Full wwPDB EM Validation Report

Jul 18, 2024 – 10:43 pm BST

PDB ID	:	8QZP
EMDB ID	:	EMD-18779
Title	:	Structure of the non-mitochondrial citrate synthase from Ananas comosus
Authors	:	Lo, Y.K.; Bohn, S.; Sendker, F.L.; Schuller, J.M.; Hochberg, G.
Deposited on	:	2023-10-28
Resolution	:	4.15 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 ⓘ 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 ⓘ) were used in the production of this report:

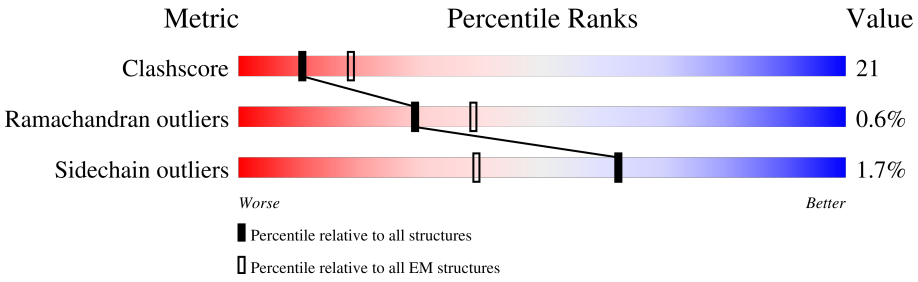
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 4.15 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	521	51% 27% · 21%
1	B	521	46% 33% · 21%
1	C	521	48% 30% · 20%
1	D	521	53% 31% 15%
1	E	521	7% 48% 28% · 23%
1	F	521	41% 33% · 24%
1	G	521	11% 49% 27% 24%
1	H	521	13% 39% 36% 24%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 25393 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 Citrate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	413	Total	C	N	O	S	0	0
			3201	2052	556	579	14		
1	B	414	Total	C	N	O	S	0	0
			3208	2057	557	580	14		
1	C	416	Total	C	N	O	S	0	0
			3217	2062	559	582	14		
1	D	441	Total	C	N	O	S	0	0
			3407	2179	593	621	14		
1	E	401	Total	C	N	O	S	0	0
			3112	1993	543	562	14		
1	F	397	Total	C	N	O	S	0	0
			3090	1981	538	557	14		
1	G	394	Total	C	N	O	S	0	0
			3068	1968	535	551	14		
1	H	397	Total	C	N	O	S	0	0
			3090	1981	538	557	14		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	514	LEU	-	expression tag	UNP A0A6P5F0R3
A	515	GLU	-	expression tag	UNP A0A6P5F0R3
A	516	HIS	-	expression tag	UNP A0A6P5F0R3
A	517	HIS	-	expression tag	UNP A0A6P5F0R3
A	518	HIS	-	expression tag	UNP A0A6P5F0R3
A	519	HIS	-	expression tag	UNP A0A6P5F0R3
A	520	HIS	-	expression tag	UNP A0A6P5F0R3
A	521	HIS	-	expression tag	UNP A0A6P5F0R3
B	514	LEU	-	expression tag	UNP A0A6P5F0R3
B	515	GLU	-	expression tag	UNP A0A6P5F0R3
B	516	HIS	-	expression tag	UNP A0A6P5F0R3
B	517	HIS	-	expression tag	UNP A0A6P5F0R3
B	518	HIS	-	expression tag	UNP A0A6P5F0R3
B	519	HIS	-	expression tag	UNP A0A6P5F0R3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	520	HIS	-	expression tag	UNP A0A6P5F0R3
B	521	HIS	-	expression tag	UNP A0A6P5F0R3
C	514	LEU	-	expression tag	UNP A0A6P5F0R3
C	515	GLU	-	expression tag	UNP A0A6P5F0R3
C	516	HIS	-	expression tag	UNP A0A6P5F0R3
C	517	HIS	-	expression tag	UNP A0A6P5F0R3
C	518	HIS	-	expression tag	UNP A0A6P5F0R3
C	519	HIS	-	expression tag	UNP A0A6P5F0R3
C	520	HIS	-	expression tag	UNP A0A6P5F0R3
C	521	HIS	-	expression tag	UNP A0A6P5F0R3
D	514	LEU	-	expression tag	UNP A0A6P5F0R3
D	515	GLU	-	expression tag	UNP A0A6P5F0R3
D	516	HIS	-	expression tag	UNP A0A6P5F0R3
D	517	HIS	-	expression tag	UNP A0A6P5F0R3
D	518	HIS	-	expression tag	UNP A0A6P5F0R3
D	519	HIS	-	expression tag	UNP A0A6P5F0R3
D	520	HIS	-	expression tag	UNP A0A6P5F0R3
D	521	HIS	-	expression tag	UNP A0A6P5F0R3
E	514	LEU	-	expression tag	UNP A0A6P5F0R3
E	515	GLU	-	expression tag	UNP A0A6P5F0R3
E	516	HIS	-	expression tag	UNP A0A6P5F0R3
E	517	HIS	-	expression tag	UNP A0A6P5F0R3
E	518	HIS	-	expression tag	UNP A0A6P5F0R3
E	519	HIS	-	expression tag	UNP A0A6P5F0R3
E	520	HIS	-	expression tag	UNP A0A6P5F0R3
E	521	HIS	-	expression tag	UNP A0A6P5F0R3
F	510	LEU	-	expression tag	UNP A0A6P5F0R3
F	511	GLU	-	expression tag	UNP A0A6P5F0R3
F	512	HIS	-	expression tag	UNP A0A6P5F0R3
F	513	HIS	-	expression tag	UNP A0A6P5F0R3
F	514	HIS	-	expression tag	UNP A0A6P5F0R3
F	515	HIS	-	expression tag	UNP A0A6P5F0R3
F	516	HIS	-	expression tag	UNP A0A6P5F0R3
F	517	HIS	-	expression tag	UNP A0A6P5F0R3
G	510	LEU	-	expression tag	UNP A0A6P5F0R3
G	511	GLU	-	expression tag	UNP A0A6P5F0R3
G	512	HIS	-	expression tag	UNP A0A6P5F0R3
G	513	HIS	-	expression tag	UNP A0A6P5F0R3
G	514	HIS	-	expression tag	UNP A0A6P5F0R3
G	515	HIS	-	expression tag	UNP A0A6P5F0R3
G	516	HIS	-	expression tag	UNP A0A6P5F0R3
G	517	HIS	-	expression tag	UNP A0A6P5F0R3

Continued on next page...

Continued from previous page...

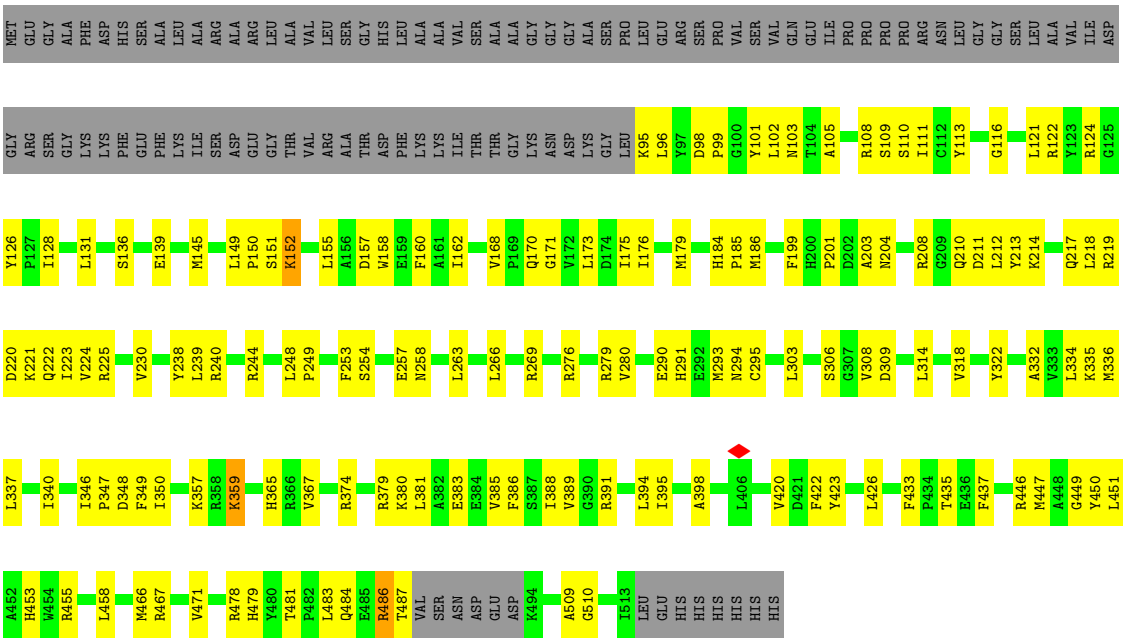
Chain	Residue	Modelled	Actual	Comment	Reference
H	510	LEU	-	expression tag	UNP A0A6P5F0R3
H	511	GLU	-	expression tag	UNP A0A6P5F0R3
H	512	HIS	-	expression tag	UNP A0A6P5F0R3
H	513	HIS	-	expression tag	UNP A0A6P5F0R3
H	514	HIS	-	expression tag	UNP A0A6P5F0R3
H	515	HIS	-	expression tag	UNP A0A6P5F0R3
H	516	HIS	-	expression tag	UNP A0A6P5F0R3
H	517	HIS	-	expression tag	UNP A0A6P5F0R3

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.

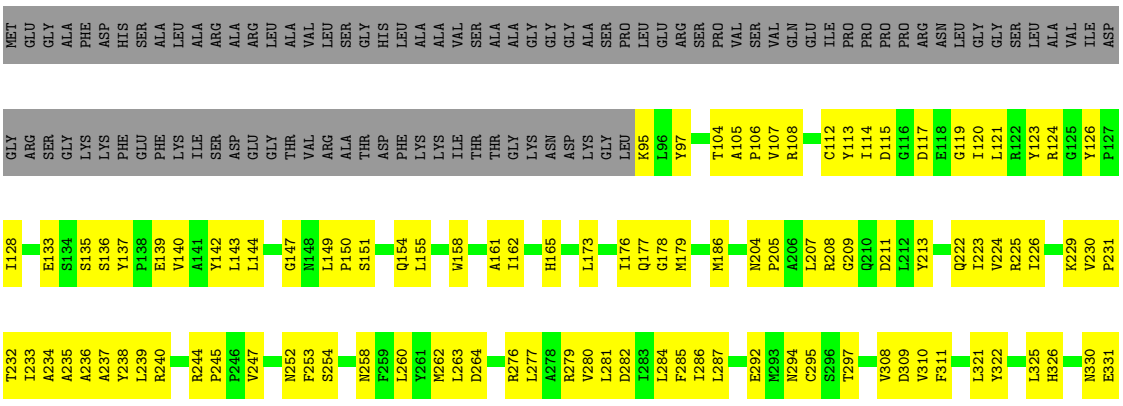
- Molecule 1: Citrate synthase

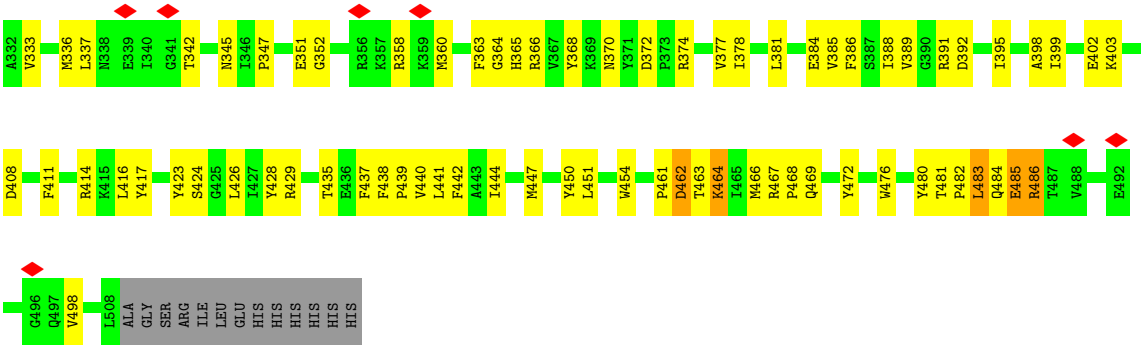
Chain A:



- Molecule 1: Citrate synthase

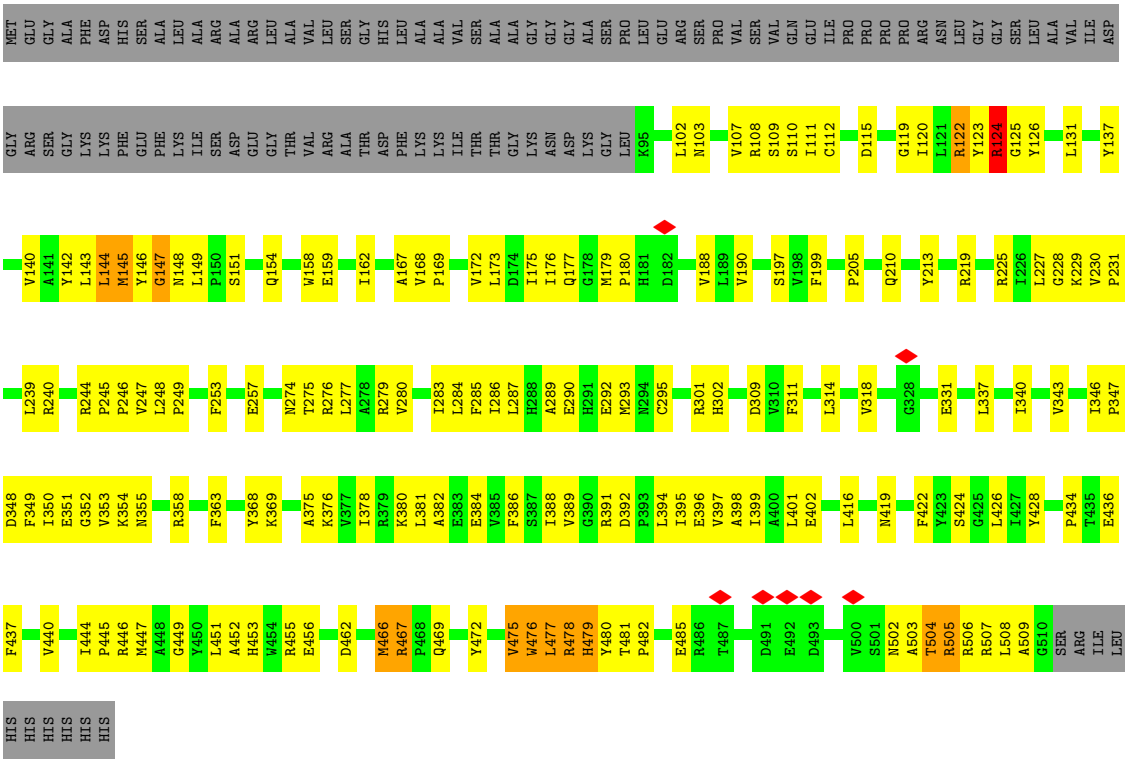
Chain B:





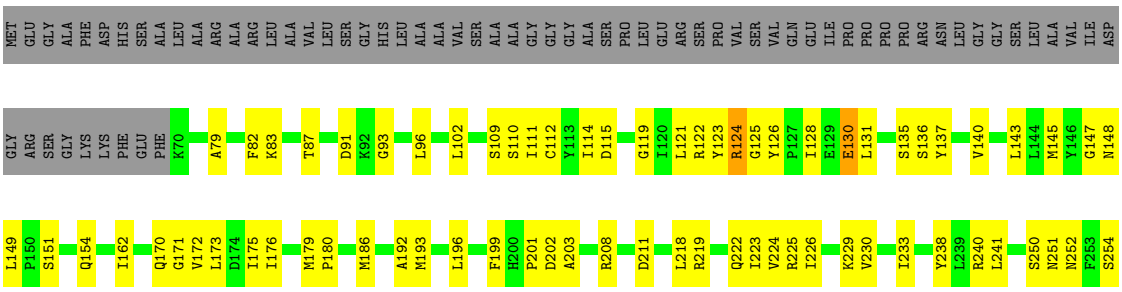
• Molecule 1: Citrate synthase

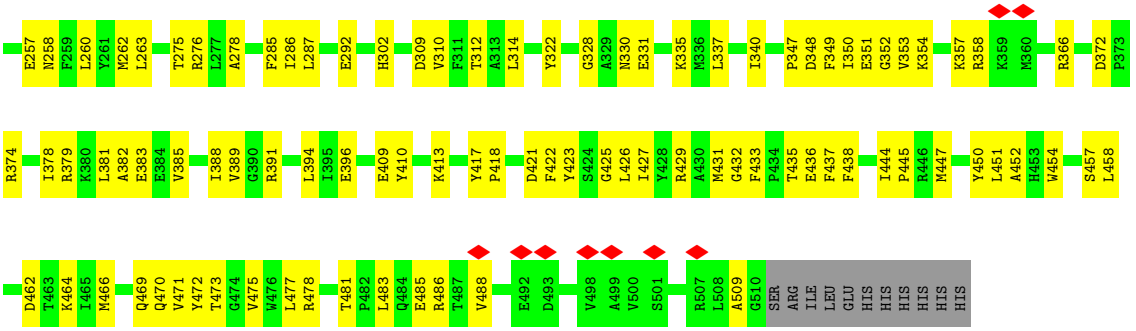
Chain C:



• Molecule 1: Citrate synthase

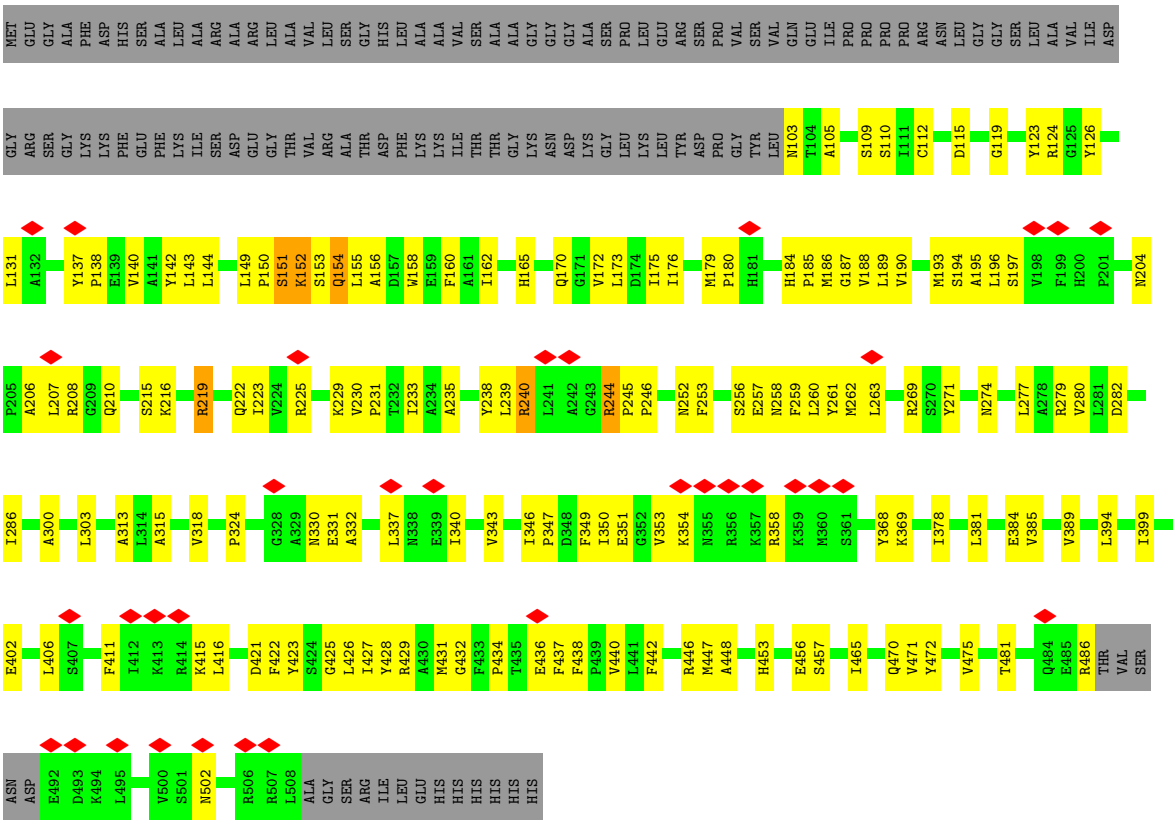
Chain D:





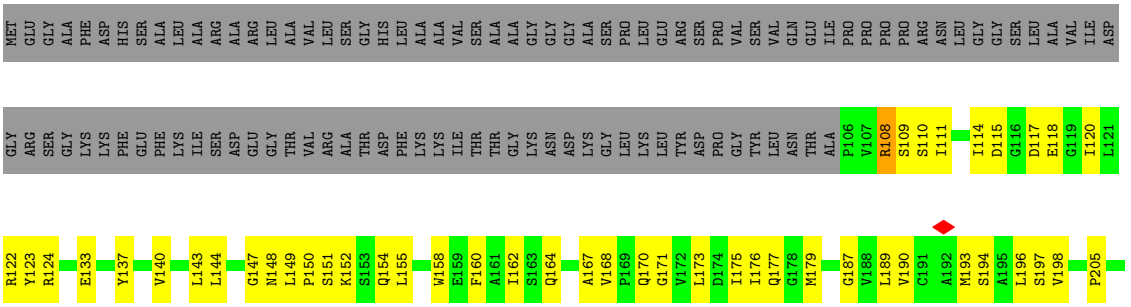
• Molecule 1: Citrate synthase

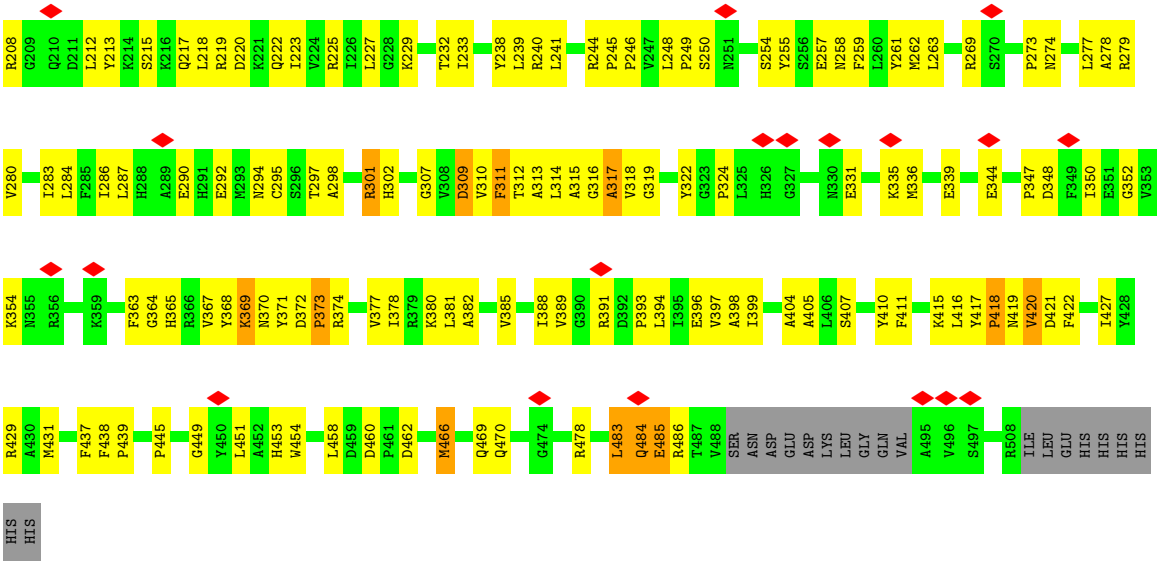
Chain E:



• Molecule 1: Citrate synthase

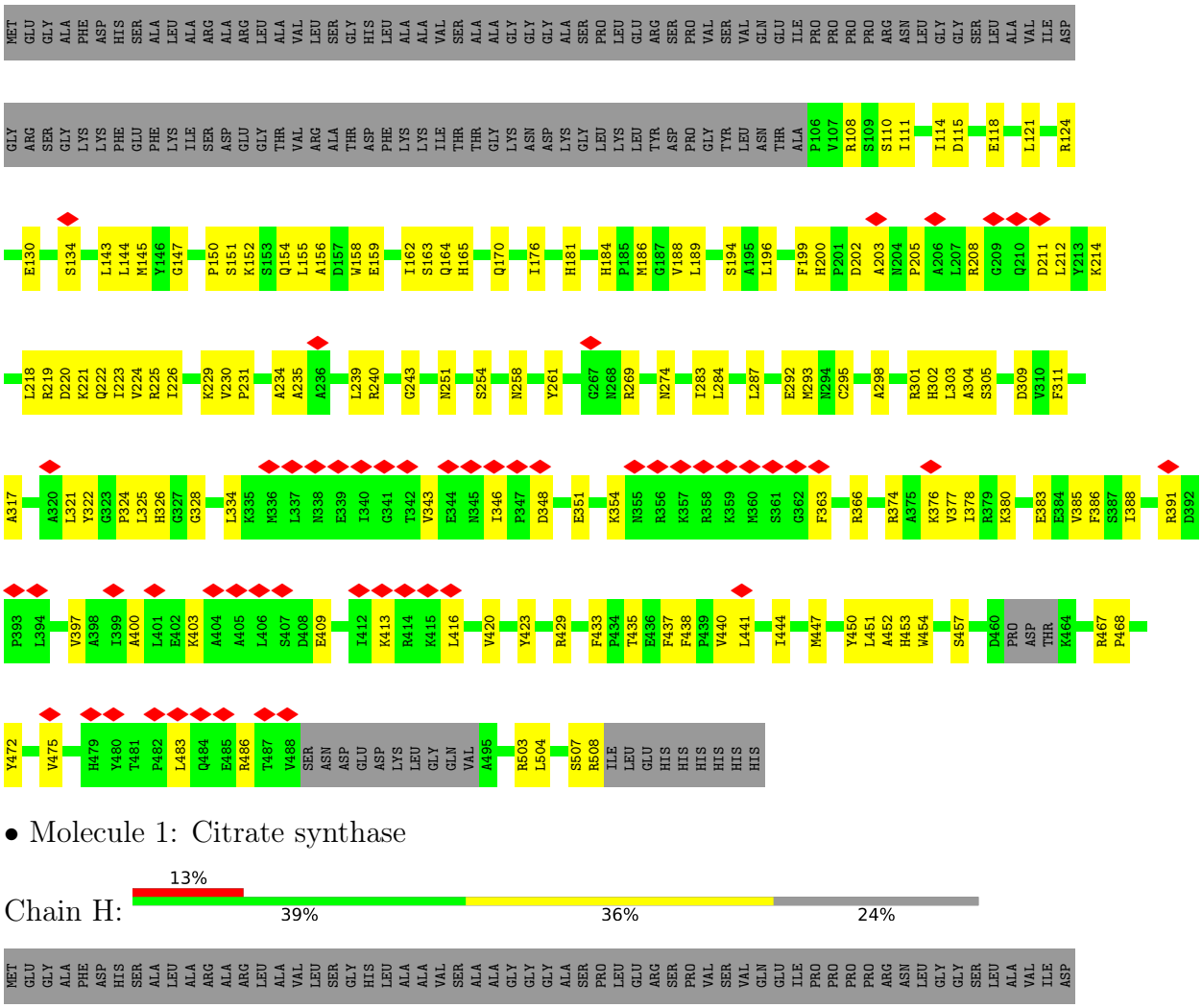
Chain F:





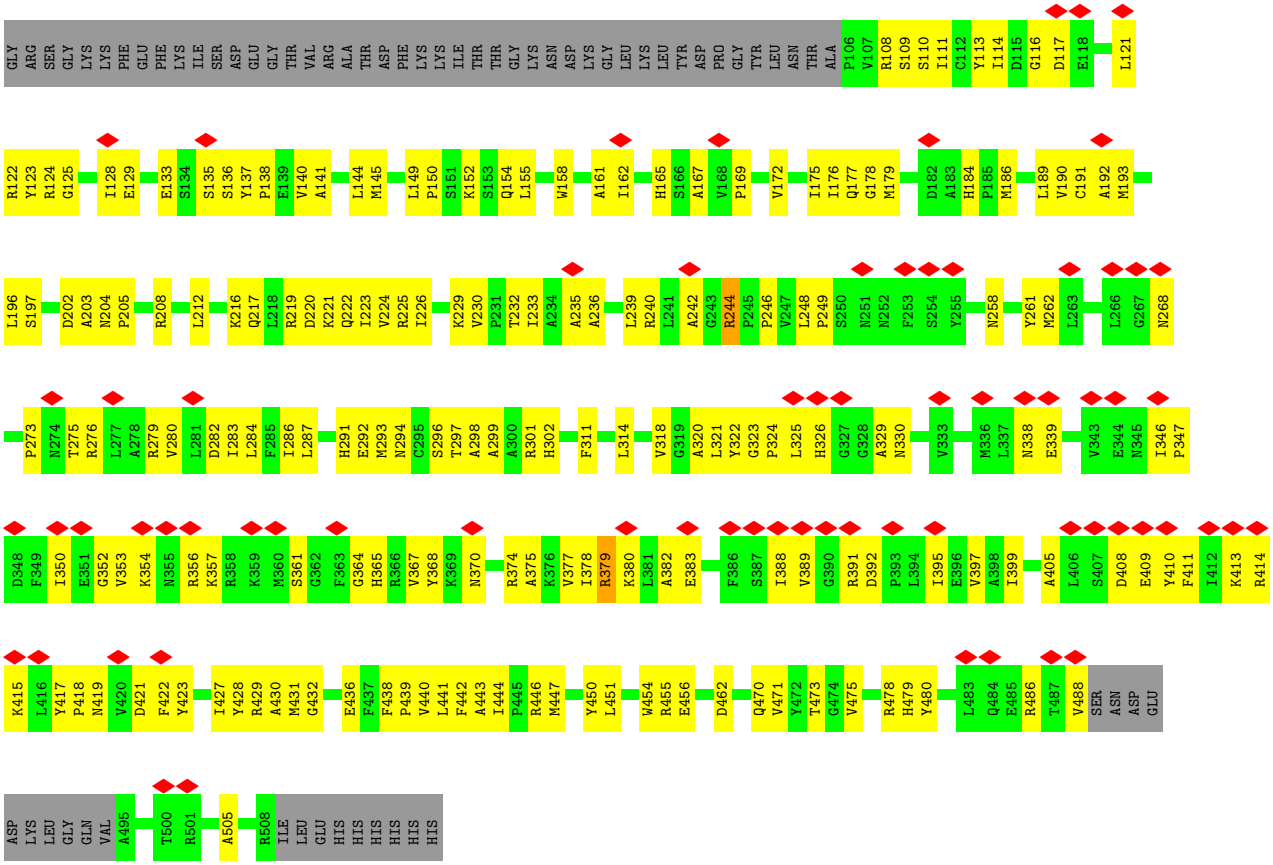
• Molecule 1: Citrate synthase

Chain G:



• Molecule 1: Citrate synthase

Chain H:


GLY ARG SER GLY LYS LYS PHE GLU PHE LYS ILE SER ASP GLU GLY THR VAL ARG ALA THR ASP PHE LYS LYS ILE THR THR GLY LYS ASN ASP LYS GLY LEU LYS LEU TYR ASP PRO GLY TYR LEU ASN THR ALA P106 V107 R108 S109 S110 I111 C112 Y113 I114 D115 G116 D117 E118 L121
R122 Y123 R124 G125 I128 E129 E133 S134 S135 S136 Y137 P138 E139 V140 A141 L144 M145 L149 P150 S151 K152 S153 Q154 L155 W158 A161 I162 H165 S166 A167 V168 P169 V172 I175 I176 Q177 G178 M179 D182 A183 H184 P185 M186 L189 V190 C191 A192 M193
L196 S197 D202 A203 N204 P205 R208 L212 K216 Q217 F218 R219 D220 K221 Q222 I223 V224 R225 I226 K229 V230 P231 T232 I233 A234 A235 A236 L239 R240 L241 A242 G243 R244 P245 P246 V247 L248 P249 S250 N251 N252 F253 S254 Y255 N258 Y261 M262 L263 L266 G267 N268
P273 N274 T275 R276 L277 A278 R279 V280 L281 D282 I283 L284 F285 I286 L287 H291 E292 M293 N294 C295 S296 T297 A298 A299 A300 R301 H302 F311 L314 V318 G319 A320 L321 Y322 G323 P324 L325 H326 G327 G328 A329 N330 V333 M336 L337 N338 E339 V343 E344 N345 I346 P347
D348 F349 I350 E351 G352 V353 K354 N355 R356 K357 R358 K359 M360 S361 G362 F363 G364 H365 R366 V367 Y368 K369 N370 R374 A375 K376 V377 I378 R379 K380 L381 A382 E383 F386 S387 I388 V389 G390 R391 D392 P393 L394 I395 E396 V397 A398 I399 A405 L406 S407 D408 E409 Y410 F411 I412 K413 R414
K415 L416 Y417 P418 N419 V420 D421 F422 Y423 I427 Y428 R429 A430 M431 G432 E436 F437 F438 P439 V440 L441 F442 A443 I444 P445 R446 M447 Y450 L451 W454 R455 E456 D462 Q470 V471 Y472 T473 G474 V475 R478 H479 Y480 L483 Q484 E485 R486 T487 V488 SER ASN ASP GLU
ASP LYS LEU GLY GLN VAL A495 T500 R501 A505 R508 ILE LEU GLU HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108304	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 ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.557	Depositor
Minimum map value	-1.651	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	218.0, 218.0, 218.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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	0.28	0/3280	0.51	0/4453
1	B	0.35	0/3288	0.56	0/4467
1	C	0.35	0/3297	0.53	0/4479
1	D	0.31	0/3488	0.52	0/4733
1	E	0.27	0/3188	0.54	0/4327
1	F	0.31	0/3166	0.55	0/4296
1	G	0.26	0/3142	0.52	0/4260
1	H	0.29	0/3166	0.55	0/4296
All	All	0.30	0/26015	0.54	0/35311

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3201	0	3150	121	0
1	B	3208	0	3150	164	0
1	C	3217	0	3158	154	0
1	D	3407	0	3358	137	0
1	E	3112	0	3066	131	0
1	F	3090	0	3056	178	0
1	G	3068	0	3037	116	0
1	H	3090	0	3056	158	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	25393	0	25031	1062	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 21.

All (1062) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:LYS:HB3	1:F:483:LEU:HD21	1.49	0.94
1:G:189:LEU:HD11	1:G:440:VAL:HG22	1.47	0.93
1:F:411:PHE:HD1	1:F:416:LEU:HB2	1.37	0.90
1:C:111:ILE:HA	1:C:124:ARG:HH21	1.37	0.88
1:D:475:VAL:HG11	1:D:478:ARG:HD3	1.56	0.86
1:F:411:PHE:CD1	1:F:416:LEU:HB2	2.10	0.86
1:H:242:ALA:HB3	1:H:244:ARG:HH12	1.42	0.84
1:G:386:PHE:HE1	1:G:391:ARG:HD3	1.41	0.83
1:H:365:HIS:HB2	1:H:368:TYR:HB2	1.60	0.81
1:C:168:VAL:HA	1:C:229:LYS:HZ1	1.47	0.80
1:C:480:TYR:HA	1:D:126:TYR:HE1	1.46	0.80
1:F:483:LEU:HA	1:F:486:ARG:HG2	1.63	0.80
1:F:248:LEU:HD12	1:F:249:PRO:HD2	1.62	0.80
1:C:467:ARG:HE	1:D:366:ARG:HH21	1.29	0.80
1:B:151:SER:H	1:B:154:GLN:NE2	1.79	0.79
1:C:177:GLN:HA	1:C:240:ARG:HE	1.47	0.78
1:F:118:GLU:HA	1:F:370:ASN:HB2	1.65	0.78
1:B:173:LEU:HA	1:B:176:ILE:HD12	1.64	0.78
1:H:208:ARG:HB2	1:H:212:LEU:HD11	1.65	0.78
1:C:293:MET:HE3	1:D:470:GLN:HB3	1.66	0.78
1:H:223:ILE:HD12	1:H:226:ILE:HD11	1.67	0.77
1:H:428:TYR:CE2	1:H:441:LEU:HD13	2.19	0.77
1:E:193:MET:HA	1:E:196:LEU:HD12	1.66	0.77
1:A:280:VAL:HG13	1:A:381:LEU:HD12	1.66	0.77
1:C:169:PRO:HD3	1:C:229:LYS:HZ1	1.49	0.77
1:H:172:VAL:HG21	1:H:192:ALA:HA	1.67	0.77
1:A:290:GLU:HB2	1:A:449:GLY:HA3	1.67	0.77
1:A:467:ARG:HH21	1:B:295:CYS:H	1.32	0.75
1:G:181:HIS:HA	1:G:240:ARG:HH12	1.52	0.75
1:D:137:TYR:HA	1:D:286:ILE:HD11	1.69	0.75
1:D:130:GLU:HG2	1:D:131:LEU:N	2.02	0.74
1:G:205:PRO:HA	1:G:212:LEU:HD21	1.69	0.74
1:A:162:ILE:HD13	1:A:224:VAL:HG13	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:ARG:HG3	1:F:147:GLY:HA2	1.70	0.73
1:F:249:PRO:HA	1:F:262:MET:SD	2.29	0.73
1:C:179:MET:O	1:C:240:ARG:NH2	2.22	0.72
1:C:199:PHE:HE1	1:D:180:PRO:HD3	1.54	0.72
1:H:176:ILE:HG22	1:H:177:GLN:H	1.54	0.72
1:D:394:LEU:HD12	1:D:429:ARG:HH12	1.55	0.71
1:E:179:MET:O	1:E:240:ARG:NH2	2.24	0.71
1:D:331:GLU:HB2	1:D:335:LYS:NZ	2.05	0.71
1:E:481:THR:O	1:E:486:ARG:NH2	2.24	0.71
1:A:199:PHE:HE1	1:B:179:MET:HG3	1.55	0.70
1:C:388:ILE:HG23	1:C:389:VAL:HG13	1.72	0.70
1:B:426:LEU:HD23	1:B:429:ARG:HH22	1.57	0.70
1:D:382:ALA:HA	1:D:427:ILE:HD11	1.73	0.70
1:G:189:LEU:HD22	1:G:234:ALA:HB1	1.71	0.70
1:E:349:PHE:HA	1:E:358:ARG:HD2	1.74	0.69
1:H:179:MET:O	1:H:240:ARG:NH2	2.25	0.69
1:D:179:MET:O	1:D:240:ARG:NH2	2.25	0.69
1:B:486:ARG:HG3	1:B:486:ARG:HH11	1.58	0.69
1:E:239:LEU:HD11	1:E:246:PRO:HA	1.74	0.69
1:C:274:ASN:HD22	1:C:277:LEU:HD23	1.57	0.69
1:C:167:ALA:O	1:C:229:LYS:NZ	2.24	0.69
1:C:467:ARG:HE	1:D:366:ARG:NH2	1.90	0.69
1:G:155:LEU:HD12	1:H:486:ARG:HH22	1.57	0.69
1:F:173:LEU:O	1:F:177:GLN:NE2	2.26	0.69
1:D:394:LEU:HB2	1:D:429:ARG:HH22	1.58	0.68
1:C:280:VAL:HG13	1:C:381:LEU:HD21	1.74	0.68
1:H:225:ARG:O	1:H:229:LYS:N	2.26	0.68
1:H:192:ALA:HB1	1:H:233:ILE:HG21	1.76	0.68
1:F:396:GLU:HA	1:F:399:ILE:HG12	1.76	0.68
1:H:320:ALA:O	1:H:326:HIS:NE2	2.27	0.68
1:D:275:THR:HG23	1:D:276:ARG:HE	1.58	0.68
1:F:133:GLU:O	1:F:279:ARG:NH2	2.26	0.68
1:G:435:THR:O	1:G:438:PHE:HB3	1.93	0.68
1:G:451:LEU:O	1:G:454:TRP:HB3	1.94	0.68
1:C:225:ARG:O	1:C:229:LYS:HG2	1.93	0.68
1:D:83:LYS:HD2	1:D:93:GLY:HA3	1.74	0.68
1:E:149:LEU:HD12	1:F:486:ARG:CZ	2.24	0.68
1:F:483:LEU:CA	1:F:486:ARG:HG2	2.24	0.67
1:H:301:ARG:NH2	1:H:456:GLU:OE1	2.25	0.67
1:D:122:ARG:HA	1:D:126:TYR:O	1.94	0.67
1:E:152:LYS:HE2	1:F:486:ARG:HB2	1.74	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:380:LYS:O	1:H:383:GLU:HG3	1.95	0.67
1:H:391:ARG:HA	1:H:395:ILE:HD11	1.74	0.67
1:B:230:VAL:O	1:B:231:PRO:C	2.27	0.67
1:A:303:LEU:HD12	1:A:308:VAL:HG21	1.77	0.67
1:D:481:THR:O	1:D:486:ARG:NH2	2.28	0.67
1:H:379:ARG:O	1:H:382:ALA:HB3	1.94	0.67
1:F:365:HIS:CE1	1:F:367:VAL:HG22	2.30	0.67
1:H:122:ARG:HD3	1:H:125:GLY:HA2	1.77	0.67
1:B:363:PHE:HB3	1:B:416:LEU:HB3	1.76	0.66
1:G:324:PRO:HA	1:G:328:GLY:H	1.60	0.66
1:H:229:LYS:NZ	1:H:232:THR:OG1	2.27	0.66
1:B:179:MET:O	1:B:240:ARG:NH1	2.23	0.66
1:B:411:PHE:HA	1:B:416:LEU:HD12	1.78	0.66
1:F:218:LEU:O	1:F:222:GLN:NE2	2.29	0.66
1:E:204:ASN:ND2	1:F:322:TYR:OH	2.29	0.66
1:A:467:ARG:NH2	1:B:295:CYS:SG	2.69	0.66
1:B:466:MET:N	1:B:466:MET:SD	2.69	0.65
1:F:483:LEU:HA	1:F:486:ARG:NE	2.12	0.65
1:D:225:ARG:O	1:D:229:LYS:HG2	1.96	0.65
1:F:363:PHE:HB3	1:F:416:LEU:HB3	1.79	0.65
1:G:150:PRO:O	1:H:486:ARG:NH1	2.30	0.65
1:D:257:GLU:HG3	1:D:278:ALA:HB1	1.77	0.65
1:H:275:THR:OG1	1:H:276:ARG:NH1	2.29	0.65
1:B:483:LEU:O	1:B:486:ARG:HB3	1.97	0.65
1:B:95:LYS:HG3	1:B:97:TYR:H	1.60	0.65
1:A:386:PHE:HB3	1:A:391:ARG:HH11	1.62	0.65
1:E:486:ARG:HB2	1:F:152:LYS:HE3	1.78	0.64
1:H:176:ILE:HG22	1:H:240:ARG:HG3	1.77	0.64
1:A:483:LEU:HD22	1:A:486:ARG:HH21	1.62	0.64
1:B:143:LEU:HD12	1:B:149:LEU:HB3	1.79	0.64
1:F:310:VAL:O	1:F:313:ALA:HB3	1.97	0.64
1:B:162:ILE:HD13	1:B:224:VAL:HG13	1.78	0.64
1:F:170:GLN:N	1:F:170:GLN:OE1	2.30	0.64
1:G:170:GLN:OE1	1:G:170:GLN:N	2.31	0.64
1:A:483:LEU:O	1:A:486:ARG:HB2	1.98	0.64
1:C:108:ARG:NH2	1:C:462:ASP:OD2	2.29	0.64
1:G:163:SER:HB2	1:G:251:ASN:HB2	1.77	0.64
1:H:197:SER:HA	1:H:311:PHE:CD2	2.33	0.64
1:G:472:TYR:HA	1:H:109:SER:HB3	1.80	0.63
1:F:309:ASP:OD2	1:F:311:PHE:HB2	1.99	0.63
1:H:172:VAL:HG23	1:H:175:ILE:HD12	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:204:ASN:O	1:H:208:ARG:NH2	2.30	0.63
1:G:205:PRO:HB2	1:H:324:PRO:HD3	1.80	0.62
1:B:435:THR:HA	1:B:438:PHE:CE2	2.34	0.62
1:C:210:GLN:OE1	1:C:210:GLN:N	2.28	0.62
1:F:371:TYR:HD2	1:F:373:PRO:HD3	1.65	0.62
1:G:114:ILE:HD11	1:G:292:GLU:H	1.63	0.62
1:C:346:ILE:HG22	1:C:401:LEU:HD23	1.80	0.62
1:B:281:LEU:HD23	1:B:284:LEU:HD12	1.80	0.62
1:E:337:LEU:HG	1:E:394:LEU:HD22	1.81	0.62
1:G:225:ARG:O	1:G:229:LYS:NZ	2.31	0.62
1:H:330:ASN:HD21	1:H:422:PHE:HA	1.65	0.62
1:B:352:GLY:HA3	1:B:358:ARG:HE	1.64	0.62
1:C:151:SER:H	1:C:154:GLN:HB2	1.64	0.62
1:E:207:LEU:HD12	1:E:208:ARG:HG3	1.81	0.62
1:A:374:ARG:HB2	1:A:420:VAL:HG11	1.82	0.62
1:C:274:ASN:HD21	1:C:276:ARG:HB2	1.63	0.62
1:E:112:CYS:HG	1:E:123:TYR:HD1	1.47	0.62
1:E:179:MET:SD	1:E:180:PRO:HD2	2.39	0.62
1:F:223:ILE:HG12	1:F:451:LEU:HD22	1.79	0.62
1:G:108:ARG:HA	1:H:470:GLN:HA	1.80	0.62
1:A:179:MET:O	1:A:240:ARG:NH2	2.25	0.62
1:B:112:CYS:SG	1:B:113:TYR:N	2.72	0.62
1:G:343:VAL:O	1:G:346:ILE:HG13	2.00	0.61
1:A:337:LEU:HD21	1:A:394:LEU:HB3	1.82	0.61
1:D:258:ASN:O	1:D:262:MET:HG3	1.99	0.61
1:B:176:ILE:HG22	1:B:240:ARG:HD2	1.81	0.61
1:G:176:ILE:O	1:G:240:ARG:NE	2.33	0.61
1:A:176:ILE:O	1:A:240:ARG:NH1	2.34	0.61
1:F:388:ILE:HG23	1:F:389:VAL:HG23	1.83	0.61
1:H:258:ASN:O	1:H:262:MET:HG3	2.01	0.61
1:B:222:GLN:OE1	1:B:225:ARG:NH1	2.33	0.61
1:C:503:ALA:O	1:C:505:ARG:N	2.31	0.61
1:D:238:TYR:CD2	1:D:263:LEU:HD11	2.36	0.61
1:E:453:HIS:O	1:E:457:SER:N	2.28	0.61
1:F:223:ILE:HG23	1:F:451:LEU:HD13	1.82	0.61
1:G:293:MET:SD	1:G:366:ARG:NH2	2.74	0.61
1:A:186:MET:HG2	1:A:322:TYR:CE2	2.36	0.60
1:B:115:ASP:HB3	1:B:120:ILE:HB	1.83	0.60
1:B:321:LEU:HD12	1:B:326:HIS:HB3	1.83	0.60
1:D:254:SER:O	1:D:258:ASN:N	2.28	0.60
1:D:378:ILE:HD12	1:D:423:TYR:HB2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LEU:HD22	1:A:128:ILE:HD13	1.82	0.60
1:F:385:VAL:HA	1:F:388:ILE:HG22	1.83	0.60
1:D:126:TYR:HB3	1:D:131:LEU:HD11	1.84	0.60
1:E:235:ALA:HB3	1:E:262:MET:HG3	1.84	0.60
1:C:346:ILE:HG13	1:C:347:PRO:HD3	1.84	0.60
1:H:389:VAL:HG21	1:H:430:ALA:HB1	1.83	0.60
1:D:162:ILE:HD13	1:D:224:VAL:HG13	1.83	0.60
1:A:210:GLN:HE21	1:B:325:LEU:HG	1.66	0.60
1:C:168:VAL:HA	1:C:229:LYS:NZ	2.16	0.60
1:E:238:TYR:HB2	1:E:437:PHE:CZ	2.37	0.60
1:E:303:LEU:HD13	1:E:313:ALA:HA	1.82	0.60
1:C:131:LEU:HB3	1:C:286:ILE:HD11	1.84	0.60
1:G:351:GLU:HA	1:G:354:LYS:HD3	1.83	0.60
1:C:102:LEU:O	1:D:469:GLN:NE2	2.25	0.59
1:E:470:GLN:NE2	1:F:292:GLU:OE2	2.35	0.59
1:F:167:ALA:HA	1:F:249:PRO:HG3	1.84	0.59
1:B:330:ASN:OD1	1:B:331:GLU:N	2.35	0.59
1:B:391:ARG:HH21	1:B:395:ILE:HG22	1.67	0.59
1:A:204:ASN:ND2	1:B:322:TYR:OH	2.24	0.59
1:H:110:SER:O	1:H:124:ARG:NH1	2.35	0.59
1:H:189:LEU:O	1:H:193:MET:HG3	2.03	0.59
1:D:331:GLU:HB2	1:D:335:LYS:HZ1	1.67	0.59
1:G:261:TYR:OH	1:G:269:ARG:O	2.21	0.59
1:H:161:ALA:O	1:H:165:HIS:ND1	2.35	0.59
1:B:292:GLU:O	1:B:294:ASN:ND2	2.35	0.59
1:C:103:ASN:ND2	1:D:79:ALA:O	2.36	0.59
1:C:348:ASP:OD1	1:C:349:PHE:N	2.36	0.58
1:C:476:TRP:HD1	1:C:477:LEU:H	1.51	0.58
1:A:152:LYS:HZ2	1:B:486:ARG:HD2	1.66	0.58
1:C:126:TYR:HB3	1:C:131:LEU:HD11	1.85	0.58
1:D:124:ARG:HB2	1:D:143:LEU:HD21	1.85	0.58
1:H:236:ALA:HA	1:H:239:LEU:HB2	1.86	0.58
1:A:239:LEU:HD11	1:A:244:ARG:HB2	1.86	0.58
1:C:502:ASN:C	1:C:504:THR:N	2.55	0.58
1:G:143:LEU:O	1:G:147:GLY:N	2.35	0.58
1:A:223:ILE:HD13	1:A:451:LEU:HD12	1.85	0.58
1:C:337:LEU:HB3	1:C:394:LEU:HD22	1.84	0.58
1:D:425:GLY:HA2	1:D:438:PHE:HE2	1.68	0.58
1:E:351:GLU:HA	1:E:354:LYS:HD2	1.85	0.58
1:F:213:TYR:O	1:F:219:ARG:NH2	2.36	0.58
1:G:386:PHE:CE1	1:G:391:ARG:HD3	2.30	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:VAL:HG13	1:A:173:LEU:HD11	1.84	0.58
1:D:374:ARG:O	1:D:378:ILE:HG12	2.03	0.58
1:F:377:VAL:HA	1:F:380:LYS:HE3	1.85	0.58
1:C:111:ILE:HA	1:C:124:ARG:NH2	2.16	0.58
1:H:165:HIS:HB3	1:H:225:ARG:HG2	1.86	0.58
1:H:395:ILE:O	1:H:399:ILE:HG13	2.04	0.58
1:A:466:MET:HB2	1:B:295:CYS:SG	2.44	0.58
1:C:190:VAL:HG22	1:C:318:VAL:HG13	1.84	0.58
1:C:197:SER:HA	1:C:311:PHE:HD2	1.68	0.58
1:A:483:LEU:HD22	1:A:486:ARG:NH2	2.18	0.57
1:G:205:PRO:HB3	1:G:212:LEU:HD11	1.86	0.57
1:B:483:LEU:H	1:B:483:LEU:HD13	1.69	0.57
1:G:433:PHE:HD2	1:G:441:LEU:HD21	1.69	0.57
1:A:332:ALA:HA	1:A:335:LYS:HE2	1.85	0.57
1:E:279:ARG:NH1	1:E:384:GLU:OE2	2.37	0.57
1:C:142:TYR:HD1	1:C:158:TRP:CE2	2.23	0.57
1:E:204:ASN:OD1	1:E:208:ARG:NH1	2.36	0.57
1:B:230:VAL:HB	1:B:231:PRO:HD3	1.86	0.57
1:E:204:ASN:O	1:E:208:ARG:NH1	2.37	0.57
1:F:194:SER:HA	1:F:312:THR:HG22	1.86	0.57
1:F:280:VAL:HG23	1:F:381:LEU:HD13	1.87	0.57
1:A:484:GLN:N	1:A:484:GLN:OE1	2.38	0.57
1:F:314:LEU:O	1:F:315:ALA:C	2.41	0.57
1:C:122:ARG:HD2	1:D:477:LEU:HD13	1.87	0.57
1:C:302:HIS:CE1	1:C:466:MET:HG3	2.40	0.57
1:H:226:ILE:HG22	1:H:311:PHE:CE1	2.40	0.57
1:B:480:TYR:OH	1:B:483:LEU:HB3	2.05	0.57
1:E:259:PHE:O	1:E:263:LEU:N	2.36	0.57
1:B:232:THR:O	1:B:235:ALA:HB3	2.05	0.56
1:D:192:ALA:HB1	1:D:233:ILE:HD13	1.87	0.56
1:G:186:MET:HA	1:G:189:LEU:HD12	1.87	0.56
1:B:234:ALA:O	1:B:235:ALA:C	2.42	0.56
1:C:173:LEU:HA	1:C:176:ILE:HG22	1.85	0.56
1:C:466:MET:SD	1:C:466:MET:N	2.78	0.56
1:D:172:VAL:HG21	1:D:196:LEU:HD22	1.86	0.56
1:F:225:ARG:O	1:F:229:LYS:HG2	2.05	0.56
1:H:111:ILE:HD11	1:H:144:LEU:HB3	1.86	0.56
1:C:274:ASN:OD1	1:C:275:THR:N	2.38	0.56
1:D:111:ILE:HA	1:D:124:ARG:HD3	1.86	0.56
1:F:123:TYR:HB3	1:F:144:LEU:HD13	1.88	0.56
1:B:136:SER:N	1:B:139:GLU:OE1	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:TYR:O	1:C:219:ARG:NH2	2.37	0.56
1:E:189:LEU:HD13	1:E:233:ILE:HG22	1.87	0.56
1:G:287:LEU:HD13	1:G:378:ILE:HG22	1.87	0.56
1:B:133:GLU:O	1:B:279:ARG:NH2	2.39	0.56
1:B:235:ALA:O	1:B:236:ALA:C	2.41	0.56
1:D:385:VAL:HA	1:D:388:ILE:HG22	1.88	0.56
1:G:218:LEU:HA	1:G:221:LYS:HE2	1.88	0.56
1:D:385:VAL:O	1:D:389:VAL:HG12	2.06	0.56
1:H:135:SER:OG	1:H:136:SER:N	2.38	0.56
1:C:469:GLN:NE2	1:D:102:LEU:O	2.37	0.56
1:F:316:GLY:O	1:F:319:GLY:N	2.39	0.56
1:C:350:ILE:O	1:C:354:LYS:N	2.33	0.56
1:F:173:LEU:HA	1:F:176:ILE:HG22	1.87	0.56
1:G:447:MET:O	1:G:450:TYR:HB2	2.06	0.56
1:B:482:PRO:O	1:B:486:ARG:N	2.39	0.55
1:F:427:ILE:O	1:F:431:MET:HG2	2.06	0.55
1:H:145:MET:HE3	1:H:455:ARG:HB2	1.88	0.55
1:G:111:ILE:HG21	1:G:453:HIS:CE1	2.41	0.55
1:G:239:LEU:O	1:G:243:GLY:N	2.34	0.55
1:A:116:GLY:HA3	1:A:367:VAL:HG12	1.87	0.55
1:F:140:VAL:HG11	1:F:286:ILE:HD11	1.87	0.55
1:H:408:ASP:HB2	1:H:411:PHE:HD2	1.70	0.55
1:A:230:VAL:HG21	1:A:447:MET:SD	2.46	0.55
1:C:145:MET:O	1:C:147:GLY:N	2.39	0.55
1:C:244:ARG:HG3	1:C:245:PRO:HD2	1.89	0.55
1:A:219:ARG:O	1:A:223:ILE:HG12	2.07	0.55
1:B:423:TYR:HA	1:B:426:LEU:HD12	1.88	0.55
1:C:169:PRO:HD3	1:C:229:LYS:NZ	2.18	0.55
1:D:87:THR:H	1:D:91:ASP:HB3	1.70	0.55
1:F:114:ILE:HD11	1:F:292:GLU:H	1.71	0.55
1:F:118:GLU:HA	1:F:370:ASN:CB	2.34	0.55
1:F:171:GLY:O	1:F:175:ILE:HG12	2.06	0.55
1:G:152:LYS:HE2	1:H:488:VAL:H	1.71	0.55
1:C:108:ARG:HG2	1:D:471:VAL:HB	1.89	0.55
1:C:284:LEU:HB3	1:C:428:TYR:OH	2.05	0.55
1:F:111:ILE:HG21	1:F:453:HIS:CE1	2.42	0.55
1:H:117:ASP:O	1:H:370:ASN:ND2	2.40	0.55
1:C:301:ARG:NH2	1:C:456:GLU:OE2	2.38	0.55
1:F:257:GLU:OE2	1:F:257:GLU:N	2.29	0.55
1:E:215:SER:O	1:E:219:ARG:NE	2.40	0.55
1:B:208:ARG:NH2	1:B:211:ASP:OD2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:GLU:OE1	1:D:436:GLU:N	2.29	0.55
1:E:274:ASN:ND2	1:H:505:ALA:O	2.34	0.55
1:H:392:ASP:OD2	1:H:429:ARG:NH1	2.40	0.55
1:E:185:PRO:O	1:E:188:VAL:HB	2.07	0.54
1:F:483:LEU:O	1:F:486:ARG:HG2	2.07	0.54
1:H:314:LEU:HD21	1:H:447:MET:SD	2.47	0.54
1:A:151:SER:HA	1:B:486:ARG:HD3	1.88	0.54
1:H:301:ARG:HH21	1:H:456:GLU:HB3	1.72	0.54
1:A:111:ILE:HD12	1:A:124:ARG:HE	1.71	0.54
1:D:462:ASP:O	1:D:464:LYS:NZ	2.33	0.54
1:E:465:ILE:HG13	1:F:295:CYS:HB3	1.90	0.54
1:F:197:SER:HA	1:F:311:PHE:CG	2.42	0.54
1:A:213:TYR:OH	1:A:309:ASP:OD1	2.24	0.54
1:B:158:TRP:O	1:B:162:ILE:HG12	2.08	0.54
1:C:348:ASP:O	1:C:352:GLY:N	2.32	0.54
1:G:346:ILE:HD11	1:G:400:ALA:HB1	1.90	0.54
1:A:347:PRO:HA	1:A:350:ILE:HG22	1.88	0.54
1:B:424:SER:O	1:B:428:TYR:HD1	1.89	0.54
1:C:382:ALA:HB1	1:C:386:PHE:HE2	1.72	0.54
1:C:507:ARG:O	1:C:509:ALA:N	2.35	0.54
1:E:103:ASN:HA	1:F:469:GLN:HG2	1.89	0.54
1:F:219:ARG:HH21	1:F:458:LEU:HD13	1.72	0.54
1:H:196:LEU:HD11	1:H:233:ILE:HG13	1.89	0.54
1:A:152:LYS:HE2	1:B:484:GLN:HA	1.89	0.54
1:A:171:GLY:HA3	1:A:199:PHE:HE2	1.73	0.54
1:B:428:TYR:CE2	1:B:441:LEU:HD22	2.42	0.54
1:C:175:ILE:HD12	1:D:175:ILE:HG23	1.88	0.54
1:D:378:ILE:HA	1:D:381:LEU:HD12	1.90	0.54
1:C:351:GLU:O	1:C:355:ASN:N	2.39	0.54
1:D:330:ASN:HB3	1:D:421:ASP:OD1	2.08	0.54
1:F:160:PHE:O	1:F:164:GLN:HG2	2.08	0.54
1:F:250:SER:OG	1:F:258:ASN:OD1	2.26	0.54
1:B:439:PRO:HA	1:B:442:PHE:HD2	1.73	0.53
1:E:300:ALA:HA	1:E:303:LEU:HD12	1.90	0.53
1:G:186:MET:HG3	1:G:322:TYR:HD2	1.73	0.53
1:D:379:ARG:NH2	1:D:383:GLU:OE2	2.40	0.53
1:G:145:MET:HG3	1:G:158:TRP:HH2	1.73	0.53
1:C:436:GLU:OE2	1:C:436:GLU:N	2.36	0.53
1:D:309:ASP:OD1	1:D:312:THR:HG22	2.08	0.53
1:H:186:MET:O	1:H:189:LEU:HG	2.09	0.53
1:A:219:ARG:HD3	1:A:458:LEU:HD22	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:THR:OG1	1:B:345:ASN:OD1	2.20	0.53
1:C:115:ASP:O	1:C:119:GLY:N	2.42	0.53
1:E:172:VAL:O	1:E:175:ILE:HG22	2.09	0.53
1:F:312:THR:O	1:F:313:ALA:C	2.46	0.53
1:C:199:PHE:CE1	1:D:180:PRO:HD3	2.39	0.53
1:G:453:HIS:O	1:G:457:SER:N	2.37	0.53
1:H:108:ARG:NH1	1:H:462:ASP:OD2	2.41	0.53
1:H:370:ASN:O	1:H:415:LYS:NZ	2.32	0.53
1:H:375:ALA:O	1:H:379:ARG:N	2.37	0.53
1:B:140:VAL:O	1:B:144:LEU:HG	2.08	0.53
1:F:168:VAL:HG23	1:F:229:LYS:HD2	1.91	0.53
1:G:202:ASP:OD2	1:G:225:ARG:NE	2.42	0.53
1:H:189:LEU:HD22	1:H:440:VAL:HG23	1.91	0.53
1:B:229:LYS:O	1:B:230:VAL:C	2.45	0.53
1:C:110:SER:HA	1:D:472:TYR:CE1	2.44	0.53
1:C:140:VAL:HG11	1:C:286:ILE:HG13	1.91	0.53
1:A:510:GLY:O	1:F:274:ASN:N	2.42	0.53
1:C:472:TYR:OH	1:C:475:VAL:O	2.27	0.53
1:B:485:GLU:O	1:B:486:ARG:C	2.46	0.53
1:C:295:CYS:SG	1:D:302:HIS:HB3	2.49	0.53
1:E:186:MET:HE3	1:E:318:VAL:HG22	1.90	0.52
1:A:152:LYS:HE3	1:B:486:ARG:HD2	1.90	0.52
1:D:429:ARG:O	1:D:432:GLY:N	2.41	0.52
1:E:253:PHE:O	1:E:258:ASN:ND2	2.42	0.52
1:H:217:GLN:OE1	1:H:217:GLN:N	2.39	0.52
1:B:205:PRO:O	1:B:209:GLY:N	2.41	0.52
1:B:280:VAL:HG23	1:B:381:LEU:HD13	1.91	0.52
1:C:375:ALA:HA	1:C:378:ILE:HG22	1.91	0.52
1:E:244:ARG:HD3	1:E:245:PRO:O	2.09	0.52
1:E:282:ASP:O	1:E:286:ILE:HG12	2.10	0.52
1:G:186:MET:HG3	1:G:322:TYR:CD2	2.44	0.52
1:G:348:ASP:OD1	1:G:348:ASP:N	2.41	0.52
1:H:284:LEU:HB3	1:H:428:TYR:OH	2.09	0.52
1:C:110:SER:HB2	1:D:473:THR:OG1	2.10	0.52
1:D:126:TYR:CE2	1:D:143:LEU:HD11	2.43	0.52
1:D:135:SER:OG	1:D:136:SER:N	2.40	0.52
1:G:254:SER:O	1:G:258:ASN:N	2.36	0.52
1:C:502:ASN:C	1:C:504:THR:H	2.12	0.52
1:D:483:LEU:HA	1:D:486:ARG:NE	2.25	0.52
1:E:330:ASN:OD1	1:E:331:GLU:N	2.40	0.52
1:B:337:LEU:HD13	1:B:398:ALA:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:PRO:O	1:D:208:ARG:NH1	2.42	0.52
1:F:261:TYR:OH	1:F:269:ARG:O	2.27	0.52
1:G:184:HIS:CE1	1:G:186:MET:HB2	2.45	0.52
1:H:282:ASP:O	1:H:286:ILE:HG12	2.09	0.52
1:A:105:ALA:HA	1:B:469:GLN:HB2	1.92	0.52
1:B:482:PRO:HB2	1:B:485:GLU:HB3	1.91	0.52
1:B:483:LEU:C	1:B:486:ARG:HB3	2.30	0.52
1:E:187:GLY:HA2	1:E:190:VAL:HG22	1.91	0.52
1:E:280:VAL:HG12	1:E:381:LEU:HG	1.92	0.52
1:C:279:ARG:HH12	1:C:283:ILE:HG12	1.74	0.52
1:C:285:PHE:HE1	1:C:444:ILE:HB	1.74	0.52
1:C:337:LEU:HD11	1:C:398:ALA:HB2	1.91	0.52
1:C:467:ARG:O	1:C:467:ARG:HG2	2.10	0.52
1:H:428:TYR:HE2	1:H:441:LEU:HD13	1.72	0.52
1:A:481:THR:HG23	1:A:486:ARG:CZ	2.39	0.52
1:C:126:TYR:CB	1:C:131:LEU:HD11	2.40	0.52
1:A:340:ILE:HG13	1:A:346:ILE:HG12	1.92	0.52
1:G:383:GLU:O	1:G:386:PHE:HB3	2.10	0.52
1:H:226:ILE:HG22	1:H:311:PHE:HE1	1.75	0.52
1:A:101:TYR:HE1	1:B:106:PRO:HB3	1.75	0.51
1:D:331:GLU:HB2	1:D:335:LYS:HZ3	1.73	0.51
1:F:208:ARG:HG2	1:F:212:LEU:HD13	1.92	0.51
1:H:446:ARG:NE	1:H:450:TYR:OH	2.40	0.51
1:C:476:TRP:O	1:C:477:LEU:C	2.47	0.51
1:F:309:ASP:O	1:F:313:ALA:HB2	2.10	0.51
1:B:233:ILE:O	1:B:234:ALA:C	2.47	0.51
1:F:363:PHE:CB	1:F:416:LEU:HB3	2.40	0.51
1:C:126:TYR:CD2	1:C:143:LEU:HD21	2.46	0.51
1:G:144:LEU:HD12	1:G:145:MET:HE2	1.92	0.51
1:H:186:MET:HG3	1:H:322:TYR:HB2	1.91	0.51
1:C:340:ILE:HG12	1:C:401:LEU:HD21	1.93	0.51
1:C:424:SER:O	1:C:428:TYR:HD2	1.94	0.51
1:B:287:LEU:HD12	1:B:374:ARG:HD2	1.92	0.51
1:H:162:ILE:HG22	1:H:224:VAL:HG13	1.91	0.51
1:D:121:LEU:HD23	1:D:128:ILE:HG12	1.92	0.51
1:G:151:SER:H	1:G:154:GLN:HB2	1.76	0.51
1:H:178:GLY:H	1:H:240:ARG:HE	1.59	0.51
1:B:364:GLY:O	1:B:366:ARG:NH1	2.44	0.51
1:B:392:ASP:OD1	1:B:395:ILE:N	2.35	0.51
1:A:175:ILE:HD11	1:B:178:GLY:HA3	1.93	0.50
1:B:230:VAL:HB	1:B:231:PRO:CD	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ARG:NH1	1:C:122:ARG:HB2	2.26	0.50
1:E:486:ARG:O	1:F:152:LYS:NZ	2.37	0.50
1:A:365:HIS:CE1	1:A:367:VAL:HB	2.45	0.50
1:B:254:SER:O	1:B:258:ASN:N	2.40	0.50
1:C:396:GLU:OE2	1:C:396:GLU:N	2.30	0.50
1:E:225:ARG:O	1:E:229:LYS:HG2	2.10	0.50
1:G:298:ALA:O	1:G:301:ARG:HG3	2.11	0.50
1:E:423:TYR:O	1:E:427:ILE:HG12	2.12	0.50
1:C:230:VAL:HG21	1:C:447:MET:HG3	1.94	0.50
1:F:283:ILE:HA	1:F:286:ILE:HG22	1.92	0.50
1:F:350:ILE:O	1:F:354:LYS:NZ	2.43	0.50
1:H:203:ALA:O	1:H:204:ASN:ND2	2.45	0.50
1:H:296:SER:HA	1:H:299:ALA:HB3	1.93	0.50
1:A:244:ARG:HH12	1:A:266:LEU:HA	1.76	0.50
1:B:365:HIS:HB2	1:B:368:TYR:HB2	1.93	0.50
1:B:428:TYR:HE2	1:B:441:LEU:HD22	1.75	0.50
1:D:349:PHE:O	1:D:358:ARG:HD2	2.11	0.50
1:F:239:LEU:HD22	1:F:246:PRO:HA	1.93	0.50
1:H:353:VAL:HG22	1:H:410:TYR:CE2	2.46	0.50
1:A:201:PRO:O	1:A:208:ARG:NH2	2.45	0.50
1:C:111:ILE:HD12	1:C:453:HIS:CE1	2.46	0.50
1:F:208:ARG:HB3	1:F:212:LEU:HB2	1.92	0.50
1:G:302:HIS:O	1:G:305:SER:OG	2.22	0.50
1:D:218:LEU:O	1:D:222:GLN:HG2	2.12	0.50
1:F:347:PRO:O	1:F:350:ILE:HB	2.11	0.50
1:A:96:LEU:O	1:B:105:ALA:N	2.35	0.50
1:B:333:VAL:O	1:B:337:LEU:HG	2.12	0.50
1:B:467:ARG:HH12	1:B:469:GLN:HA	1.77	0.50
1:G:450:TYR:O	1:G:453:HIS:HB2	2.12	0.50
1:D:151:SER:H	1:D:154:GLN:HB2	1.77	0.49
1:F:364:GLY:N	1:F:417:TYR:O	2.44	0.49
1:G:203:ALA:HB1	1:G:309:ASP:HB2	1.94	0.49
1:B:483:LEU:O	1:B:486:ARG:NE	2.45	0.49
1:C:109:SER:OG	1:C:110:SER:N	2.45	0.49
1:C:478:ARG:HB3	1:D:125:GLY:O	2.11	0.49
1:F:312:THR:HA	1:F:315:ALA:HB2	1.93	0.49
1:A:509:ALA:O	1:F:277:LEU:HG	2.12	0.49
1:B:294:ASN:H	1:B:297:THR:HB	1.77	0.49
1:B:414:ARG:HB2	1:B:416:LEU:HG	1.94	0.49
1:C:391:ARG:HA	1:C:395:ILE:HD12	1.93	0.49
1:C:502:ASN:O	1:C:504:THR:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:LEU:HA	1:E:280:VAL:HG22	1.94	0.49
1:A:253:PHE:HB3	1:A:257:GLU:HB3	1.95	0.49
1:B:213:TYR:OH	1:B:310:VAL:N	2.40	0.49
1:C:176:ILE:O	1:C:240:ARG:NE	2.45	0.49
1:C:478:ARG:CG	1:C:479:HIS:H	2.25	0.49
1:C:480:TYR:CG	1:C:481:THR:N	2.80	0.49
1:A:121:LEU:O	1:A:128:ILE:N	2.46	0.49
1:B:115:ASP:O	1:B:119:GLY:N	2.45	0.49
1:B:117:ASP:O	1:B:370:ASN:ND2	2.38	0.49
1:D:409:GLU:HG2	1:D:413:LYS:CE	2.42	0.49
1:F:294:ASN:N	1:F:297:THR:OG1	2.35	0.49
1:G:108:ARG:HB3	1:H:471:VAL:HG22	1.94	0.49
1:G:130:GLU:O	1:G:134:SER:OG	2.31	0.49
1:B:223:ILE:HG23	1:B:451:LEU:HD23	1.95	0.49
1:B:258:ASN:O	1:B:262:MET:HE3	2.13	0.49
1:B:438:PHE:HB3	1:B:442:PHE:HE2	1.77	0.49
1:B:467:ARG:NH1	1:B:469:GLN:OE1	2.45	0.49
1:B:482:PRO:HD2	1:B:485:GLU:HG2	1.95	0.49
1:D:352:GLY:HA2	1:D:357:LYS:NZ	2.28	0.49
1:F:417:TYR:O	1:F:418:PRO:C	2.51	0.49
1:A:348:ASP:OD1	1:A:349:PHE:N	2.46	0.49
1:B:260:LEU:HD13	1:B:281:LEU:HD12	1.94	0.49
1:E:257:GLU:OE1	1:E:257:GLU:N	2.46	0.49
1:E:472:TYR:HA	1:F:110:SER:HA	1.94	0.49
1:F:115:ASP:HB2	1:F:122:ARG:HH21	1.77	0.49
1:F:238:TYR:CD2	1:F:263:LEU:HD11	2.47	0.49
1:G:374:ARG:HA	1:G:377:VAL:HG22	1.94	0.49
1:H:330:ASN:ND2	1:H:422:PHE:HA	2.28	0.49
1:H:443:ALA:O	1:H:447:MET:HG3	2.12	0.49
1:A:276:ARG:NH1	1:A:388:ILE:HD13	2.28	0.49
1:C:274:ASN:ND2	1:C:276:ARG:HB2	2.27	0.49
1:E:151:SER:O	1:E:154:GLN:HB2	2.13	0.49
1:E:261:TYR:HA	1:E:271:TYR:HE2	1.78	0.49
1:E:343:VAL:HA	1:E:346:ILE:HG12	1.94	0.49
1:F:312:THR:O	1:F:315:ALA:HB3	2.13	0.49
1:H:279:ARG:HE	1:H:283:ILE:HG23	1.78	0.49
1:B:258:ASN:O	1:B:262:MET:HG2	2.13	0.49
1:D:140:VAL:HG21	1:D:286:ILE:HD12	1.95	0.49
1:D:347:PRO:O	1:D:351:GLU:HG2	2.12	0.49
1:E:470:GLN:HB2	1:F:109:SER:H	1.78	0.49
1:G:295:CYS:HB2	1:G:326:HIS:NE2	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LYS:NZ	1:B:486:ARG:HD2	2.28	0.49
1:E:131:LEU:HD23	1:E:140:VAL:HG12	1.95	0.49
1:F:466:MET:SD	1:F:466:MET:N	2.82	0.49
1:B:232:THR:O	1:B:233:ILE:C	2.50	0.48
1:B:232:THR:OG1	1:B:233:ILE:N	2.43	0.48
1:E:447:MET:SD	1:E:448:ALA:N	2.86	0.48
1:G:231:PRO:O	1:G:235:ALA:N	2.46	0.48
1:A:220:ASP:OD1	1:A:455:ARG:NH2	2.46	0.48
1:A:385:VAL:HA	1:A:388:ILE:HG22	1.95	0.48
1:D:186:MET:HB2	1:D:322:TYR:CE2	2.49	0.48
1:E:152:LYS:N	1:F:483:LEU:HD11	2.28	0.48
1:F:344:GLU:O	1:F:347:PRO:HD2	2.13	0.48
1:F:365:HIS:HB3	1:F:368:TYR:O	2.12	0.48
1:G:162:ILE:HA	1:G:224:VAL:HG23	1.94	0.48
1:G:475:VAL:HG13	1:H:125:GLY:HA3	1.93	0.48
1:H:364:GLY:N	1:H:419:ASN:HB3	2.28	0.48
1:B:399:ILE:O	1:B:402:GLU:HG3	2.12	0.48
1:E:193:MET:HE2	1:E:315:ALA:HA	1.94	0.48
1:E:425:GLY:HA2	1:E:428:TYR:HD2	1.78	0.48
1:G:110:SER:HB2	1:H:473:THR:HG23	1.95	0.48
1:H:475:VAL:HG12	1:H:478:ARG:HH21	1.79	0.48
1:A:170:GLN:HA	1:A:173:LEU:HD12	1.95	0.48
1:A:337:LEU:O	1:A:340:ILE:HG22	2.14	0.48
1:B:364:GLY:N	1:B:417:TYR:O	2.38	0.48
1:F:269:ARG:HH12	1:H:268:ASN:HD21	1.62	0.48
1:F:393:PRO:HA	1:F:396:GLU:OE2	2.12	0.48
1:G:230:VAL:HB	1:G:231:PRO:HD3	1.96	0.48
1:B:236:ALA:O	1:B:239:LEU:HG	2.14	0.48
1:B:236:ALA:O	1:B:237:ALA:C	2.49	0.48
1:F:257:GLU:HB2	1:F:273:PRO:HG3	1.95	0.48
1:F:315:ALA:O	1:F:318:VAL:HG12	2.14	0.48
1:F:405:ALA:HB1	1:F:411:PHE:CE2	2.48	0.48
1:D:124:ARG:CZ	1:D:147:GLY:HA2	2.43	0.48
1:B:142:TYR:HD2	1:B:158:TRP:CE3	2.32	0.48
1:C:144:LEU:HD23	1:C:144:LEU:HA	1.69	0.48
1:E:152:LYS:HD3	1:F:483:LEU:HD21	1.95	0.48
1:E:219:ARG:O	1:E:222:GLN:HG2	2.14	0.48
1:F:382:ALA:HA	1:F:385:VAL:HG12	1.95	0.48
1:G:124:ARG:HE	1:G:144:LEU:HA	1.78	0.48
1:G:200:HIS:CE1	1:G:225:ARG:HH11	2.31	0.48
1:H:479:HIS:ND1	1:H:480:TYR:O	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HD22	1:B:128:ILE:HB	1.96	0.48
1:C:107:VAL:HG21	1:C:301:ARG:NH1	2.28	0.48
1:C:125:GLY:HA3	1:D:478:ARG:NH1	2.29	0.48
1:A:334:LEU:HD22	1:A:435:THR:HG21	1.95	0.48
1:C:503:ALA:C	1:C:505:ARG:N	2.67	0.48
1:D:111:ILE:O	1:D:124:ARG:N	2.36	0.48
1:D:202:ASP:N	1:D:202:ASP:OD1	2.46	0.48
1:D:509:ALA:O	1:G:274:ASN:N	2.47	0.48
1:H:248:LEU:HD12	1:H:249:PRO:HD2	1.96	0.48
1:E:256:SER:O	1:E:260:LEU:HG	2.13	0.48
1:G:184:HIS:O	1:G:188:VAL:HG23	2.14	0.48
1:H:347:PRO:HA	1:H:350:ILE:HG22	1.95	0.48
1:B:226:ILE:O	1:B:230:VAL:HG23	2.14	0.47
1:F:117:ASP:OD1	1:F:118:GLU:N	2.47	0.47
1:H:140:VAL:HG21	1:H:286:ILE:HD12	1.96	0.47
1:H:261:TYR:HB2	1:H:273:PRO:HB3	1.96	0.47
1:H:388:ILE:HG23	1:H:389:VAL:HG13	1.96	0.47
1:B:186:MET:HG2	1:B:322:TYR:CD1	2.49	0.47
1:D:287:LEU:HD12	1:D:374:ARG:HB3	1.95	0.47
1:E:158:TRP:CE2	1:E:162:ILE:HD11	2.49	0.47
1:G:343:VAL:HG12	1:G:397:VAL:HA	1.95	0.47
1:G:467:ARG:NH2	1:G:468:PRO:O	2.47	0.47
1:B:161:ALA:O	1:B:165:HIS:ND1	2.36	0.47
1:B:486:ARG:HH11	1:B:486:ARG:CG	2.26	0.47
1:C:477:LEU:HD23	1:D:122:ARG:HH11	1.79	0.47
1:D:171:GLY:O	1:D:175:ILE:HG12	2.14	0.47
1:E:119:GLY:HA2	1:E:368:TYR:HE1	1.79	0.47
1:G:124:ARG:NH2	1:G:144:LEU:O	2.36	0.47
1:H:223:ILE:HA	1:H:226:ILE:HG12	1.95	0.47
1:A:238:TYR:HB2	1:A:437:PHE:CZ	2.49	0.47
1:A:276:ARG:HA	1:A:279:ARG:NH1	2.29	0.47
1:E:252:ASN:HD21	1:E:269:ARG:NH2	2.13	0.47
1:F:118:GLU:HB3	1:F:120:ILE:HG13	1.96	0.47
1:E:235:ALA:HB2	1:E:259:PHE:CE1	2.49	0.47
1:F:254:SER:HB3	1:F:257:GLU:OE1	2.15	0.47
1:H:137:TYR:HB3	1:H:138:PRO:HD3	1.97	0.47
1:H:294:ASN:N	1:H:297:THR:OG1	2.42	0.47
1:A:218:LEU:HD13	1:A:221:LYS:HD2	1.96	0.47
1:A:481:THR:O	1:A:486:ARG:NH2	2.48	0.47
1:B:107:VAL:HG21	1:B:463:THR:HG21	1.97	0.47
1:D:126:TYR:CD1	1:D:131:LEU:HD21	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:ASP:OD1	1:D:211:ASP:N	2.48	0.47
1:E:422:PHE:O	1:E:426:LEU:HG	2.14	0.47
1:F:150:PRO:HB2	1:F:155:LEU:HB2	1.95	0.47
1:H:428:TYR:CD2	1:H:441:LEU:HD13	2.48	0.47
1:A:109:SER:OG	1:A:110:SER:N	2.47	0.47
1:A:336:MET:HB2	1:A:359:LYS:NZ	2.30	0.47
1:A:379:ARG:NH2	1:A:423:TYR:OH	2.46	0.47
1:A:483:LEU:HA	1:A:486:ARG:HE	1.79	0.47
1:C:285:PHE:HD1	1:C:445:PRO:HB3	1.79	0.47
1:F:378:ILE:HD11	1:F:420:VAL:HA	1.95	0.47
1:G:194:SER:HB2	1:H:191:CYS:HA	1.96	0.47
1:H:165:HIS:CD2	1:H:221:LYS:HE2	2.50	0.47
1:H:357:LYS:HA	1:H:357:LYS:HE2	1.97	0.47
1:H:365:HIS:N	1:H:368:TYR:O	2.43	0.47
1:C:159:GLU:HA	1:C:162:ILE:HG22	1.96	0.47
1:G:385:VAL:HA	1:G:388:ILE:HG12	1.95	0.47
1:H:150:PRO:HB2	1:H:154:GLN:HB2	1.97	0.47
1:H:192:ALA:O	1:H:196:LEU:HG	2.15	0.47
1:H:205:PRO:HA	1:H:212:LEU:HD12	1.97	0.47
1:H:409:GLU:O	1:H:413:LYS:HG3	2.14	0.47
1:A:150:PRO:O	1:B:486:ARG:NH1	2.47	0.47
1:E:378:ILE:HD12	1:E:423:TYR:HB2	1.96	0.47
1:F:354:LYS:HD3	1:F:410:TYR:HB2	1.96	0.47
1:F:369:LYS:O	1:F:370:ASN:C	2.51	0.47
1:A:157:ASP:HA	1:A:160:PHE:HB3	1.96	0.47
1:A:291:HIS:CE1	1:A:446:ARG:HH12	2.33	0.47
1:E:423:TYR:HA	1:E:426:LEU:HD12	1.97	0.47
1:F:238:TYR:HB2	1:F:437:PHE:CZ	2.50	0.47
1:G:200:HIS:ND1	1:G:225:ARG:HD3	2.29	0.47
1:F:292:GLU:O	1:F:294:ASN:ND2	2.48	0.46
1:F:311:PHE:C	1:F:313:ALA:N	2.63	0.46
1:H:137:TYR:HA	1:H:286:ILE:HD11	1.96	0.46
1:B:126:TYR:HE2	1:B:149:LEU:HD23	1.79	0.46
1:B:244:ARG:HE	1:B:245:PRO:HD2	1.80	0.46
1:D:123:TYR:O	1:D:124:ARG:C	2.52	0.46
1:D:423:TYR:HA	1:D:426:LEU:HD12	1.97	0.46
1:E:123:TYR:HB3	1:E:144:LEU:HD21	1.97	0.46
1:E:434:PRO:HB2	1:E:436:GLU:CD	2.35	0.46
1:F:158:TRP:O	1:F:162:ILE:HG12	2.14	0.46
1:H:323:GLY:H	1:H:326:HIS:CE1	2.33	0.46
1:H:374:ARG:O	1:H:377:VAL:HG22	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ASP:O	1:B:286:ILE:HG12	2.16	0.46
1:E:330:ASN:HB2	1:E:438:PHE:HD2	1.80	0.46
1:F:363:PHE:CD2	1:F:418:PRO:HD3	2.50	0.46
1:A:365:HIS:CD2	1:A:367:VAL:H	2.34	0.46
1:B:176:ILE:O	1:B:240:ARG:NH1	2.49	0.46
1:B:239:LEU:HD22	1:B:247:VAL:HG13	1.96	0.46
1:B:386:PHE:HB3	1:B:391:ARG:HD2	1.98	0.46
1:D:173:LEU:HD23	1:D:176:ILE:HD12	1.96	0.46
1:G:200:HIS:HB2	1:G:311:PHE:HE2	1.81	0.46
1:H:405:ALA:HA	1:H:411:PHE:CD2	2.50	0.46
1:B:447:MET:HA	1:B:450:TYR:CD2	2.51	0.46
1:D:151:SER:N	1:D:154:GLN:OE1	2.48	0.46
1:D:172:VAL:HG23	1:D:199:PHE:CD2	2.49	0.46
1:E:153:SER:O	1:E:154:GLN:C	2.54	0.46
1:F:371:TYR:CD2	1:F:373:PRO:HD3	2.46	0.46
1:H:354:LYS:HD3	1:H:410:TYR:HB3	1.97	0.46
1:B:135:SER:OG	1:B:139:GLU:OE1	2.32	0.46
1:E:486:ARG:HH22	1:F:149:LEU:HD22	1.80	0.46
1:F:118:GLU:HG3	1:F:371:TYR:CE1	2.51	0.46
1:F:316:GLY:O	1:F:317:ALA:C	2.54	0.46
1:C:349:PHE:O	1:C:353:VAL:N	2.44	0.46
1:D:347:PRO:HA	1:D:350:ILE:HG12	1.97	0.46
1:E:399:ILE:O	1:E:402:GLU:HG2	2.15	0.46
1:A:254:SER:O	1:A:258:ASN:N	2.32	0.46
1:A:276:ARG:O	1:A:280:VAL:HG23	2.16	0.46
1:B:372:ASP:OD2	1:B:374:ARG:NE	2.49	0.46
1:C:392:ASP:H	1:C:395:ILE:HD12	1.81	0.46
1:C:480:TYR:HA	1:D:126:TYR:CE1	2.37	0.46
1:D:145:MET:SD	1:D:452:ALA:HA	2.56	0.46
1:E:150:PRO:O	1:F:486:ARG:HG3	2.16	0.46
1:F:151:SER:N	1:F:154:GLN:HB2	2.31	0.46
1:H:405:ALA:O	1:H:418:PRO:HD3	2.16	0.46
1:A:218:LEU:HA	1:A:221:LYS:HG2	1.98	0.46
1:A:314:LEU:HD11	1:A:450:TYR:HB3	1.97	0.46
1:C:239:LEU:HD11	1:C:247:VAL:HG23	1.98	0.46
1:E:274:ASN:HB3	1:E:277:LEU:HG	1.97	0.46
1:F:284:LEU:HA	1:F:287:LEU:HD23	1.98	0.46
1:A:96:LEU:HB3	1:B:104:THR:HA	1.98	0.46
1:A:184:HIS:CD2	1:A:186:MET:H	2.33	0.46
1:B:403:LYS:HD2	1:B:403:LYS:HA	1.76	0.46
1:E:105:ALA:HB2	1:F:469:GLN:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:ILE:O	1:C:350:ILE:HG23	2.15	0.45
1:C:349:PHE:HA	1:C:358:ARG:HH11	1.81	0.45
1:D:111:ILE:HG12	1:D:112:CYS:SG	2.56	0.45
1:F:196:LEU:HG	1:F:311:PHE:CE1	2.51	0.45
1:G:164:GLN:NE2	1:G:165:HIS:HB2	2.31	0.45
1:H:177:GLN:H	1:H:240:ARG:HG3	1.81	0.45
1:A:263:LEU:HD11	1:A:433:PHE:CE1	2.51	0.45
1:B:150:PRO:HG2	1:B:155:LEU:HD12	1.97	0.45
1:C:290:GLU:HG3	1:C:449:GLY:HA3	1.97	0.45
1:E:184:HIS:CD2	1:E:186:MET:HB3	2.52	0.45
1:G:145:MET:HG3	1:G:158:TRP:CH2	2.51	0.45
1:H:338:ASN:O	1:H:339:GLU:HG3	2.17	0.45
1:G:303:LEU:HD12	1:G:304:ALA:N	2.31	0.45
1:A:217:GLN:HG2	1:A:218:LEU:HD22	1.99	0.45
1:B:285:PHE:HE1	1:B:441:LEU:HD21	1.80	0.45
1:E:350:ILE:O	1:E:353:VAL:HG12	2.16	0.45
1:F:484:GLN:H	1:F:484:GLN:CD	2.20	0.45
1:H:184:HIS:HD2	1:H:436:GLU:HB2	1.80	0.45
1:H:293:MET:HB2	1:H:298:ALA:HB2	1.98	0.45
1:D:381:LEU:O	1:D:385:VAL:HG23	2.17	0.45
1:E:244:ARG:NH1	1:E:245:PRO:O	2.49	0.45
1:E:385:VAL:O	1:E:389:VAL:HG12	2.17	0.45
1:F:290:GLU:OE1	1:F:449:GLY:HA3	2.16	0.45
1:F:364:GLY:HA2	1:F:417:TYR:CD1	2.52	0.45
1:G:196:LEU:HA	1:G:199:PHE:CD2	2.51	0.45
1:G:503:ARG:O	1:G:507:SER:N	2.50	0.45
1:H:418:PRO:HB2	1:H:423:TYR:CE1	2.51	0.45
1:H:444:ILE:HA	1:H:447:MET:HE3	1.97	0.45
1:A:158:TRP:O	1:A:162:ILE:HG12	2.17	0.45
1:E:124:ARG:HG3	1:E:143:LEU:O	2.17	0.45
1:E:230:VAL:HG23	1:E:231:PRO:HD3	1.99	0.45
1:F:314:LEU:O	1:F:316:GLY:N	2.49	0.45
1:F:398:ALA:HB1	1:F:422:PHE:CE1	2.51	0.45
1:H:378:ILE:O	1:H:382:ALA:N	2.46	0.45
1:H:410:TYR:CE1	1:H:414:ARG:HD2	2.51	0.45
1:A:381:LEU:O	1:A:385:VAL:HG23	2.17	0.45
1:C:228:GLY:O	1:C:231:PRO:HD2	2.16	0.45
1:C:363:PHE:HB3	1:C:416:LEU:HB3	1.97	0.45
1:D:126:TYR:CB	1:D:131:LEU:HD11	2.45	0.45
1:F:263:LEU:HD12	1:F:263:LEU:HA	1.76	0.45
1:F:280:VAL:O	1:F:284:LEU:HG	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:419:ASN:OD1	1:F:421:ASP:HB3	2.16	0.45
1:B:276:ARG:HD3	1:B:384:GLU:OE2	2.17	0.45
1:B:308:VAL:HG22	1:B:309:ASP:OD1	2.17	0.45
1:D:352:GLY:HA2	1:D:357:LYS:HZ2	1.82	0.45
1:D:466:MET:SD	1:D:466:MET:N	2.88	0.45
1:E:411:PHE:O	1:E:416:LEU:N	2.42	0.45
1:F:483:LEU:HA	1:F:486:ARG:CG	2.41	0.45
1:G:121:LEU:HD23	1:G:121:LEU:H	1.82	0.45
1:H:141:ALA:O	1:H:145:MET:HB2	2.17	0.45
1:A:314:LEU:O	1:A:318:VAL:HG23	2.17	0.45
1:B:114:ILE:HG13	1:B:292:GLU:HG2	1.98	0.45
1:C:123:TYR:CZ	1:C:289:ALA:HB3	2.52	0.45
1:D:251:ASN:OD1	1:D:252:ASN:N	2.49	0.45
1:F:175:ILE:HG22	1:F:179:MET:HE1	1.97	0.45
1:F:205:PRO:HD2	1:F:309:ASP:HB3	1.98	0.45
1:F:259:PHE:O	1:F:262:MET:HB2	2.17	0.45
1:F:485:GLU:O	1:F:486:ARG:C	2.55	0.45
1:B:204:ASN:ND2	1:B:207:LEU:HG	2.32	0.45
1:C:369:LYS:HD3	1:C:369:LYS:HA	1.71	0.45
1:F:404:ALA:O	1:F:407:SER:OG	2.30	0.45
1:G:154:GLN:HA	1:G:154:GLN:OE1	2.17	0.45
1:H:223:ILE:HG13	1:H:451:LEU:HD23	1.99	0.45
1:B:309:ASP:OD1	1:B:309:ASP:N	2.50	0.44
1:E:172:VAL:O	1:E:176:ILE:HG12	2.17	0.44
1:H:152:LYS:HA	1:H:155:LEU:HD12	1.98	0.44
1:A:152:LYS:CE	1:B:486:ARG:HD2	2.47	0.44
1:B:235:ALA:O	1:B:238:TYR:N	2.51	0.44
1:B:408:ASP:HB3	1:B:411:PHE:CD2	2.51	0.44
1:B:464:LYS:HB2	1:B:464:LYS:HE2	1.57	0.44
1:C:123:TYR:O	1:C:124:ARG:C	2.54	0.44
1:C:440:VAL:O	1:C:444:ILE:HG12	2.18	0.44
1:E:131:LEU:HD21	1:E:143:LEU:HD13	1.99	0.44
1:E:175:ILE:HD11	1:F:175:ILE:HG23	1.99	0.44
1:F:254:SER:OG	1:F:255:TYR:N	2.50	0.44
1:G:376:LYS:HG2	1:G:380:LYS:HE2	1.97	0.44
1:G:486:ARG:NE	1:H:149:LEU:HD22	2.32	0.44
1:H:242:ALA:HB3	1:H:244:ARG:NH1	2.22	0.44
1:B:236:ALA:HA	1:B:239:LEU:HG	1.99	0.44
1:B:385:VAL:HA	1:B:388:ILE:HG22	2.00	0.44
1:C:173:LEU:HD12	1:C:246:PRO:HG3	1.98	0.44
1:C:422:PHE:CE2	1:C:426:LEU:HD11	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ILE:HD12	1:D:292:GLU:HB2	1.99	0.44
1:D:337:LEU:O	1:D:340:ILE:HG22	2.17	0.44
1:E:109:SER:HB3	1:F:470:GLN:HG3	1.98	0.44
1:E:152:LYS:HD3	1:F:483:LEU:CD2	2.47	0.44
1:E:330:ASN:ND2	1:E:438:PHE:HB3	2.32	0.44
1:F:187:GLY:HA2	1:F:190:VAL:HG22	1.99	0.44
1:F:391:ARG:HH12	1:F:399:ILE:HD13	1.81	0.44
1:G:151:SER:HB3	1:H:488:VAL:HA	1.99	0.44
1:G:208:ARG:HB2	1:G:212:LEU:HD23	1.99	0.44
1:B:277:LEU:HA	1:B:280:VAL:HG12	1.98	0.44
1:B:347:PRO:O	1:B:351:GLU:HG2	2.17	0.44
1:D:180:PRO:C	1:D:240:ARG:HH22	2.20	0.44
1:D:203:ALA:HB2	1:D:222:GLN:HE22	1.83	0.44
1:F:316:GLY:O	1:F:318:VAL:N	2.51	0.44
1:F:377:VAL:O	1:F:381:LEU:HG	2.17	0.44
1:G:115:ASP:OD2	1:G:118:GLU:HB2	2.17	0.44
1:G:226:ILE:O	1:G:230:VAL:HG23	2.17	0.44
1:A:102:LEU:HD22	1:B:467:ARG:HB3	1.98	0.44
1:A:293:MET:O	1:A:294:ASN:ND2	2.50	0.44
1:F:348:ASP:O	1:F:352:GLY:N	2.44	0.44
1:G:111:ILE:HG21	1:G:453:HIS:NE2	2.32	0.44
1:G:211:ASP:HA	1:G:214:LYS:HD3	2.00	0.44
1:C:398:ALA:HA	1:C:401:LEU:HD12	1.99	0.44
1:E:472:TYR:OH	1:E:475:VAL:O	2.26	0.44
1:F:393:PRO:HA	1:F:396:GLU:CD	2.38	0.44
1:G:283:ILE:O	1:G:287:LEU:HG	2.17	0.44
1:H:190:VAL:HG22	1:H:318:VAL:HG13	1.99	0.44
1:H:226:ILE:HG13	1:H:451:LEU:HD21	2.00	0.44
1:H:329:ALA:HB3	1:H:421:ASP:HB3	1.99	0.44
1:H:438:PHE:HB2	1:H:439:PRO:HD3	2.00	0.44
1:C:279:ARG:HH12	1:C:283:ILE:CG1	2.30	0.44
1:C:506:ARG:O	1:C:507:ARG:C	2.55	0.44
1:E:151:SER:O	1:E:152:LYS:C	2.55	0.44
1:E:152:LYS:CE	1:F:486:ARG:HB2	2.46	0.44
1:F:331:GLU:C	1:F:335:LYS:HZ2	2.21	0.44
1:A:186:MET:HG2	1:A:322:TYR:CD2	2.52	0.44
1:B:121:LEU:HD21	1:B:123:TYR:CE1	2.53	0.44
1:D:417:TYR:HB2	1:D:418:PRO:HD2	2.00	0.44
1:E:140:VAL:HG21	1:E:286:ILE:HD12	1.98	0.44
1:E:324:PRO:HD2	1:F:307:GLY:O	2.17	0.44
1:E:427:ILE:HG22	1:E:431:MET:HE1	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:TYR:O	1:F:241:LEU:HB3	2.18	0.44
1:H:202:ASP:HA	1:H:208:ARG:HH12	1.82	0.44
1:C:137:TYR:HA	1:C:140:VAL:HG12	1.98	0.44
1:E:149:LEU:H	1:E:149:LEU:HD23	1.82	0.44
1:F:301:ARG:NH1	1:F:302:HIS:HB2	2.33	0.44
1:A:211:ASP:N	1:A:211:ASP:OD1	2.51	0.43
1:B:177:GLN:O	1:B:240:ARG:NH2	2.51	0.43
1:B:385:VAL:O	1:B:389:VAL:HG12	2.17	0.43
1:C:169:PRO:CD	1:C:229:LYS:HZ1	2.27	0.43
1:D:429:ARG:C	1:D:432:GLY:H	2.21	0.43
1:E:340:ILE:HD11	1:E:349:PHE:HB2	2.00	0.43
1:E:429:ARG:NH1	1:E:432:GLY:HA2	2.32	0.43
1:B:230:VAL:HG21	1:B:447:MET:SD	2.59	0.43
1:B:381:LEU:O	1:B:385:VAL:HG23	2.18	0.43
1:D:372:ASP:OD1	1:D:374:ARG:HG3	2.18	0.43
1:G:317:ALA:HB1	1:G:450:TYR:HE2	1.82	0.43
1:A:95:LYS:HA	1:A:95:LYS:HD3	1.85	0.43
1:A:203:ALA:O	1:A:213:TYR:OH	2.34	0.43
1:B:139:GLU:HG3	1:B:155:LEU:HD11	2.01	0.43
1:B:252:ASN:OD1	1:B:253:PHE:N	2.52	0.43
1:B:441:LEU:HA	1:B:444:ILE:HG12	2.01	0.43
1:C:115:ASP:HB3	1:C:120:ILE:HB	2.00	0.43
1:C:142:TYR:C	1:C:144:LEU:N	2.72	0.43
1:C:289:ALA:O	1:C:446:ARG:HA	2.19	0.43
1:C:376:LYS:HB3	1:C:380:LYS:NZ	2.33	0.43
1:E:151:SER:H	1:E:154:GLN:HB2	1.84	0.43
1:H:223:ILE:HD13	1:H:454:TRP:CZ3	2.53	0.43
1:A:98:ASP:OD2	1:A:101:TYR:HA	2.19	0.43
1:A:380:LYS:O	1:A:383:GLU:HG3	2.18	0.43
1:C:477:LEU:HD22	1:C:478:ARG:H	1.83	0.43
1:C:482:PRO:HB2	1:C:485:GLU:HG3	1.99	0.43
1:D:170:GLN:OE1	1:D:170:GLN:HA	2.17	0.43
1:D:223:ILE:HG13	1:D:451:LEU:HD12	2.01	0.43
1:F:168:VAL:HG21	1:F:233:ILE:HD11	2.00	0.43
1:H:114:ILE:HG23	1:H:368:TYR:CZ	2.53	0.43
1:H:220:ASP:O	1:H:223:ILE:HG22	2.18	0.43
1:B:467:ARG:NH1	1:B:468:PRO:O	2.52	0.43
1:C:314:LEU:HD13	1:C:314:LEU:HA	1.86	0.43
1:E:110:SER:HB2	1:E:456:GLU:OE1	2.18	0.43
1:F:374:ARG:HA	1:F:377:VAL:HG12	2.00	0.43
1:G:220:ASP:OD1	1:G:221:LYS:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:429:ARG:NH2	1:G:433:PHE:O	2.52	0.43
1:A:184:HIS:CG	1:A:185:PRO:HD2	2.54	0.43
1:A:221:LYS:HD3	1:A:225:ARG:NH2	2.34	0.43
1:C:503:ALA:O	1:C:507:ARG:N	2.50	0.43
1:D:82:PHE:HD2	1:D:96:LEU:HD21	1.82	0.43
1:F:394:LEU:HA	1:F:397:VAL:HG22	1.99	0.43
1:G:124:ARG:HG3	1:G:147:GLY:HA2	1.99	0.43
1:G:163:SER:O	1:G:251:ASN:ND2	2.51	0.43
1:B:234:ALA:O	1:B:237:ALA:N	2.51	0.43
1:C:172:VAL:N	1:C:199:PHE:HE2	2.16	0.43
1:E:126:TYR:CZ	1:F:478:ARG:HD2	2.54	0.43
1:E:502:ASN:HA	1:H:432:GLY:HA2	2.00	0.43
1:F:244:ARG:HG3	1:F:245:PRO:HD2	2.01	0.43
1:F:277:LEU:HA	1:F:280:VAL:HG12	2.00	0.43
1:G:287:LEU:O	1:G:374:ARG:NH1	2.47	0.43
1:G:374:ARG:O	1:G:378:ILE:HG12	2.18	0.43
1:H:193:MET:HE1	1:H:318:VAL:HG11	2.01	0.43
1:A:150:PRO:HD2	1:B:486:ARG:HH12	1.83	0.43
1:C:115:ASP:HB3	1:C:120:ILE:H	1.83	0.43
1:E:437:PHE:CE1	1:E:440:VAL:HG21	2.54	0.43
1:F:143:LEU:HA	1:F:148:ASN:O	2.19	0.43
1:H:235:ALA:HB2	1:H:262:MET:SD	2.59	0.43
1:H:446:ARG:HA	1:H:446:ARG:HD2	1.88	0.43
1:A:481:THR:HG23	1:A:486:ARG:NE	2.34	0.43
1:C:279:ARG:O	1:C:283:ILE:HG12	2.19	0.43
1:C:478:ARG:HD2	1:D:125:GLY:O	2.19	0.43
1:D:447:MET:HA	1:D:450:TYR:HD2	1.84	0.43
1:G:219:ARG:O	1:G:223:ILE:HG12	2.18	0.43
1:G:437:PHE:CE1	1:G:440:VAL:HG21	2.53	0.43
1:A:391:ARG:HB3	1:A:395:ILE:HB	2.01	0.43
1:C:451:LEU:O	1:C:455:ARG:N	2.38	0.43
1:E:196:LEU:HD11	1:E:233:ILE:CD1	2.49	0.43
1:E:219:ARG:O	1:E:223:ILE:HG12	2.19	0.43
1:G:504:LEU:O	1:G:508:ARG:N	2.52	0.43
1:H:123:TYR:HB3	1:H:144:LEU:HD21	2.01	0.43
1:D:148:ASN:OD1	1:D:149:LEU:N	2.51	0.42
1:E:137:TYR:HB3	1:E:138:PRO:HD3	2.01	0.42
1:F:137:TYR:OH	1:F:445:PRO:HA	2.19	0.42
1:H:129:GLU:O	1:H:133:GLU:HG3	2.19	0.42
1:H:222:GLN:O	1:H:226:ILE:HG23	2.19	0.42
1:H:230:VAL:HG21	1:H:447:MET:HE1	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:350:ILE:HD12	1:H:350:ILE:HA	1.92	0.42
1:A:145:MET:HG3	1:A:158:TRP:HH2	1.83	0.42
1:B:336:MET:HE1	1:B:360:MET:HA	2.01	0.42
1:C:180:PRO:HD2	1:D:199:PHE:HE1	1.84	0.42
1:D:226:ILE:O	1:D:230:VAL:HG23	2.20	0.42
1:F:229:LYS:O	1:F:232:THR:OG1	2.30	0.42
1:A:478:ARG:O	1:A:479:HIS:ND1	2.52	0.42
1:C:331:GLU:N	1:C:331:GLU:OE1	2.53	0.42
1:C:397:VAL:O	1:C:401:LEU:HG	2.18	0.42
1:E:206:ALA:HB1	1:F:322:TYR:O	2.20	0.42
1:E:216:LYS:HA	1:E:219:ARG:HE	1.83	0.42
1:F:460:ASP:HB2	1:F:462:ASP:OD1	2.19	0.42
1:G:222:GLN:O	1:G:226:ILE:HG12	2.19	0.42
1:B:229:LYS:O	1:B:232:THR:N	2.52	0.42
1:C:419:ASN:OD1	1:C:422:PHE:N	2.50	0.42
1:D:353:VAL:HA	1:D:358:ARG:O	2.20	0.42
1:E:112:CYS:SG	1:E:123:TYR:HD1	2.42	0.42
1:G:151:SER:HA	1:H:486:ARG:HD2	2.00	0.42
1:H:121:LEU:O	1:H:128:ILE:HG23	2.18	0.42
1:H:167:ALA:HA	1:H:232:THR:HG21	2.01	0.42
1:H:364:GLY:H	1:H:419:ASN:HB3	1.83	0.42
1:A:214:LYS:HA	1:A:214:LYS:HD3	1.86	0.42
1:C:248:LEU:HG	1:C:249:PRO:HD2	1.99	0.42
1:C:283:ILE:HA	1:C:286:ILE:HG22	2.02	0.42
1:F:483:LEU:O	1:F:484:GLN:C	2.56	0.42
1:A:199:PHE:CE1	1:B:179:MET:HG3	2.45	0.42
1:A:422:PHE:CE2	1:A:426:LEU:HD11	2.54	0.42
1:D:435:THR:HA	1:D:438:PHE:CD1	2.54	0.42
1:E:151:SER:HB3	1:E:154:GLN:HG2	2.01	0.42
1:E:235:ALA:CB	1:E:262:MET:HG3	2.48	0.42
1:E:421:ASP:OD1	1:E:422:PHE:N	2.52	0.42
1:G:186:MET:SD	1:G:189:LEU:HD12	2.59	0.42
1:G:378:ILE:HD12	1:G:423:TYR:HB2	2.01	0.42
1:H:114:ILE:HD11	1:H:291:HIS:HA	2.01	0.42
1:H:177:GLN:OE1	1:H:246:PRO:HG3	2.19	0.42
1:A:136:SER:N	1:A:139:GLU:OE2	2.52	0.42
1:A:208:ARG:HE	1:A:212:LEU:HD22	1.85	0.42
1:C:126:TYR:CE1	1:D:478:ARG:HG3	2.55	0.42
1:C:350:ILE:HA	1:C:353:VAL:HB	2.02	0.42
1:C:449:GLY:O	1:C:452:ALA:HB3	2.19	0.42
1:D:454:TRP:O	1:D:457:SER:OG	2.21	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:437:PHE:CZ	1:E:440:VAL:HG21	2.55	0.42
1:F:196:LEU:O	1:F:197:SER:C	2.56	0.42
1:G:156:ALA:O	1:G:159:GLU:HG3	2.20	0.42
1:G:334:LEU:HD11	1:G:435:THR:HG21	2.02	0.42
1:H:158:TRP:O	1:H:162:ILE:HG23	2.19	0.42
1:A:108:ARG:HG2	1:B:97:TYR:OH	2.20	0.42
1:B:151:SER:OG	1:B:154:GLN:OE1	2.36	0.42
1:D:250:SER:OG	1:D:251:ASN:N	2.53	0.42
1:D:328:GLY:HA2	1:D:331:GLU:OE1	2.20	0.42
1:F:151:SER:H	1:F:154:GLN:HB2	1.85	0.42
1:G:145:MET:HE1	1:G:452:ALA:N	2.34	0.42
1:B:461:PRO:O	1:B:462:ASP:C	2.58	0.42
1:C:253:PHE:HB3	1:C:257:GLU:HB3	2.01	0.42
1:D:109:SER:OG	1:D:110:SER:N	2.53	0.42
1:F:217:GLN:HG3	1:F:218:LEU:HD22	2.02	0.42
1:F:411:PHE:CE1	1:F:416:LEU:HB2	2.52	0.42
1:G:444:ILE:O	1:G:447:MET:HG2	2.20	0.42
1:H:325:LEU:HD11	1:H:361:SER:HB2	2.00	0.42
1:A:357:LYS:HE2	1:A:357:LYS:HB3	1.68	0.42
1:A:398:ALA:HB1	1:A:422:PHE:HZ	1.85	0.42
1:B:437:PHE:O	1:B:440:VAL:HG12	2.20	0.42
1:C:122:ARG:HB2	1:C:122:ARG:HH11	1.84	0.42
1:C:399:ILE:O	1:C:402:GLU:HG3	2.20	0.42
1:D:238:TYR:O	1:D:241:LEU:HB3	2.20	0.42
1:D:354:LYS:HG2	1:D:410:TYR:CD2	2.55	0.42
1:F:115:ASP:HB2	1:F:122:ARG:NH2	2.34	0.42
1:G:284:LEU:HD23	1:G:287:LEU:HD12	2.02	0.42
1:H:356:ARG:HE	1:H:414:ARG:CZ	2.31	0.42
1:H:441:LEU:HD12	1:H:442:PHE:N	2.34	0.42
1:A:276:ARG:HG2	1:A:279:ARG:HH22	1.85	0.41
1:B:310:VAL:HG13	1:B:311:PHE:HD1	1.85	0.41
1:C:119:GLY:HA2	1:C:368:TYR:CE1	2.55	0.41
1:C:162:ILE:HD11	1:C:227:LEU:HG	2.02	0.41
1:D:122:ARG:HB3	1:D:126:TYR:H	1.85	0.41
1:E:172:VAL:HG12	1:E:195:ALA:HB3	2.01	0.41
1:F:393:PRO:O	1:F:397:VAL:HG13	2.19	0.41
1:F:419:ASN:C	1:F:421:ASP:N	2.72	0.41
1:G:409:GLU:OE1	1:G:413:LYS:NZ	2.53	0.41
1:A:152:LYS:O	1:A:155:LEU:HG	2.20	0.41
1:B:244:ARG:NE	1:B:245:PRO:HD2	2.35	0.41
1:D:83:LYS:HA	1:D:93:GLY:HA3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:ASN:ND2	1:D:438:PHE:HD2	2.18	0.41
1:E:331:GLU:HG2	1:E:332:ALA:N	2.35	0.41
1:F:215:SER:OG	1:F:217:GLN:HG2	2.20	0.41
1:F:280:VAL:HG23	1:F:381:LEU:HB3	2.01	0.41
1:H:216:LYS:HZ2	1:H:220:ASP:HB2	1.85	0.41
1:A:218:LEU:O	1:A:222:GLN:HG2	2.20	0.41
1:B:482:PRO:O	1:B:485:GLU:HG3	2.21	0.41
1:D:348:ASP:N	1:D:348:ASP:OD1	2.53	0.41
1:E:184:HIS:NE2	1:E:186:MET:HB3	2.35	0.41
1:F:189:LEU:O	1:F:193:MET:HE3	2.20	0.41
1:H:116:GLY:HA3	1:H:367:VAL:HG22	2.02	0.41
1:A:113:TYR:HB2	1:B:472:TYR:CD2	2.55	0.41
1:A:471:VAL:HB	1:B:108:ARG:HG2	2.03	0.41
1:B:230:VAL:HA	1:B:233:ILE:HG22	2.03	0.41
1:B:426:LEU:HD23	1:B:429:ARG:NH2	2.30	0.41
1:C:384:GLU:OE1	1:C:384:GLU:N	2.49	0.41
1:C:467:ARG:HD3	1:D:102:LEU:HD21	2.03	0.41
1:D:125:GLY:O	1:D:126:TYR:CG	2.74	0.41
1:E:156:ALA:O	1:E:160:PHE:HD1	2.03	0.41
1:F:162:ILE:HD12	1:F:227:LEU:HD23	2.01	0.41
1:F:176:ILE:HG13	1:F:240:ARG:HD3	2.02	0.41
1:H:202:ASP:OD1	1:H:202:ASP:N	2.52	0.41
1:H:216:LYS:HA	1:H:219:ARG:HH21	1.85	0.41
1:B:124:ARG:CZ	1:B:147:GLY:HA2	2.50	0.41
1:D:285:PHE:HD1	1:D:445:PRO:HB3	1.85	0.41
1:D:432:GLY:O	1:D:433:PHE:C	2.59	0.41
1:E:422:PHE:CE2	1:E:426:LEU:HD11	2.55	0.41
1:E:471:VAL:HG23	1:F:108:ARG:HG2	2.01	0.41
1:F:197:SER:O	1:F:198:VAL:C	2.56	0.41
1:G:295:CYS:SG	1:G:325:LEU:HD11	2.61	0.41
1:H:184:HIS:NE2	1:H:436:GLU:O	2.53	0.41
1:H:405:ALA:O	1:H:417:TYR:HA	2.20	0.41
1:A:122:ARG:NE	1:B:476:TRP:O	2.53	0.41
1:A:126:TYR:HB3	1:A:131:LEU:HD21	2.02	0.41
1:A:248:LEU:HG	1:A:249:PRO:HD2	2.02	0.41
1:B:263:LEU:HD23	1:B:264:ASP:CG	2.41	0.41
1:C:176:ILE:HG13	1:C:188:VAL:CG1	2.50	0.41
1:C:280:VAL:O	1:C:284:LEU:HD23	2.21	0.41
1:D:193:MET:CE	1:D:230:VAL:HG22	2.51	0.41
1:D:219:ARG:NH1	1:D:458:LEU:HD23	2.35	0.41
1:D:481:THR:OG1	1:D:485:GLU:OE2	2.32	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:PRO:HA	1:E:350:ILE:HG12	2.02	0.41
1:F:117:ASP:O	1:F:370:ASN:HB2	2.20	0.41
1:F:118:GLU:HG3	1:F:371:TYR:CZ	2.55	0.41
1:F:197:SER:HB2	1:F:312:THR:HG23	2.02	0.41
1:F:257:GLU:HB3	1:F:278:ALA:HB1	2.01	0.41
1:F:311:PHE:O	1:F:312:THR:C	2.54	0.41
1:G:321:LEU:HA	1:G:326:HIS:CE1	2.54	0.41
1:G:378:ILE:HD13	1:G:420:VAL:HG13	2.02	0.41
1:E:165:HIS:CD2	1:E:225:ARG:HA	2.55	0.41
1:E:170:GLN:OE1	1:E:173:LEU:HB2	2.21	0.41
1:E:172:VAL:O	1:E:176:ILE:HG23	2.20	0.41
1:F:336:MET:HA	1:F:339:GLU:HG2	2.02	0.41
1:H:114:ILE:HD12	1:H:292:GLU:H	1.85	0.41
1:C:142:TYR:C	1:C:144:LEU:H	2.23	0.41
1:C:149:LEU:HB3	1:D:486:ARG:NH1	2.35	0.41
1:C:274:ASN:HB3	1:C:277:LEU:HB2	2.02	0.41
1:C:283:ILE:O	1:C:287:LEU:HD23	2.21	0.41
1:C:478:ARG:CD	1:C:479:HIS:H	2.34	0.41
1:D:260:LEU:HD12	1:D:260:LEU:HA	1.88	0.41
1:E:142:TYR:CD1	1:E:150:PRO:HB3	2.56	0.41
1:E:402:GLU:O	1:E:406:LEU:HG	2.21	0.41
1:G:155:LEU:HD23	1:G:155:LEU:HA	1.91	0.41
1:H:293:MET:N	1:H:293:MET:SD	2.94	0.41
1:H:299:ALA:HA	1:H:302:HIS:CE1	2.55	0.41
1:H:321:LEU:HD23	1:H:321:LEU:HA	1.91	0.41
1:H:353:VAL:HG22	1:H:410:TYR:HE2	1.84	0.41
1:A:303:LEU:O	1:A:306:SER:OG	2.34	0.41
1:B:365:HIS:CE1	1:B:374:ARG:HH21	2.38	0.41
1:B:378:ILE:HD11	1:B:423:TYR:HD2	1.86	0.41
1:C:205:PRO:HD2	1:C:309:ASP:HB3	2.02	0.41
1:C:343:VAL:O	1:C:346:ILE:HG12	2.21	0.41
1:C:391:ARG:HG2	1:C:395:ILE:HG21	2.02	0.41
1:C:434:PRO:HG2	1:C:437:PHE:HB2	2.02	0.41
1:D:285:PHE:HE1	1:D:444:ILE:HB	1.85	0.41
1:D:422:PHE:CE1	1:D:426:LEU:HD11	2.56	0.41
1:E:194:SER:O	1:E:197:SER:HB2	2.21	0.41
1:E:411:PHE:HA	1:E:416:LEU:HB2	2.03	0.41
1:F:176:ILE:HD11	1:F:240:ARG:HE	1.86	0.41
1:F:284:LEU:O	1:F:287:LEU:HG	2.20	0.41
1:F:311:PHE:O	1:F:313:ALA:N	2.53	0.41
1:G:400:ALA:O	1:G:403:LYS:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:409:GLU:O	1:G:413:LYS:HG2	2.20	0.41
1:G:472:TYR:CE1	1:H:113:TYR:HB2	2.55	0.41
1:H:280:VAL:HA	1:H:283:ILE:HG12	2.03	0.41
1:H:427:ILE:O	1:H:431:MET:HG2	2.20	0.41
1:B:137:TYR:CD1	1:B:285:PHE:HB3	2.56	0.41
1:D:238:TYR:HB2	1:D:437:PHE:CZ	2.56	0.41
1:D:391:ARG:NH2	1:D:396:GLU:HG3	2.36	0.41
1:E:210:GLN:HG2	1:F:324:PRO:HG2	2.02	0.41
1:E:369:LYS:HB3	1:E:415:LYS:HB3	2.03	0.41
1:G:363:PHE:HB3	1:G:416:LEU:HD11	2.02	0.41
1:A:111:ILE:HG21	1:A:453:HIS:CE1	2.56	0.40
1:A:295:CYS:HB3	1:B:466:MET:SD	2.61	0.40
1:B:365:HIS:HE1	1:B:372:ASP:OD2	2.04	0.40
1:D:115:ASP:O	1:D:119:GLY:N	2.54	0.40
1:D:310:VAL:HG22	1:D:314:LEU:HD23	2.02	0.40
1:D:475:VAL:CG1	1:D:478:ARG:HD3	2.39	0.40
1:E:165:HIS:CD2	1:E:225:ARG:HG3	2.56	0.40
1:F:283:ILE:O	1:F:286:ILE:HG22	2.21	0.40
1:B:377:VAL:O	1:B:381:LEU:HG	2.21	0.40
1:C:124:ARG:HA	1:C:124:ARG:HD3	1.50	0.40
1:E:115:ASP:O	1:E:119:GLY:N	2.54	0.40
1:E:176:ILE:CG2	1:E:188:VAL:HG13	2.52	0.40
1:E:442:PHE:O	1:E:446:ARG:HG3	2.22	0.40
1:F:438:PHE:N	1:F:439:PRO:HD2	2.37	0.40
1:H:186:MET:O	1:H:190:VAL:HG23	2.21	0.40
1:C:112:CYS:HB3	1:C:292:GLU:OE2	2.20	0.40
1:D:172:VAL:O	1:D:176:ILE:HG13	2.21	0.40
1:D:409:GLU:HG2	1:D:413:LYS:HE2	2.02	0.40
1:E:152:LYS:O	1:E:156:ALA:N	2.42	0.40
1:F:213:TYR:CE2	1:F:454:TRP:HZ2	2.40	0.40
1:F:298:ALA:O	1:F:301:ARG:HD3	2.22	0.40
1:G:295:CYS:HB2	1:G:326:HIS:HE2	1.86	0.40
1:G:483:LEU:HD12	1:G:486:ARG:HB2	2.04	0.40
1:H:216:LYS:NZ	1:H:220:ASP:HB2	2.36	0.40
1:H:284:LEU:HD13	1:H:287:LEU:HD23	2.03	0.40
1:A:151:SER:O	1:A:152:LYS:C	2.60	0.40
1:H:352:GLY:O	1:H:356:ARG:N	2.55	0.40
1:A:121:LEU:HB3	1:A:128:ILE:HB	2.03	0.40
1:A:149:LEU:HB2	1:B:486:ARG:HH12	1.86	0.40
1:A:385:VAL:O	1:A:389:VAL:HG12	2.21	0.40
1:A:483:LEU:HD11	1:B:139:GLU:OE2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:LEU:O	1:B:454:TRP:HB3	2.21	0.40
1:F:372:ASP:O	1:F:374:ARG:N	2.54	0.40
1:G:322:TYR:O	1:G:322:TYR:CD1	2.74	0.40
1:H:346:ILE:HD11	1:H:397:VAL:HG13	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	409/521 (78%)	383 (94%)	24 (6%)	2 (0%)	29 68
1	B	412/521 (79%)	378 (92%)	33 (8%)	1 (0%)	47 80
1	C	414/521 (80%)	374 (90%)	32 (8%)	8 (2%)	8 41
1	D	439/521 (84%)	404 (92%)	34 (8%)	1 (0%)	47 80
1	E	397/521 (76%)	365 (92%)	32 (8%)	0	100 100
1	F	393/521 (75%)	362 (92%)	26 (7%)	5 (1%)	12 48
1	G	388/521 (74%)	360 (93%)	28 (7%)	0	100 100
1	H	393/521 (75%)	340 (86%)	52 (13%)	1 (0%)	41 76
All	All	3245/4168 (78%)	2966 (91%)	261 (8%)	18 (1%)	29 64

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	PRO
1	C	146	TYR
1	F	311	PHE
1	C	145	MET
1	C	147	GLY
1	C	476	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	504	THR
1	C	505	ARG
1	D	488	VAL
1	F	418	PRO
1	C	124	ARG
1	F	317	ALA
1	C	508	LEU
1	A	103	ASN
1	B	498	VAL
1	F	373	PRO
1	F	420	VAL
1	H	169	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	328/427 (77%)	323 (98%)	5 (2%)	65 79
1	B	328/427 (77%)	322 (98%)	6 (2%)	59 76
1	C	328/427 (77%)	318 (97%)	10 (3%)	41 63
1	D	349/427 (82%)	346 (99%)	3 (1%)	78 88
1	E	320/427 (75%)	313 (98%)	7 (2%)	52 70
1	F	319/427 (75%)	308 (97%)	11 (3%)	37 60
1	G	316/427 (74%)	316 (100%)	0	100 100
1	H	319/427 (75%)	317 (99%)	2 (1%)	86 92
All	All	2607/3416 (76%)	2563 (98%)	44 (2%)	62 78

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	LYS
1	A	269	ARG
1	A	359	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	486	ARG
1	A	487	THR
1	B	462	ASP
1	B	464	LYS
1	B	481	THR
1	B	483	LEU
1	B	485	GLU
1	B	486	ARG
1	C	122	ARG
1	C	124	ARG
1	C	144	LEU
1	C	148	ASN
1	C	466	MET
1	C	467	ARG
1	C	475	VAL
1	C	477	LEU
1	C	478	ARG
1	C	479	HIS
1	D	124	ARG
1	D	130	GLU
1	D	431	MET
1	E	151	SER
1	E	152	LYS
1	E	154	GLN
1	E	155	LEU
1	E	219	ARG
1	E	240	ARG
1	E	244	ARG
1	F	108	ARG
1	F	220	ASP
1	F	301	ARG
1	F	309	ASP
1	F	369	LYS
1	F	415	LYS
1	F	429	ARG
1	F	466	MET
1	F	483	LEU
1	F	484	GLN
1	F	485	GLU
1	H	244	ARG
1	H	379	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	365	HIS
1	B	294	ASN
1	B	365	HIS
1	D	302	HIS
1	E	170	GLN
1	E	204	ASN
1	F	177	GLN
1	F	355	ASN
1	H	204	ASN
1	H	330	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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.

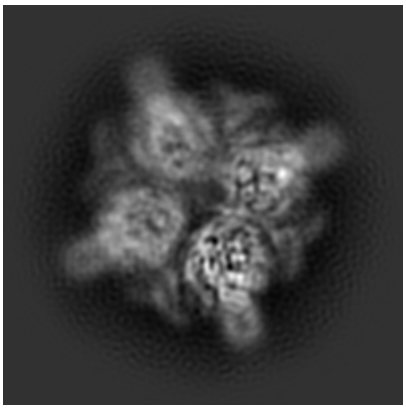
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18779. These allow visual inspection of the internal detail of the map and identification of artifacts.

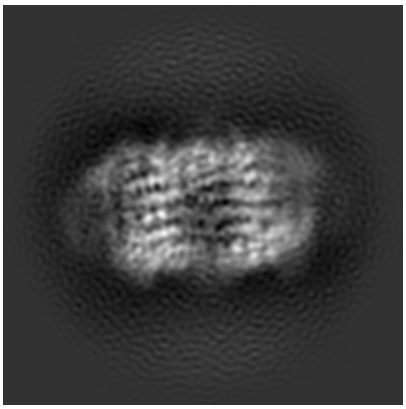
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

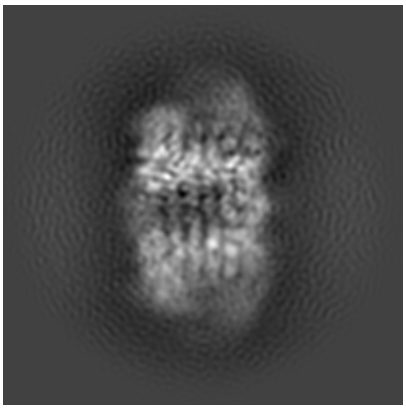
6.1.1 Primary map



X

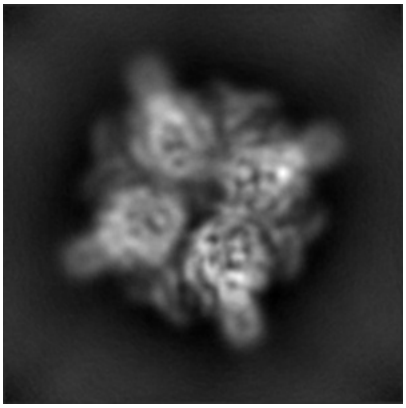


Y

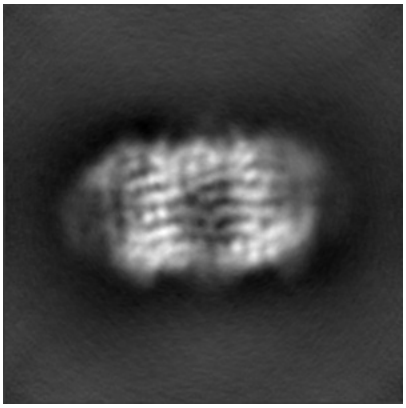


Z

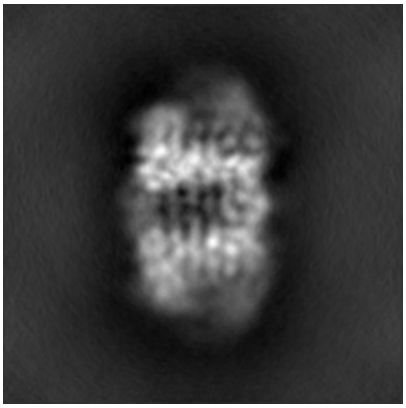
6.1.2 Raw map



X



Y

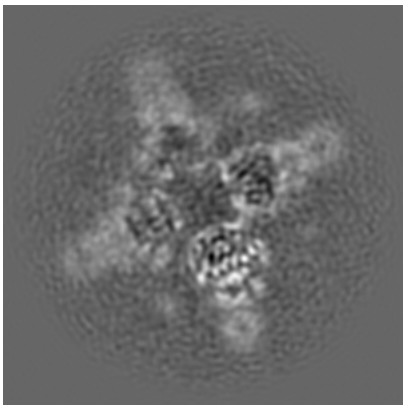


Z

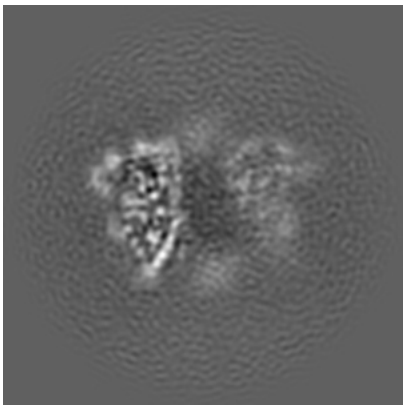
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

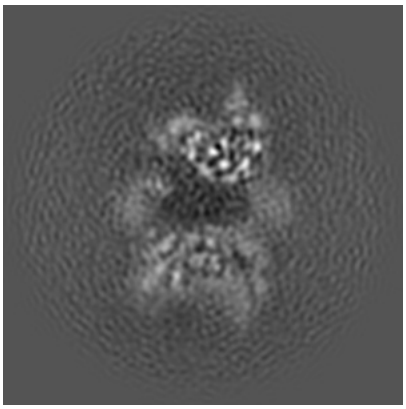
6.2.1 Primary map



X Index: 100

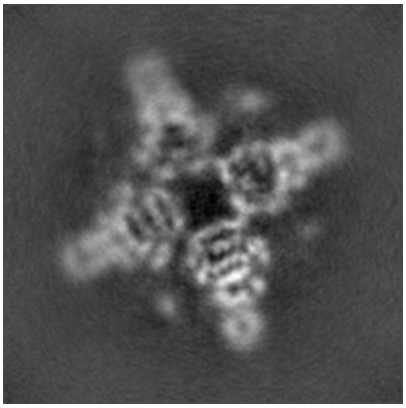


Y Index: 100

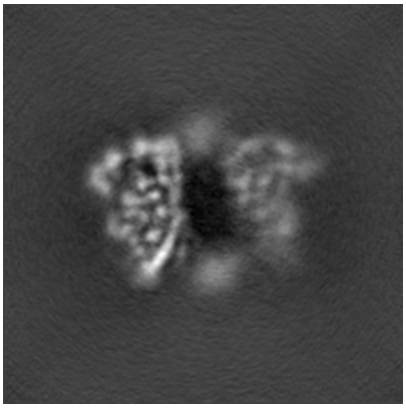


Z Index: 100

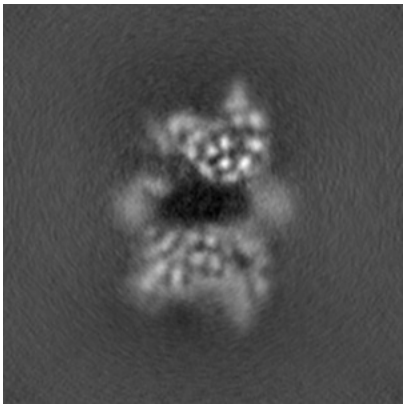
6.2.2 Raw map



X Index: 100



Y Index: 100

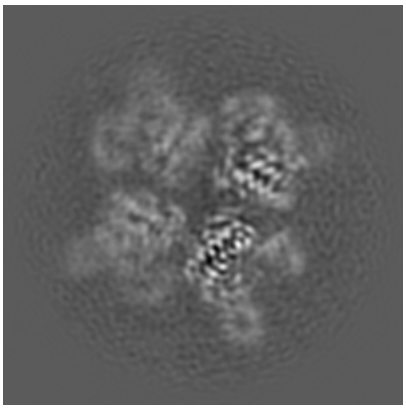


Z Index: 100

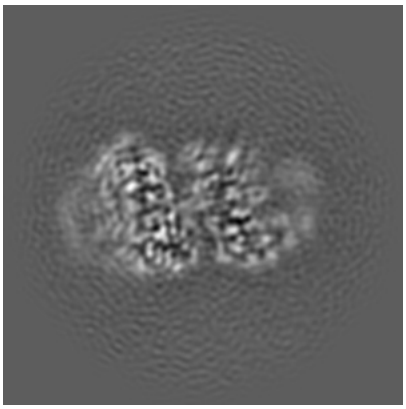
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

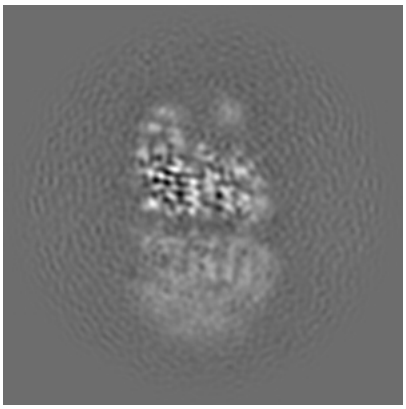
6.3.1 Primary map



X Index: 86

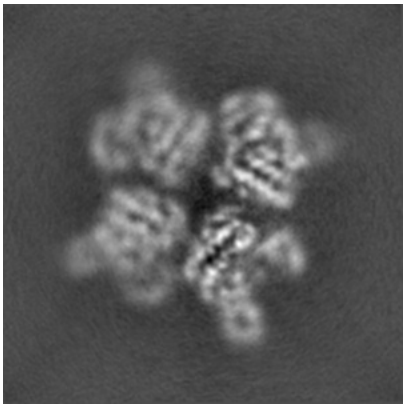


Y Index: 118

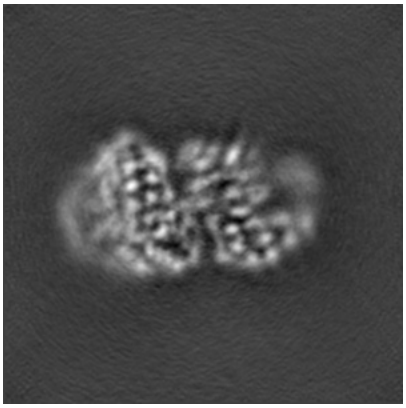


Z Index: 79

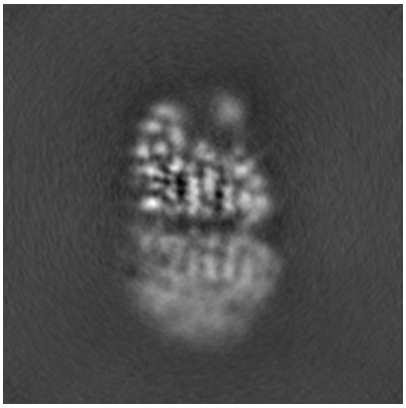
6.3.2 Raw map



X Index: 86



Y Index: 118

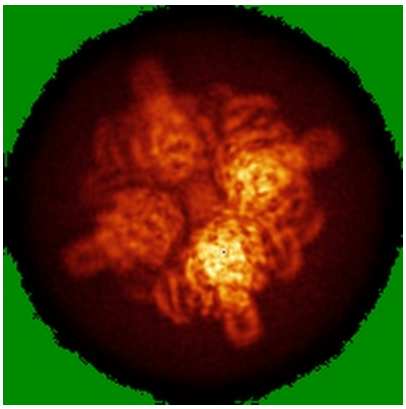


Z Index: 79

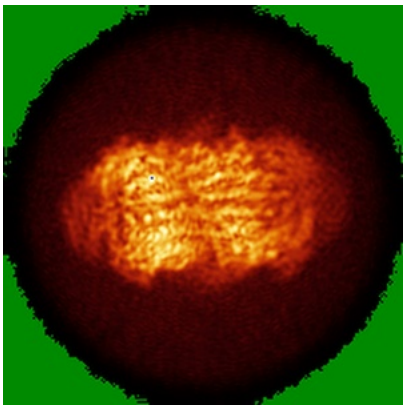
The images above show the largest variance slices of the map in three orthogonal directions.

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

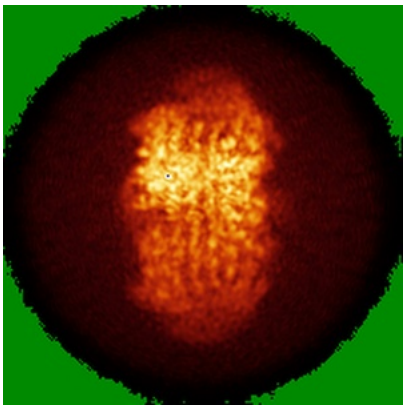
6.4.1 Primary map



X

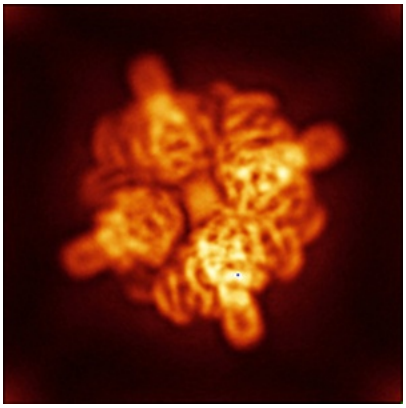


Y

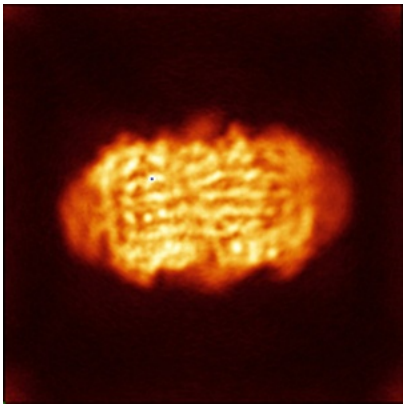


Z

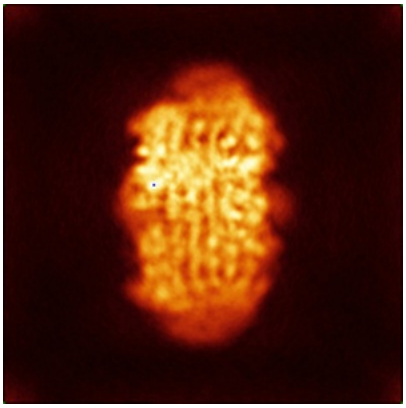
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

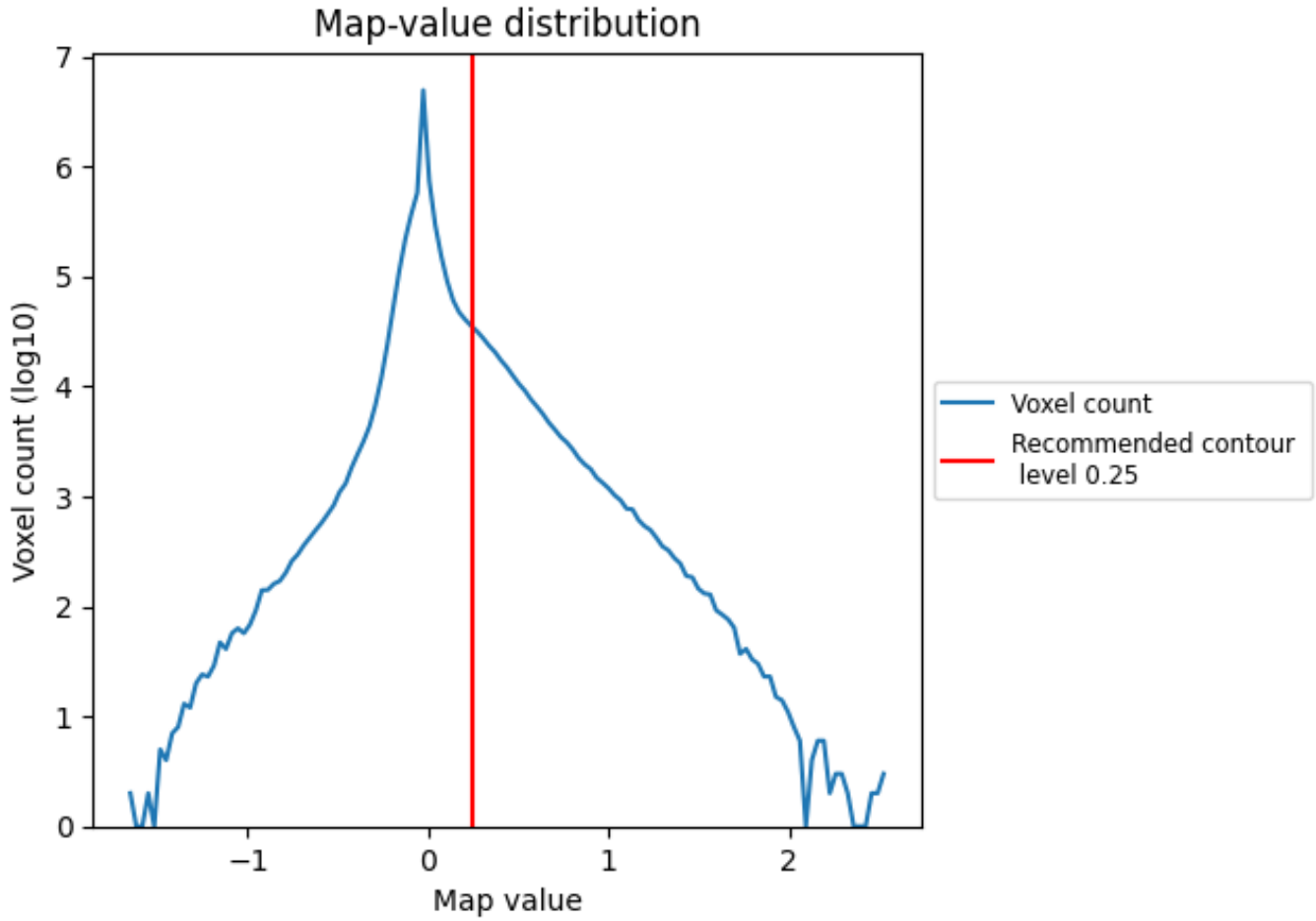
6.6 Mask visualisation (i)

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

7 Map analysis

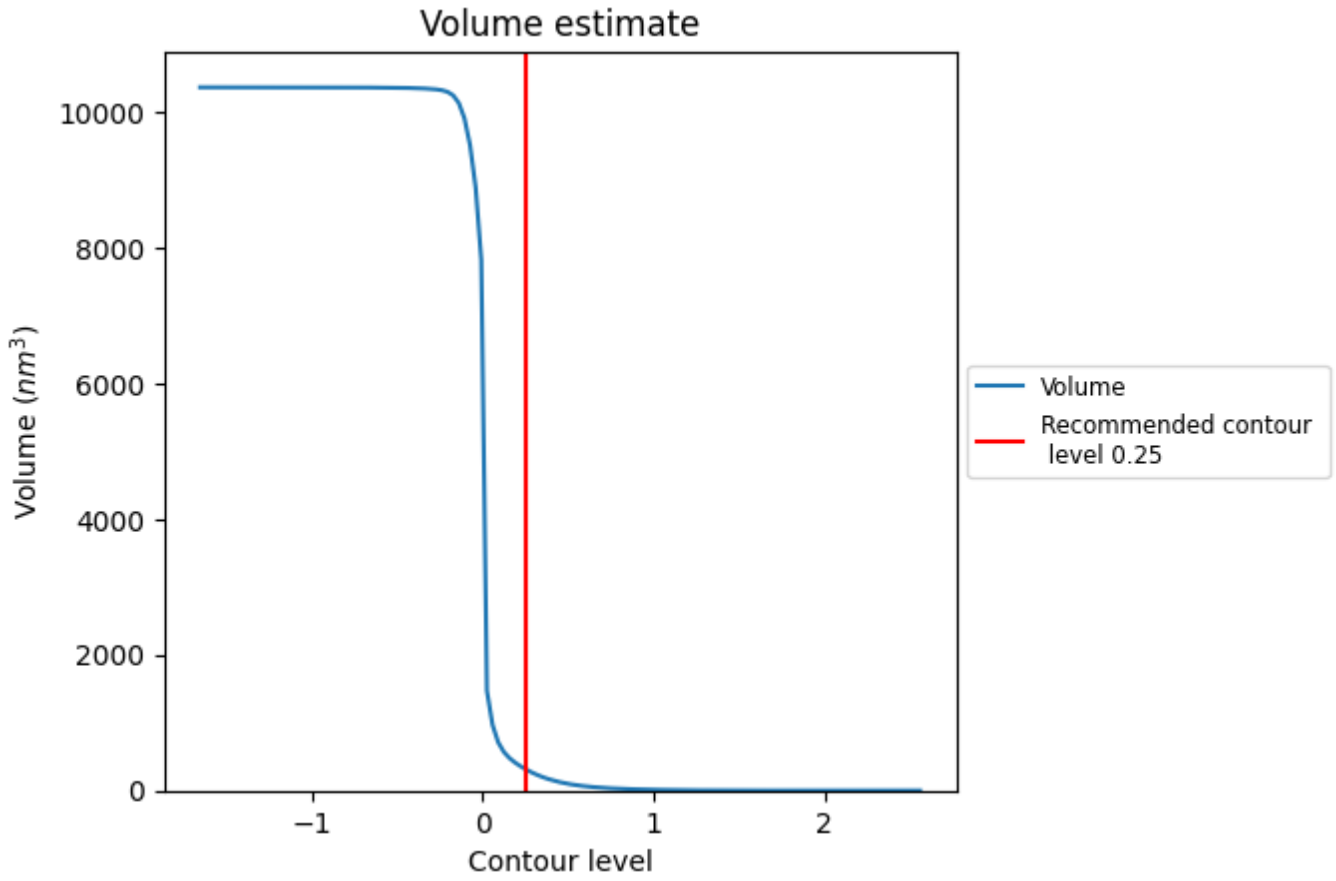
This section contains the results of statistical analysis of the map.

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.

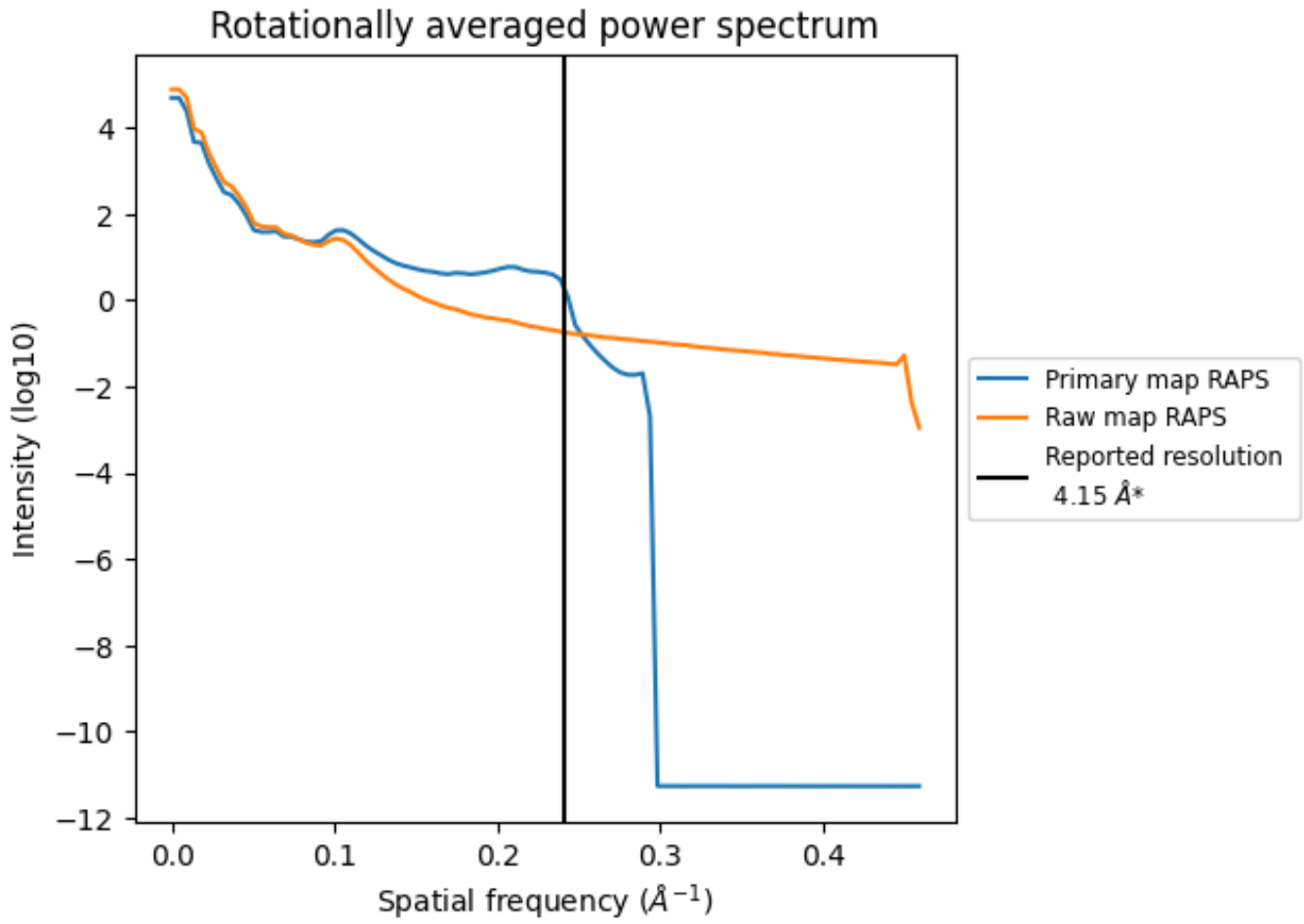
7.2 Volume estimate



The volume at the recommended contour level is 317 nm^3; this corresponds to an approximate mass of 286 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)

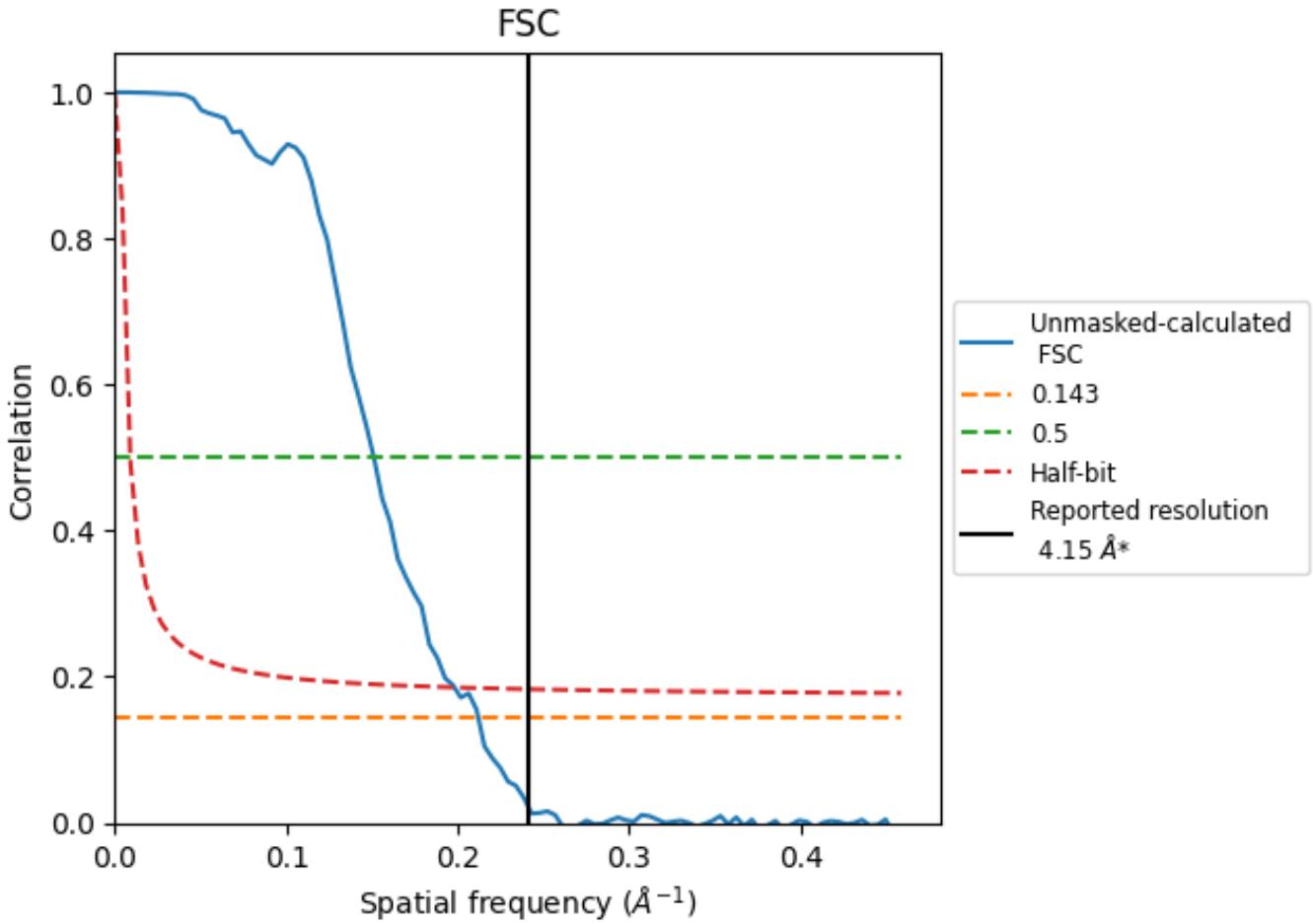


*Reported resolution corresponds to spatial frequency of 0.241 Å^{-1}

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 0.241 Å^{-1}

8.2 Resolution estimates (i)

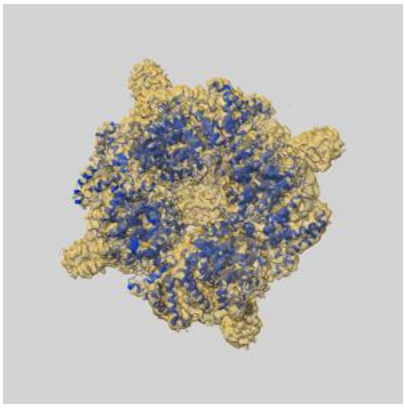
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.71	6.62	5.05

*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 4.71 differs from the reported value 4.15 by more than 10 %

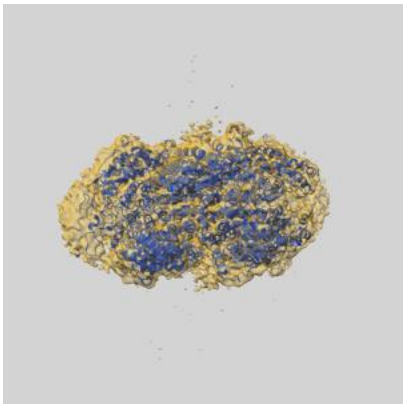
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18779 and PDB model 8QZP. Per-residue inclusion information can be found in section 3 on page 6.

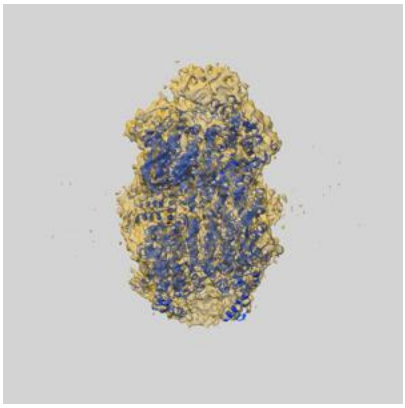
9.1 Map-model overlay



X



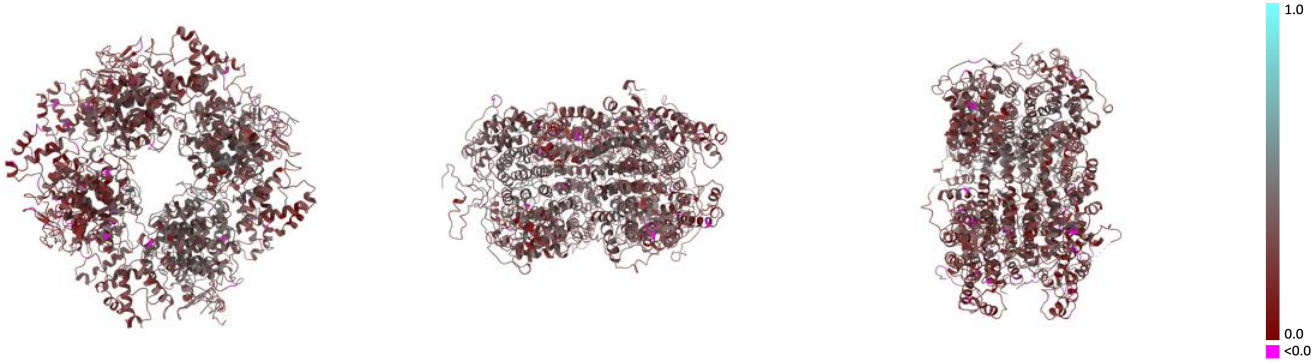
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

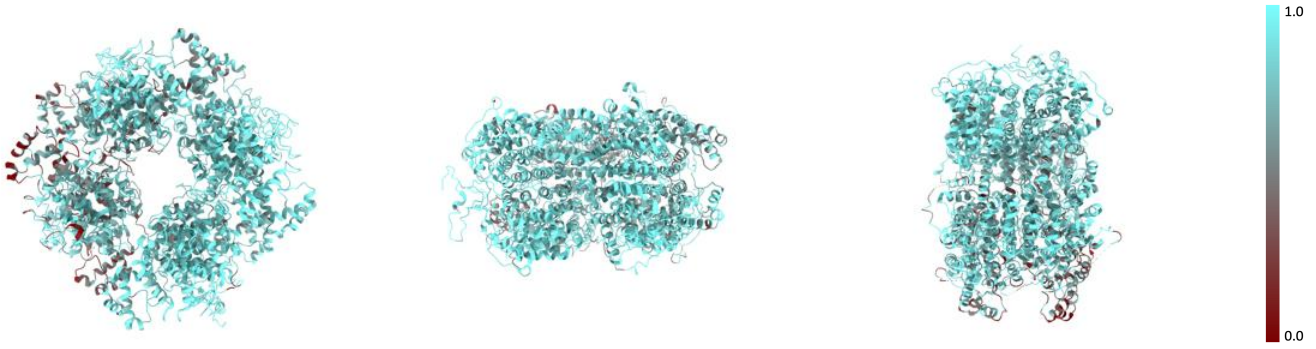
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

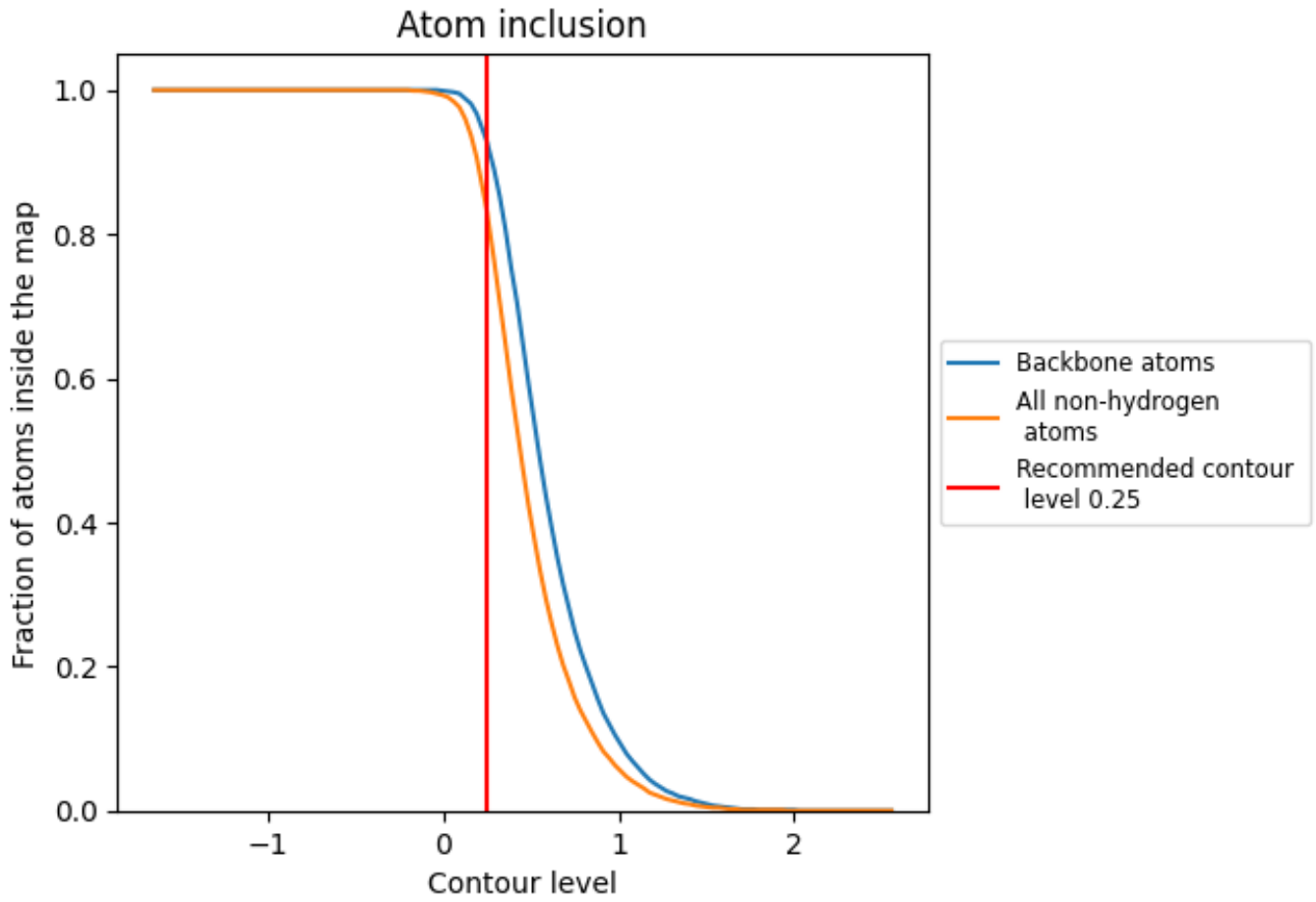
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 83% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8290	0.3040
A	0.8910	0.3290
B	0.8980	0.3230
C	0.9150	0.3620
D	0.9040	0.3540
E	0.7660	0.2590
F	0.7900	0.2840
G	0.7520	0.2710
H	0.6980	0.2450