	0.51
1:D:264:ARG:NH1	1:D:424:LEU:HD13	2.26	0.51
1:E:295:SER:OG	1:E:377:PRO:HD3	2.10	0.51
1:E:441:LEU:N	1:E:442:PRO:HD3	2.24	0.51
1:A:132:PRO:HD3	1:A:553:TYR:CE2	2.46	0.51
1:A:138:MET:HB3	1:A:254:ARG:NH1	2.26	0.51
1:A:451:PHE:CE1	1:B:97:GLN:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:PHE:O	1:B:237:HIS:HB3	2.09	0.51
1:C:264:ARG:NH1	1:C:424:LEU:HD13	2.26	0.51
1:C:452:ARG:NH2	1:D:99:ASN:HD22	2.07	0.51
1:C:547:ARG:O	1:C:548:ARG:HB2	2.11	0.51
1:D:451:PHE:CE1	1:E:97:GLN:HB2	2.46	0.51
1:A:125:THR:HG22	1:A:524:THR:HG23	1.92	0.50
1:A:494:HIS:C	1:A:496:PHE:N	2.64	0.50
1:B:135:ASN:HA	1:B:172:GLU:HG2	1.93	0.50
1:A:98:ASN:ND2	1:E:452:ARG:HE	2.08	0.50
1:A:556:LYS:HZ3	1:E:436:GLN:CD	2.14	0.50
1:B:427:THR:HG23	1:B:428:PRO:HD2	1.94	0.50
1:B:451:PHE:CE1	1:C:97:GLN:HG3	2.47	0.50
1:C:266:PRO:C	1:C:268:GLN:H	2.15	0.50
1:C:567:SER:CB	1:D:49:THR:HG21	2.41	0.50
1:D:233:ASN:O	1:D:233:ASN:OD1	2.30	0.50
1:D:451:PHE:HE1	1:E:97:GLN:HG3	1.76	0.50
1:D:520:VAL:HG23	1:D:521:PRO:HD2	1.92	0.50
1:E:430:VAL:HG23	1:E:517:SER:HB2	1.93	0.50
1:A:547:ARG:O	1:A:548:ARG:HB2	2.11	0.50
1:D:197:ARG:HG3	1:D:198:GLN:HG2	1.93	0.50
1:D:243:LEU:CD2	1:D:403:TYR:HD2	2.24	0.50
1:E:138:MET:HB3	1:E:254:ARG:NH1	2.26	0.50
1:A:233:ASN:O	1:A:233:ASN:OD1	2.30	0.50
1:A:451:PHE:HE1	1:B:97:GLN:HG3	1.76	0.50
1:B:60:LEU:O	1:B:61:ALA:CB	2.59	0.50
1:D:60:LEU:O	1:D:61:ALA:CB	2.59	0.50
1:D:436:GLN:CD	1:E:556:LYS:HZ3	2.14	0.50
1:E:192:TYR:CD2	1:E:193:LEU:HD23	2.47	0.50
1:A:197:ARG:HG3	1:A:198:GLN:HG2	1.93	0.50
1:A:451:PHE:CE1	1:B:97:GLN:HG3	2.47	0.50
1:C:135:ASN:HA	1:C:172:GLU:HG2	1.94	0.50
1:C:266:PRO:O	1:C:268:GLN:N	2.43	0.50
1:C:451:PHE:CE1	1:D:97:GLN:HG3	2.47	0.50
1:C:544:THR:HG22	1:C:545:ASP:N	2.27	0.50
1:D:567:SER:CB	1:E:49:THR:HG21	2.41	0.50
1:E:211:ASP:HA	1:E:508:PRO:HG2	1.89	0.50
1:E:243:LEU:CD2	1:E:403:TYR:HD2	2.24	0.50
1:A:97:GLN:HG3	1:E:451:PHE:CE1	2.47	0.50
1:A:243:LEU:CD2	1:A:403:TYR:HD2	2.24	0.50
1:A:266:PRO:C	1:A:268:GLN:H	2.15	0.50
1:A:491:SER:O	1:A:492:LEU:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:THR:O	1:C:181:ILE:N	2.45	0.50
1:C:192:TYR:CD2	1:C:193:LEU:HD23	2.47	0.50
1:D:192:TYR:CD2	1:D:193:LEU:HD23	2.47	0.50
1:D:427:THR:HG23	1:D:428:PRO:HD2	1.94	0.50
1:E:243:LEU:CD2	1:E:244:PRO:HD3	2.42	0.50
1:E:427:THR:HG23	1:E:428:PRO:HD2	1.94	0.50
1:A:178:THR:O	1:A:181:ILE:N	2.45	0.50
1:A:544:THR:HG22	1:A:545:ASP:N	2.27	0.50
1:A:567:SER:CB	1:B:49:THR:HG21	2.41	0.50
1:B:61:ALA:HB1	1:B:62:PRO:CD	2.42	0.50
1:B:491:SER:O	1:B:492:LEU:O	2.29	0.50
1:B:544:THR:HG22	1:B:545:ASP:N	2.26	0.50
1:B:547:ARG:O	1:B:548:ARG:HB2	2.11	0.50
1:B:567:SER:CB	1:C:49:THR:HG21	2.41	0.50
1:C:451:PHE:HE1	1:D:97:GLN:HG3	1.77	0.50
1:D:237:HIS:ND1	1:D:238:PRO:O	2.45	0.50
1:A:61:ALA:HB1	1:A:62:PRO:CD	2.42	0.50
1:B:243:LEU:CD2	1:B:244:PRO:HD3	2.42	0.50
1:B:266:PRO:C	1:B:268:GLN:H	2.15	0.50
1:B:395:SER:C	1:B:397:ASP:H	2.14	0.50
1:B:425:LEU:HD12	1:B:426:CYS:N	2.26	0.50
1:C:61:ALA:HB1	1:C:62:PRO:CD	2.42	0.50
1:C:233:ASN:O	1:C:233:ASN:OD1	2.30	0.50
1:D:114:ASP:OD1	1:D:115:ASP:N	2.45	0.50
1:D:135:ASN:HA	1:D:172:GLU:HG2	1.94	0.50
1:D:451:PHE:CE1	1:E:97:GLN:HG3	2.47	0.50
1:D:491:SER:O	1:D:492:LEU:O	2.29	0.50
1:E:61:ALA:HB1	1:E:62:PRO:CD	2.42	0.50
1:A:192:TYR:CD2	1:A:193:LEU:HD23	2.47	0.50
1:B:233:ASN:O	1:B:233:ASN:OD1	2.30	0.50
1:B:386:SER:O	1:B:387:LYS:CB	2.57	0.50
1:B:436:GLN:CD	1:C:556:LYS:HZ3	2.16	0.50
1:C:114:ASP:OD1	1:C:115:ASP:N	2.45	0.50
1:C:243:LEU:CD2	1:C:244:PRO:HD3	2.42	0.50
1:D:395:SER:C	1:D:397:ASP:H	2.14	0.50
1:E:178:THR:O	1:E:181:ILE:N	2.45	0.50
1:E:266:PRO:C	1:E:268:GLN:H	2.14	0.50
1:E:266:PRO:O	1:E:268:GLN:N	2.43	0.50
1:E:547:ARG:O	1:E:548:ARG:HB2	2.11	0.50
1:A:49:THR:HG21	1:E:567:SER:CB	2.42	0.49
1:A:425:LEU:HD12	1:A:426:CYS:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:THR:O	1:B:181:ILE:N	2.45	0.49
1:B:494:HIS:C	1:B:496:PHE:N	2.64	0.49
1:D:178:THR:O	1:D:181:ILE:N	2.45	0.49
1:D:197:ARG:HG3	1:D:198:GLN:HG3	1.94	0.49
1:E:544:THR:HG22	1:E:545:ASP:N	2.26	0.49
1:A:126:ILE:HG23	1:A:523:LEU:HD23	1.94	0.49
1:A:394:ILE:HG22	1:A:400:PHE:O	2.12	0.49
1:A:486:ILE:HD11	1:E:485:LEU:HD11	1.94	0.49
1:B:481:VAL:HG21	1:C:482:TYR:OH	2.12	0.49
1:C:197:ARG:HG3	1:C:198:GLN:HG2	1.93	0.49
1:D:243:LEU:HD22	1:D:244:PRO:CD	2.43	0.49
1:D:266:PRO:C	1:D:268:GLN:H	2.15	0.49
1:D:436:GLN:NE2	1:E:556:LYS:HZ3	2.09	0.49
1:B:171:PRO:O	1:B:175:TYR:OH	2.25	0.49
1:B:212:THR:HG23	1:B:508:PRO:HB3	1.94	0.49
1:C:444:MET:HE3	1:C:561:VAL:HG21	1.94	0.49
1:D:126:ILE:HG23	1:D:523:LEU:HD23	1.94	0.49
1:D:212:THR:HG23	1:D:508:PRO:HB3	1.94	0.49
1:D:243:LEU:CD2	1:D:244:PRO:HD3	2.42	0.49
1:D:544:THR:HG22	1:D:545:ASP:N	2.26	0.49
1:E:114:ASP:OD1	1:E:115:ASP:N	2.45	0.49
1:A:243:LEU:CD2	1:A:244:PRO:HD3	2.42	0.49
1:A:395:SER:C	1:A:397:ASP:H	2.14	0.49
1:A:430:VAL:HG23	1:A:517:SER:HB2	1.93	0.49
1:B:129:THR:HG22	1:B:553:TYR:O	2.13	0.49
1:D:61:ALA:HB1	1:D:62:PRO:CD	2.42	0.49
1:E:444:MET:CE	1:E:561:VAL:HG21	2.43	0.49
1:E:491:SER:O	1:E:492:LEU:O	2.29	0.49
1:A:129:THR:HG22	1:A:553:TYR:O	2.13	0.49
1:A:436:GLN:CD	1:B:556:LYS:HZ3	2.15	0.49
1:A:481:VAL:HG21	1:B:482:TYR:OH	2.13	0.49
1:A:485:LEU:HD11	1:B:486:ILE:HD11	1.95	0.49
1:C:91:PHE:CD2	1:C:91:PHE:N	2.81	0.49
1:C:237:HIS:ND1	1:C:238:PRO:O	2.45	0.49
1:C:243:LEU:HD22	1:C:244:PRO:CD	2.43	0.49
1:E:67:THR:OG1	1:E:68:ARG:N	2.45	0.49
1:B:114:ASP:OD1	1:B:115:ASP:N	2.45	0.49
1:B:243:LEU:CD2	1:B:403:TYR:HD2	2.24	0.49
1:B:262:ARG:HH11	1:C:130:ASN:HD22	1.55	0.49
1:C:212:THR:HG23	1:C:508:PRO:HB3	1.94	0.49
1:E:60:LEU:O	1:E:61:ALA:CB	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:THR:HG22	1:E:526:HIS:NE2	2.28	0.49
1:E:135:ASN:HA	1:E:172:GLU:HG2	1.94	0.49
1:E:394:ILE:HG22	1:E:400:PHE:O	2.12	0.49
1:A:114:ASP:OD1	1:A:115:ASP:N	2.45	0.49
1:A:262:ARG:HH11	1:B:130:ASN:HD22	1.56	0.49
1:B:197:ARG:HG3	1:B:198:GLN:HG2	1.93	0.49
1:B:394:ILE:HG22	1:B:400:PHE:O	2.12	0.49
1:C:394:ILE:HG22	1:C:400:PHE:O	2.13	0.49
1:D:444:MET:CE	1:D:561:VAL:HG21	2.43	0.49
1:E:129:THR:HG22	1:E:553:TYR:O	2.13	0.49
1:E:243:LEU:HD22	1:E:244:PRO:CD	2.43	0.49
1:A:97:GLN:HG3	1:E:451:PHE:HE1	1.77	0.49
1:A:452:ARG:HE	1:B:98:ASN:ND2	2.08	0.49
1:B:451:PHE:HE1	1:C:97:GLN:HG3	1.76	0.49
1:D:67:THR:OG1	1:D:68:ARG:N	2.45	0.49
1:E:126:ILE:HG23	1:E:523:LEU:HD23	1.94	0.49
1:E:211:ASP:OD1	1:E:213:ARG:HG2	2.13	0.49
1:E:233:ASN:O	1:E:233:ASN:OD1	2.30	0.49
1:B:243:LEU:HD22	1:B:244:PRO:CD	2.43	0.49
1:B:430:VAL:HG23	1:B:517:SER:HB2	1.93	0.49
1:C:197:ARG:HG3	1:C:198:GLN:HG3	1.94	0.49
1:C:430:VAL:HG23	1:C:517:SER:HB2	1.93	0.49
1:E:449:VAL:HG12	1:E:450:THR:HG23	1.95	0.49
1:A:197:ARG:HG3	1:A:198:GLN:HG3	1.94	0.49
1:A:451:PHE:HE2	1:A:462:VAL:HG23	1.78	0.49
1:B:192:TYR:CD2	1:B:193:LEU:HD23	2.47	0.49
1:B:452:ARG:HE	1:C:98:ASN:ND2	2.08	0.49
1:C:427:THR:HG23	1:C:428:PRO:HD2	1.94	0.49
1:D:125:THR:HG22	1:D:526:HIS:NE2	2.28	0.49
1:D:129:THR:HG22	1:D:553:TYR:O	2.13	0.49
1:D:481:VAL:HG21	1:E:482:TYR:OH	2.13	0.49
1:A:212:THR:HG23	1:A:508:PRO:HB3	1.94	0.48
1:A:427:THR:HG23	1:A:428:PRO:HD2	1.94	0.48
1:B:444:MET:CE	1:B:561:VAL:HG21	2.43	0.48
1:C:243:LEU:CD2	1:C:403:TYR:HD2	2.24	0.48
1:D:69:VAL:HG22	1:D:561:VAL:HB	1.95	0.48
1:D:203:GLU:O	1:D:205:ASP:N	2.46	0.48
1:D:214:ASN:HD21	1:D:216:ARG:HG2	1.78	0.48
1:D:444:MET:HE3	1:D:561:VAL:HG21	1.94	0.48
1:A:441:LEU:HB2	1:A:445:MET:HE2	1.95	0.48
1:A:482:TYR:OH	1:E:481:VAL:HG21	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ASN:HD22	1:B:99:ASN:N	2.11	0.48
1:B:545:ASP:OD1	1:B:549:ARG:HG2	2.13	0.48
1:C:69:VAL:HG22	1:C:561:VAL:HB	1.95	0.48
1:C:203:GLU:O	1:C:205:ASP:N	2.46	0.48
1:C:449:VAL:HG12	1:C:450:THR:HG23	1.95	0.48
1:D:66:THR:HA	1:D:563:PRO:O	2.13	0.48
1:D:211:ASP:HA	1:D:508:PRO:HG2	1.89	0.48
1:E:203:GLU:O	1:E:205:ASP:N	2.46	0.48
1:A:125:THR:HG22	1:A:526:HIS:NE2	2.28	0.48
1:A:243:LEU:HD22	1:A:244:PRO:CD	2.43	0.48
1:A:449:VAL:HG12	1:A:450:THR:HG23	1.95	0.48
1:B:67:THR:OG1	1:B:68:ARG:N	2.45	0.48
1:B:237:HIS:ND1	1:B:238:PRO:O	2.45	0.48
1:C:211:ASP:OD1	1:C:213:ARG:HG2	2.13	0.48
1:C:292:TYR:HA	1:C:377:PRO:HG3	1.90	0.48
1:C:389:ARG:CD	1:C:502:ASN:HD22	2.23	0.48
1:D:91:PHE:N	1:D:91:PHE:CD2	2.81	0.48
1:A:91:PHE:N	1:A:91:PHE:CD2	2.81	0.48
1:A:214:ASN:HD21	1:A:216:ARG:HG2	1.78	0.48
1:C:444:MET:CE	1:C:561:VAL:HG21	2.43	0.48
1:C:451:PHE:HE2	1:C:462:VAL:HG23	1.78	0.48
1:C:481:VAL:HG21	1:D:482:TYR:OH	2.12	0.48
1:D:476:TYR:HD1	1:D:513:ILE:HD12	1.79	0.48
1:D:545:ASP:OD1	1:D:549:ARG:HG2	2.13	0.48
1:A:66:THR:HA	1:A:563:PRO:O	2.14	0.48
1:A:545:ASP:OD1	1:A:549:ARG:HG2	2.13	0.48
1:B:485:LEU:HD11	1:C:486:ILE:HD11	1.94	0.48
1:C:66:THR:HA	1:C:563:PRO:O	2.13	0.48
1:C:126:ILE:HG23	1:C:523:LEU:HD23	1.94	0.48
1:C:452:ARG:HE	1:D:98:ASN:ND2	2.08	0.48
1:D:394:ILE:HG22	1:D:400:PHE:O	2.13	0.48
1:D:452:ARG:HE	1:E:98:ASN:ND2	2.08	0.48
1:E:69:VAL:HG22	1:E:561:VAL:HB	1.95	0.48
1:E:212:THR:HG23	1:E:508:PRO:HB3	1.94	0.48
1:E:451:PHE:HE2	1:E:462:VAL:HG23	1.78	0.48
1:A:67:THR:OG1	1:A:68:ARG:N	2.45	0.48
1:B:197:ARG:HG3	1:B:198:GLN:HG3	1.94	0.48
1:B:211:ASP:OD1	1:B:213:ARG:HG2	2.13	0.48
1:B:292:TYR:HA	1:B:377:PRO:HG3	1.90	0.48
1:C:129:THR:HG22	1:C:553:TYR:O	2.13	0.48
1:D:485:LEU:HD11	1:E:486:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ILE:HD13	1:E:449:VAL:HG11	1.96	0.48
1:A:243:LEU:CD2	1:A:403:TYR:CE2	2.96	0.48
1:A:444:MET:CE	1:A:561:VAL:HG21	2.43	0.48
1:B:66:THR:HA	1:B:563:PRO:O	2.13	0.48
1:B:197:ARG:C	1:B:199:ASN:H	2.17	0.48
1:C:98:ASN:HD22	1:C:99:ASN:N	2.11	0.48
1:C:125:THR:HG22	1:C:526:HIS:NE2	2.28	0.48
1:C:545:ASP:OD1	1:C:549:ARG:HG2	2.13	0.48
1:D:243:LEU:HD22	1:D:244:PRO:HD2	1.96	0.48
1:D:538:VAL:HG23	1:D:538:VAL:O	2.14	0.48
1:E:214:ASN:HD21	1:E:216:ARG:HG2	1.78	0.48
1:E:237:HIS:ND1	1:E:238:PRO:O	2.45	0.48
1:A:135:ASN:HA	1:A:172:GLU:HG2	1.94	0.48
1:A:243:LEU:HD22	1:A:244:PRO:HD2	1.96	0.48
1:A:431:THR:O	1:A:432:CYS:HB2	2.14	0.48
1:B:126:ILE:HG23	1:B:523:LEU:HD23	1.94	0.48
1:E:98:ASN:HD22	1:E:99:ASN:N	2.11	0.48
1:E:243:LEU:HD22	1:E:244:PRO:HD2	1.96	0.48
1:A:389:ARG:CD	1:A:502:ASN:HD22	2.23	0.48
1:B:476:TYR:HD1	1:B:513:ILE:HD12	1.79	0.48
1:B:538:VAL:O	1:B:538:VAL:HG23	2.14	0.48
1:D:171:PRO:O	1:D:175:TYR:OH	2.25	0.48
1:E:395:SER:C	1:E:397:ASP:H	2.14	0.48
1:B:125:THR:HG22	1:B:526:HIS:NE2	2.28	0.48
1:B:203:GLU:HA	1:B:206:ILE:HG13	1.96	0.48
1:B:203:GLU:O	1:B:205:ASP:N	2.46	0.48
1:B:214:ASN:HD21	1:B:216:ARG:HG2	1.79	0.48
1:C:243:LEU:CD2	1:C:403:TYR:CE2	2.96	0.48
1:D:211:ASP:OD1	1:D:213:ARG:HG2	2.13	0.48
1:E:75:LYS:HZ2	1:E:94:THR:HG23	1.79	0.48
1:E:91:PHE:CD2	1:E:91:PHE:N	2.81	0.48
1:A:130:ASN:HD22	1:E:262:ARG:HH11	1.55	0.47
1:A:197:ARG:C	1:A:199:ASN:H	2.17	0.47
1:A:203:GLU:O	1:A:205:ASP:N	2.46	0.47
1:A:538:VAL:HG23	1:A:538:VAL:O	2.14	0.47
1:E:197:ARG:HG3	1:E:198:GLN:HG3	1.94	0.47
1:E:410:TYR:O	1:E:420:ARG:HD3	2.14	0.47
1:E:538:VAL:HG23	1:E:538:VAL:O	2.14	0.47
1:A:83:ASN:OD1	1:A:83:ASN:N	2.26	0.47
1:A:436:GLN:OE1	1:A:436:GLN:N	2.38	0.47
1:A:449:VAL:HG11	1:B:111:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:PHE:N	1:B:500:PRO:CD	2.77	0.47
1:C:214:ASN:HD21	1:C:216:ARG:HG2	1.78	0.47
1:C:410:TYR:O	1:C:420:ARG:HD3	2.14	0.47
1:D:430:VAL:CG2	1:D:431:THR:N	2.77	0.47
1:D:449:VAL:HG12	1:D:450:THR:HG23	1.95	0.47
1:D:499:PHE:N	1:D:500:PRO:CD	2.78	0.47
1:D:508:PRO:HA	1:D:509:PRO:HD3	1.73	0.47
1:E:545:ASP:OD1	1:E:549:ARG:HG2	2.13	0.47
1:A:211:ASP:OD1	1:A:213:ARG:HG2	2.13	0.47
1:A:410:TYR:O	1:A:420:ARG:HD3	2.14	0.47
1:B:243:LEU:HD22	1:B:244:PRO:HD2	1.96	0.47
1:B:431:THR:O	1:B:432:CYS:HB2	2.14	0.47
1:B:451:PHE:HE2	1:B:462:VAL:HG23	1.78	0.47
1:C:243:LEU:HD22	1:C:244:PRO:HD2	1.96	0.47
1:A:203:GLU:HA	1:A:206:ILE:HG13	1.96	0.47
1:A:405:SER:HB3	1:A:408:LEU:HB2	1.97	0.47
1:B:430:VAL:CG2	1:B:431:THR:N	2.77	0.47
1:D:98:ASN:HD22	1:D:99:ASN:N	2.12	0.47
1:D:263:LYS:HZ3	1:D:268:GLN:HB2	1.77	0.47
1:E:66:THR:HA	1:E:563:PRO:O	2.14	0.47
1:E:476:TYR:HD1	1:E:513:ILE:HD12	1.79	0.47
1:A:430:VAL:CG2	1:A:431:THR:N	2.77	0.47
1:A:499:PHE:N	1:A:500:PRO:CD	2.78	0.47
1:C:149:VAL:CG2	1:C:195:VAL:HG11	2.45	0.47
1:C:413:GLY:O	1:C:414:ASP:C	2.53	0.47
1:C:431:THR:O	1:C:432:CYS:HB2	2.14	0.47
1:C:485:LEU:HD11	1:D:486:ILE:HD11	1.94	0.47
1:D:216:ARG:HG3	1:D:216:ARG:O	2.15	0.47
1:E:216:ARG:HG3	1:E:216:ARG:O	2.15	0.47
1:E:243:LEU:CD2	1:E:403:TYR:CE2	2.96	0.47
1:E:431:THR:O	1:E:432:CYS:HB2	2.14	0.47
1:A:69:VAL:HG22	1:A:561:VAL:HB	1.95	0.47
1:A:78:ASP:OD1	1:A:94:THR:HG22	2.15	0.47
1:A:98:ASN:HD22	1:A:99:ASN:N	2.11	0.47
1:A:216:ARG:HG3	1:A:216:ARG:O	2.15	0.47
1:A:476:TYR:HD1	1:A:513:ILE:HD12	1.79	0.47
1:C:558:LEU:HD23	1:C:558:LEU:HA	1.62	0.47
1:D:405:SER:HB3	1:D:408:LEU:HB2	1.97	0.47
1:D:413:GLY:O	1:D:414:ASP:C	2.53	0.47
1:B:69:VAL:HG22	1:B:561:VAL:HB	1.95	0.47
1:B:216:ARG:O	1:B:216:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:TYR:O	1:B:420:ARG:HD3	2.14	0.47
1:B:413:GLY:O	1:B:414:ASP:C	2.53	0.47
1:B:449:VAL:HG12	1:B:450:THR:HG23	1.95	0.47
1:B:449:VAL:HG11	1:C:111:ILE:HD13	1.95	0.47
1:C:131:MET:HA	1:C:553:TYR:CD2	2.50	0.47
1:C:449:VAL:HG11	1:D:111:ILE:HD13	1.96	0.47
1:D:131:MET:HA	1:D:553:TYR:CD2	2.50	0.47
1:D:410:TYR:O	1:D:420:ARG:HD3	2.14	0.47
1:E:74:ASN:HD22	1:E:556:LYS:HZ1	1.61	0.47
1:E:180:THR:HG21	1:E:258:LEU:HD23	1.97	0.47
1:E:197:ARG:C	1:E:199:ASN:H	2.17	0.47
1:A:74:ASN:HD22	1:A:556:LYS:HZ1	1.62	0.47
1:C:197:ARG:C	1:C:199:ASN:H	2.17	0.47
1:D:449:VAL:HG11	1:E:111:ILE:HD13	1.96	0.47
1:E:131:MET:HA	1:E:553:TYR:CD2	2.50	0.47
1:E:261:ILE:HD12	1:E:406:TRP:CE3	2.50	0.47
1:A:60:LEU:HD21	1:E:451:PHE:O	2.15	0.47
1:A:261:ILE:HD12	1:A:406:TRP:CE3	2.50	0.47
1:C:389:ARG:HH11	1:C:389:ARG:CG	2.28	0.47
1:D:451:PHE:HE2	1:D:462:VAL:HG23	1.78	0.47
1:E:389:ARG:HH11	1:E:389:ARG:CG	2.28	0.47
1:E:430:VAL:CG2	1:E:431:THR:N	2.77	0.47
1:B:91:PHE:CD2	1:B:91:PHE:N	2.81	0.47
1:B:233:ASN:OD1	1:B:233:ASN:C	2.54	0.47
1:C:78:ASP:OD1	1:C:94:THR:HG22	2.14	0.47
1:C:265:GLN:HA	1:C:266:PRO:HD2	1.57	0.47
1:C:430:VAL:CG2	1:C:431:THR:N	2.78	0.47
1:D:203:GLU:HA	1:D:206:ILE:HG13	1.96	0.47
1:D:389:ARG:HH11	1:D:389:ARG:CG	2.28	0.47
1:E:405:SER:HB3	1:E:408:LEU:HB2	1.97	0.47
1:B:130:ASN:HA	1:B:519:ASN:CG	2.36	0.46
1:B:131:MET:HA	1:B:553:TYR:CD2	2.50	0.46
1:B:261:ILE:HD12	1:B:406:TRP:CE3	2.50	0.46
1:B:405:SER:HB3	1:B:408:LEU:HB2	1.97	0.46
1:C:203:GLU:HA	1:C:206:ILE:HG13	1.96	0.46
1:A:130:ASN:HA	1:A:519:ASN:CG	2.36	0.46
1:A:131:MET:HA	1:A:553:TYR:CD2	2.50	0.46
1:A:237:HIS:ND1	1:A:238:PRO:O	2.45	0.46
1:A:413:GLY:O	1:A:414:ASP:C	2.53	0.46
1:A:450:THR:HG21	1:B:96:ILE:CD1	2.46	0.46
1:A:451:PHE:O	1:B:60:LEU:HD21	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:TYR:HD1	1:C:513:ILE:HD12	1.79	0.46
1:D:138:MET:HB3	1:D:254:ARG:HH11	1.80	0.46
1:D:197:ARG:O	1:D:199:ASN:N	2.43	0.46
1:D:292:TYR:HA	1:D:377:PRO:HG3	1.90	0.46
1:A:180:THR:HG21	1:A:258:LEU:HD23	1.97	0.46
1:A:389:ARG:HH11	1:A:389:ARG:CG	2.29	0.46
1:A:436:GLN:HE22	1:B:556:LYS:HZ3	1.63	0.46
1:B:83:ASN:OD1	1:B:83:ASN:N	2.26	0.46
1:B:508:PRO:HA	1:B:509:PRO:HD3	1.73	0.46
1:C:180:THR:HG21	1:C:258:LEU:HD23	1.97	0.46
1:D:261:ILE:HD12	1:D:406:TRP:CE3	2.50	0.46
1:E:138:MET:HB3	1:E:254:ARG:HH11	1.80	0.46
1:A:96:ILE:CD1	1:E:450:THR:HG21	2.46	0.46
1:B:441:LEU:HB2	1:B:445:MET:HE2	1.98	0.46
1:C:113:LEU:HD23	1:C:113:LEU:HA	1.71	0.46
1:C:130:ASN:HA	1:C:519:ASN:CG	2.36	0.46
1:C:215:PHE:O	1:C:216:ARG:HB3	2.15	0.46
1:D:78:ASP:OD1	1:D:94:THR:HG22	2.14	0.46
1:E:203:GLU:HA	1:E:206:ILE:HG13	1.96	0.46
1:A:51:GLY:HA3	1:A:116:ARG:HH12	1.81	0.46
1:A:513:ILE:HD12	1:A:513:ILE:N	2.31	0.46
1:B:68:ARG:NH1	1:B:68:ARG:CG	2.66	0.46
1:B:211:ASP:C	1:B:212:THR:CG2	2.84	0.46
1:B:376:LYS:CB	1:B:377:PRO:HD2	2.32	0.46
1:C:451:PHE:O	1:D:60:LEU:HD21	2.16	0.46
1:D:146:ARG:HE	1:D:246:CYS:HA	1.80	0.46
1:D:410:TYR:CE2	1:E:172:GLU:OE1	2.69	0.46
1:D:450:THR:HG21	1:E:96:ILE:CD1	2.46	0.46
1:D:451:PHE:O	1:E:60:LEU:HD21	2.16	0.46
1:E:146:ARG:HE	1:E:246:CYS:HA	1.79	0.46
1:E:211:ASP:C	1:E:212:THR:CG2	2.84	0.46
1:E:413:GLY:O	1:E:414:ASP:C	2.53	0.46
1:A:427:THR:HA	1:A:428:PRO:HD3	1.75	0.46
1:B:51:GLY:HA3	1:B:116:ARG:HH12	1.81	0.46
1:B:78:ASP:OD1	1:B:94:THR:HG22	2.15	0.46
1:B:180:THR:HG21	1:B:258:LEU:HD23	1.97	0.46
1:B:202:LEU:O	1:B:205:ASP:OD1	2.34	0.46
1:C:51:GLY:HA3	1:C:116:ARG:HH12	1.81	0.46
1:C:244:PRO:HA	1:C:275:TYR:CE2	2.51	0.46
1:C:538:VAL:HG23	1:C:538:VAL:O	2.14	0.46
1:D:211:ASP:C	1:D:212:THR:CG2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:ASP:OD1	1:E:94:THR:HG22	2.14	0.46
1:A:146:ARG:HE	1:A:246:CYS:HA	1.80	0.46
1:A:178:THR:O	1:A:180:THR:N	2.49	0.46
1:A:544:THR:HG23	1:A:549:ARG:N	2.31	0.46
1:B:436:GLN:NE2	1:C:556:LYS:HZ3	2.14	0.46
1:B:450:THR:HG21	1:C:96:ILE:CD1	2.45	0.46
1:C:138:MET:HB3	1:C:254:ARG:HH11	1.80	0.46
1:C:146:ARG:HE	1:C:246:CYS:HA	1.80	0.46
1:C:178:THR:O	1:C:180:THR:N	2.49	0.46
1:C:216:ARG:HG3	1:C:216:ARG:O	2.15	0.46
1:D:130:ASN:HA	1:D:519:ASN:CG	2.36	0.46
1:D:178:THR:O	1:D:180:THR:N	2.49	0.46
1:E:215:PHE:O	1:E:216:ARG:HB3	2.15	0.46
1:A:73:ASP:OD1	1:A:73:ASP:N	2.42	0.46
1:A:132:PRO:HD3	1:A:553:TYR:CD2	2.51	0.46
1:A:233:ASN:OD1	1:A:233:ASN:C	2.54	0.46
1:B:135:ASN:HB2	1:B:172:GLU:OE2	2.16	0.46
1:B:151:ARG:NH1	1:B:205:ASP:OD2	2.49	0.46
1:B:215:PHE:O	1:B:216:ARG:HB3	2.15	0.46
1:C:261:ILE:HD12	1:C:406:TRP:CE3	2.50	0.46
1:C:544:THR:HG23	1:C:549:ARG:N	2.31	0.46
1:E:295:SER:CB	1:E:377:PRO:HG3	2.36	0.46
1:A:135:ASN:HB2	1:A:172:GLU:OE2	2.16	0.46
1:A:138:MET:HB3	1:A:254:ARG:HH11	1.80	0.46
1:A:211:ASP:C	1:A:212:THR:CG2	2.84	0.46
1:A:215:PHE:O	1:A:216:ARG:HB3	2.15	0.46
1:A:468:LEU:HA	1:A:469:PRO:HD3	1.76	0.46
1:B:146:ARG:HE	1:B:246:CYS:HA	1.80	0.46
1:B:244:PRO:HA	1:B:275:TYR:CE2	2.51	0.46
1:B:382:LEU:HD12	1:B:382:LEU:HA	1.75	0.46
1:C:211:ASP:C	1:C:212:THR:CG2	2.84	0.46
1:C:513:ILE:HD12	1:C:513:ILE:N	2.31	0.46
1:D:51:GLY:HA3	1:D:116:ARG:HH12	1.81	0.46
1:D:132:PRO:HD3	1:D:553:TYR:CD2	2.51	0.46
1:D:215:PHE:O	1:D:216:ARG:HB3	2.15	0.46
1:D:295:SER:CB	1:D:377:PRO:HG3	2.36	0.46
1:E:202:LEU:O	1:E:205:ASP:OD1	2.34	0.46
1:B:178:THR:O	1:B:180:THR:N	2.49	0.46
1:B:225:LEU:HD22	1:B:285:ALA:O	2.16	0.46
1:B:237:HIS:CD2	1:B:425:LEU:CD1	2.97	0.46
1:B:389:ARG:HH11	1:B:389:ARG:CG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ASN:OD1	1:C:233:ASN:C	2.54	0.46
1:C:405:SER:HB3	1:C:408:LEU:HB2	1.97	0.46
1:C:499:PHE:N	1:C:500:PRO:CD	2.77	0.46
1:D:135:ASN:HB2	1:D:172:GLU:OE2	2.16	0.46
1:D:202:LEU:O	1:D:205:ASP:OD1	2.34	0.46
1:E:178:THR:O	1:E:180:THR:N	2.49	0.46
1:A:225:LEU:HD22	1:A:285:ALA:O	2.16	0.45
1:B:132:PRO:HD3	1:B:553:TYR:CD2	2.51	0.45
1:B:493:THR:CG2	1:B:494:HIS:N	2.79	0.45
1:B:513:ILE:HD12	1:B:513:ILE:N	2.31	0.45
1:C:67:THR:OG1	1:C:68:ARG:N	2.45	0.45
1:C:151:ARG:NH1	1:C:205:ASP:OD2	2.49	0.45
1:C:295:SER:CB	1:C:377:PRO:HG3	2.36	0.45
1:C:450:THR:HG21	1:D:96:ILE:CD1	2.46	0.45
1:D:197:ARG:CG	1:D:198:GLN:H	2.29	0.45
1:D:244:PRO:HA	1:D:275:TYR:CE2	2.51	0.45
1:A:93:THR:HG22	1:A:94:THR:O	2.16	0.45
1:A:151:ARG:NH1	1:A:205:ASP:OD2	2.49	0.45
1:A:493:THR:HG22	1:A:494:HIS:O	2.16	0.45
1:B:451:PHE:O	1:C:60:LEU:HD21	2.16	0.45
1:C:135:ASN:HA	1:C:172:GLU:CG	2.46	0.45
1:D:431:THR:O	1:D:432:CYS:HB2	2.14	0.45
1:D:544:THR:HG23	1:D:549:ARG:N	2.31	0.45
1:E:233:ASN:OD1	1:E:233:ASN:C	2.54	0.45
1:E:244:PRO:HA	1:E:275:TYR:CE2	2.51	0.45
1:E:493:THR:HG22	1:E:494:HIS:O	2.16	0.45
1:E:544:THR:HG23	1:E:549:ARG:N	2.31	0.45
1:A:382:LEU:HD12	1:A:382:LEU:HA	1.75	0.45
1:A:410:TYR:CE2	1:B:172:GLU:OE1	2.69	0.45
1:B:135:ASN:HA	1:B:172:GLU:CG	2.47	0.45
1:C:436:GLN:HE21	1:D:558:LEU:HD11	1.81	0.45
1:C:493:THR:HG22	1:C:494:HIS:O	2.16	0.45
1:C:493:THR:CG2	1:C:494:HIS:N	2.80	0.45
1:D:195:VAL:HG12	1:D:196:GLY:N	2.32	0.45
1:D:197:ARG:C	1:D:199:ASN:H	2.17	0.45
1:D:436:GLN:HE21	1:E:558:LEU:HD11	1.81	0.45
1:D:493:THR:CG2	1:D:494:HIS:N	2.80	0.45
1:E:135:ASN:HA	1:E:172:GLU:CG	2.46	0.45
1:E:441:LEU:HB2	1:E:445:MET:HE2	1.97	0.45
1:A:558:LEU:HD11	1:E:436:GLN:HE21	1.81	0.45
1:C:146:ARG:HB2	1:C:165:TRP:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ARG:CG	1:C:198:GLN:H	2.29	0.45
1:E:51:GLY:HA3	1:E:116:ARG:HH12	1.81	0.45
1:E:93:THR:HG22	1:E:94:THR:O	2.16	0.45
1:A:135:ASN:HA	1:A:172:GLU:CG	2.47	0.45
1:A:295:SER:CB	1:A:377:PRO:HG3	2.36	0.45
1:B:135:ASN:N	1:B:140:THR:OG1	2.47	0.45
1:B:265:GLN:HA	1:B:266:PRO:HD2	1.57	0.45
1:B:436:GLN:HE21	1:C:558:LEU:HD11	1.81	0.45
1:C:68:ARG:NH1	1:C:68:ARG:CG	2.66	0.45
1:C:202:LEU:O	1:C:205:ASP:OD1	2.34	0.45
1:C:225:LEU:HD22	1:C:285:ALA:O	2.16	0.45
1:C:237:HIS:CD2	1:C:425:LEU:CD1	2.97	0.45
1:D:135:ASN:HA	1:D:172:GLU:CG	2.47	0.45
1:D:146:ARG:HB2	1:D:165:TRP:CD2	2.52	0.45
1:D:170:LEU:HB3	1:D:171:PRO:HD2	1.99	0.45
1:D:225:LEU:HD22	1:D:285:ALA:O	2.16	0.45
1:D:446:GLN:O	1:D:448:PRO:HD3	2.17	0.45
1:E:130:ASN:HA	1:E:519:ASN:CG	2.36	0.45
1:E:170:LEU:HB3	1:E:171:PRO:HD2	1.99	0.45
1:E:195:VAL:HG12	1:E:196:GLY:N	2.32	0.45
1:E:225:LEU:HD22	1:E:285:ALA:O	2.16	0.45
1:A:146:ARG:HB2	1:A:165:TRP:CD2	2.52	0.45
1:A:202:LEU:O	1:A:205:ASP:OD1	2.34	0.45
1:B:93:THR:HG22	1:B:94:THR:O	2.16	0.45
1:B:243:LEU:CD2	1:B:403:TYR:CE2	2.96	0.45
1:B:529:LEU:HD21	1:C:68:ARG:HE	1.82	0.45
1:D:151:ARG:NH1	1:D:205:ASP:OD2	2.49	0.45
1:D:441:LEU:HB2	1:D:445:MET:HE2	1.99	0.45
1:E:135:ASN:HB2	1:E:172:GLU:OE2	2.16	0.45
1:A:436:GLN:HE21	1:B:558:LEU:HD11	1.81	0.45
1:B:527:GLY:HA3	1:C:68:ARG:NH2	2.32	0.45
1:C:132:PRO:HD3	1:C:553:TYR:CD2	2.51	0.45
1:C:463:VAL:HB	1:C:529:LEU:HD13	1.99	0.45
1:D:74:ASN:ND2	1:D:556:LYS:HZ1	2.13	0.45
1:D:180:THR:HG21	1:D:258:LEU:HD23	1.97	0.45
1:D:243:LEU:HD23	1:D:244:PRO:HD3	1.99	0.45
1:D:513:ILE:HD12	1:D:513:ILE:N	2.31	0.45
1:E:132:PRO:HD3	1:E:553:TYR:CD2	2.51	0.45
1:E:202:LEU:O	1:E:203:GLU:C	2.55	0.45
1:E:446:GLN:O	1:E:448:PRO:HD3	2.17	0.45
1:E:499:PHE:N	1:E:500:PRO:CD	2.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:GLN:O	1:A:448:PRO:HD3	2.17	0.45
1:B:197:ARG:CG	1:B:198:GLN:H	2.30	0.45
1:B:544:THR:HG23	1:B:549:ARG:N	2.31	0.45
1:C:135:ASN:HB2	1:C:172:GLU:OE2	2.16	0.45
1:C:436:GLN:OE1	1:C:436:GLN:N	2.38	0.45
1:D:63:LEU:HD12	1:D:63:LEU:HA	1.82	0.45
1:D:250:PHE:O	1:D:252:HIS:N	2.50	0.45
1:E:258:LEU:HD12	1:E:258:LEU:C	2.37	0.45
1:E:513:ILE:HD12	1:E:513:ILE:N	2.31	0.45
1:E:525:ASP:OD1	1:E:525:ASP:O	2.35	0.45
1:A:243:LEU:HD23	1:A:244:PRO:HD3	1.99	0.45
1:A:292:TYR:HA	1:A:377:PRO:HG3	1.91	0.45
1:B:195:VAL:HG12	1:B:196:GLY:N	2.32	0.45
1:D:233:ASN:OD1	1:D:233:ASN:C	2.54	0.45
1:D:525:ASP:OD1	1:D:525:ASP:O	2.35	0.45
1:E:493:THR:CG2	1:E:494:HIS:N	2.80	0.45
1:B:129:THR:HB	1:B:130:ASN:H	1.65	0.45
1:B:138:MET:HB3	1:B:254:ARG:HH11	1.80	0.45
1:B:149:VAL:CG2	1:B:195:VAL:HG11	2.45	0.45
1:C:195:VAL:HG12	1:C:196:GLY:N	2.32	0.45
1:C:225:LEU:HD13	1:C:287:LEU:HA	1.99	0.45
1:C:533:ASN:OD1	1:C:533:ASN:N	2.50	0.45
1:D:529:LEU:HD21	1:E:68:ARG:HE	1.82	0.45
1:E:476:TYR:HD1	1:E:513:ILE:CD1	2.30	0.45
1:A:74:ASN:ND2	1:A:556:LYS:NZ	2.66	0.44
1:A:75:LYS:NZ	1:A:94:THR:HG23	2.33	0.44
1:A:197:ARG:O	1:A:199:ASN:N	2.43	0.44
1:A:250:PHE:O	1:A:252:HIS:N	2.50	0.44
1:A:525:ASP:OD1	1:A:525:ASP:O	2.35	0.44
1:B:146:ARG:HB2	1:B:165:TRP:CD2	2.52	0.44
1:B:170:LEU:HB3	1:B:171:PRO:HD2	1.99	0.44
1:B:203:GLU:C	1:B:205:ASP:N	2.71	0.44
1:B:295:SER:CB	1:B:377:PRO:HG3	2.36	0.44
1:B:493:THR:HG22	1:B:494:HIS:O	2.16	0.44
1:C:217:LEU:CB	1:C:232:THR:HG21	2.46	0.44
1:C:525:ASP:OD1	1:C:525:ASP:O	2.35	0.44
1:E:151:ARG:NH1	1:E:205:ASP:OD2	2.49	0.44
1:A:172:GLU:OE1	1:E:410:TYR:CE2	2.68	0.44
1:C:229:GLY:O	1:C:286:LEU:HD13	2.18	0.44
1:D:258:LEU:HD12	1:D:258:LEU:C	2.37	0.44
1:D:493:THR:HG22	1:D:494:HIS:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:PHE:O	1:E:252:HIS:N	2.50	0.44
1:E:389:ARG:CD	1:E:502:ASN:HD22	2.23	0.44
1:E:420:ARG:HG3	1:E:420:ARG:O	2.17	0.44
1:E:533:ASN:OD1	1:E:533:ASN:N	2.50	0.44
1:A:476:TYR:HD1	1:A:513:ILE:CD1	2.30	0.44
1:A:529:LEU:HD21	1:B:68:ARG:HE	1.82	0.44
1:B:225:LEU:HD13	1:B:287:LEU:HA	2.00	0.44
1:B:229:GLY:O	1:B:286:LEU:HD13	2.18	0.44
1:D:75:LYS:NZ	1:D:94:THR:HG23	2.32	0.44
1:D:217:LEU:CB	1:D:232:THR:HG21	2.46	0.44
1:D:389:ARG:CD	1:D:502:ASN:HD22	2.23	0.44
1:E:68:ARG:NH1	1:E:68:ARG:CG	2.66	0.44
1:E:75:LYS:NZ	1:E:94:THR:HG23	2.32	0.44
1:E:243:LEU:HD23	1:E:244:PRO:HD3	1.99	0.44
1:A:229:GLY:O	1:A:286:LEU:HD13	2.18	0.44
1:A:441:LEU:HD12	1:A:445:MET:CE	2.48	0.44
1:A:533:ASN:OD1	1:A:533:ASN:N	2.50	0.44
1:B:243:LEU:HD23	1:B:244:PRO:HD3	1.99	0.44
1:B:476:TYR:HD1	1:B:513:ILE:CD1	2.30	0.44
1:C:75:LYS:NZ	1:C:94:THR:HG23	2.32	0.44
1:C:93:THR:HG22	1:C:94:THR:O	2.17	0.44
1:C:203:GLU:C	1:C:205:ASP:N	2.70	0.44
1:C:262:ARG:NH1	1:D:130:ASN:ND2	2.55	0.44
1:C:410:TYR:CE2	1:D:172:GLU:OE1	2.68	0.44
1:C:527:GLY:HA3	1:D:68:ARG:NH2	2.32	0.44
1:D:203:GLU:C	1:D:205:ASP:N	2.70	0.44
1:D:265:GLN:HA	1:D:266:PRO:HD2	1.57	0.44
1:E:63:LEU:HA	1:E:63:LEU:HD12	1.82	0.44
1:A:195:VAL:HG12	1:A:196:GLY:N	2.32	0.44
1:A:203:GLU:C	1:A:205:ASP:N	2.70	0.44
1:A:429:ASP:OD1	1:A:432:CYS:N	2.51	0.44
1:B:74:ASN:ND2	1:B:556:LYS:NZ	2.65	0.44
1:B:75:LYS:NZ	1:B:94:THR:HG23	2.32	0.44
1:B:250:PHE:O	1:B:252:HIS:N	2.50	0.44
1:B:446:GLN:O	1:B:448:PRO:HD3	2.17	0.44
1:C:63:LEU:HD12	1:C:63:LEU:HA	1.82	0.44
1:C:250:PHE:O	1:C:252:HIS:N	2.50	0.44
1:C:468:LEU:HD12	1:C:468:LEU:C	2.38	0.44
1:D:93:THR:HG22	1:D:94:THR:O	2.17	0.44
1:D:295:SER:O	1:D:296:LEU:CB	2.64	0.44
1:D:429:ASP:OD1	1:D:432:CYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:ARG:HB2	1:E:165:TRP:CD2	2.52	0.44
1:E:229:GLY:O	1:E:286:LEU:HD13	2.18	0.44
1:E:441:LEU:HD12	1:E:445:MET:CE	2.48	0.44
1:B:558:LEU:HA	1:B:558:LEU:HD23	1.62	0.44
1:C:243:LEU:HD23	1:C:244:PRO:HD3	1.99	0.44
1:A:560:ILE:HD11	1:E:465:ALA:HB3	2.00	0.44
1:B:258:LEU:HD12	1:B:258:LEU:C	2.38	0.44
1:B:261:ILE:HD12	1:B:406:TRP:CZ3	2.53	0.44
1:B:436:GLN:OE1	1:B:436:GLN:N	2.39	0.44
1:B:463:VAL:HB	1:B:529:LEU:HD13	1.99	0.44
1:C:264:ARG:HG3	1:C:264:ARG:O	2.18	0.44
1:E:128:HIS:HD2	1:E:555:TYR:HD2	1.66	0.44
1:E:468:LEU:HD12	1:E:468:LEU:C	2.38	0.44
1:A:68:ARG:HE	1:E:529:LEU:HD21	1.82	0.44
1:A:83:ASN:ND2	1:A:92:LEU:O	2.51	0.44
1:A:197:ARG:CG	1:A:198:GLN:H	2.30	0.44
1:A:391:TYR:O	1:A:392:ASN:C	2.57	0.44
1:B:420:ARG:HG3	1:B:420:ARG:O	2.17	0.44
1:C:83:ASN:ND2	1:C:92:LEU:O	2.51	0.44
1:C:128:HIS:HD2	1:C:555:TYR:HD2	1.66	0.44
1:C:420:ARG:O	1:C:420:ARG:HG3	2.17	0.44
1:D:533:ASN:OD1	1:D:533:ASN:N	2.50	0.44
1:E:225:LEU:HD13	1:E:287:LEU:HA	1.99	0.44
1:E:261:ILE:HD12	1:E:406:TRP:CZ3	2.53	0.44
1:A:68:ARG:NH2	1:E:527:GLY:HA3	2.32	0.44
1:A:170:LEU:HB3	1:A:171:PRO:HD2	1.99	0.44
1:B:525:ASP:OD1	1:B:525:ASP:O	2.35	0.44
1:C:170:LEU:HB3	1:C:171:PRO:HD2	1.99	0.44
1:C:446:GLN:O	1:C:448:PRO:HD3	2.17	0.44
1:E:83:ASN:ND2	1:E:92:LEU:O	2.51	0.44
1:A:130:ASN:ND2	1:E:262:ARG:NH1	2.55	0.43
1:A:420:ARG:HG3	1:A:420:ARG:O	2.17	0.43
1:A:493:THR:CG2	1:A:494:HIS:N	2.79	0.43
1:A:527:GLY:HA3	1:B:68:ARG:NH2	2.32	0.43
1:B:467:LEU:HD12	1:B:467:LEU:HA	1.83	0.43
1:C:202:LEU:O	1:C:203:GLU:C	2.55	0.43
1:C:258:LEU:HD12	1:C:258:LEU:C	2.37	0.43
1:C:261:ILE:HD12	1:C:406:TRP:CZ3	2.53	0.43
1:D:83:ASN:ND2	1:D:92:LEU:O	2.51	0.43
1:D:106:ALA:C	1:D:108:THR:N	2.71	0.43
1:D:135:ASN:N	1:D:140:THR:OG1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:ARG:HG3	1:D:420:ARG:O	2.17	0.43
1:E:436:GLN:OE1	1:E:436:GLN:N	2.39	0.43
1:A:202:LEU:O	1:A:203:GLU:C	2.55	0.43
1:A:225:LEU:HD13	1:A:287:LEU:HA	1.99	0.43
1:A:258:LEU:HD12	1:A:258:LEU:C	2.37	0.43
1:A:264:ARG:HG3	1:A:264:ARG:O	2.18	0.43
1:A:468:LEU:HD12	1:A:468:LEU:C	2.38	0.43
1:B:533:ASN:OD1	1:B:533:ASN:N	2.50	0.43
1:D:261:ILE:HD12	1:D:406:TRP:CZ3	2.53	0.43
1:D:444:MET:HB2	1:D:539:GLN:CD	2.39	0.43
1:D:468:LEU:HD12	1:D:468:LEU:C	2.38	0.43
1:D:527:GLY:HA3	1:E:68:ARG:NH2	2.33	0.43
1:E:74:ASN:ND2	1:E:556:LYS:NZ	2.66	0.43
1:A:106:ALA:C	1:A:108:THR:H	2.22	0.43
1:A:244:PRO:HA	1:A:275:TYR:CE2	2.51	0.43
1:A:393:LEU:N	1:A:393:LEU:CD1	2.81	0.43
1:A:467:LEU:HD13	1:B:126:ILE:HG21	2.01	0.43
1:B:83:ASN:ND2	1:B:92:LEU:O	2.51	0.43
1:C:429:ASP:OD1	1:C:432:CYS:N	2.51	0.43
1:C:524:THR:OG1	1:C:525:ASP:N	2.52	0.43
1:E:264:ARG:HG3	1:E:264:ARG:O	2.18	0.43
1:A:463:VAL:HB	1:A:529:LEU:HD13	1.99	0.43
1:B:202:LEU:O	1:B:203:GLU:C	2.55	0.43
1:C:391:TYR:O	1:C:392:ASN:C	2.57	0.43
1:D:225:LEU:HD13	1:D:287:LEU:HA	1.99	0.43
1:D:262:ARG:HH11	1:E:130:ASN:HD22	1.55	0.43
1:E:197:ARG:CG	1:E:198:GLN:H	2.29	0.43
1:E:444:MET:HB2	1:E:539:GLN:CD	2.39	0.43
1:A:237:HIS:CD2	1:A:425:LEU:CD1	2.97	0.43
1:B:411:ASN:OD1	1:C:172:GLU:N	2.52	0.43
1:B:467:LEU:HD13	1:C:126:ILE:HG21	2.00	0.43
1:B:497:ASN:O	1:B:500:PRO:HD3	2.19	0.43
1:C:74:ASN:ND2	1:C:556:LYS:NZ	2.66	0.43
1:C:395:SER:C	1:C:397:ASP:N	2.71	0.43
1:C:419:ILE:C	1:C:421:SER:N	2.72	0.43
1:D:229:GLY:O	1:D:286:LEU:HD13	2.18	0.43
1:A:419:ILE:C	1:A:421:SER:N	2.72	0.43
1:A:481:VAL:O	1:A:482:TYR:C	2.57	0.43
1:A:497:ASN:O	1:A:500:PRO:HD3	2.19	0.43
1:A:524:THR:OG1	1:A:525:ASP:N	2.52	0.43
1:A:527:GLY:HA3	1:B:68:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LEU:N	1:B:393:LEU:CD1	2.81	0.43
1:B:419:ILE:C	1:B:421:SER:N	2.72	0.43
1:B:465:ALA:HB3	1:C:560:ILE:HD11	2.00	0.43
1:C:106:ALA:C	1:C:108:THR:N	2.71	0.43
1:C:476:TYR:HD1	1:C:513:ILE:CD1	2.30	0.43
1:C:527:GLY:HA3	1:D:68:ARG:HH21	1.84	0.43
1:D:74:ASN:ND2	1:D:556:LYS:NZ	2.66	0.43
1:E:149:VAL:CG2	1:E:195:VAL:HG11	2.45	0.43
1:A:68:ARG:NH1	1:A:562:SER:CB	2.79	0.43
1:A:419:ILE:O	1:A:421:SER:N	2.52	0.43
1:A:508:PRO:HA	1:A:509:PRO:HD3	1.73	0.43
1:B:262:ARG:NH1	1:C:130:ASN:ND2	2.55	0.43
1:B:429:ASP:OD1	1:B:432:CYS:N	2.51	0.43
1:C:444:MET:HB2	1:C:539:GLN:CD	2.39	0.43
1:D:463:VAL:HB	1:D:529:LEU:HD13	1.99	0.43
1:E:391:TYR:O	1:E:392:ASN:C	2.57	0.43
1:E:427:THR:HA	1:E:428:PRO:HD3	1.75	0.43
1:A:126:ILE:HG21	1:E:467:LEU:HD13	2.00	0.43
1:C:441:LEU:HB2	1:C:445:MET:HE2	2.00	0.43
1:C:465:ALA:HB3	1:D:560:ILE:HD11	2.00	0.43
1:C:529:LEU:HD21	1:D:68:ARG:HE	1.82	0.43
1:D:243:LEU:CD2	1:D:403:TYR:CE2	2.96	0.43
1:D:436:GLN:OE1	1:D:436:GLN:N	2.38	0.43
1:E:106:ALA:C	1:E:108:THR:H	2.22	0.43
1:C:481:VAL:O	1:C:482:TYR:C	2.57	0.43
1:D:74:ASN:HD22	1:D:556:LYS:HZ1	1.67	0.43
1:D:393:LEU:N	1:D:393:LEU:CD1	2.81	0.43
1:E:217:LEU:CB	1:E:232:THR:HG21	2.46	0.43
1:E:463:VAL:HB	1:E:529:LEU:HD13	1.99	0.43
1:A:128:HIS:HD2	1:A:555:TYR:HD2	1.66	0.43
1:A:214:ASN:O	1:A:216:ARG:N	2.50	0.43
1:A:261:ILE:HD12	1:A:406:TRP:CZ3	2.53	0.43
1:A:444:MET:HB2	1:A:539:GLN:CD	2.39	0.43
1:B:264:ARG:HG3	1:B:264:ARG:O	2.18	0.43
1:B:524:THR:OG1	1:B:525:ASP:N	2.52	0.43
1:C:197:ARG:O	1:C:199:ASN:N	2.43	0.43
1:D:264:ARG:HG3	1:D:264:ARG:O	2.18	0.43
1:E:68:ARG:NH1	1:E:562:SER:CB	2.79	0.43
1:E:275:TYR:CE1	1:E:404:ARG:HD2	2.54	0.43
1:E:419:ILE:O	1:E:421:SER:N	2.52	0.43
1:A:279:GLU:O	1:A:280:GLY:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:TYR:O	1:B:392:ASN:C	2.57	0.42
1:B:527:GLY:HA3	1:C:68:ARG:HH21	1.84	0.42
1:C:194:LYS:O	1:C:194:LYS:HG2	2.19	0.42
1:C:419:ILE:O	1:C:421:SER:N	2.52	0.42
1:D:65:ASP:O	1:D:66:THR:C	2.57	0.42
1:D:202:LEU:O	1:D:203:GLU:C	2.55	0.42
1:D:394:ILE:HG23	1:D:395:SER:N	2.34	0.42
1:E:65:ASP:O	1:E:66:THR:C	2.58	0.42
1:E:265:GLN:HA	1:E:266:PRO:HD2	1.57	0.42
1:E:481:VAL:O	1:E:482:TYR:C	2.57	0.42
1:E:497:ASN:O	1:E:500:PRO:HD3	2.19	0.42
1:A:451:PHE:CE1	1:B:97:GLN:CB	3.03	0.42
1:B:419:ILE:O	1:B:421:SER:N	2.52	0.42
1:B:468:LEU:HD12	1:B:468:LEU:C	2.38	0.42
1:D:68:ARG:NH1	1:D:562:SER:CB	2.79	0.42
1:D:275:TYR:CE1	1:D:404:ARG:HD2	2.54	0.42
1:D:476:TYR:HD1	1:D:513:ILE:CD1	2.30	0.42
1:B:106:ALA:C	1:B:108:THR:H	2.22	0.42
1:C:65:ASP:O	1:C:66:THR:C	2.58	0.42
1:C:411:ASN:OD1	1:D:172:GLU:N	2.51	0.42
1:C:430:VAL:O	1:C:432:CYS:N	2.53	0.42
1:C:467:LEU:HD12	1:C:467:LEU:HA	1.83	0.42
1:D:75:LYS:HZ2	1:D:94:THR:HG23	1.84	0.42
1:D:106:ALA:C	1:D:108:THR:H	2.22	0.42
1:D:128:HIS:HD2	1:D:555:TYR:HD2	1.66	0.42
1:D:278:LEU:CD2	1:D:419:ILE:HD12	2.38	0.42
1:D:441:LEU:HD12	1:D:445:MET:CE	2.47	0.42
1:E:106:ALA:C	1:E:108:THR:N	2.71	0.42
1:A:53:ASN:O	1:A:54:SER:O	2.38	0.42
1:B:128:HIS:HD2	1:B:555:TYR:HD2	1.66	0.42
1:B:389:ARG:CD	1:B:502:ASN:HD22	2.23	0.42
1:B:410:TYR:CE2	1:C:172:GLU:OE1	2.68	0.42
1:B:444:MET:HB2	1:B:539:GLN:CD	2.39	0.42
1:B:481:VAL:O	1:B:482:TYR:C	2.57	0.42
1:C:75:LYS:HZ2	1:C:94:THR:HG23	1.83	0.42
1:C:497:ASN:O	1:C:500:PRO:HD3	2.19	0.42
1:D:149:VAL:CG2	1:D:195:VAL:HG11	2.45	0.42
1:D:411:ASN:OD1	1:E:172:GLU:N	2.52	0.42
1:E:203:GLU:H	1:E:203:GLU:HG2	1.69	0.42
1:E:419:ILE:C	1:E:421:SER:N	2.72	0.42
1:A:106:ALA:C	1:A:108:THR:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLU:N	1:E:411:ASN:OD1	2.52	0.42
1:B:451:PHE:CE1	1:C:97:GLN:CB	3.03	0.42
1:C:393:LEU:N	1:C:393:LEU:CD1	2.81	0.42
1:D:419:ILE:O	1:D:421:SER:N	2.52	0.42
1:E:203:GLU:C	1:E:205:ASP:N	2.71	0.42
1:E:237:HIS:CD2	1:E:425:LEU:CD1	2.97	0.42
1:A:558:LEU:HD23	1:A:558:LEU:HA	1.62	0.42
1:B:194:LYS:O	1:B:194:LYS:HG2	2.19	0.42
1:B:230:VAL:HG13	1:B:503:GLN:NE2	2.35	0.42
1:B:275:TYR:CE1	1:B:404:ARG:HD2	2.54	0.42
1:B:295:SER:O	1:B:296:LEU:CB	2.64	0.42
1:C:230:VAL:HG13	1:C:503:GLN:NE2	2.35	0.42
1:C:275:TYR:CE1	1:C:404:ARG:HD2	2.54	0.42
1:C:478:ASP:C	1:C:480:ALA:N	2.73	0.42
1:D:93:THR:CG2	1:D:94:THR:N	2.83	0.42
1:D:230:VAL:HG13	1:D:503:GLN:NE2	2.35	0.42
1:D:502:ASN:C	1:D:504:ILE:H	2.23	0.42
1:E:53:ASN:O	1:E:54:SER:O	2.38	0.42
1:E:93:THR:CG2	1:E:94:THR:N	2.83	0.42
1:E:135:ASN:N	1:E:140:THR:OG1	2.47	0.42
1:E:230:VAL:HG13	1:E:503:GLN:NE2	2.35	0.42
1:A:230:VAL:HG13	1:A:503:GLN:NE2	2.35	0.42
1:A:395:SER:C	1:A:397:ASP:N	2.71	0.42
1:A:465:ALA:HB3	1:B:560:ILE:HD11	2.00	0.42
1:B:237:HIS:NE2	1:B:425:LEU:CD1	2.83	0.42
1:B:441:LEU:HD12	1:B:445:MET:CE	2.47	0.42
1:C:106:ALA:C	1:C:108:THR:H	2.22	0.42
1:C:502:ASN:C	1:C:504:ILE:H	2.23	0.42
1:D:279:GLU:O	1:D:280:GLY:O	2.37	0.42
1:D:467:LEU:HD13	1:E:126:ILE:HG21	2.01	0.42
1:D:524:THR:OG1	1:D:525:ASP:N	2.52	0.42
1:D:527:GLY:HA3	1:E:68:ARG:HH21	1.84	0.42
1:E:145:ALA:HB3	1:E:168:PHE:CE1	2.44	0.42
1:A:65:ASP:O	1:A:66:THR:C	2.58	0.42
1:A:411:ASN:OD1	1:B:172:GLU:N	2.52	0.42
1:A:430:VAL:O	1:A:432:CYS:N	2.53	0.42
1:A:502:ASN:C	1:A:504:ILE:H	2.23	0.42
1:C:279:GLU:O	1:C:280:GLY:O	2.38	0.42
1:D:406:TRP:HE1	1:D:419:ILE:HG21	1.85	0.42
1:D:451:PHE:CE1	1:E:97:GLN:CB	3.03	0.42
1:D:465:ALA:HB3	1:E:560:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:497:ASN:O	1:D:500:PRO:HD3	2.19	0.42
1:E:475:PHE:CD1	1:E:475:PHE:N	2.88	0.42
1:A:68:ARG:HH21	1:E:527:GLY:HA3	1.84	0.42
1:B:65:ASP:O	1:B:66:THR:C	2.57	0.42
1:B:197:ARG:O	1:B:199:ASN:N	2.43	0.42
1:B:279:GLU:O	1:B:280:GLY:O	2.38	0.42
1:C:441:LEU:HD12	1:C:445:MET:CE	2.48	0.42
1:D:53:ASN:O	1:D:54:SER:O	2.38	0.42
1:D:391:TYR:O	1:D:392:ASN:C	2.57	0.42
1:E:178:THR:C	1:E:180:THR:N	2.73	0.42
1:E:194:LYS:O	1:E:194:LYS:HG2	2.19	0.42
1:A:180:THR:O	1:A:181:ILE:C	2.58	0.42
1:A:237:HIS:NE2	1:A:425:LEU:CD1	2.83	0.42
1:B:68:ARG:NH1	1:B:562:SER:CB	2.79	0.42
1:B:475:PHE:N	1:B:475:PHE:CD1	2.88	0.42
1:B:502:ASN:C	1:B:504:ILE:H	2.23	0.42
1:C:406:TRP:HE1	1:C:419:ILE:HG21	1.85	0.42
1:C:467:LEU:HD13	1:D:126:ILE:HG21	2.01	0.42
1:D:178:THR:C	1:D:180:THR:N	2.73	0.42
1:D:194:LYS:O	1:D:194:LYS:HG2	2.19	0.42
1:D:237:HIS:NE2	1:D:425:LEU:CD1	2.83	0.42
1:E:430:VAL:O	1:E:432:CYS:N	2.53	0.42
1:E:501:GLU:O	1:E:501:GLU:HG2	2.20	0.42
1:E:524:THR:OG1	1:E:525:ASP:N	2.52	0.42
1:A:149:VAL:CG2	1:A:195:VAL:HG11	2.45	0.41
1:D:68:ARG:NH1	1:D:68:ARG:CG	2.66	0.41
1:D:129:THR:HB	1:D:130:ASN:H	1.65	0.41
1:E:131:MET:HA	1:E:132:PRO:HD3	1.87	0.41
1:A:194:LYS:HG2	1:A:194:LYS:O	2.19	0.41
1:B:53:ASN:O	1:B:54:SER:O	2.38	0.41
1:B:75:LYS:HZ2	1:B:94:THR:HG23	1.84	0.41
1:B:154:THR:HG1	1:B:160:GLU:HB2	1.83	0.41
1:B:211:ASP:C	1:B:212:THR:HG23	2.41	0.41
1:B:394:ILE:HG23	1:B:395:SER:N	2.34	0.41
1:B:406:TRP:HE1	1:B:419:ILE:HG21	1.85	0.41
1:B:430:VAL:O	1:B:432:CYS:N	2.53	0.41
1:B:468:LEU:HA	1:B:469:PRO:HD3	1.76	0.41
1:C:180:THR:O	1:C:181:ILE:C	2.58	0.41
1:D:430:VAL:O	1:D:432:CYS:N	2.53	0.41
1:E:279:GLU:O	1:E:280:GLY:O	2.38	0.41
1:E:376:LYS:CB	1:E:377:PRO:HD2	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:THR:HG1	1:A:160:GLU:HB2	1.81	0.41
1:A:178:THR:C	1:A:180:THR:N	2.73	0.41
1:A:275:TYR:CE1	1:A:404:ARG:HD2	2.54	0.41
1:B:93:THR:CG2	1:B:94:THR:N	2.83	0.41
1:B:450:THR:HG21	1:C:96:ILE:HD13	2.03	0.41
1:C:178:THR:C	1:C:180:THR:N	2.73	0.41
1:C:214:ASN:O	1:C:216:ARG:N	2.50	0.41
1:C:419:ILE:HG22	1:C:423:THR:HG22	2.02	0.41
1:C:451:PHE:CE1	1:D:97:GLN:CB	3.03	0.41
1:D:383:THR:C	1:D:384:GLU:HG3	2.41	0.41
1:D:481:VAL:O	1:D:482:TYR:C	2.57	0.41
1:E:149:VAL:O	1:E:149:VAL:HG22	2.21	0.41
1:E:243:LEU:HD23	1:E:243:LEU:HA	1.92	0.41
1:E:406:TRP:HE1	1:E:419:ILE:HG21	1.85	0.41
1:B:88:HIS:CD2	1:B:555:TYR:O	2.74	0.41
1:B:180:THR:O	1:B:181:ILE:C	2.58	0.41
1:C:135:ASN:N	1:C:140:THR:OG1	2.47	0.41
1:C:211:ASP:C	1:C:212:THR:HG23	2.41	0.41
1:C:237:HIS:NE2	1:C:425:LEU:CD1	2.83	0.41
1:C:501:GLU:O	1:C:501:GLU:HG2	2.20	0.41
1:D:501:GLU:HG2	1:D:501:GLU:O	2.20	0.41
1:D:530:PRO:HG3	1:E:66:THR:O	2.21	0.41
1:E:237:HIS:NE2	1:E:425:LEU:CD1	2.83	0.41
1:E:287:LEU:HD23	1:E:288:ASP:C	2.41	0.41
1:E:383:THR:C	1:E:384:GLU:HG3	2.41	0.41
1:A:135:ASN:N	1:A:140:THR:OG1	2.47	0.41
1:B:106:ALA:C	1:B:108:THR:N	2.71	0.41
1:C:88:HIS:CD2	1:C:555:TYR:O	2.74	0.41
1:C:382:LEU:HA	1:C:382:LEU:HD12	1.75	0.41
1:D:214:ASN:O	1:D:216:ARG:N	2.50	0.41
1:D:265:GLN:NE2	1:D:268:GLN:NE2	2.68	0.41
1:D:382:LEU:HD12	1:D:382:LEU:HA	1.75	0.41
1:E:211:ASP:C	1:E:212:THR:HG23	2.41	0.41
1:E:395:SER:C	1:E:397:ASP:N	2.71	0.41
1:B:287:LEU:HD23	1:B:288:ASP:C	2.41	0.41
1:B:395:SER:C	1:B:397:ASP:N	2.71	0.41
1:B:530:PRO:HG3	1:C:66:THR:O	2.21	0.41
1:C:211:ASP:OD1	1:C:212:THR:N	2.35	0.41
1:C:475:PHE:CD1	1:C:475:PHE:N	2.88	0.41
1:E:197:ARG:O	1:E:199:ASN:N	2.43	0.41
1:E:255:LEU:HD23	1:E:255:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:502:ASN:C	1:E:504:ILE:H	2.23	0.41
1:E:508:PRO:HA	1:E:509:PRO:HD3	1.73	0.41
1:A:153:LEU:HD23	1:A:159:VAL:HG12	2.03	0.41
1:A:203:GLU:H	1:A:203:GLU:HG2	1.69	0.41
1:A:287:LEU:HD23	1:A:288:ASP:C	2.41	0.41
1:A:406:TRP:HE1	1:A:419:ILE:HG21	1.85	0.41
1:A:419:ILE:HG22	1:A:423:THR:HG22	2.02	0.41
1:A:430:VAL:HG23	1:A:431:THR:N	2.36	0.41
1:A:530:PRO:HG3	1:B:66:THR:O	2.21	0.41
1:B:478:ASP:C	1:B:480:ALA:N	2.73	0.41
1:C:149:VAL:HG22	1:C:149:VAL:O	2.21	0.41
1:C:265:GLN:NE2	1:C:268:GLN:NE2	2.68	0.41
1:D:478:ASP:C	1:D:480:ALA:N	2.73	0.41
1:E:214:ASN:O	1:E:216:ARG:N	2.50	0.41
1:E:265:GLN:NE2	1:E:268:GLN:NE2	2.68	0.41
1:E:393:LEU:N	1:E:393:LEU:CD1	2.81	0.41
1:E:429:ASP:OD1	1:E:432:CYS:N	2.51	0.41
1:A:97:GLN:CB	1:E:451:PHE:CE1	3.03	0.41
1:A:211:ASP:C	1:A:212:THR:HG23	2.41	0.41
1:A:475:PHE:CD1	1:A:475:PHE:N	2.88	0.41
1:B:214:ASN:O	1:B:216:ARG:N	2.50	0.41
1:B:383:THR:C	1:B:384:GLU:HG3	2.41	0.41
1:C:180:THR:HG21	1:C:258:LEU:HD21	2.03	0.41
1:C:430:VAL:HG23	1:C:431:THR:N	2.36	0.41
1:C:450:THR:HG21	1:D:96:ILE:HD13	2.03	0.41
1:D:395:SER:C	1:D:397:ASP:N	2.71	0.41
1:E:113:LEU:HD23	1:E:113:LEU:HA	1.71	0.41
1:E:478:ASP:C	1:E:480:ALA:N	2.73	0.41
1:A:93:THR:CG2	1:A:94:THR:N	2.83	0.41
1:A:96:ILE:HD13	1:E:450:THR:HG21	2.03	0.41
1:A:265:GLN:NE2	1:A:268:GLN:NE2	2.68	0.41
1:A:501:GLU:HG2	1:A:501:GLU:O	2.20	0.41
1:B:113:LEU:HD23	1:B:113:LEU:HA	1.71	0.41
1:B:185:ASN:O	1:B:188:ILE:HB	2.21	0.41
1:B:243:LEU:CD1	1:B:403:TYR:HE2	2.33	0.41
1:B:381:PRO:HG2	1:B:381:PRO:O	2.21	0.41
1:C:68:ARG:NH1	1:C:562:SER:CB	2.79	0.41
1:C:504:ILE:C	1:C:506:ALA:H	2.25	0.41
1:D:134:VAL:HG21	1:D:175:TYR:CE2	2.56	0.41
1:D:153:LEU:HD23	1:D:159:VAL:HG12	2.03	0.41
1:D:180:THR:O	1:D:181:ILE:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:ASP:C	1:D:212:THR:HG23	2.41	0.41
1:D:287:LEU:HD23	1:D:288:ASP:C	2.41	0.41
1:D:394:ILE:CG2	1:D:398:SER:HB2	2.51	0.41
1:D:475:PHE:CD1	1:D:475:PHE:N	2.88	0.41
1:E:88:HIS:CD2	1:E:555:TYR:O	2.74	0.41
1:E:129:THR:HB	1:E:130:ASN:H	1.65	0.41
1:E:153:LEU:HD23	1:E:159:VAL:HG12	2.03	0.41
1:E:180:THR:O	1:E:181:ILE:C	2.58	0.41
1:A:66:THR:O	1:E:530:PRO:HG3	2.21	0.41
1:A:217:LEU:CB	1:A:232:THR:HG21	2.46	0.41
1:B:178:THR:C	1:B:180:THR:N	2.73	0.41
1:B:430:VAL:HG23	1:B:431:THR:N	2.36	0.41
1:C:53:ASN:O	1:C:54:SER:O	2.38	0.41
1:C:131:MET:HA	1:C:132:PRO:HD3	1.87	0.41
1:D:96:ILE:HD13	1:D:96:ILE:HA	1.87	0.41
1:D:131:MET:HA	1:D:132:PRO:HD3	1.87	0.41
1:D:149:VAL:HG22	1:D:149:VAL:O	2.21	0.41
1:D:290:ASP:O	1:D:291:ALA:C	2.60	0.41
1:E:295:SER:O	1:E:296:LEU:CB	2.64	0.41
1:A:383:THR:C	1:A:384:GLU:HG3	2.41	0.40
1:B:63:LEU:HA	1:B:63:LEU:HD12	1.82	0.40
1:B:153:LEU:HD23	1:B:159:VAL:HG12	2.03	0.40
1:B:501:GLU:HG2	1:B:501:GLU:O	2.20	0.40
1:C:93:THR:CG2	1:C:94:THR:N	2.83	0.40
1:C:96:ILE:HG22	1:C:98:ASN:H	1.86	0.40
1:D:96:ILE:HG22	1:D:98:ASN:H	1.86	0.40
1:D:430:VAL:HG23	1:D:431:THR:N	2.36	0.40
1:D:542:THR:O	1:D:542:THR:HG22	2.21	0.40
1:E:468:LEU:HA	1:E:469:PRO:HD3	1.76	0.40
1:A:220:ASP:HA	1:A:221:PRO:HD2	1.89	0.40
1:C:129:THR:HB	1:C:130:ASN:H	1.65	0.40
1:C:153:LEU:HD23	1:C:159:VAL:HG12	2.03	0.40
1:C:383:THR:C	1:C:384:GLU:HG3	2.41	0.40
1:D:180:THR:HG21	1:D:258:LEU:HD21	2.03	0.40
1:D:198:GLN:H	1:D:198:GLN:HG3	1.63	0.40
1:D:419:ILE:C	1:D:421:SER:N	2.72	0.40
1:A:180:THR:HG21	1:A:258:LEU:HD21	2.03	0.40
1:B:132:PRO:HD2	1:B:135:ASN:HD22	1.86	0.40
1:C:508:PRO:HA	1:C:509:PRO:HD3	1.73	0.40
1:C:530:PRO:HG3	1:D:66:THR:O	2.21	0.40
1:D:75:LYS:HB3	1:D:78:ASP:OD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:ASN:O	1:E:188:ILE:HB	2.21	0.40
1:B:75:LYS:HB3	1:B:78:ASP:OD2	2.22	0.40
1:B:96:ILE:HG22	1:B:98:ASN:H	1.86	0.40
1:B:265:GLN:NE2	1:B:268:GLN:NE2	2.68	0.40
1:C:73:ASP:OD1	1:C:73:ASP:N	2.42	0.40
1:C:134:VAL:HG21	1:C:175:TYR:CE2	2.56	0.40
1:D:145:ALA:HB3	1:D:168:PHE:CE1	2.44	0.40
1:E:243:LEU:CG	1:E:403:TYR:CE2	3.05	0.40
1:E:419:ILE:HA	1:E:422:TRP:NE1	2.37	0.40
1:A:134:VAL:HG21	1:A:175:TYR:CE2	2.56	0.40
1:A:149:VAL:HG22	1:A:149:VAL:O	2.21	0.40
1:A:211:ASP:OD1	1:A:212:THR:N	2.35	0.40
1:B:278:LEU:CD2	1:B:419:ILE:HD12	2.38	0.40
1:B:481:VAL:HG13	1:B:482:TYR:N	2.37	0.40
1:C:381:PRO:HG2	1:C:381:PRO:O	2.21	0.40
1:D:88:HIS:CD2	1:D:555:TYR:O	2.74	0.40
1:D:113:LEU:HD23	1:D:113:LEU:HA	1.71	0.40
1:D:154:THR:HG1	1:D:160:GLU:HB2	1.83	0.40
1:E:290:ASP:O	1:E:291:ALA:C	2.60	0.40
1:E:394:ILE:HG23	1:E:395:SER:N	2.34	0.40
1:E:468:LEU:HD12	1:E:469:PRO:N	2.37	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	A	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	0 8
1	B	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	0 8
1	C	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	0 8
1	D	444/523 (85%)	323 (73%)	75 (17%)	46 (10%)	0 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	0 8
All	All	2220/2615 (85%)	1619 (73%)	371 (17%)	230 (10%)	1 8

All (230) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	59	GLU
1	A	130	ASN
1	A	137	PHE
1	A	296	LEU
1	A	375	LYS
1	A	378	VAL
1	A	379	ILE
1	A	449	VAL
1	A	469	PRO
1	A	492	LEU
1	A	506	ALA
1	B	54	SER
1	B	59	GLU
1	B	130	ASN
1	B	137	PHE
1	B	296	LEU
1	B	375	LYS
1	B	378	VAL
1	B	379	ILE
1	B	449	VAL
1	B	469	PRO
1	B	492	LEU
1	B	506	ALA
1	C	54	SER
1	C	59	GLU
1	C	130	ASN
1	C	137	PHE
1	C	296	LEU
1	C	375	LYS
1	C	378	VAL
1	C	379	ILE
1	C	449	VAL
1	C	469	PRO
1	C	492	LEU
1	C	506	ALA

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Mol	Chain	Res	Type
1	D	54	SER
1	D	59	GLU
1	D	130	ASN
1	D	137	PHE
1	D	296	LEU
1	D	375	LYS
1	D	378	VAL
1	D	379	ILE
1	D	449	VAL
1	D	469	PRO
1	D	492	LEU
1	D	506	ALA
1	E	54	SER
1	E	59	GLU
1	E	130	ASN
1	E	137	PHE
1	E	296	LEU
1	E	375	LYS
1	E	378	VAL
1	E	379	ILE
1	E	449	VAL
1	E	469	PRO
1	E	492	LEU
1	E	506	ALA
1	A	50	GLY
1	A	79	VAL
1	A	157	LYS
1	A	196	GLY
1	A	204	SER
1	A	212	THR
1	A	216	ARG
1	A	251	THR
1	A	267	PHE
1	A	280	GLY
1	A	386	SER
1	A	527	GLY
1	B	50	GLY
1	B	79	VAL
1	B	157	LYS
1	B	196	GLY
1	B	204	SER
1	B	212	THR

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Mol	Chain	Res	Type
1	B	216	ARG
1	B	251	THR
1	B	267	PHE
1	B	280	GLY
1	B	386	SER
1	B	527	GLY
1	C	50	GLY
1	C	79	VAL
1	C	157	LYS
1	C	196	GLY
1	C	204	SER
1	C	212	THR
1	C	216	ARG
1	C	251	THR
1	C	267	PHE
1	C	280	GLY
1	C	386	SER
1	C	527	GLY
1	D	50	GLY
1	D	79	VAL
1	D	157	LYS
1	D	196	GLY
1	D	204	SER
1	D	212	THR
1	D	216	ARG
1	D	251	THR
1	D	267	PHE
1	D	280	GLY
1	D	386	SER
1	D	527	GLY
1	E	50	GLY
1	E	79	VAL
1	E	157	LYS
1	E	196	GLY
1	E	204	SER
1	E	212	THR
1	E	216	ARG
1	E	251	THR
1	E	267	PHE
1	E	280	GLY
1	E	386	SER
1	E	527	GLY

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Mol	Chain	Res	Type
1	A	66	THR
1	A	74	ASN
1	A	198	GLN
1	A	199	ASN
1	A	215	PHE
1	A	233	ASN
1	A	392	ASN
1	A	414	ASP
1	A	428	PRO
1	A	431	THR
1	A	479	GLN
1	B	66	THR
1	B	74	ASN
1	B	198	GLN
1	B	199	ASN
1	B	215	PHE
1	B	233	ASN
1	B	392	ASN
1	B	414	ASP
1	B	428	PRO
1	B	431	THR
1	B	479	GLN
1	C	66	THR
1	C	74	ASN
1	C	198	GLN
1	C	199	ASN
1	C	215	PHE
1	C	233	ASN
1	C	392	ASN
1	C	414	ASP
1	C	428	PRO
1	C	431	THR
1	C	479	GLN
1	D	66	THR
1	D	74	ASN
1	D	198	GLN
1	D	199	ASN
1	D	215	PHE
1	D	233	ASN
1	D	392	ASN
1	D	414	ASP
1	D	428	PRO

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Mol	Chain	Res	Type
1	D	431	THR
1	D	479	GLN
1	E	66	THR
1	E	74	ASN
1	E	198	GLN
1	E	199	ASN
1	E	215	PHE
1	E	233	ASN
1	E	392	ASN
1	E	414	ASP
1	E	428	PRO
1	E	431	THR
1	E	479	GLN
1	A	388	LYS
1	B	388	LYS
1	C	388	LYS
1	D	388	LYS
1	E	388	LYS
1	A	155	LYS
1	A	179	MET
1	A	232	THR
1	A	490	THR
1	A	513	ILE
1	B	155	LYS
1	B	179	MET
1	B	232	THR
1	B	490	THR
1	B	513	ILE
1	C	155	LYS
1	C	179	MET
1	C	266	PRO
1	C	490	THR
1	C	513	ILE
1	D	155	LYS
1	D	179	MET
1	D	490	THR
1	D	513	ILE
1	E	155	LYS
1	E	179	MET
1	E	490	THR
1	E	513	ILE
1	A	61	ALA

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Mol	Chain	Res	Type
1	A	237	HIS
1	A	266	PRO
1	B	61	ALA
1	B	237	HIS
1	B	266	PRO
1	C	61	ALA
1	C	232	THR
1	C	237	HIS
1	D	61	ALA
1	D	232	THR
1	D	237	HIS
1	D	266	PRO
1	E	61	ALA
1	E	232	THR
1	E	237	HIS
1	E	266	PRO
1	A	486	ILE
1	B	486	ILE
1	C	486	ILE
1	D	486	ILE
1	E	486	ILE
1	B	195	VAL
1	C	195	VAL
1	D	195	VAL
1	A	195	VAL
1	E	195	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	404/451 (90%)	369 (91%)	35 (9%)	10	31
1	B	404/451 (90%)	369 (91%)	35 (9%)	10	31
1	C	404/451 (90%)	369 (91%)	35 (9%)	10	31
1	D	404/451 (90%)	369 (91%)	35 (9%)	10	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	404/451 (90%)	369 (91%)	35 (9%)	10	31
All	All	2020/2255 (90%)	1845 (91%)	175 (9%)	14	31

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	76	SER
1	A	83	ASN
1	A	98	ASN
1	A	100	ASP
1	A	102	SER
1	A	146	ARG
1	A	153	LEU
1	A	166	VAL
1	A	214	ASN
1	A	223	THR
1	A	232	THR
1	A	233	ASN
1	A	238	PRO
1	A	249	ASP
1	A	256	SER
1	A	258	LEU
1	A	271	PHE
1	A	287	LEU
1	A	401	THR
1	A	420	ARG
1	A	429	ASP
1	A	440	SER
1	A	446	GLN
1	A	459	ASN
1	A	468	LEU
1	A	482	TYR
1	A	501	GLU
1	A	512	THR
1	A	525	ASP
1	A	528	THR
1	A	531	LEU
1	A	533	ASN
1	A	534	SER
1	A	562	SER
1	B	58	SER

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Mol	Chain	Res	Type
1	B	76	SER
1	B	83	ASN
1	B	98	ASN
1	B	100	ASP
1	B	102	SER
1	B	146	ARG
1	B	153	LEU
1	B	166	VAL
1	B	214	ASN
1	B	223	THR
1	B	232	THR
1	B	233	ASN
1	B	238	PRO
1	B	249	ASP
1	B	256	SER
1	B	258	LEU
1	B	271	PHE
1	B	287	LEU
1	B	401	THR
1	B	420	ARG
1	B	429	ASP
1	B	440	SER
1	B	446	GLN
1	B	459	ASN
1	B	468	LEU
1	B	482	TYR
1	B	501	GLU
1	B	512	THR
1	B	525	ASP
1	B	528	THR
1	B	531	LEU
1	B	533	ASN
1	B	534	SER
1	B	562	SER
1	C	58	SER
1	C	76	SER
1	C	83	ASN
1	C	98	ASN
1	C	100	ASP
1	C	102	SER
1	C	146	ARG
1	C	153	LEU

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Mol	Chain	Res	Type
1	C	166	VAL
1	C	214	ASN
1	C	223	THR
1	C	232	THR
1	C	233	ASN
1	C	238	PRO
1	C	249	ASP
1	C	256	SER
1	C	258	LEU
1	C	271	PHE
1	C	287	LEU
1	C	401	THR
1	C	420	ARG
1	C	429	ASP
1	C	440	SER
1	C	446	GLN
1	C	459	ASN
1	C	468	LEU
1	C	482	TYR
1	C	501	GLU
1	C	512	THR
1	C	525	ASP
1	C	528	THR
1	C	531	LEU
1	C	533	ASN
1	C	534	SER
1	C	562	SER
1	D	58	SER
1	D	76	SER
1	D	83	ASN
1	D	98	ASN
1	D	100	ASP
1	D	102	SER
1	D	146	ARG
1	D	153	LEU
1	D	166	VAL
1	D	214	ASN
1	D	223	THR
1	D	232	THR
1	D	233	ASN
1	D	238	PRO
1	D	249	ASP

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Mol	Chain	Res	Type
1	D	256	SER
1	D	258	LEU
1	D	271	PHE
1	D	287	LEU
1	D	401	THR
1	D	420	ARG
1	D	429	ASP
1	D	440	SER
1	D	446	GLN
1	D	459	ASN
1	D	468	LEU
1	D	482	TYR
1	D	501	GLU
1	D	512	THR
1	D	525	ASP
1	D	528	THR
1	D	531	LEU
1	D	533	ASN
1	D	534	SER
1	D	562	SER
1	E	58	SER
1	E	76	SER
1	E	83	ASN
1	E	98	ASN
1	E	100	ASP
1	E	102	SER
1	E	146	ARG
1	E	153	LEU
1	E	166	VAL
1	E	214	ASN
1	E	223	THR
1	E	232	THR
1	E	233	ASN
1	E	238	PRO
1	E	249	ASP
1	E	256	SER
1	E	258	LEU
1	E	271	PHE
1	E	287	LEU
1	E	401	THR
1	E	420	ARG
1	E	429	ASP

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Mol	Chain	Res	Type
1	E	440	SER
1	E	446	GLN
1	E	459	ASN
1	E	468	LEU
1	E	482	TYR
1	E	501	GLU
1	E	512	THR
1	E	525	ASP
1	E	528	THR
1	E	531	LEU
1	E	533	ASN
1	E	534	SER
1	E	562	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	86	ASN
1	A	98	ASN
1	A	99	ASN
1	A	128	HIS
1	A	130	ASN
1	A	214	ASN
1	A	265	GLN
1	A	282	ASN
1	A	402	GLN
1	A	459	ASN
1	A	471	HIS
1	B	74	ASN
1	B	86	ASN
1	B	98	ASN
1	B	99	ASN
1	B	128	HIS
1	B	130	ASN
1	B	214	ASN
1	B	265	GLN
1	B	282	ASN
1	B	402	GLN
1	B	459	ASN
1	B	471	HIS
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	86	ASN
1	C	98	ASN
1	C	99	ASN
1	C	128	HIS
1	C	130	ASN
1	C	214	ASN
1	C	265	GLN
1	C	282	ASN
1	C	402	GLN
1	C	459	ASN
1	C	471	HIS
1	D	74	ASN
1	D	86	ASN
1	D	98	ASN
1	D	99	ASN
1	D	128	HIS
1	D	130	ASN
1	D	199	ASN
1	D	214	ASN
1	D	265	GLN
1	D	282	ASN
1	D	402	GLN
1	D	459	ASN
1	D	471	HIS
1	E	74	ASN
1	E	86	ASN
1	E	98	ASN
1	E	99	ASN
1	E	128	HIS
1	E	130	ASN
1	E	214	ASN
1	E	265	GLN
1	E	282	ASN
1	E	402	GLN
1	E	459	ASN
1	E	471	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

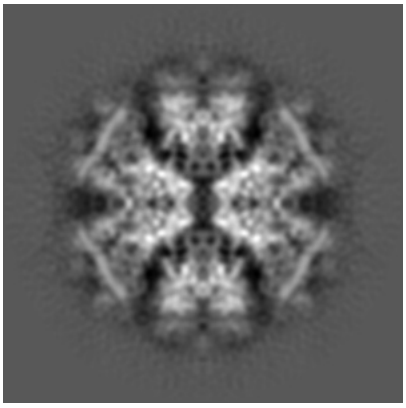
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1178. These allow visual inspection of the internal detail of the map and identification of artifacts.

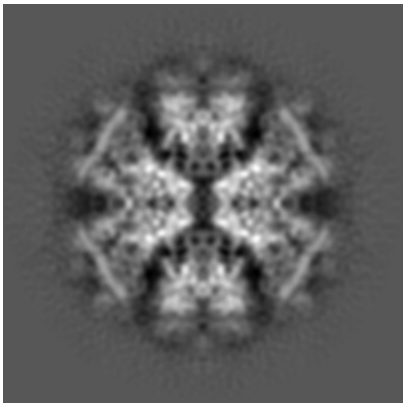
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

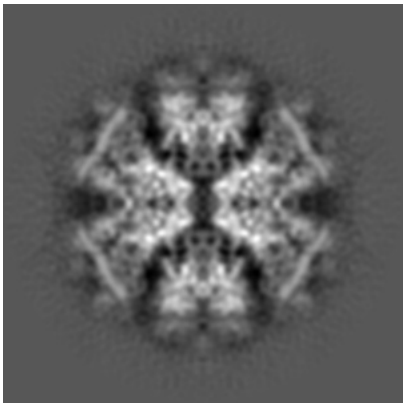
6.1.1 Primary map



X



Y

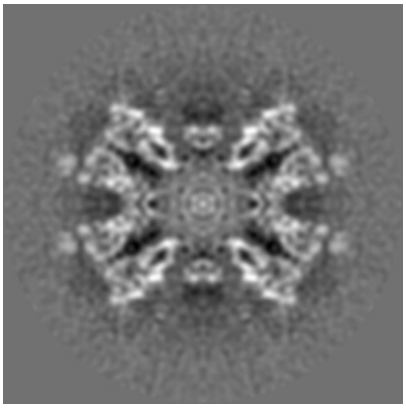


Z

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

6.2 Central slices (i)

6.2.1 Primary map



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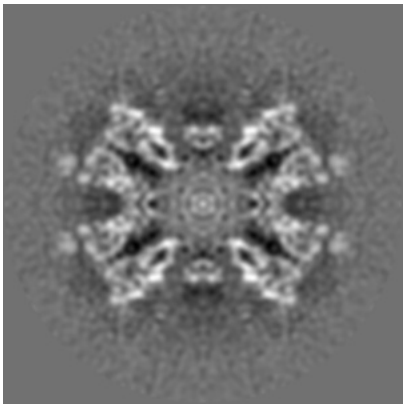
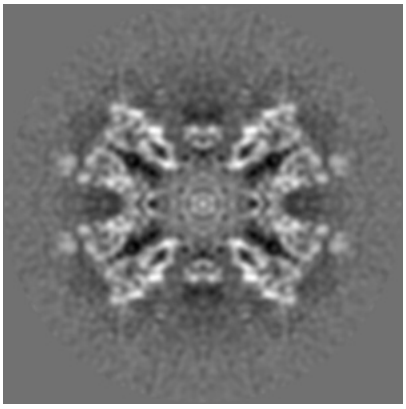


Y Index: 139

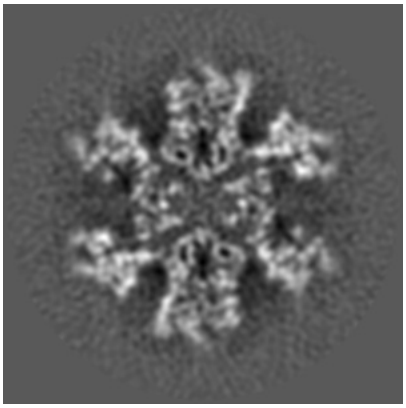


Z Index: 139

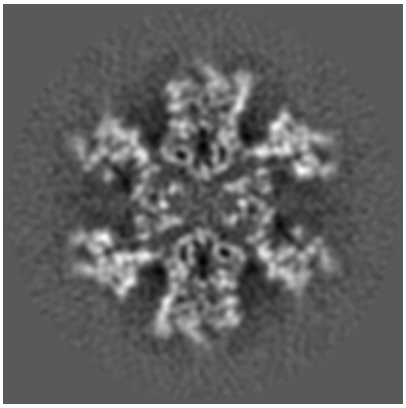
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

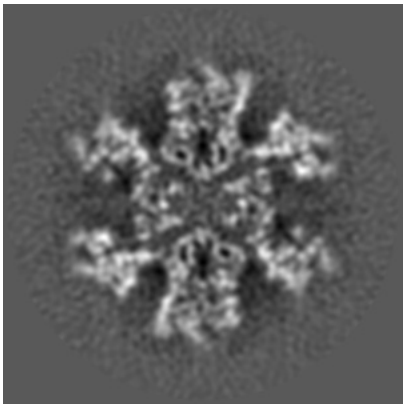
6.3.1 Primary map



X Index: 164



Y Index: 164

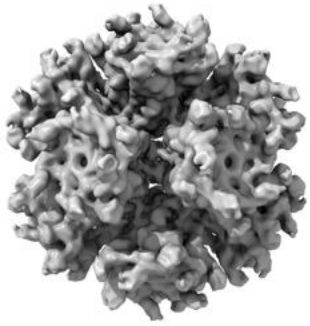


Z Index: 164

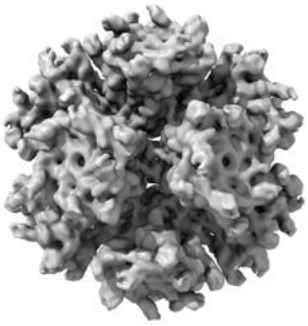
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

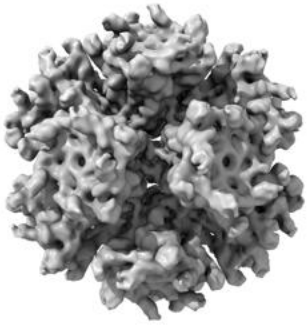
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 91.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

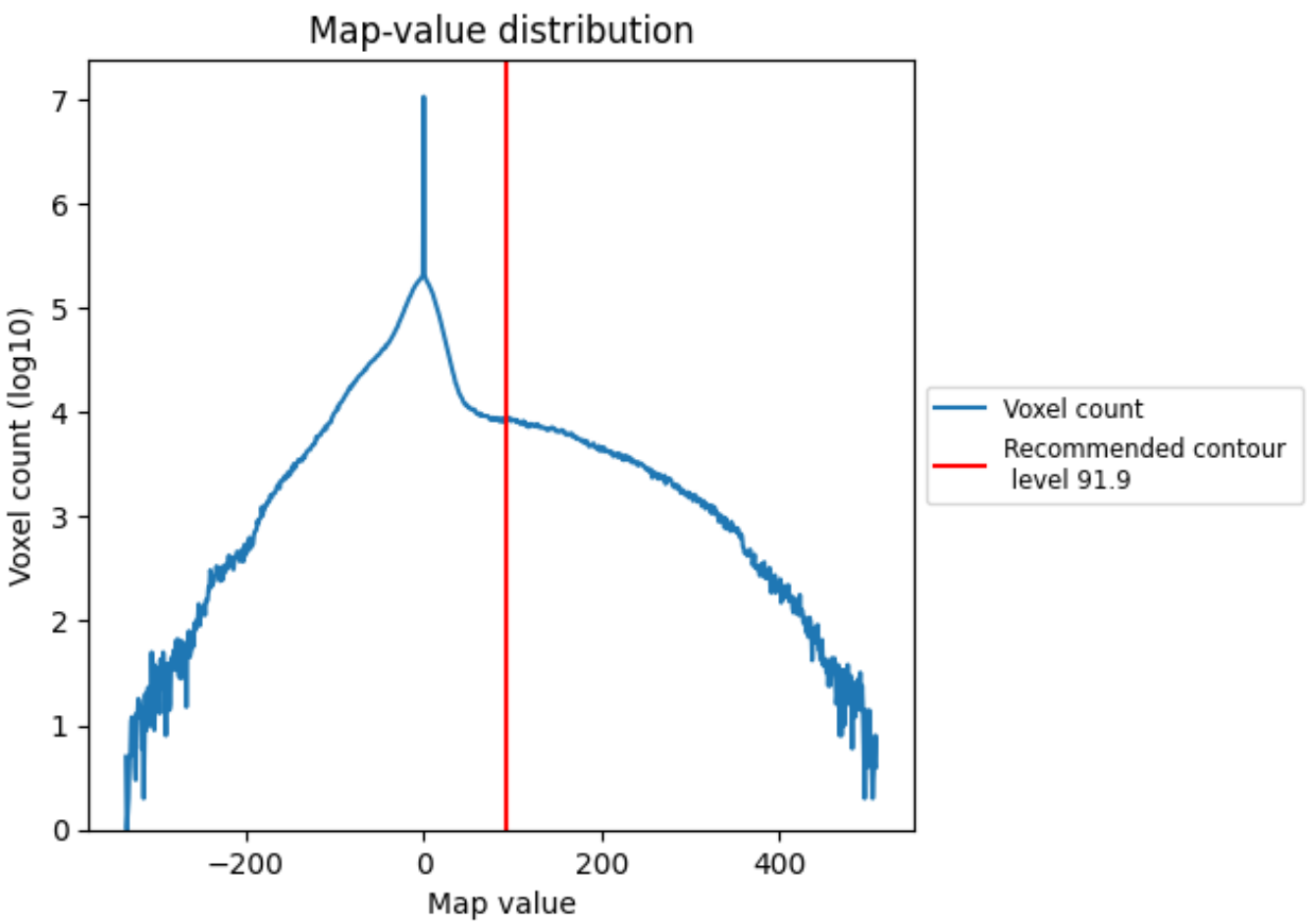
6.5 Mask visualisation (i)

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

7 Map analysis (i)

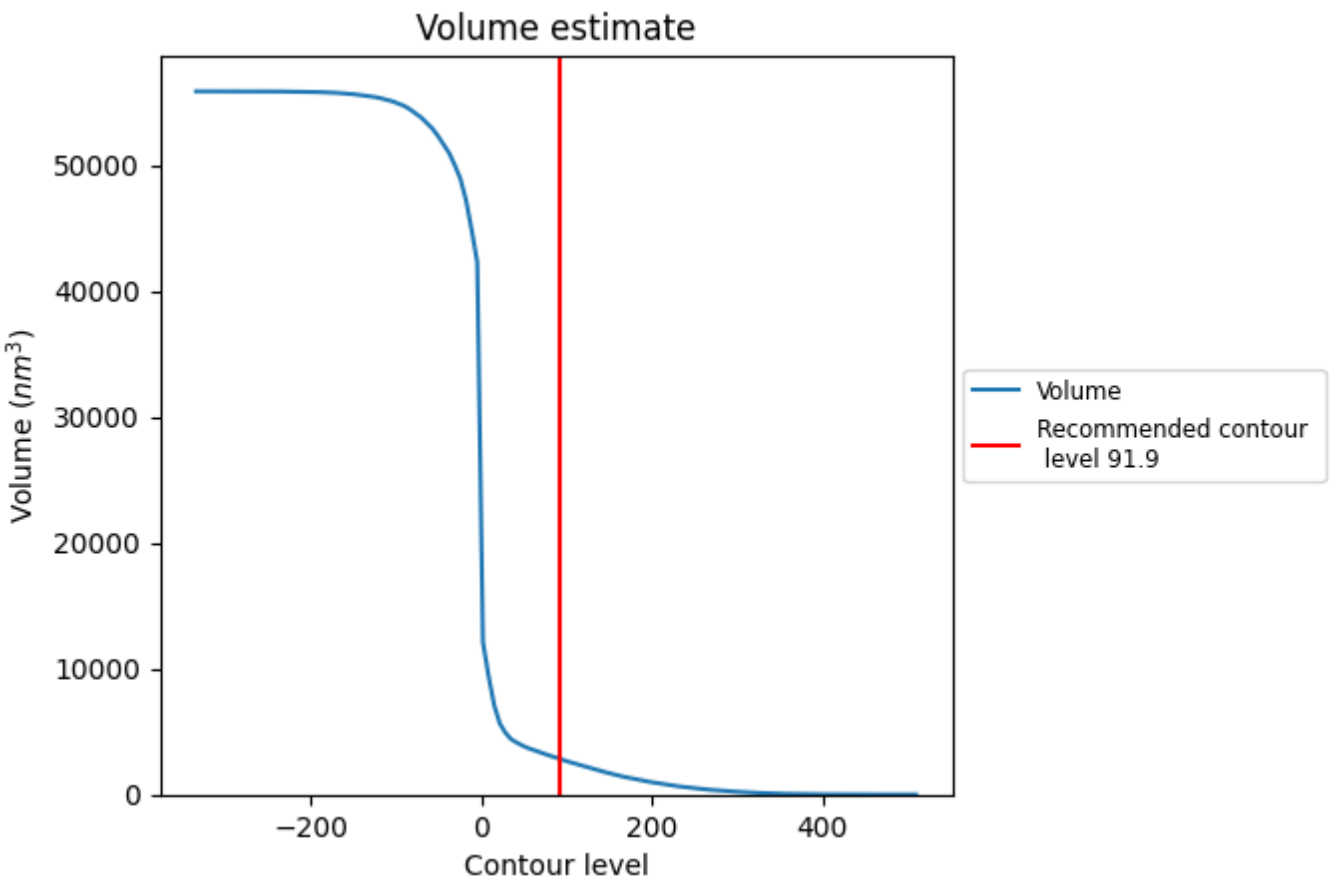
This section contains the results of statistical analysis of the map.

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.

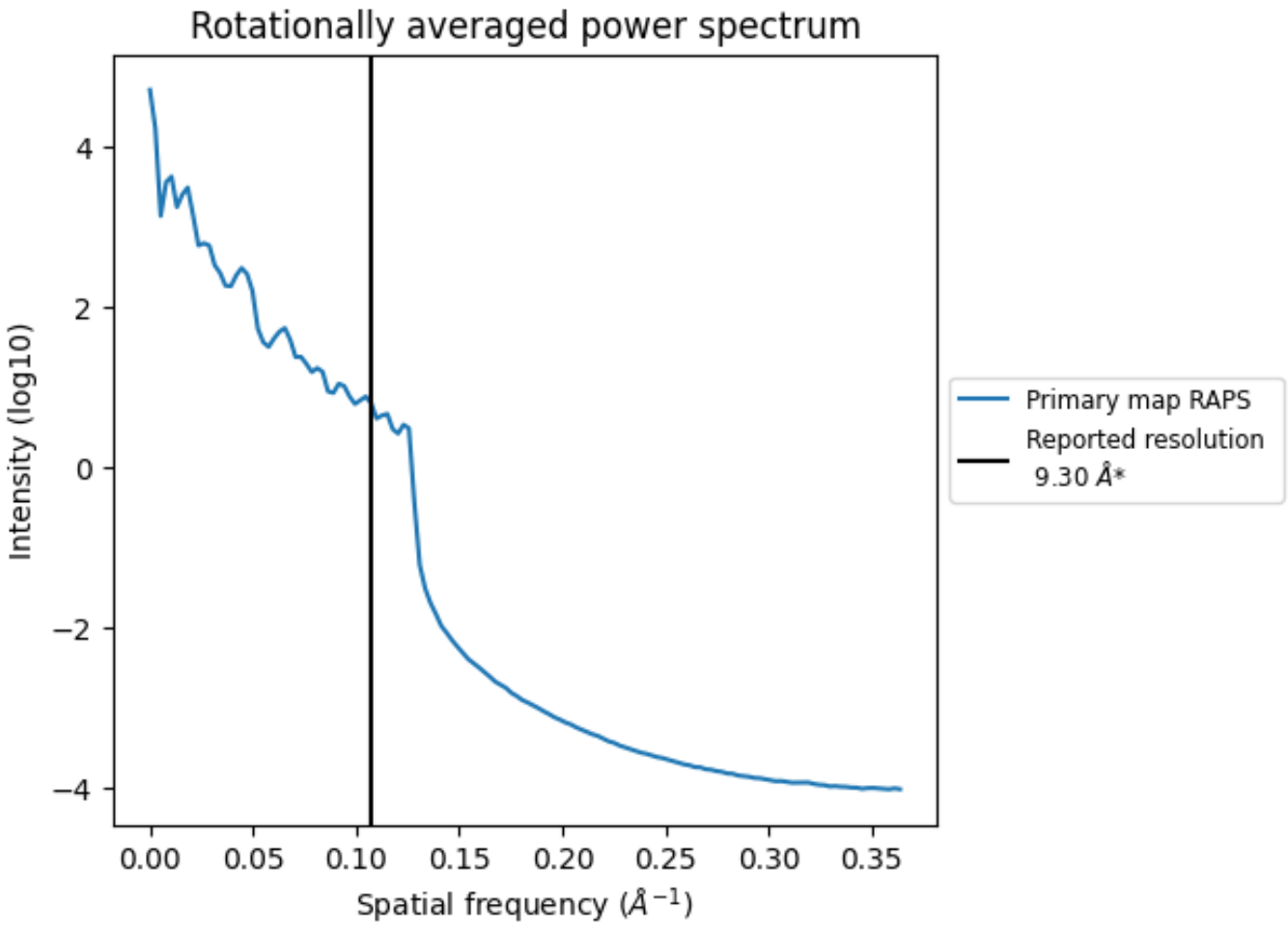
7.2 Volume estimate (i)



The volume at the recommended contour level is 2826 nm^3; this corresponds to an approximate mass of 2552 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 0.108 Å^{-1}

8 Fourier-Shell correlation (i)

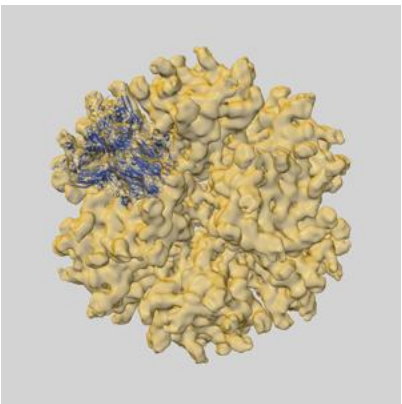
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

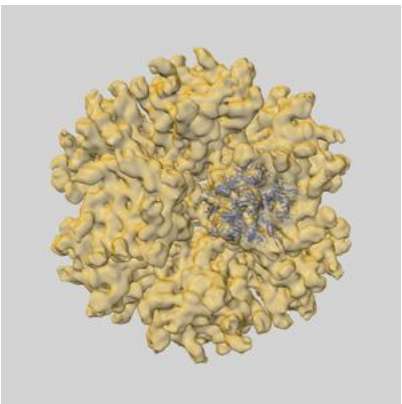
This section contains information regarding the fit between EMDB map EMD-1178 and PDB model 2C9G. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

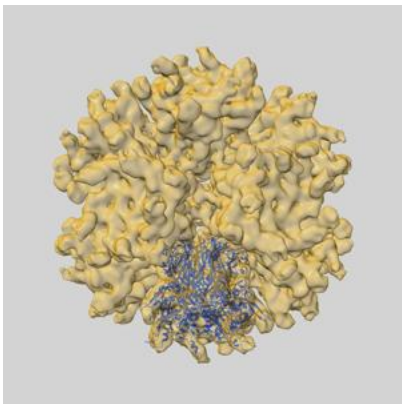
9.1.1 Map-model overlay (i)



X

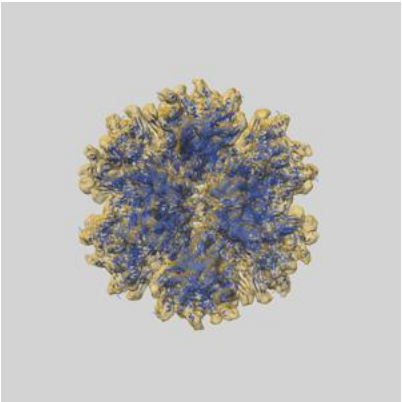


Y

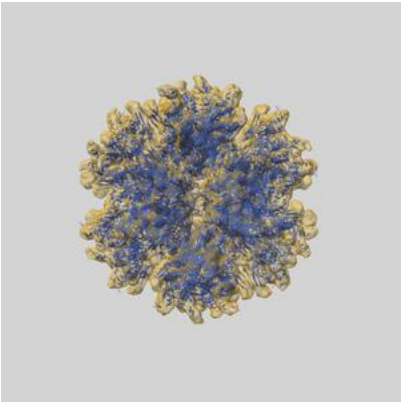


Z

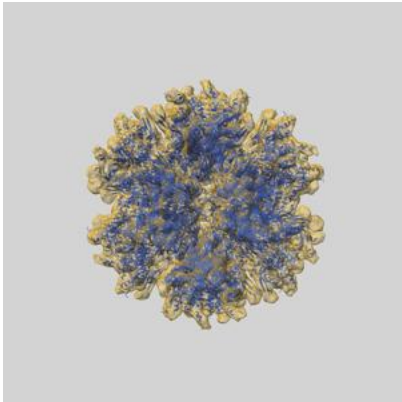
9.1.2 Map-model assembly overlay (i)



X



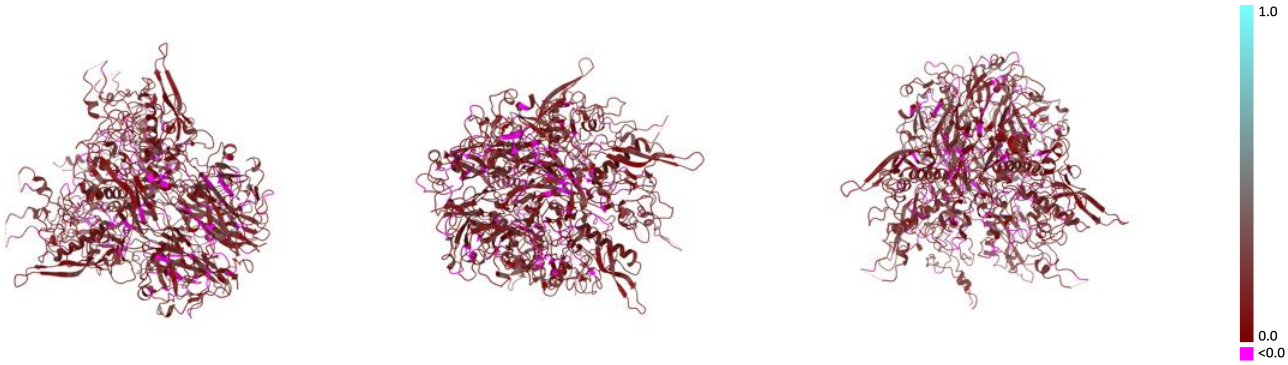
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 91.9 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.

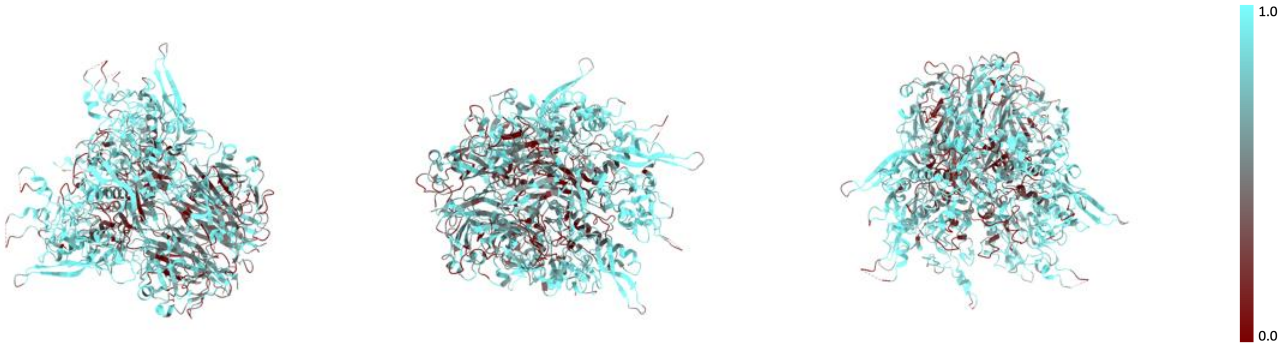
9.2 Q-score mapped to coordinate model (i)



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.

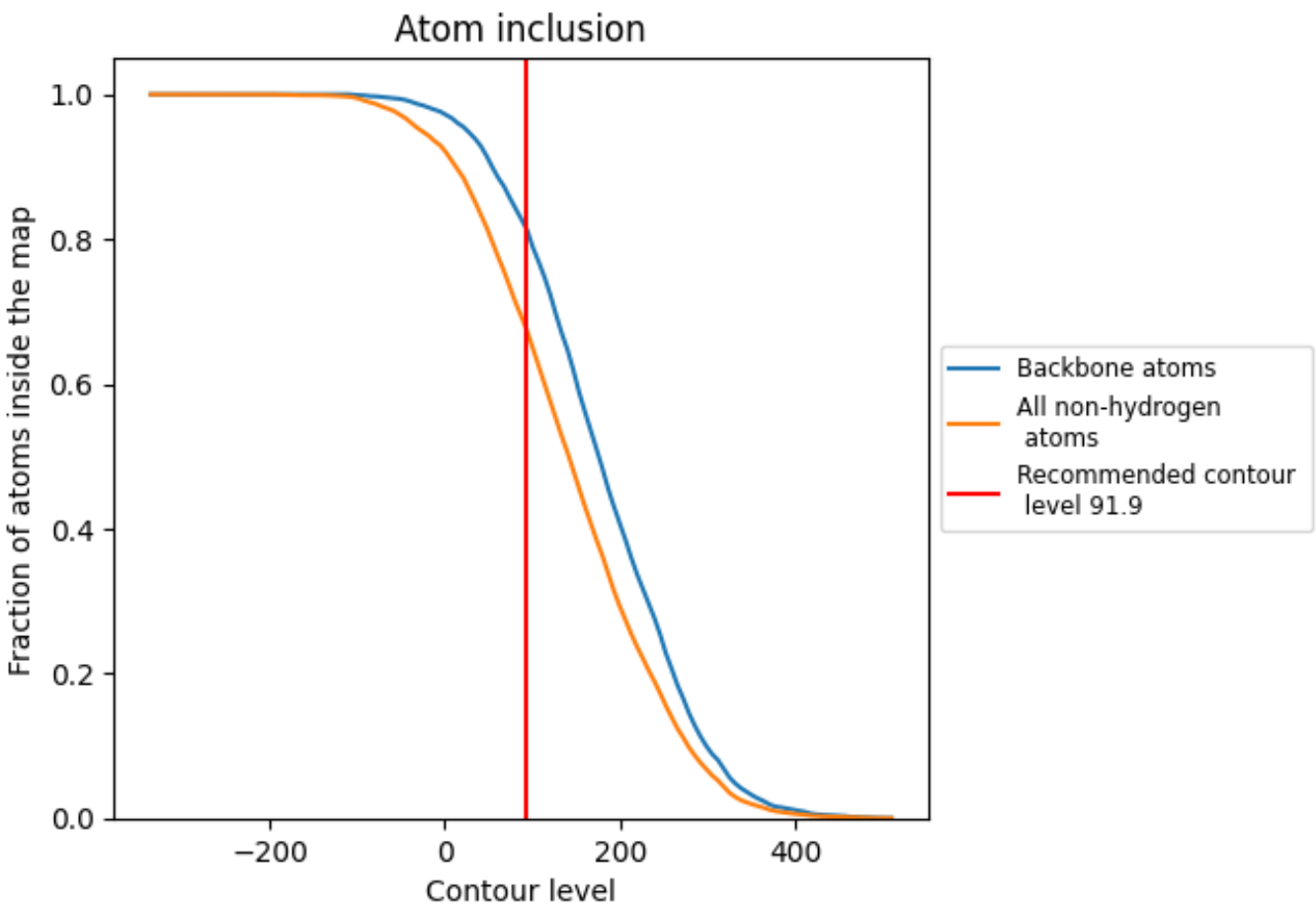
9.3 Atom inclusion mapped to coordinate model (i)



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 (91.9).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 68% 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 (91.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6784	0.1170
A	0.6753	0.1170
B	0.6833	0.1170
C	0.6767	0.1170
D	0.6778	0.1170
E	0.6787	0.1180