Full wwPDB EM Validation Report (i)

Nov 13, 2022 – 05:52 PM EST

PDB ID	:	7JGG
EMDB ID	:	EMD-22326
Title	:	Cryo-EM structure of P. falciparum VAR2CSA NF45 DBL5 and DBL6 domains at 4.88 A
Authors	:	Ma, R.; Tolia, N.H.
Deposited on	:	2020-07-19
Resolution	:	4.88 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

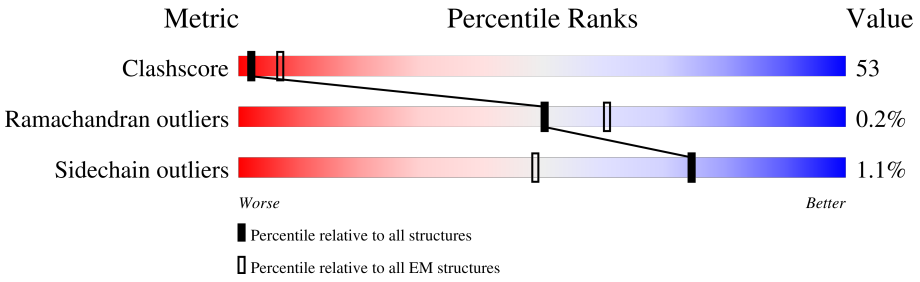
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.88 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	2653	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4210 atoms, of which 28 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 Erythrocyte membrane protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	506	4210	2643	28	713	799	27	0	0

There are 11 discrepancies between the modelled and reference sequences:

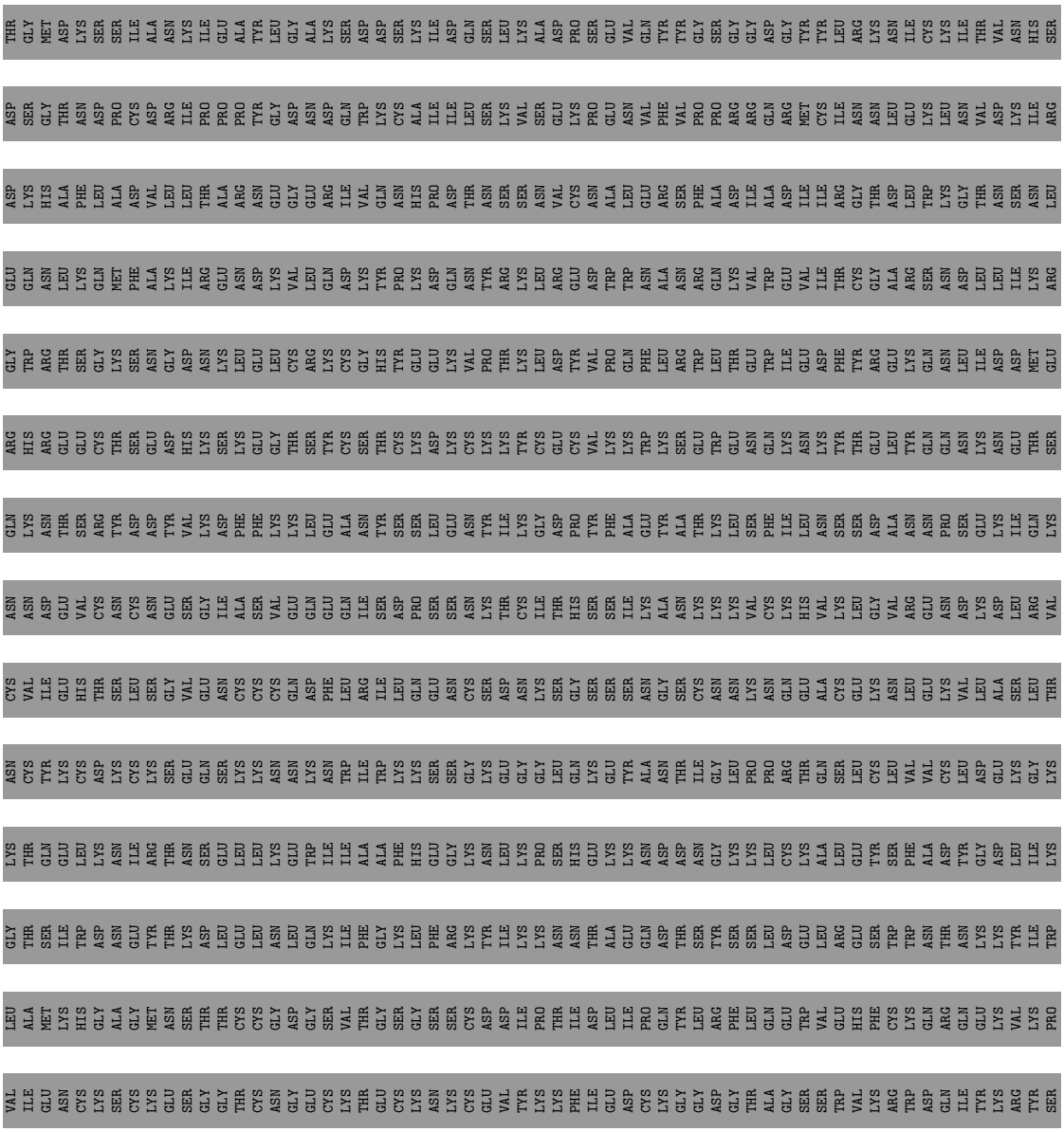
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	THR	-	expression tag	UNP W7K270
A	0	GLY	-	expression tag	UNP W7K270
A	2643	GLY	-	expression tag	UNP W7K270
A	2644	THR	-	expression tag	UNP W7K270
A	2645	LYS	-	expression tag	UNP W7K270
A	2646	HIS	-	expression tag	UNP W7K270
A	2647	HIS	-	expression tag	UNP W7K270
A	2648	HIS	-	expression tag	UNP W7K270
A	2649	HIS	-	expression tag	UNP W7K270
A	2650	HIS	-	expression tag	UNP W7K270
A	2651	HIS	-	expression tag	UNP W7K270

3 Residue-property plots (i)

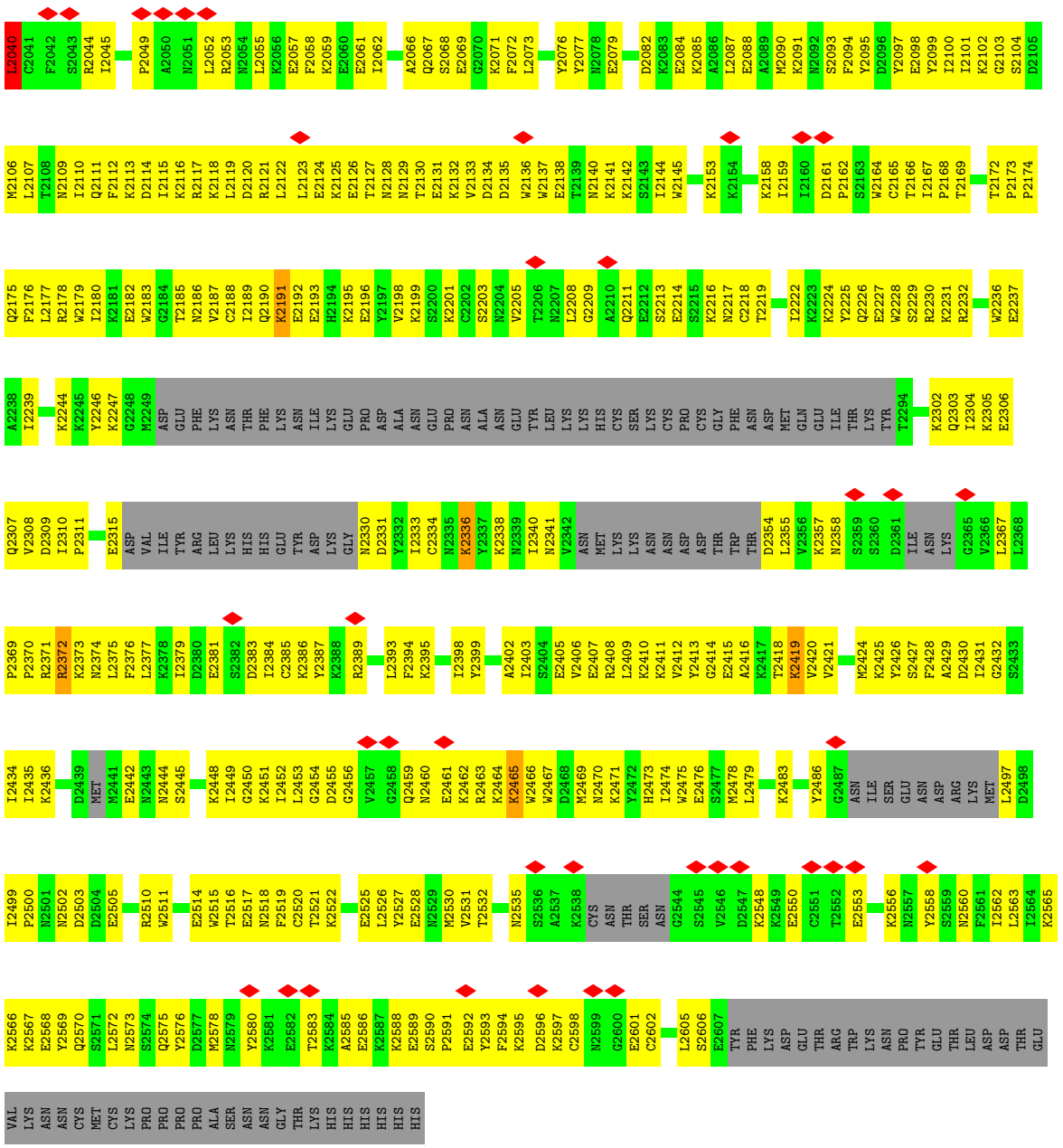
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Erythrocyte membrane protein 1

Chain A:



E2015
W2016
N2017
D2018
W2019
D2020
M2021
R2022
D2023
P2024
Y2025
N2026
K2027
Y2028
K2029
L2032
I2033
P2034
P2035
R2036
R2037
R2038
Q2039


L2040 C2041 F2042 S2043 R2044 I2045 P2049 A2050 M2051 L2052 R2053 N2054 L2055 K2056 E2057 F2058 K2059 E2060 E2061 I2062 A2066 Q2067 S2068 E2069 G2070 K2071 F2072 L2073 Y2076 Y2077 N2078 E2079 D2082 K2083 E2084 K2085 A2086 L2087 E2088 A2089 M2090 K2091 N2092 S2093 F2094 Y2095 D2096 Y2097 E2098 Y2099 I2100 I2101 K2102 G2103 S2104 D2105
M2106 L2107 T2108 N2109 I2110 Q2111 F2112 K2113 D2114 I2115 K2116 R2117 K2118 L2119 D2120 R2121 L2122 L2123 E2124 K2125 E2126 T2127 N2128 N2129 T2130 E2131 K2132 V2133 D2134 D2135 W2136 W2137 E2138 T2139 N2140 K2141 K2142 S2143 I2144 W2145 K2153 K2154 K2158 I2159 I2160 D2161 P2162 S2163 W2164 C2165 T2166 I2167 P2168 T2169 T2172 P2173 P2174
Q2175 F2176 L2177 R2178 W2179 I2180 K2181 E2182 W2183 G2184 T2185 N2186 V2187 C2188 I2189 Q2190 K2191 E2192 E2193 H2194 K2195 E2196 Y2197 V2198 K2199 S2200 K2201 C2202 S2203 N2204 V2205 T2206 N2207 L2208 G2209 A2210 Q2211 E2212 S2213 E2214 S2215 K2216 N2217 C2218 T2219 I2222 K2223 K2224 Y2225 Q2226 E2227 W2228 S2229 R2230 K2231 R2232 W2236 E2237
A2238 I2239 K2244 K2245 Y2246 K2247 G2248 M2249 ASP GLU PHE LYS ASN THR PHE LYS ASN ILE LYS GLU PRO ASP ALA ASN GLU PRO ASN ALA ASN GLU TYR LEU LYS LYS HIS CYS SER LYS CYS PRO CYS GLY PHE ASN ASP MET GLN GLU ILE THR LYS TYR T2294 K2302 Q2303 I2304 K2305 E2306
Q2307 V2308 D2309 I2310 P2311 E2315 ASP VAL ILE TYR ARG LEU LYS HIS HIS GLU TYR ASP LYS GLY N2330 D2331 Y2332 I2333 C2334 N2335 K2336 Y2337 K2338 N2339 I2340 N2341 V2342 ASN MET LYS LYS ASN ASN ASP ASP THR TRP THR D2354 L2355 V2356 K2357 N2358 S2359 S2360 D2361 ILE ASN LYS G2365 V2366 L2367 L2368
P2369 P2370 R2371 R2372 K2373 N2374 L2375 F2376 L2377 K2378 I2379 D2380 E2381 S2382 D2383 I2384 C2385 K2386 Y2387 K2388 R2389 L2393 F2394 K2395 I2398 Y2399 A2402 I2403 S2404 E2405 V2406 E2407 R2408 L2409 K2410 K2411 V2412 Y2413 G2414 E2415 A2416 K2417 T2418 R2419 V2420 V2421 M2424 K2425 Y2426 S2427 F2428 A2429 D2430 I2431 G2432 S2433
I2434 I2435 K2436 D2439 MET M2441 E2442 N2443 N2444 S2445 K2448 I2449 G2450 K2451 I2452 L2453 G2454 D2455 G2456 V2457 G2458 G2459 N2460 E2461 K2462 R2463 K2464 K2465 W2466 W2467 D2468 M2469 N2470 K2471 Y2472 H2473 I2474 W2475 E2476 S2477 M2478 L2479 K2483 Y2486 G2487 ASN ILE SER GLU ASN ASP ARG LYS MET L2497 D2498
I2499 P2500 N2501 N2502 D2503 D2504 E2505 R2510 W2511 E2514 W2515 T2516 E2517 N2518 F2519 C2520 T2521 K2522 E2525 L2526 Y2527 E2528 N2529 M2530 V2531 T2532 N2535 S2536 A2537 K2538 CYS ASN THR SER ASN G2544 S2545 V2546 D2547 K2548 K2549 E2550 C2551 T2552 E2553 K2556 N2557 Y2558 S2559 N2560 F2561 I2562 L2563 I2564 K2565
K2566 K2567 E2568 Y2569 Q2570 S2571 L2572 N2573 S2574 Q2575 Y2576 D2577 M2578 N2579 Y2580 K2581 E2582 T2583 K2584 A2585 E2586 K2587 K2588 E2589 S2590 P2591 E2592 Y2593 F2594 K2595 D2596 K2597 C2598 N2599 G2600 E2601 C2602 L2605 S2606 E2607 TYR PHE LYS ASP GLU THR ARG TRP LYS ASN PRO TYR GLU THR LEU ASP ASP THR GLU
VAL LYS ASN ASN CYS MET CYS LYS PRO PRO PRO ALA SER ASN ASN GLY THR LYS 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	157702	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 ($e^-/Å^2$)	57	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	29.549	Depositor
Minimum map value	-4.473	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.0	Depositor
Map size (Å)	317.4, 317.4, 317.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	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	0.24	0/4264	0.38	1/5710 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2040	LEU	CB-CG-CD1	5.92	121.06	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2039	GLN	Peptide

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	4182	28	4095	440	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4182	28	4095	440	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 53.

All (440) 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:A:2548:LYS:HE3	1:A:2550:GLU:HB3	1.38	1.04
1:A:2244:LYS:HG2	1:A:2247:LYS:HE2	1.37	1.03
1:A:2198:VAL:HG21	1:A:2222:ILE:HD13	1.42	1.01
1:A:2369:PRO:HG2	1:A:2372:ARG:HB3	1.44	0.98
1:A:2407:GLU:HA	1:A:2410:LYS:HZ3	1.27	0.98
1:A:2159:ILE:HG13	1:A:2167:ILE:HG22	1.47	0.97
1:A:2460:ASN:HB2	1:A:2463:ARG:HB2	1.43	0.96
1:A:2562:ILE:HG22	1:A:2566:LYS:HZ3	1.32	0.92
1:A:2386:LYS:HE3	1:A:2393:LEU:HD13	1.48	0.92
1:A:2034:PRO:HG2	1:A:2037:ARG:HB3	1.55	0.88
1:A:2103:GLY:HA2	1:A:2175:GLN:HE22	1.38	0.88
1:A:2111:GLN:HB3	1:A:2115:ILE:HD13	1.57	0.87
1:A:2563:LEU:HA	1:A:2566:LYS:HE2	1.56	0.85
1:A:2383:ASP:HA	1:A:2386:LYS:HD3	1.57	0.85
1:A:2224:LYS:O	1:A:2227:GLU:HG3	1.78	0.83
1:A:2188:CYS:O	1:A:2191:LYS:HG3	1.77	0.83
1:A:2406:VAL:HG11	1:A:2474:ILE:HD12	1.61	0.81
1:A:2569:TYR:HA	1:A:2572:LEU:HD12	1.62	0.80
1:A:2199:LYS:O	1:A:2203:SER:OG	1.99	0.80
1:A:2562:ILE:HG22	1:A:2566:LYS:NZ	1.98	0.78
1:A:2516:THR:HG22	1:A:2605:LEU:HD22	1.66	0.78
1:A:2023:ASP:HB3	1:A:2024:PRO:HD3	1.64	0.78
1:A:2176:PHE:CZ	1:A:2180:ILE:HD11	2.19	0.78
1:A:2021:MET:HE1	1:A:2032:LEU:HD12	1.66	0.78
1:A:2436:LYS:HE2	1:A:2464:LYS:HA	1.66	0.78
1:A:2052:LEU:HD23	1:A:2057:GLU:HG2	1.66	0.77
1:A:2135:ASP:O	1:A:2138:GLU:HG3	1.84	0.77
1:A:2602:CYS:HA	1:A:2605:LEU:HG	1.65	0.76
1:A:2044:ARG:HE	1:A:2045:ILE:H	1.30	0.76
1:A:2588:LYS:HZ3	1:A:2592:GLU:HB3	1.51	0.76
1:A:2376:PHE:HB2	1:A:2405:GLU:HG2	1.67	0.75
1:A:2053:ARG:HH21	1:A:2057:GLU:HG3	1.48	0.75
1:A:2465:LYS:HD2	1:A:2469:MET:HE2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2236:TRP:O	1:A:2239:ILE:HG22	1.86	0.75
1:A:2379:ILE:HD11	1:A:2444:ASN:HB2	1.69	0.74
1:A:2179:TRP:O	1:A:2182:GLU:HG3	1.88	0.74
1:A:2558:TYR:CE2	1:A:2562:ILE:HD11	2.22	0.74
1:A:2058:PHE:O	1:A:2061:GLU:HG3	1.87	0.73
1:A:2462:LYS:O	1:A:2465:LYS:HG3	1.88	0.73
1:A:2100:ILE:O	1:A:2113:LYS:NZ	2.21	0.73
1:A:2044:ARG:HH21	1:A:2045:ILE:HG12	1.54	0.73
1:A:2222:ILE:HG21	1:A:2308:VAL:HG21	1.70	0.73
1:A:2521:THR:OG1	1:A:2522:LYS:NZ	2.20	0.73
1:A:2602:CYS:SG	1:A:2605:LEU:HD12	2.30	0.72
1:A:2069:GLU:O	1:A:2073:LEU:HG	1.89	0.72
1:A:2355:LEU:HD21	1:A:2374:ASN:HD22	1.55	0.72
1:A:2453:LEU:HD22	1:A:2455:ASP:OD1	1.89	0.72
1:A:2186:ASN:O	1:A:2190:GLN:HG2	1.89	0.72
1:A:2084:GLU:OE2	1:A:2085:LYS:NZ	2.23	0.71
1:A:2132:LYS:HA	1:A:2135:ASP:OD2	1.90	0.71
1:A:2370:PRO:O	1:A:2373:LYS:NZ	2.23	0.71
1:A:2173:PRO:HD2	1:A:2178:ARG:HD2	1.73	0.70
1:A:2435:ILE:HD11	1:A:2467:TRP:HB2	1.74	0.70
1:A:2394:PHE:CZ	1:A:2398:ILE:HD11	2.26	0.69
1:A:2407:GLU:HB3	1:A:2411:LYS:NZ	2.08	0.69
1:A:2588:LYS:NZ	1:A:2592:GLU:HB3	2.07	0.69
1:A:2455:ASP:OD2	1:A:2463:ARG:NH1	2.26	0.69
1:A:2456:GLY:H	1:A:2459:GLN:HE21	1.41	0.69
1:A:2381:GLU:HA	1:A:2384:ILE:HG12	1.73	0.68
1:A:2572:LEU:HD23	1:A:2575:GLN:OE1	1.94	0.68
1:A:2066:ALA:HB1	1:A:2144:ILE:HD13	1.76	0.68
1:A:2517:GLU:O	1:A:2521:THR:HG23	1.93	0.68
1:A:2059:LYS:O	1:A:2062:ILE:HG22	1.93	0.68
1:A:2153:LYS:HD2	1:A:2164:TRP:HA	1.75	0.68
1:A:2017:ASN:HB2	1:A:2020:ASP:HB3	1.75	0.68
1:A:2384:ILE:HD12	1:A:2451:LYS:HD2	1.76	0.67
1:A:2306:GLU:HA	1:A:2309:ASP:OD2	1.95	0.67
1:A:2471:LYS:HE3	1:A:2499:ILE:HG21	1.76	0.67
1:A:2058:PHE:HE2	1:A:2116:LYS:HD3	1.60	0.67
1:A:2330:ASN:OD1	1:A:2331:ASP:N	2.27	0.67
1:A:2130:THR:O	1:A:2133:VAL:HG22	1.94	0.67
1:A:2208:LEU:O	1:A:2211:GLN:NE2	2.28	0.67
1:A:2219:THR:O	1:A:2222:ILE:HG22	1.95	0.67
1:A:2450:GLY:HA2	1:A:2454:GLY:HA2	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2588:LYS:HZ3	1:A:2592:GLU:CB	2.08	0.67
1:A:2566:LYS:O	1:A:2570:GLN:N	2.22	0.66
1:A:2189:ILE:O	1:A:2193:GLU:HG2	1.94	0.66
1:A:2562:ILE:O	1:A:2565:LYS:HB3	1.95	0.66
1:A:2421:VAL:HA	1:A:2424:MET:CE	2.26	0.66
1:A:2053:ARG:NH2	1:A:2057:GLU:HG3	2.11	0.66
1:A:2575:GLN:HA	1:A:2578:MET:CE	2.26	0.66
1:A:2416:ALA:HB3	1:A:2419:LYS:CG	2.26	0.66
1:A:2174:PRO:HG2	1:A:2177:LEU:HD12	1.79	0.65
1:A:2355:LEU:HA	1:A:2358:ASN:OD1	1.96	0.65
1:A:2589:GLU:O	1:A:2593:TYR:N	2.25	0.65
1:A:2305:LYS:HG2	1:A:2307:GLN:H	1.61	0.65
1:A:2035:PRO:HA	1:A:2038:ARG:HG2	1.78	0.65
1:A:2479:LEU:HD21	1:A:2497:LEU:HD22	1.77	0.65
1:A:2084:GLU:O	1:A:2087:LEU:HG	1.97	0.65
1:A:2460:ASN:O	1:A:2464:LYS:N	2.29	0.65
1:A:2129:ASN:ND2	1:A:2131:GLU:HB2	2.12	0.64
1:A:2158:LYS:HD2	1:A:2167:ILE:HG23	1.79	0.64
1:A:2453:LEU:HD23	1:A:2453:LEU:O	1.97	0.64
1:A:2138:GLU:O	1:A:2142:LYS:HG2	1.98	0.64
1:A:2421:VAL:HA	1:A:2424:MET:HE2	1.79	0.64
1:A:2067:GLN:O	1:A:2071:LYS:HG2	1.98	0.64
1:A:2394:PHE:CE2	1:A:2398:ILE:HD11	2.33	0.64
1:A:2432:GLY:O	1:A:2436:LYS:HG2	1.98	0.64
1:A:2455:ASP:OD2	1:A:2463:ARG:HD2	1.98	0.64
1:A:2465:LYS:CD	1:A:2469:MET:HE2	2.27	0.64
1:A:2191:LYS:HE3	1:A:2192:GLU:OE2	1.97	0.63
1:A:2372:ARG:HB2	1:A:2430:ASP:OD1	1.98	0.63
1:A:2594:PHE:O	1:A:2597:LYS:HG2	1.98	0.63
1:A:2474:ILE:HG22	1:A:2478:MET:CE	2.29	0.63
1:A:2176:PHE:O	1:A:2180:ILE:HG13	1.99	0.62
1:A:2590:SER:HB2	1:A:2591:PRO:HD3	1.81	0.62
1:A:2018:ASP:O	1:A:2022:ARG:HG2	2.00	0.62
1:A:2161:ASP:HB2	1:A:2164:TRP:O	2.00	0.62
1:A:2088:GLU:HA	1:A:2091:LYS:HE3	1.80	0.62
1:A:2575:GLN:HA	1:A:2578:MET:HE2	1.82	0.62
1:A:2474:ILE:O	1:A:2478:MET:HE2	2.00	0.62
1:A:2435:ILE:O	1:A:2463:ARG:NE	2.25	0.61
1:A:2141:LYS:O	1:A:2144:ILE:HG22	1.99	0.61
1:A:2407:GLU:HA	1:A:2410:LYS:NZ	2.11	0.61
1:A:2405:GLU:O	1:A:2409:LEU:HD23	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2415:GLU:OE2	1:A:2486:TYR:OH	2.08	0.61
1:A:2103:GLY:HA2	1:A:2175:GLN:NE2	2.12	0.61
1:A:2228:TRP:CZ3	1:A:2231:LYS:HD2	2.36	0.61
1:A:2522:LYS:O	1:A:2526:LEU:HD23	2.01	0.61
1:A:2099:TYR:CE1	1:A:2178:ARG:HB3	2.36	0.61
1:A:2124:GLU:HG3	1:A:2132:LYS:HD3	1.82	0.61
1:A:2103:GLY:CA	1:A:2175:GLN:HE22	2.12	0.61
1:A:2563:LEU:HA	1:A:2566:LYS:CE	2.28	0.60
1:A:2429:ALA:HB2	1:A:2510:ARG:HH12	1.65	0.60
1:A:2119:LEU:HD12	1:A:2120:ASP:N	2.17	0.60
1:A:2121:ARG:HA	1:A:2128:ASN:HB3	1.82	0.60
1:A:2053:ARG:HH22	1:A:2061:GLU:HG2	1.66	0.60
1:A:2473:HIS:O	1:A:2476:GLU:HG3	2.02	0.60
1:A:2058:PHE:CE2	1:A:2116:LYS:HD3	2.36	0.60
1:A:2073:LEU:HD13	1:A:2093:SER:HB2	1.84	0.59
1:A:2116:LYS:O	1:A:2119:LEU:HG	2.01	0.59
1:A:2413:TYR:HB3	1:A:2420:VAL:HG22	1.84	0.59
1:A:2416:ALA:HB3	1:A:2419:LYS:HG3	1.83	0.59
1:A:2475:TRP:O	1:A:2478:MET:HG2	2.02	0.59
1:A:2099:TYR:HE1	1:A:2178:ARG:HB3	1.68	0.59
1:A:2448:LYS:HE3	1:A:2451:LYS:HZ1	1.68	0.59
1:A:2518:ASN:O	1:A:2522:LYS:HG2	2.03	0.59
1:A:2183:TRP:NE1	1:A:2239:ILE:HG21	2.17	0.59
1:A:2518:ASN:OD1	1:A:2519:PHE:N	2.35	0.59
1:A:2034:PRO:HG2	1:A:2037:ARG:CB	2.28	0.59
1:A:2021:MET:HE1	1:A:2032:LEU:HA	1.85	0.59
1:A:2137:TRP:HA	1:A:2140:ASN:ND2	2.18	0.58
1:A:2124:GLU:HG3	1:A:2132:LYS:CD	2.33	0.58
1:A:2033:ILE:O	1:A:2038:ARG:NH2	2.35	0.58
1:A:2190:GLN:HB3	1:A:2232:ARG:HH22	1.68	0.58
1:A:2385:CYS:SG	1:A:2389:ARG:NE	2.76	0.58
1:A:2502:ASN:O	1:A:2510:ARG:HD3	2.02	0.58
1:A:2408:ARG:NH1	1:A:2412:VAL:HG11	2.18	0.58
1:A:2516:THR:HG21	1:A:2605:LEU:HB3	1.85	0.58
1:A:2407:GLU:HG2	1:A:2410:LYS:NZ	2.19	0.58
1:A:2408:ARG:O	1:A:2412:VAL:HG22	2.04	0.58
1:A:2428:PHE:O	1:A:2431:ILE:HG12	2.04	0.58
1:A:2114:ASP:O	1:A:2118:LYS:HD3	2.03	0.57
1:A:2336:LYS:NZ	1:A:2476:GLU:OE2	2.26	0.57
1:A:2460:ASN:CB	1:A:2463:ARG:HB2	2.27	0.57
1:A:2516:THR:CG2	1:A:2605:LEU:HD13	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2418:THR:O	1:A:2421:VAL:HG12	2.04	0.57
1:A:2511:TRP:O	1:A:2514:GLU:HG2	2.04	0.57
1:A:2213:SER:HA	1:A:2216:LYS:HD3	1.86	0.56
1:A:2407:GLU:HB3	1:A:2411:LYS:HZ1	1.69	0.56
1:A:2053:ARG:NH2	1:A:2061:GLU:HG2	2.20	0.56
1:A:2372:ARG:HH21	1:A:2442:GLU:HB3	1.70	0.56
1:A:2098:GLU:HA	1:A:2101:ILE:HG12	1.88	0.56
1:A:2173:PRO:HD2	1:A:2178:ARG:HH11	1.69	0.56
1:A:2305:LYS:O	1:A:2308:VAL:HG12	2.06	0.56
1:A:2414:GLY:HA3	1:A:2419:LYS:NZ	2.20	0.56
1:A:2173:PRO:HD2	1:A:2178:ARG:CD	2.36	0.56
1:A:2442:GLU:HG3	1:A:2445:SER:HB3	1.87	0.56
1:A:2525:GLU:O	1:A:2528:GLU:HG3	2.06	0.56
1:A:2069:GLU:HB3	1:A:2097:TYR:OH	2.06	0.56
1:A:2055:LEU:HB2	1:A:2123:LEU:HD22	1.86	0.56
1:A:2427:SER:O	1:A:2431:ILE:HG23	2.05	0.56
1:A:2434:ILE:HD11	1:A:2442:GLU:HG3	1.86	0.56
1:A:2448:LYS:HE3	1:A:2451:LYS:NZ	2.21	0.56
1:A:2049:PRO:HB2	1:A:2052:LEU:HB3	1.88	0.55
1:A:2124:GLU:HB3	1:A:2132:LYS:NZ	2.20	0.55
1:A:2367:LEU:HB3	1:A:2567:LYS:NZ	2.21	0.55
1:A:2188:CYS:SG	1:A:2189:ILE:N	2.79	0.55
1:A:2449:ILE:HG23	1:A:2455:ASP:OD2	2.06	0.55
1:A:2531:VAL:HA	1:A:2535:ASN:OD1	2.05	0.55
1:A:2340:ILE:HD12	1:A:2403:ILE:HD11	1.88	0.55
1:A:2448:LYS:O	1:A:2451:LYS:HG2	2.06	0.55
1:A:2566:LYS:O	1:A:2570:GLN:HG2	2.06	0.55
1:A:2183:TRP:HE1	1:A:2239:ILE:HG21	1.72	0.55
1:A:2435:ILE:HD11	1:A:2467:TRP:CD1	2.42	0.55
1:A:2528:GLU:HA	1:A:2531:VAL:HG22	1.88	0.55
1:A:2118:LYS:O	1:A:2122:LEU:HD23	2.07	0.54
1:A:2158:LYS:HB3	1:A:2167:ILE:HG23	1.88	0.54
1:A:2182:GLU:O	1:A:2185:THR:HG22	2.07	0.54
1:A:2586:GLU:OE2	1:A:2590:SER:OG	2.23	0.54
1:A:2055:LEU:HG	1:A:2059:LYS:NZ	2.23	0.54
1:A:2059:LYS:HG2	1:A:2136:TRP:CZ2	2.42	0.54
1:A:2413:TYR:O	1:A:2419:LYS:NZ	2.40	0.54
1:A:2470:ASN:O	1:A:2474:ILE:HG12	2.08	0.54
1:A:2137:TRP:HA	1:A:2140:ASN:HD22	1.73	0.54
1:A:2602:CYS:HA	1:A:2605:LEU:CG	2.38	0.54
1:A:2355:LEU:HD22	1:A:2373:LYS:HZ3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2576:TYR:O	1:A:2580:TYR:N	2.41	0.54
1:A:2017:ASN:ND2	1:A:2020:ASP:OD1	2.40	0.53
1:A:2196:GLU:HA	1:A:2199:LYS:HG2	1.91	0.53
1:A:2409:LEU:HD12	1:A:2413:TYR:CZ	2.43	0.53
1:A:2479:LEU:HD11	1:A:2483:LYS:HE3	1.89	0.53
1:A:2021:MET:CE	1:A:2032:LEU:HA	2.39	0.53
1:A:2461:GLU:HG2	1:A:2462:LYS:N	2.24	0.53
1:A:2027:LYS:NZ	1:A:2029:LYS:HB2	2.23	0.53
1:A:2205:VAL:O	1:A:2209:GLY:HA3	2.08	0.53
1:A:2465:LYS:HD2	1:A:2469:MET:CE	2.39	0.53
1:A:2475:TRP:CH2	1:A:2500:PRO:HD2	2.43	0.53
1:A:2118:LYS:NZ	1:A:2121:ARG:HH12	2.07	0.52
1:A:2111:GLN:O	1:A:2115:ILE:HG12	2.09	0.52
1:A:2159:ILE:HD12	1:A:2168:PRO:CD	2.39	0.52
1:A:2033:ILE:HG13	1:A:2038:ARG:HB3	1.90	0.52
1:A:2336:LYS:O	1:A:2340:ILE:HG12	2.09	0.52
1:A:2589:GLU:O	1:A:2593:TYR:HB2	2.09	0.52
1:A:2153:LYS:HG3	1:A:2165:CYS:N	2.25	0.52
1:A:2173:PRO:HD2	1:A:2178:ARG:CG	2.40	0.52
1:A:2244:LYS:O	1:A:2247:LYS:HG2	2.09	0.52
1:A:2101:ILE:HB	1:A:2137:TRP:CE3	2.44	0.52
1:A:2407:GLU:CA	1:A:2410:LYS:HZ3	2.13	0.52
1:A:2449:ILE:HA	1:A:2452:ILE:HD11	1.91	0.52
1:A:2021:MET:CE	1:A:2032:LEU:HD12	2.37	0.52
1:A:2158:LYS:HD2	1:A:2167:ILE:CG2	2.40	0.52
1:A:2471:LYS:HE3	1:A:2499:ILE:HD13	1.92	0.52
1:A:2379:ILE:HA	1:A:2448:LYS:NZ	2.25	0.52
1:A:2598:CYS:HB3	1:A:2601:GLU:H	1.75	0.52
1:A:2461:GLU:HG2	1:A:2462:LYS:H	1.75	0.51
1:A:2052:LEU:CD2	1:A:2057:GLU:HG2	2.38	0.51
1:A:2227:GLU:HA	1:A:2230:ARG:HD2	1.91	0.51
1:A:2357:LYS:HD2	1:A:2357:LYS:N	2.24	0.51
1:A:2039:GLN:O	1:A:2040:LEU:CD1	2.59	0.51
1:A:2355:LEU:HD13	1:A:2374:ASN:HB3	1.93	0.51
1:A:2402:ALA:O	1:A:2406:VAL:HG13	2.10	0.51
1:A:2403:ILE:O	1:A:2406:VAL:HG22	2.11	0.51
1:A:2575:GLN:HA	1:A:2578:MET:HE3	1.93	0.51
1:A:2195:LYS:HA	1:A:2198:VAL:HG12	1.93	0.51
1:A:2138:GLU:O	1:A:2142:LYS:NZ	2.34	0.51
1:A:2435:ILE:CD1	1:A:2467:TRP:HB2	2.40	0.51
1:A:2308:VAL:O	1:A:2311:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2474:ILE:HG22	1:A:2478:MET:HE2	1.92	0.51
1:A:2213:SER:HA	1:A:2216:LYS:CD	2.40	0.51
1:A:2381:GLU:HA	1:A:2384:ILE:CG1	2.41	0.51
1:A:2044:ARG:NH2	1:A:2045:ILE:HG12	2.24	0.50
1:A:2069:GLU:HB3	1:A:2097:TYR:CZ	2.46	0.50
1:A:2355:LEU:HD11	1:A:2374:ASN:ND2	2.26	0.50
1:A:2386:LYS:HE3	1:A:2393:LEU:CD1	2.31	0.50
1:A:2530:MET:SD	1:A:2531:VAL:HG13	2.51	0.50
1:A:2568:GLU:O	1:A:2572:LEU:HG	2.11	0.50
1:A:2407:GLU:O	1:A:2411:LYS:HE2	2.11	0.50
1:A:2516:THR:CG2	1:A:2605:LEU:HB3	2.41	0.50
1:A:2409:LEU:HA	1:A:2412:VAL:HG22	1.93	0.50
1:A:2371:ARG:HG3	1:A:2426:TYR:HD2	1.76	0.50
1:A:2431:ILE:HA	1:A:2434:ILE:HG22	1.92	0.50
1:A:2569:TYR:HA	1:A:2572:LEU:HB2	1.93	0.50
1:A:2436:LYS:HB3	1:A:2460:ASN:ND2	2.27	0.50
1:A:2126:GLU:O	1:A:2127:THR:OG1	2.28	0.50
1:A:2159:ILE:HB	1:A:2166:THR:O	2.12	0.50
1:A:2428:PHE:CZ	1:A:2478:MET:HE1	2.47	0.50
1:A:2449:ILE:HG12	1:A:2463:ARG:NH2	2.26	0.50
1:A:2176:PHE:HB2	1:A:2246:TYR:HE2	1.77	0.50
1:A:2116:LYS:HA	1:A:2119:LEU:CD2	2.41	0.49
1:A:2076:TYR:O	1:A:2079:GLU:HB3	2.12	0.49
1:A:2173:PRO:CD	1:A:2178:ARG:HH11	2.25	0.49
1:A:2304:ILE:HG21	1:A:2308:VAL:HG11	1.93	0.49
1:A:2385:CYS:O	1:A:2389:ARG:HG3	2.12	0.49
1:A:2102:LYS:NZ	1:A:2134:ASP:O	2.46	0.49
1:A:2087:LEU:HD12	1:A:2088:GLU:N	2.27	0.49
1:A:2414:GLY:HA3	1:A:2419:LYS:HZ2	1.77	0.49
1:A:2466:TRP:HA	1:A:2469:MET:HE3	1.95	0.49
1:A:2121:ARG:HA	1:A:2128:ASN:HD22	1.77	0.49
1:A:2109:ASN:HB3	1:A:2112:PHE:HD1	1.77	0.48
1:A:2145:TRP:CZ2	1:A:2169:THR:HA	2.48	0.48
1:A:2055:LEU:O	1:A:2059:LYS:HG3	2.13	0.48
1:A:2431:ILE:O	1:A:2435:ILE:HG23	2.14	0.48
1:A:2505:GLU:HB2	1:A:2510:ARG:HG3	1.95	0.48
1:A:2159:ILE:HD12	1:A:2168:PRO:HD3	1.95	0.48
1:A:2436:LYS:CE	1:A:2464:LYS:HA	2.40	0.48
1:A:2431:ILE:O	1:A:2434:ILE:HG22	2.12	0.48
1:A:2044:ARG:HE	1:A:2045:ILE:N	2.05	0.48
1:A:2106:MET:O	1:A:2107:LEU:HD22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2407:GLU:HB3	1:A:2411:LYS:HZ3	1.76	0.48
1:A:2164:TRP:NE1	1:A:2166:THR:OG1	2.41	0.48
1:A:2387:TYR:CD1	1:A:2394:PHE:HB2	2.49	0.48
1:A:2528:GLU:O	1:A:2532:THR:HG22	2.13	0.48
1:A:2018:ASP:OD2	1:A:2018:ASP:N	2.45	0.47
1:A:2125:LYS:HE3	1:A:2128:ASN:HA	1.96	0.47
1:A:2338:LYS:HA	1:A:2341:ASN:OD1	2.14	0.47
1:A:2164:TRP:CZ2	1:A:2166:THR:HG21	2.49	0.47
1:A:2183:TRP:O	1:A:2187:VAL:HG12	2.14	0.47
1:A:2394:PHE:O	1:A:2398:ILE:HG13	2.14	0.47
1:A:2104:SER:H	1:A:2117:ARG:HH22	1.61	0.47
1:A:2158:LYS:N	1:A:2165:CYS:SG	2.83	0.47
1:A:2172:THR:HG23	1:A:2172:THR:O	2.14	0.47
1:A:2428:PHE:HZ	1:A:2478:MET:HE1	1.79	0.47
1:A:2435:ILE:HD11	1:A:2467:TRP:CB	2.43	0.47
1:A:2516:THR:HG22	1:A:2605:LEU:HD13	1.96	0.47
1:A:2355:LEU:HB3	1:A:2373:LYS:NZ	2.29	0.47
1:A:2426:TYR:HA	1:A:2514:GLU:OE1	2.14	0.47
1:A:2153:LYS:HG3	1:A:2165:CYS:H	1.80	0.47
1:A:2052:LEU:HD23	1:A:2052:LEU:O	2.15	0.47
1:A:2110:ILE:H	1:A:2110:ILE:HD12	1.80	0.47
1:A:2116:LYS:HA	1:A:2119:LEU:HD21	1.96	0.47
1:A:2141:LYS:HB3	1:A:2142:LYS:NZ	2.30	0.46
1:A:2217:ASN:OD1	1:A:2218:CYS:N	2.48	0.46
1:A:2449:ILE:HG12	1:A:2463:ARG:CZ	2.44	0.46
1:A:2035:PRO:CA	1:A:2038:ARG:HG2	2.45	0.46
1:A:2082:ASP:HB3	1:A:2085:LYS:HB2	1.96	0.46
1:A:2479:LEU:O	1:A:2483:LYS:HG3	2.16	0.46
1:A:2124:GLU:HB3	1:A:2132:LYS:HZ2	1.80	0.46
1:A:2201:LYS:HZ1	1:A:2218:CYS:HA	1.80	0.46
1:A:2371:ARG:HG3	1:A:2426:TYR:CD2	2.50	0.46
1:A:2421:VAL:HA	1:A:2424:MET:HE3	1.97	0.46
1:A:2475:TRP:HA	1:A:2478:MET:CE	2.45	0.46
1:A:2379:ILE:HD13	1:A:2448:LYS:HD2	1.97	0.46
1:A:2449:ILE:HA	1:A:2452:ILE:CD1	2.45	0.46
1:A:2588:LYS:NZ	1:A:2596:ASP:OD2	2.41	0.46
1:A:2315:GLU:N	1:A:2315:GLU:OE1	2.49	0.46
1:A:2409:LEU:HD12	1:A:2413:TYR:CE2	2.50	0.46
1:A:2583:THR:O	1:A:2583:THR:HG23	2.15	0.46
1:A:2128:ASN:OD1	1:A:2132:LYS:HE3	2.16	0.46
1:A:2216:LYS:O	1:A:2219:THR:OG1	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2173:PRO:CD	1:A:2178:ARG:HD2	2.44	0.46
1:A:2403:ILE:O	1:A:2407:GLU:HG3	2.16	0.46
1:A:2515:TRP:HZ3	1:A:2575:GLN:NE2	2.14	0.46
1:A:2553:GLU:HA	1:A:2556:LYS:HD3	1.98	0.46
1:A:2205:VAL:HG21	1:A:2311:PRO:HG3	1.97	0.45
1:A:2569:TYR:O	1:A:2573:ASN:N	2.37	0.45
1:A:2027:LYS:HZ2	1:A:2029:LYS:HB2	1.81	0.45
1:A:2053:ARG:HH22	1:A:2058:PHE:HA	1.80	0.45
1:A:2425:LYS:HG3	1:A:2503:ASP:OD1	2.16	0.45
1:A:2035:PRO:HA	1:A:2038:ARG:HD2	1.97	0.45
1:A:2442:GLU:O	1:A:2442:GLU:HG2	2.16	0.45
1:A:2591:PRO:O	1:A:2595:LYS:HG2	2.16	0.45
1:A:2016:TRP:HD1	1:A:2038:ARG:HH12	1.63	0.45
1:A:2141:LYS:NZ	1:A:2145:TRP:HB2	2.31	0.45
1:A:2527:TYR:OH	1:A:2558:TYR:OH	2.35	0.45
1:A:2409:LEU:HD12	1:A:2413:TYR:OH	2.16	0.45
1:A:2141:LYS:HZ1	1:A:2145:TRP:HB2	1.82	0.45
1:A:2475:TRP:HA	1:A:2478:MET:HG2	1.98	0.45
1:A:2370:PRO:O	1:A:2373:LYS:HG2	2.16	0.45
1:A:2099:TYR:HE1	1:A:2178:ARG:HE	1.65	0.45
1:A:2304:ILE:CG2	1:A:2308:VAL:HG11	2.47	0.44
1:A:2073:LEU:HD13	1:A:2093:SER:CB	2.47	0.44
1:A:2515:TRP:HZ3	1:A:2575:GLN:HE22	1.65	0.44
1:A:2033:ILE:HD12	1:A:2038:ARG:HA	1.99	0.44
1:A:2188:CYS:O	1:A:2192:GLU:OE1	2.36	0.44
1:A:2205:VAL:HG21	1:A:2311:PRO:CG	2.47	0.44
1:A:2237:GLU:HA	1:A:2237:GLU:OE1	2.16	0.44
1:A:2244:LYS:HG2	1:A:2247:LYS:CE	2.27	0.44
1:A:2029:LYS:HD2	1:A:2029:LYS:HA	1.76	0.44
1:A:2303:GLN:C	1:A:2304:ILE:HD13	2.38	0.44
1:A:2333:ILE:HG13	1:A:2334:CYS:N	2.33	0.44
1:A:2035:PRO:O	1:A:2038:ARG:HG2	2.18	0.44
1:A:2077:TYR:HE2	1:A:2090:MET:CE	2.29	0.44
1:A:2077:TYR:HE2	1:A:2090:MET:HE1	1.83	0.44
1:A:2090:MET:SD	1:A:2094:PHE:CZ	3.11	0.44
1:A:2159:ILE:HD12	1:A:2168:PRO:HD2	2.00	0.44
1:A:2357:LYS:HD2	1:A:2357:LYS:H	1.82	0.44
1:A:2418:THR:HG23	1:A:2419:LYS:N	2.33	0.44
1:A:2069:GLU:HB3	1:A:2097:TYR:CE2	2.53	0.44
1:A:2176:PHE:CE2	1:A:2180:ILE:HD11	2.51	0.44
1:A:2376:PHE:CZ	1:A:2408:ARG:HD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2068:SER:O	1:A:2072:PHE:CD1	2.71	0.43
1:A:2102:LYS:NZ	1:A:2137:TRP:HB2	2.33	0.43
1:A:2522:LYS:HA	1:A:2522:LYS:HD3	1.87	0.43
1:A:2595:LYS:HA	1:A:2595:LYS:HE3	2.00	0.43
1:A:2053:ARG:HA	1:A:2053:ARG:NE	2.33	0.43
1:A:2304:ILE:HG22	1:A:2305:LYS:N	2.33	0.43
1:A:2528:GLU:HA	1:A:2531:VAL:CG2	2.47	0.43
1:A:2068:SER:HB2	1:A:2072:PHE:CZ	2.53	0.43
1:A:2310:ILE:HD12	1:A:2310:ILE:H	1.83	0.43
1:A:2355:LEU:HD11	1:A:2374:ASN:HD22	1.82	0.43
1:A:2527:TYR:O	1:A:2530:MET:HG3	2.18	0.43
1:A:2569:TYR:O	1:A:2572:LEU:HB2	2.17	0.43
1:A:2211:GLN:HE21	1:A:2214:GLU:CB	2.32	0.43
1:A:2310:ILE:HB	1:A:2311:PRO:HD3	1.98	0.43
1:A:2191:LYS:HD3	1:A:2195:LYS:NZ	2.33	0.43
1:A:2161:ASP:HB3	1:A:2162:PRO:HD2	2.00	0.43
1:A:2230:ARG:HG2	1:A:2302:LYS:NZ	2.33	0.43
1:A:2424:MET:HB3	1:A:2428:PHE:CZ	2.54	0.43
1:A:2520:CYS:HB2	1:A:2605:LEU:CD2	2.49	0.43
1:A:2035:PRO:HA	1:A:2038:ARG:CG	2.46	0.43
1:A:2055:LEU:HB2	1:A:2123:LEU:CD2	2.49	0.43
1:A:2528:GLU:O	1:A:2531:VAL:HG22	2.18	0.43
1:A:2025:TYR:HB3	1:A:2027:LYS:HG2	2.00	0.43
1:A:2377:LEU:O	1:A:2377:LEU:HG	2.18	0.43
1:A:2456:GLY:N	1:A:2459:GLN:HE21	2.11	0.43
1:A:2213:SER:O	1:A:2216:LYS:NZ	2.51	0.42
1:A:2395:LYS:HE2	1:A:2399:TYR:OH	2.19	0.42
1:A:2515:TRP:O	1:A:2518:ASN:OD1	2.37	0.42
1:A:2039:GLN:O	1:A:2040:LEU:HD13	2.19	0.42
1:A:2073:LEU:HD11	1:A:2097:TYR:CE2	2.54	0.42
1:A:2153:LYS:HG3	1:A:2165:CYS:HB3	2.00	0.42
1:A:2222:ILE:HD12	1:A:2225:TYR:HB2	2.01	0.42
1:A:2226:GLN:O	1:A:2229:SER:OG	2.35	0.42
1:A:2354:ASP:OD2	1:A:2357:LYS:HB2	2.20	0.42
1:A:2475:TRP:CZ3	1:A:2499:ILE:HG23	2.54	0.42
1:A:2190:GLN:HB2	1:A:2232:ARG:HH12	1.84	0.42
1:A:2020:ASP:O	1:A:2024:PRO:HD2	2.20	0.42
1:A:2466:TRP:HE3	1:A:2469:MET:HE1	1.85	0.42
1:A:2097:TYR:O	1:A:2101:ILE:HG12	2.19	0.42
1:A:2375:LEU:HB3	1:A:2377:LEU:HD22	2.02	0.42
1:A:2098:GLU:HA	1:A:2101:ILE:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2448:LYS:O	1:A:2452:ILE:HG12	2.19	0.42
1:A:2022:ARG:NE	1:A:2022:ARG:HA	2.35	0.41
1:A:2090:MET:O	1:A:2093:SER:OG	2.32	0.41
1:A:2569:TYR:HA	1:A:2572:LEU:CD1	2.42	0.41
1:A:2594:PHE:HD2	1:A:2606:SER:HG	1.66	0.41
1:A:2211:GLN:HG2	1:A:2211:GLN:O	2.20	0.41
1:A:2420:VAL:HG12	1:A:2424:MET:HE2	2.02	0.41
1:A:2230:ARG:HG2	1:A:2302:LYS:HZ3	1.83	0.41
1:A:2367:LEU:HB3	1:A:2567:LYS:HZ3	1.84	0.41
1:A:2384:ILE:HD12	1:A:2451:LYS:CD	2.46	0.41
1:A:2516:THR:HG22	1:A:2605:LEU:CD2	2.44	0.41
1:A:2035:PRO:HA	1:A:2038:ARG:CD	2.51	0.41
1:A:2331:ASP:CG	1:A:2334:CYS:HB3	2.41	0.41
1:A:2384:ILE:CD1	1:A:2451:LYS:HE3	2.51	0.41
1:A:2442:GLU:CG	1:A:2445:SER:HB3	2.51	0.41
1:A:2017:ASN:HB2	1:A:2020:ASP:CB	2.47	0.41
1:A:2435:ILE:HD11	1:A:2467:TRP:CG	2.56	0.41
1:A:2475:TRP:HA	1:A:2478:MET:SD	2.61	0.41
1:A:2355:LEU:HB3	1:A:2373:LYS:HZ1	1.86	0.41
1:A:2377:LEU:H	1:A:2377:LEU:HD23	1.84	0.41
1:A:2053:ARG:NH2	1:A:2058:PHE:HA	2.35	0.41
1:A:2191:LYS:HD3	1:A:2195:LYS:HZ1	1.86	0.41
1:A:2218:CYS:SG	1:A:2219:THR:N	2.94	0.41
1:A:2413:TYR:HE1	1:A:2424:MET:HG2	1.85	0.41
1:A:2449:ILE:O	1:A:2452:ILE:HG12	2.21	0.41
1:A:2195:LYS:HA	1:A:2198:VAL:CG1	2.51	0.41
1:A:2464:LYS:HZ2	1:A:2467:TRP:HZ3	1.69	0.41
1:A:2037:ARG:O	1:A:2037:ARG:HD2	2.21	0.40
1:A:2399:TYR:O	1:A:2403:ILE:HG13	2.21	0.40
1:A:2185:THR:O	1:A:2189:ILE:HG12	2.21	0.40
1:A:2035:PRO:HA	1:A:2038:ARG:HH11	1.86	0.40
1:A:2179:TRP:HA	1:A:2182:GLU:CG	2.51	0.40
1:A:2560:ASN:O	1:A:2563:LEU:HB3	2.22	0.40
1:A:2091:LYS:HB2	1:A:2095:TYR:CZ	2.56	0.40
1:A:2585:ALA:O	1:A:2586:GLU:HG3	2.22	0.40
1:A:2141:LYS:HZ3	1:A:2144:ILE:HG23	1.86	0.40
1:A:2455:ASP:CG	1:A:2463:ARG:HD2	2.42	0.40
1:A:2528:GLU:CA	1:A:2531:VAL:HG22	2.52	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	490/2653 (18%)	473 (96%)	16 (3%)	1 (0%)	47 81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2040	LEU

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	461/2419 (19%)	456 (99%)	5 (1%)	73 85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2191	LYS
1	A	2336	LYS
1	A	2372	ARG
1	A	2419	LYS
1	A	2465	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	2140	ASN
1	A	2175	GLN
1	A	2374	ASN
1	A	2459	GLN
1	A	2506	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

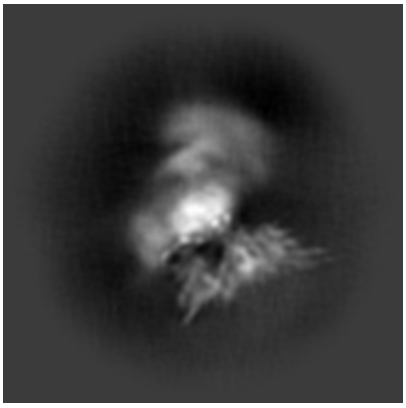
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22326. These allow visual inspection of the internal detail of the map and identification of artifacts.

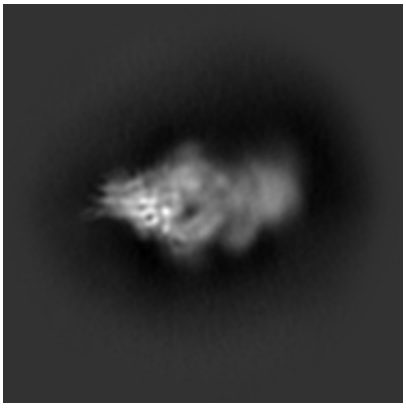
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

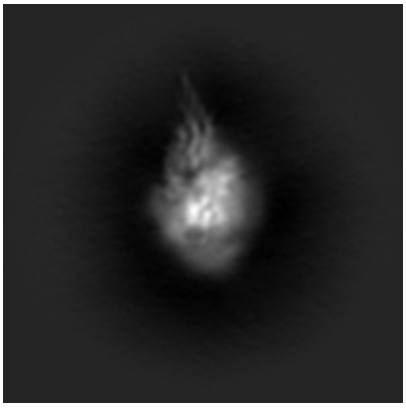
6.1.1 Primary map



X



Y

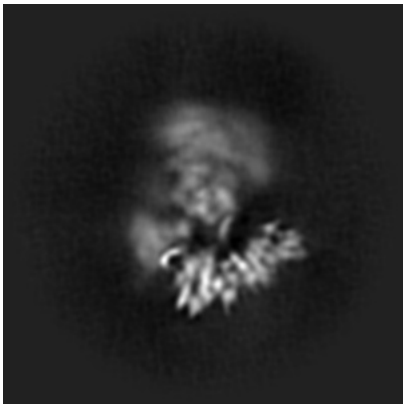


Z

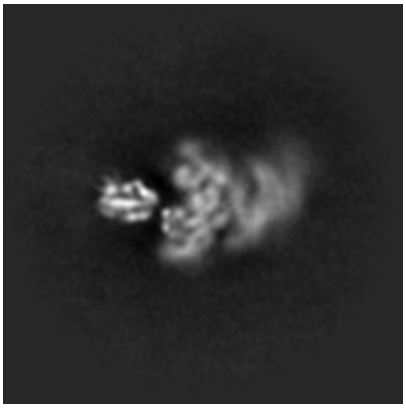
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

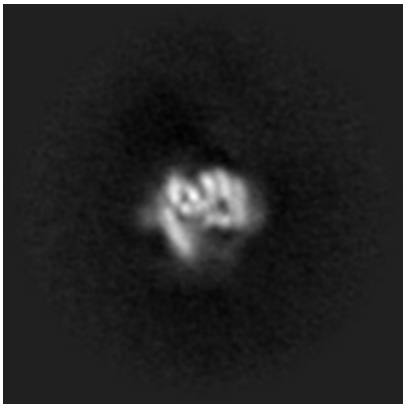
6.2.1 Primary map



X Index: 150



Y Index: 150

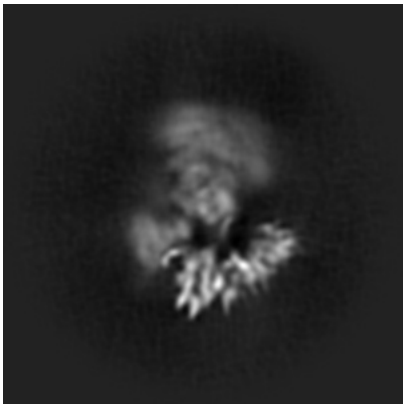


Z Index: 150

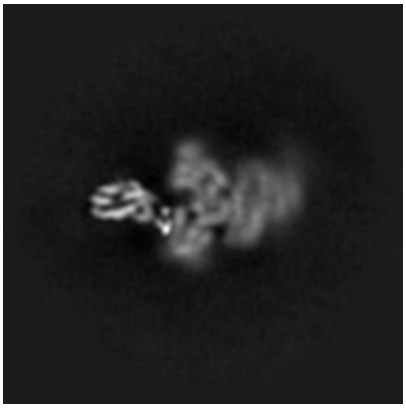
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

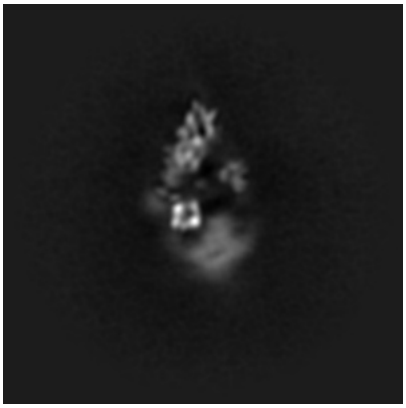
6.3.1 Primary map



X Index: 152



Y Index: 144

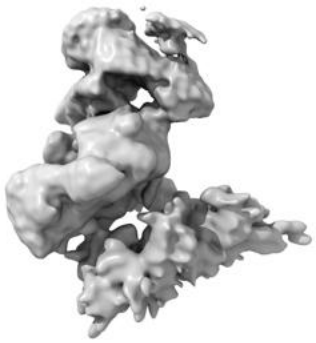


Z Index: 122

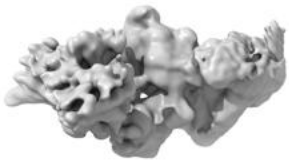
The images above show the largest variance slices of the map in three orthogonal directions.

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 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

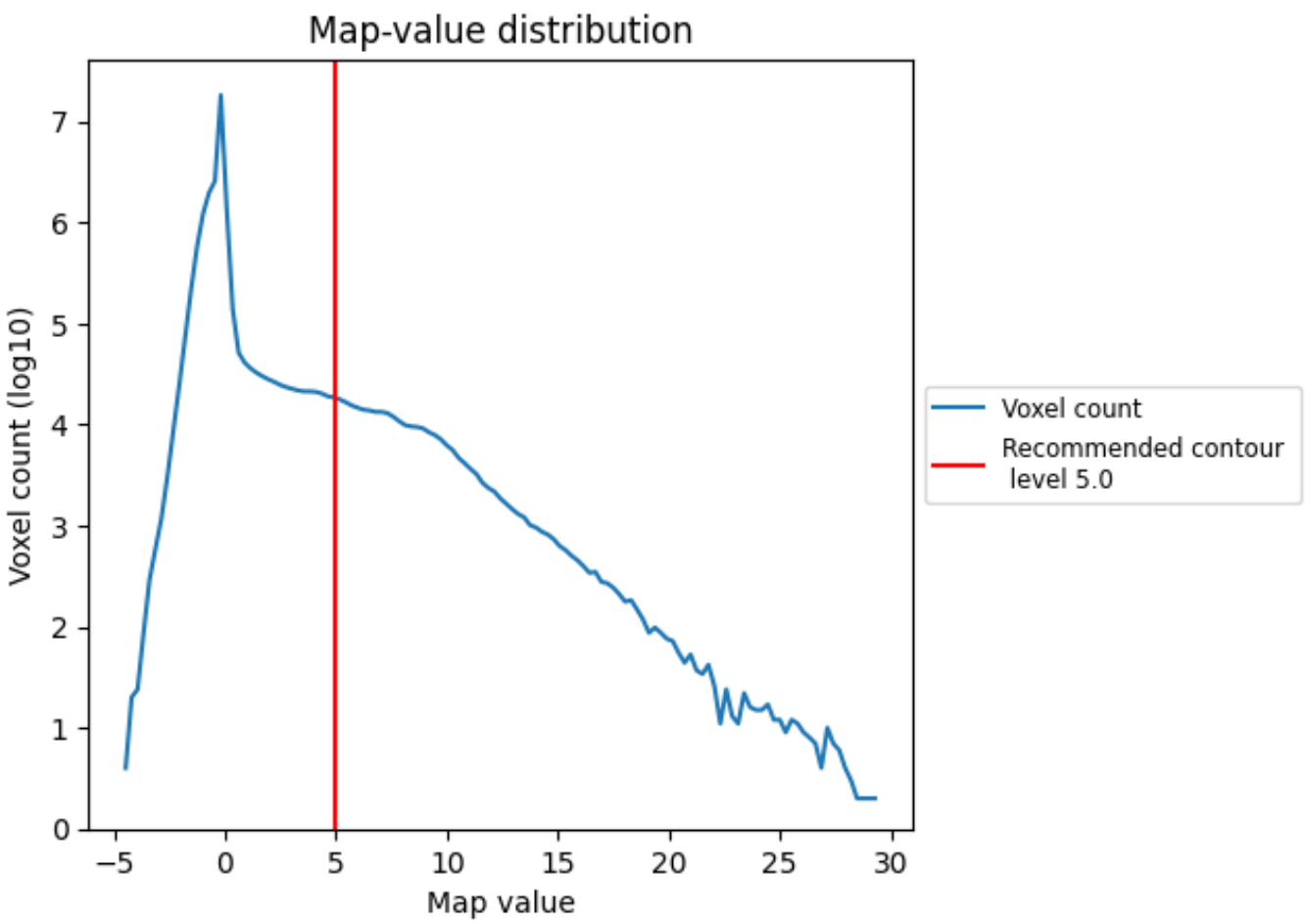
6.5 Mask visualisation (i)

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

7 Map analysis (i)

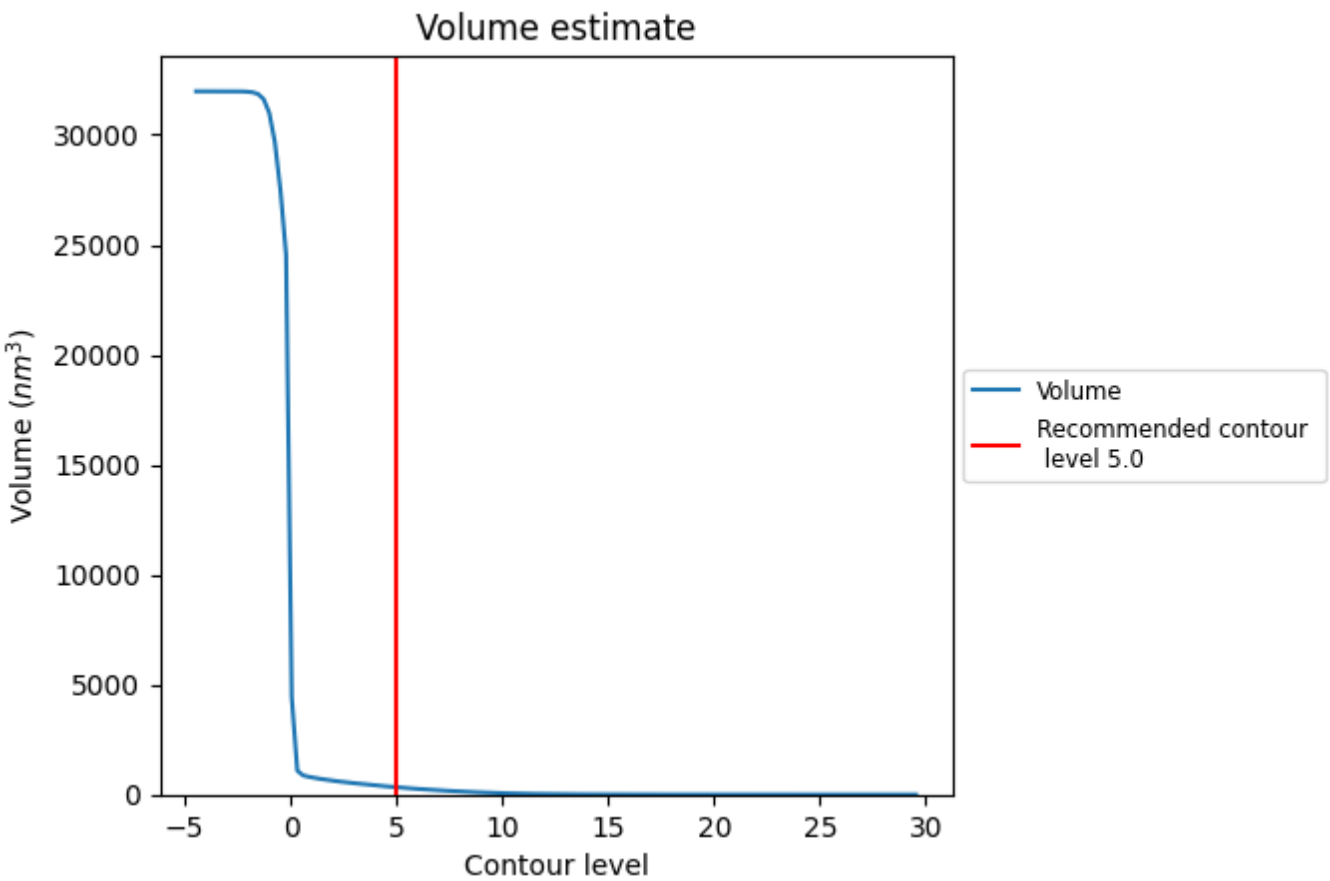
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

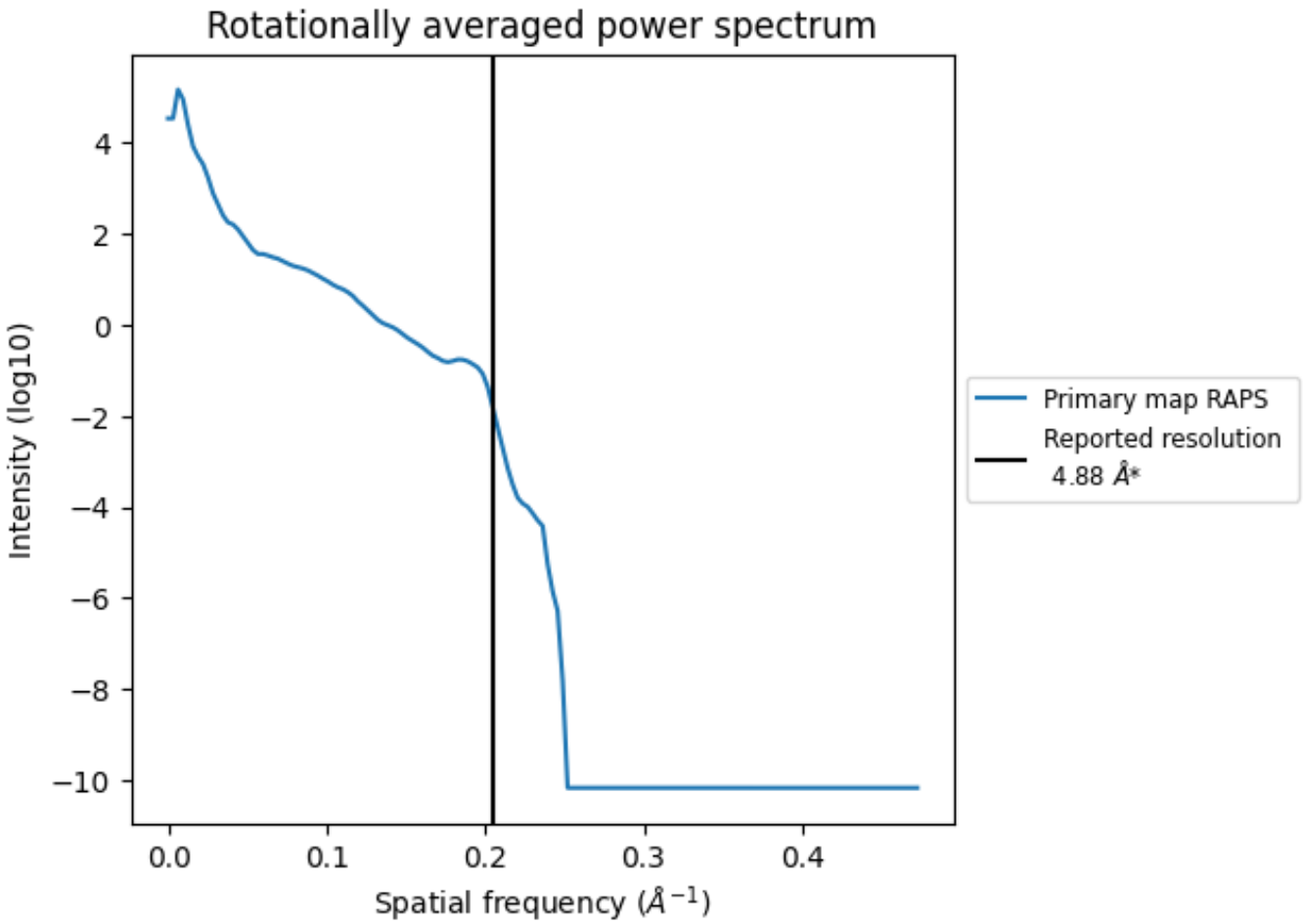
7.2 Volume estimate (i)



The volume at the recommended contour level is 332 nm^3; this corresponds to an approximate mass of 300 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 0.205 Å^{-1}

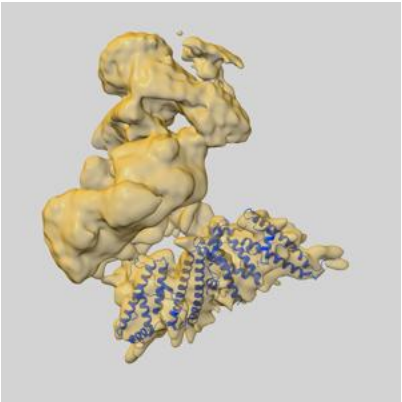
8 Fourier-Shell correlation (i)

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

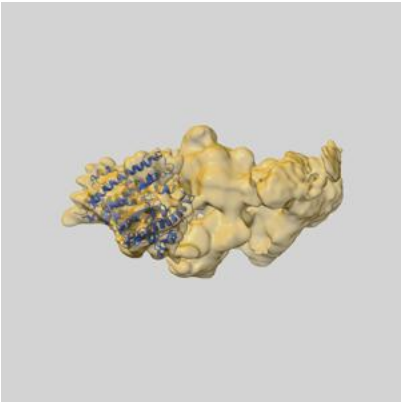
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22326 and PDB model 7JGG. Per-residue inclusion information can be found in section 3 on page 4.

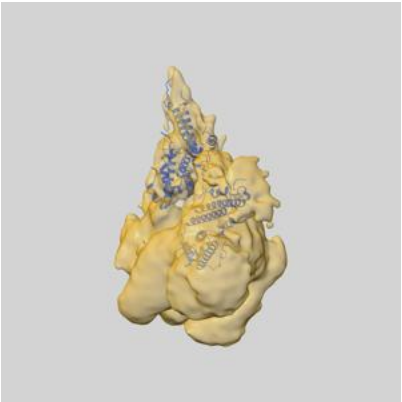
9.1 Map-model overlay (i)



X



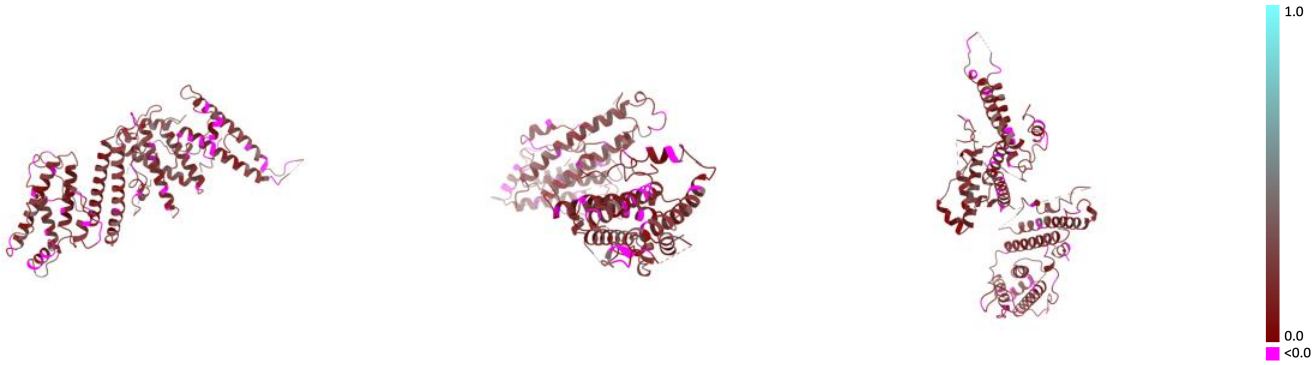
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0 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.

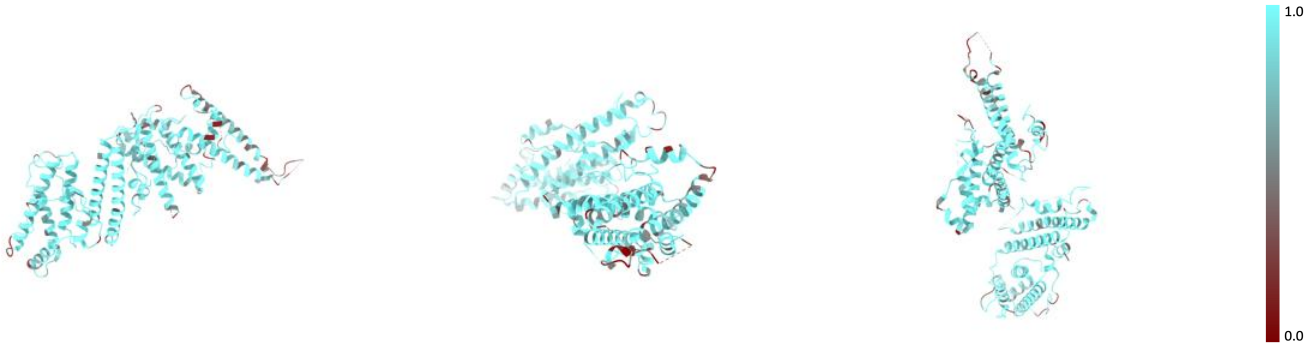
9.2 Q-score mapped to coordinate model (i)



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.

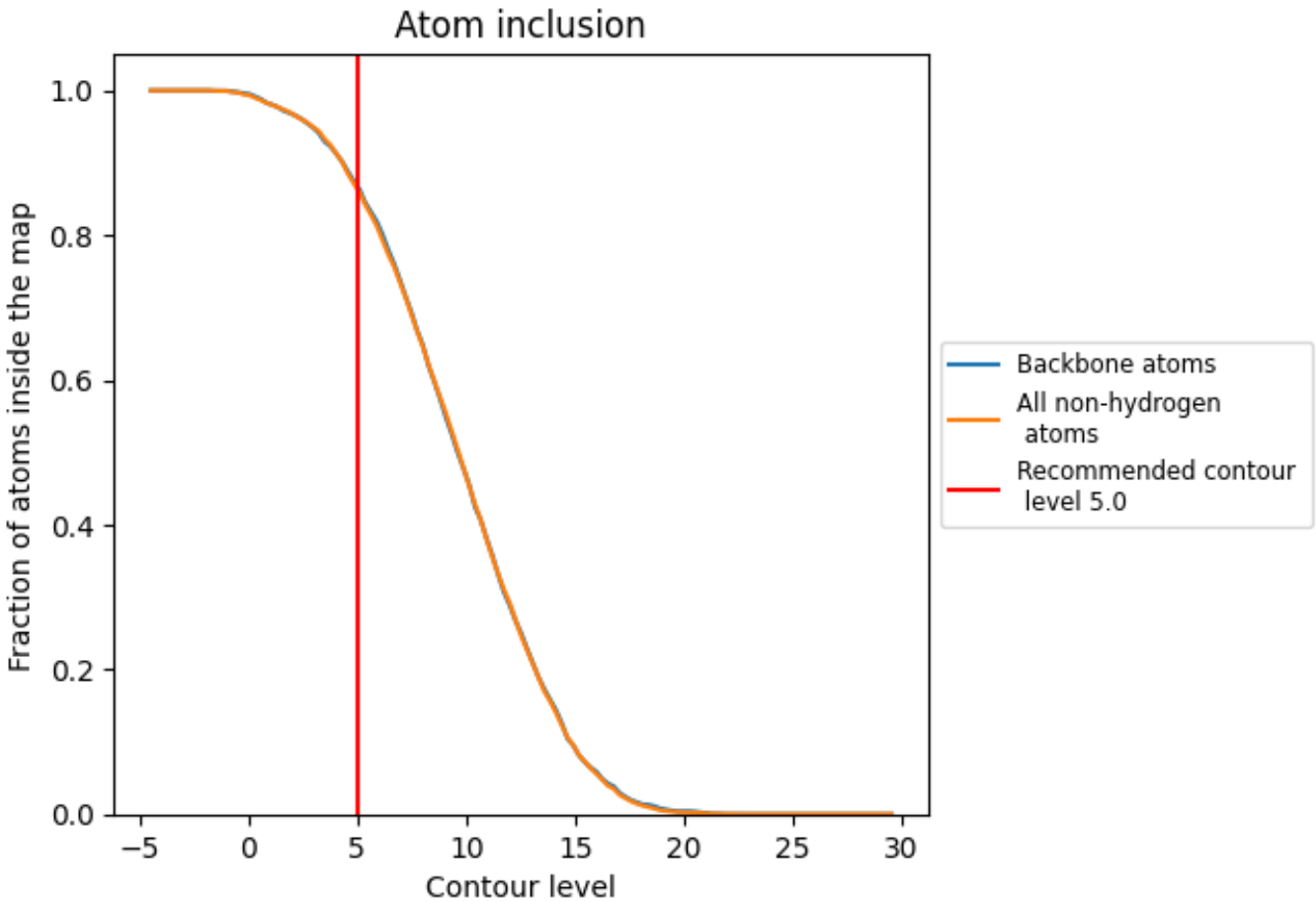
9.3 Atom inclusion mapped to coordinate model (i)



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 (5.0).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (5.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8638	0.1540
A	0.8660	0.1540