wwPDB EM Validation Summary Report

Feb 6, 2025 – 03:45 pm GMT

PDB ID	:	8RDE
EMDB ID	:	EMD-19070
Title	:	STRUCTURE OF THE MOUSE FCGBP DIMER PROTEIN IN ITS COMPACT CONFORMATION
Authors	:	Gallego, P.; Hansson, G.C.; Johansson, M.E.V.
Deposited on	:	2023-12-08
Resolution	:	3.70 Å(reported)

This is a wwPDB EM Validation Summary 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:

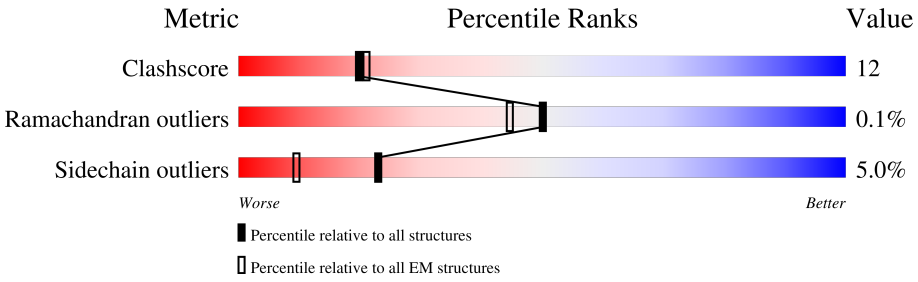
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	2587	38% 13% · 48%
1	D	2587	38% 14% · 48%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20050 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.

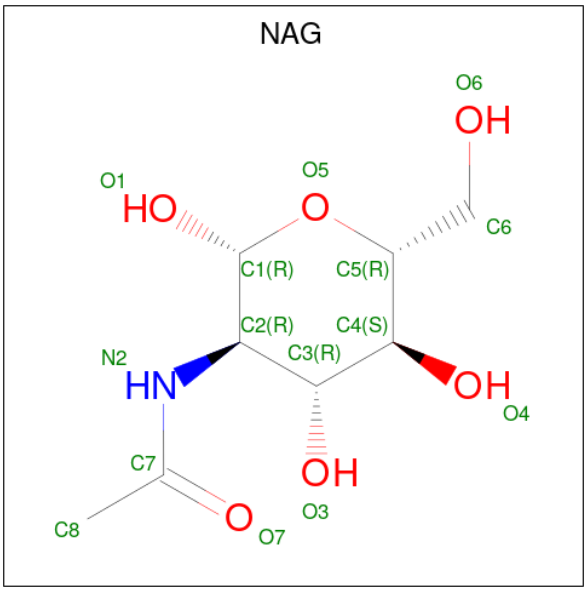
- Molecule 1 is a protein called Fc fragment of IgG binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1342	Total	C	N	O	S	1	0
			9937	6174	1721	1921	121		
1	D	1342	Total	C	N	O	S	1	0
			9937	6174	1721	1921	121		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2584	THR	-	expression tag	UNP E9Q0B5
A	2585	ARG	-	expression tag	UNP E9Q0B5
A	2586	THR	-	expression tag	UNP E9Q0B5
A	2587	ARG	-	expression tag	UNP E9Q0B5
D	2584	THR	-	expression tag	UNP E9Q0B5
D	2585	ARG	-	expression tag	UNP E9Q0B5
D	2586	THR	-	expression tag	UNP E9Q0B5
D	2587	ARG	-	expression tag	UNP E9Q0B5

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

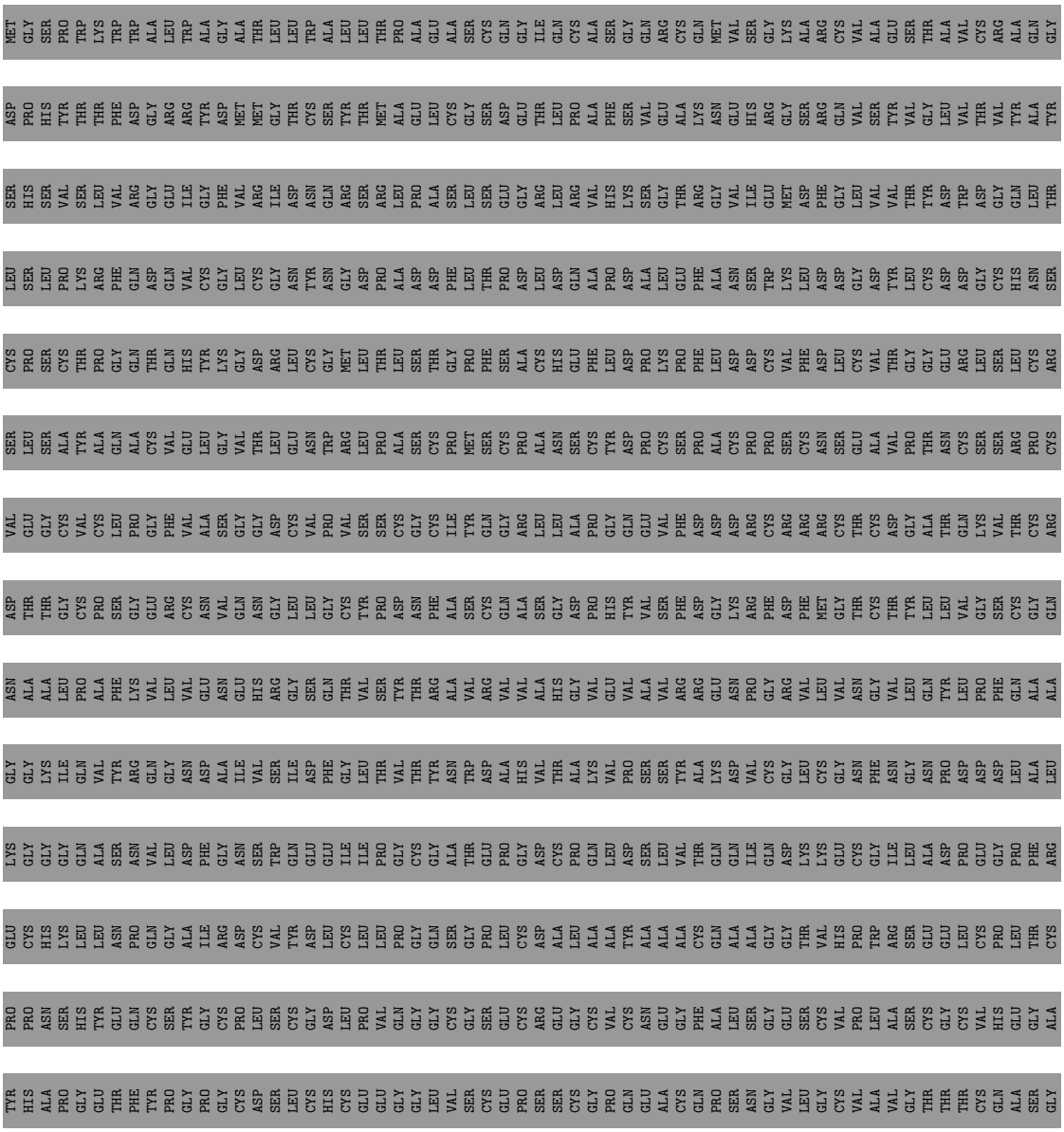
Mol	Chain	Residues	Atoms	AltConf
3	A	4	Total Ca 4 4	0
3	D	4	Total Ca 4 4	0

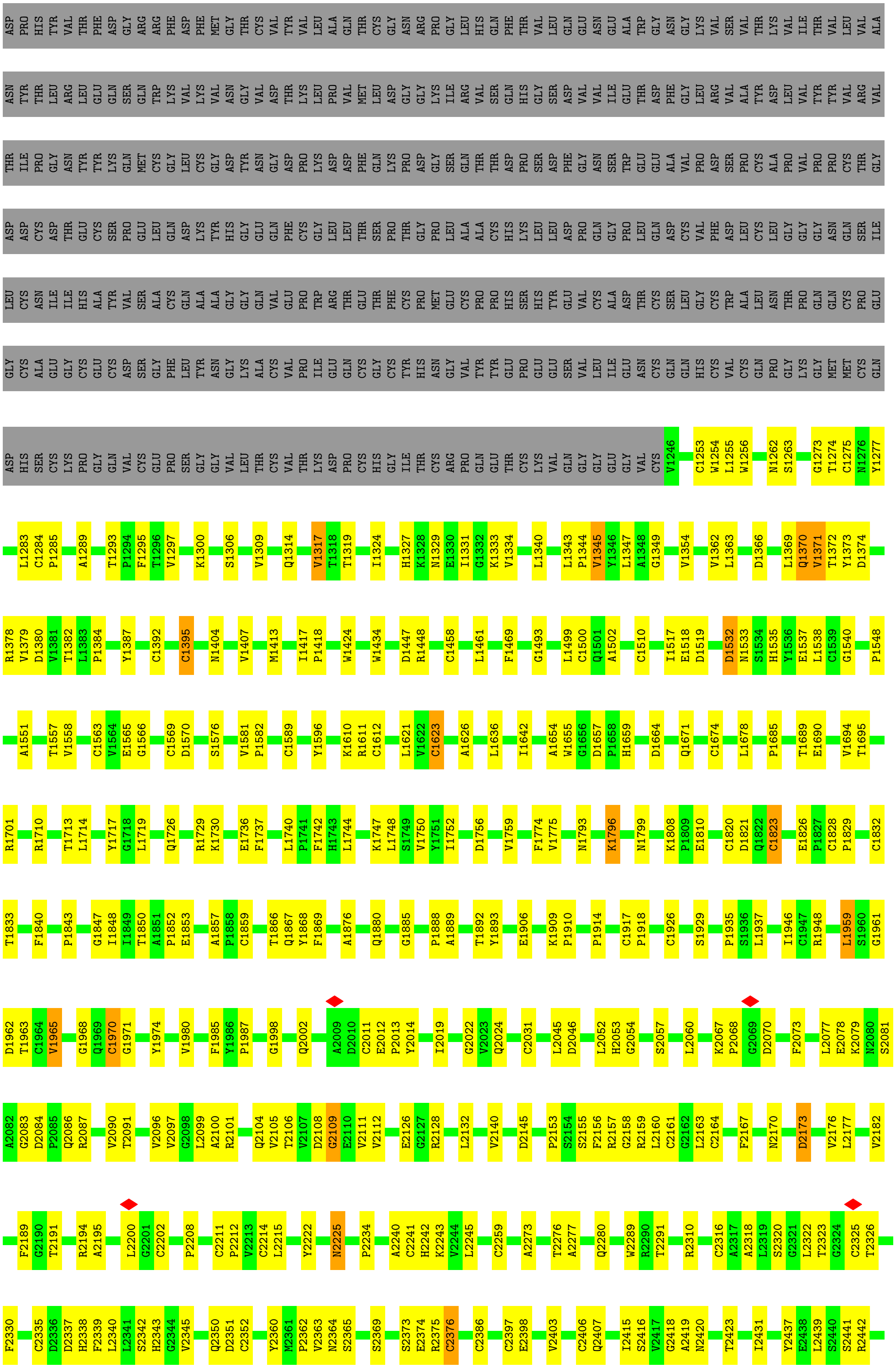
3 Residue-property plots (i)

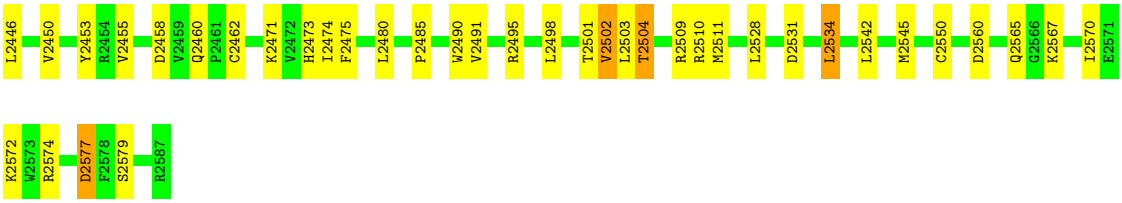
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:

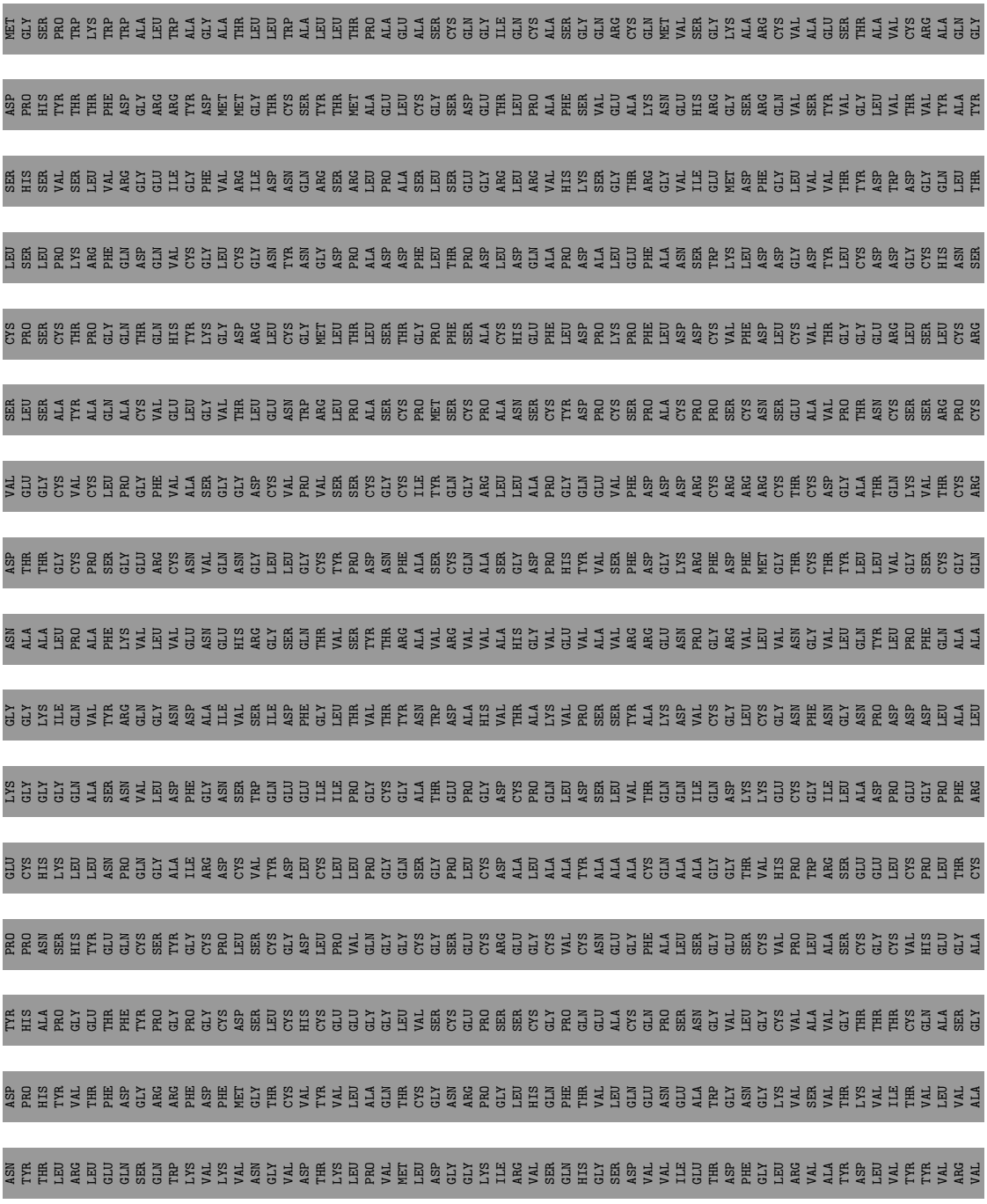


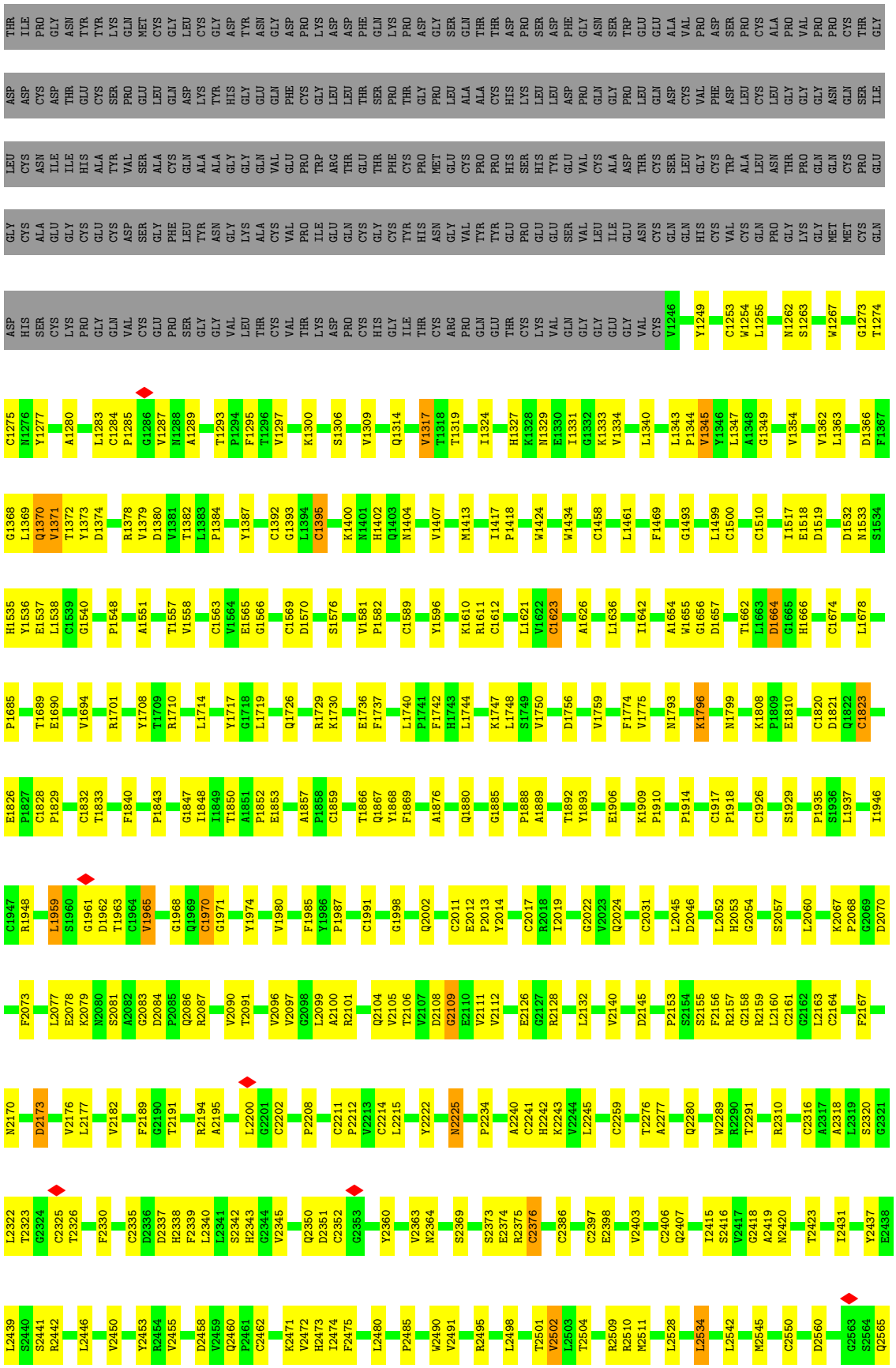

ASP PRO HIS TYR VAL THR PHE ASP GLY ARG ARG PHE ASP PHE MET GLY THR CYS VAL TYR VAL LEU ALA GLN THR CYS GLY ASN ARG PRO GLY LEU HIS GLN PHE THR VAL LEU GLN GLU ASN GLU ALA TRP GLY ASN GLY LYS VAL SER VAL THR LYS VAL ILE THR VAL LEU VAL ALA
ASN TYR THR LEU ARG LEU GLU GLN SER GLN TRP LYS VAL LYS VAL ASN GLY VAL ASP THR LYS LEU PRO VAL MET LEU ASP GLY GLY LYS ILE ARG VAL SER GLN HIS GLY SER ASP VAL VAL ILE GLU THR ASP PHE GLY LEU ARG VAL ALA TYR ASP LEU VAL TYR TYR VAL ARG VAL
THR ILE PRO GLY ASN TYR TYR LYS GLN MET CYS GLY LEU CYS GLY ASP TYR ASN GLY ASP PRO LYS ASP ASP PHE GLN LYS PRO ASP GLY SER GLN THR THR ASP PRO SER ASP PHE GLY ASN SER TRP GLU GLU ALA VAL PRO ASP SER PRO CYS ALA PRO VAL PRO PRO CYS THR GLY
ASP ASP CYS ASP THR GLU CYS SER PRO GLU LEU GLN ASP LYS TYR HIS GLY GLU GLN PHE CYS GLY LEU LEU THR SER PRO THR GLY PRO LEU ALA ALA CYS HIS LYS LEU LEU ASP PRO GLN GLY PRO LEU GLN ASP CYS VAL PHE ASP LEU CYS LEU GLY GLY GLY ASN GLN SER ILE
LEU CYS ASN ILE ILE HIS ALA TYR VAL SER ALA CYS GLN ALA ALA GLY GLN VAL GLU PRO TRP ARG THR GLU THR PHE CYS PRO MET GLU CYS PRO PRO HIS SER HIS TYR GLU VAL CYS ALA ASP THR CYS SER LEU GLY CYS TRP ALA LEU ASN THR PRO GLN GLN CYS PRO GLU
GLY CYS ALA GLU GLY CYS GLU CYS ASP SER GLY PHE LEU TYR ASN GLY LYS ALA CYS VAL PRO ILE GLU GLN CYS GLY CYS TYR HIS ASN GLY VAL TYR TYR GLU PRO GLU GLU SER VAL LEU ILE GLU ASN CYS GLN GLN HIS CYS VAL CYS GLN PRO GLY LYS GLY MET MET CYS GLN
ASP HIS SER CYS LYS PRO GLY GLN VAL CYS GLU PRO SER GLY GLY VAL LEU THR CYS VAL THR LYS ASP PRO CYS HIS GLY ILE THR CYS ARG PRO GLN GLU THR CYS LYS VAL GLN GLY GLY GLU GLY VAL CYS V1246 C1253 W1254 L1255 W1256 N1262 S1263 G1273 T1274 C1275 N1276 Y1277
L1283 C1284 P1285 A1289 T1293 P1294 F1295 T1296 V1297 K1300 S1306 V1309 Q1314 V1317 T1318 T1319 T1324 H1327 K1328 N1329 E1330 I1331 G1332 K1333 V1334 L1340 L1343 P1344 V1345 Y1346 L1347 A1348 G1349 V1354 V1362 L1363 D1366 L1369 Q1370 V1371 T1372 Y1373 D1374
R1378 V1379 D1380 V1381 T1382 L1383 P1384 Y1387 C1392 C1395 N1404 V1407 M1413 I1417 P1418 W1424 W1434 D1447 R1448 C1458 L1461 F1469 G1493 L1499 C1500 Q1501 A1502 C1510 I1517 E1518 D1519 D1532 N1533 S1534 H1535 Y1536 E1537 L1538 C1539 G1540 P1548
A1551 T1557 V1558 C1563 V1564 E1565 G1566 C1569 D1570 S1576 V1581 P1582 C1589 Y1596 K1610 R1611 C1612 L1621 V1622 C1623 A1626 L1636 I1642 A1654 W1655 G1656 D1657 P1658 H1659 D1664 Q1671 C1674 L1678 P1685 T1689 E1690 V1694 T1695
R1701 R1710 T1713 L1714 Y1717 G1718 L1719 Q1726 R1729 K1730 E1736 F1737 L1740 P1741 F1742 H1743 L1744 K1747 L1748 S1749 V1750 Y1751 I1752 D1756 V1759 F1774 V1775 N1793 K1796 N1799 K1808 P1809 E1810 C1820 D1821 Q1822 C1823 E1826 P1827 C1828 P1829 C1832
T1833 F1840 P1843 G1847 I1848 I1849 T1850 A1851 P1852 E1853 A1857 P1858 C1859 T1866 Q1867 Y1868 F1869 A1876 Q1880 G1885 P1888 A1889 T1892 Y1893 E1906 K1909 P1910 P1914 C1917 P1918 C1926 S1929 P1935 S1936 L1937 I1946 C1947 R1948 L1959 S1960 G1961
D1962 T1963 C1964 V1965 G1968 Q1969 C1970 G1971 Y1974 V1980 F1985 Y1986 P1987 G1998 Q2002 A2009 D2010 C2011 E2012 P2013 Y2014 I2019 G2022 V2023 Q2024 C2031 L2045 D2046 L2052 H2053 G2054 S2057 L2060 K2067 P2068 G2069 D2070 F2073 L2077 E2078 K2079 N2080 S2081
A2082 G2083 D2084 P2085 Q2086 R2087 V2090 T2091 V2096 V2097 G2098 L2099 A2100 R2101 Q2104 V2105 T2106 V2107 D2108 G2109 E2110 V2111 V2112 E2126 G2127 R2128 L2132 V2140 D2145 P2153 S2154 S2155 F2156 R2157 G2158 R2159 L2160 C2161 G2162 L2163 C2164 F2167 N2170 D2173 V2176 L2177 V2182
F2189 G2190 T2191 R2194 A2195 L2200 G2201 C2202 P2208 C2211 P2212 V2213 C2214 L2215 Y2222 N2225 P2234 A2240 C2241 H2242 K2243 V2244 L2245 C2259 A2273 T2276 A2277 Q2280 W2289 R2290 T2291 R2310 C2316 A2317 A2318 L2319 S2320 G2321 L2322 T2323 G2324 C2325 T2326
F2330 C2335 D2336 D2337 H2338 F2339 L2340 L2341 S2342 H2343 G2344 V2345 Q2350 D2351 C2352 Y2360 M2361 P2362 V2363 N2364 S2365 S2369 S2373 E2374 R2375 C2376 C2386 C2397 E2398 V2403 C2406 Q2407 I2415 S2416 V2417 G2418 A2419 N2420 T2423 I2431 Y2437 E2438 L2439 S2440 S2441 R2442



• Molecule 1: Fc fragment of IgG binding protein

Chain D:




THR ILE PRO GLY ASN TYR TYR LYS GLN MET CYS GLY LEU CYS GLY ASP TYR ASN GLY ASP PRO LYS ASP ASP PHE GLN LYS PRO ASP GLY SER GLN THR THR ASP PRO SER ASP PHE GLY ASN SER TRP GLU GLU ALA VAL PRO ASP SER PRO CYS ALA PRO VAL PRO PRO CYS THR GLY
ASP ASP CYS ASP THR GLU CYS SER PRO GLU LEU GLN ASP LYS TYR HIS ALA TYR VAL SER ALA CYS GLN ALA ALA CYS HIS LYS LEU LEU ASP PRO GLN GLY PRO LEU GLN LEU CYS LEU GLY GLY GLY ASN GLN SER ILE
LEU CYS ASN ILE ILE HIS ALA TYR VAL SER ALA CYS GLN VAL GLU PHE CYS GLY GLY GLN VAL GLU PRO TRP ARG THR GLU THR PHE CYS PRO MET GLU CYS PRO PRO HIS SER HIS TYR GLU VAL CYS ALA ASP THR CYS SER LEU GLY CYS VAL PHE ASP LEU ALA LEU CYS ASN THR PRO GLN GLN GLY PRO GLU
GLY CYS ALA GLU GLY CYS GLU CYS ASP SER GLY PHE LEU TYR ASN GLY LYS ALA CYS VAL PRO ILE GLU GLN CYS GLY TYR HIS ASN GLY VAL TYR TYR GLU PRO GLU GLU SER VAL LEU ILE GLU ASN CYS GLN GLN HIS CYS VAL CYS GLN PRO GLY LYS GLY MET MET CYS GLN
ASP HIS SER CYS LYS PRO GLY GLN VAL CYS GLU PRO SER GLY GLY VAL LEU THR CYS VAL THR LYS ASP PRO CYS GLY THR HIS GLY ILE THR CYS ARG PRO GLN GLU GLY CYS LYS VAL GLN GLY GLU GLY VAL CYS V1246 Y1249 C1253 W1254 L1255 N1262 S1263 W1267 G1273 T1274
C1275 N1276 Y1277 A1280 L1283 C1284 P1285 G1286 V1287 N1288 A1289 T1293 P1294 F1295 T1296 V1297 K1300 S1306 V1309 Q1314 V1317 T1318 T1319 I1324 H1327 K1328 N1329 E1330 I1331 G1332 K1333 V1334 L1340 L1343 P1344 V1345 Y1346 L1347 A1348 G1349 V1354 V1362 L1363 D1366 F1367
G1368 L1369 Q1370 V1371 T1372 Y1373 D1374 R1378 V1379 D1380 V1381 T1382 L1383 P1384 Y1387 C1392 G1393 L1394 C1395 K1400 N1401 H1402 Q1403 N1404 V1407 M1413 I1417 P1418 W1424 W1434 C1458 L1461 F1469 G1493 L1499 C1500 C1510 I1517 E1518 D1519 D1532 N1533 S1534
H1535 Y1536 E1537 L1538 C1539 G1540 P1548 A1551 T1557 V1558 C1563 V1564 E1565 G1566 C1569 D1570 S1576 V1581 P1582 C1589 Y1596 K1610 R1611 C1612 L1621 V1622 C1623 A1626 L1636 I1642 A1654 W1655 G1656 D1657 T1662 L1663 D1664 G1665 H1666 C1674 L1678
P1685 T1689 E1690 V1694 R1701 Y1708 T1709 R1710 L1714 Y1717 G1718 L1719 Q1726 R1729 K1730 E1736 F1737 L1740 P1741 F1742 H1743 L1744 K1747 L1748 S1749 V1750 D1756 V1759 F1774 V1775 N1793 K1796 N1799 K1808 P1809 E1810 C1820 D1821 Q1822 C1823
E1826 P1827 C1828 P1829 C1832 T1833 F1840 P1843 G1847 I1848 T1849 T1850 A1851 P1852 E1853 A1857 P1858 C1859 T1866 Q1867 Y1868 F1869 A1876 Q1880 G1885 P1888 A1889 T1892 Y1893 E1906 K1909 P1910 P1914 C1917 P1918 C1926 S1929 P1935 S1936 L1937 I1946
C1947 R1948 L1959 S1960 G1961 D1962 T1963 C1964 V1965 G1968 Q1969 C1970 G1971 Y1974 V1980 F1985 Y1986 P1987 C1991 G1998 Q2002 C2011 E2012 P2013 Y2014 C2017 R2018 I2019 G2022 V2023 Q2024 C2031 L2045 D2046 L2052 H2053 G2054 S2057 L2060 K2067 P2068 G2069 D2070
F2073 L2077 E2078 K2079 N2080 S2081 A2082 G2083 D2084 P2085 Q2086 R2087 V2090 T2091 V2096 V2097 G2098 L2099 A2100 R2101 Q2104 V2105 T2106 V2107 D2108 G2109 E2110 V2111 V2112 E2126 G2127 R2128 L2132 V2140 D2145 P2153 S2154 S2155 F2156 R2157 G2158 R2159 L2160 C2161 G2162 L2163 C2164 F2167
N2170 D2173 V2176 L2177 V2182 F2189 G2190 T2191 R2194 A2195 L2200 G2201 C2202 P2208 C2211 P2212 V2213 C2214 L2215 Y2222 N2225 P2234 A2240 C2241 H2242 K2243 V2244 L2245 C2259 T2276 A2277 Q2280 W2289 R2290 T2291 R2310 C2316 A2317 A2318 L2319 S2320 G2321
L2322 T2323 G2324 C2325 T2326 F2330 C2335 D2336 D2337 H2338 F2339 L2340 L2341 S2342 H2343 G2344 V2345 Q2350 D2351 C2352 G2353 Y2360 V2363 N2364 S2369 S2373 E2374 R2375 C2376 C2386 C2397 E2398 V2403 C2406 Q2407 I2415 S2416 V2417 G2418 A2419 N2420 T2423 I2431 Y2437 E2438
L2439 S2440 S2441 R2442 L2446 V2450 Y2453 R2454 V2455 D2458 V2459 Q2460 P2461 C2462 K2471 V2472 H2473 I2474 F2475 L2480 P2485 W2490 V2491 R2495 L2498 T2501 V2502 L2503 T2504 R2509 R2510 M2511 L2528 L2534 L2542 M2545 C2550 D2560 G2563 S2564 Q2565


G2566
K2567
I2570
E2571
K2572
W2573
R2574
D2577
R2587

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	184178	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.340	Depositor
Minimum map value	-0.132	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0495	Depositor
Map size (Å)	302.72, 302.72, 302.72	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA

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	0.34	2/10201 (0.0%)	0.56	2/13926 (0.0%)
1	D	0.34	2/10201 (0.0%)	0.56	1/13926 (0.0%)
All	All	0.34	4/20402 (0.0%)	0.56	3/27852 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1582	PRO	N-CD	9.10	1.60	1.47
1	D	1582	PRO	N-CD	9.07	1.60	1.47
1	A	2234	PRO	N-CD	-7.97	1.36	1.47
1	D	2234	PRO	N-CD	-7.96	1.36	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1582	PRO	CA-N-CD	-5.02	104.47	111.50
1	D	1582	PRO	CA-N-CD	-5.02	104.47	111.50
1	A	2234	PRO	CA-N-CD	5.01	118.72	111.70

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	9937	0	9279	233	0
1	D	9937	0	9279	239	0
2	A	84	0	78	7	0
2	D	84	0	78	7	0
3	A	4	0	0	0	0
3	D	4	0	0	0	0
All	All	20050	0	18714	471	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 12.

The worst 5 of 471 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:2316:CYS:SG	1:A:2360:TYR:CE1	2.29	1.26
1:D:2316:CYS:SG	1:D:2360:TYR:CE1	2.28	1.26
1:A:1621:LEU:HD12	1:A:1621:LEU:O	1.50	1.11
1:D:1621:LEU:HD12	1:D:1621:LEU:O	1.50	1.10
1:D:2352:CYS:SG	1:D:2360:TYR:OH	2.27	0.92

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	1337/2587 (52%)	1253 (94%)	83 (6%)	1 (0%)	48 78
1	D	1337/2587 (52%)	1253 (94%)	83 (6%)	1 (0%)	48 78
All	All	2674/5174 (52%)	2506 (94%)	166 (6%)	2 (0%)	50 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2109	GLY
1	D	2109	GLY

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	1085/2113 (51%)	1031 (95%)	54 (5%)	20	47
1	D	1085/2113 (51%)	1031 (95%)	54 (5%)	20	47
All	All	2170/4226 (51%)	2062 (95%)	108 (5%)	23	47

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1370	GLN
1	D	1796	LYS
1	D	2462	CYS
1	D	1395	CYS
1	D	1557	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1880	GLN
1	D	1880	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	5603	1	14,14,15	0.34	0	17,19,21	0.68	0
2	NAG	A	5601	1	14,14,15	0.81	1 (7%)	17,19,21	0.95	1 (5%)
2	NAG	A	5607	1	14,14,15	0.88	1 (7%)	17,19,21	1.25	1 (5%)
2	NAG	A	5608	1	14,14,15	0.70	1 (7%)	17,19,21	0.86	0
2	NAG	D	5607	1	14,14,15	0.89	1 (7%)	17,19,21	1.25	1 (5%)
2	NAG	A	5603	1	14,14,15	0.34	0	17,19,21	0.68	0
2	NAG	D	5601	1	14,14,15	0.81	1 (7%)	17,19,21	0.95	1 (5%)
2	NAG	D	5608	1	14,14,15	0.70	1 (7%)	17,19,21	0.86	0
2	NAG	D	5609	1	14,14,15	0.26	0	17,19,21	0.42	0
2	NAG	A	5609	1	14,14,15	0.27	0	17,19,21	0.42	0
2	NAG	A	5610	1	14,14,15	0.30	0	17,19,21	0.42	0
2	NAG	D	5610	1	14,14,15	0.30	0	17,19,21	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	5603	1	-	0/6/23/26	0/1/1/1
2	NAG	A	5601	1	-	2/6/23/26	0/1/1/1
2	NAG	A	5607	1	-	2/6/23/26	0/1/1/1
2	NAG	A	5608	1	-	3/6/23/26	0/1/1/1
2	NAG	D	5607	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	5603	1	-	0/6/23/26	0/1/1/1
2	NAG	D	5601	1	-	2/6/23/26	0/1/1/1
2	NAG	D	5608	1	-	3/6/23/26	0/1/1/1
2	NAG	D	5609	1	-	1/6/23/26	0/1/1/1
2	NAG	A	5609	1	-	1/6/23/26	0/1/1/1
2	NAG	A	5610	1	-	1/6/23/26	0/1/1/1
2	NAG	D	5610	1	-	1/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5607	NAG	O5-C1	3.17	1.48	1.43
2	A	5607	NAG	O5-C1	3.14	1.48	1.43
2	D	5601	NAG	O5-C1	2.58	1.47	1.43
2	A	5601	NAG	O5-C1	2.58	1.47	1.43
2	D	5608	NAG	O5-C1	-2.38	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	5607	NAG	C1-O5-C5	4.95	118.90	112.19
2	A	5607	NAG	C1-O5-C5	4.92	118.86	112.19
2	D	5601	NAG	C1-O5-C5	3.68	117.18	112.19
2	A	5601	NAG	C1-O5-C5	3.66	117.15	112.19

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5601	NAG	C4-C5-C6-O6
2	D	5601	NAG	C4-C5-C6-O6
2	A	5601	NAG	O5-C5-C6-O6
2	D	5601	NAG	O5-C5-C6-O6
2	A	5607	NAG	O5-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5601	NAG	1	0

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Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5607	NAG	3	0
2	A	5608	NAG	2	0
2	D	5607	NAG	3	0
2	D	5608	NAG	3	0
2	D	5609	NAG	1	0
2	A	5609	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	1657:ASP	C	1658:PRO	N	7.71
1	A	1657:ASP	C	1658:PRO	N	7.58
1	A	1258:ASP	C	1259:PRO	N	5.18
1	D	1258:ASP	C	1259:PRO	N	5.03

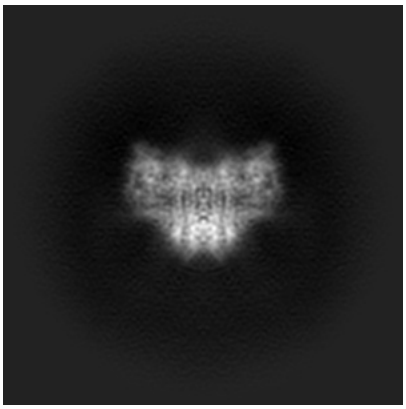
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19070. These allow visual inspection of the internal detail of the map and identification of artifacts.

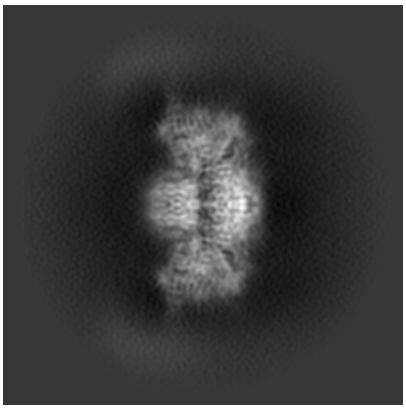
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

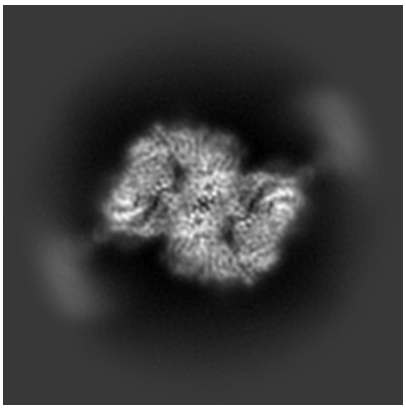
6.1.1 Primary map



X

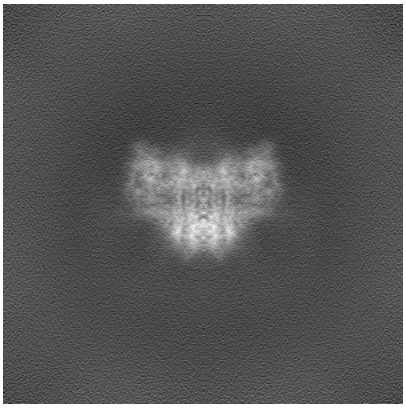


Y

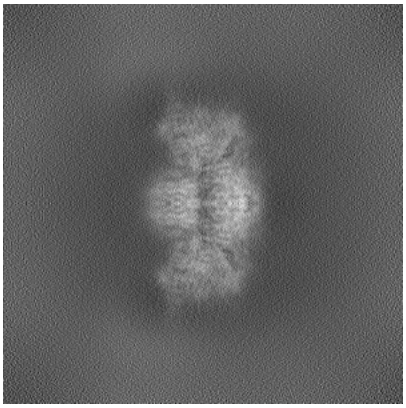


Z

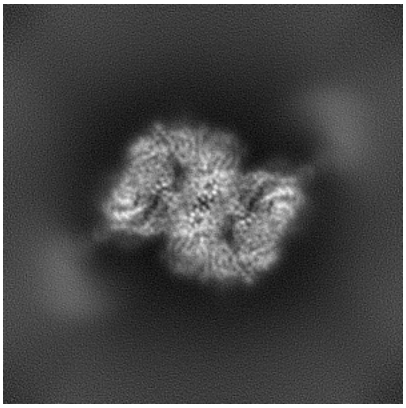
6.1.2 Raw map



X



Y



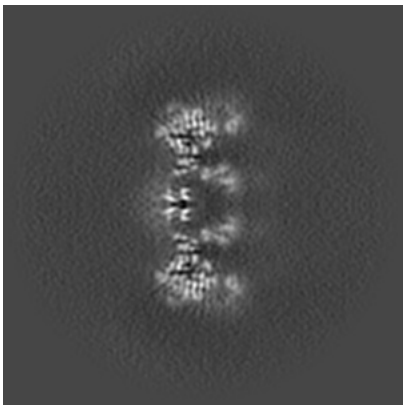
Z

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

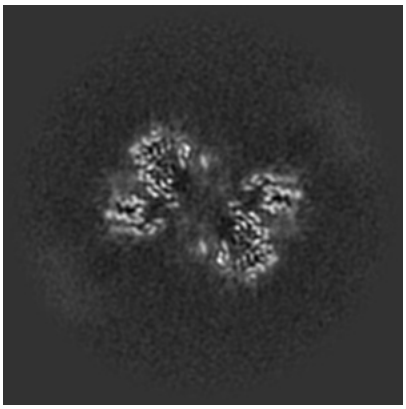
6.2 Central slices (i)

6.2.1 Primary map

X Index: 176

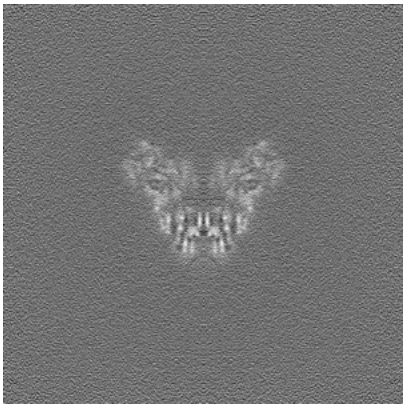


Y Index: 176

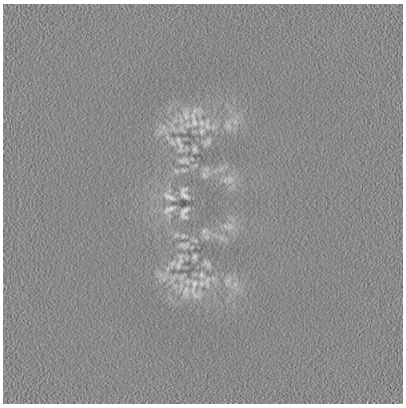


Z Index: 176

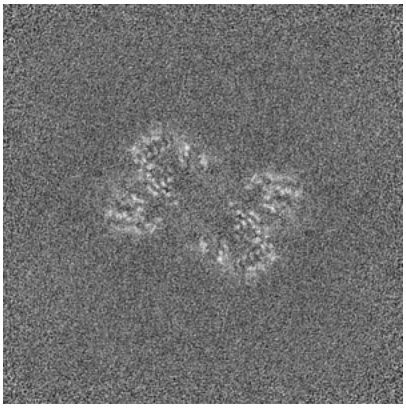
6.2.2 Raw map



X Index: 176



Y Index: 176



Z Index: 176

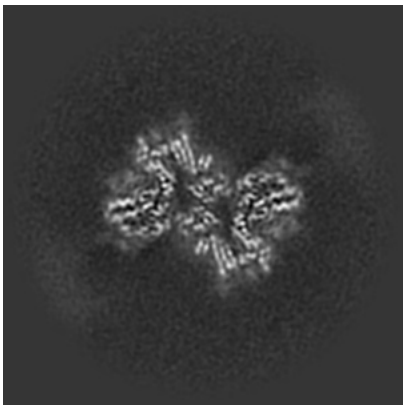
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

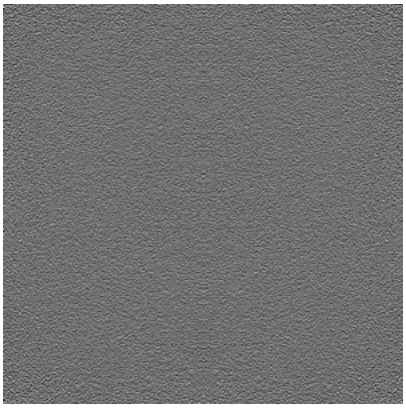
X Index: 176

Y Index: 186

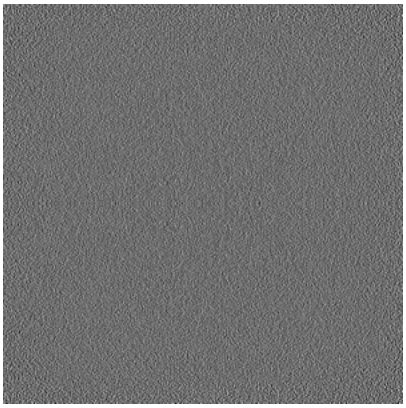


Z Index: 168

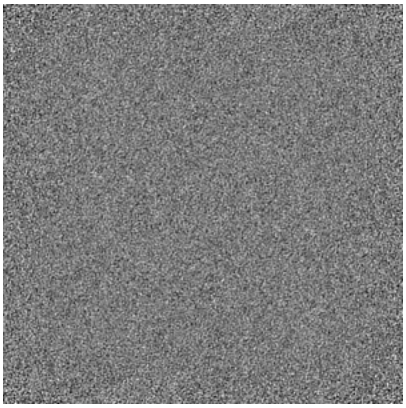
6.3.2 Raw map



X Index: 0



Y Index: 0

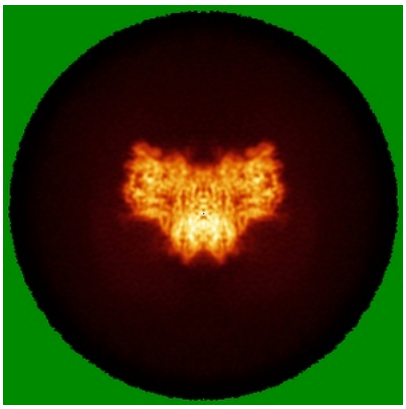


Z Index: 351

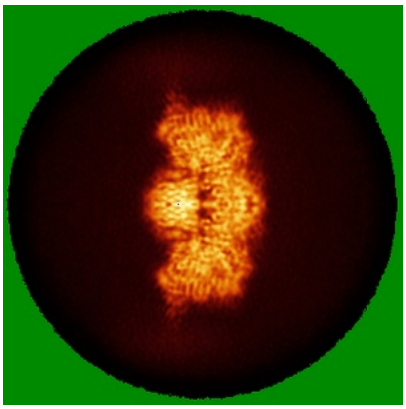
The images above show the largest variance slices of the map in three orthogonal directions.

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

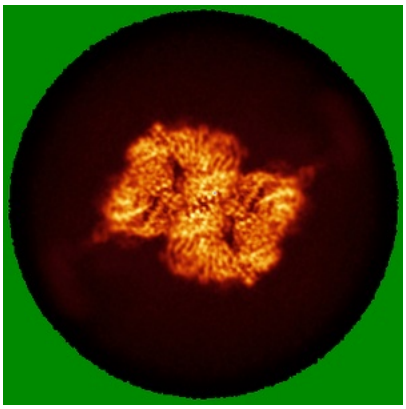
6.4.1 Primary map



X

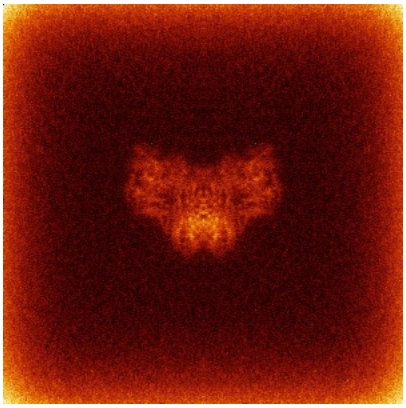


Y

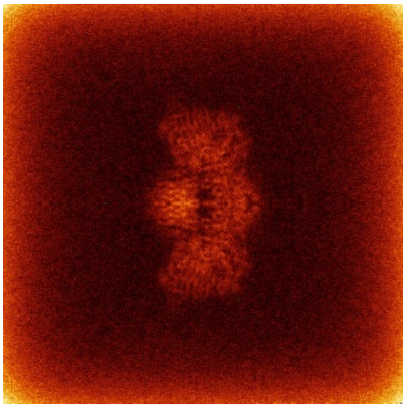


Z

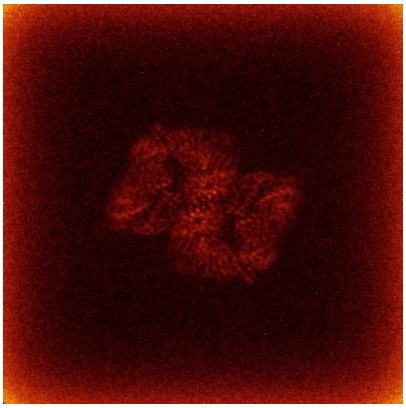
6.4.2 Raw map



X



Y

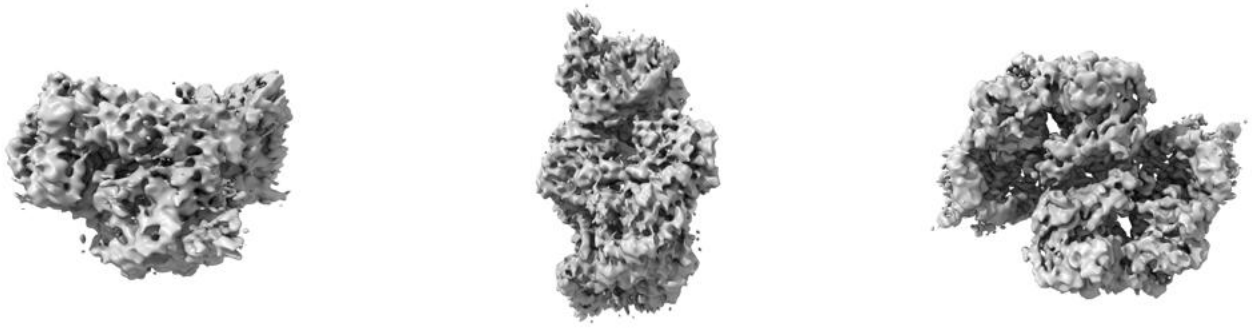


Z

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)

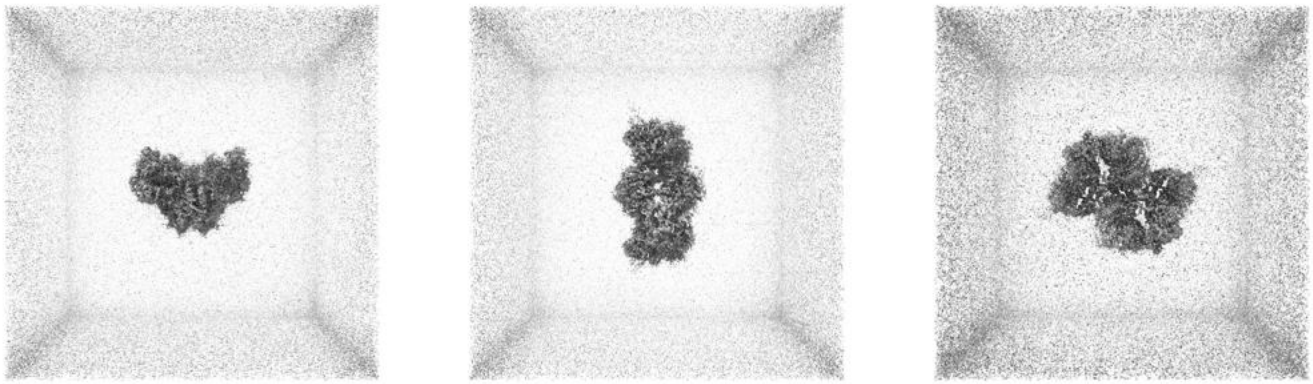
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0495. 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.

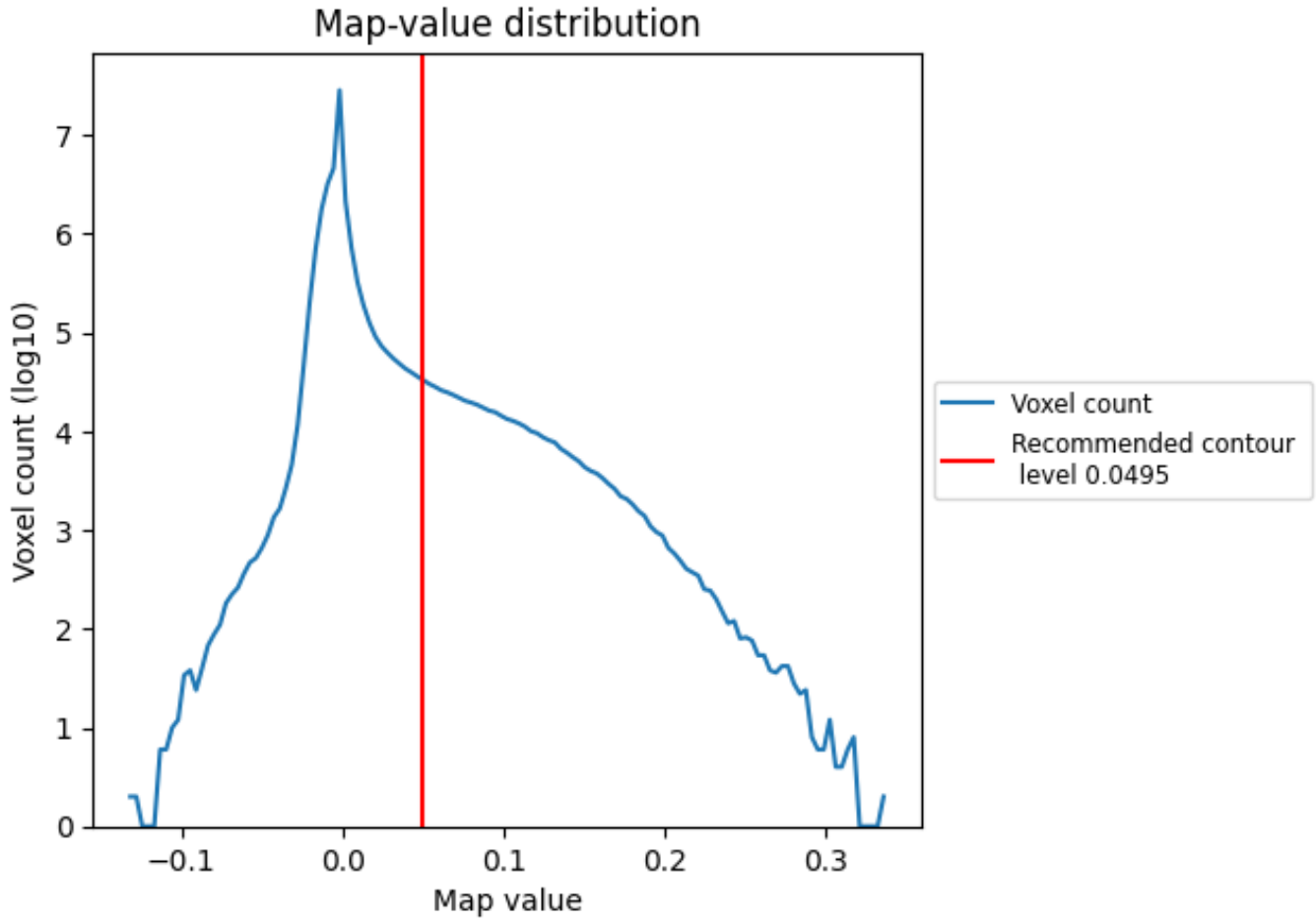
6.6 Mask visualisation (i)

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

7 Map analysis

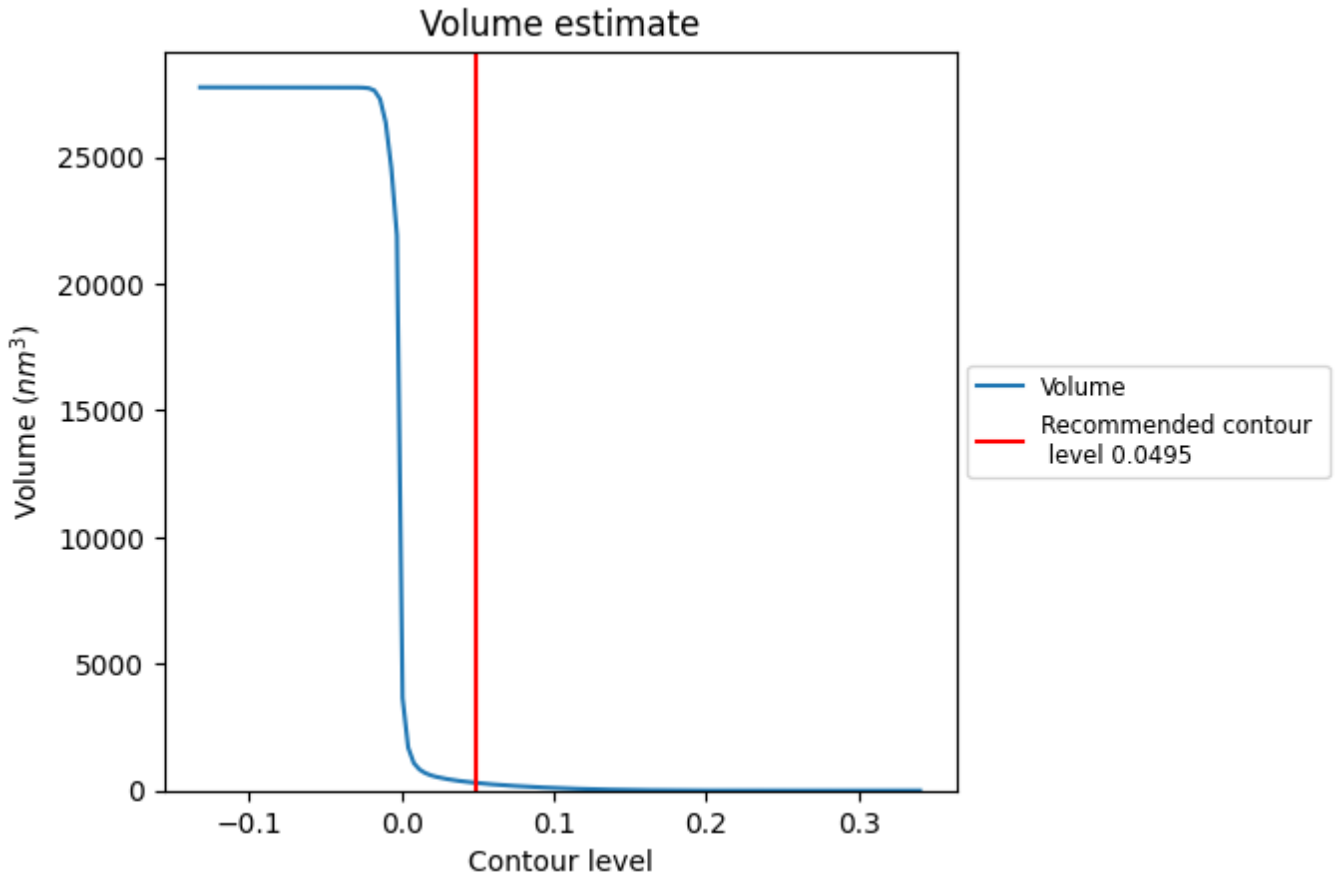
This section contains the results of statistical analysis of the map.

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.

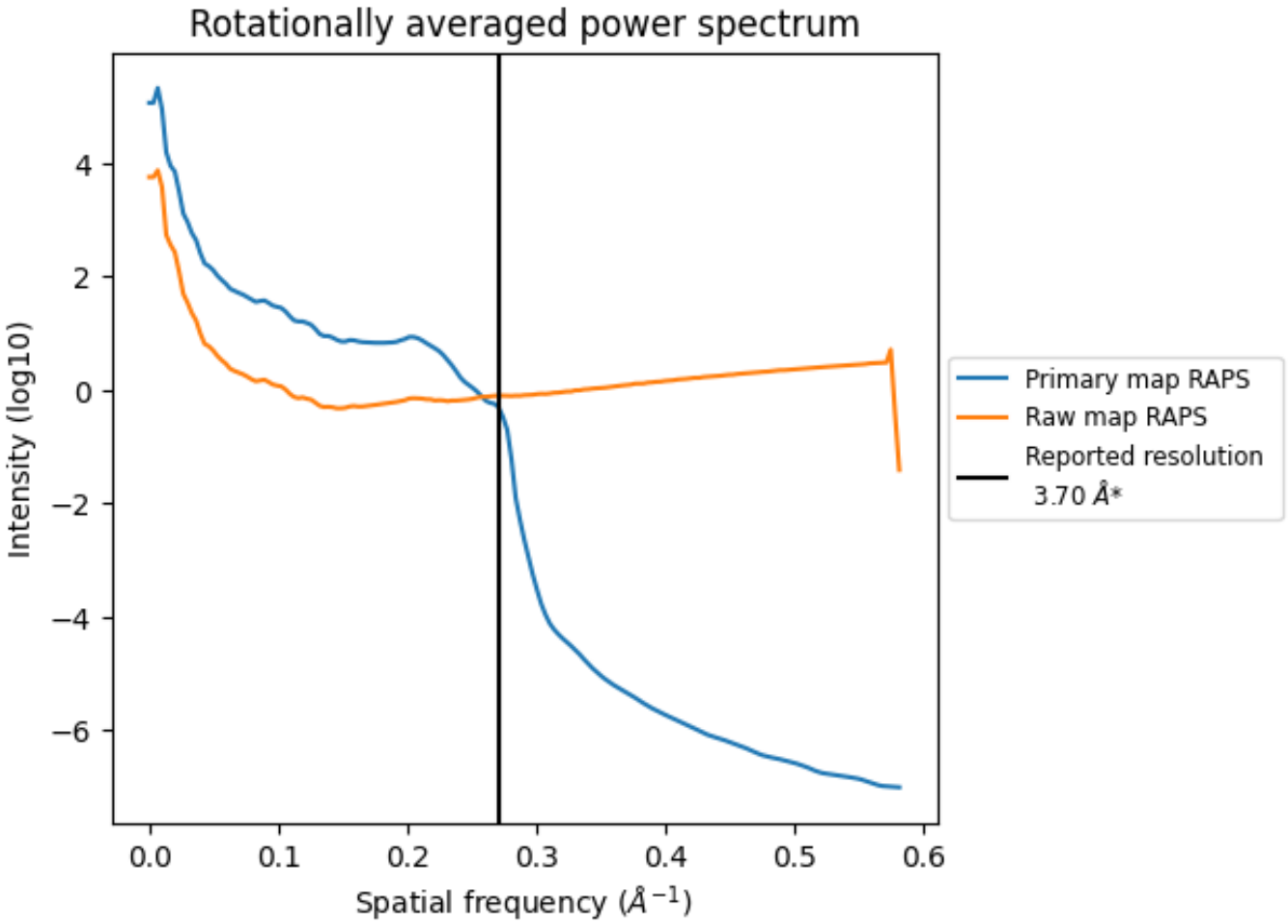
7.2 Volume estimate (i)



The volume at the recommended contour level is 300 nm^3; this corresponds to an approximate mass of 271 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)

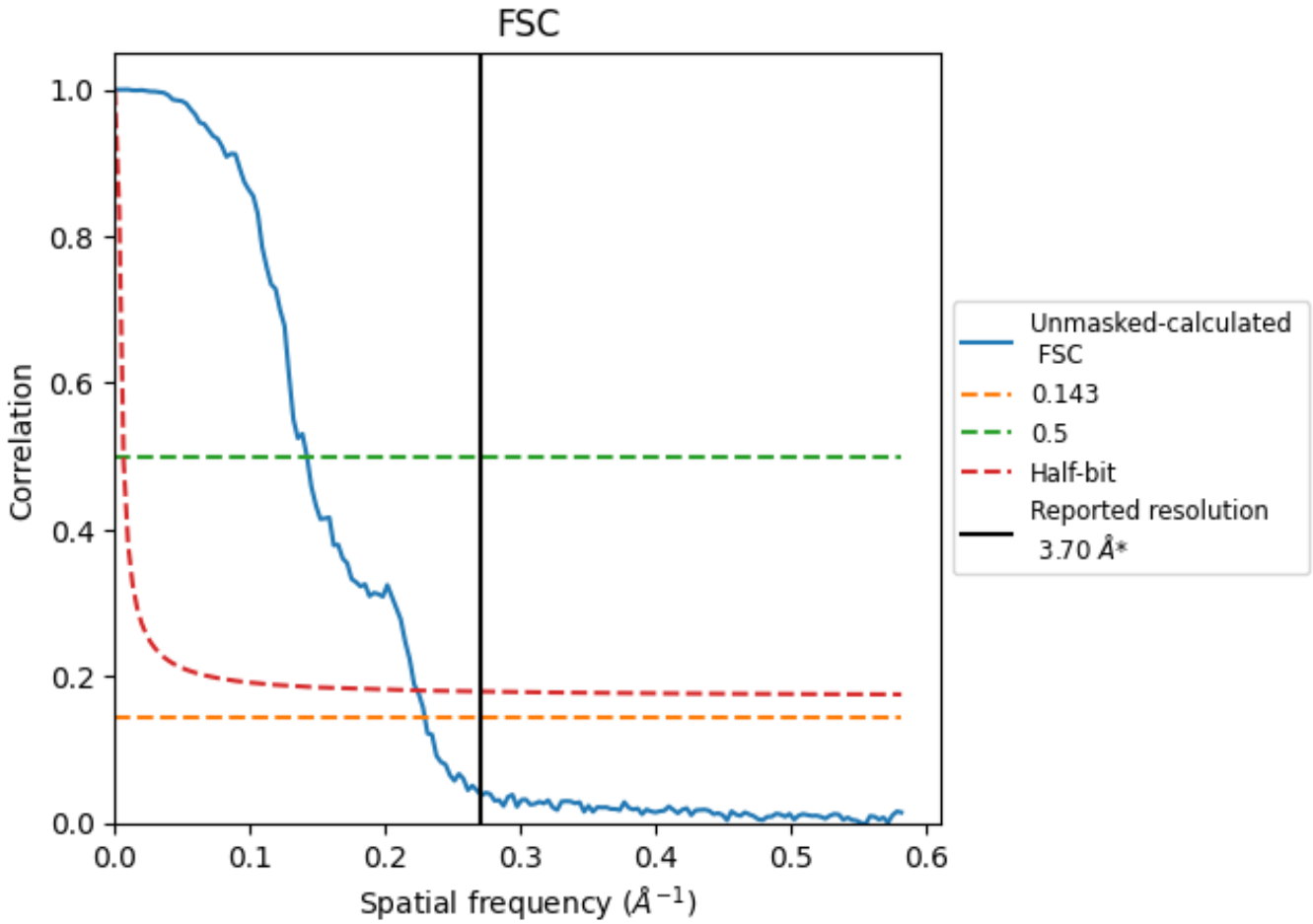


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

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 0.270 Å^{-1}

8.2 Resolution estimates (i)

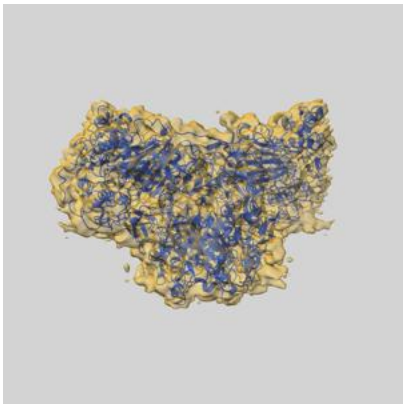
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.36	7.04	4.47

*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 4.36 differs from the reported value 3.7 by more than 10 %

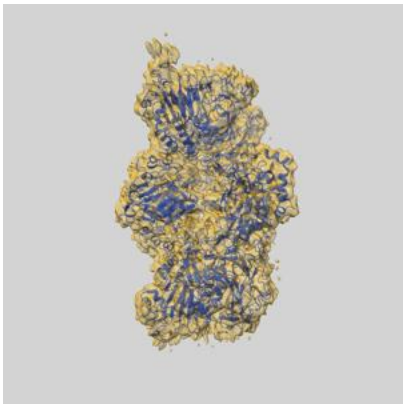
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19070 and PDB model 8RDE. Per-residue inclusion information can be found in section 3 on page 6.

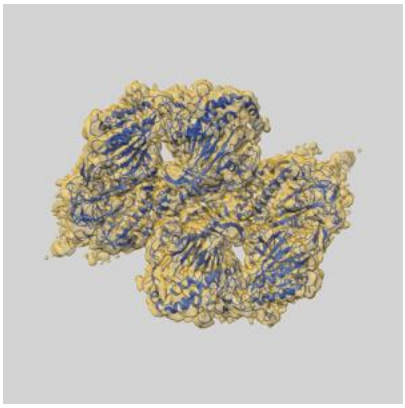
9.1 Map-model overlay



X



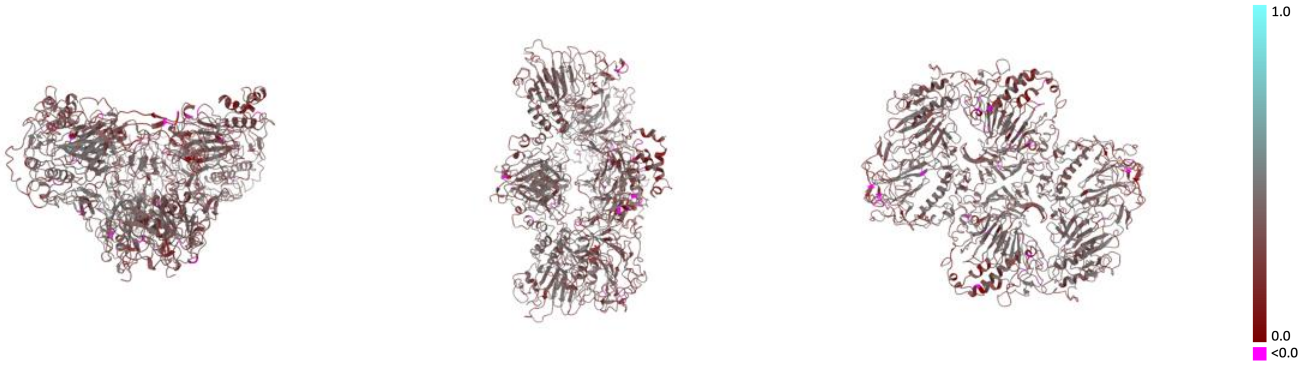
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0495 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

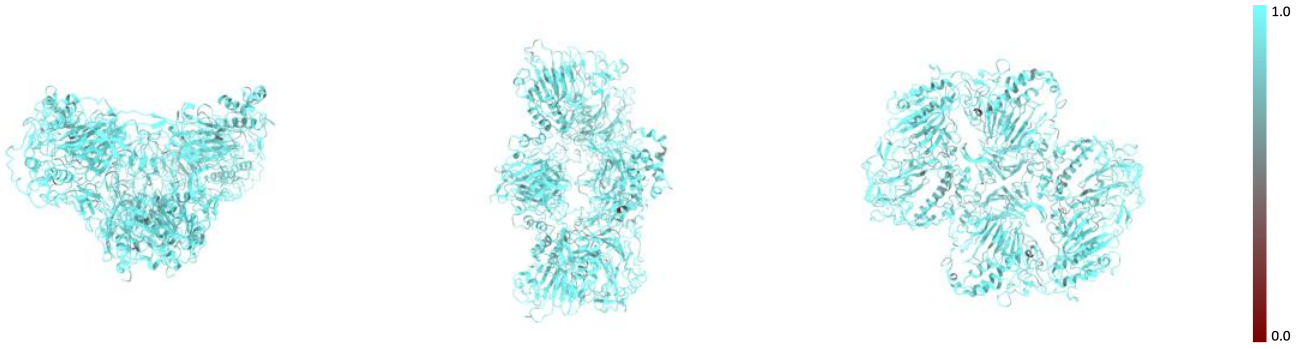
9.2 Q-score mapped to coordinate model



X Y Z

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

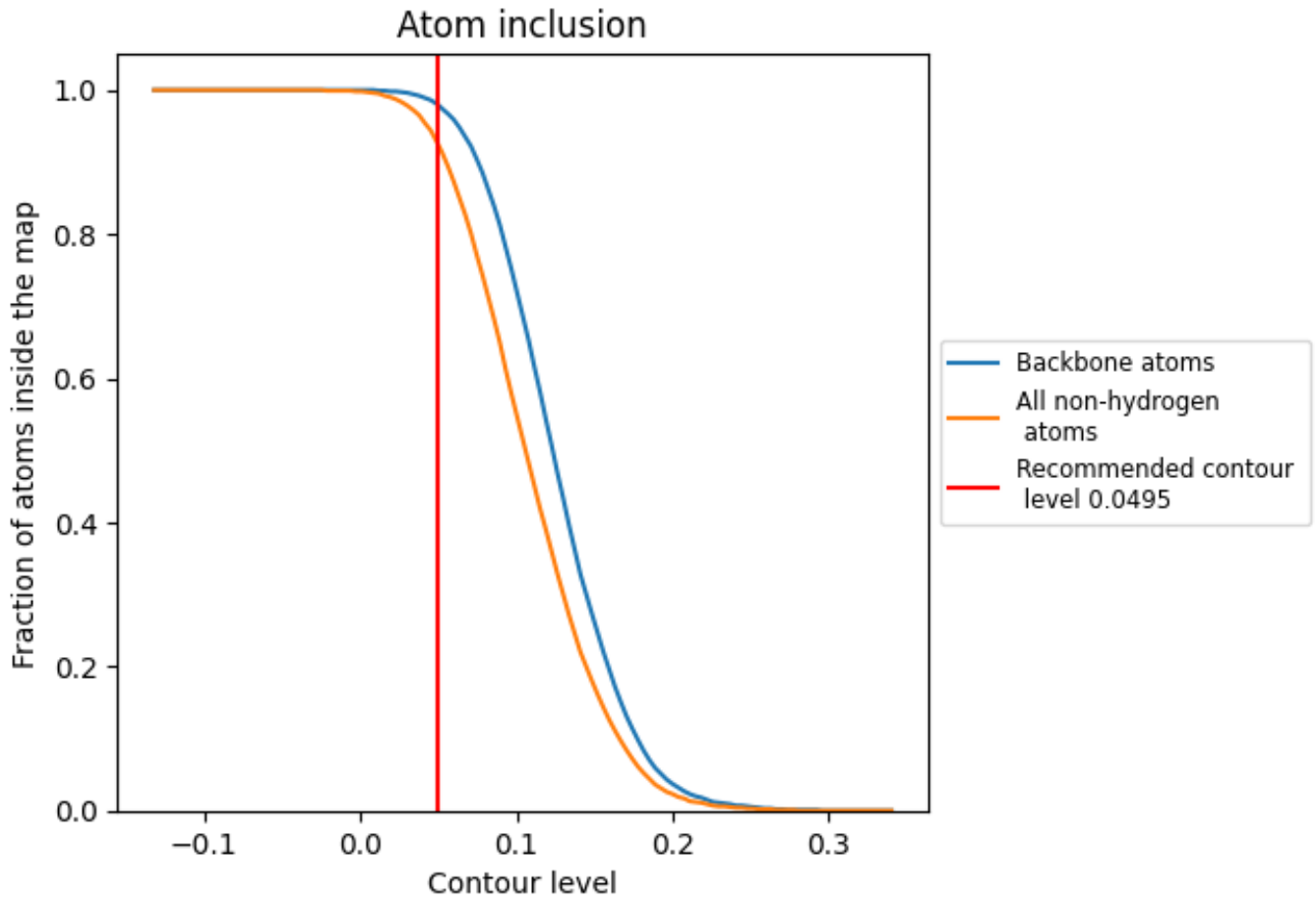
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0495).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.0495) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9260	0.3430
A	0.9230	0.3390
D	0.9290	0.3470