Full wwPDB EM Validation Report (i)

Dec 18, 2022 – 01:29 pm GMT

PDB ID	:	7AKV
EMDB ID	:	EMD-11814
Title	:	The cryo-EM structure of the Vag8-C1 inhibitor complex
Authors	:	Johnson, S.; Lea, S.M.; Deme, J.C.; Furlong, E.; Dhillon, A.
Deposited on	:	2020-10-02
Resolution	:	3.60 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:

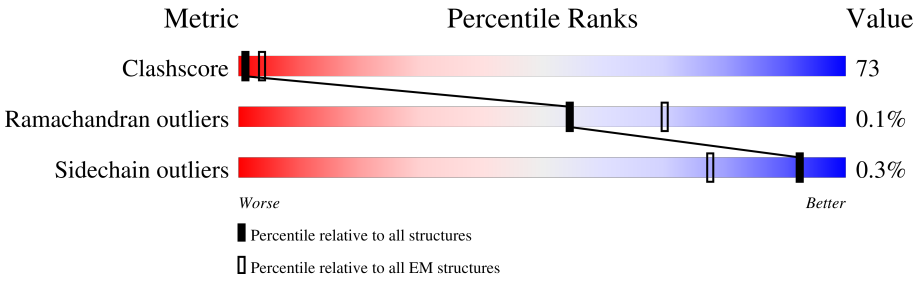
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	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	403	
2	G	877	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6201 atoms, of which 245 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 Plasma protease C1 inhibitor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	378	2979	1915	494	554	16	0	0

- Molecule 2 is a protein called Vag8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	G	421	3222	1806	245	558	609	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

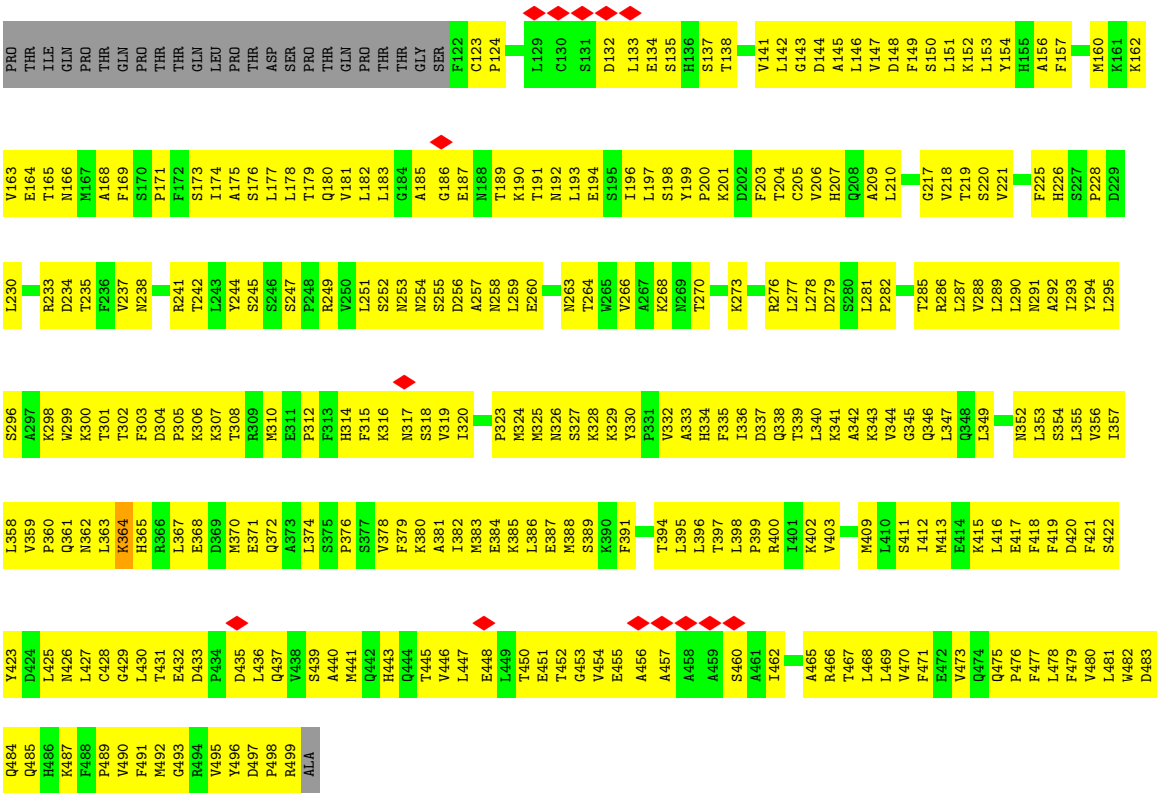
Chain	Residue	Modelled	Actual	Comment	Reference
G	107	VAL	LEU	conflict	UNP O66044
G	108	VAL	GLY	conflict	UNP O66044

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.

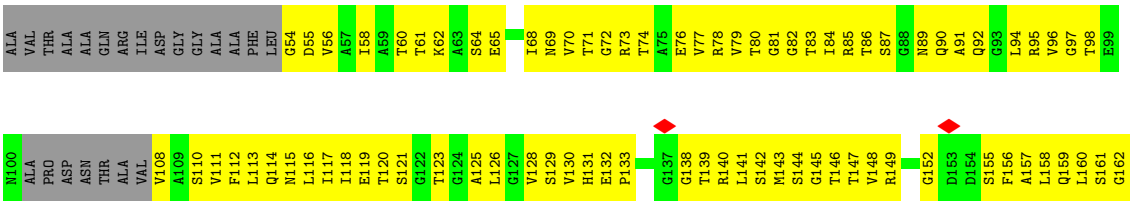
- Molecule 1: Plasma protease C1 inhibitor

Chain A:



- Molecule 2: Vag8

Chain G:



P163 A164 S165 A166 T167 L168 N169 D170 V171 A172 L173 E174 T175 A176 G177 Q178 Q179 A180 P181 A182 V183 V184 L185 W186 Q187 G188 A189 Q190 L191 N192 A193 Q194 G195 L196 V197 V198 Q199 V200 N201 G202 A203 G204 V205 S206 A207 I208 H209 A210 Q211 D212 A213 G214 S215 F216 T217 L218 S219 G220 S221 D222
I223 T224 A225 R226 G227 L228 E229 V230 V231 G232 I233 Y234 V235 Q236 E237 G238 M239 L243 T244 G245 T246 R247 V248 T249 T250 Q251 G252 D253 T254 A255 P256 A257 L258 Q259 V260 E261 D262 A263 G264 T265 H266 V267 S268 M269 N270 G271 G272 A273 L274 S277 G278 A279 N280 S281 P282 A283 L286
L287 A288 G289 G290 S291 A292 Q293 F294 R295 D296 L299 R300 T301 V302 A305 S306 H307 G308 V309 D310 V311 A312 A313 H314 S315 E316 V317 E318 L319 A320 H321 V324 D327 G328 Q329 G330 A331 H332 G333 L334 V335 V336 T337 R338 S339 M342 V343 R344 A345 G346 S347 L348 V349 E350 S351
T352 G355 A356 A357 A358 L359 L360 E361 S362 L365 T366 V367 V371 V372 H373 G374 H375 G376 A377 A378 G379 L380 E381 V382 D383 G384 E385 S386 N387 V388 S389 L390 L391 N392 G393 A394 R395 L396 Q400 P401 T402 A403 I404 R405 L406 I407 D408 P409 R410 S411 V412 L413 N414 L415 D416 I417
K418 D419 R420 A421 Q422 L423 L424 G425 D426 I427 A428 P429 E430 A431 Q432 Q433 PRO ASP GLY SER P434 E435 Q436 A437 R438 V439 R440 V441 A442 L443 A444 D445 G446 G447 T448 W449 R452 T453 D454 G455 ALA V456 H457 T458 V459 R460 L461 L462 D463 R464 G465 V466 W467 T468 V469 T470 G471 D472 S473
R474 V475 A476 E477 V478 K479 L480 E481 GLY GLY THR LEU ALA PHE ALA PRO PRO ALA GLN PRO LYS GLY ALA PHE LYS THR LEU VAL ALA THR GLN GLY ILE SER GLY THR GLY THR ILE VAL MET ASN ALA HIS LEU PRO SER GLY THR ALA ASP VAL LEU PRO GLY PHE GLY
ASP ARG GLN VAL LEU VAL VAL ASN ASN THR ASP ASP GLY THR GLU SER GLY ALA THR LYS VAL PRO LEU ILE GLU ASP GLU GLN GLN GLY HIS THR ALA PHE THR LEU GLY ASN MET GLY GLY ARG VAL ASP ALA GLY ALA ARG GLN TYR GLU LEU THR ALA SER GLU ALA GLN ALA ASP LYS
ALA ARG THR TRP GLN LEU THR THR PRO THR ASN GLU LEU SER THR THR ALA THR ALA ALA VAL ASN ALA MET ALA ILE ALA ALA SER GLN ARG ILE TRP GLN ALA GLU MET ASP VAL LEU LEU ARG HIS MET SER GLY LEU HIS SER ILE GLY SER PRO GLY GLY PHE TRP ALA ARG GLU LEU
SER GLN ARG GLN ARG LEU ASP THR GLY TYR GLY PRO TRP GLN LYS GLN THR VAL SER GLY ILE GLU LEU GLY LEU ASP ARG ARG ARG VAL ALA GLY GLY ALA THR THR ALA TRP SER VAL GLY MET LEU ALA GLY TYR SER GLU THR ARG ARG ASP GLY GLY GLY ALA TYR ARG ALA GLY
HIS SER ALA HIS VAL GLY ALA TYR VAL SER TYR LEU ASN ASP SER GLY TYR VAL ASP ARG PHE ARG HIS GLY PHE ASP ILE ARG THR THR ASP LEU LYS ARG VAL ASP ALA LYS HIS ARG SER HIS GLY LEU GLY GLY ALA LEU LEU ARG GLY GLY HIS ARG
ILE ASP ILE ASP GLY GLY TRP TYR VAL GLU PRO GLN ALA SER VAL ALA TRP PHE HIS ALA GLY GLY SER ARG TYR GLU ALA SER ARG GLY LEU ARG VAL ARG ALA ASP GLY ALA HIS SER TRP VAL LEU ARG ALA ARG ALA GLY ALA GLU ALA GLY ARG GLN MET ARG LEU ALA ASN GLY ASN ILE
VAL GLU PRO TYR ALA ARG LEU GLY TRP ALA GLN GLU LEU GLY ALA ASP ASN ALA VAL TYR THR ASN GLY ILE ARG HIS VAL THR ARG SER ARG GLY GLY GLY PHE ALA GLU ALA ARG VAL GLY VAL GLY ALA ALA LEU LEU GLY LYS ARG HIS ALA LEU TYR ALA ASP TYR GLU TYR ALA LYS
ALA ARG PHE GLU ALA PRO TRP THR LEU GLN LEU GLY TYR ARG SER TRP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	687883	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0122	Depositor
Map size (Å)	271.584, 271.584, 271.584	wwPDB
Map dimensions	328, 328, 328	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82800007, 0.82800007, 0.82800007	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	0.28	0/3043	0.43	0/4127
2	G	0.27	0/3008	0.53	1/4091 (0.0%)
All	All	0.27	0/6051	0.49	1/8218 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	163	PRO	N-CA-CB	6.47	111.06	103.30

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	2979	0	3025	375	0
2	G	2977	245	2914	501	0
All	All	5956	245	5939	872	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 73.

All (872) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:131:HIS:HB2	2:G:161:SER:HB2	1.26	1.12
2:G:417:ILE:HG23	2:G:421:ALA:HB3	1.25	1.10
1:A:402:LYS:HG2	1:A:448:GLU:HG3	1.35	1.07
2:G:132:GLU:HG2	2:G:133:PRO:HD2	1.33	1.07
2:G:252:GLY:HA3	2:G:278:GLY:HA3	1.35	1.04
2:G:348:LEU:HD21	2:G:350:GLU:HG3	1.04	1.03
1:A:430:LEU:HG	1:A:431:THR:HG23	1.38	1.03
2:G:168:LEU:HD13	2:G:171:VAL:HG21	1.38	1.01
2:G:158:LEU:HB2	2:G:183:VAL:HG12	1.43	1.01
2:G:78:ARG:HD3	2:G:112:PHE:HB2	1.40	1.00
2:G:171:VAL:HG11	2:G:173:LEU:HD23	1.43	0.99
1:A:301:THR:HG23	1:A:457:ALA:HB3	1.44	0.98
2:G:193:ALA:HB1	2:G:196:LEU:HD11	1.46	0.97
2:G:129:SER:HB2	2:G:159:GLN:HG3	1.44	0.95
2:G:179:GLN:HA	2:G:204:GLY:HA2	1.47	0.95
2:G:403:ALA:HB2	2:G:425:GLY:HA3	1.49	0.94
1:A:346:GLN:HB2	1:A:386:LEU:HD21	1.47	0.94
1:A:359:VAL:HG21	1:A:473:VAL:HG12	1.48	0.93
2:G:160:LEU:HD22	2:G:164:ALA:HB1	1.51	0.93
2:G:262:ASP:HB2	2:G:265:THR:HG23	1.50	0.92
1:A:221:VAL:HG21	1:A:270:THR:HG22	1.51	0.91
2:G:348:LEU:CD2	2:G:350:GLU:HG3	1.99	0.91
2:G:61:THR:HB	2:G:86:THR:HG22	1.51	0.91
1:A:395:LEU:HB3	1:A:470:VAL:HG23	1.53	0.89
1:A:483:ASP:O	1:A:484:GLN:HG2	1.74	0.88
2:G:467:TRP:HH2	2:G:475:VAL:HG21	1.39	0.88
2:G:235:VAL:HG23	2:G:260:VAL:HG13	1.54	0.88
2:G:116:LEU:O	2:G:146:THR:HA	1.73	0.87
2:G:400:GLN:HG2	2:G:401:PRO:HD2	1.57	0.86
1:A:185:ALA:HA	1:A:427:LEU:HD23	1.58	0.85
1:A:180:GLN:HG2	1:A:244:TYR:CE1	2.12	0.85
2:G:140:ARG:NH1	2:G:165:SER:OG	2.10	0.85
2:G:262:ASP:CB	2:G:265:THR:HG23	2.06	0.85
2:G:452:ARG:HH21	2:G:471:GLY:HA3	1.42	0.84
2:G:319:LEU:HD11	2:G:324:VAL:HG21	1.59	0.84
2:G:210:ALA:HB1	2:G:239:MET:CE	2.08	0.84
2:G:269:MET:HE1	2:G:274:LEU:HD11	1.57	0.83
1:A:310:MET:HE1	1:A:323:PRO:HG3	1.61	0.83
2:G:207:ALA:HB3	2:G:232:GLY:O	1.80	0.81
1:A:123:CYS:SG	1:A:233:ARG:NH1	2.53	0.81
2:G:193:ALA:HB1	2:G:196:LEU:CD1	2.09	0.81
2:G:208:ILE:HB	2:G:233:ILE:HD13	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:237:GLU:HA	2:G:262:ASP:OD1	1.80	0.81
1:A:162:LYS:HB2	1:A:165:THR:HG21	1.63	0.81
2:G:143:MET:HB2	2:G:168:LEU:HD22	1.62	0.81
2:G:360:LEU:HD23	2:G:380:LEU:HD11	1.63	0.81
1:A:259:LEU:HD12	1:A:281:LEU:HB2	1.62	0.80
2:G:183:VAL:HG22	2:G:208:ILE:HG12	1.62	0.80
2:G:360:LEU:HD21	2:G:365:LEU:HD22	1.64	0.80
1:A:367:LEU:HD23	1:A:496:TYR:HE1	1.45	0.80
1:A:235:THR:HA	1:A:238:ASN:HD21	1.45	0.80
1:A:144:ASP:OD1	1:A:145:ALA:N	2.15	0.80
1:A:353:LEU:HD22	1:A:481:LEU:HD21	1.63	0.80
2:G:173:LEU:HG	2:G:198:VAL:HG12	1.64	0.79
1:A:134:GLU:OE1	1:A:137:SER:OG	2.01	0.79
2:G:160:LEU:HB2	2:G:185:LEU:HD23	1.64	0.79
2:G:300:ARG:NH1	2:G:327:ASP:OD2	2.15	0.79
2:G:383:ASP:OD1	2:G:407:ILE:N	2.15	0.79
2:G:243:LEU:HD23	2:G:246:THR:HG21	1.64	0.79
2:G:449:TRP:HH2	2:G:453:THR:HB	1.47	0.78
2:G:274:LEU:HD12	2:G:299:LEU:CD2	2.13	0.78
2:G:438:ARG:CZ	2:G:438:ARG:HA	2.12	0.78
2:G:342:MET:HE1	2:G:344:ARG:HE	1.46	0.78
2:G:261:GLU:O	2:G:261:GLU:HG2	1.82	0.78
2:G:413:LEU:CD2	2:G:415:LEU:HB2	2.13	0.78
2:G:183:VAL:HG23	2:G:208:ILE:HG23	1.64	0.77
2:G:351:SER:OG	2:G:355:GLY:O	2.03	0.77
2:G:417:ILE:CG2	2:G:421:ALA:HB3	2.12	0.77
1:A:310:MET:HE2	1:A:323:PRO:HA	1.65	0.77
2:G:477:GLU:OE1	2:G:479:LYS:HE2	1.85	0.77
1:A:317:ASN:OD1	1:A:318:SER:N	2.18	0.77
2:G:348:LEU:HD21	2:G:350:GLU:CG	2.00	0.76
2:G:407:ILE:HA	2:G:430:GLU:HG2	1.66	0.76
2:G:168:LEU:HB3	2:G:171:VAL:HG23	1.68	0.76
2:G:313:ALA:HA	2:G:338:ARG:HG3	1.67	0.76
1:A:156:ALA:HB2	1:A:416:LEU:HD21	1.68	0.76
1:A:304:ASP:OD2	1:A:307:LYS:N	2.19	0.76
1:A:142:LEU:HD13	1:A:203:PHE:HE1	1.50	0.76
1:A:142:LEU:HD21	1:A:210:LEU:HD22	1.68	0.76
1:A:160:MET:CE	1:A:415:LYS:HG2	2.16	0.76
1:A:327:SER:HB3	1:A:330:TYR:HB2	1.68	0.76
2:G:405:ARG:NH1	2:G:429:PRO:O	2.19	0.76
2:G:348:LEU:HD23	2:G:349:VAL:N	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PRO:HD2	1:A:428:CYS:SG	2.26	0.75
2:G:337:THR:OG1	2:G:361:GLU:OE2	2.04	0.75
2:G:332:HIS:ND1	2:G:356:ALA:O	2.18	0.75
2:G:296:ASP:OD1	2:G:321:HIS:ND1	2.19	0.75
2:G:168:LEU:HB3	2:G:171:VAL:CG2	2.16	0.75
2:G:402:THR:HG21	2:G:405:ARG:HH21	1.52	0.74
1:A:181:VAL:CG2	1:A:289:LEU:HD21	2.17	0.74
1:A:329:LYS:HD3	1:A:465:ALA:HB3	1.69	0.74
1:A:324:MET:HE3	1:A:399:PRO:HD3	1.68	0.74
1:A:259:LEU:HD12	1:A:281:LEU:CB	2.17	0.74
1:A:378:VAL:O	1:A:382:ILE:HG13	1.86	0.74
2:G:65:GLU:HA	2:G:91:ALA:CB	2.17	0.74
2:G:249:THR:HG22	2:G:250:THR:H	1.52	0.74
1:A:346:GLN:HE21	1:A:354:SER:HB2	1.52	0.74
2:G:168:LEU:CD1	2:G:171:VAL:HG21	2.15	0.74
2:G:342:MET:SD	2:G:344:ARG:HB2	2.28	0.74
2:G:184:VAL:HG23	2:G:209:HIS:HD2	1.53	0.74
2:G:199:GLN:OE1	2:G:226:ARG:NH1	2.21	0.73
1:A:299:TRP:O	1:A:454:VAL:N	2.17	0.73
2:G:360:LEU:HD11	2:G:365:LEU:HB2	1.71	0.73
1:A:368:GLU:O	1:A:372:GLN:HG3	1.90	0.72
1:A:173:SER:HB3	1:A:291:ASN:HD21	1.53	0.72
1:A:175:ALA:O	1:A:179:THR:HG23	1.88	0.72
2:G:190:GLN:HG2	2:G:215:SER:HB3	1.71	0.72
2:G:274:LEU:HD12	2:G:299:LEU:HD21	1.72	0.72
1:A:254:ASN:O	1:A:258:ASN:ND2	2.22	0.71
2:G:417:ILE:HG23	2:G:421:ALA:CB	2.13	0.71
2:G:402:THR:HA	2:G:426:ASP:HB2	1.72	0.71
1:A:447:LEU:HD11	1:A:491:PHE:CD2	2.25	0.71
2:G:380:LEU:HG	2:G:382:VAL:HG23	1.73	0.71
2:G:208:ILE:HB	2:G:233:ILE:CD1	2.20	0.71
2:G:446:GLY:O	2:G:448:THR:HG23	1.90	0.71
1:A:206:VAL:HG22	1:A:210:LEU:HD23	1.73	0.71
1:A:443:HIS:NE2	1:A:445:THR:OG1	2.22	0.71
2:G:110:SER:HA	2:G:140:ARG:O	1.90	0.71
2:G:197:VAL:HA	2:G:222:ASP:OD1	1.90	0.71
2:G:79:VAL:HB	2:G:113:LEU:HD13	1.72	0.70
1:A:150:SER:HB2	1:A:492:MET:HE2	1.73	0.70
2:G:404:ILE:CD1	2:G:423:LEU:HD11	2.21	0.70
2:G:116:LEU:HD23	2:G:117:ILE:N	2.07	0.70
2:G:94:LEU:HD23	2:G:128:VAL:HB	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:221:SER:O	2:G:246:THR:HA	1.90	0.70
2:G:234:TYR:CZ	2:G:236:GLN:HG2	2.26	0.70
2:G:171:VAL:CG1	2:G:173:LEU:HD23	2.18	0.70
2:G:449:TRP:CH2	2:G:453:THR:HB	2.27	0.70
1:A:226:HIS:HB2	1:A:230:LEU:HD23	1.74	0.70
2:G:412:VAL:HA	2:G:438:ARG:O	1.92	0.70
1:A:149:PHE:CD1	1:A:197:LEU:HA	2.26	0.70
1:A:206:VAL:HA	1:A:209:ALA:HB3	1.74	0.70
2:G:236:GLN:HA	2:G:265:THR:HG21	1.74	0.70
2:G:71:THR:HA	2:G:97:GLY:O	1.92	0.69
2:G:299:LEU:HD12	2:G:324:VAL:HG22	1.74	0.69
2:G:382:VAL:HG11	2:G:386:SER:HB3	1.73	0.69
2:G:173:LEU:O	2:G:198:VAL:HA	1.92	0.69
2:G:287:LEU:HD23	2:G:312:ALA:CB	2.21	0.69
2:G:442:ALA:O	2:G:443:LEU:HD12	1.92	0.69
1:A:203:PHE:CD1	1:A:206:VAL:HB	2.28	0.69
1:A:368:GLU:HA	1:A:371:GLU:OE1	1.93	0.69
2:G:184:VAL:HG23	2:G:209:HIS:CD2	2.27	0.69
2:G:260:VAL:HB	2:G:286:LEU:HD13	1.75	0.69
1:A:481:LEU:HD22	1:A:490:VAL:CG1	2.22	0.69
2:G:210:ALA:HB1	2:G:239:MET:HE2	1.75	0.69
2:G:269:MET:HE2	2:G:274:LEU:HD21	1.74	0.69
2:G:160:LEU:HD22	2:G:164:ALA:CB	2.22	0.69
1:A:352:ASN:ND2	1:A:485:GLN:OE1	2.25	0.69
1:A:367:LEU:HD23	1:A:496:TYR:CE1	2.26	0.69
2:G:382:VAL:HB	2:G:413:LEU:HD12	1.73	0.69
1:A:200:PRO:O	1:A:203:PHE:HB2	1.93	0.69
2:G:155:SER:O	2:G:180:ALA:HB1	1.92	0.69
2:G:453:THR:OG1	2:G:456:VAL:HG23	1.93	0.69
1:A:304:ASP:OD2	1:A:307:LYS:HG2	1.93	0.69
2:G:390:LEU:HB2	2:G:417:ILE:HD13	1.73	0.69
1:A:174:ILE:O	1:A:178:LEU:HD23	1.94	0.68
1:A:185:ALA:HA	1:A:427:LEU:CD2	2.22	0.68
1:A:346:GLN:HB3	1:A:386:LEU:HD11	1.76	0.68
1:A:481:LEU:HD22	1:A:490:VAL:HG11	1.76	0.68
2:G:168:LEU:HD13	2:G:171:VAL:CG2	2.21	0.68
2:G:400:GLN:CG	2:G:401:PRO:HD2	2.22	0.68
2:G:404:ILE:HB	2:G:427:ILE:CD1	2.24	0.68
2:G:312:ALA:O	2:G:315:SER:OG	2.08	0.68
2:G:235:VAL:CG2	2:G:260:VAL:HG13	2.22	0.68
2:G:269:MET:CE	2:G:274:LEU:HD21	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:390:LEU:HD21	2:G:396:LEU:HB2	1.74	0.68
2:G:125:ALA:O	2:G:155:SER:HA	1.94	0.68
1:A:253:ASN:OD1	1:A:254:ASN:N	2.27	0.68
1:A:327:SER:CB	1:A:330:TYR:HB2	2.24	0.68
1:A:194:GLU:OE1	1:A:199:TYR:HB2	1.93	0.68
2:G:140:ARG:HH11	2:G:165:SER:HG	1.40	0.68
2:G:382:VAL:CG1	2:G:386:SER:HB3	2.24	0.68
2:G:96:VAL:HB	2:G:130:VAL:HG23	1.75	0.67
2:G:152:GLY:O	2:G:177:GLY:HA3	1.94	0.67
2:G:442:ALA:C	2:G:443:LEU:HD12	2.14	0.67
1:A:192:ASN:O	1:A:196:ILE:HG12	1.94	0.67
1:A:251:LEU:HB3	1:A:258:ASN:ND2	2.08	0.67
2:G:287:LEU:HD23	2:G:312:ALA:HB3	1.76	0.67
2:G:210:ALA:HB1	2:G:239:MET:HE1	1.77	0.67
1:A:329:LYS:HD3	1:A:465:ALA:CB	2.26	0.66
2:G:61:THR:CB	2:G:86:THR:HG22	2.24	0.66
2:G:393:GLY:N	2:G:420:ARG:HB3	2.08	0.66
1:A:466:ARG:HG3	2:G:234:TYR:CD1	2.29	0.66
1:A:482:TRP:NE1	1:A:487:LYS:HA	2.11	0.66
2:G:62:LYS:HE3	2:G:64:SER:OG	1.93	0.66
2:G:262:ASP:HB2	2:G:265:THR:CG2	2.26	0.66
1:A:353:LEU:HD22	1:A:481:LEU:CD2	2.26	0.66
2:G:371:VAL:HG21	2:G:395:ARG:NH2	2.10	0.66
1:A:187:GLU:O	1:A:191:THR:HG23	1.95	0.66
1:A:277:LEU:HD23	1:A:290:LEU:HD11	1.78	0.66
2:G:437:ALA:O	2:G:438:ARG:NH1	2.28	0.66
1:A:384:GLU:O	1:A:387:GLU:HG3	1.96	0.66
1:A:420:ASP:O	1:A:425:LEU:HB2	1.96	0.66
1:A:206:VAL:HG22	1:A:210:LEU:CD2	2.27	0.65
1:A:233:ARG:NE	1:A:432:GLU:OE2	2.23	0.65
2:G:456:VAL:HG11	2:G:459:VAL:HG22	1.78	0.65
2:G:415:LEU:HD23	2:G:416:ASP:N	2.11	0.65
2:G:129:SER:HB2	2:G:159:GLN:CG	2.23	0.65
2:G:416:ASP:OD2	2:G:418:LYS:HG3	1.97	0.65
1:A:148:ASP:O	1:A:152:LYS:HG3	1.96	0.64
2:G:56:VAL:HG12	2:G:80:THR:CG2	2.27	0.64
2:G:319:LEU:HD11	2:G:324:VAL:CG2	2.27	0.64
1:A:299:TRP:HH2	1:A:355:LEU:HD23	1.63	0.64
2:G:56:VAL:HG12	2:G:80:THR:HG21	1.78	0.64
2:G:402:THR:HG21	2:G:405:ARG:NH2	2.11	0.64
1:A:238:ASN:O	1:A:242:THR:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:84:ILE:HD12	2:G:116:LEU:CD2	2.27	0.64
2:G:131:HIS:CB	2:G:161:SER:HB2	2.15	0.64
2:G:360:LEU:HD21	2:G:365:LEU:CD2	2.28	0.64
1:A:301:THR:HB	1:A:330:TYR:CZ	2.33	0.64
1:A:300:LYS:HA	1:A:454:VAL:HG12	1.78	0.64
1:A:324:MET:HG2	1:A:399:PRO:CA	2.27	0.64
2:G:263:ALA:HA	2:G:289:GLY:HA3	1.80	0.64
2:G:333:GLY:H	2:G:357:ALA:HA	1.62	0.64
1:A:469:LEU:HD12	1:A:469:LEU:O	1.98	0.64
2:G:216:PHE:HD2	2:G:218:LEU:HD13	1.63	0.63
1:A:411:SER:O	1:A:415:LYS:HD3	1.98	0.63
1:A:314:HIS:ND1	1:A:319:VAL:HG22	2.13	0.63
1:A:332:VAL:CG2	1:A:396:LEU:HD22	2.28	0.63
2:G:225:ALA:O	2:G:226:ARG:HD2	1.99	0.63
1:A:180:GLN:HG2	1:A:244:TYR:CD1	2.33	0.63
2:G:315:SER:O	2:G:339:SER:HB2	1.99	0.63
1:A:201:LYS:HD2	1:A:201:LYS:N	2.14	0.63
2:G:96:VAL:HB	2:G:130:VAL:CG2	2.28	0.63
2:G:388:VAL:HG12	2:G:415:LEU:HA	1.81	0.63
1:A:177:LEU:HD22	1:A:291:ASN:HB2	1.79	0.63
1:A:300:LYS:HA	1:A:454:VAL:CG1	2.29	0.63
2:G:246:THR:O	2:G:272:GLY:HA2	1.98	0.63
1:A:454:VAL:HG13	1:A:455:GLU:HG3	1.81	0.62
2:G:262:ASP:HB3	2:G:264:GLY:H	1.64	0.62
1:A:157:PHE:CE1	1:A:412:ILE:HG13	2.34	0.62
2:G:390:LEU:HD23	2:G:394:ALA:HB3	1.81	0.62
2:G:92:GLN:HB3	2:G:126:LEU:HD23	1.81	0.62
2:G:452:ARG:NH2	2:G:471:GLY:HA3	2.13	0.62
2:G:118:ILE:HB	2:G:148:VAL:HG22	1.81	0.62
1:A:218:VAL:HG23	1:A:295:LEU:HA	1.79	0.62
1:A:324:MET:HG2	1:A:399:PRO:HA	1.81	0.62
2:G:94:LEU:CD2	2:G:113:LEU:HG	2.29	0.62
1:A:340:LEU:HD11	1:A:374:LEU:HD13	1.81	0.62
1:A:478:LEU:HD12	1:A:493:GLY:O	2.01	0.61
2:G:69:ASN:HA	2:G:95:ARG:O	2.00	0.61
2:G:443:LEU:HD23	2:G:447:GLY:O	2.00	0.61
2:G:236:GLN:OE1	2:G:237:GLU:HG2	2.00	0.61
2:G:404:ILE:HD11	2:G:423:LEU:HD11	1.80	0.61
1:A:341:LYS:C	1:A:361:GLN:HG3	2.21	0.61
1:A:298:LYS:HE3	1:A:452:THR:O	2.00	0.61
1:A:447:LEU:HD11	1:A:491:PHE:HD2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:173:LEU:HD11	2:G:182:ALA:HB1	1.83	0.61
2:G:311:VAL:HG21	2:G:317:VAL:CG1	2.30	0.61
2:G:419:ASP:O	2:G:420:ARG:NE	2.33	0.61
1:A:234:ASP:O	1:A:238:ASN:ND2	2.34	0.61
1:A:475:GLN:HB2	1:A:476:PRO:HD2	1.82	0.61
2:G:409:PRO:O	2:G:437:ALA:HB1	2.00	0.61
2:G:443:LEU:HD21	2:G:449:TRP:H	1.65	0.61
2:G:173:LEU:CG	2:G:198:VAL:HG12	2.30	0.61
2:G:183:VAL:CG2	2:G:208:ILE:HG12	2.29	0.61
1:A:219:THR:O	1:A:293:ILE:HG13	2.01	0.61
2:G:362:SER:HA	2:G:385:GLU:O	2.01	0.61
2:G:457:HIS:O	2:G:476:ALA:HB3	2.00	0.61
1:A:304:ASP:HB3	1:A:307:LYS:HG2	1.83	0.61
2:G:337:THR:HG22	2:G:338:ARG:HG2	1.83	0.61
1:A:335:PHE:O	1:A:336:ILE:HD13	2.00	0.60
2:G:84:ILE:HD12	2:G:116:LEU:HD21	1.83	0.60
1:A:398:LEU:HD23	1:A:399:PRO:O	2.02	0.60
2:G:65:GLU:HA	2:G:91:ALA:HB1	1.83	0.60
2:G:92:GLN:HB3	2:G:126:LEU:CD2	2.32	0.60
1:A:220:SER:HB2	1:A:293:ILE:HD12	1.82	0.60
2:G:332:HIS:HB2	2:G:335:VAL:CG2	2.32	0.60
2:G:271:GLY:HA2	2:G:296:ASP:O	2.01	0.60
1:A:196:ILE:HG13	1:A:418:PHE:HD1	1.67	0.60
1:A:310:MET:HE2	1:A:323:PRO:CA	2.31	0.60
1:A:420:ASP:HA	1:A:423:TYR:O	2.01	0.60
1:A:305:PRO:O	1:A:308:THR:HG22	2.02	0.60
2:G:80:THR:O	2:G:114:GLN:HB3	2.02	0.60
2:G:132:GLU:HG2	2:G:133:PRO:CD	2.21	0.60
2:G:422:GLN:N	2:G:422:GLN:OE1	2.34	0.60
1:A:183:LEU:HB2	1:A:207:HIS:NE2	2.16	0.60
1:A:241:ARG:CD	1:A:247:SER:HB3	2.32	0.60
2:G:296:ASP:HA	2:G:321:HIS:O	2.01	0.60
1:A:225:PHE:CD2	1:A:249:ARG:HB3	2.37	0.59
2:G:294:PHE:CE2	2:G:299:LEU:HD11	2.36	0.59
1:A:169:PHE:CE1	1:A:171:PRO:HG3	2.37	0.59
1:A:169:PHE:HE1	1:A:171:PRO:HG3	1.67	0.59
2:G:309:VAL:HB	2:G:334:LEU:HD12	1.84	0.59
2:G:108:VAL:N	2:G:139:THR:HA	2.17	0.59
2:G:338:ARG:HA	2:G:362:SER:O	2.01	0.59
1:A:163:VAL:HG13	1:A:164:GLU:H	1.67	0.59
1:A:204:THR:HG23	1:A:205:CYS:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:452:ARG:HH21	2:G:471:GLY:CA	2.12	0.59
2:G:144:SER:O	2:G:146:THR:HG23	2.02	0.59
2:G:161:SER:HA	2:G:186:TRP:HB2	1.84	0.59
2:G:463:ASP:HB3	2:G:464:ARG:NH1	2.17	0.59
1:A:476:PRO:HB3	1:A:496:TYR:HA	1.83	0.59
2:G:360:LEU:HD23	2:G:380:LEU:CD1	2.32	0.59
1:A:360:PRO:HD2	1:A:475:GLN:NE2	2.18	0.59
2:G:208:ILE:CD1	2:G:218:LEU:HD21	2.32	0.59
2:G:320:ALA:HA	2:G:344:ARG:O	2.03	0.59
2:G:162:GLY:HA2	2:G:187:GLN:O	2.03	0.59
2:G:263:ALA:HA	2:G:289:GLY:O	2.03	0.59
1:A:285:THR:HG23	1:A:439:SER:HB2	1.84	0.59
2:G:94:LEU:HD22	2:G:113:LEU:HG	1.85	0.59
2:G:112:PHE:CD1	2:G:142:SER:HB3	2.38	0.58
2:G:226:ARG:HG3	2:G:251:GLN:CG	2.33	0.58
2:G:301:THR:HG22	2:G:306:SER:OG	2.03	0.58
1:A:163:VAL:HG13	1:A:164:GLU:N	2.17	0.58
1:A:228:PRO:HD3	1:A:251:LEU:O	2.03	0.58
1:A:362:ASN:HD21	1:A:364:LYS:HB3	1.67	0.58
2:G:191:LEU:HD21	2:G:193:ALA:HB2	1.83	0.58
2:G:402:THR:H	2:G:426:ASP:HB2	1.69	0.58
2:G:440:ARG:O	2:G:441:VAL:HG23	2.03	0.58
1:A:409:MET:HG3	1:A:441:MET:HE2	1.84	0.58
1:A:466:ARG:HG3	2:G:234:TYR:CE1	2.37	0.58
2:G:55:ASP:HB2	2:G:79:VAL:HG22	1.85	0.58
2:G:404:ILE:HD11	2:G:423:LEU:CD1	2.33	0.58
1:A:394:THR:HG23	1:A:469:LEU:O	2.04	0.58
1:A:217:GLY:O	1:A:296:SER:OG	2.18	0.58
1:A:301:THR:HG23	1:A:457:ALA:CB	2.28	0.58
2:G:71:THR:HG23	2:G:72:GLY:N	2.19	0.58
2:G:198:VAL:CG2	2:G:223:ILE:HD12	2.33	0.58
2:G:302:VAL:HG13	2:G:302:VAL:O	2.03	0.58
2:G:404:ILE:HB	2:G:427:ILE:HD12	1.85	0.58
1:A:149:PHE:CD1	1:A:197:LEU:HD13	2.39	0.58
1:A:409:MET:HB2	1:A:441:MET:HG2	1.86	0.58
2:G:54:GLY:HA2	2:G:77:VAL:O	2.03	0.58
2:G:228:LEU:HB2	2:G:253:ASP:HB3	1.86	0.58
2:G:453:THR:HG23	2:G:454:ASP:N	2.19	0.58
1:A:427:LEU:HD13	1:A:430:LEU:HD23	1.85	0.58
1:A:497:ASP:OD2	1:A:499:ARG:HG2	2.03	0.58
2:G:459:VAL:HG12	2:G:459:VAL:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:TRP:HE1	1:A:487:LYS:HA	1.68	0.58
1:A:305:PRO:HA	1:A:451:GLU:HG2	1.86	0.57
1:A:360:PRO:HB3	1:A:365:HIS:HB3	1.87	0.57
2:G:249:THR:O	2:G:250:THR:OG1	2.14	0.57
1:A:164:GLU:HA	1:A:496:TYR:CD2	2.39	0.57
1:A:315:PHE:HE1	1:A:320:ILE:HG23	1.67	0.57
1:A:343:LYS:HE2	1:A:471:PHE:CE1	2.39	0.57
1:A:466:ARG:O	1:A:468:LEU:HD12	2.04	0.57
2:G:130:VAL:O	2:G:160:LEU:HD23	2.04	0.57
1:A:466:ARG:HD2	2:G:231:VAL:CB	2.34	0.57
2:G:259:GLN:HE21	2:G:287:LEU:HD12	1.68	0.57
2:G:407:ILE:HG12	2:G:430:GLU:CG	2.35	0.57
2:G:460:ARG:HG3	2:G:460:ARG:O	2.05	0.57
1:A:182:LEU:HA	1:A:185:ALA:HB2	1.86	0.57
1:A:225:PHE:HE2	1:A:249:ARG:HD2	1.70	0.57
2:G:336:VAL:HG13	2:G:339:SER:OG	2.05	0.57
2:G:410:ARG:HG2	2:G:438:ARG:HG2	1.86	0.57
2:G:452:ARG:HD3	2:G:472:ASP:O	2.05	0.57
2:G:413:LEU:HD23	2:G:415:LEU:HB2	1.87	0.57
2:G:226:ARG:HG3	2:G:251:GLN:HG3	1.85	0.57
1:A:341:LYS:HE2	1:A:365:HIS:CE1	2.40	0.57
2:G:262:ASP:O	2:G:263:ALA:HB3	2.05	0.57
1:A:342:ALA:HB2	1:A:370:MET:SD	2.45	0.56
2:G:438:ARG:HH12	2:G:457:HIS:CG	2.23	0.56
1:A:162:LYS:HB2	1:A:165:THR:CG2	2.35	0.56
1:A:182:LEU:CD1	1:A:190:LYS:HG3	2.35	0.56
1:A:221:VAL:CG2	1:A:270:THR:HG22	2.30	0.56
1:A:477:PHE:CE2	1:A:495:VAL:HB	2.40	0.56
2:G:65:GLU:CB	2:G:91:ALA:HA	2.35	0.56
2:G:336:VAL:HB	2:G:360:LEU:HD13	1.87	0.56
1:A:218:VAL:HG22	1:A:293:ILE:HG12	1.87	0.56
1:A:415:LYS:HD2	1:A:415:LYS:N	2.20	0.56
2:G:157:ALA:HB3	2:G:182:ALA:O	2.06	0.56
2:G:188:GLY:O	2:G:214:GLY:HA2	2.05	0.56
2:G:200:VAL:O	2:G:201:ASN:ND2	2.37	0.56
1:A:266:VAL:O	1:A:270:THR:HG23	2.05	0.56
2:G:82:GLY:C	2:G:116:LEU:HG	2.25	0.56
1:A:304:ASP:HB3	1:A:307:LYS:CG	2.36	0.56
2:G:402:THR:CA	2:G:426:ASP:HB2	2.35	0.56
1:A:132:ASP:OD1	1:A:135:SER:HB2	2.04	0.56
1:A:357:ILE:HD11	1:A:471:PHE:HE2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:MET:HE1	1:A:415:LYS:HG2	1.88	0.56
1:A:174:ILE:HD11	1:A:443:HIS:ND1	2.21	0.56
2:G:237:GLU:HA	2:G:237:GLU:OE1	2.06	0.56
2:G:263:ALA:HA	2:G:289:GLY:C	2.25	0.56
2:G:116:LEU:HD22	2:G:118:ILE:CD1	2.35	0.55
2:G:356:ALA:HB2	2:G:378:ALA:HB3	1.87	0.55
2:G:373:HIS:HD2	2:G:395:ARG:HH22	1.53	0.55
2:G:438:ARG:HA	2:G:438:ARG:NE	2.20	0.55
1:A:150:SER:HB2	1:A:492:MET:CE	2.36	0.55
1:A:285:THR:HG23	1:A:439:SER:CB	2.35	0.55
2:G:147:THR:O	2:G:149:ARG:HG3	2.07	0.55
1:A:285:THR:CG2	1:A:288:VAL:HG23	2.36	0.55
2:G:358:ALA:HB3	2:G:380:LEU:HA	1.88	0.55
1:A:305:PRO:CA	1:A:451:GLU:HG2	2.37	0.55
2:G:92:GLN:OE1	2:G:126:LEU:HD21	2.07	0.55
2:G:141:LEU:HD12	2:G:142:SER:H	1.72	0.55
2:G:443:LEU:O	2:G:462:LEU:HB2	2.05	0.55
1:A:302:THR:HB	1:A:456:ALA:HA	1.87	0.55
2:G:94:LEU:HG	2:G:94:LEU:O	2.07	0.55
2:G:96:VAL:HB	2:G:130:VAL:CB	2.37	0.55
2:G:118:ILE:CG1	2:G:148:VAL:HG22	2.37	0.55
2:G:216:PHE:CD2	2:G:218:LEU:HD13	2.41	0.55
2:G:388:VAL:CG1	2:G:415:LEU:HA	2.36	0.55
2:G:406:LEU:HD12	2:G:411:SER:OG	2.07	0.55
1:A:419:PHE:O	1:A:422:SER:N	2.36	0.55
2:G:78:ARG:HD3	2:G:112:PHE:CB	2.26	0.55
2:G:108:VAL:N	2:G:138:GLY:O	2.40	0.55
2:G:143:MET:O	2:G:144:SER:OG	2.21	0.55
2:G:260:VAL:HG12	2:G:265:THR:OG1	2.06	0.55
1:A:147:VAL:HG22	1:A:489:PRO:HD3	1.89	0.55
1:A:186:GLY:O	1:A:190:LYS:HB2	2.07	0.55
1:A:277:LEU:CD2	1:A:290:LEU:HD21	2.37	0.55
2:G:179:GLN:HA	2:G:204:GLY:CA	2.31	0.55
1:A:206:VAL:O	1:A:210:LEU:N	2.28	0.55
1:A:186:GLY:O	1:A:190:LYS:HD2	2.07	0.54
2:G:435:GLU:OE2	2:G:435:GLU:N	2.35	0.54
2:G:467:TRP:HD1	2:G:467:TRP:O	1.89	0.54
1:A:287:LEU:HD12	1:A:288:VAL:H	1.72	0.54
2:G:250:THR:HG21	2:G:255:ALA:O	2.07	0.54
2:G:347:SER:O	2:G:348:LEU:HB2	2.08	0.54
1:A:235:THR:HA	1:A:238:ASN:ND2	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:212:ASP:HA	2:G:237:GLU:O	2.07	0.54
2:G:283:ALA:HB3	2:G:308:GLY:O	2.08	0.54
1:A:153:LEU:HD22	1:A:169:PHE:CD1	2.43	0.54
1:A:312:PRO:HB3	1:A:319:VAL:CG1	2.36	0.54
1:A:316:LYS:HG3	1:A:317:ASN:H	1.72	0.54
1:A:320:ILE:HG21	1:A:499:ARG:HH12	1.72	0.54
2:G:158:LEU:HD12	2:G:183:VAL:CG1	2.38	0.54
2:G:72:GLY:O	2:G:73:ARG:HG2	2.07	0.54
2:G:384:GLY:O	2:G:411:SER:HB2	2.08	0.54
1:A:337:ASP:OD2	1:A:339:THR:OG1	2.25	0.54
1:A:460:SER:OG	1:A:462:ILE:HG12	2.08	0.54
2:G:478:VAL:O	2:G:479:LYS:HD3	2.08	0.54
2:G:94:LEU:O	2:G:128:VAL:HG23	2.08	0.54
2:G:194:GLN:HG3	2:G:219:SER:HB2	1.89	0.54
2:G:269:MET:CE	2:G:274:LEU:HD11	2.34	0.54
2:G:342:MET:HE1	2:G:344:ARG:NE	2.21	0.54
1:A:154:TYR:CE1	1:A:478:LEU:HD11	2.43	0.53
1:A:277:LEU:CD2	1:A:290:LEU:HD11	2.38	0.53
1:A:403:VAL:CG1	1:A:447:LEU:HB2	2.38	0.53
1:A:403:VAL:HG12	1:A:447:LEU:HB2	1.90	0.53
1:A:428:CYS:SG	1:A:429:GLY:N	2.81	0.53
1:A:181:VAL:HG21	1:A:289:LEU:HD21	1.90	0.53
1:A:416:LEU:O	1:A:417:GLU:HB2	2.07	0.53
1:A:173:SER:HB3	1:A:291:ASN:ND2	2.23	0.53
2:G:178:GLN:O	2:G:204:GLY:N	2.41	0.53
2:G:262:ASP:HB3	2:G:265:THR:HG23	1.87	0.53
2:G:96:VAL:HB	2:G:130:VAL:HB	1.90	0.53
2:G:200:VAL:HG12	2:G:201:ASN:N	2.24	0.53
2:G:254:THR:HA	2:G:280:ASN:O	2.08	0.53
2:G:60:THR:O	2:G:61:THR:OG1	2.22	0.53
2:G:147:THR:O	2:G:147:THR:HG23	2.08	0.53
2:G:175:THR:HG23	2:G:200:VAL:HG13	1.89	0.53
2:G:373:HIS:CD2	2:G:395:ARG:HH22	2.27	0.53
1:A:197:LEU:O	1:A:198:SER:OG	2.26	0.53
1:A:255:SER:HA	1:A:258:ASN:HB2	1.90	0.53
1:A:384:GLU:HG3	1:A:385:LYS:N	2.23	0.53
2:G:94:LEU:HB3	2:G:128:VAL:HB	1.91	0.53
1:A:255:SER:O	1:A:258:ASN:HB2	2.09	0.53
1:A:315:PHE:CE1	1:A:320:ILE:HG23	2.43	0.53
2:G:119:GLU:HG3	2:G:119:GLU:O	2.09	0.53
1:A:233:ARG:HE	1:A:432:GLU:CD	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LEU:HD23	1:A:470:VAL:CG2	2.39	0.53
2:G:263:ALA:HA	2:G:289:GLY:CA	2.39	0.53
1:A:398:LEU:HG	1:A:399:PRO:HD2	1.90	0.52
1:A:164:GLU:HA	1:A:496:TYR:CE2	2.44	0.52
1:A:359:VAL:CG1	1:A:475:GLN:HE21	2.21	0.52
1:A:302:THR:HA	1:A:453:GLY:HA3	1.92	0.52
1:A:324:MET:CE	1:A:397:THR:HG22	2.40	0.52
1:A:332:VAL:O	1:A:391:PHE:HA	2.10	0.52
1:A:446:VAL:O	1:A:447:LEU:HD22	2.09	0.52
2:G:318:GLU:HG3	2:G:318:GLU:O	2.08	0.52
1:A:381:ALA:HA	1:A:384:GLU:HG2	1.90	0.52
2:G:351:SER:O	2:G:352:THR:OG1	2.23	0.52
2:G:459:VAL:O	2:G:461:LEU:HG	2.10	0.52
1:A:312:PRO:HB3	1:A:319:VAL:HG11	1.91	0.52
1:A:332:VAL:HG21	1:A:396:LEU:HD22	1.90	0.52
1:A:497:ASP:OD1	1:A:499:ARG:NE	2.43	0.52
2:G:90:GLN:O	2:G:90:GLN:HG2	2.10	0.52
1:A:225:PHE:O	1:A:287:LEU:HD12	2.10	0.52
1:A:304:ASP:CB	1:A:307:LYS:HG2	2.40	0.52
1:A:308:THR:HA	1:A:324:MET:O	2.10	0.52
2:G:229:GLU:HG3	2:G:254:THR:OG1	2.08	0.52
2:G:263:ALA:N	2:G:288:ALA:O	2.42	0.52
2:G:410:ARG:CG	2:G:438:ARG:HG2	2.39	0.52
2:G:426:ASP:O	2:G:427:ILE:HD13	2.10	0.52
1:A:153:LEU:HD22	1:A:169:PHE:CE1	2.44	0.52
2:G:247:ARG:HB3	2:G:247:ARG:NH1	2.25	0.52
2:G:367:VAL:O	2:G:391:LEU:HD23	2.10	0.52
1:A:205:CYS:O	1:A:209:ALA:N	2.24	0.52
1:A:340:LEU:HD11	1:A:374:LEU:CD1	2.39	0.52
2:G:250:THR:HG22	2:G:251:GLN:N	2.23	0.52
2:G:319:LEU:HD23	2:G:320:ALA:N	2.25	0.52
1:A:314:HIS:CD2	1:A:363:LEU:HD21	2.45	0.52
2:G:117:ILE:HG13	2:G:147:THR:HG22	1.92	0.52
1:A:164:GLU:HG2	1:A:496:TYR:CD2	2.45	0.51
1:A:299:TRP:HB2	1:A:453:GLY:HA2	1.92	0.51
1:A:329:LYS:NZ	1:A:465:ALA:HB3	2.25	0.51
1:A:359:VAL:HG12	1:A:475:GLN:HE21	1.75	0.51
1:A:413:MET:CE	1:A:421:PHE:HB2	2.39	0.51
2:G:83:THR:HA	2:G:116:LEU:CD2	2.40	0.51
2:G:311:VAL:HG21	2:G:317:VAL:HG11	1.91	0.51
1:A:181:VAL:HG22	1:A:289:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LYS:HB2	1:A:349:LEU:O	2.10	0.51
1:A:455:GLU:OE2	1:A:457:ALA:HB2	2.11	0.51
2:G:132:GLU:OE1	2:G:138:GLY:HA2	2.10	0.51
1:A:225:PHE:CE2	1:A:249:ARG:HD2	2.45	0.51
1:A:241:ARG:CG	1:A:247:SER:HB3	2.41	0.51
1:A:276:ARG:NH1	1:A:279:ASP:OD1	2.38	0.51
1:A:418:PHE:CE2	1:A:420:ASP:HB2	2.45	0.51
2:G:249:THR:HG22	2:G:250:THR:N	2.23	0.51
2:G:434:PRO:HD2	2:G:435:GLU:OE1	2.09	0.51
1:A:204:THR:HG23	1:A:205:CYS:H	1.76	0.51
2:G:70:VAL:HG21	2:G:77:VAL:HG11	1.93	0.51
2:G:83:THR:CA	2:G:116:LEU:HD21	2.41	0.51
2:G:198:VAL:HG22	2:G:223:ILE:CD1	2.40	0.51
2:G:306:SER:O	2:G:307:HIS:ND1	2.42	0.51
2:G:358:ALA:O	2:G:380:LEU:HD12	2.10	0.51
2:G:380:LEU:HD22	2:G:388:VAL:HG21	1.93	0.51
1:A:189:THR:HG21	1:A:426:ASN:O	2.11	0.51
1:A:260:GLU:OE2	1:A:264:THR:HG21	2.10	0.51
2:G:118:ILE:O	2:G:120:THR:N	2.40	0.51
2:G:371:VAL:HG13	2:G:371:VAL:O	2.11	0.51
2:G:386:SER:OG	2:G:413:LEU:HG	2.11	0.51
1:A:360:PRO:HA	1:A:370:MET:SD	2.51	0.51
2:G:167:THR:O	2:G:168:LEU:HD23	2.11	0.51
2:G:412:VAL:HG22	2:G:438:ARG:CB	2.41	0.51
1:A:241:ARG:O	1:A:245:SER:HA	2.11	0.51
1:A:335:PHE:CZ	1:A:344:VAL:HG11	2.46	0.51
1:A:384:GLU:HG3	1:A:385:LYS:H	1.76	0.51
1:A:166:ASN:HB3	1:A:496:TYR:H	1.76	0.51
1:A:329:LYS:CD	1:A:465:ALA:HB3	2.38	0.51
2:G:348:LEU:HD23	2:G:349:VAL:CA	2.41	0.51
1:A:341:LYS:O	1:A:361:GLN:HG3	2.11	0.51
2:G:83:THR:HG22	2:G:85:ARG:HG3	1.93	0.51
2:G:210:ALA:CB	2:G:239:MET:HE2	2.41	0.51
2:G:76:GLU:HA	2:G:110:SER:O	2.10	0.50
2:G:329:GLN:HG3	2:G:330:GLY:H	1.75	0.50
1:A:359:VAL:HG13	1:A:360:PRO:HD2	1.93	0.50
2:G:94:LEU:HD23	2:G:128:VAL:CB	2.40	0.50
2:G:367:VAL:HG21	2:G:372:VAL:HG21	1.92	0.50
1:A:234:ASP:OD1	1:A:235:THR:N	2.45	0.50
1:A:252:SER:N	1:A:258:ASN:OD1	2.29	0.50
2:G:70:VAL:HG12	2:G:70:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:238:GLY:H	2:G:265:THR:HG22	1.76	0.50
2:G:301:THR:HG22	2:G:301:THR:O	2.11	0.50
2:G:419:ASP:HA	2:G:445:ASP:O	2.10	0.50
2:G:183:VAL:CG2	2:G:208:ILE:HG23	2.37	0.50
2:G:382:VAL:HG11	2:G:386:SER:CB	2.40	0.50
2:G:419:ASP:O	2:G:419:ASP:OD2	2.29	0.50
1:A:413:MET:HG2	1:A:418:PHE:HB3	1.92	0.50
2:G:84:ILE:HD13	2:G:118:ILE:HD12	1.92	0.50
2:G:219:SER:HA	2:G:244:THR:O	2.12	0.50
1:A:156:ALA:HB2	1:A:416:LEU:CD2	2.40	0.50
1:A:343:LYS:HE2	1:A:471:PHE:HE1	1.76	0.50
1:A:431:THR:OG1	1:A:436:LEU:HD21	2.12	0.50
2:G:257:ALA:HB3	2:G:283:ALA:O	2.12	0.50
1:A:123:CYS:SG	1:A:124:PRO:HD2	2.52	0.50
2:G:117:ILE:C	2:G:118:ILE:HD13	2.31	0.50
2:G:238:GLY:N	2:G:265:THR:HG22	2.27	0.50
1:A:332:VAL:HG12	1:A:333:ALA:N	2.26	0.49
1:A:399:PRO:HD3	1:A:473:VAL:HG23	1.94	0.49
2:G:228:LEU:HD23	2:G:228:LEU:H	1.76	0.49
2:G:402:THR:N	2:G:426:ASP:HB2	2.26	0.49
1:A:286:ARG:HB2	1:A:437:GLN:HE21	1.76	0.49
1:A:304:ASP:CG	1:A:307:LYS:HG2	2.31	0.49
2:G:181:PRO:HA	2:G:206:SER:O	2.12	0.49
2:G:208:ILE:HD12	2:G:233:ILE:HD11	1.94	0.49
1:A:194:GLU:CD	1:A:199:TYR:HB2	2.33	0.49
1:A:290:LEU:HD23	1:A:291:ASN:N	2.27	0.49
1:A:447:LEU:HD11	1:A:491:PHE:CE2	2.47	0.49
2:G:84:ILE:HD12	2:G:116:LEU:HD22	1.95	0.49
2:G:469:VAL:HG22	2:G:470:THR:N	2.27	0.49
2:G:82:GLY:O	2:G:83:THR:OG1	2.28	0.49
2:G:305:ALA:HA	2:G:330:GLY:O	2.12	0.49
2:G:467:TRP:CH2	2:G:475:VAL:HG21	2.32	0.49
2:G:453:THR:HG23	2:G:454:ASP:H	1.78	0.49
1:A:328:LYS:HE2	1:A:328:LYS:HA	1.94	0.49
1:A:398:LEU:HG	1:A:473:VAL:HG21	1.95	0.49
2:G:65:GLU:HB3	2:G:91:ALA:HA	1.95	0.49
2:G:198:VAL:HG22	2:G:223:ILE:HD12	1.94	0.49
2:G:256:PRO:HA	2:G:282:PRO:O	2.13	0.49
1:A:281:LEU:HD23	1:A:282:PRO:O	2.12	0.49
1:A:303:PHE:CE2	1:A:327:SER:HB2	2.48	0.49
2:G:237:GLU:CA	2:G:262:ASP:OD1	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:294:PHE:O	2:G:295:ARG:HG2	2.12	0.49
2:G:406:LEU:O	2:G:429:PRO:HA	2.13	0.49
1:A:160:MET:HE3	1:A:415:LYS:HG2	1.93	0.49
2:G:196:LEU:N	2:G:196:LEU:HD12	2.27	0.49
1:A:189:THR:HA	1:A:420:ASP:OD2	2.13	0.49
2:G:235:VAL:HG22	2:G:260:VAL:HG22	1.94	0.49
2:G:311:VAL:HG12	2:G:315:SER:OG	2.13	0.49
1:A:396:LEU:HD13	1:A:471:PHE:HB3	1.95	0.49
2:G:419:ASP:OD2	2:G:420:ARG:NH2	2.46	0.49
2:G:407:ILE:HG12	2:G:430:GLU:HG3	1.95	0.48
2:G:260:VAL:HB	2:G:286:LEU:CD1	2.40	0.48
2:G:292:ALA:HB1	2:G:294:PHE:CE1	2.48	0.48
1:A:181:VAL:O	1:A:185:ALA:N	2.46	0.48
1:A:340:LEU:HD12	1:A:382:ILE:HD11	1.94	0.48
2:G:210:ALA:HB3	2:G:235:VAL:HG12	1.95	0.48
1:A:259:LEU:HD12	1:A:281:LEU:HB3	1.94	0.48
1:A:305:PRO:N	1:A:451:GLU:HG2	2.28	0.48
1:A:433:ASP:OD1	1:A:435:ASP:N	2.46	0.48
1:A:149:PHE:HD1	1:A:197:LEU:HA	1.77	0.48
1:A:367:LEU:HD22	1:A:476:PRO:C	2.33	0.48
2:G:226:ARG:O	2:G:230:VAL:HG11	2.13	0.48
2:G:380:LEU:HG	2:G:382:VAL:CG2	2.42	0.48
1:A:183:LEU:O	1:A:183:LEU:HD12	2.13	0.48
1:A:256:ASP:OD1	1:A:257:ALA:N	2.42	0.48
1:A:273:LYS:HG3	1:A:294:TYR:CZ	2.49	0.48
1:A:346:GLN:CB	1:A:386:LEU:HD11	2.42	0.48
1:A:352:ASN:ND2	1:A:485:GLN:HB2	2.29	0.48
2:G:94:LEU:HG	2:G:128:VAL:HG23	1.96	0.48
2:G:128:VAL:HG13	2:G:158:LEU:CD2	2.44	0.48
2:G:396:LEU:O	2:G:396:LEU:HD23	2.13	0.48
2:G:456:VAL:CG1	2:G:457:HIS:N	2.76	0.48
1:A:281:LEU:HD23	1:A:282:PRO:N	2.29	0.48
1:A:335:PHE:C	1:A:336:ILE:HD13	2.34	0.48
2:G:118:ILE:CB	2:G:148:VAL:HG22	2.44	0.48
2:G:212:ASP:OD2	2:G:237:GLU:HB3	2.14	0.48
2:G:459:VAL:HG11	2:G:467:TRP:CE3	2.49	0.48
1:A:385:LYS:O	1:A:388:MET:HG3	2.13	0.48
2:G:81:GLY:C	2:G:116:LEU:HD12	2.34	0.48
2:G:94:LEU:HD21	2:G:113:LEU:CD2	2.44	0.48
2:G:141:LEU:HD12	2:G:142:SER:N	2.29	0.48
2:G:173:LEU:O	2:G:173:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:295:ARG:HH12	2:G:296:ASP:CG	2.17	0.48
2:G:250:THR:CG2	2:G:251:GLN:N	2.77	0.47
2:G:431:ALA:HB3	2:G:433:GLN:OE1	2.14	0.47
2:G:77:VAL:HG23	2:G:78:ARG:N	2.28	0.47
2:G:85:ARG:HG2	2:G:119:GLU:CG	2.44	0.47
2:G:190:GLN:CG	2:G:215:SER:HB3	2.42	0.47
2:G:460:ARG:NE	2:G:462:LEU:HD11	2.29	0.47
1:A:123:CYS:CB	1:A:233:ARG:HH12	2.27	0.47
1:A:164:GLU:HG2	1:A:496:TYR:CE2	2.49	0.47
2:G:194:GLN:O	2:G:196:LEU:HD12	2.14	0.47
2:G:332:HIS:HB2	2:G:335:VAL:HG22	1.96	0.47
2:G:403:ALA:CB	2:G:425:GLY:HA3	2.32	0.47
1:A:300:LYS:CA	1:A:454:VAL:HG12	2.44	0.47
2:G:156:PHE:CE1	2:G:181:PRO:HD2	2.50	0.47
2:G:393:GLY:H	2:G:420:ARG:HB3	1.78	0.47
1:A:325:MET:SD	1:A:398:LEU:O	2.73	0.47
1:A:376:PRO:O	1:A:380:LYS:HG3	2.15	0.47
2:G:56:VAL:HA	2:G:80:THR:OG1	2.14	0.47
2:G:58:ILE:HD12	2:G:58:ILE:H	1.79	0.47
2:G:173:LEU:CD1	2:G:198:VAL:HG12	2.45	0.47
2:G:200:VAL:HG12	2:G:201:ASN:H	1.80	0.47
1:A:176:SER:O	1:A:179:THR:OG1	2.27	0.47
2:G:145:GLY:H	2:G:170:ASP:HB3	1.80	0.47
1:A:490:VAL:HG13	1:A:491:PHE:N	2.29	0.47
1:A:320:ILE:CG2	1:A:499:ARG:HH12	2.28	0.47
2:G:130:VAL:HG13	2:G:160:LEU:CD2	2.45	0.47
2:G:207:ALA:O	2:G:208:ILE:C	2.53	0.47
2:G:466:VAL:HG12	2:G:468:THR:OG1	2.15	0.47
1:A:346:GLN:OE1	1:A:386:LEU:HG	2.16	0.46
2:G:438:ARG:HA	2:G:438:ARG:NH1	2.30	0.46
1:A:386:LEU:O	1:A:389:SER:HB2	2.15	0.46
1:A:446:VAL:C	1:A:447:LEU:HD22	2.35	0.46
2:G:274:LEU:HB2	2:G:299:LEU:HD23	1.98	0.46
2:G:319:LEU:CD1	2:G:324:VAL:HG21	2.39	0.46
2:G:382:VAL:HB	2:G:413:LEU:CD1	2.41	0.46
2:G:83:THR:HA	2:G:116:LEU:HD21	1.97	0.46
1:A:340:LEU:CD1	1:A:374:LEU:HD13	2.45	0.46
1:A:400:ARG:NH2	1:A:451:GLU:OE1	2.47	0.46
1:A:151:LEU:HD21	1:A:379:PHE:CD2	2.50	0.46
2:G:201:ASN:HD21	2:G:226:ARG:HH11	1.62	0.46
1:A:384:GLU:HA	1:A:387:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:65:GLU:H	2:G:65:GLU:CD	2.18	0.46
2:G:159:GLN:HA	2:G:184:VAL:O	2.15	0.46
2:G:289:GLY:HA2	2:G:314:HIS:O	2.15	0.46
1:A:218:VAL:HG22	1:A:293:ILE:CG1	2.46	0.46
1:A:218:VAL:HG21	1:A:491:PHE:CZ	2.51	0.46
1:A:299:TRP:CE3	1:A:349:LEU:HD23	2.51	0.46
1:A:413:MET:SD	1:A:421:PHE:HB2	2.56	0.46
2:G:433:GLN:HB3	2:G:435:GLU:OE2	2.16	0.46
1:A:324:MET:HE1	1:A:397:THR:HG22	1.98	0.46
1:A:367:LEU:HD22	1:A:476:PRO:O	2.16	0.46
2:G:187:GLN:CD	2:G:187:GLN:H	2.19	0.46
1:A:335:PHE:CE1	1:A:344:VAL:HG11	2.51	0.46
2:G:416:ASP:O	2:G:417:ILE:HG12	2.16	0.46
1:A:178:LEU:HD12	1:A:193:LEU:HD21	1.98	0.45
1:A:154:TYR:OH	1:A:478:LEU:HD13	2.16	0.45
2:G:130:VAL:CG1	2:G:160:LEU:HD21	2.46	0.45
2:G:196:LEU:HB2	2:G:221:SER:HB2	1.97	0.45
2:G:222:ASP:CB	2:G:247:ARG:HG2	2.46	0.45
2:G:301:THR:HG22	2:G:306:SER:CB	2.46	0.45
2:G:460:ARG:CZ	2:G:462:LEU:HD11	2.47	0.45
1:A:241:ARG:HG2	1:A:247:SER:HB3	1.99	0.45
2:G:234:TYR:CE2	2:G:236:GLN:HG2	2.51	0.45
2:G:405:ARG:HG2	2:G:430:GLU:OE2	2.17	0.45
2:G:477:GLU:HG2	2:G:478:VAL:N	2.30	0.45
1:A:226:HIS:CB	1:A:230:LEU:HD23	2.42	0.45
1:A:447:LEU:HD21	1:A:491:PHE:CE2	2.52	0.45
2:G:74:THR:O	2:G:74:THR:HG22	2.17	0.45
2:G:191:LEU:C	2:G:191:LEU:HD23	2.37	0.45
2:G:321:HIS:H	2:G:346:GLY:HA2	1.80	0.45
2:G:452:ARG:HE	2:G:471:GLY:CA	2.29	0.45
1:A:203:PHE:O	1:A:206:VAL:HG12	2.16	0.45
1:A:362:ASN:ND2	1:A:364:LYS:HB3	2.29	0.45
2:G:193:ALA:HB1	2:G:196:LEU:HD21	1.97	0.45
2:G:380:LEU:HB3	2:G:404:ILE:HG13	1.99	0.45
2:G:390:LEU:HD23	2:G:394:ALA:CB	2.46	0.45
2:G:402:THR:CG2	2:G:405:ARG:HH21	2.25	0.45
1:A:347:LEU:HD12	1:A:347:LEU:N	2.32	0.45
2:G:158:LEU:CB	2:G:183:VAL:HG12	2.30	0.45
2:G:453:THR:O	2:G:454:ASP:HB2	2.17	0.45
1:A:479:PHE:CE1	1:A:495:VAL:HG23	2.52	0.45
2:G:158:LEU:HD12	2:G:183:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ASP:OD1	1:A:382:ILE:HG12	2.17	0.45
1:A:276:ARG:HG3	1:A:276:ARG:HH11	1.81	0.45
1:A:304:ASP:OD1	1:A:306:LYS:HE2	2.17	0.45
2:G:410:ARG:HG2	2:G:410:ARG:O	2.17	0.45
1:A:162:LYS:HE2	1:A:165:THR:HG21	1.98	0.44
2:G:71:THR:O	2:G:98:THR:HB	2.17	0.44
2:G:85:ARG:HG2	2:G:119:GLU:HG2	1.98	0.44
2:G:90:GLN:N	2:G:123:THR:O	2.49	0.44
2:G:238:GLY:CA	2:G:265:THR:HG22	2.48	0.44
2:G:262:ASP:O	2:G:263:ALA:CB	2.64	0.44
1:A:182:LEU:HD12	1:A:190:LYS:HG3	1.98	0.44
1:A:286:ARG:HB2	1:A:437:GLN:NE2	2.32	0.44
1:A:420:ASP:HB3	1:A:425:LEU:HD12	1.99	0.44
2:G:380:LEU:H	2:G:396:LEU:HD21	1.81	0.44
1:A:166:ASN:HB2	1:A:495:VAL:HA	1.99	0.44
2:G:72:GLY:C	2:G:73:ARG:HG2	2.38	0.44
2:G:77:VAL:HG22	2:G:111:VAL:HB	1.99	0.44
2:G:201:ASN:ND2	2:G:226:ARG:HH11	2.16	0.44
2:G:82:GLY:N	2:G:116:LEU:HG	2.33	0.44
2:G:365:LEU:HD12	2:G:366:THR:N	2.33	0.44
1:A:144:ASP:OD1	1:A:144:ASP:C	2.56	0.44
1:A:206:VAL:O	1:A:210:LEU:HD23	2.17	0.44
2:G:65:GLU:CG	2:G:91:ALA:HA	2.47	0.44
2:G:261:GLU:HB3	2:G:287:LEU:HB2	2.00	0.44
2:G:301:THR:HG22	2:G:306:SER:HG	1.81	0.44
2:G:309:VAL:HB	2:G:334:LEU:CD1	2.48	0.44
1:A:225:PHE:HA	1:A:249:ARG:O	2.18	0.44
2:G:112:PHE:HA	2:G:142:SER:O	2.17	0.44
2:G:197:VAL:HG12	2:G:197:VAL:O	2.18	0.44
2:G:216:PHE:HD2	2:G:218:LEU:CD1	2.28	0.44
1:A:266:VAL:HG11	1:A:277:LEU:HD23	2.00	0.43
1:A:291:ASN:OD1	1:A:292:ALA:N	2.51	0.43
2:G:158:LEU:HB2	2:G:183:VAL:CG1	2.31	0.43
2:G:209:HIS:NE2	2:G:211:GLN:OE1	2.49	0.43
2:G:260:VAL:HG21	2:G:267:VAL:HG21	2.00	0.43
2:G:456:VAL:HG12	2:G:457:HIS:N	2.33	0.43
1:A:447:LEU:HD21	1:A:491:PHE:CD2	2.54	0.43
2:G:263:ALA:CA	2:G:289:GLY:HA3	2.46	0.43
1:A:138:THR:O	1:A:141:VAL:N	2.50	0.43
1:A:316:LYS:HD2	1:A:316:LYS:HA	1.86	0.43
1:A:344:VAL:HG23	1:A:358:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LEU:HD13	1:A:430:LEU:CD2	2.48	0.43
2:G:115:ASN:HA	2:G:144:SER:O	2.17	0.43
1:A:298:LYS:NZ	1:A:452:THR:HB	2.34	0.43
1:A:338:GLN:O	1:A:341:LYS:N	2.51	0.43
1:A:383:MET:HG2	1:A:482:TRP:CH2	2.54	0.43
2:G:58:ILE:HG23	2:G:83:THR:O	2.18	0.43
2:G:467:TRP:C	2:G:467:TRP:CD1	2.92	0.43
1:A:142:LEU:HD13	1:A:203:PHE:CE1	2.39	0.43
1:A:178:LEU:HD12	1:A:193:LEU:HD11	2.01	0.43
1:A:241:ARG:HD2	1:A:247:SER:HB3	2.00	0.43
1:A:266:VAL:HG21	1:A:277:LEU:HB3	2.00	0.43
2:G:238:GLY:O	2:G:239:MET:HG2	2.18	0.43
1:A:142:LEU:O	1:A:146:LEU:HG	2.18	0.43
1:A:153:LEU:HD21	1:A:157:PHE:CE1	2.54	0.43
1:A:206:VAL:HG13	1:A:207:HIS:N	2.33	0.43
1:A:259:LEU:HD11	1:A:279:ASP:O	2.17	0.43
2:G:89:ASN:O	2:G:90:GLN:HB3	2.19	0.43
2:G:94:LEU:HD23	2:G:128:VAL:CG2	2.48	0.43
2:G:193:ALA:HB1	2:G:196:LEU:CD2	2.49	0.43
2:G:463:ASP:O	2:G:464:ARG:HB2	2.19	0.43
1:A:299:TRP:CE3	1:A:299:TRP:HA	2.53	0.43
2:G:395:ARG:HG3	2:G:424:LEU:HD12	2.01	0.43
2:G:434:PRO:HD2	2:G:435:GLU:CD	2.39	0.43
2:G:463:ASP:HB3	2:G:464:ARG:CZ	2.49	0.43
1:A:206:VAL:CA	1:A:209:ALA:HB3	2.45	0.43
2:G:97:GLY:HA3	2:G:131:HIS:O	2.18	0.43
2:G:183:VAL:HG23	2:G:183:VAL:O	2.19	0.43
2:G:243:LEU:HD12	2:G:243:LEU:N	2.34	0.43
2:G:412:VAL:HG22	2:G:438:ARG:HB3	2.01	0.43
1:A:304:ASP:C	1:A:451:GLU:HG2	2.39	0.43
1:A:403:VAL:HG13	1:A:403:VAL:O	2.18	0.43
1:A:149:PHE:CE1	1:A:197:LEU:HD13	2.54	0.42
1:A:226:HIS:O	1:A:251:LEU:HB2	2.18	0.42
1:A:263:ASN:ND2	1:A:278:LEU:O	2.46	0.42
1:A:310:MET:CE	1:A:323:PRO:HG3	2.43	0.42
1:A:466:ARG:HA	2:G:234:TYR:CZ	2.53	0.42
1:A:182:LEU:HD11	1:A:190:LYS:HG3	2.00	0.42
2:G:68:ILE:O	2:G:94:LEU:HA	2.20	0.42
2:G:230:VAL:O	2:G:255:ALA:HB1	2.19	0.42
2:G:457:HIS:ND1	2:G:458:THR:HG23	2.34	0.42
1:A:259:LEU:C	1:A:259:LEU:HD23	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LEU:HB3	1:A:430:LEU:HB3	2.00	0.42
2:G:238:GLY:H	2:G:265:THR:CG2	2.32	0.42
2:G:381:GLU:HG2	2:G:405:ARG:HB3	2.02	0.42
2:G:469:VAL:HG22	2:G:470:THR:H	1.84	0.42
2:G:252:GLY:HA2	2:G:277:SER:O	2.20	0.42
1:A:134:GLU:HA	1:A:137:SER:OG	2.19	0.42
1:A:327:SER:OG	1:A:330:TYR:HB2	2.20	0.42
1:A:400:ARG:HH21	1:A:450:THR:HB	1.84	0.42
2:G:352:THR:HA	2:G:376:GLY:HA3	2.02	0.42
2:G:464:ARG:O	2:G:466:VAL:HG23	2.20	0.42
1:A:362:ASN:CG	1:A:364:LYS:H	2.23	0.42
1:A:483:ASP:O	1:A:484:GLN:CG	2.57	0.42
1:A:219:THR:OG1	1:A:294:TYR:CE1	2.72	0.42
1:A:276:ARG:NH1	1:A:276:ARG:HG3	2.34	0.42
1:A:298:LYS:HB3	1:A:452:THR:O	2.20	0.42
1:A:427:LEU:HD23	1:A:427:LEU:HA	1.89	0.42
1:A:480:VAL:HG22	1:A:492:MET:HG3	2.00	0.42
1:A:277:LEU:HD21	1:A:290:LEU:HD21	2.02	0.42
2:G:56:VAL:HG12	2:G:80:THR:HG23	2.00	0.42
2:G:478:VAL:HG12	2:G:479:LYS:N	2.34	0.42
1:A:142:LEU:HD12	1:A:142:LEU:HA	1.82	0.41
1:A:345:GLY:O	1:A:357:ILE:HG12	2.20	0.41
1:A:462:ILE:N	1:A:462:ILE:HD13	2.36	0.41
1:A:467:THR:O	1:A:467:THR:HG23	2.19	0.41
2:G:228:LEU:CG	2:G:229:GLU:OE2	2.69	0.41
2:G:266:HIS:NE2	2:G:268:SER:OG	2.53	0.41
1:A:204:THR:CG2	1:A:205:CYS:N	2.83	0.41
2:G:114:GLN:OE1	2:G:115:ASN:N	2.53	0.41
2:G:226:ARG:HG3	2:G:251:GLN:HG2	2.01	0.41
2:G:260:VAL:CG2	2:G:267:VAL:HG21	2.50	0.41
2:G:400:GLN:HG2	2:G:401:PRO:CD	2.40	0.41
2:G:404:ILE:HD13	2:G:423:LEU:HD21	2.02	0.41
1:A:133:LEU:HG	1:A:134:GLU:OE2	2.20	0.41
1:A:307:LYS:O	1:A:326:ASN:ND2	2.54	0.41
1:A:497:ASP:CG	1:A:499:ARG:HG2	2.40	0.41
2:G:65:GLU:HG3	2:G:91:ALA:HA	2.01	0.41
2:G:349:VAL:HG12	2:G:357:ALA:HB1	2.02	0.41
2:G:395:ARG:O	2:G:395:ARG:HG2	2.19	0.41
1:A:288:VAL:HG13	1:A:440:ALA:O	2.21	0.41
1:A:496:TYR:O	1:A:498:PRO:HD3	2.20	0.41
2:G:158:LEU:HD12	2:G:183:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:259:GLN:HG2	2:G:261:GLU:OE1	2.20	0.41
2:G:404:ILE:HB	2:G:427:ILE:HD13	2.01	0.41
1:A:383:MET:HE1	1:A:482:TRP:CG	2.55	0.41
2:G:295:ARG:HB3	2:G:295:ARG:NH1	2.35	0.41
1:A:233:ARG:O	1:A:237:VAL:HG23	2.21	0.41
1:A:356:VAL:HG22	1:A:386:LEU:CD2	2.51	0.41
2:G:228:LEU:HG	2:G:229:GLU:OE2	2.21	0.41
2:G:468:THR:HG22	2:G:468:THR:O	2.19	0.41
2:G:475:VAL:HG12	2:G:477:GLU:H	1.86	0.41
1:A:143:GLY:O	1:A:147:VAL:HG23	2.20	0.41
1:A:218:VAL:O	1:A:218:VAL:HG13	2.19	0.41
1:A:310:MET:HE1	1:A:323:PRO:CG	2.41	0.41
1:A:346:GLN:HE21	1:A:354:SER:CB	2.25	0.41
1:A:295:LEU:HB3	1:A:447:LEU:HD13	2.03	0.41
1:A:334:HIS:CE1	1:A:336:ILE:HD11	2.55	0.41
1:A:398:LEU:HD23	1:A:399:PRO:N	2.35	0.41
2:G:87:SER:HA	2:G:121:SER:O	2.21	0.41
2:G:266:HIS:HA	2:G:291:SER:O	2.21	0.41
2:G:269:MET:HG2	2:G:270:ASN:N	2.35	0.41
2:G:311:VAL:HG21	2:G:317:VAL:HG12	2.02	0.41
2:G:311:VAL:CG1	2:G:315:SER:OG	2.69	0.41
2:G:390:LEU:HD23	2:G:394:ALA:O	2.21	0.41
1:A:157:PHE:CZ	1:A:409:MET:HE1	2.55	0.41
1:A:307:LYS:HB3	1:A:326:ASN:HB2	2.03	0.41
1:A:481:LEU:HD23	1:A:482:TRP:N	2.36	0.41
2:G:114:GLN:O	2:G:115:ASN:C	2.58	0.41
2:G:202:GLY:O	2:G:227:GLY:HA3	2.20	0.41
2:G:319:LEU:HD22	2:G:343:VAL:HG13	2.03	0.41
2:G:406:LEU:O	2:G:406:LEU:HG	2.20	0.41
1:A:189:THR:HA	1:A:192:ASN:OD1	2.21	0.41
2:G:324:VAL:O	2:G:349:VAL:HA	2.21	0.41
1:A:157:PHE:HA	1:A:412:ILE:HD11	2.03	0.40
1:A:332:VAL:CG1	1:A:333:ALA:N	2.83	0.40
2:G:178:GLN:O	2:G:204:GLY:CA	2.68	0.40
2:G:243:LEU:HB3	2:G:246:THR:CG2	2.51	0.40
2:G:407:ILE:HG12	2:G:430:GLU:CD	2.41	0.40
2:G:460:ARG:NH2	2:G:462:LEU:HD11	2.36	0.40
1:A:168:ALA:HB2	1:A:403:VAL:HG11	2.04	0.40
1:A:409:MET:HB3	1:A:441:MET:HE1	2.03	0.40
2:G:365:LEU:HD12	2:G:366:THR:H	1.86	0.40
1:A:480:VAL:HG22	1:A:492:MET:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:77:VAL:CG2	2:G:111:VAL:HB	2.51	0.40
2:G:225:ALA:HB1	2:G:230:VAL:CG2	2.51	0.40
2:G:235:VAL:CG2	2:G:260:VAL:HG22	2.52	0.40
2:G:382:VAL:O	2:G:406:LEU:HA	2.21	0.40
2:G:474:ARG:NE	2:G:474:ARG:HA	2.35	0.40
2:G:65:GLU:HG3	2:G:91:ALA:CA	2.51	0.40
2:G:117:ILE:O	2:G:118:ILE:HD13	2.21	0.40
2:G:373:HIS:ND1	2:G:375:HIS:HB2	2.36	0.40
2:G:413:LEU:HD21	2:G:415:LEU:HB2	2.01	0.40
2:G:417:ILE:HG22	2:G:447:GLY:HA3	2.03	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	376/403 (93%)	339 (90%)	37 (10%)	0	100	100
2	G	417/877 (48%)	313 (75%)	103 (25%)	1 (0%)	47	79
All	All	793/1280 (62%)	652 (82%)	140 (18%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	163	PRO

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	343/366 (94%)	341 (99%)	2 (1%)	86 94
2	G	302/637 (47%)	302 (100%)	0	100 100
All	All	645/1003 (64%)	643 (100%)	2 (0%)	92 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	LYS
1	A	364	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	ASN
1	A	271	ASN
1	A	334	HIS
1	A	346	GLN
1	A	475	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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-11814. These allow visual inspection of the internal detail of the map and identification of artifacts.

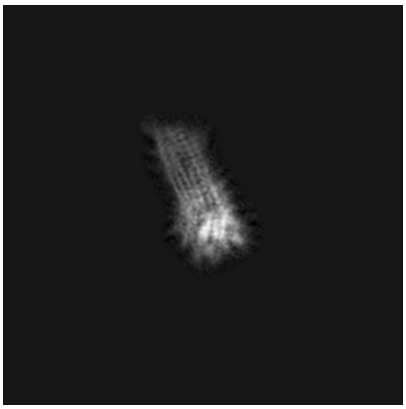
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map

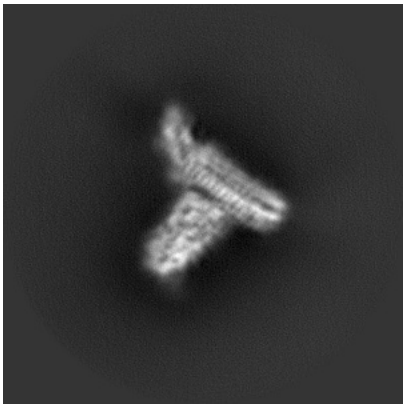
X

Y

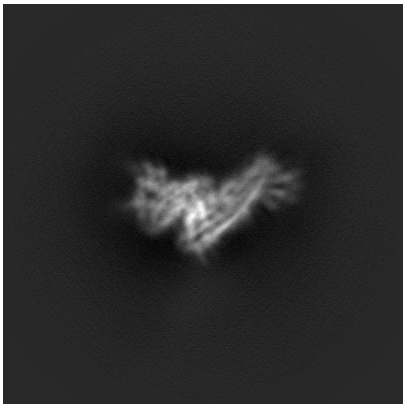


Z

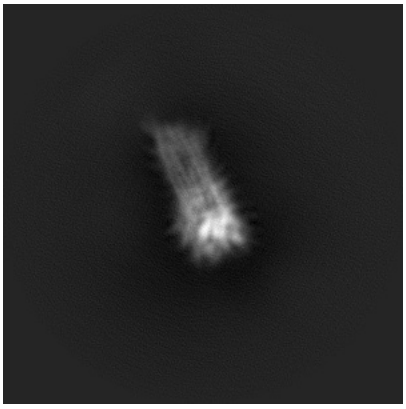
6.1.2 Raw map



X



Y

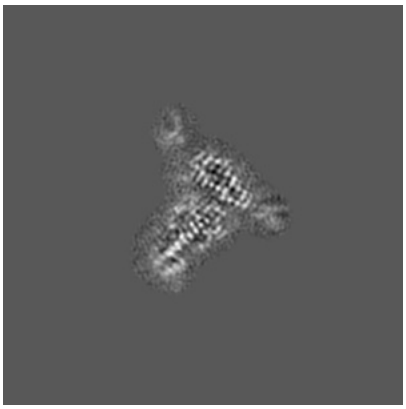


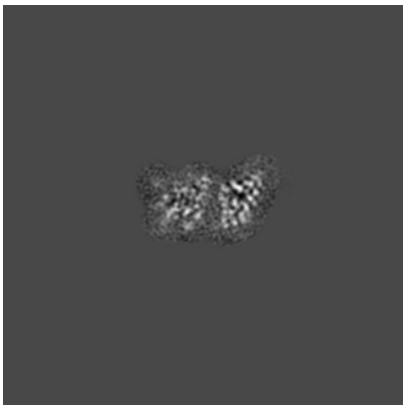
Z

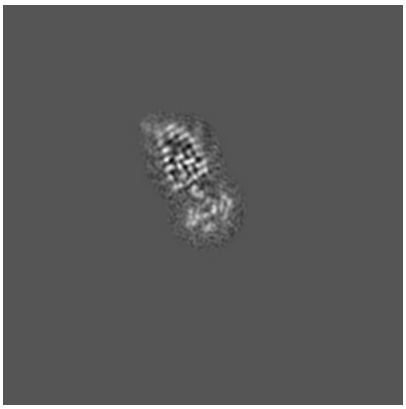
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

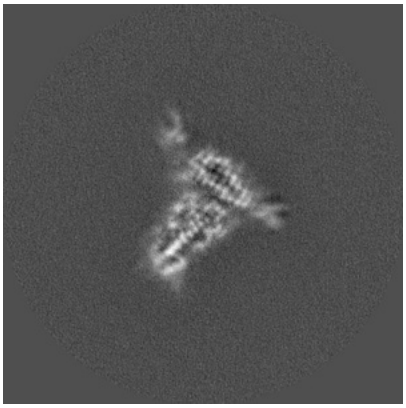
6.2.1 Primary map

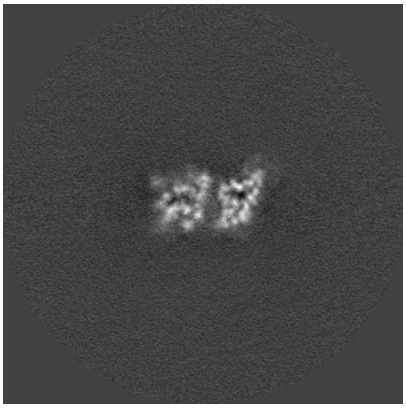

X Index: 164

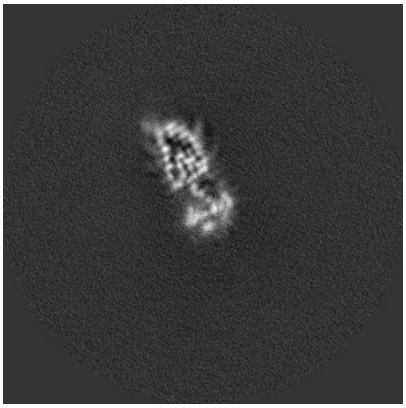

Y Index: 164


Z Index: 164

6.2.2 Raw map


X Index: 164

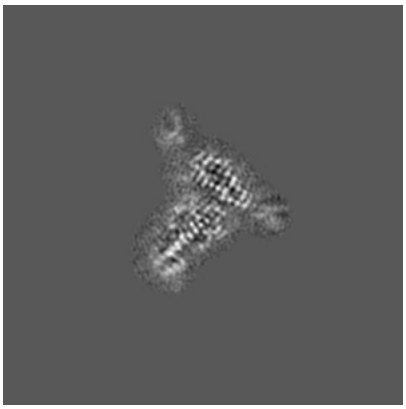

Y Index: 164

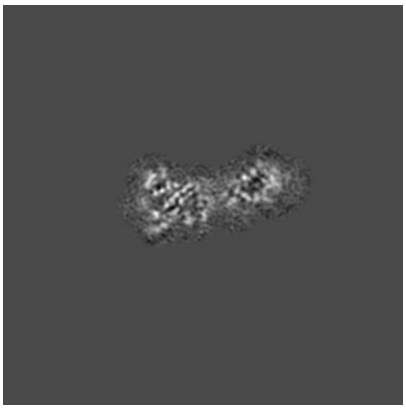

Z Index: 164

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

6.3 Largest variance slices (i)

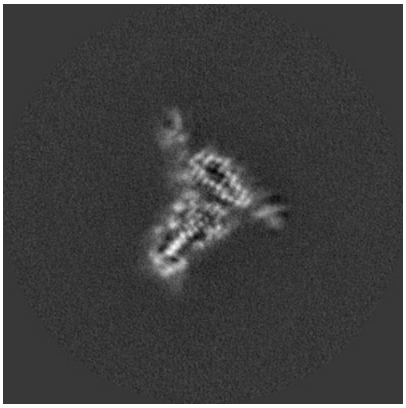
6.3.1 Primary map

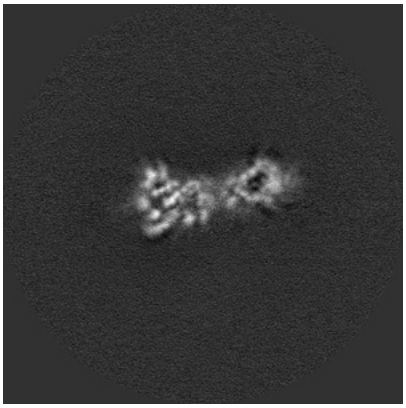

X Index: 164

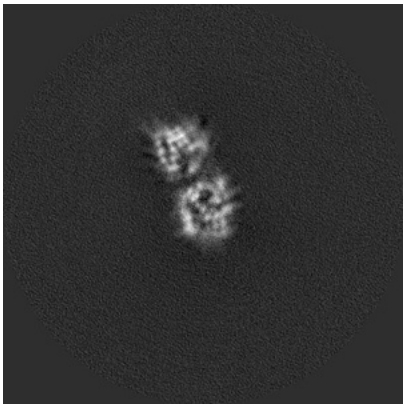

Y Index: 149

Z Index: 163

6.3.2 Raw map


X Index: 165

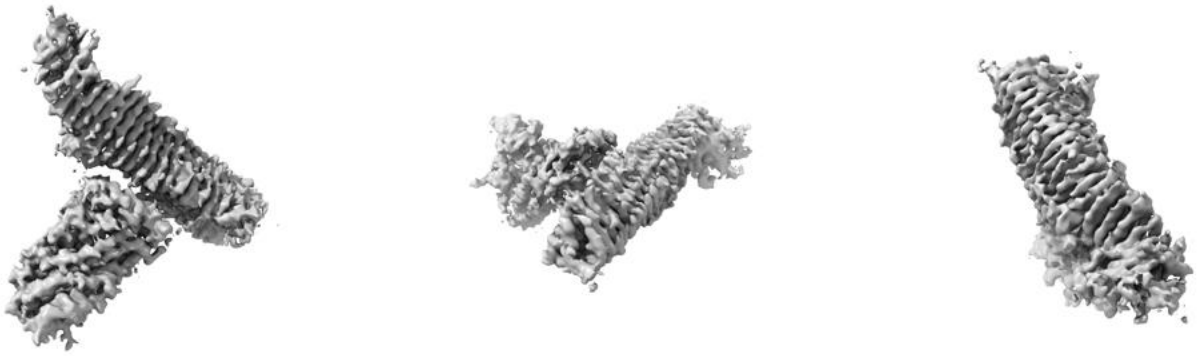

Y Index: 148


Z Index: 154

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 0.0122. 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.

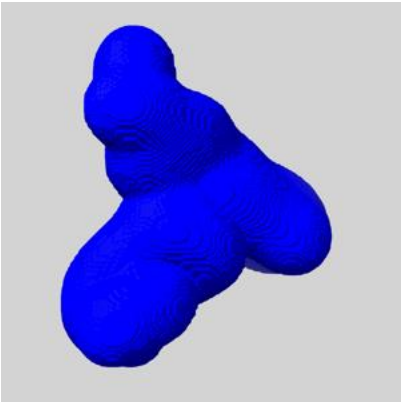
6.5 Mask visualisation (i)

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

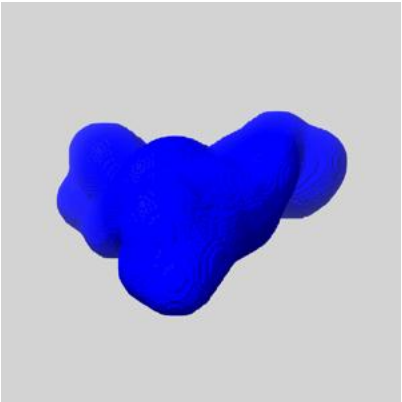
A mask typically either:

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

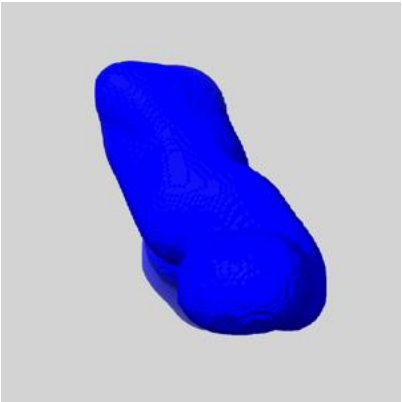
6.5.1 emd_11814_msk_1.map (i)



X



Y

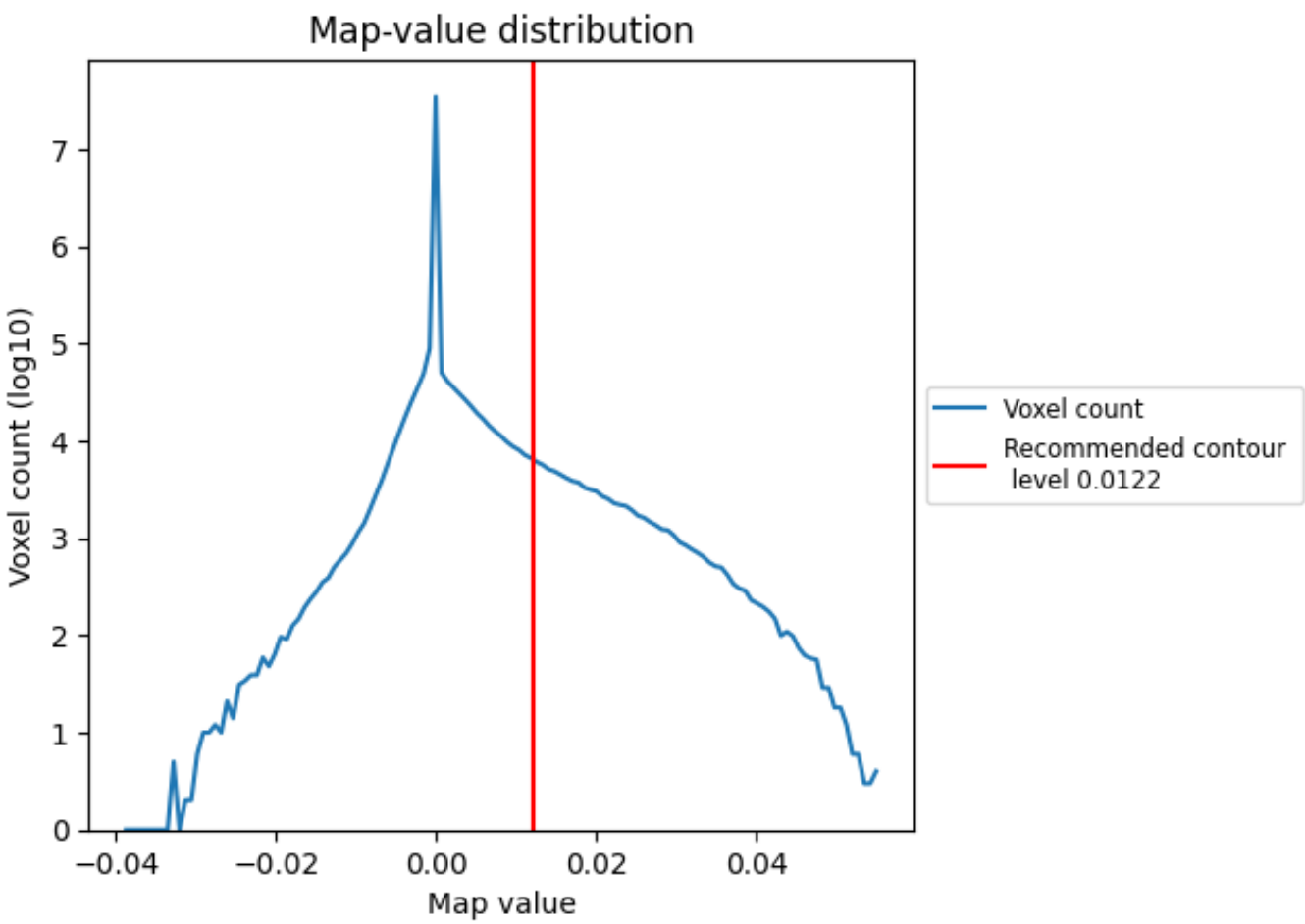


Z

7 Map analysis (i)

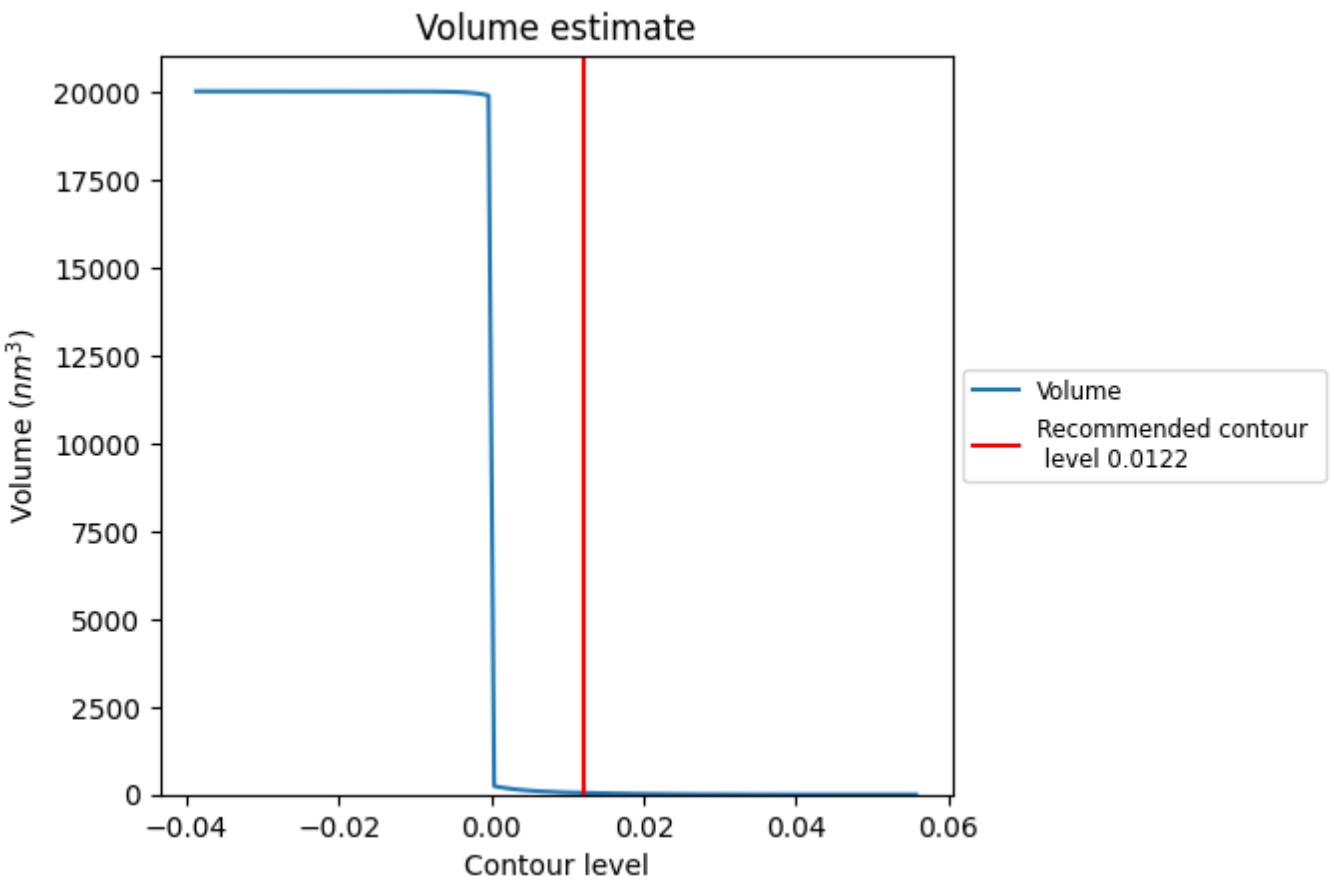
This section contains the results of statistical analysis of the map.

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.

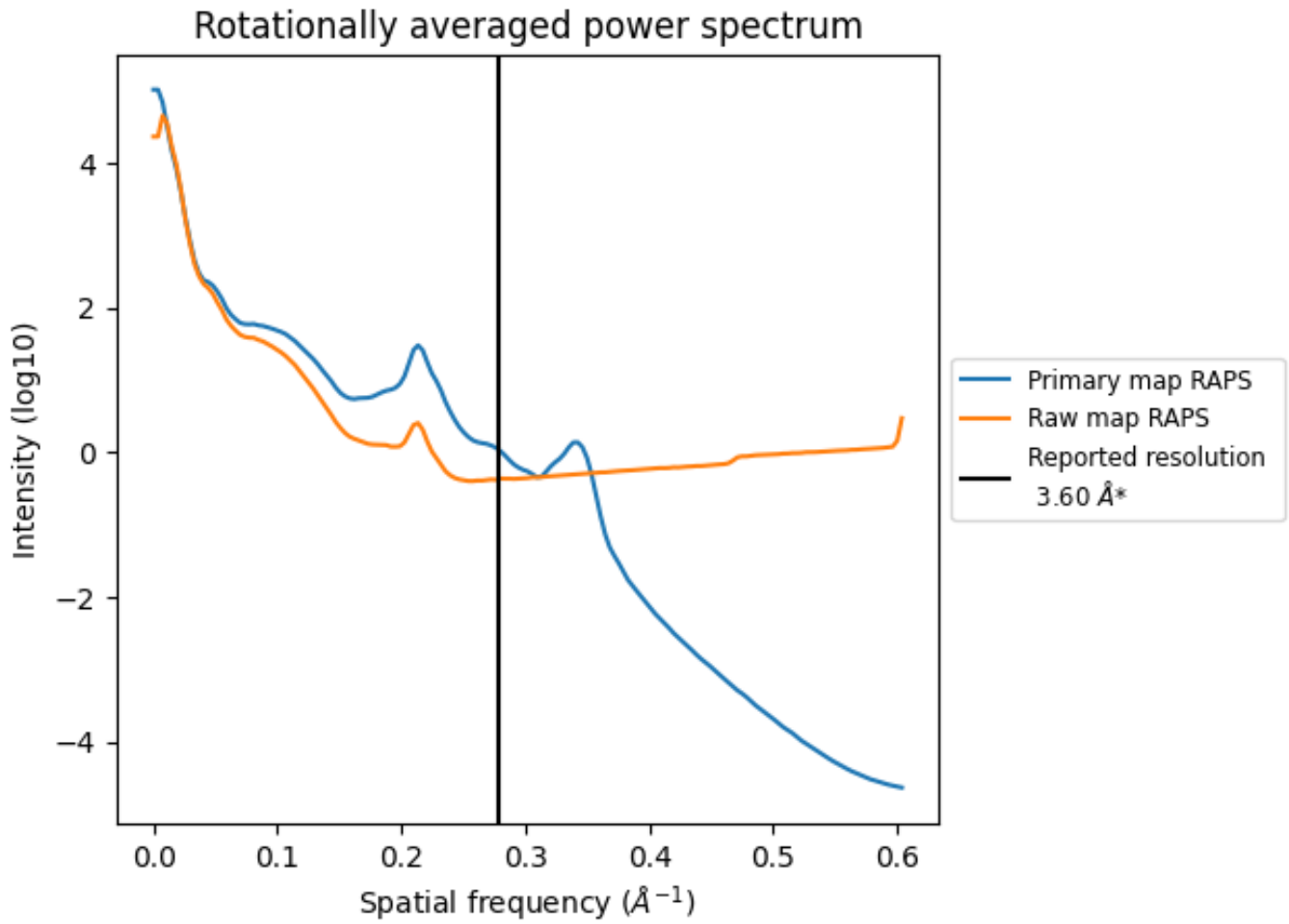
7.2 Volume estimate (i)



The volume at the recommended contour level is 47 nm^3; this corresponds to an approximate mass of 42 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)

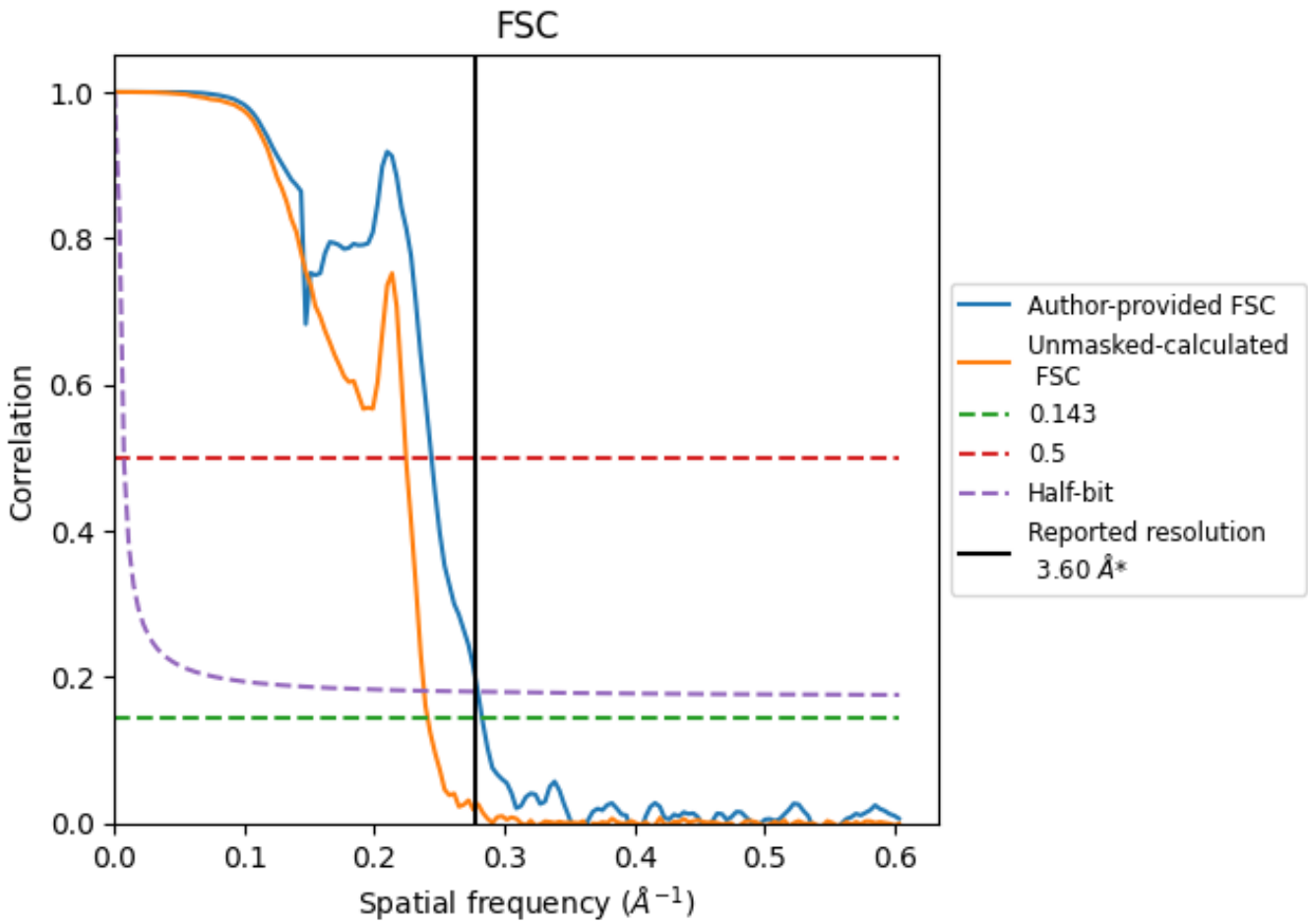


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

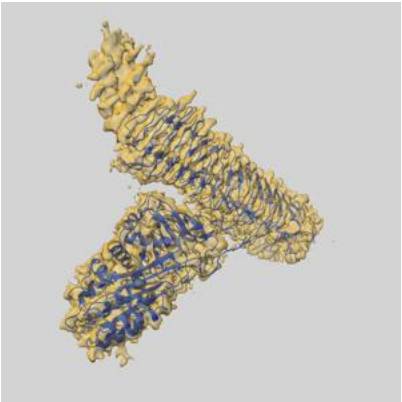
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.53	4.10	3.58
Unmasked-calculated*	4.15	4.46	4.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.6 by more than 10 %

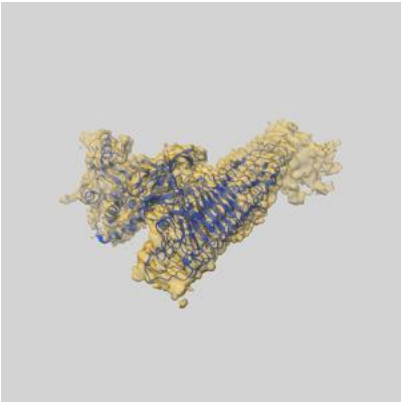
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11814 and PDB model 7AKV. Per-residue inclusion information can be found in section 3 on page 4.

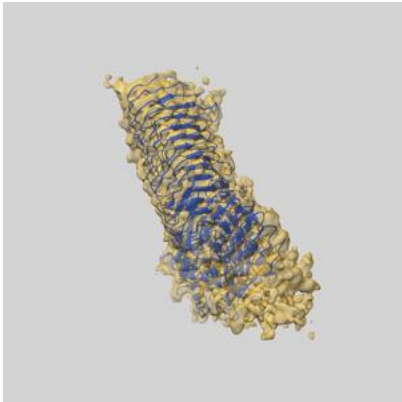
9.1 Map-model overlay (i)



X



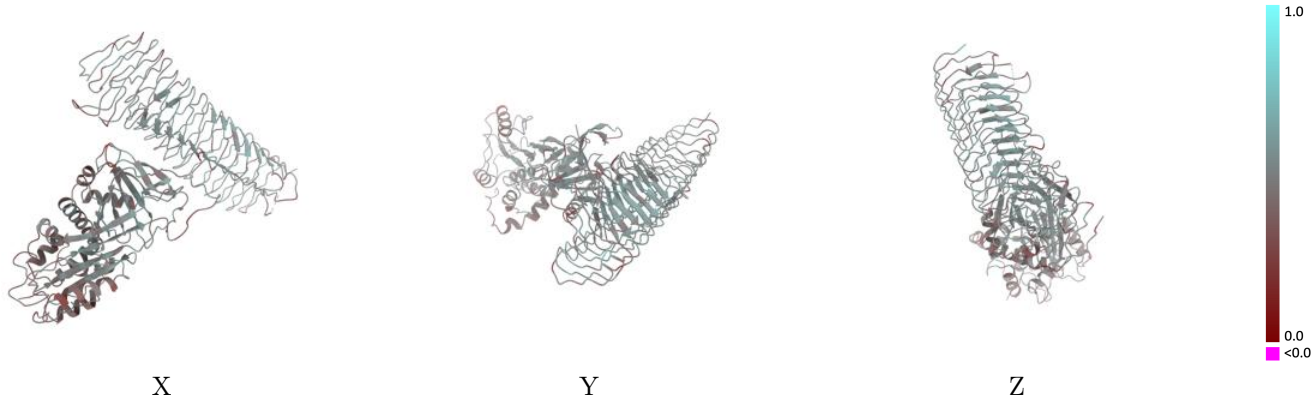
Y



Z

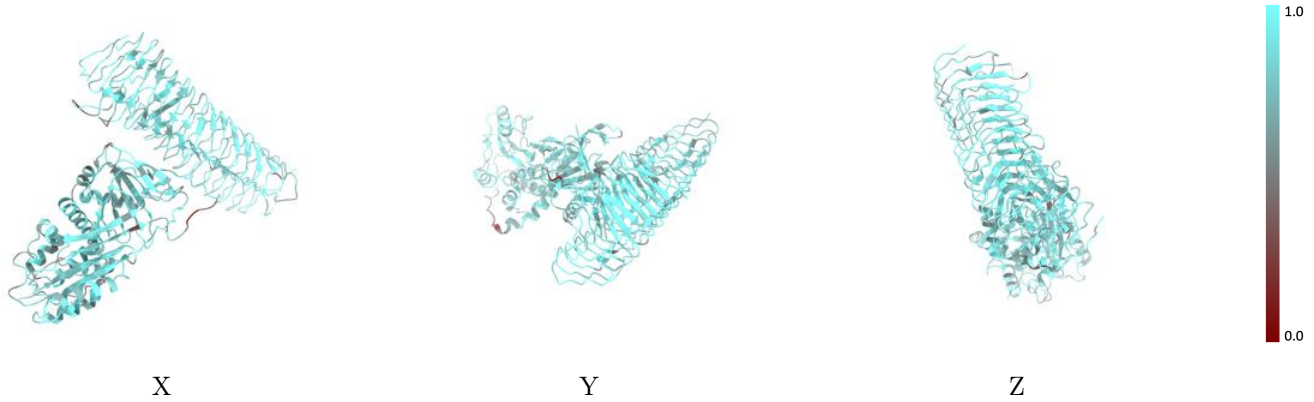
The images above show the 3D surface view of the map at the recommended contour level 0.0122 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



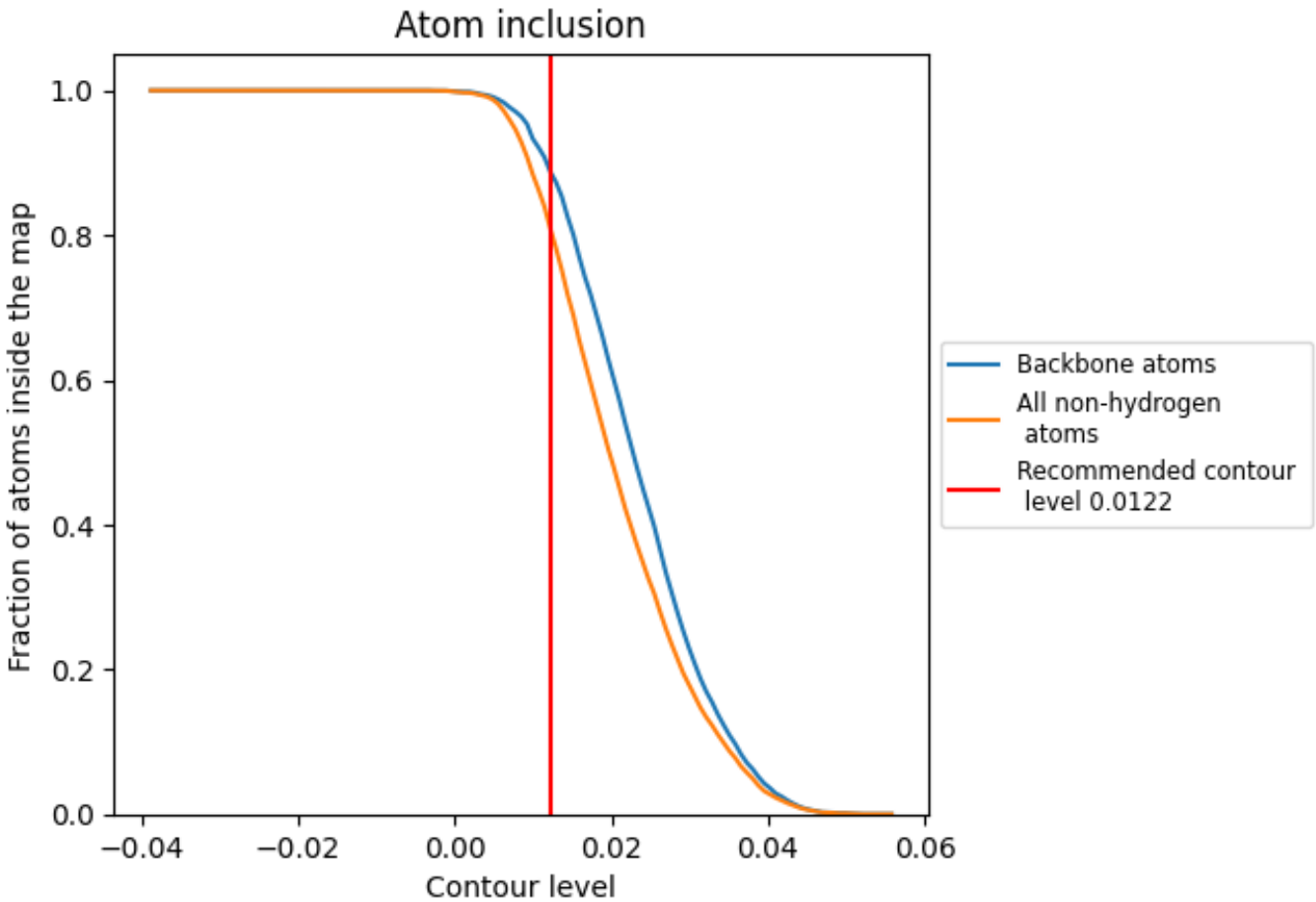
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.0122).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0122) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8092	0.4770
A	0.7957	0.4570
G	0.8317	0.4970