WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Dec 17, 2022 – 08:35 pm GMT

PDB ID	:	6YAF
EMDB ID	:	EMD-10748
Title	:	AP2 on a membrane containing tyrosine-based cargo peptide
Authors	:	Kovtun, O.; Kane Dickson, V.; Kelly, B.T.; Owen, D.; Briggs, J.A.G.
Deposited on	:	2020-03-12
Resolution	:	9.10 Å(reported)
Based on initial model	:	2XA7

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)	:	2.31.3

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 9.10 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.
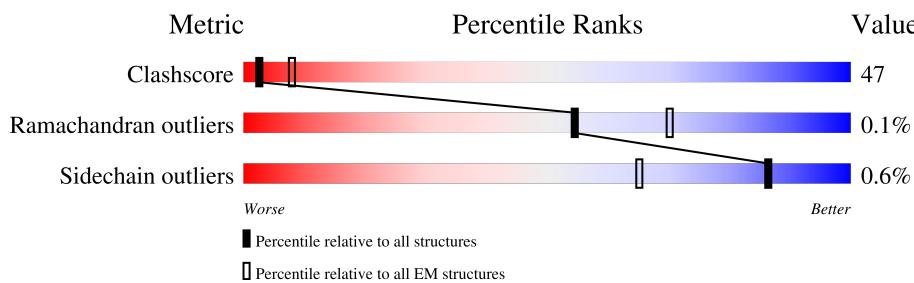
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	628	
2	B	944	
3	M	446	
4	P	16	
5	S	142	
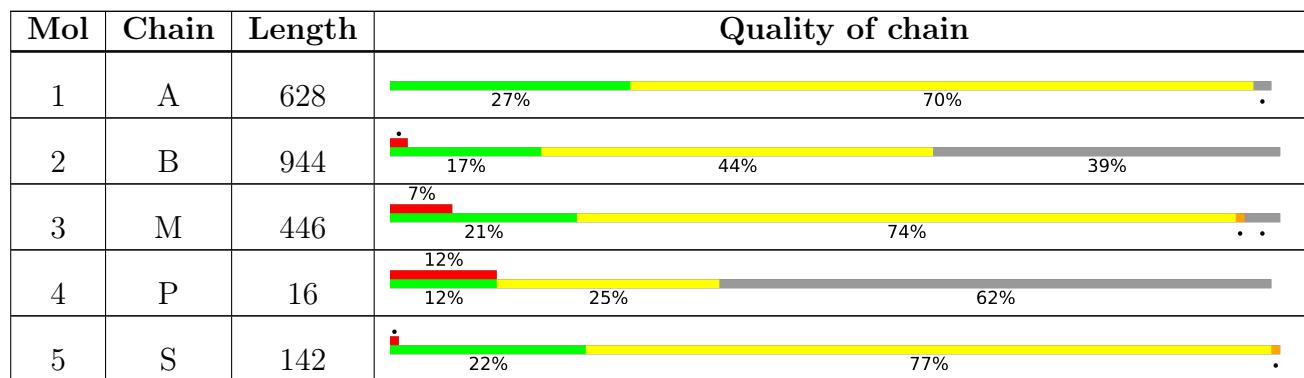
2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 14145 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 AP-2 complex subunit alpha-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	613	Total 4837	C 3081	N 833	O 902	S 21	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASP	GLU	conflict	UNP P18484
A	272	GLU	-	insertion	UNP P18484
A	622	GLY	PRO	conflict	UNP P18484
A	624	GLY	-	expression tag	UNP P18484
A	625	LEU	-	expression tag	UNP P18484
A	626	VAL	-	expression tag	UNP P18484
A	627	PRO	-	expression tag	UNP P18484
A	628	ARG	-	expression tag	UNP P18484

- Molecule 2 is a protein called AP-2 complex subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	579	Total 4597	C 2928	N 763	O 881	S 25	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	MET	-	initiating methionine	UNP P63010
B	-5	HIS	-	expression tag	UNP P63010
B	-4	HIS	-	expression tag	UNP P63010
B	-3	HIS	-	expression tag	UNP P63010
B	-2	HIS	-	expression tag	UNP P63010
B	-1	HIS	-	expression tag	UNP P63010
B	0	HIS	-	expression tag	UNP P63010

- Molecule 3 is a protein called AP-2 complex subunit mu.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	428	Total 3454	C 2208	N 601	O 625	S 20	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	237	MET	-	insertion	UNP P84092
M	238	GLU	-	insertion	UNP P84092
M	239	GLN	-	insertion	UNP P84092
M	240	LYS	-	insertion	UNP P84092
M	241	LEU	-	insertion	UNP P84092
M	242	ILE	-	insertion	UNP P84092
M	243	SER	-	insertion	UNP P84092
M	244	GLU	-	insertion	UNP P84092
M	245	GLU	-	insertion	UNP P84092
M	246	ASP	-	insertion	UNP P84092
M	247	LEU	-	insertion	UNP P84092

- Molecule 4 is a protein called Tyrosine type cargo signal derived from TGN38.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	P	6	Total 57	C 34	N 11	O 12	0	0

- Molecule 5 is a protein called AP-2 complex subunit sigma.

| Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	142	Total 1200	C 778	N 200	O 215	S 7	0	0

3 Residue-property plots ⓘ

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: AP-2 complex subunit alpha-2

Chain A:

• Molecule 2: AP-2 complex subunit beta

Chain B:

17%   44%   39%

MET HIS HIS HIS HIS HIS MET THR ASP S4 K5 Y6 F7 T8 T9 N10 K11 K12 G13 E14 I15 F16 E17 L18 K19 A20 E21 L22 N23 N24 E25 K26 K27 E28 K29 R30 K31 E32 A33 V34 K35 K36 V37 I38 A39 A40 M41 T42 V43 G44 K45 D46 V47 S48 S49 L50 F51 P52 D53

V54 V55 N56 C57 M58 Q59 T60 D61 N62 L63 E64 L65 K66 K67 L68 V69 Y70 L71 Y72 L73 M74 N75 Y76 A77 K78 S79 Q80 P81 D82 A87 V88 N89 S90 K93 D94 D97 P98 N99 P100 L101 I102 R103 A104 L105 A106 V107 R108 T109 M110 G111 C112 I113 R114 V115 D116 K117 I118

Y121 L122 C123 E124 P125 L126 R127 K128 K131 D132 E133 D134 P135 Y136 V137 R138 K139 T140 V143 C144 V145 A146 K147 L148 H149 D150 I151 N152 A153 E157 D158 Q159 L162 L165 R166 D167 L168 N173 P174 M175 V176 V177 A178 N179 A180 V181 A182 A183 L184 S185 E186 I187 S188

E189 S190 H191 P192 N195 L196 L197 D198 L199 N200 P201 Q202 N203 I204 N205 K206 L207 T208 T209 A210 L211 N212 E213 C214 W217 G218 Q219 I220 F221 I222 L223 D224 C225 L226 S227 N228 Y229 D233 D234 R235 E236 A237 Q238 S239 I240 C241 E242 R243 V244 T245 P246 R247 L248 S249 H250 A251 N252

S253 A254 V255 V256 L257 S258 K261 V262 L263 M264 K265 F266 L267 E268 L269 L270 P271 D275 Y276 Y277 N278 M279 L280 L281 K282 K283 L284 A285 P286 P287 L288 V289 T290 L291 L292 S293 G294 E295 P296 E297 V298 Q299 Y300 V301 A302 L303 R304 N305 I306 N307 L308 I309 V310 Q311 K312 R313 P314 E315

I316 L317 K318 K322 V323 F324 F325 V326 K327 D330 P331 I332 Y333 V334 K335 L336 E337 K338 L339 D340 I341 M342 I343 R344 L345 A346 S347 Q348 A349 N350 I351 A352 Q353 V354 L355 A356 E357 L358 K359 E360 Y361 A362 T363 E364 V365 D366 V367 D368 F369 V370 R371 K372 A373 V374 R375 A376 I377 G378

R379 C380 A381 I382 K383 Q386 R390 L395 L396 D397 L398 I399 Q400 T401 K402 V403 N404 Y405 V406 V407 Q408 I411 V412 V413 I414 R415 D416 I417 F418 R419 K420 Y421 P422 N423 K424 Y425 E426 S427 I428 L432 L436 L439 D440 E441 P442 D443 A444 R445 A446 A447 M448 I449 W450

I451 V452 G453 E454 Y455 A456 E457 R458 I459 D460 N461 A462 D463 E464 L465 L466 E467 S468 F469 L470 E471 G472 F473 E476 S477 T478 Q479 V480 Q481 L482 L485 T486 A487 I488 V489 K490 L491 F492 L493 K494 K495 P496 S497 E498 T499 Q500 E501 L502 V503 Q504 D505 V506 L507 S508 L509 A510 T511 Q512

D513 S514 D515 N516 P517 D518 L519 R520 D521 R522 G523 Y524 I525 Y526 W527 R528 S531 T532 D533 P534 A537 K538 E539 V540 V541 L542 S543 S544 K545 E550 E551 T552 D553 L554 I555 E556 P557 T558 L559 L560 D561 E562 L563 I564 C565 H566 I567 G568 S569 L570 A571 S572 V573 Y574 H575 K576 P577

P578 N579 A580 F581 V582 GLU GLY SER HIS ILE HIS ARG LYS HIS PRO ILE HIS HIS GLY SER THR ASP GLY ASP SER PRO VAL THR THR ALA THR ASN LEU GLU PRO GLN ILE PRO GLN GLY ASP LEU LEU GLY ASP LEU ASN LEU ASP LEU GLY

PRO PRO VAL ASN VAL PRO GLN VAL VAL SER SER MET GLN MET GLY ALA VAL ASP LEU LEU GLY GLY LEU ASP ASP SER LEU VAL GLY GLN SER GLY PHE ILE PRO SER SER VAL PRO ALA THR PHE ALA PRO SER PRO THR PRO ALA VAL VAL SER SER GLY LEU ASN ASP LEU PHE GLU LEU SER

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

ASN LYS ASN SER PHE GLY VAL ILE PRO SER THR PRO LEU ALA ILE HIS THR PRO LEU MET PRO ASN GLN SER ILE VAL ASP PHE GLU LEU PRO LEU ASN THR LEU GLY VAL PRO VAL MET LYS MET GLU MET ASN PHE THR ASN LYS ALA LEU VAL ALA VAL LYS ASN ASN ILE ASP VAL PHE ALA ILE ALA

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

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

• Molecule 3: AP-2 complex subunit mu

Chain M:

7%   21%   74%

• Molecule 4: Tyrosine type cargo signal derived from TGN38

Chain P:

• Molecule 5: AP-2 complex subunit sigma

Chain S:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	100556	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction in novaCTF with by multiplication	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/Å^2)$	3.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	6500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	4.546	Depositor
Minimum map value	-3.015	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.259	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	227.84, 227.84, 227.84	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.78, 1.78, 1.78	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.31	0/4922	0.46	0/6669
2	B	0.31	0/4669	0.46	0/6331
3	M	0.33	0/3520	0.51	0/4735
4	P	0.34	0/57	0.76	0/74
5	S	0.33	0/1224	0.51	0/1650
All	All	0.32	0/14392	0.48	0/19459

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	191	HIS	Peptide
2	B	251	ALA	Peptide

5.2 Too-close contacts ⓘ

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	4837	0	4952	440	0
2	B	4597	0	4715	442	0
3	M	3454	0	3536	389	0
4	P	57	0	53	7	0
5	S	1200	0	1195	124	0
All	All	14145	0	14451	1349	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 47.

All (1349) 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)
3:M:2:ILE:H	3:M:119:GLY:HA3	1.29	0.98
2:B:54:VAL:O	2:B:58:MET:HB2	1.70	0.91
1:A:273:ASP:H	1:A:277:ARG:HD2	1.33	0.91
3:M:433:VAL:HG12	4:P:5:LEU:HD22	1.51	0.90
3:M:170:ARG:HH21	3:M:430:ILE:HG12	1.32	0.90
3:M:322:PHE:H	3:M:372:MET:H	1.21	0.87
1:A:271:PRO:HA	1:A:277:ARG:HD3	1.56	0.86
2:B:108:ARG:NH2	2:B:140:THR:OG1	2.09	0.85
3:M:312:LEU:HB2	3:M:383:LEU:HD11	1.54	0.85
1:A:518:SER:H	1:A:522:GLN:HE22	1.24	0.85
2:B:350:ASN:HB3	2:B:353:GLN:HE21	1.43	0.84
2:B:540:VAL:O	2:B:545:LYS:NZ	2.12	0.83
3:M:33:ARG:O	3:M:37:ILE:HB	1.78	0.83
3:M:268:PHE:O	3:M:272:ARG:N	2.11	0.82
3:M:174:PHE:HA	3:M:432:TRP:HB2	1.63	0.81
3:M:32:PHE:CE1	3:M:55:PHE:CZ	2.69	0.80
5:S:42:ARG:NH1	5:S:59:TYR:OH	2.15	0.79
5:S:7:ILE:HD13	5:S:16:LEU:HD23	1.63	0.79
2:B:122:LEU:O	2:B:126:LEU:N	2.14	0.79
1:A:43:LYS:HE3	1:A:49:ALA:HA	1.63	0.79
3:M:432:TRP:HE1	4:P:4:ARG:HE	1.31	0.78
3:M:319:LYS:NZ	3:M:320:SER:O	2.15	0.78
3:M:213:LYS:HB2	3:M:416:LYS:HB2	1.64	0.77
1:A:240:ALA:HA	1:A:253:PRO:HB3	1.65	0.77
3:M:331:ILE:HB	3:M:366:ILE:HB	1.67	0.77
1:A:399:ARG:HG3	1:A:435:TYR:HB3	1.66	0.77
2:B:496:PRO:O	2:B:500:GLN:NE2	2.18	0.77
3:M:250:GLN:HE21	3:M:408:SER:HA	1.50	0.76
1:A:383:VAL:HB	1:A:387:GLN:HE22	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:323:LYS:HB3	3:M:326:LEU:HG	1.66	0.76
5:S:13:LYS:HB2	5:S:15:ARG:HH21	1.47	0.76
1:A:257:LEU:HA	1:A:260:LYS:HD2	1.66	0.76
3:M:370:ALA:HB3	3:M:373:LYS:HE2	1.66	0.76
3:M:260:HIS:NE2	3:M:284:GLU:OE1	2.18	0.76
3:M:32:PHE:CZ	3:M:55:PHE:CE1	2.74	0.76
2:B:115:VAL:HG13	2:B:116:ASP:H	1.51	0.75
1:A:285:GLU:HA	1:A:329:ARG:HH12	1.51	0.75
2:B:361:TYR:HA	2:B:364:GLU:HG2	1.68	0.75
1:A:83:LEU:O	1:A:91:LYS:NZ	2.17	0.75
2:B:229:TYR:O	2:B:265:LYS:NZ	2.18	0.75
3:M:351:GLY:HA3	3:M:366:ILE:HG12	1.69	0.74
3:M:60:ARG:NH1	3:M:86:CYS:SG	2.61	0.73
3:M:153:SER:O	3:M:157:GLY:N	2.17	0.73
2:B:124:GLU:HG3	2:B:128:LYS:HE3	1.69	0.73
2:B:214:CYS:O	2:B:219:GLN:NE2	2.22	0.73
1:A:469:VAL:O	1:A:476:GLN:NE2	2.21	0.73
3:M:264:ARG:H	3:M:274:ILE:HB	1.53	0.73
1:A:527:HIS:HA	1:A:530:PHE:HB2	1.70	0.72
2:B:111:GLY:O	2:B:114:ARG:NH1	2.19	0.72
3:M:349:MET:HG3	3:M:376:GLN:H	1.53	0.72
3:M:323:LYS:NZ	3:M:325:SER:OG	2.20	0.72
5:S:102:ASP:O	5:S:106:ASN:ND2	2.21	0.72
1:A:62:LEU:HB3	1:A:72:ILE:HG13	1.71	0.72
1:A:147:PHE:HB3	1:A:151:ILE:HG12	1.71	0.72
1:A:66:PHE:HD1	1:A:71:ASP:HA	1.54	0.72
2:B:98:PRO:O	2:B:103:ARG:NH2	2.23	0.72
1:A:41:ARG:O	1:A:45:LYS:N	2.15	0.72
2:B:149:HIS:HA	2:B:153:ALA:HB2	1.72	0.72
1:A:380:GLU:HG3	1:A:382:ASP:H	1.54	0.72
2:B:485:LEU:HB2	2:B:522:ARG:HH21	1.55	0.72
3:M:4:GLY:HA2	3:M:19:VAL:HA	1.72	0.72
1:A:43:LYS:HA	1:A:47:ASP:HB2	1.71	0.72
2:B:516:ASN:OD1	2:B:519:LEU:N	2.23	0.72
2:B:543:SER:O	2:B:545:LYS:NZ	2.22	0.72
3:M:1:MET:N	3:M:118:PHE:O	2.21	0.72
2:B:404:ASN:O	2:B:408:GLN:N	2.23	0.72
2:B:175:MET:HE1	3:M:156:THR:HA	1.71	0.71
3:M:342:SER:HB2	3:M:382:GLU:HB2	1.72	0.71
1:A:520:LEU:HD13	1:A:555:VAL:HG23	1.70	0.71
3:M:95:LYS:NZ	3:M:97:SER:OG	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:100:ASN:O	3:M:104:ASN:ND2	2.19	0.71
3:M:180:SER:HA	3:M:438:ARG:HB3	1.70	0.71
5:S:42:ARG:O	5:S:61:ARG:NH1	2.21	0.71
2:B:364:GLU:HB2	2:B:369:PHE:HZ	1.54	0.71
5:S:7:ILE:HB	5:S:16:LEU:HB3	1.72	0.71
2:B:457:GLU:HA	2:B:495:LYS:HE2	1.71	0.71
3:M:347:ILE:HB	3:M:378:SER:H	1.54	0.71
1:A:365:ALA:O	1:A:368:THR:OG1	2.08	0.71
1:A:384:SER:O	1:A:388:ARG:NH1	2.24	0.71
2:B:492:PHE:HD1	2:B:499:THR:HB	1.56	0.71
3:M:320:SER:N	3:M:373:LYS:O	2.23	0.71
1:A:77:MET:SD	1:A:77:MET:N	2.63	0.71
1:A:519:PRO:O	1:A:523:PHE:HB2	1.91	0.71
3:M:304:VAL:HG22	3:M:314:VAL:HG13	1.72	0.71
1:A:194:HIS:HA	1:A:197:ASN:HD22	1.56	0.70
1:A:198:ASP:O	1:A:232:ARG:NH2	2.21	0.70
1:A:550:ASN:HB3	1:A:599:LEU:HD22	1.73	0.70
2:B:304:ARG:HH21	2:B:574:TYR:HA	1.56	0.70
1:A:398:ASP:H	1:A:401:ASN:HD21	1.37	0.70
2:B:210:ALA:O	2:B:214:CYS:N	2.24	0.70
1:A:193:VAL:O	1:A:197:ASN:ND2	2.25	0.70
2:B:135:PRO:O	2:B:139:LYS:HB2	1.90	0.70
2:B:185:SER:O	2:B:188:SER:OG	2.10	0.70
2:B:309:ILE:O	2:B:313:ARG:N	2.19	0.70
1:A:59:VAL:HG21	1:A:82:LEU:HD11	1.74	0.70
1:A:79:ALA:HA	1:A:82:LEU:HD12	1.72	0.70
3:M:144:THR:H	3:M:147:GLU:HB3	1.57	0.70
5:S:51:GLU:HA	5:S:56:LYS:HA	1.74	0.70
3:M:60:ARG:HH12	3:M:83:TYR:HA	1.55	0.70
3:M:337:THR:HG22	3:M:362:ILE:HG13	1.74	0.70
2:B:234:ASP:OD1	2:B:235:ARG:NH1	2.25	0.70
2:B:166:ARG:HH12	2:B:197:LEU:H	1.39	0.69
3:M:214:PHE:HA	3:M:415:LEU:HA	1.73	0.69
3:M:255:ASP:OD2	3:M:291:THR:N	2.22	0.69
2:B:6:TYR:HB3	3:M:102:LYS:HG2	1.74	0.69
3:M:115:ILE:O	3:M:122:GLN:N	2.25	0.69
2:B:249:SER:HA	2:B:252:ASN:HD21	1.58	0.69
3:M:304:VAL:HG13	3:M:314:VAL:HG22	1.75	0.69
2:B:264:MET:HA	2:B:267:LEU:HB2	1.75	0.69
2:B:476:GLU:O	2:B:481:GLN:NE2	2.25	0.69
2:B:19:LYS:O	2:B:23:ASN:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:2:ILE:N	3:M:119:GLY:HA3	2.07	0.69
2:B:28:GLU:HG2	2:B:29:LYS:H	1.57	0.68
3:M:309:ARG:NH1	3:M:387:ASN:O	2.26	0.68
1:A:78:GLU:N	1:A:78:GLU:OE1	2.24	0.68
1:A:448:ASN:HB3	1:A:451:ARG:HH21	1.58	0.68
2:B:184:LEU:HB2	2:B:196:LEU:HD11	1.74	0.68
1:A:335:GLY:O	1:A:339:GLN:NE2	2.27	0.68
2:B:32:GLU:HA	2:B:35:LYS:HD2	1.74	0.68
3:M:90:ALA:O	3:M:94:GLY:N	2.26	0.68
3:M:170:ARG:HG3	3:M:172:GLU:HG3	1.76	0.68
1:A:21:ARG:O	1:A:24:LYS:NZ	2.23	0.68
2:B:43:VAL:HG23	2:B:45:LYS:HG2	1.76	0.68
2:B:305:ASN:HD21	2:B:573:VAL:HG22	1.59	0.68
2:B:34:VAL:HG11	2:B:68:LEU:HD22	1.74	0.68
1:A:455:ASP:OD2	1:A:493:HIS:ND1	2.26	0.68
2:B:135:PRO:HB3	2:B:173:ASN:HD21	1.58	0.68
1:A:334:LEU:HD13	1:A:353:MET:HG3	1.75	0.67
1:A:519:PRO:O	1:A:523:PHE:CB	2.41	0.67
5:S:119:LEU:HD22	5:S:124:ARG:HD2	1.75	0.67
3:M:268:PHE:HA	3:M:273:SER:H	1.59	0.67
2:B:401:THR:HG22	3:M:389:LYS:HD3	1.75	0.67
1:A:481:LYS:O	1:A:516:ARG:NH2	2.27	0.67
1:A:533:CYS:SG	1:A:538:ARG:NH1	2.68	0.67
2:B:166:ARG:NH2	2:B:197:LEU:O	2.27	0.67
1:A:534:SER:O	1:A:537:THR:OG1	2.12	0.67
3:M:267:LYS:NZ	3:M:271:GLU:OE2	2.28	0.67
1:A:19:ASP:OD1	1:A:20:ILE:N	2.28	0.67
1:A:364:GLU:N	1:A:364:GLU:OE1	2.28	0.67
3:M:48:THR:HB	3:M:55:PHE:HB2	1.77	0.66
3:M:319:LYS:HD2	3:M:374:GLU:HB2	1.76	0.66
2:B:212:ASN:O	3:M:264:ARG:NH1	2.28	0.66
2:B:47:VAL:HG23	2:B:72:TYR:HE1	1.61	0.66
2:B:264:MET:HG3	2:B:312:LYS:HZ1	1.59	0.66
3:M:74:ASN:OD1	3:M:77:MET:N	2.24	0.66
5:S:8:GLN:HG3	5:S:66:TYR:HB2	1.76	0.66
5:S:60:ARG:N	5:S:67:PHE:O	2.28	0.66
1:A:89:THR:N	5:S:142:GLU:OXT	2.20	0.66
1:A:432:ALA:O	1:A:436:ALA:N	2.29	0.66
1:A:431:LEU:HA	1:A:434:LYS:HD2	1.78	0.66
3:M:329:GLN:NE2	3:M:402:GLU:OE2	2.28	0.66
1:A:444:ASP:OD1	1:A:478:TYR:OH	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:LEU:O	2:B:54:VAL:N	2.21	0.66
5:S:118:PHE:HA	5:S:124:ARG:H	1.61	0.65
2:B:37:VAL:HG13	2:B:47:VAL:HG21	1.78	0.65
3:M:356:LYS:HG3	3:M:359:GLU:HB3	1.77	0.65
1:A:533:CYS:O	1:A:538:ARG:NH2	2.30	0.65
2:B:245:THR:OG1	2:B:276:TYR:OH	2.13	0.65
5:S:103:LEU:O	5:S:107:PHE:N	2.29	0.65
1:A:106:SER:OG	1:A:110:ARG:NH1	2.30	0.65
2:B:450:TRP:O	2:B:454:GLU:HG2	1.97	0.65
3:M:161:TRP:HB2	3:M:279:PRO:HB3	1.77	0.65
3:M:443:GLU:OE1	3:M:443:GLU:N	2.29	0.65
2:B:492:PHE:CD1	2:B:499:THR:HB	2.31	0.65
3:M:97:SER:H	3:M:100:ASN:HB2	1.61	0.65
5:S:106:ASN:OD1	5:S:109:LYS:NZ	2.27	0.65
3:M:311:LYS:HE3	3:M:382:GLU:HG2	1.78	0.65
3:M:350:LYS:NZ	3:M:368:ARG:O	2.29	0.65
3:M:356:LYS:HB3	3:M:361:ALA:HB3	1.79	0.65
1:A:119:ASP:HB3	1:A:127:PHE:HB3	1.78	0.65
3:M:9:ASN:ND2	3:M:13:GLU:O	2.30	0.64
3:M:212:CYS:HB3	3:M:417:VAL:HG12	1.78	0.64
1:A:173:LEU:HG	1:A:177:ARG:HH21	1.62	0.64
2:B:234:ASP:O	2:B:238:GLN:N	2.29	0.64
5:S:5:ILE:N	5:S:18:LYS:O	2.25	0.64
1:A:316:LEU:O	1:A:320:HIS:NE2	2.29	0.64
1:A:503:ILE:O	1:A:507:PHE:N	2.29	0.64
1:A:285:GLU:OE2	1:A:329:ARG:NH1	2.31	0.64
1:A:585:ARG:NH1	2:B:543:SER:OG	2.31	0.64
2:B:364:GLU:HB2	2:B:369:PHE:CZ	2.33	0.64
3:M:405:PHE:N	3:M:437:GLY:H	1.96	0.64
2:B:250:HIS:CE1	3:M:265:LEU:HD12	2.33	0.63
2:B:501:GLU:OE1	2:B:501:GLU:N	2.30	0.63
3:M:32:PHE:CZ	3:M:55:PHE:HE1	2.15	0.63
3:M:335:ILE:O	3:M:362:ILE:N	2.25	0.63
5:S:3:ARG:HB2	5:S:70:CYS:HB3	1.79	0.63
1:A:564:ARG:HE	1:A:588:THR:HG1	1.46	0.63
2:B:41:MET:SD	2:B:75:ASN:ND2	2.71	0.63
1:A:162:ASP:HA	1:A:203:VAL:HG13	1.79	0.63
1:A:205:THR:HA	1:A:257:LEU:HD13	1.79	0.63
1:A:462:TRP:HA	1:A:465:VAL:HG12	1.81	0.63
3:M:161:TRP:NE1	3:M:277:ILE:O	2.32	0.63
3:M:337:THR:N	3:M:360:ASN:O	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:TYR:HA	2:B:336:LEU:HD12	1.80	0.63
2:B:343:ILE:HG13	2:B:376:ALA:HB1	1.80	0.63
1:A:339:GLN:O	1:A:341:ARG:NH1	2.32	0.63
1:A:502:TYR:O	1:A:547:LYS:NZ	2.32	0.63
2:B:211:LEU:HD21	2:B:247:ARG:HD2	1.80	0.63
1:A:96:LEU:O	1:A:100:VAL:N	2.28	0.63
3:M:336:PRO:O	3:M:445:ARG:NH1	2.32	0.62
5:S:93:GLU:O	5:S:96:HIS:ND1	2.31	0.62
5:S:116:GLU:O	5:S:124:ARG:NH1	2.27	0.62
1:A:87:ARG:N	1:A:90:GLU:OE1	2.32	0.62
1:A:343:THR:HG23	5:S:45:LYS:HE3	1.81	0.62
2:B:416:ASP:HA	2:B:419:ARG:HD3	1.80	0.62
3:M:18:ARG:HG3	3:M:20:TYR:CE2	2.34	0.62
3:M:306:GLU:OE1	3:M:309:ARG:NE	2.33	0.62
5:S:10:ARG:N	5:S:64:GLY:O	2.32	0.62
2:B:53:ASP:HA	2:B:56:ASN:HD21	1.65	0.62
2:B:344:ARG:HH12	2:B:552:THR:HB	1.64	0.62
3:M:7:ILE:H	3:M:16:ILE:HG22	1.63	0.62
3:M:130:LYS:H	3:M:162:ARG:HH22	1.47	0.62
2:B:134:ASP:OD2	2:B:137:VAL:N	2.28	0.62
2:B:249:SER:HB3	3:M:259:PHE:HD2	1.65	0.62
3:M:126:THR:OG1	3:M:162:ARG:NH2	2.30	0.62
1:A:615:LYS:O	1:A:618:LYS:HG2	1.99	0.62
3:M:170:ARG:NH1	3:M:171:ASN:H	1.98	0.62
5:S:7:ILE:O	5:S:15:ARG:N	2.33	0.62
2:B:348:GLN:N	2:B:348:GLN:OE1	2.32	0.62
5:S:84:ILE:O	5:S:88:VAL:HG23	2.00	0.62
2:B:327:LYS:N	2:B:330:ASP:OD2	2.33	0.62
4:P:3:GLN:HE22	4:P:5:LEU:HB2	1.65	0.62
1:A:25:SER:O	1:A:28:ALA:N	2.33	0.61
1:A:382:ASP:O	1:A:386:ARG:NH1	2.32	0.61
3:M:8:TYR:HE1	3:M:33:ARG:HH21	1.48	0.61
1:A:137:ASN:OD1	1:A:138:VAL:N	2.32	0.61
2:B:90:SER:HA	2:B:93:LYS:HD2	1.82	0.61
2:B:465:LEU:O	2:B:468:SER:OG	2.13	0.61
2:B:481:GLN:OE1	2:B:481:GLN:N	2.33	0.61
2:B:524:TYR:HA	2:B:527:TRP:NE1	2.15	0.61
2:B:263:LEU:O	2:B:267:LEU:N	2.34	0.61
3:M:114:GLU:O	3:M:122:GLN:NE2	2.20	0.61
3:M:199:ARG:HA	3:M:287:ARG:HA	1.82	0.61
5:S:7:ILE:HG13	5:S:67:PHE:HA	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:ASN:OD1	1:A:577:GLN:NE2	2.33	0.61
1:A:347:TYR:OH	1:A:388:ARG:NH2	2.34	0.61
1:A:468:ILE:O	1:A:472:ARG:N	2.34	0.61
1:A:124:ASN:HD21	1:A:127:PHE:H	1.48	0.61
1:A:573:ASP:OD2	1:A:576:LEU:N	2.27	0.61
1:A:299:LYS:HB2	1:A:302:HIS:CD2	2.35	0.61
1:A:518:SER:N	1:A:522:GLN:HE22	1.96	0.61
2:B:99:ASN:ND2	3:M:143:GLN:OE1	2.34	0.61
2:B:362:ALA:O	3:M:390:LYS:NZ	2.33	0.61
2:B:563:LEU:HD13	2:B:572:SER:HA	1.81	0.61
3:M:223:GLU:HG2	3:M:246:ASP:HA	1.83	0.61
5:S:10:ARG:HB2	5:S:64:GLY:HA2	1.82	0.61
2:B:453:GLY:O	2:B:494:LYS:NZ	2.28	0.61
3:M:221:VAL:HG23	3:M:247:LEU:HA	1.82	0.61
5:S:3:ARG:N	5:S:70:CYS:O	2.34	0.61
1:A:357:ALA:HB2	1:A:392:LEU:HD12	1.81	0.61
1:A:498:LYS:HD3	1:A:537:THR:HG22	1.82	0.61
2:B:412:VAL:HG21	2:B:443:ASP:HB2	1.83	0.61
3:M:58:VAL:O	3:M:65:LEU:N	2.34	0.61
1:A:27:GLU:HG2	1:A:31:LYS:HE2	1.81	0.60
1:A:99:SER:OG	1:A:134:CYS:SG	2.59	0.60
1:A:549:VAL:HG13	1:A:556:LYS:HB2	1.82	0.60
3:M:59:LYS:HA	3:M:64:TRP:HA	1.82	0.60
3:M:126:THR:O	3:M:162:ARG:NE	2.34	0.60
3:M:161:TRP:HE1	3:M:277:ILE:HG22	1.66	0.60
5:S:42:ARG:NH1	5:S:46:HIS:HB3	2.16	0.60
1:A:326:LEU:HD13	1:A:329:ARG:HD3	1.82	0.60
3:M:69:THR:OG1	3:M:71:GLN:OE1	2.18	0.60
1:A:585:ARG:HD3	2:B:540:VAL:HG13	1.83	0.60
3:M:200:VAL:N	3:M:284:GLU:OE2	2.34	0.60
1:A:514:ASP:O	1:A:517:SER:OG	2.11	0.60
2:B:110:MET:O	2:B:113:ILE:HG12	2.01	0.60
2:B:267:LEU:O	2:B:313:ARG:NH2	2.34	0.60
2:B:412:VAL:HG13	2:B:415:ARG:HH21	1.66	0.60
2:B:487:ALA:HA	2:B:490:LYS:HE2	1.84	0.60
2:B:493:LEU:HB3	2:B:542:LEU:HD11	1.82	0.60
1:A:430:ILE:HG12	1:A:434:LYS:HE3	1.84	0.60
5:S:52:PHE:CE1	5:S:57:ILE:HG23	2.36	0.60
2:B:411:ILE:HG22	2:B:447:ALA:HB3	1.83	0.60
2:B:308:LEU:HD21	2:B:575:HIS:HD1	1.67	0.60
3:M:238:GLU:OE2	3:M:240:LYS:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:331:ILE:N	3:M:366:ILE:O	2.35	0.60
1:A:572:ALA:O	2:B:419:ARG:NH2	2.24	0.60
1:A:548:PHE:O	1:A:552:PHE:N	2.34	0.60
2:B:398:LEU:HA	2:B:401:THR:HG23	1.83	0.60
3:M:170:ARG:NH2	3:M:430:ILE:HG12	2.13	0.60
2:B:105:LEU:HD12	2:B:108:ARG:HD2	1.84	0.59
5:S:58:ILE:N	5:S:69:ILE:O	2.34	0.59
3:M:48:THR:O	3:M:55:PHE:N	2.35	0.59
3:M:336:PRO:HA	3:M:361:ALA:HA	1.83	0.59
5:S:18:LYS:NZ	5:S:19:TRP:O	2.28	0.59
5:S:47:THR:HG23	5:S:49:PHE:H	1.67	0.59
3:M:117:ASP:N	3:M:122:GLN:HE22	2.00	0.59
1:A:159:ASP:HA	1:A:165:LYS:HE3	1.83	0.59
1:A:360:GLU:HA	1:A:363:HIS:CD2	2.37	0.59
2:B:32:GLU:O	2:B:36:LYS:HG3	2.02	0.59
2:B:457:GLU:HB3	2:B:494:LYS:HD3	1.84	0.59
2:B:556:GLU:HB3	2:B:559:LEU:HB3	1.85	0.59
1:A:567:SER:OG	1:A:568:GLN:OE1	2.19	0.59
2:B:207:LEU:HD13	2:B:222:ILE:HG23	1.84	0.59
2:B:407:VAL:O	2:B:411:ILE:HG13	2.01	0.59
2:B:415:ARG:NH2	2:B:443:ASP:O	2.36	0.59
3:M:329:GLN:HA	3:M:368:ARG:HA	1.85	0.59
3:M:213:LYS:N	3:M:416:LYS:O	2.31	0.59
3:M:268:PHE:HA	3:M:273:SER:N	2.17	0.59
3:M:432:TRP:HE1	4:P:4:ARG:NE	2.00	0.59
5:S:3:ARG:HD3	5:S:21:MET:HE3	1.85	0.59
1:A:32:ARG:HD2	1:A:35:LYS:HE3	1.84	0.58
1:A:360:GLU:HA	1:A:363:HIS:HD2	1.68	0.58
3:M:217:ASN:ND2	3:M:244:GLU:OE2	2.31	0.58
1:A:390:VAL:O	1:A:394:TYR:HB2	2.03	0.58
2:B:70:TYR:OH	2:B:94:ASP:OD2	2.21	0.58
2:B:116:ASP:N	2:B:116:ASP:OD1	2.31	0.58
2:B:199:LEU:HD12	2:B:229:TYR:HD1	1.67	0.58
1:A:394:TYR:CZ	1:A:431:LEU:HG	2.39	0.58
1:A:154:ILE:O	1:A:165:LYS:NZ	2.36	0.58
1:A:542:LEU:HB3	1:A:583:TYR:CE2	2.38	0.58
1:A:212:THR:HG22	1:A:216:GLN:HE21	1.67	0.58
1:A:606:PRO:HB2	1:A:608:ARG:HH12	1.68	0.58
3:M:32:PHE:CE1	3:M:55:PHE:CE1	2.91	0.58
1:A:205:THR:HG22	1:A:257:LEU:HB2	1.85	0.58
1:A:354:CYS:HA	1:A:357:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:524:TYR:HB3	2:B:528:ARG:CZ	2.34	0.58
1:A:235:ARG:NH1	1:A:238:THR:OG1	2.37	0.58
1:A:314:ILE:O	1:A:318:ILE:N	2.35	0.58
2:B:341:ILE:O	2:B:345:LEU:N	2.35	0.58
2:B:463:ASP:OD1	2:B:463:ASP:N	2.35	0.58
1:A:564:ARG:HH21	1:A:588:THR:HA	1.68	0.58
2:B:213:GLU:HA	3:M:264:ARG:HH22	1.68	0.58
2:B:7:PHE:HZ	2:B:32:GLU:HG3	1.68	0.58
2:B:139:LYS:O	2:B:179:ASN:ND2	2.36	0.58
2:B:175:MET:SD	2:B:175:MET:N	2.77	0.58
3:M:298:PHE:HD2	3:M:442:TYR:CZ	2.21	0.58
3:M:335:ILE:HB	3:M:362:ILE:HB	1.84	0.58
3:M:397:ILE:H	3:M:445:ARG:HB2	1.69	0.58
1:A:105:ASN:HD22	1:A:108:LEU:HD12	1.69	0.57
3:M:188:GLN:HG3	3:M:303:LEU:HD11	1.85	0.57
2:B:124:GLU:OE2	2:B:131:LYS:NZ	2.31	0.57
2:B:240:ILE:O	2:B:244:VAL:HG23	2.04	0.57
3:M:394:ARG:HB3	3:M:446:CYS:HB3	1.86	0.57
5:S:36:HIS:O	5:S:40:THR:HG23	2.04	0.57
3:M:214:PHE:HE2	3:M:216:MET:HB2	1.69	0.57
1:A:460:GLU:N	1:A:460:GLU:OE1	2.32	0.57
1:A:608:ARG:NH2	2:B:512:GLN:O	2.37	0.57
2:B:398:LEU:O	2:B:401:THR:OG1	2.12	0.57
2:B:486:THR:OG1	2:B:490:LYS:NZ	2.36	0.57
5:S:91:LEU:HD22	5:S:95:PHE:HE2	1.69	0.57
1:A:459:GLU:HA	1:A:462:TRP:NE1	2.19	0.57
2:B:118:ILE:HD12	2:B:121:TYR:HB2	1.86	0.57
4:P:5:LEU:HG	4:P:6:ASN:H	1.70	0.57
2:B:192:PRO:HD2	2:B:195:ASN:HD21	1.70	0.57
3:M:32:PHE:CZ	3:M:55:PHE:CZ	2.92	0.57
3:M:337:THR:H	3:M:361:ALA:HA	1.69	0.57
1:A:341:ARG:O	1:A:346:ARG:NH2	2.38	0.57
2:B:18:LEU:HD21	2:B:50:LEU:HD11	1.87	0.57
3:M:78:VAL:O	3:M:82:LEU:HG	2.05	0.57
3:M:174:PHE:HD2	3:M:434:ARG:HH12	1.53	0.57
3:M:186:SER:HB3	3:M:192:LEU:HD21	1.85	0.57
1:A:106:SER:O	1:A:110:ARG:N	2.34	0.57
1:A:214:LEU:O	1:A:218:ASN:N	2.38	0.57
1:A:303:SER:O	1:A:307:ASN:ND2	2.38	0.57
2:B:11:LYS:HG2	2:B:12:LYS:HG3	1.87	0.57
1:A:273:ASP:OD1	1:A:276:VAL:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:491:LEU:O	2:B:495:LYS:N	2.27	0.57
3:M:116:LEU:HD12	3:M:121:PRO:HB3	1.87	0.57
3:M:405:PHE:H	3:M:437:GLY:H	1.51	0.57
1:A:341:ARG:H	1:A:341:ARG:HD2	1.70	0.56
1:A:431:LEU:HD23	1:A:434:LYS:HD2	1.87	0.56
1:A:526:LEU:O	1:A:530:PHE:N	2.38	0.56
2:B:88:VAL:HG12	2:B:118:ILE:HD13	1.86	0.56
3:M:186:SER:N	3:M:190:GLN:O	2.32	0.56
5:S:13:LYS:HB2	5:S:15:ARG:NH2	2.19	0.56
2:B:302:ALA:O	2:B:306:ILE:HG12	2.05	0.56
2:B:557:PRO:O	2:B:561:ASP:N	2.24	0.56
1:A:465:VAL:HA	1:A:468:ILE:HD12	1.87	0.56
2:B:7:PHE:HD2	2:B:36:LYS:HG2	1.69	0.56
2:B:396:LEU:HA	2:B:399:ILE:HD12	1.86	0.56
2:B:481:GLN:O	2:B:485:LEU:HG	2.04	0.56
3:M:299:ARG:N	3:M:319:LYS:O	2.25	0.56
2:B:279:MET:HA	2:B:282:LYS:HE3	1.87	0.56
3:M:95:LYS:NZ	3:M:100:ASN:OD1	2.32	0.56
2:B:375:ARG:HD2	2:B:413:VAL:HG22	1.86	0.56
2:B:386:GLN:O	2:B:390:ARG:NH1	2.38	0.56
2:B:418:PHE:HB3	2:B:450:TRP:HH2	1.71	0.56
2:B:146:ALA:HA	2:B:149:HIS:CD2	2.41	0.56
1:A:560:GLN:O	1:A:564:ARG:HD3	2.06	0.56
2:B:249:SER:HA	2:B:252:ASN:ND2	2.20	0.56
5:S:124:ARG:NH1	5:S:125:GLU:OE1	2.39	0.56
1:A:560:GLN:O	1:A:563:LEU:HD23	2.06	0.56
3:M:292:LYS:NZ	3:M:293:ASP:OD1	2.29	0.56
1:A:75:GLY:O	1:A:79:ALA:N	2.39	0.56
1:A:99:SER:HB3	1:A:137:ASN:ND2	2.21	0.56
2:B:366:ASP:HB3	2:B:369:PHE:CD1	2.40	0.56
3:M:10:HIS:NE2	3:M:62:ASN:HB2	2.21	0.56
1:A:163:SER:HA	1:A:166:GLN:NE2	2.22	0.55
2:B:61:ASP:OD1	2:B:61:ASP:N	2.38	0.55
3:M:209:MET:HB2	3:M:421:LYS:NZ	2.21	0.55
1:A:136:ALA:O	1:A:174:ARG:NE	2.39	0.55
1:A:147:PHE:HA	1:A:150:GLU:HB3	1.88	0.55
2:B:28:GLU:HA	2:B:31:LYS:HE2	1.88	0.55
2:B:82:ASP:OD1	2:B:82:ASP:N	2.38	0.55
2:B:307:ASN:OD1	2:B:308:LEU:N	2.39	0.55
2:B:330:ASP:OD2	2:B:338:LYS:NZ	2.37	0.55
2:B:368:ASP:O	2:B:372:LYS:HG2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:56:PHE:HB2	3:M:67:ALA:HB3	1.87	0.55
1:A:341:ARG:HD2	1:A:341:ARG:N	2.20	0.55
2:B:21:GLU:HB2	2:B:29:LYS:HB3	1.88	0.55
2:B:213:GLU:O	3:M:158:GLN:NE2	2.40	0.55
2:B:443:ASP:OD1	2:B:444:ALA:N	2.39	0.55
3:M:178:LEU:HA	3:M:436:ILE:HG13	1.88	0.55
3:M:222:ILE:HG12	3:M:249:LYS:N	2.19	0.55
5:S:135:LEU:O	5:S:139:GLN:N	2.40	0.55
1:A:244:LEU:HD13	1:A:247:TYR:CD2	2.42	0.55
2:B:33:ALA:O	2:B:37:VAL:HG23	2.05	0.55
2:B:301:VAL:HG13	2:B:573:VAL:HG11	1.89	0.55
3:M:172:GLU:HG2	3:M:430:ILE:HB	1.89	0.55
1:A:460:GLU:HA	1:A:463:TYR:HB2	1.89	0.55
1:A:471:ASN:HA	1:A:604:PRO:HB3	1.88	0.55
3:M:396:PRO:HA	3:M:445:ARG:N	2.22	0.55
3:M:411:LYS:HG2	3:M:435:TYR:CZ	2.42	0.55
1:A:34:ASN:HA	1:A:37:LEU:HD12	1.87	0.55
1:A:63:LEU:O	1:A:67:LEU:HG	2.07	0.55
1:A:402:ALA:HA	1:A:405:ILE:HB	1.87	0.55
2:B:296:PRO:O	2:B:300:TYR:HB2	2.05	0.55
3:M:49:ASN:HA	3:M:53:THR:O	2.06	0.55
5:S:59:TYR:HA	5:S:68:CYS:HA	1.89	0.55
5:S:118:PHE:HD1	5:S:123:ILE:HA	1.71	0.55
1:A:459:GLU:HA	1:A:462:TRP:CE2	2.42	0.55
2:B:118:ILE:HA	2:B:121:TYR:CD2	2.42	0.55
2:B:501:GLU:O	2:B:504:GLN:HG2	2.05	0.55
3:M:184:LEU:H	3:M:193:SER:HB3	1.72	0.55
5:S:8:GLN:HA	5:S:15:ARG:H	1.72	0.55
1:A:337:PHE:HA	1:A:340:HIS:NE2	2.21	0.55
2:B:127:ARG:NH2	2:B:157:GLU:OE1	2.38	0.55
2:B:357:GLU:O	2:B:360:GLU:HB3	2.07	0.55
3:M:151:ILE:O	3:M:154:GLN:HG2	2.07	0.55
3:M:310:THR:O	3:M:383:LEU:N	2.24	0.55
3:M:332:GLU:HB2	3:M:365:LYS:HD3	1.89	0.55
1:A:112:ILE:O	1:A:116:ILE:HG12	2.06	0.55
3:M:214:PHE:CE2	3:M:216:MET:HB2	2.42	0.55
1:A:176:TYR:OH	1:A:217:LYS:HG3	2.06	0.55
1:A:176:TYR:HD1	1:A:183:VAL:HG21	1.71	0.55
1:A:581:VAL:HG11	2:B:545:LYS:HE3	1.89	0.55
5:S:32:ILE:O	5:S:36:HIS:ND1	2.40	0.55
2:B:127:ARG:O	2:B:131:LYS:N	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:GLN:O	2:B:206:LYS:HE3	2.07	0.54
2:B:252:ASN:O	2:B:255:VAL:N	2.40	0.54
3:M:99:GLU:HA	3:M:102:LYS:HD2	1.88	0.54
5:S:100:GLU:O	5:S:104:VAL:HG23	2.06	0.54
1:A:359:SER:O	1:A:363:HIS:N	2.41	0.54
1:A:542:LEU:HB3	1:A:583:TYR:HE2	1.69	0.54
2:B:239:SER:O	2:B:243:ARG:HG2	2.07	0.54
2:B:324:PHE:HA	2:B:338:LYS:HG2	1.88	0.54
2:B:371:ARG:NH2	2:B:405:TYR:O	2.41	0.54
2:B:351:ILE:HA	2:B:354:VAL:HB	1.90	0.54
3:M:129:LEU:HA	3:M:132:PHE:CE1	2.42	0.54
1:A:564:ARG:NE	1:A:588:THR:OG1	2.25	0.54
2:B:499:THR:HG22	2:B:503:VAL:HG13	1.90	0.54
3:M:216:MET:O	3:M:413:ARG:NH2	2.40	0.54
3:M:338:PRO:HD2	3:M:381:ILE:HG13	1.89	0.54
2:B:51:PHE:HE1	2:B:73:LEU:HD12	1.73	0.54
3:M:126:THR:HG1	3:M:162:ARG:HH21	1.52	0.54
3:M:203:LYS:NZ	3:M:204:SER:O	2.40	0.54
1:A:116:ILE:O	1:A:120:LEU:HG	2.07	0.54
1:A:324:PRO:HA	1:A:327:LEU:HD12	1.90	0.54
3:M:201:VAL:HA	3:M:284:GLU:HA	1.90	0.54
5:S:39:VAL:HG13	5:S:61:ARG:HD3	1.88	0.54
1:A:525:LEU:O	1:A:528:SER:OG	2.17	0.54
2:B:485:LEU:HB2	2:B:522:ARG:NH2	2.20	0.54
3:M:200:VAL:O	3:M:285:LEU:N	2.39	0.54
3:M:315:LYS:NZ	3:M:378:SER:OG	2.41	0.54
5:S:25:ASP:OD1	5:S:25:ASP:N	2.40	0.54
5:S:62:TYR:N	5:S:65:LEU:O	2.41	0.54
2:B:135:PRO:O	2:B:139:LYS:CB	2.55	0.54
2:B:395:LEU:HA	2:B:398:LEU:HD12	1.89	0.54
5:S:26:ASP:N	5:S:26:ASP:OD1	2.41	0.54
1:A:466:ILE:HD11	1:A:499:VAL:HG22	1.88	0.54
3:M:9:ASN:HD21	3:M:13:GLU:HG2	1.73	0.54
3:M:55:PHE:HB3	3:M:57:HIS:NE2	2.22	0.54
1:A:252:VAL:HG23	1:A:255:PRO:HD3	1.88	0.53
2:B:226:LEU:O	2:B:265:LYS:NZ	2.39	0.53
2:B:450:TRP:NE1	2:B:454:GLU:OE2	2.40	0.53
5:S:78:LEU:O	5:S:82:GLU:HG2	2.08	0.53
1:A:398:ASP:H	1:A:401:ASN:ND2	2.05	0.53
1:A:518:SER:H	1:A:522:GLN:NE2	2.01	0.53
2:B:361:TYR:HB3	2:B:369:PHE:HE2	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:TYR:HB3	2:B:424:LYS:HD2	1.89	0.53
2:B:479:GLN:HA	2:B:482:LEU:HD12	1.90	0.53
2:B:521:ASP:OD1	2:B:528:ARG:NH2	2.42	0.53
5:S:1:MET:HG2	5:S:3:ARG:NH2	2.23	0.53
3:M:117:ASP:H	3:M:122:GLN:HE22	1.55	0.53
1:A:30:ILE:HG22	1:A:34:ASN:HD21	1.74	0.53
1:A:585:ARG:NH2	2:B:539:GLU:O	2.41	0.53
3:M:215:GLY:O	3:M:413:ARG:N	2.41	0.53
3:M:299:ARG:HH11	3:M:321:ASN:HB2	1.74	0.53
1:A:32:ARG:NH1	1:A:36:GLU:HG2	2.23	0.53
1:A:244:LEU:HD13	1:A:247:TYR:HD2	1.74	0.53
1:A:362:SER:O	1:A:366:VAL:HG23	2.09	0.53
1:A:399:ARG:O	1:A:403:GLN:NE2	2.31	0.53
3:M:268:PHE:HB2	3:M:274:ILE:HG23	1.91	0.53
3:M:249:LYS:HZ3	3:M:409:GLY:HA3	1.73	0.53
5:S:1:MET:N	5:S:3:ARG:HH21	2.05	0.53
5:S:52:PHE:O	5:S:53:ARG:HG2	2.09	0.53
1:A:170:LEU:HD12	5:S:119:LEU:HB3	1.90	0.53
1:A:526:LEU:HA	1:A:529:LYS:HD2	1.90	0.53
2:B:578:PRO:HA	2:B:581:PHE:CZ	2.43	0.53
3:M:59:LYS:HG2	3:M:64:TRP:CG	2.43	0.53
3:M:299:ARG:O	3:M:319:LYS:HB3	2.09	0.53
3:M:311:LYS:HA	3:M:382:GLU:HA	1.91	0.53
1:A:81:ASN:O	1:A:85:SER:HB2	2.09	0.53
1:A:103:ASN:ND2	1:A:109:ILE:HG12	2.24	0.53
1:A:105:ASN:O	1:A:108:LEU:N	2.42	0.53
1:A:276:VAL:HG13	1:A:279:ARG:NH2	2.24	0.53
3:M:307:VAL:HB	3:M:311:LYS:HB3	1.90	0.53
2:B:518:ASP:O	2:B:522:ARG:HB2	2.08	0.53
3:M:218:ASP:HB3	3:M:219:LYS:HD2	1.90	0.53
1:A:51:ASP:O	1:A:55:LYS:HB2	2.09	0.53
2:B:297:GLU:OE1	2:B:297:GLU:N	2.31	0.53
2:B:524:TYR:HA	2:B:527:TRP:CD1	2.44	0.53
3:M:32:PHE:CE2	3:M:55:PHE:HE1	2.27	0.53
3:M:254:ILE:HD11	3:M:288:TYR:HB2	1.91	0.53
2:B:159:GLN:HA	2:B:162:LEU:HD12	1.91	0.52
2:B:201:PRO:HA	2:B:204:ILE:HD12	1.90	0.52
2:B:296:PRO:HA	2:B:299:GLN:HE21	1.74	0.52
2:B:541:VAL:O	2:B:545:LYS:NZ	2.36	0.52
3:M:129:LEU:HD23	3:M:132:PHE:HE1	1.73	0.52
3:M:221:VAL:HA	3:M:251:SER:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:98:VAL:HG23	5:S:102:ASP:HB2	1.92	0.52
1:A:495:ASN:HA	1:A:498:LYS:HE2	1.90	0.52
1:A:210:LEU:O	1:A:214:LEU:HG	2.09	0.52
2:B:525:ILE:HG13	2:B:528:ARG:HH21	1.75	0.52
3:M:41:GLN:HE22	3:M:43:VAL:HG23	1.74	0.52
3:M:296:LEU:HB2	3:M:299:ARG:CZ	2.39	0.52
1:A:15:VAL:O	1:A:18:SER:OG	2.23	0.52
1:A:463:TYR:CE1	2:B:516:ASN:HA	2.44	0.52
2:B:62:ASN:HB3	2:B:65:LEU:HB3	1.91	0.52
2:B:287:PRO:O	2:B:290:THR:OG1	2.21	0.52
2:B:360:GLU:O	2:B:363:THR:OG1	2.19	0.52
1:A:167:SER:OG	5:S:124:ARG:NE	2.37	0.52
1:A:444:ASP:HA	1:A:447:LEU:HD12	1.91	0.52
3:M:167:LYS:HA	3:M:207:SER:HB3	1.90	0.52
5:S:5:ILE:HG23	5:S:69:ILE:HG12	1.91	0.52
1:A:150:GLU:HA	1:A:153:LYS:HE2	1.91	0.52
1:A:472:ARG:HB2	1:A:476:GLN:HE22	1.74	0.52
2:B:211:LEU:HG	2:B:219:GLN:HG2	1.92	0.52
3:M:213:LYS:HE3	3:M:275:SER:HA	1.91	0.52
1:A:13:LEU:HB2	1:A:57:LYS:HG3	1.92	0.52
1:A:417:ASP:HB3	1:A:420:ILE:HG12	1.92	0.52
2:B:166:ARG:HH12	2:B:197:LEU:N	2.05	0.52
1:A:325:ASN:O	1:A:329:ARG:HG3	2.09	0.52
3:M:251:SER:HB2	3:M:410:LEU:HD13	1.92	0.52
3:M:329:GLN:N	3:M:402:GLU:OE2	2.43	0.52
5:S:55:PHE:HB2	5:S:72:ASP:HA	1.91	0.52
3:M:304:VAL:HB	3:M:394:ARG:NH2	2.25	0.52
5:S:138:LEU:HD22	5:S:141:LEU:HD11	1.92	0.52
1:A:259:VAL:HA	1:A:312:GLU:HG2	1.91	0.51
2:B:166:ARG:HH22	2:B:197:LEU:HB2	1.75	0.51
3:M:125:GLU:OE2	3:M:161:TRP:N	2.25	0.51
3:M:185:MET:HA	3:M:191:VAL:HA	1.92	0.51
3:M:260:HIS:CD2	3:M:286:MET:HA	2.45	0.51
1:A:132:LEU:HD22	1:A:168:ALA:HA	1.93	0.51
1:A:250:TYR:CE2	1:A:301:GLN:HG3	2.46	0.51
2:B:10:ASN:ND2	2:B:40:ALA:HA	2.24	0.51
2:B:404:ASN:HB2	2:B:408:GLN:HE21	1.76	0.51
3:M:203:LYS:HA	3:M:282:GLU:HA	1.92	0.51
1:A:243:ASP:HA	1:A:245:GLN:NE2	2.26	0.51
1:A:303:SER:HA	1:A:306:LYS:HE3	1.92	0.51
2:B:135:PRO:N	2:B:138:ARG:HH21	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:GLU:OE1	2:B:189:GLU:N	2.44	0.51
2:B:261:LYS:HE3	2:B:567:ILE:O	2.10	0.51
2:B:382:ILE:HA	2:B:421:TYR:HE2	1.75	0.51
1:A:181:ASP:OD1	1:A:182:LEU:N	2.43	0.51
3:M:172:GLU:HB3	3:M:432:TRP:HZ3	1.75	0.51
1:A:213:THR:O	1:A:217:LYS:HG2	2.10	0.51
1:A:233:LEU:O	1:A:237:VAL:HG23	2.11	0.51
1:A:342:GLU:HA	5:S:45:LYS:NZ	2.26	0.51
1:A:380:GLU:C	1:A:381:ARG:HD2	2.31	0.51
1:A:387:GLN:HB2	1:A:388:ARG:NH1	2.25	0.51
1:A:430:ILE:O	1:A:433:GLU:HG3	2.10	0.51
3:M:262:CYS:O	3:M:276:PHE:HA	2.11	0.51
3:M:426:ASP:OD1	3:M:426:ASP:N	2.42	0.51
1:A:377:LEU:O	1:A:386:ARG:NE	2.41	0.51
1:A:544:THR:HA	1:A:547:LYS:HE3	1.92	0.51
1:A:565:SER:OG	1:A:567:SER:OG	2.28	0.51
5:S:43:ASP:OD1	5:S:46:HIS:NE2	2.43	0.51
1:A:64:PHE:HA	1:A:67:LEU:HD12	1.93	0.51
1:A:75:GLY:HA2	1:A:78:GLU:HB2	1.92	0.51
1:A:472:ARG:HB3	1:A:474:ASP:OD1	2.11	0.51
2:B:556:GLU:OE1	2:B:559:LEU:N	2.25	0.51
3:M:184:LEU:HB3	3:M:193:SER:HB3	1.93	0.51
1:A:43:LYS:HG2	1:A:58:TYR:HE2	1.76	0.51
1:A:65:ILE:HG22	1:A:70:HIS:HB2	1.93	0.51
1:A:79:ALA:O	1:A:83:LEU:HG	2.11	0.51
1:A:443:VAL:O	1:A:447:LEU:HG	2.10	0.51
1:A:566:ASP:O	1:A:570:LYS:N	2.43	0.51
2:B:521:ASP:O	2:B:524:TYR:HB2	2.10	0.51
3:M:209:MET:HB2	3:M:421:LYS:HZ2	1.74	0.51
5:S:75:ASP:HB3	5:S:80:TYR:CE2	2.46	0.51
1:A:58:TYR:O	1:A:62:LEU:HG	2.11	0.51
1:A:225:SER:O	1:A:228:LEU:HG	2.11	0.51
1:A:280:LEU:O	1:A:284:LEU:HG	2.10	0.51
1:A:414:GLU:OE1	1:A:415:THR:HG23	2.11	0.51
2:B:74:MET:O	2:B:78:LYS:HG2	2.11	0.51
2:B:199:LEU:HD23	2:B:199:LEU:H	1.75	0.51
2:B:287:PRO:O	2:B:291:LEU:HG	2.11	0.51
2:B:297:GLU:O	2:B:301:VAL:HG23	2.11	0.51
2:B:456:ALA:HB1	2:B:491:LEU:HD13	1.92	0.51
2:B:581:PHE:HA	3:M:52:ARG:NE	2.25	0.51
3:M:80:GLU:HB3	3:M:84:LYS:NZ	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:327:LEU:O	3:M:329:GLN:NE2	2.38	0.51
3:M:354:LYS:HD3	3:M:363:VAL:HG11	1.92	0.51
1:A:279:ARG:HA	1:A:282:GLU:CD	2.32	0.51
2:B:574:TYR:CD2	2:B:576:LYS:HB2	2.46	0.51
3:M:10:HIS:HA	3:M:64:TRP:CZ2	2.46	0.51
3:M:102:LYS:HA	3:M:105:PHE:CZ	2.46	0.51
3:M:215:GLY:HA3	3:M:414:TYR:CD2	2.47	0.51
3:M:405:PHE:N	3:M:435:TYR:O	2.43	0.51
2:B:5:LYS:HD2	2:B:6:TYR:O	2.11	0.50
2:B:94:ASP:OD2	2:B:106:ALA:HB2	2.11	0.50
3:M:27:ASN:OD1	3:M:28:ALA:N	2.44	0.50
5:S:56:LYS:HG3	5:S:71:VAL:HG23	1.92	0.50
1:A:109:ILE:HA	1:A:112:ILE:HD12	1.93	0.50
2:B:510:ALA:O	2:B:514:SER:HB2	2.10	0.50
3:M:18:ARG:HG3	3:M:20:TYR:HE2	1.76	0.50
3:M:211:GLU:OE2	3:M:276:PHE:N	2.45	0.50
3:M:212:CYS:HB2	3:M:276:PHE:CE2	2.46	0.50
3:M:350:LYS:H	3:M:364:TRP:HZ2	1.59	0.50
3:M:364:TRP:NE1	3:M:375:SER:OG	2.43	0.50
5:S:23:PHE:HB2	5:S:28:LYS:NZ	2.26	0.50
5:S:49:PHE:HA	5:S:57:ILE:O	2.11	0.50
5:S:116:GLU:CD	5:S:124:ARG:HH12	2.14	0.50
1:A:605:PHE:CD1	1:A:606:PRO:HD2	2.46	0.50
2:B:11:LYS:HB3	2:B:12:LYS:HZ3	1.77	0.50
2:B:350:ASN:HB3	2:B:354:VAL:HG23	1.93	0.50
2:B:357:GLU:HB3	2:B:361:TYR:CZ	2.45	0.50
2:B:375:ARG:HH21	2:B:379:ARG:N	2.10	0.50
5:S:123:ILE:HG21	5:S:126:THR:HG23	1.92	0.50
1:A:369:HIS:O	1:A:373:VAL:HG23	2.12	0.50
1:A:579:ARG:NH2	1:A:583:TYR:OH	2.42	0.50
2:B:341:ILE:HG22	2:B:345:LEU:HG	1.93	0.50
3:M:26:ARG:HH12	3:M:30:ASP:N	2.09	0.50
3:M:128:ALA:HB3	3:M:154:GLN:NE2	2.26	0.50
5:S:99:CYS:N	5:S:102:ASP:OD2	2.41	0.50
1:A:99:SER:HB3	1:A:137:ASN:HD21	1.76	0.50
1:A:353:MET:O	1:A:357:ALA:N	2.45	0.50
1:A:612:ILE:HA	1:A:615:LYS:HE3	1.93	0.50
2:B:7:PHE:O	2:B:9:THR:HG23	2.12	0.50
2:B:386:GLN:CD	2:B:386:GLN:H	2.15	0.50
3:M:75:ALA:HB1	3:M:79:PHE:CZ	2.46	0.50
3:M:161:TRP:HZ2	3:M:277:ILE:HB	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:364:TRP:HB2	3:M:377:ILE:HD13	1.94	0.50
2:B:234:ASP:HB2	2:B:238:GLN:HE21	1.77	0.50
2:B:289:VAL:O	2:B:293:SER:N	2.45	0.50
2:B:354:VAL:O	2:B:358:LEU:HG	2.12	0.50
3:M:254:ILE:HG21	3:M:257:CYS:HB3	1.93	0.50
2:B:315:GLU:O	2:B:317:LEU:N	2.44	0.50
2:B:461:ASN:OD1	2:B:461:ASN:N	2.45	0.50
3:M:218:ASP:HB2	3:M:413:ARG:HH12	1.77	0.50
1:A:156:VAL:HG11	1:A:191:ARG:HE	1.77	0.50
1:A:380:GLU:HB3	1:A:386:ARG:NH2	2.27	0.50
2:B:67:LYS:HD3	2:B:105:LEU:HD21	1.94	0.50
2:B:206:LYS:O	2:B:209:THR:OG1	2.28	0.50
2:B:436:LEU:HD22	2:B:469:PHE:HZ	1.77	0.50
3:M:146:GLU:O	3:M:150:GLN:HB2	2.12	0.50
2:B:99:ASN:ND2	3:M:148:GLN:HE22	2.10	0.50
3:M:322:PHE:O	3:M:372:MET:HG2	2.12	0.50
1:A:381:ARG:H	1:A:386:ARG:NH2	2.10	0.49
1:A:430:ILE:HA	1:A:433:GLU:HG3	1.94	0.49
2:B:132:ASP:O	2:B:138:ARG:HD3	2.12	0.49
2:B:261:LYS:HB2	2:B:567:ILE:HG23	1.93	0.49
2:B:564:ILE:O	2:B:567:ILE:HG22	2.12	0.49
1:A:196:LEU:O	1:A:232:ARG:NE	2.45	0.49
1:A:397:CYS:SG	1:A:398:ASP:N	2.86	0.49
1:A:402:ALA:O	1:A:406:VAL:HG23	2.12	0.49
2:B:312:LYS:HG2	2:B:313:ARG:HG2	1.94	0.49
2:B:355:LEU:HD12	2:B:358:LEU:HB2	1.93	0.49
3:M:80:GLU:HB3	3:M:84:LYS:HZ1	1.76	0.49
1:A:156:VAL:HG21	1:A:191:ARG:HH21	1.77	0.49
2:B:73:LEU:HD11	2:B:87:ALA:HB2	1.95	0.49
2:B:497:SER:C	2:B:500:GLN:HE22	2.15	0.49
5:S:60:ARG:O	5:S:67:PHE:N	2.39	0.49
1:A:216:GLN:HB2	1:A:217:LYS:HZ2	1.77	0.49
1:A:343:THR:HA	1:A:346:ARG:HH21	1.77	0.49
1:A:484:PHE:HB3	1:A:516:ARG:NH2	2.27	0.49
2:B:125:PRO:HA	2:B:128:LYS:HD2	1.94	0.49
2:B:135:PRO:HB3	2:B:173:ASN:ND2	2.26	0.49
2:B:277:TYR:O	2:B:281:LEU:HG	2.11	0.49
3:M:181:VAL:O	3:M:441:ILE:HB	2.12	0.49
1:A:57:LYS:HG2	1:A:58:TYR:CD1	2.48	0.49
1:A:91:LYS:HE2	1:A:127:PHE:CZ	2.47	0.49
1:A:171:CYS:O	1:A:175:LEU:HG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASP:OD1	1:A:277:ARG:N	2.38	0.49
2:B:324:PHE:HD1	2:B:338:LYS:HA	1.77	0.49
5:S:47:THR:O	5:S:59:TYR:OH	2.27	0.49
5:S:49:PHE:CE1	5:S:58:ILE:HG23	2.48	0.49
1:A:161:MET:SD	1:A:163:SER:N	2.85	0.49
2:B:258:SER:O	2:B:262:VAL:HG23	2.12	0.49
2:B:290:THR:HA	2:B:293:SER:HB2	1.93	0.49
3:M:13:GLU:HA	3:M:33:ARG:CZ	2.42	0.49
3:M:223:GLU:HG2	3:M:247:LEU:H	1.78	0.49
5:S:19:TRP:HB3	5:S:23:PHE:CD2	2.46	0.49
1:A:124:ASN:ND2	1:A:127:PHE:H	2.11	0.49
1:A:523:PHE:CZ	1:A:559:ILE:HG12	2.48	0.49
2:B:582:VAL:HB	3:M:52:ARG:NH1	2.28	0.49
3:M:356:LYS:N	3:M:361:ALA:O	2.41	0.49
1:A:616:LEU:HA	1:A:619:LYS:HD3	1.94	0.49
2:B:21:GLU:OE2	2:B:36:LYS:NZ	2.39	0.49
3:M:144:THR:O	3:M:148:GLN:N	2.31	0.49
3:M:321:ASN:HA	3:M:372:MET:HA	1.95	0.49
1:A:52:GLY:HA2	1:A:90:GLU:OE2	2.13	0.49
1:A:277:ARG:HA	1:A:280:LEU:HB3	1.94	0.49
1:A:371:GLU:HA	1:A:374:ILE:HD12	1.95	0.49
1:A:535:VAL:HG13	1:A:576:LEU:HD11	1.95	0.49
2:B:403:VAL:HB	2:B:405:TYR:CZ	2.48	0.49
3:M:64:TRP:N	3:M:64:TRP:CD1	2.80	0.49
3:M:97:SER:N	3:M:100:ASN:OD1	2.46	0.49
3:M:345:GLN:OE1	3:M:380:GLU:HB2	2.13	0.49
5:S:95:PHE:HB3	5:S:98:VAL:HB	1.94	0.49
1:A:88:TYR:CD2	5:S:141:LEU:HB3	2.48	0.49
1:A:384:SER:OG	1:A:385:VAL:N	2.46	0.49
1:A:565:SER:O	1:A:569:LEU:HG	2.13	0.49
2:B:26:LYS:HZ2	2:B:27:LYS:HG2	1.78	0.49
3:M:305:ARG:HD3	3:M:313:GLU:O	2.13	0.49
3:M:322:PHE:HB3	3:M:326:LEU:HD12	1.95	0.49
1:A:450:ILE:HG21	1:A:496:LEU:HB2	1.95	0.48
2:B:428:ILE:O	2:B:432:LEU:HG	2.13	0.48
2:B:468:SER:OG	2:B:469:PHE:N	2.46	0.48
3:M:396:PRO:HB2	3:M:443:GLU:HB2	1.95	0.48
1:A:325:ASN:OD1	1:A:326:LEU:N	2.44	0.48
1:A:573:ASP:OD1	1:A:576:LEU:HB2	2.13	0.48
2:B:46:ASP:HA	2:B:76:TYR:CE1	2.49	0.48
2:B:306:ILE:O	2:B:310:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:527:TRP:O	2:B:531:SER:N	2.39	0.48
5:S:20:TYR:CD2	5:S:121:GLY:HA2	2.48	0.48
1:A:20:ILE:HA	1:A:23:CYS:SG	2.53	0.48
1:A:246:ASP:HB3	5:S:130:LYS:NZ	2.28	0.48
1:A:380:GLU:HG3	1:A:382:ASP:N	2.27	0.48
1:A:547:LYS:HA	1:A:599:LEU:HD21	1.95	0.48
2:B:52:PRO:O	2:B:56:ASN:ND2	2.45	0.48
3:M:221:VAL:HG12	3:M:251:SER:H	1.78	0.48
1:A:18:SER:O	1:A:22:ASN:ND2	2.47	0.48
2:B:581:PHE:HA	3:M:52:ARG:HE	1.77	0.48
3:M:143:GLN:NE2	3:M:148:GLN:HA	2.28	0.48
5:S:54:ASN:N	5:S:54:ASN:OD1	2.47	0.48
5:S:67:PHE:CE2	5:S:88:VAL:HG22	2.49	0.48
1:A:97:PHE:O	1:A:101:LEU:N	2.31	0.48
1:A:115:ALA:HA	1:A:118:ASN:HD22	1.77	0.48
1:A:199:GLN:N	1:A:199:GLN:OE1	2.47	0.48
2:B:199:LEU:HD12	2:B:229:TYR:CD1	2.48	0.48
1:A:10:MET:HB2	1:A:57:LYS:HB2	1.95	0.48
1:A:299:LYS:HB2	1:A:302:HIS:HD2	1.77	0.48
1:A:330:ALA:HA	1:A:333:GLN:NE2	2.28	0.48
1:A:342:GLU:HB3	1:A:345:LEU:HG	1.95	0.48
1:A:558:THR:O	1:A:562:VAL:HG13	2.13	0.48
1:A:563:LEU:C	1:A:568:GLN:HE21	2.17	0.48
1:A:612:ILE:HG23	1:A:615:LYS:NZ	2.28	0.48
2:B:66:LYS:HZ3	2:B:102:ILE:HG23	1.78	0.48
2:B:441:GLU:O	2:B:445:ARG:HG3	2.13	0.48
1:A:156:VAL:HG21	1:A:191:ARG:NH2	2.29	0.48
1:A:360:GLU:OE1	1:A:360:GLU:N	2.38	0.48
2:B:182:ALA:HB2	2:B:221:PHE:CE2	2.49	0.48
1:A:87:ARG:HB2	1:A:90:GLU:HG3	1.94	0.48
1:A:363:HIS:O	1:A:367:LYS:HG3	2.13	0.48
1:A:381:ARG:H	1:A:386:ARG:HH22	1.62	0.48
1:A:563:LEU:HD11	1:A:584:LEU:HA	1.96	0.48
2:B:53:ASP:HA	2:B:56:ASN:ND2	2.26	0.48
2:B:285:ALA:HB3	2:B:286:PRO:HD3	1.95	0.48
2:B:333:TYR:O	2:B:336:LEU:HB2	2.14	0.48
2:B:417:ILE:O	2:B:421:TYR:N	2.45	0.48
2:B:579:ASN:O	3:M:52:ARG:NH2	2.47	0.48
5:S:8:GLN:HB3	5:S:14:THR:HA	1.96	0.48
1:A:364:GLU:O	1:A:368:THR:HG23	2.13	0.48
2:B:249:SER:HB3	3:M:259:PHE:CD2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:9:ASN:HB3	3:M:15:LEU:HD21	1.96	0.48
3:M:50:ILE:HB	3:M:55:PHE:CE2	2.49	0.48
3:M:50:ILE:HB	3:M:55:PHE:HE2	1.78	0.48
5:S:19:TRP:HB3	5:S:23:PHE:CE2	2.49	0.48
1:A:235:ARG:O	1:A:239:SER:N	2.28	0.48
1:A:413:LEU:HD21	1:A:424:ILE:HG21	1.94	0.48
3:M:25:GLY:O	3:M:29:VAL:HG23	2.14	0.48
3:M:211:GLU:HG2	3:M:277:ILE:HG13	1.95	0.48
3:M:264:ARG:HB2	3:M:275:SER:H	1.78	0.48
1:A:445:THR:O	1:A:449:LEU:HG	2.14	0.47
2:B:47:VAL:HG23	2:B:72:TYR:CE1	2.47	0.47
2:B:54:VAL:O	2:B:58:MET:CB	2.53	0.47
2:B:139:LYS:HB3	2:B:139:LYS:HE2	1.72	0.47
2:B:442:PRO:HG3	2:B:445:ARG:HH22	1.78	0.47
3:M:34:VAL:HA	3:M:38:HIS:HD2	1.78	0.47
3:M:171:ASN:O	3:M:429:VAL:HA	2.14	0.47
1:A:163:SER:OG	5:S:124:ARG:NH2	2.47	0.47
1:A:333:GLN:HB3	1:A:337:PHE:CZ	2.49	0.47
2:B:203:ASN:O	2:B:206:LYS:HG2	2.14	0.47
2:B:456:ALA:HB3	2:B:494:LYS:HD2	1.94	0.47
1:A:384:SER:O	1:A:388:ARG:HG2	2.13	0.47
1:A:476:GLN:N	1:A:476:GLN:OE1	2.47	0.47
1:A:543:SER:O	1:A:546:ILE:HG22	2.15	0.47
2:B:6:TYR:CD1	3:M:102:LYS:HD3	2.49	0.47
2:B:135:PRO:HD2	3:M:152:THR:HG23	1.97	0.47
3:M:97:SER:O	3:M:101:ILE:HG12	2.14	0.47
3:M:132:PHE:HE2	3:M:154:GLN:HE22	1.63	0.47
3:M:170:ARG:HH22	3:M:428:ASP:C	2.18	0.47
1:A:418:TYR:O	1:A:421:ARG:HB3	2.14	0.47
2:B:6:TYR:HB3	3:M:102:LYS:CG	2.42	0.47
3:M:166:ILE:O	3:M:208:GLY:N	2.26	0.47
2:B:104:ALA:O	2:B:140:THR:HG21	2.15	0.47
3:M:364:TRP:HE1	3:M:375:SER:HG	1.62	0.47
3:M:405:PHE:CE2	3:M:407:PRO:HA	2.49	0.47
1:A:475:VAL:O	1:A:479:ALA:N	2.29	0.47
1:A:483:VAL:O	1:A:487:LEU:HG	2.15	0.47
1:A:485:GLU:HA	1:A:488:GLN:NE2	2.30	0.47
1:A:503:ILE:HG23	1:A:507:PHE:HD2	1.79	0.47
2:B:66:LYS:NZ	2:B:102:ILE:HG23	2.29	0.47
3:M:101:ILE:HG22	3:M:105:PHE:HE1	1.79	0.47
3:M:338:PRO:HB3	3:M:383:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ASP:HB3	1:A:420:ILE:CG1	2.45	0.47
1:A:474:ASP:N	1:A:476:GLN:OE1	2.48	0.47
2:B:28:GLU:HG2	2:B:29:LYS:N	2.25	0.47
2:B:48:SER:OG	2:B:80:GLN:HG2	2.15	0.47
2:B:108:ARG:HA	2:B:144:CYS:SG	2.55	0.47
2:B:187:ILE:O	2:B:190:SER:OG	2.18	0.47
2:B:404:ASN:OD1	2:B:404:ASN:N	2.46	0.47
2:B:555:ILE:HG21	2:B:560:LEU:HD13	1.96	0.47
3:M:116:LEU:HA	3:M:121:PRO:HA	1.95	0.47
3:M:171:ASN:HB3	3:M:206:LEU:HG	1.97	0.47
1:A:304:ASN:ND2	5:S:82:GLU:OE2	2.45	0.47
1:A:426:LEU:HD23	1:A:615:LYS:NZ	2.30	0.47
1:A:552:PHE:HB3	1:A:554:GLU:OE2	2.15	0.47
1:A:598:VAL:HG22	2:B:528:ARG:HG3	1.97	0.47
2:B:375:ARG:NH1	2:B:413:VAL:HA	2.30	0.47
2:B:464:GLU:HG2	2:B:465:LEU:N	2.29	0.47
3:M:20:TYR:HB3	3:M:118:PHE:HA	1.97	0.47
3:M:320:SER:O	3:M:373:LYS:N	2.48	0.47
5:S:48:ASN:ND2	5:S:60:ARG:HA	2.30	0.47
1:A:244:LEU:HB3	1:A:247:TYR:HB2	1.97	0.47
1:A:314:ILE:O	1:A:318:ILE:HG12	2.15	0.47
1:A:442:TYR:O	1:A:446:ILE:HG12	2.15	0.47
2:B:32:GLU:OE1	2:B:32:GLU:N	2.48	0.47
2:B:166:ARG:NH1	2:B:198:ASP:OD1	2.48	0.47
2:B:177:VAL:O	2:B:181:VAL:HG23	2.15	0.47
3:M:287:ARG:HH12	3:M:289:ARG:HB3	1.80	0.47
3:M:397:ILE:HG13	3:M:445:ARG:HE	1.79	0.47
5:S:65:LEU:HB3	5:S:67:PHE:CE1	2.50	0.47
1:A:139:GLY:HA3	1:A:174:ARG:NH2	2.30	0.47
1:A:249:TYR:O	1:A:252:VAL:HG22	2.14	0.47
1:A:519:PRO:O	1:A:523:PHE:HB3	2.15	0.47
2:B:415:ARG:HA	2:B:450:TRP:CZ3	2.49	0.47
3:M:81:PHE:HZ	3:M:115:ILE:HG23	1.79	0.47
3:M:199:ARG:HB2	3:M:284:GLU:OE2	2.15	0.47
3:M:347:ILE:HG13	3:M:378:SER:HB2	1.96	0.47
3:M:411:LYS:HG2	3:M:435:TYR:CE2	2.50	0.47
1:A:149:GLY:HA2	1:A:152:PRO:HG2	1.97	0.46
1:A:544:THR:HG22	1:A:548:PHE:CE1	2.49	0.46
2:B:17:GLU:O	2:B:21:GLU:HG2	2.15	0.46
2:B:304:ARG:CZ	2:B:575:HIS:HD2	2.29	0.46
2:B:471:GLU:HG2	2:B:472:GLY:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:270:SER:O	3:M:272:ARG:NH1	2.48	0.46
1:A:330:ALA:HA	1:A:333:GLN:HE21	1.79	0.46
2:B:304:ARG:NE	2:B:573:VAL:O	2.48	0.46
2:B:375:ARG:O	2:B:375:ARG:NE	2.42	0.46
3:M:116:LEU:HD21	3:M:119:GLY:HA2	1.97	0.46
3:M:311:LYS:HE2	3:M:380:GLU:HB3	1.96	0.46
5:S:127:SER:O	5:S:131:VAL:HG23	2.16	0.46
5:S:28:LYS:HA	5:S:31:LEU:HD12	1.97	0.46
5:S:119:LEU:HB2	5:S:124:ARG:HB2	1.96	0.46
1:A:212:THR:OG1	1:A:264:LEU:HD12	2.16	0.46
1:A:303:SER:HA	1:A:306:LYS:HG2	1.97	0.46
2:B:26:LYS:NZ	2:B:27:LYS:HG2	2.29	0.46
3:M:202:MET:N	3:M:283:PHE:O	2.29	0.46
3:M:357:ALA:C	3:M:359:GLU:H	2.18	0.46
1:A:430:ILE:HG23	1:A:434:LYS:NZ	2.31	0.46
2:B:99:ASN:HD22	3:M:148:GLN:HE22	1.63	0.46
2:B:186:GLU:O	2:B:189:GLU:HB2	2.15	0.46
2:B:244:VAL:HA	2:B:247:ARG:HG2	1.97	0.46
1:A:272:GLU:H	1:A:277:ARG:CD	2.27	0.46
1:A:482:THR:HA	1:A:485:GLU:CD	2.36	0.46
2:B:34:VAL:O	2:B:38:ILE:HG12	2.16	0.46
2:B:415:ARG:HD3	2:B:447:ALA:HA	1.96	0.46
2:B:439:LEU:HB3	2:B:445:ARG:HG2	1.98	0.46
2:B:491:LEU:HA	2:B:494:LYS:HG2	1.97	0.46
3:M:32:PHE:CE1	3:M:55:PHE:HZ	2.30	0.46
3:M:170:ARG:HH11	3:M:171:ASN:H	1.63	0.46
3:M:258:THR:OG1	3:M:287:ARG:HB3	2.15	0.46
5:S:92:ASN:HD22	5:S:98:VAL:HG12	1.81	0.46
1:A:13:LEU:O	1:A:17:ILE:HG12	2.16	0.46
1:A:281:THR:O	1:A:285:GLU:HG2	2.16	0.46
1:A:574:VAL:O	1:A:577:GLN:HB2	2.15	0.46
2:B:128:LYS:HA	2:B:131:LYS:HB2	1.97	0.46
2:B:241:CYS:O	2:B:276:TYR:OH	2.32	0.46
2:B:339:LEU:O	2:B:343:ILE:HG12	2.16	0.46
2:B:464:GLU:HA	2:B:467:GLU:OE1	2.16	0.46
3:M:170:ARG:NH1	3:M:428:ASP:O	2.42	0.46
3:M:257:CYS:HB2	3:M:286:MET:HE3	1.96	0.46
1:A:454:GLY:O	1:A:493:HIS:HB3	2.16	0.46
1:A:478:TYR:CZ	1:A:482:THR:HG21	2.51	0.46
2:B:238:GLN:O	2:B:242:GLU:HG2	2.16	0.46
2:B:457:GLU:OE2	2:B:458:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:525:ILE:HA	2:B:528:ARG:HG2	1.97	0.46
3:M:71:GLN:O	3:M:73:VAL:HG13	2.16	0.46
3:M:298:PHE:HD1	3:M:320:SER:HA	1.81	0.46
3:M:372:MET:O	3:M:373:LYS:HD3	2.16	0.46
1:A:83:LEU:O	1:A:91:LYS:HG2	2.16	0.46
1:A:448:ASN:HA	1:A:451:ARG:HE	1.81	0.46
2:B:570:LEU:HD12	3:M:72:ASN:HA	1.97	0.46
3:M:107:LEU:HD23	3:M:133:ILE:HG22	1.98	0.46
3:M:179:GLU:OE2	3:M:179:GLU:N	2.49	0.46
5:S:47:THR:OG1	5:S:48:ASN:N	2.48	0.46
5:S:50:VAL:HG12	5:S:59:TYR:CD2	2.51	0.46
1:A:276:VAL:O	1:A:279:ARG:HG2	2.15	0.46
1:A:530:PHE:HB3	1:A:531:HIS:CD2	2.51	0.46
2:B:382:ILE:HG22	2:B:550:GLU:OE1	2.15	0.46
2:B:411:ILE:HD12	2:B:444:ALA:HB1	1.97	0.46
3:M:131:THR:OG1	3:M:132:PHE:N	2.49	0.46
3:M:143:GLN:NE2	3:M:151:ILE:HD12	2.31	0.46
1:A:161:MET:SD	1:A:164:VAL:HG22	2.56	0.45
2:B:100:PRO:HD2	3:M:148:GLN:OE1	2.15	0.45
2:B:307:ASN:HD21	2:B:575:HIS:CE1	2.35	0.45
2:B:507:LEU:O	2:B:511:THR:OG1	2.20	0.45
3:M:129:LEU:HD23	3:M:132:PHE:CE1	2.51	0.45
3:M:244:GLU:OE2	3:M:413:ARG:HA	2.16	0.45
3:M:256:ASP:HB2	3:M:289:ARG:HG2	1.97	0.45
3:M:264:ARG:HD3	3:M:264:ARG:HA	1.76	0.45
5:S:32:ILE:HG23	5:S:36:HIS:CE1	2.51	0.45
1:A:18:SER:HA	1:A:21:ARG:NH2	2.30	0.45
1:A:91:LYS:HE2	1:A:127:PHE:CE2	2.52	0.45
1:A:192:VAL:HB	1:A:211:ILE:HD11	1.98	0.45
2:B:189:GLU:HA	2:B:191:HIS:CE1	2.51	0.45
2:B:284:LEU:O	2:B:288:LEU:HG	2.17	0.45
3:M:101:ILE:HG22	3:M:105:PHE:CE1	2.50	0.45
3:M:252:ILE:HG12	3:M:253:ALA:N	2.31	0.45
5:S:49:PHE:CZ	5:S:81:LEU:HB2	2.51	0.45
1:A:318:ILE:HD12	1:A:356:LEU:HD13	1.98	0.45
1:A:393:LEU:HA	1:A:396:MET:HG2	1.98	0.45
1:A:527:HIS:NE2	1:A:545:TYR:HE2	2.14	0.45
2:B:10:ASN:ND2	2:B:45:LYS:HB2	2.32	0.45
2:B:101:LEU:HD22	2:B:136:TYR:HD2	1.80	0.45
2:B:103:ARG:O	2:B:107:VAL:HG23	2.16	0.45
2:B:533:ASP:N	2:B:533:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:575:HIS:O	2:B:576:LYS:HD3	2.15	0.45
3:M:15:LEU:HD12	3:M:63:ILE:HG23	1.99	0.45
1:A:480:ALA:O	1:A:504:LEU:HD21	2.17	0.45
2:B:221:PHE:HA	2:B:224:ASP:OD2	2.16	0.45
2:B:246:PRO:HG2	2:B:247:ARG:HE	1.81	0.45
2:B:250:HIS:N	2:B:252:ASN:OD1	2.49	0.45
2:B:374:VAL:HG13	2:B:395:LEU:HD22	1.98	0.45
3:M:8:TYR:HB2	3:M:64:TRP:HB2	1.99	0.45
3:M:23:ASP:OD1	3:M:24:ILE:N	2.49	0.45
3:M:184:LEU:N	3:M:193:SER:HB3	2.30	0.45
3:M:238:GLU:HB3	4:P:6:ASN:HB2	1.98	0.45
5:S:94:TYR:CD2	5:S:135:LEU:HD21	2.52	0.45
1:A:124:ASN:HD21	1:A:127:PHE:HD1	1.64	0.45
1:A:299:LYS:HB3	1:A:301:GLN:CD	2.37	0.45
1:A:554:GLU:OE1	1:A:554:GLU:N	2.43	0.45
3:M:287:ARG:NH1	3:M:289:ARG:HB3	2.31	0.45
5:S:35:VAL:O	5:S:39:VAL:HG23	2.15	0.45
1:A:374:ILE:O	1:A:377:LEU:HG	2.17	0.45
1:A:587:SER:OG	1:A:588:THR:N	2.50	0.45
2:B:108:ARG:HB3	2:B:140:THR:HG23	1.98	0.45
2:B:165:LEU:HA	2:B:168:LEU:HB2	1.98	0.45
2:B:295:GLU:H	2:B:298:VAL:CG2	2.29	0.45
3:M:324:PRO:HA	3:M:371:GLY:H	1.82	0.45
2:B:217:TRP:CZ2	3:M:121:PRO:HB2	2.52	0.45
2:B:477:SER:HB3	2:B:479:GLN:HE22	1.81	0.45
3:M:173:LEU:O	3:M:432:TRP:HE3	2.00	0.45
3:M:245:GLU:OE1	3:M:245:GLU:N	2.49	0.45
5:S:109:LYS:O	5:S:113:VAL:HG13	2.16	0.45
1:A:216:GLN:HB2	1:A:217:LYS:NZ	2.31	0.45
1:A:273:ASP:OD1	1:A:275:ALA:N	2.50	0.45
1:A:566:ASP:OD1	1:A:566:ASP:N	2.49	0.45
2:B:28:GLU:OE1	2:B:28:GLU:N	2.44	0.45
2:B:366:ASP:HB3	2:B:369:PHE:HD1	1.81	0.45
2:B:426:GLU:OE1	2:B:426:GLU:N	2.37	0.45
3:M:33:ARG:HG3	3:M:37:ILE:HD12	1.99	0.45
1:A:209:SER:HB3	1:A:260:LYS:NZ	2.32	0.45
1:A:471:ASN:OD1	1:A:605:PHE:N	2.50	0.45
1:A:481:LYS:HG2	1:A:516:ARG:HH21	1.80	0.45
2:B:331:PRO:HG2	2:B:334:VAL:HB	1.98	0.45
2:B:567:ILE:HA	2:B:572:SER:OG	2.16	0.45
3:M:21:ARG:HB3	3:M:23:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:86:CYS:HA	3:M:89:MET:SD	2.57	0.45
3:M:106:VAL:HG13	3:M:107:LEU:HD12	1.98	0.45
3:M:151:ILE:O	3:M:155:VAL:HG23	2.16	0.45
3:M:185:MET:HG2	3:M:190:GLN:H	1.82	0.45
3:M:363:VAL:HG12	3:M:365:LYS:HB2	1.99	0.45
1:A:13:LEU:HD22	1:A:57:LYS:HA	1.98	0.45
1:A:422:GLU:O	1:A:426:LEU:HD13	2.17	0.45
1:A:493:HIS:O	1:A:497:VAL:HG23	2.16	0.45
1:A:550:ASN:HB3	1:A:599:LEU:CD2	2.46	0.45
1:A:552:PHE:O	1:A:555:VAL:HG12	2.17	0.45
2:B:54:VAL:HG21	2:B:72:TYR:CE2	2.52	0.45
2:B:341:ILE:HA	2:B:344:ARG:HB2	1.99	0.45
2:B:380:CYS:HA	2:B:383:LYS:HB2	1.98	0.45
3:M:296:LEU:HB2	3:M:299:ARG:NH2	2.31	0.45
1:A:64:PHE:HD1	1:A:67:LEU:HD12	1.83	0.44
1:A:424:ILE:O	1:A:427:LYS:HG2	2.17	0.44
2:B:400:GLN:HA	2:B:402:LYS:NZ	2.31	0.44
2:B:524:TYR:HA	2:B:527:TRP:HE1	1.81	0.44
3:M:214:PHE:HD1	3:M:415:LEU:HD13	1.81	0.44
3:M:249:LYS:HB3	3:M:408:SER:O	2.17	0.44
3:M:251:SER:CB	3:M:410:LEU:HD13	2.47	0.44
3:M:336:PRO:HD2	3:M:397:ILE:HG12	2.00	0.44
5:S:24:ASP:O	5:S:28:LYS:N	2.36	0.44
1:A:56:LYS:HD3	1:A:87:ARG:HH11	1.81	0.44
1:A:480:ALA:HB2	1:A:507:PHE:HB3	2.00	0.44
1:A:612:ILE:HG23	1:A:615:LYS:HZ1	1.82	0.44
2:B:243:ARG:O	2:B:246:PRO:HD2	2.18	0.44
2:B:408:GLN:HB3	2:B:441:GLU:OE1	2.17	0.44
2:B:551:GLU:HG3	2:B:554:LEU:HD12	1.99	0.44
3:M:167:LYS:NZ	3:M:168:TYR:O	2.45	0.44
3:M:255:ASP:HB2	3:M:290:THR:HA	1.98	0.44
5:S:108:TYR:CE2	5:S:109:LYS:HG3	2.52	0.44
2:B:545:LYS:N	2:B:545:LYS:HD2	2.32	0.44
3:M:127:GLY:O	3:M:162:ARG:HD3	2.17	0.44
3:M:259:PHE:CE2	3:M:265:LEU:HD21	2.53	0.44
3:M:349:MET:HG2	3:M:376:GLN:O	2.18	0.44
5:S:86:ASN:HA	5:S:89:GLU:CD	2.38	0.44
1:A:13:LEU:HD13	1:A:61:LYS:HG3	1.99	0.44
1:A:65:ILE:HA	1:A:68:LEU:HB2	1.99	0.44
1:A:358:SER:HA	1:A:363:HIS:CE1	2.53	0.44
1:A:441:TRP:HA	1:A:444:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:466:LEU:O	2:B:470:LEU:HG	2.17	0.44
3:M:7:ILE:HG22	3:M:15:LEU:HB2	1.99	0.44
5:S:81:LEU:O	5:S:85:HIS:HD2	2.00	0.44
1:A:344:ASN:O	1:A:348:LEU:HG	2.17	0.44
2:B:139:LYS:O	2:B:143:VAL:HG23	2.17	0.44
2:B:162:LEU:O	2:B:166:ARG:HB2	2.18	0.44
2:B:445:ARG:O	2:B:449:ILE:HG12	2.17	0.44
2:B:468:SER:O	2:B:471:GLU:N	2.44	0.44
3:M:7:ILE:HG23	3:M:64:TRP:O	2.17	0.44
3:M:183:LEU:O	3:M:441:ILE:HG22	2.18	0.44
1:A:259:VAL:HG23	1:A:309:VAL:HG12	1.99	0.44
2:B:285:ALA:O	2:B:289:VAL:HG23	2.17	0.44
1:A:38:ALA:O	1:A:42:SER:OG	2.17	0.44
2:B:114:ARG:HG2	2:B:148:LEU:HA	2.00	0.44
2:B:357:GLU:HB3	2:B:361:TYR:OH	2.18	0.44
2:B:422:PRO:O	2:B:424:LYS:HG3	2.18	0.44
2:B:538:LYS:HE3	2:B:538:LYS:HB3	1.84	0.44
3:M:26:ARG:NH1	3:M:29:VAL:HB	2.32	0.44
3:M:161:TRP:CZ2	3:M:277:ILE:HB	2.53	0.44
3:M:175:LEU:HB2	3:M:433:VAL:HG23	1.99	0.44
3:M:188:GLN:CD	3:M:188:GLN:H	2.21	0.44
3:M:304:VAL:HA	3:M:314:VAL:HA	2.00	0.44
3:M:311:LYS:HG3	3:M:382:GLU:HA	2.00	0.44
1:A:499:VAL:O	1:A:503:ILE:HG12	2.18	0.44
2:B:182:ALA:HB2	2:B:221:PHE:CD2	2.53	0.44
2:B:322:LYS:HA	2:B:325:PHE:CE2	2.53	0.44
2:B:331:PRO:O	2:B:335:LYS:HG3	2.17	0.44
2:B:367:VAL:O	2:B:371:ARG:HG3	2.17	0.44
3:M:49:ASN:HD21	3:M:52:ARG:H	1.66	0.44
3:M:239:GLN:OE1	3:M:243:SER:OG	2.25	0.44
1:A:26:LYS:HA	1:A:26:LYS:HD3	1.73	0.44
1:A:133:HIS:HE1	1:A:167:SER:HB3	1.82	0.44
1:A:156:VAL:HA	1:A:159:ASP:OD1	2.18	0.44
1:A:300:VAL:HG22	1:A:304:ASN:OD1	2.18	0.44
2:B:114:ARG:HH21	2:B:150:ASP:CG	2.22	0.44
2:B:233:ASP:N	2:B:236:GLU:OE2	2.40	0.44
2:B:234:ASP:HA	2:B:237:ALA:HB3	1.99	0.44
2:B:568:GLY:O	3:M:74:ASN:ND2	2.48	0.44
5:S:56:LYS:HE3	5:S:71:VAL:HG23	1.99	0.44
1:A:397:CYS:O	1:A:435:TYR:OH	2.28	0.43
2:B:225:CYS:HA	2:B:228:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:GLU:OE1	2:B:236:GLU:N	2.47	0.43
2:B:253:SER:OG	3:M:76:ALA:HB1	2.18	0.43
2:B:399:ILE:O	2:B:402:LYS:HE3	2.18	0.43
3:M:147:GLU:HA	3:M:150:GLN:HE21	1.83	0.43
3:M:395:PRO:HD2	3:M:445:ARG:HD2	1.99	0.43
5:S:91:LEU:HD22	5:S:95:PHE:CE2	2.52	0.43
1:A:77:MET:N	1:A:108:LEU:HD21	2.33	0.43
1:A:324:PRO:O	1:A:328:VAL:HG23	2.17	0.43
2:B:269:LEU:H	2:B:269:LEU:HD23	1.83	0.43
2:B:297:GLU:O	2:B:300:TYR:HB3	2.17	0.43
2:B:399:ILE:HA	2:B:407:VAL:HG22	1.99	0.43
2:B:551:GLU:OE1	2:B:551:GLU:N	2.51	0.43
3:M:254:ILE:HG12	3:M:257:CYS:HB3	2.00	0.43
3:M:419:GLU:HB2	3:M:424:TYR:CZ	2.53	0.43
5:S:103:LEU:C	5:S:106:ASN:H	2.21	0.43
2:B:58:MET:O	2:B:60:THR:HG22	2.18	0.43
2:B:308:LEU:HG	2:B:575:HIS:HE1	1.83	0.43
2:B:347:SER:O	2:B:351:ILE:HG23	2.18	0.43
3:M:188:GLN:HA	3:M:301:ILE:HG23	2.00	0.43
5:S:34:GLU:O	5:S:38:VAL:HG23	2.19	0.43
1:A:362:SER:OG	1:A:365:ALA:HB3	2.19	0.43
1:A:535:VAL:HA	1:A:538:ARG:NE	2.33	0.43
2:B:22:LEU:C	2:B:24:ASN:H	2.20	0.43
2:B:459:ILE:HG22	2:B:462:ALA:HB2	2.00	0.43
2:B:489:VAL:HG21	2:B:526:TYR:CE1	2.53	0.43
2:B:499:THR:HG23	2:B:502:LEU:HD12	2.01	0.43
2:B:563:LEU:HD21	2:B:578:PRO:HD3	2.01	0.43
3:M:11:LYS:HE2	3:M:13:GLU:OE2	2.19	0.43
3:M:107:LEU:HB2	3:M:135:GLN:HE22	1.83	0.43
5:S:95:PHE:CB	5:S:98:VAL:HB	2.48	0.43
1:A:192:VAL:O	1:A:196:LEU:HG	2.18	0.43
1:A:423:GLU:HG3	1:A:619:LYS:HZ3	1.83	0.43
1:A:509:ASN:N	1:A:509:ASN:OD1	2.50	0.43
2:B:105:LEU:HD12	2:B:105:LEU:HA	1.89	0.43
2:B:114:ARG:NH1	2:B:147:LYS:HB3	2.34	0.43
2:B:132:ASP:OD2	2:B:134:ASP:N	2.43	0.43
2:B:284:LEU:O	2:B:287:PRO:HG2	2.18	0.43
2:B:440:ASP:N	2:B:440:ASP:OD1	2.51	0.43
2:B:534:PRO:HA	2:B:537:ALA:HB3	2.00	0.43
3:M:1:MET:HG3	3:M:120:TYR:CD1	2.53	0.43
5:S:113:VAL:O	5:S:116:GLU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ASN:OD1	1:A:114:ASN:N	2.51	0.43
1:A:218:ASN:HB3	1:A:221:GLU:HB2	1.99	0.43
1:A:424:ILE:O	1:A:428:VAL:HG13	2.19	0.43
1:A:521:ILE:HA	1:A:524:ASN:HD21	1.84	0.43
1:A:533:CYS:SG	1:A:537:THR:OG1	2.75	0.43
3:M:39:ALA:HB3	3:M:44:ARG:NH1	2.33	0.43
1:A:468:ILE:HG22	1:A:472:ARG:HG2	2.00	0.43
2:B:52:PRO:O	2:B:55:VAL:HG12	2.19	0.43
3:M:37:ILE:HG23	3:M:64:TRP:CZ3	2.54	0.43
3:M:48:THR:N	3:M:55:PHE:O	2.51	0.43
3:M:177:VAL:N	3:M:434:ARG:O	2.37	0.43
5:S:87:PHE:CE2	5:S:91:LEU:HD11	2.54	0.43
1:A:16:PHE:O	1:A:20:ILE:HG22	2.19	0.43
1:A:521:ILE:HA	1:A:524:ASN:ND2	2.33	0.43
1:A:543:SER:HB3	1:A:579:ARG:NH2	2.34	0.43
1:A:600:GLU:OE2	1:A:603:PRO:HD3	2.19	0.43
1:A:605:PHE:CG	1:A:606:PRO:HD2	2.54	0.43
3:M:55:PHE:HB3	3:M:57:HIS:CD2	2.54	0.43
3:M:90:ALA:HA	3:M:94:GLY:O	2.19	0.43
5:S:87:PHE:O	5:S:91:LEU:HG	2.19	0.43
1:A:140:SER:N	1:A:143:MET:SD	2.92	0.43
1:A:150:GLU:O	1:A:154:ILE:HG12	2.18	0.43
1:A:220:GLU:OE1	1:A:220:GLU:N	2.52	0.43
2:B:66:LYS:HE3	2:B:105:LEU:HD23	2.01	0.43
2:B:143:VAL:HG12	2:B:147:LYS:NZ	2.34	0.43
3:M:2:ILE:HG23	3:M:69:THR:HB	2.00	0.43
3:M:12:GLY:O	3:M:33:ARG:NE	2.52	0.43
3:M:74:ASN:O	3:M:77:MET:HG3	2.19	0.43
1:A:445:THR:HA	1:A:448:ASN:ND2	2.34	0.43
1:A:594:ILE:HA	1:A:597:THR:HB	2.00	0.43
3:M:56:PHE:CD2	3:M:78:VAL:HG11	2.54	0.43
5:S:3:ARG:HD3	5:S:21:MET:CE	2.49	0.43
1:A:231:SER:O	1:A:235:ARG:HG2	2.19	0.42
2:B:90:SER:N	2:B:93:LYS:HZ2	2.17	0.42
2:B:134:ASP:C	2:B:138:ARG:HE	2.22	0.42
2:B:473:PHE:CZ	2:B:509:LEU:HB3	2.54	0.42
3:M:59:LYS:HG2	3:M:64:TRP:CD1	2.54	0.42
3:M:102:LYS:HA	3:M:105:PHE:CE1	2.54	0.42
3:M:352:LYS:NZ	3:M:354:LYS:HD2	2.34	0.42
5:S:4:PHE:CD1	5:S:6:LEU:HG	2.54	0.42
1:A:43:LYS:HG2	1:A:58:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:O	1:A:81:ASN:HB2	2.20	0.42
1:A:223:LYS:HA	1:A:226:VAL:HG23	2.01	0.42
2:B:31:LYS:HE2	2:B:31:LYS:HB2	1.86	0.42
2:B:262:VAL:O	2:B:265:LYS:HB3	2.19	0.42
2:B:450:TRP:CE3	2:B:451:ILE:HG12	2.53	0.42
5:S:117:MET:O	5:S:124:ARG:N	2.51	0.42
1:A:73:ASP:OD1	1:A:74:PHE:HD1	2.01	0.42
1:A:166:GLN:NE2	5:S:125:GLU:OE2	2.44	0.42
1:A:487:LEU:HD12	1:A:504:LEU:HD12	2.01	0.42
1:A:543:SER:HB3	1:A:579:ARG:HH22	1.83	0.42
2:B:382:ILE:HA	2:B:421:TYR:CE2	2.52	0.42
2:B:423:ASN:ND2	2:B:455:TYR:OH	2.52	0.42
1:A:94:GLY:O	1:A:98:ILE:HG12	2.20	0.42
1:A:380:GLU:CD	1:A:385:VAL:HG21	2.40	0.42
1:A:383:VAL:HB	1:A:387:GLN:NE2	2.26	0.42
1:A:481:LYS:HE3	1:A:481:LYS:HB3	1.89	0.42
1:A:485:GLU:HG3	1:A:516:ARG:HH22	1.84	0.42
1:A:505:GLY:O	1:A:551:LEU:HD12	2.20	0.42
2:B:257:LEU:HB3	2:B:568:GLY:HA2	2.01	0.42
2:B:367:VAL:HG23	2:B:405:TYR:CD2	2.54	0.42
3:M:111:LEU:HD21	3:M:133:ILE:HG21	2.02	0.42
3:M:250:GLN:N	3:M:408:SER:O	2.52	0.42
5:S:67:PHE:HE2	5:S:88:VAL:HG22	1.85	0.42
1:A:142:GLU:HA	1:A:145:GLU:CD	2.40	0.42
1:A:333:GLN:HB3	1:A:337:PHE:CE2	2.54	0.42
1:A:615:LYS:HG2	1:A:618:LYS:HE2	2.01	0.42
2:B:366:ASP:HB3	2:B:369:PHE:CE1	2.54	0.42
3:M:14:VAL:HG13	3:M:33:ARG:NH2	2.34	0.42
5:S:23:PHE:HB2	5:S:28:LYS:HZ3	1.85	0.42
1:A:159:ASP:HA	1:A:165:LYS:CE	2.47	0.42
1:A:197:ASN:ND2	1:A:228:LEU:HD13	2.34	0.42
1:A:462:TRP:HB2	1:A:499:VAL:HG21	2.02	0.42
1:A:467:GLN:O	1:A:471:ASN:ND2	2.52	0.42
3:M:260:HIS:O	3:M:262:CYS:N	2.45	0.42
3:M:318:ILE:O	3:M:374:GLU:HA	2.20	0.42
1:A:10:MET:HE1	1:A:56:LYS:HE2	2.00	0.42
1:A:539:ALA:HB1	1:A:579:ARG:HH12	1.84	0.42
2:B:10:ASN:O	2:B:11:LYS:HB2	2.20	0.42
2:B:105:LEU:HA	2:B:108:ARG:HG2	2.00	0.42
2:B:139:LYS:HA	2:B:179:ASN:HD21	1.85	0.42
2:B:158:ASP:OD1	2:B:159:GLN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:3:GLY:CA	3:M:21:ARG:HB2	2.50	0.42
3:M:271:GLU:HA	3:M:272:ARG:NH1	2.34	0.42
1:A:50:LEU:O	1:A:55:LYS:HG3	2.18	0.42
1:A:191:ARG:O	1:A:195:LEU:HG	2.20	0.42
1:A:409:MET:O	1:A:413:LEU:HG	2.20	0.42
1:A:464:ARG:HA	1:A:467:GLN:OE1	2.20	0.42
2:B:49:SER:O	2:B:52:PRO:HD2	2.18	0.42
2:B:492:PHE:CD1	2:B:496:PRO:HA	2.55	0.42
3:M:298:PHE:C	3:M:299:ARG:HD2	2.40	0.42
3:M:340:ASN:O	3:M:383:LEU:HD23	2.19	0.42
1:A:44:PHE:HD2	1:A:74:PHE:HE2	1.66	0.42
2:B:118:ILE:HG13	2:B:122:LEU:HD23	2.01	0.42
2:B:151:ILE:HG23	2:B:152:ASN:OD1	2.20	0.42
2:B:166:ARG:HH22	2:B:197:LEU:CB	2.32	0.42
2:B:578:PRO:HA	2:B:581:PHE:CE2	2.55	0.42
5:S:43:ASP:OD1	5:S:46:HIS:CD2	2.72	0.42
5:S:58:ILE:HD13	5:S:80:TYR:CB	2.49	0.42
1:A:18:SER:HA	1:A:21:ARG:NH1	2.35	0.42
1:A:394:TYR:OH	1:A:427:LYS:O	2.26	0.42
2:B:305:ASN:ND2	2:B:573:VAL:HG22	2.32	0.42
3:M:30:ASP:OD1	3:M:31:ALA:N	2.52	0.42
3:M:104:ASN:OD1	3:M:135:GLN:NE2	2.52	0.42
3:M:126:THR:HA	3:M:129:LEU:HG	2.02	0.42
3:M:180:SER:HB2	3:M:438:ARG:HH21	1.85	0.42
3:M:221:VAL:O	3:M:223:GLU:HG3	2.20	0.42
3:M:324:PRO:HA	3:M:371:GLY:N	2.35	0.42
5:S:110:VAL:O	5:S:114:VAL:HG23	2.19	0.42
1:A:50:LEU:O	1:A:54:SER:OG	2.38	0.41
1:A:95:TYR:HD1	1:A:134:CYS:SG	2.43	0.41
1:A:116:ILE:HG23	1:A:131:ALA:HB1	2.02	0.41
1:A:235:ARG:O	1:A:239:SER:OG	2.35	0.41
1:A:241:SER:HB3	1:A:248:THR:CG2	2.50	0.41
1:A:512:ALA:O	1:A:517:SER:OG	2.37	0.41
2:B:312:LYS:HZ3	2:B:564:ILE:HD12	1.84	0.41
2:B:374:VAL:HG21	2:B:406:VAL:HG13	2.01	0.41
2:B:408:GLN:HB3	2:B:441:GLU:CD	2.40	0.41
3:M:81:PHE:CZ	3:M:116:LEU:HB2	2.55	0.41
3:M:404:PRO:HA	3:M:436:ILE:HA	2.02	0.41
1:A:173:LEU:HD13	1:A:210:LEU:HD13	2.03	0.41
1:A:270:PRO:HB3	1:A:320:HIS:ND1	2.35	0.41
2:B:316:ILE:C	2:B:318:LYS:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:108:ILE:O	3:M:112:LEU:HD23	2.20	0.41
3:M:334:ARG:O	3:M:397:ILE:HG23	2.19	0.41
3:M:355:TYR:HE2	3:M:357:ALA:HB2	1.85	0.41
3:M:398:SER:HA	3:M:442:TYR:O	2.20	0.41
5:S:37:ALA:O	5:S:41:VAL:HG22	2.20	0.41
5:S:86:ASN:HA	5:S:89:GLU:OE2	2.21	0.41
1:A:533:CYS:SG	1:A:538:ARG:HG2	2.60	0.41
2:B:205:ASN:O	2:B:209:THR:HG23	2.21	0.41
2:B:370:VAL:O	2:B:374:VAL:HG23	2.21	0.41
2:B:525:ILE:HA	2:B:528:ARG:HE	1.85	0.41
3:M:80:GLU:HA	3:M:83:TYR:CD2	2.55	0.41
3:M:184:LEU:O	3:M:192:LEU:N	2.53	0.41
3:M:203:LYS:HA	3:M:203:LYS:HD2	1.93	0.41
5:S:49:PHE:CE1	5:S:77:ASN:HB3	2.55	0.41
5:S:138:LEU:C	5:S:140:SER:H	2.24	0.41
1:A:13:LEU:CD1	1:A:61:LYS:HG3	2.49	0.41
1:A:115:ALA:HA	1:A:118:ASN:ND2	2.34	0.41
1:A:185:MET:HA	1:A:188:TRP:CH2	2.55	0.41
1:A:613:LEU:HD12	1:A:614:ALA:N	2.35	0.41
2:B:305:ASN:O	2:B:309:ILE:HG13	2.21	0.41
2:B:350:ASN:O	2:B:353:GLN:HG3	2.19	0.41
2:B:379:ARG:O	2:B:383:LYS:HG3	2.20	0.41
2:B:400:GLN:HA	2:B:402:LYS:HZ2	1.84	0.41
2:B:500:GLN:CD	2:B:500:GLN:H	2.23	0.41
3:M:338:PRO:HG2	3:M:381:ILE:HB	2.02	0.41
1:A:29:GLU:O	1:A:33:ILE:HG13	2.20	0.41
1:A:222:PHE:O	1:A:268:TYR:OH	2.37	0.41
1:A:350:LEU:HB3	1:A:388:ARG:HB2	2.03	0.41
1:A:370:ILE:O	1:A:374:ILE:HG13	2.21	0.41
1:A:439:TYR:O	1:A:443:VAL:HG23	2.21	0.41
2:B:62:ASN:OD1	2:B:64:GLU:HG2	2.20	0.41
2:B:174:PRO:HD2	2:B:175:MET:HE2	2.02	0.41
2:B:566:HIS:CG	2:B:571:ALA:HB3	2.56	0.41
3:M:1:MET:C	3:M:21:ARG:HE	2.24	0.41
3:M:70:LYS:H	3:M:71:GLN:NE2	2.18	0.41
3:M:106:VAL:O	3:M:110:GLU:HG3	2.20	0.41
3:M:123:ASN:OD1	3:M:124:SER:N	2.53	0.41
4:P:4:ARG:CZ	4:P:4:ARG:HA	2.50	0.41
2:B:11:LYS:CG	2:B:12:LYS:HG3	2.50	0.41
2:B:190:SER:O	2:B:192:PRO:HD2	2.20	0.41
5:S:55:PHE:HD2	5:S:71:VAL:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:TYR:HB3	1:A:302:HIS:CE1	2.56	0.41
1:A:386:ARG:O	1:A:390:VAL:HG23	2.20	0.41
1:A:540:LEU:O	1:A:543:SER:OG	2.28	0.41
2:B:11:LYS:HD3	2:B:12:LYS:HZ3	1.85	0.41
2:B:26:LYS:HA	2:B:26:LYS:HD2	1.79	0.41
2:B:99:ASN:HB3	2:B:102:ILE:HB	2.02	0.41
2:B:127:ARG:HB3	2:B:131:LYS:NZ	2.36	0.41
2:B:253:SER:O	2:B:257:LEU:HG	2.19	0.41
2:B:275:ASP:O	2:B:279:MET:N	2.28	0.41
3:M:112:LEU:HA	3:M:115:ILE:HG22	2.03	0.41
3:M:268:PHE:HB2	3:M:274:ILE:CG2	2.50	0.41
5:S:86:ASN:O	5:S:90:VAL:HG23	2.20	0.41
1:A:97:PHE:CE2	1:A:101:LEU:HD22	2.55	0.41
2:B:94:ASP:HA	2:B:97:ASP:OD2	2.21	0.41
2:B:282:LYS:HG3	2:B:283:LYS:N	2.36	0.41
2:B:563:LEU:HD23	2:B:563:LEU:HA	1.80	0.41
3:M:19:VAL:HG13	3:M:24:ILE:HG13	2.03	0.41
3:M:28:ALA:HB1	3:M:32:PHE:CZ	2.56	0.41
3:M:37:ILE:HG12	3:M:64:TRP:HZ3	1.85	0.41
3:M:341:THR:HG23	3:M:381:ILE:HG23	2.03	0.41
3:M:344:VAL:HA	3:M:381:ILE:HD13	2.01	0.41
5:S:49:PHE:HZ	5:S:81:LEU:HB2	1.85	0.41
1:A:213:THR:O	1:A:217:LYS:NZ	2.36	0.41
1:A:246:ASP:OD2	5:S:130:LYS:HG3	2.21	0.41
1:A:505:GLY:HA3	1:A:544:THR:HG23	2.02	0.41
1:A:591:SER:OG	1:A:593:ASP:OD1	2.21	0.41
1:A:605:PHE:HE1	2:B:520:ARG:HD2	1.86	0.41
1:A:617:LYS:O	1:A:620:LYS:HB3	2.21	0.41
2:B:115:VAL:HG22	2:B:116:ASP:OD1	2.21	0.41
2:B:248:LEU:HB3	2:B:249:SER:H	1.74	0.41
2:B:271:PRO:HA	2:B:277:TYR:HB3	2.03	0.41
2:B:318:LYS:NZ	2:B:346:ALA:O	2.34	0.41
2:B:339:LEU:O	2:B:342:MET:HB2	2.20	0.41
2:B:379:ARG:O	2:B:383:LYS:N	2.50	0.41
2:B:423:ASN:OD1	2:B:458:ARG:NH1	2.54	0.41
2:B:455:TYR:HA	2:B:457:GLU:OE2	2.21	0.41
3:M:65:LEU:HD11	3:M:85:MET:SD	2.61	0.41
3:M:331:ILE:O	3:M:366:ILE:N	2.26	0.41
3:M:340:ASN:HD22	3:M:384:LEU:H	1.68	0.41
5:S:52:PHE:N	5:S:55:PHE:O	2.37	0.41
1:A:147:PHE:HA	1:A:150:GLU:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:O	1:A:236:ILE:HG13	2.21	0.41
1:A:321:ASP:HA	1:A:327:LEU:HD21	2.03	0.41
1:A:424:ILE:HA	1:A:427:LYS:HG2	2.01	0.41
1:A:438:ASP:CG	1:A:441:TRP:HB3	2.41	0.41
2:B:208:LEU:HD13	2:B:243:ARG:HG3	2.03	0.41
2:B:280:LEU:HA	2:B:283:LYS:CD	2.52	0.41
2:B:464:GLU:HG2	2:B:465:LEU:H	1.86	0.41
2:B:521:ASP:HA	2:B:524:TYR:CG	2.55	0.41
3:M:240:LYS:HG2	3:M:242:ILE:H	1.86	0.41
3:M:313:GLU:HG2	3:M:380:GLU:HB3	2.03	0.41
3:M:345:GLN:O	3:M:379:ALA:HA	2.20	0.41
1:A:380:GLU:HB3	1:A:386:ARG:CZ	2.51	0.40
1:A:417:ASP:O	1:A:421:ARG:HB2	2.21	0.40
1:A:610:SER:O	1:A:610:SER:OG	2.32	0.40
2:B:293:SER:OG	3:M:289:ARG:NH2	2.53	0.40
3:M:185:MET:HA	3:M:192:LEU:H	1.86	0.40
1:A:51:ASP:OD1	1:A:52:GLY:N	2.49	0.40
1:A:107:GLU:O	1:A:111:LEU:HG	2.22	0.40
1:A:231:SER:HB3	1:A:279:ARG:NH1	2.35	0.40
1:A:401:ASN:O	1:A:405:ILE:HG12	2.21	0.40
1:A:427:LYS:HA	1:A:430:ILE:HG22	2.03	0.40
1:A:559:ILE:HA	1:A:562:VAL:HG22	2.03	0.40
2:B:4:SER:OG	3:M:105:PHE:N	2.54	0.40
2:B:347:SER:O	2:B:350:ASN:N	2.54	0.40
2:B:378:GLY:HA3	2:B:413:VAL:CG1	2.52	0.40
3:M:250:GLN:NE2	3:M:408:SER:HA	2.28	0.40
1:A:170:LEU:HB3	5:S:120:ALA:HB3	2.04	0.40
1:A:504:LEU:HD23	1:A:504:LEU:HA	1.85	0.40
2:B:375:ARG:O	2:B:379:ARG:HG3	2.22	0.40
3:M:3:GLY:HA3	3:M:21:ARG:HB2	2.03	0.40
3:M:6:PHE:CD1	3:M:17:SER:HA	2.57	0.40
3:M:256:ASP:HB2	3:M:289:ARG:CD	2.51	0.40
3:M:369:MET:HG3	3:M:370:ALA:O	2.21	0.40
1:A:16:PHE:HE1	1:A:32:ARG:HG3	1.86	0.40
1:A:277:ARG:O	1:A:280:LEU:HB3	2.22	0.40
1:A:598:VAL:HG13	2:B:525:ILE:HG12	2.03	0.40
2:B:354:VAL:HA	2:B:357:GLU:OE1	2.22	0.40
2:B:492:PHE:HE1	2:B:500:GLN:HG3	1.87	0.40
2:B:501:GLU:O	2:B:505:GLN:HG3	2.22	0.40
3:M:214:PHE:CE1	3:M:412:VAL:HG22	2.56	0.40
3:M:300:VAL:HG22	3:M:318:ILE:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:4:PHE:CB	5:S:19:TRP:HA	2.51	0.40
1:A:155:LEU:HD12	1:A:165:LYS:HD3	2.04	0.40
1:A:397:CYS:SG	1:A:401:ASN:ND2	2.93	0.40
2:B:13:GLY:HA2	2:B:16:PHE:CD2	2.56	0.40
2:B:77:ALA:HA	2:B:80:GLN:HG3	2.04	0.40
3:M:77:MET:HA	3:M:80:GLU:OE2	2.22	0.40
3:M:296:LEU:HA	3:M:297:PRO:HD3	1.97	0.40
5:S:60:ARG:HB2	5:S:67:PHE:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	611/628 (97%)	546 (89%)	65 (11%)	0	100	100
2	B	577/944 (61%)	509 (88%)	67 (12%)	1 (0%)	47	81
3	M	422/446 (95%)	355 (84%)	67 (16%)	0	100	100
4	P	4/16 (25%)	3 (75%)	1 (25%)	0	100	100
5	S	140/142 (99%)	116 (83%)	24 (17%)	0	100	100
All	All	1754/2176 (81%)	1529 (87%)	224 (13%)	1 (0%)	54	86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	316	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	537/548 (98%)	533 (99%)	4 (1%)	84	90
2	B	522/840 (62%)	521 (100%)	1 (0%)	93	96
3	M	384/398 (96%)	381 (99%)	3 (1%)	81	89
4	P	6/15 (40%)	6 (100%)	0	100	100
5	S	131/131 (100%)	129 (98%)	2 (2%)	65	80
All	All	1580/1932 (82%)	1570 (99%)	10 (1%)	86	92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	273	ASP
1	A	381	ARG
1	A	564	ARG
2	B	114	ARG
3	M	272	ARG
3	M	305	ARG
3	M	322	PHE
5	S	10	ARG
5	S	36	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	34	ASN
1	A	70	HIS
1	A	105	ASN
1	A	114	ASN
1	A	118	ASN
1	A	124	ASN
1	A	194	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	197	ASN
1	A	218	ASN
1	A	302	HIS
1	A	333	GLN
1	A	363	HIS
1	A	448	ASN
1	A	495	ASN
1	A	522	GLN
1	A	531	HIS
1	A	560	GLN
1	A	577	GLN
2	B	191	HIS
2	B	195	ASN
2	B	238	GLN
2	B	305	ASN
2	B	353	GLN
2	B	423	ASN
3	M	9	ASN
3	M	35	ASN
3	M	38	HIS
3	M	72	ASN
3	M	135	GLN
3	M	148	GLN
3	M	150	GLN
3	M	154	GLN
3	M	182	ASN
3	M	250	GLN
3	M	376	GLN
4	P	3	GLN
5	S	85	HIS
5	S	92	ASN
5	S	128	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 ⓘ

This section contains visualisations of the EMDB entry EMD-10748. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

X	Y	Z

6.1.2 Raw map

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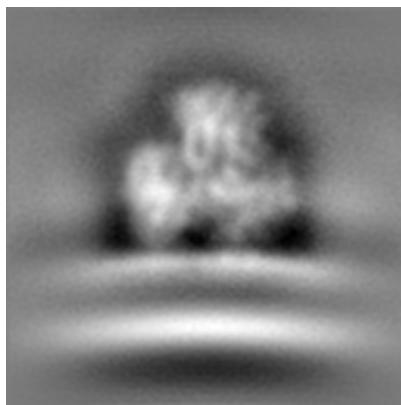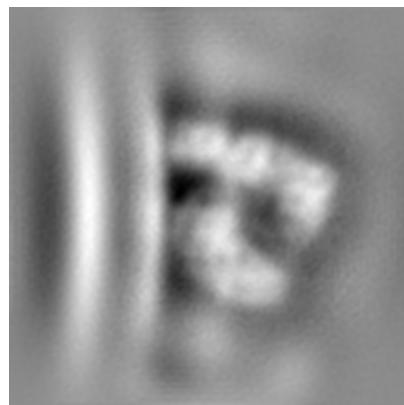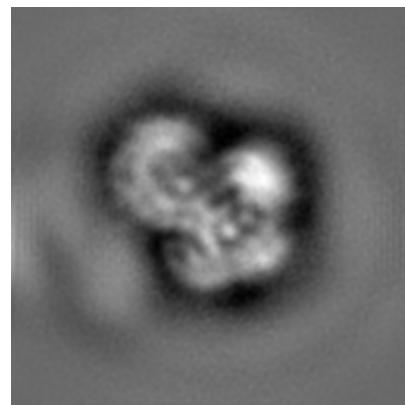
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map

X Index: 64
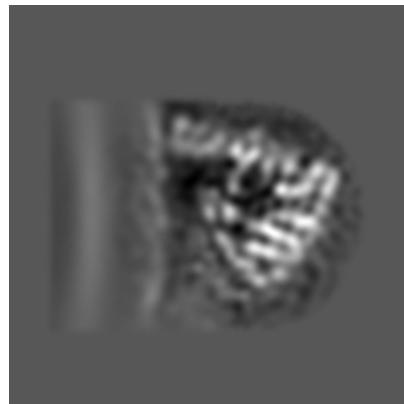
Y Index: 64

Z Index: 64

6.2.2 Raw map
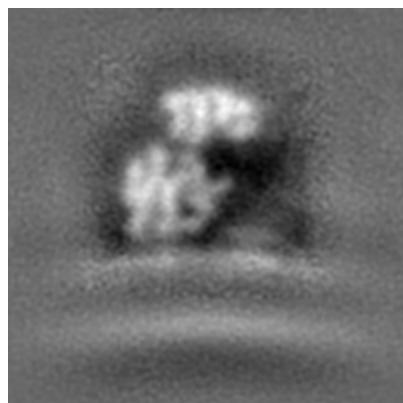
X Index: 64
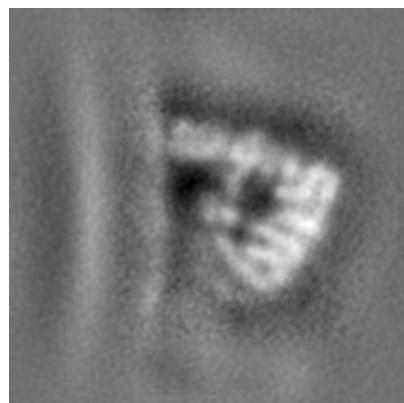
Y Index: 64
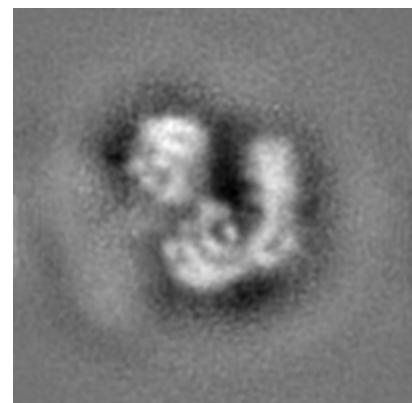
Z Index: 64

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
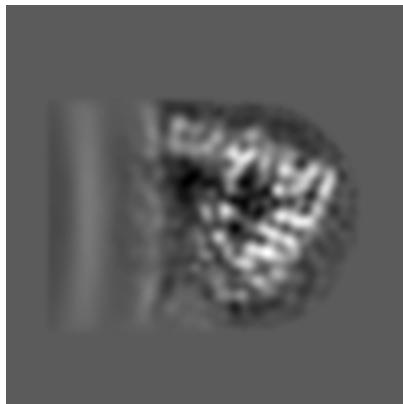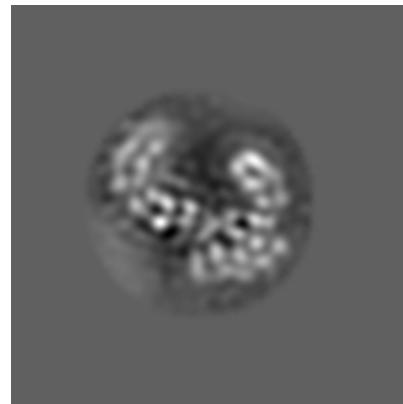
| X Index: 69 | Y Index: 65 | Z Index: 79 |

6.3.2 Raw map
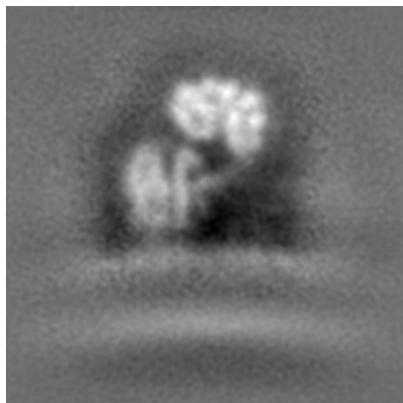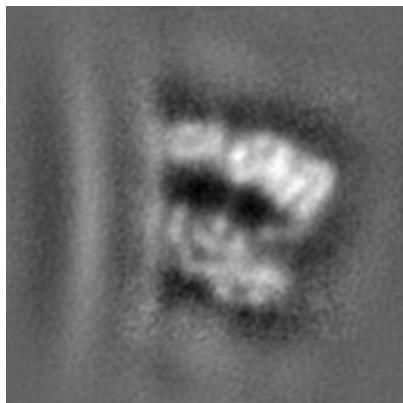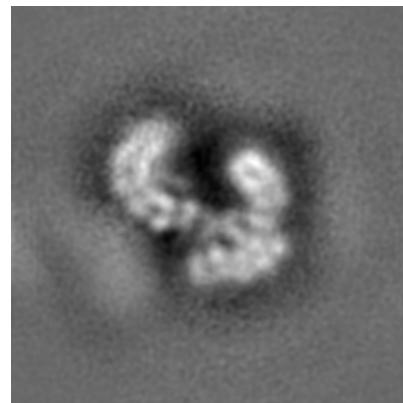
| X Index: 69 | Y Index: 72 | Z Index: 79 |

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X   Y   Z
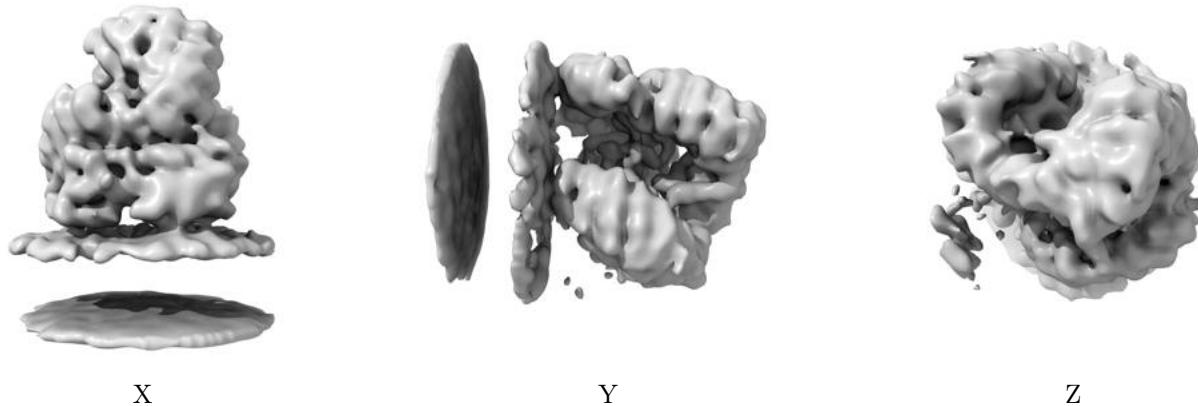
The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X   Y   Z

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

6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure

- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.5.1 emd_10748_msk_1.map (i)

X　　　　　Y　　　　　Z
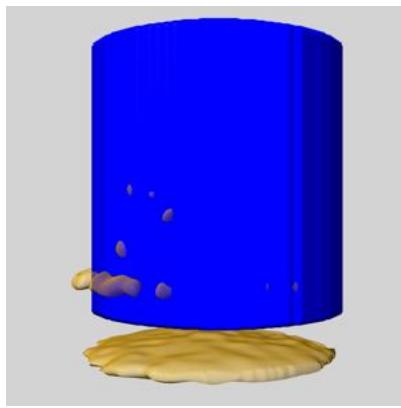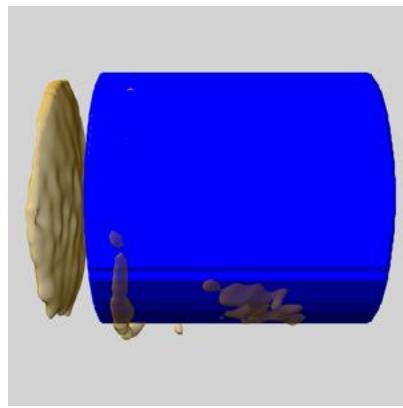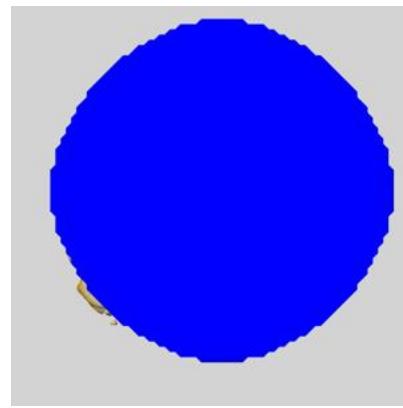
7 Map analysis ⓘ

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

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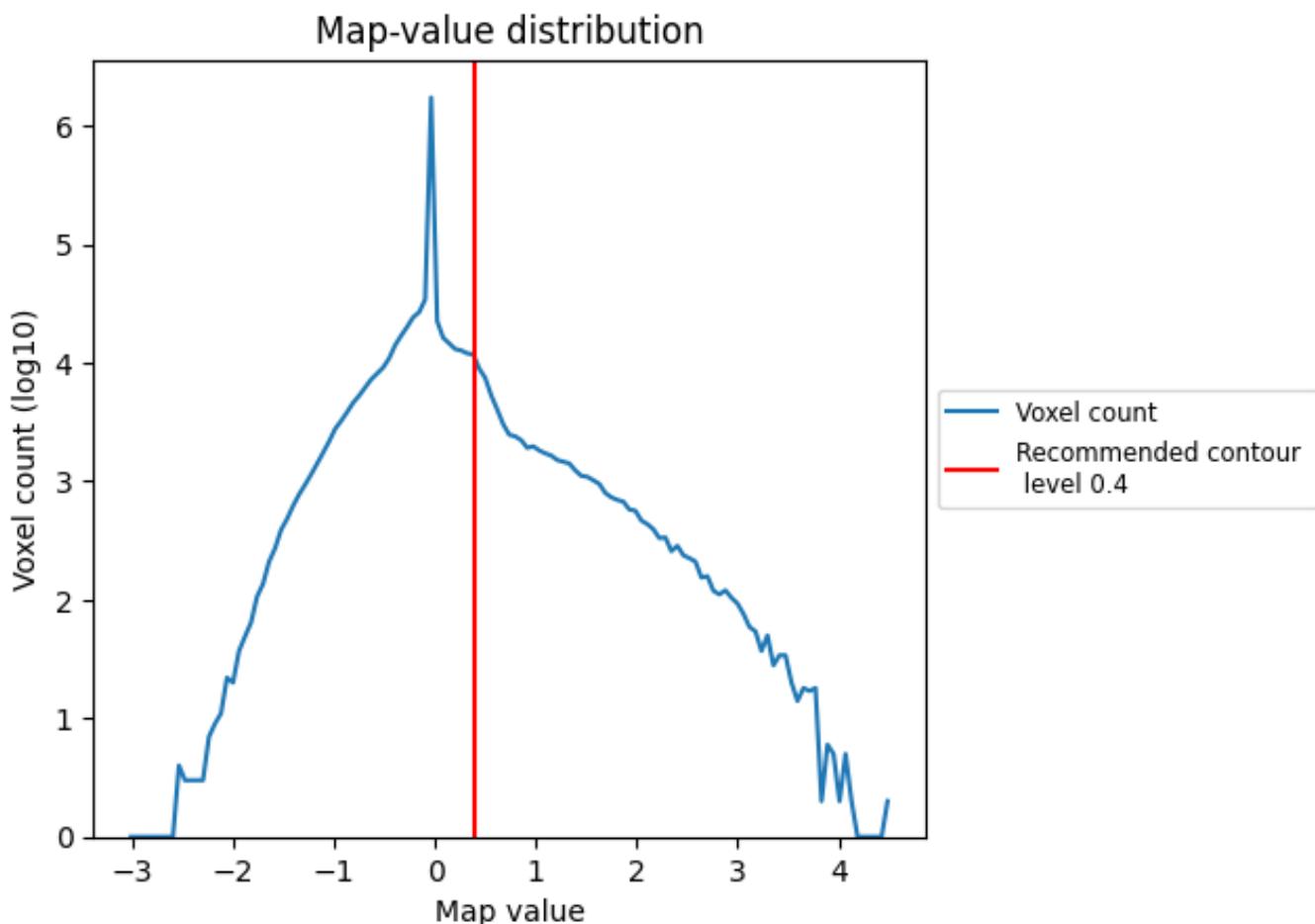
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
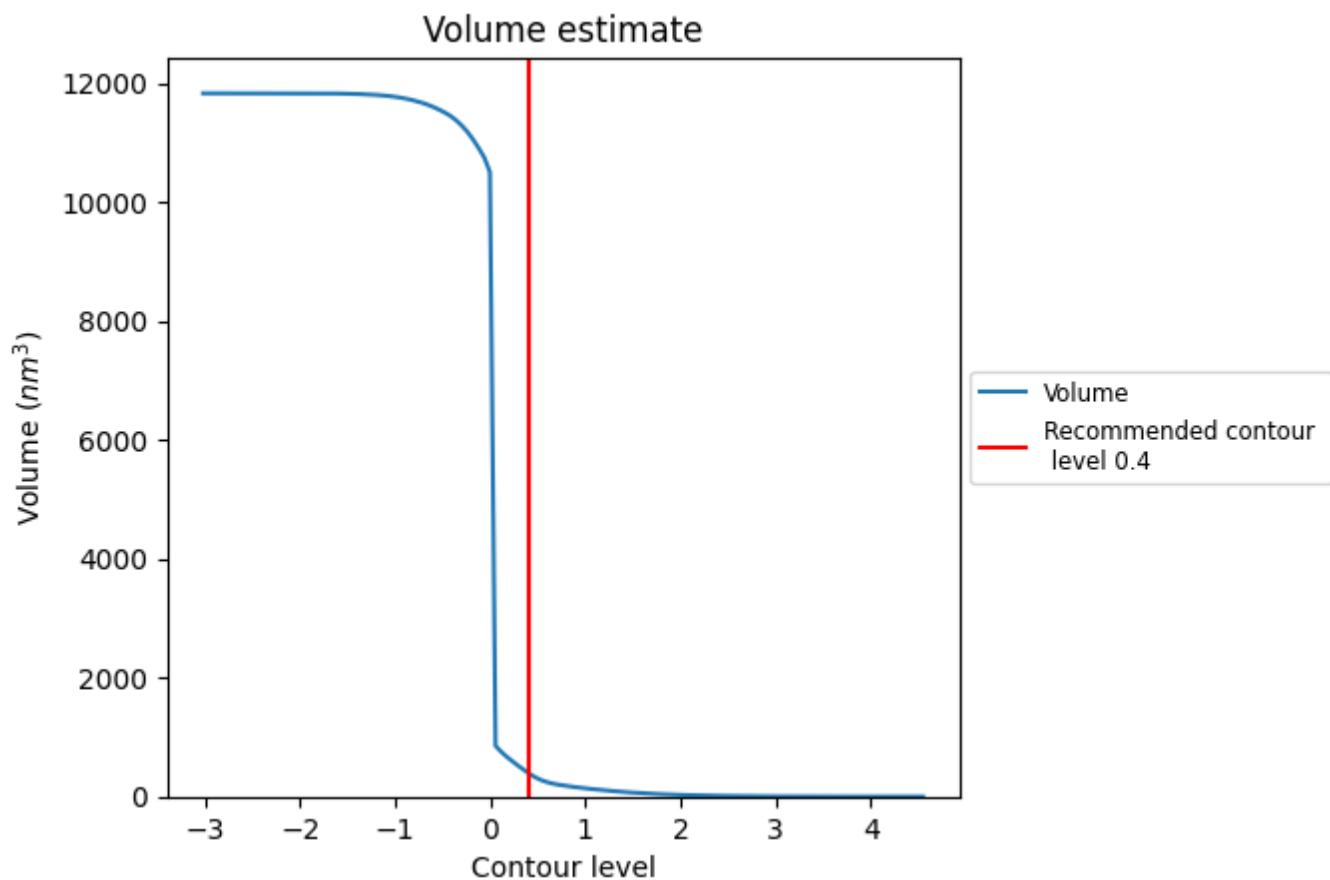
The volume at the recommended contour level is 397 nm^3; this corresponds to an approximate mass of 358 kDa.

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　ⓘ
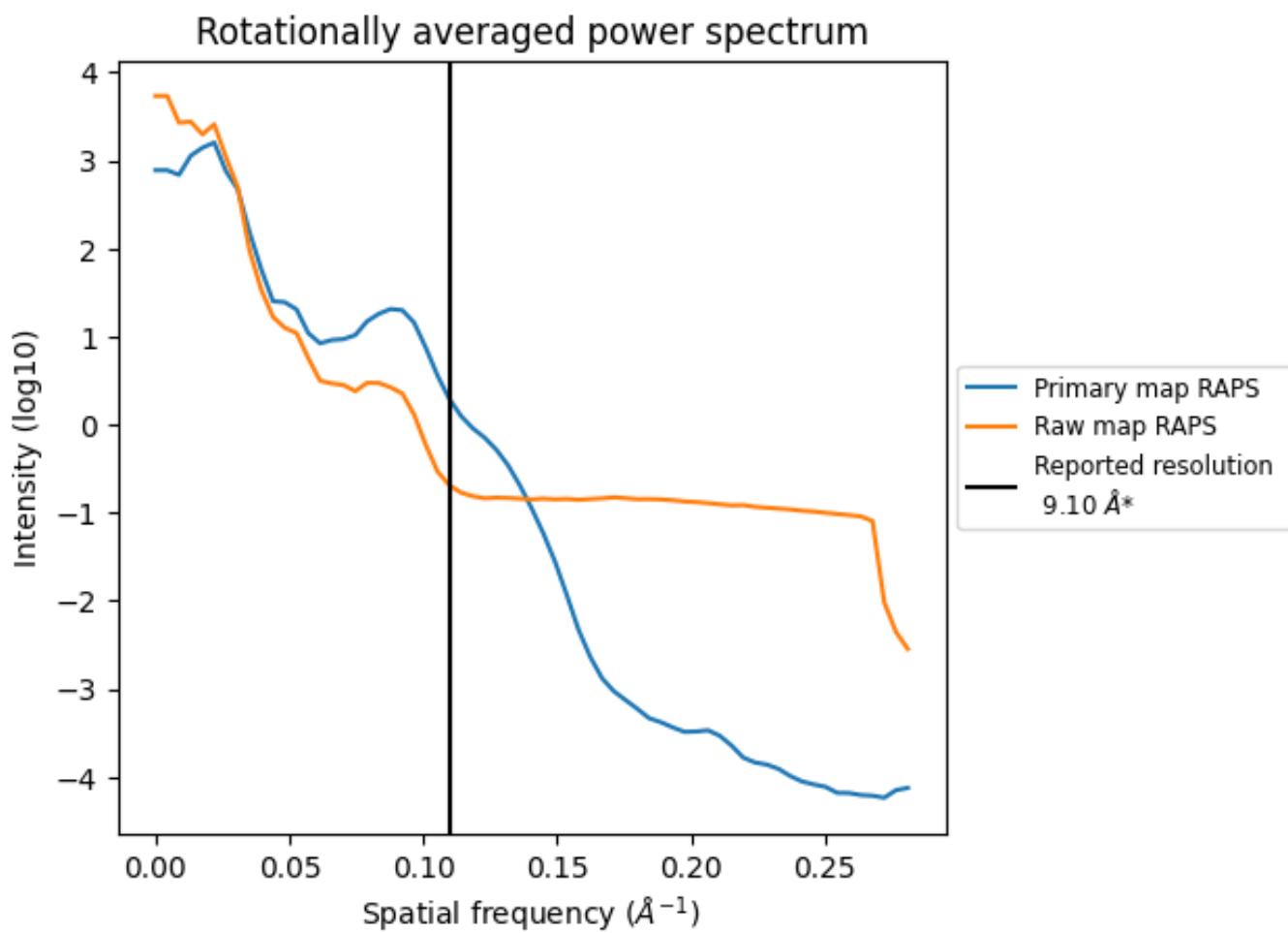
*Reported resolution corresponds to spatial frequency of 0.110 Å^{-1}

8   Fourier-Shell correlation ⓘ

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

8.1   FSC ⓘ
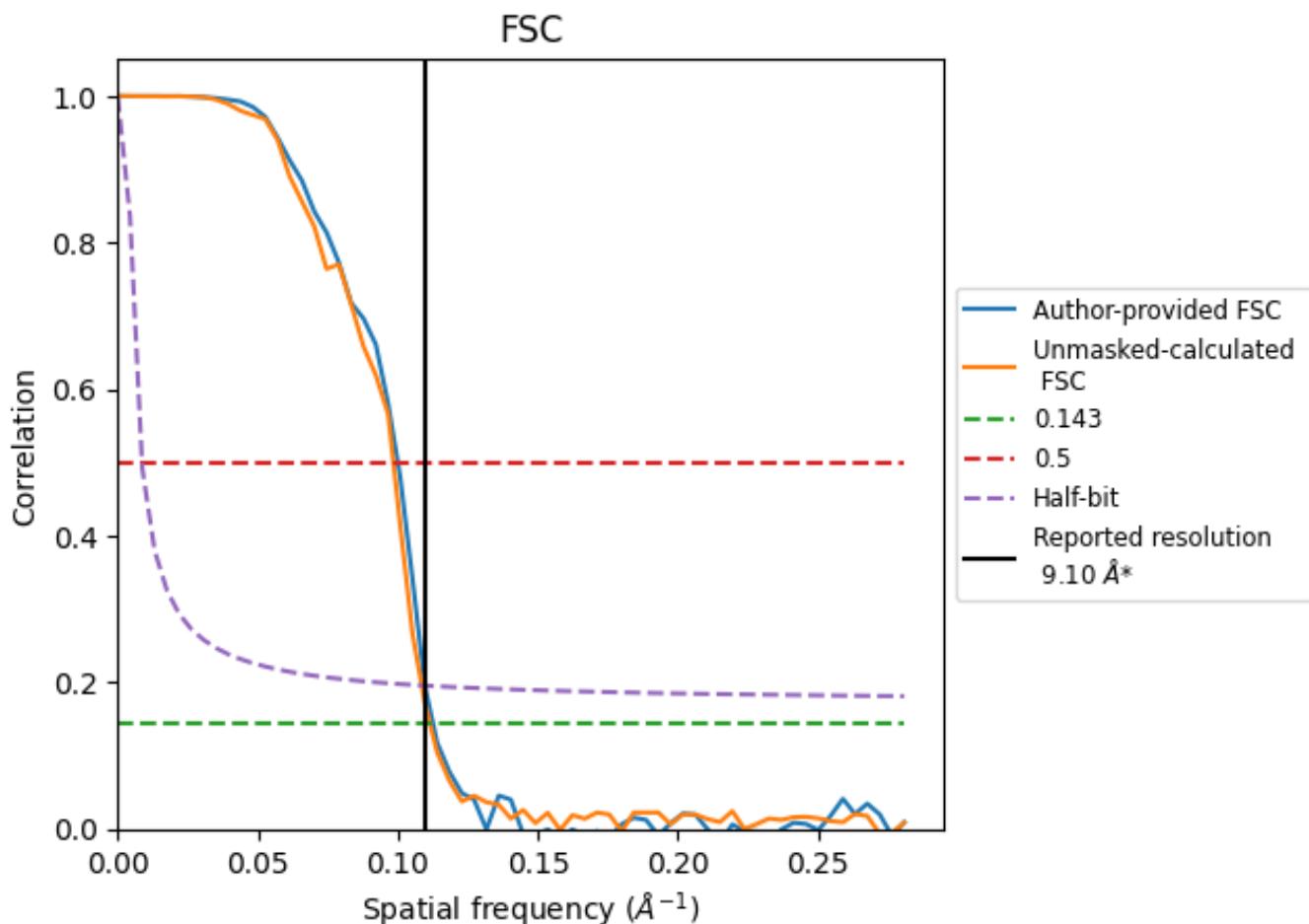
*Reported resolution corresponds to spatial frequency of 0.110 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.10	-	-
Author-provided FSC curve	8.87	9.99	9.11
Unmasked-calculated*	8.96	10.15	9.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-10748 and PDB model 6YAF. Per-residue inclusion information can be found in section 3 on page 5.

9.1   Map-model overlay ⓘ

X   Y   Z
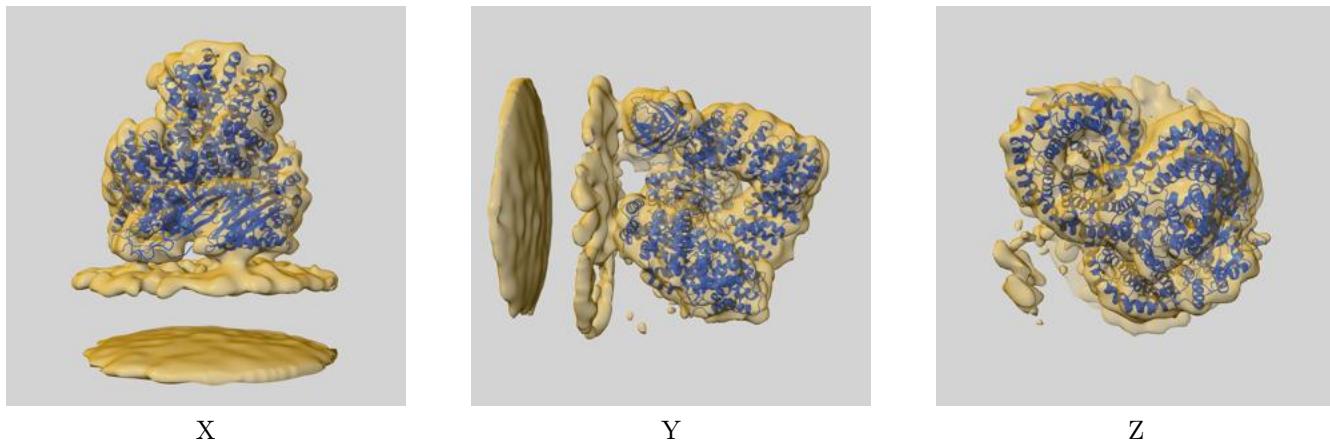
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

X   Y   Z
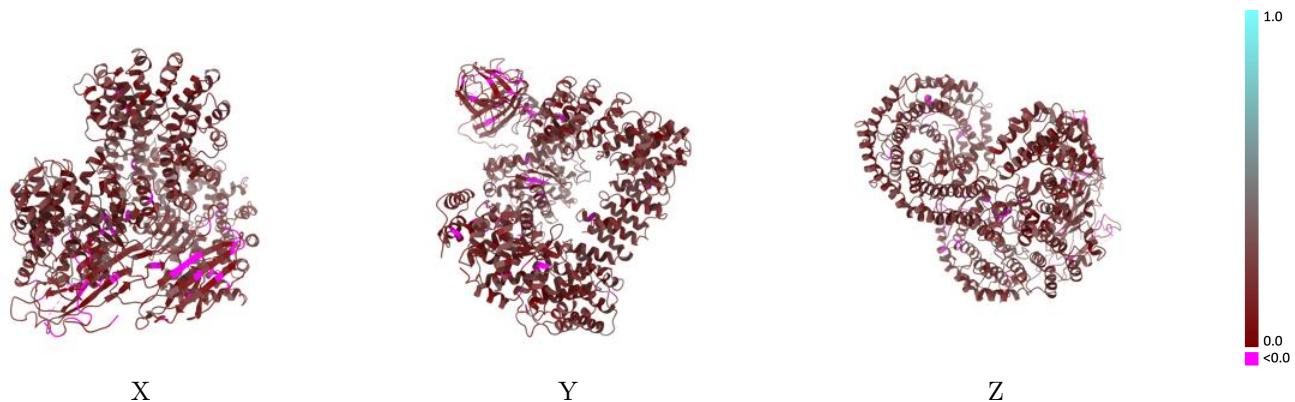
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ

X   Y   Z
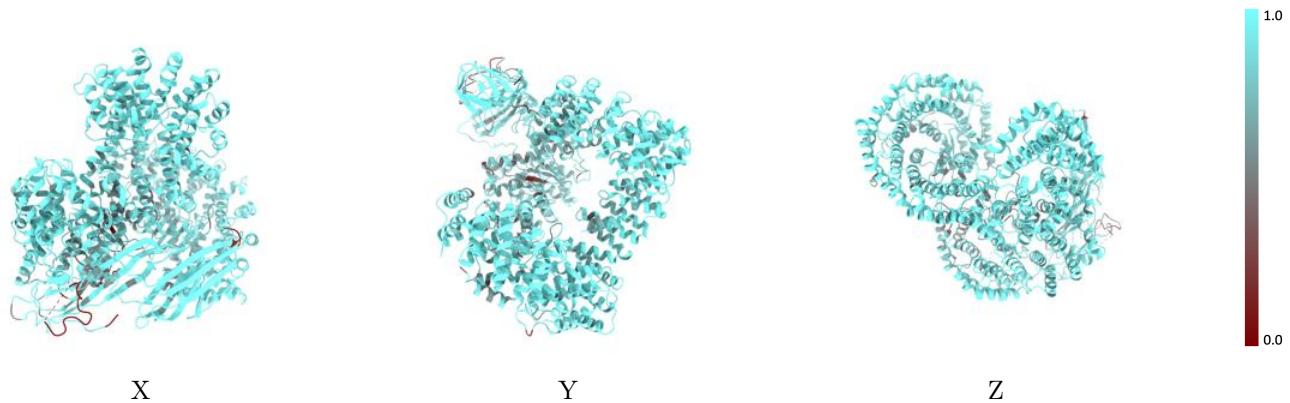
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion ⓘ
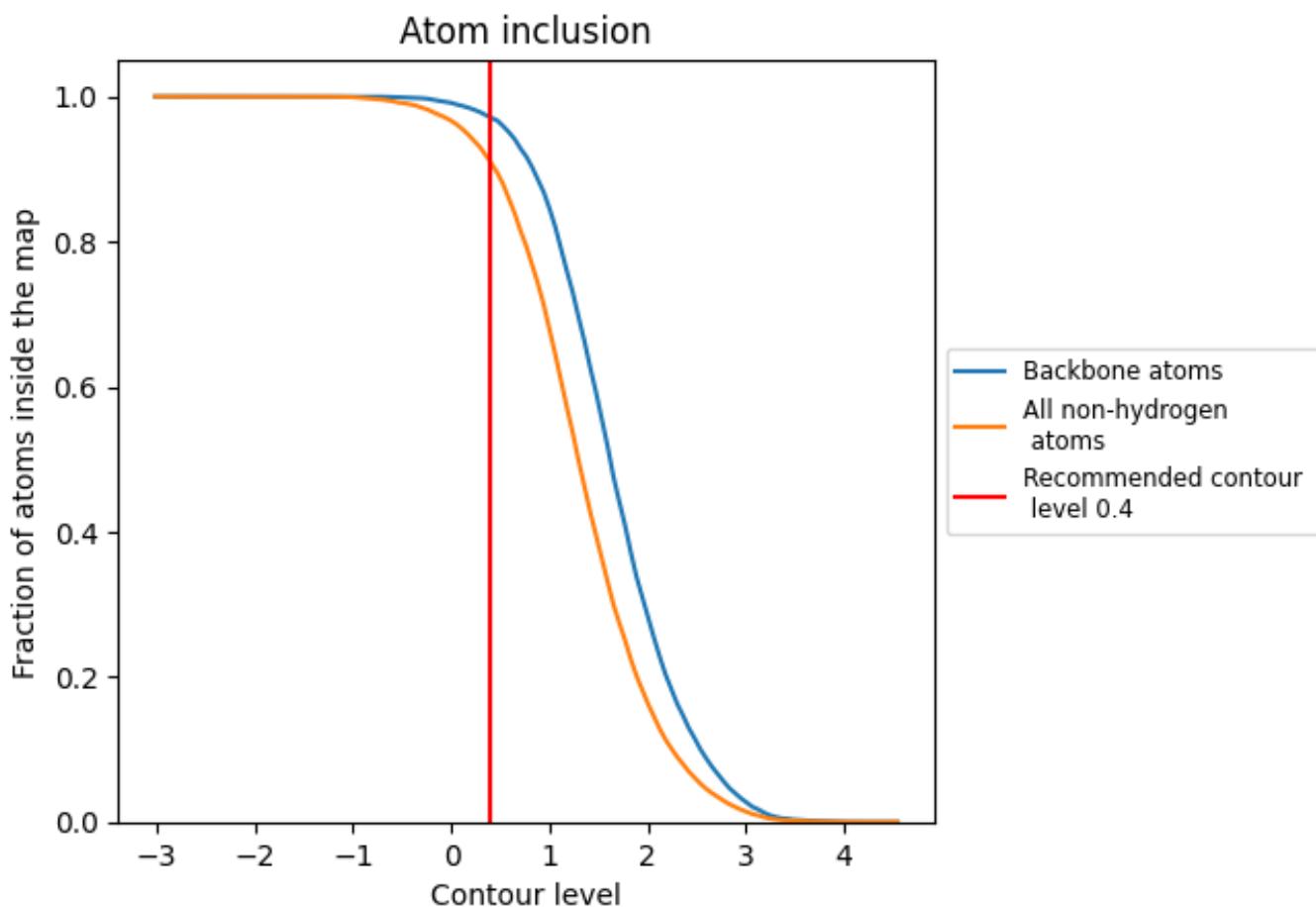
At the recommended contour level, 97% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9098	0.1980
A	0.9606	0.2110
B	0.9183	0.2080
M	0.8471	0.1740
P	0.5926	0.0620
S	0.8672	0.1880