Full wwPDB EM Validation Report (i)

Aug 5, 2026 – 10:10 AM EDT

PDB ID	:	8FD6 / pdb_00008fd6
EMDB ID	:	EMD-29003
Title	:	Engineered human dynein motor domain in the microtubule-unbound state in the buffer containing ATP-Vi
Authors	:	Ton, W.; Wang, Y.; Chai, P.
Deposited on	:	2022-12-02
Resolution	:	2.90 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:

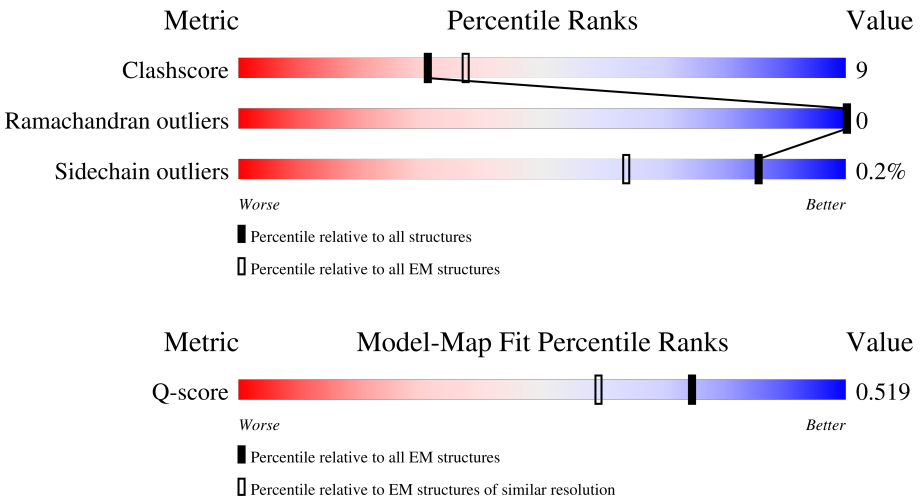
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	3126	8% 69% 19% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	VO4	A	3205	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 22170 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.

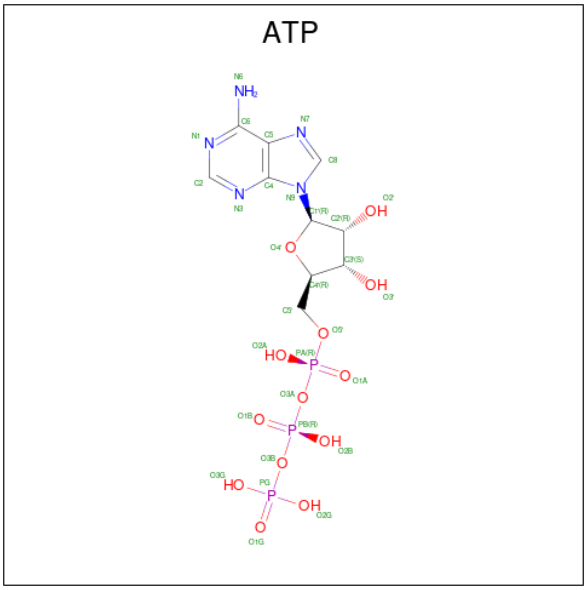
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1,Serine–tRNA ligase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2747	22052	14053	3812	4076	111	0	0

There are 4 discrepancies between the modelled and reference sequences:

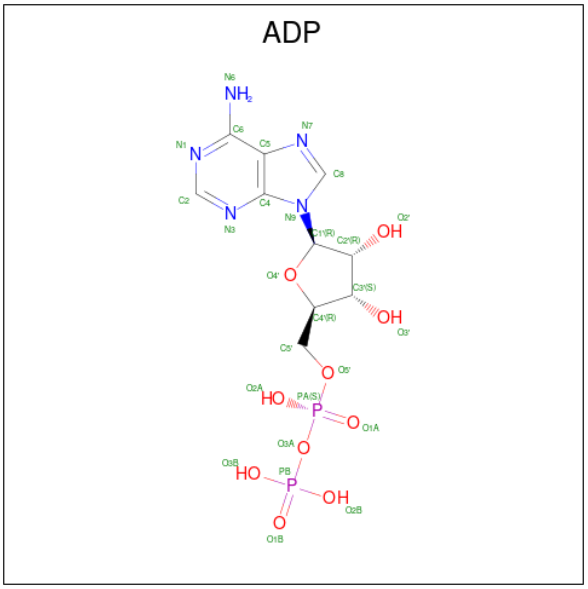
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q14204
A	2	SER	-	expression tag	UNP Q14204
A	3125	GLU	-	expression tag	UNP Q14204
A	3126	PHE	-	expression tag	UNP Q14204

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



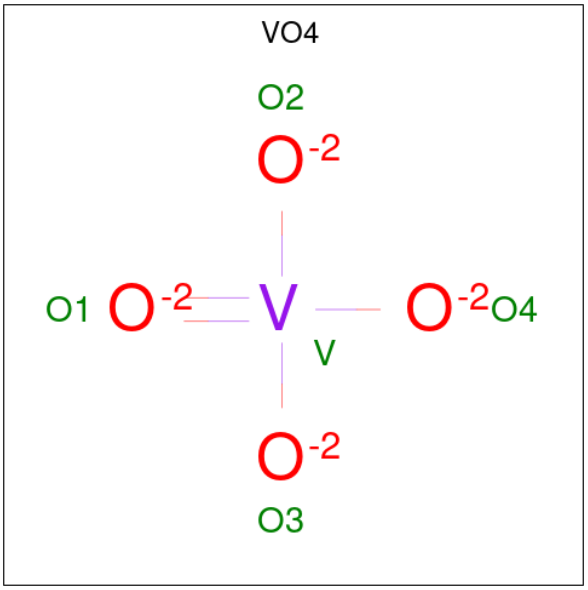
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	31	10	5	13	3	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is VANADATE ION (CCD ID: VO4) (formula: O_4V) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	O	V	
4	A	1	5	4	1	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

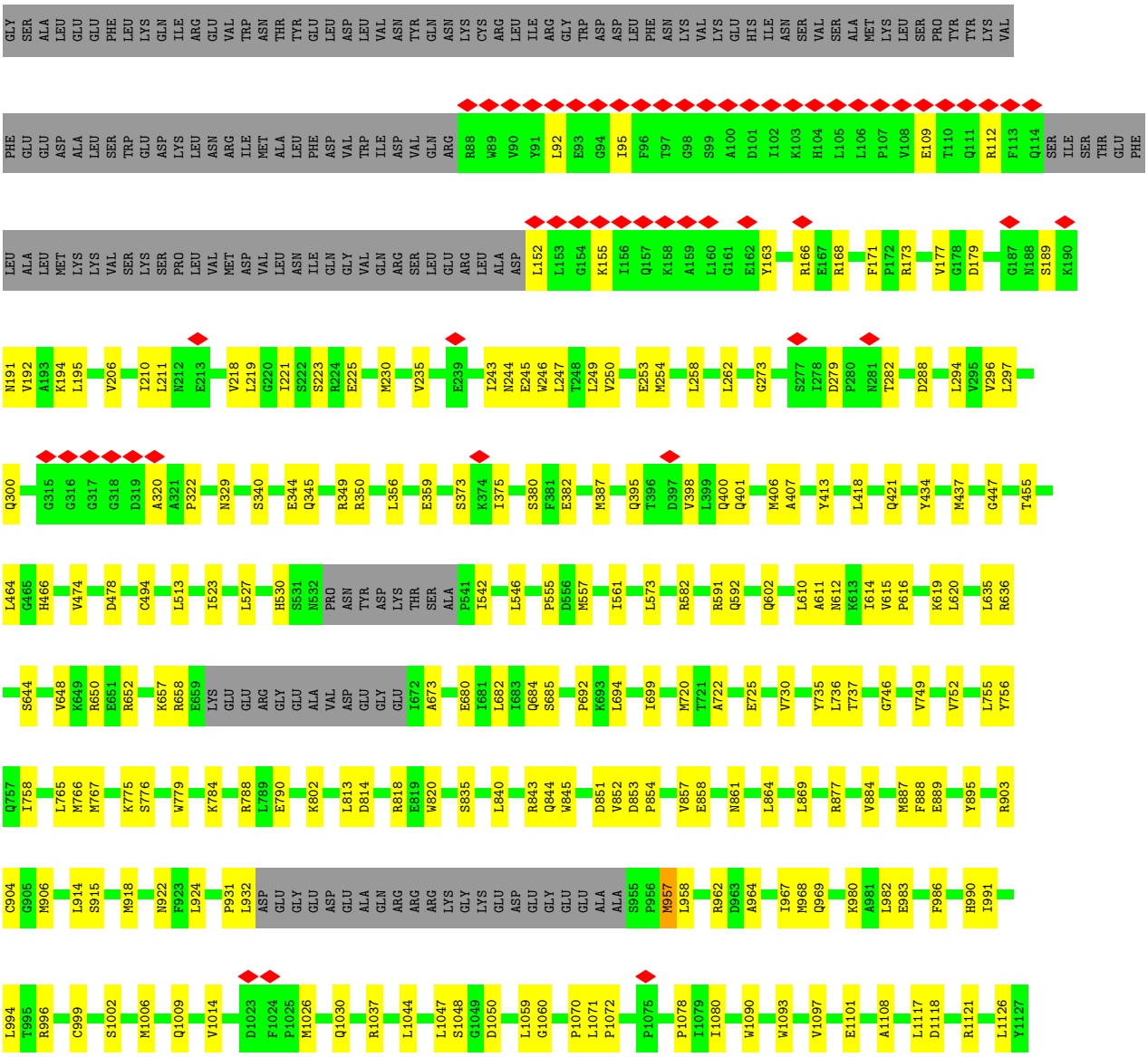
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	A	1	1	1	0

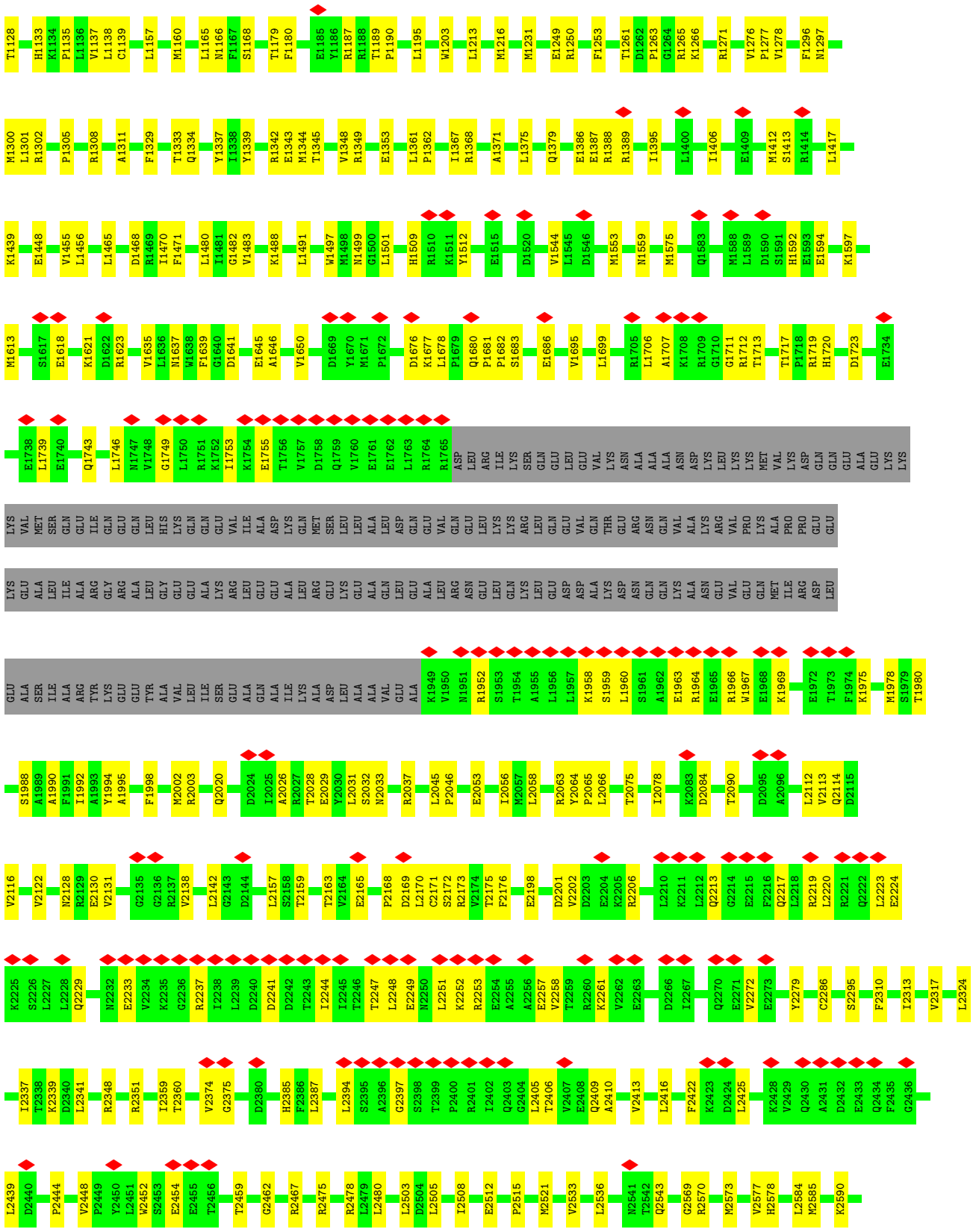
3 Residue-property plots (i)

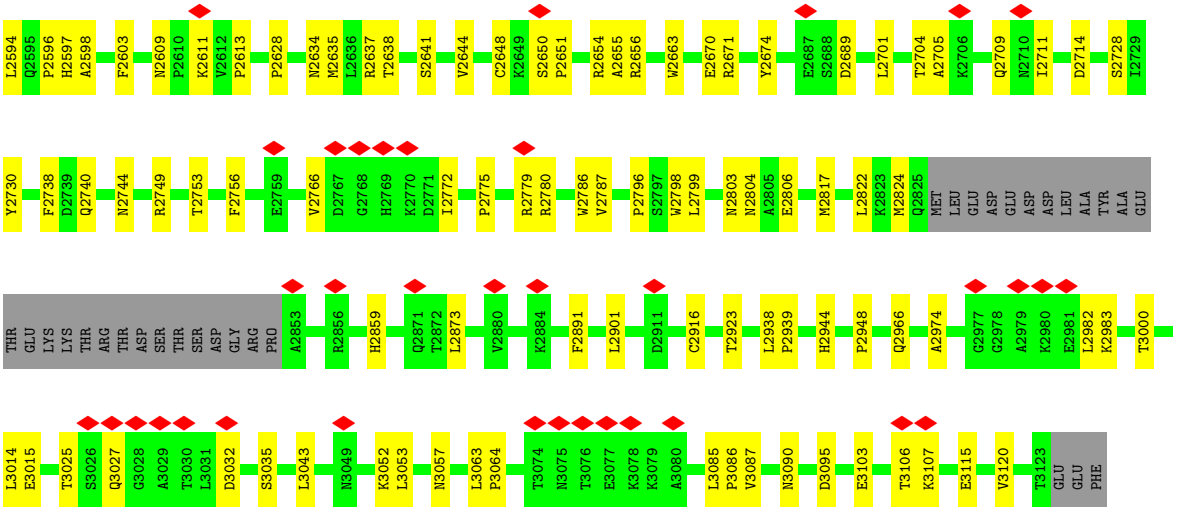
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:




T1128 H1133 K1134 P1135 L1136 V1137 L1138 C1139 L1157 M1160 L1165 N1166 F1167 S1168 T1179 F1180 E1185 Y1186 R1187 R1188 T1189 P1190 L1195 W1203 L1213 M1216 M1231 E1249 R1250 F1253 T1261 D1262 P1263 G1264 R1265 K1266 R1271 V1276 P1277 V1278 F1296 N1297
M1300 L1301 R1302 P1305 R1308 A1311 F1329 T1333 Q1334 Y1337 I1338 Y1339 R1342 E1343 M1344 T1345 V1348 R1349 E1353 L1361 P1362 I1367 R1368 A1371 L1375 Q1379 E1386 E1387 R1388 R1389 I1395 L1400 I1406 E1409 M1412 S1413 R1414 L1417
K1439 E1448 V1455 L1456 L1465 D1468 R1469 I1470 F1471 L1480 I1481 G1482 V1483 K1488 L1491 W1497 M1498 N1499 G1500 L1501 H1509 R1510 K1511 Y1512 E1515 D1520 V1544 L1545 D1546 M1553 N1559 M1575 Q1583 M1588 L1589 D1590 S1591 H1592 E1593 E1594 K1597
M1613 S1617 E1618 K1621 D1622 R1623 V1635 L1636 N1637 W1638 F1639 G1640 D1641 E1645 A1646 V1650 D1669 Y1670 M1671 P1672 D1676 K1677 L1678 P1679 Q1680 P1681 P1682 S1683 E1686 V1695 L1699 R1705 L1706 A1707 K1708 R1709 G1710 G1711 R1712 T1713 T1717 P1718 R1719 H1720 D1723 E1734
E1738 L1739 E1740 Q1743 L1746 N1747 V1748 G1749 L1750 R1751 K1752 I1753 K1754 E1755 T1756 V1757 D1758 Q1759 V1760 E1761 E1762 L1763 R1764 R1765 ASP LEU ARG ILE LYS SER GLN GLU LEU GLU VAL LYS ASN ALA ALA ALA ASN ASP LYS LEU LYS LYS MET VAL LYS ASP GLN GLN GLU ALA GLU LYS LYS
LYS VAL MET SER GLN GLU ILE GLN GLU GLN LEU HIS LYS GLN GLN GLU VAL ILE ALA ASP LYS GLN MET SER LEU LEU ALA LEU ASP GLN GLU VAL GLN GLU GLU LEU LYS LYS ARG LEU GLN GLU VAL GLN THR GLU ARG ASN GLN VAL ALA LYS ARG VAL PRO LYS ALA PRO PRO GLU GLU
LYS GLU ALA LEU ILE ALA ARG GLY ARG ALA LEU GLY GLU GLU ALA LYS ARG LEU GLU GLU ALA LEU ARG GLU LYS GLU ALA GLN LEU GLU ALA LEU ARG ASN GLU LEU GLN LYS LEU GLU ASP ALA LYS ASP ASN GLN GLN LYS ALA ASN GLU VAL GLU GLN MET ILE ARG ASP LEU
GLU ALA SER ILE ALA ARG TYR LYS GLU GLU TYR ALA VAL LEU ILE SER GLU ALA GLN ALA ILE LYS ALA ASP LEU ALA ALA VAL GLU ALA K1949 V1950 N1951 R1952 S1953 T1954 A1955 L1956 L1957 K1958 S1959 L1960 S1961 A1962 E1963 R1964 E1965 R1966 W1967 E1968 K1969 E1972 T1973 F1974 K1975 M1978 S1979 T1980
S1988 A1989 A1990 F1991 I1992 A1993 Y1994 A1995 F1998 M2002 R2003 Q2020 D2024 I2025 A2026 R2027 T2028 E2029 Y2030 L2031 S2032 N2033 R2037 L2045 P2046 E2053 I2056 M2057 L2058 R2063 Y2064 P2065 L2066 T2075 I2078 K2083 D2084 T2090 D2095 A2096 L2112 V2113 Q2114 D2115
V2116 V2122 N2128 R2129 E2130 V2131 G2135 G2136 R2137 V2138 L2142 G2143 D2144 L2157 S2158 T2159 T2163 V2164 E2165 P2168 D2169 L2170 C2171 S2172 R2173 V2174 T2175 F2176 E2198 D2201 V2202 D2203 E2204 K2205 R2206 L2210 K2211 L2212 Q2213 G2214 E2215 F2216 Q2217 L2218 R2219 L2220 R2221 Q2222 L2223 E2224
K2225 S2226 L2227 L2228 Q2229 N2232 E2233 V2234 K2235 G2236 R2237 I2238 L2239 D2240 D2241 D2242 T2243 I2244 I2245 T2246 T2247 L2248 E2249 N2250 L2251 K2252 R2253 E2254 A2255 A2256 E2257 V2258 T2259 R2260 K2261 V2262 E2263 D2266 I2267 Q2270 E2271 V2272 E2273 Y2279 C2286 S2295 F2310 I2313 V2317 L2324
I2337 T2338 K2339 D2340 L2341 R2348 R2351 I2359 T2360 V2374 G2375 D2380 H2385 F2386 L2387 L2394 S2395 A2396 G2397 S2398 T2399 P2400 R2401 I2402 Q2403 G2404 L2405 T2406 V2407 E2408 Q2409 A2410 V2413 L2416 F2422 K2423 D2424 L2425 K2428 V2429 Q2430 A2431 D2432 E2433 Q2434 F2435 G2436
L2439 D2440 P2444 V2448 P2449 Y2450 L2451 W2452 S2453 E2454 E2455 T2456 T2459 G2462 R2467 R2475 R2478 L2479 L2480 L2503 D2504 L2505 I2508 E2512 P2515 M2521 V2533 L2536 M2541 T2542 Q2543 G2569 R2570 M2573 V2577 H2578 L2584 M2585 K2590


L2594 Q2595 P2596 H2597 A2598 F2603 N2609 P2610 K2611 V2612 P2613 P2628 N2634 M2635 L2636 R2637 T2638 S2641 V2644 C2648 K2649 S2650 P2651 R2654 A2655 R2656 W2663 E2670 R2671 Y2674 E2687 S2688 D2689 L2701 T2704 A2705 K2706 Q2709 N2710 I2711 D2714 S2728 I2729
Y2730 F2738 D2739 Q2740 N2744 R2749 T2753 F2756 E2759 V2766 D2767 G2768 H2769 K2770 D2771 I2772 P2775 R2779 R2780 W2786 V2787 P2796 S2797 W2798 L2799 N2803 N2804 A2805 E2806 M2817 L2822 K2823 M2824 Q2825 MET LEU GLU ASP GLU ASP ASP LEU ALA TYR ALA GLU
THR GLU LYS LYS THR ARG THR ASP SER THR SER ASP GLY ARG PRO A2853 R2856 H2859 Q2871 T2872 L2873 V2880 K2884 F2891 L2901 D2911 C2916 T2923 L2938 P2939 H2944 P2948 Q2966 A2974 G2977 G2978 A2979 K2980 E2981 L2982 K2983 T3000
L3014 E3015 T3025 S3026 Q3027 G3028 A3029 T3030 L3031 D3032 S3035 L3043 N3049 K3052 L3053 N3057 L3063 P3064 T3074 N3075 T3076 E3077 K3078 K3079 A3080 L3085 P3086 V3087 N3090 D3095 E3103 T3106 K3107 E3115 V3120 T3123 GLU GLU PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	201707	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.842	Depositor
Minimum map value	-1.658	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	413.64, 413.64, 413.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.149, 1.149, 1.149	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: VO4, MG, ATP, ADP

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	0.35	0/22525	0.44	0/30531

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 (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	22052	0	22113	389	0
2	A	31	0	12	5	0
3	A	81	0	36	4	0
4	A	5	0	0	2	0
5	A	1	0	0	0	0
All	All	22170	0	22161	389	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 9.

All (389) 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:932:LEU:HB2	1:A:957:MET:CE	1.96	0.95
1:A:932:LEU:HB2	1:A:957:MET:HE3	1.53	0.90
1:A:406:MET:HG2	1:A:407:ALA:H	1.44	0.81
1:A:2650:SER:HB3	1:A:2651:PRO:HD2	1.63	0.81
1:A:766:MET:HG2	1:A:888:PHE:HB2	1.64	0.80
1:A:1187:ARG:HE	1:A:1195:LEU:HD13	1.45	0.80
1:A:398:VAL:HG13	1:A:400:GLN:H	1.49	0.76
1:A:1050:ASP:HB3	1:A:1278:VAL:HG13	1.67	0.76
1:A:2628:PRO:HG3	1:A:2637:ARG:HD2	1.67	0.76
1:A:2766:VAL:HG11	1:A:2772:ILE:HG12	1.65	0.76
1:A:869:LEU:HD21	1:A:877:ARG:HB3	1.68	0.74
1:A:2650:SER:HB2	1:A:2654:ARG:HE	1.51	0.74
1:A:932:LEU:HB2	1:A:957:MET:HE1	1.71	0.73
1:A:2804:ASN:ND2	1:A:3057:ASN:O	2.22	0.72
1:A:1231:MET:HE2	1:A:1253:PHE:HZ	1.53	0.71
1:A:903:ARG:NH1	4:A:3205:VO4:O4	2.24	0.71
1:A:1368:ARG:NH1	1:A:1413:SER:OG	2.24	0.70
1:A:1963:GLU:OE1	1:A:1966:ARG:NH2	2.24	0.70
1:A:109:GLU:HA	1:A:112:ARG:HB3	1.74	0.70
1:A:1101:GLU:OE2	1:A:1302:ARG:NH2	2.27	0.68
1:A:852:VAL:HG13	1:A:857:VAL:HG11	1.75	0.67
1:A:2634:ASN:ND2	1:A:2670:GLU:OE2	2.28	0.67
1:A:2439:LEU:O	1:A:2475:ARG:NH1	2.26	0.66
1:A:616:PRO:HA	1:A:619:LYS:HG2	1.76	0.66
1:A:1014:VAL:HG13	1:A:1026:MET:HE3	1.76	0.66
1:A:1379:GLN:HE21	1:A:1388:ARG:HB3	1.60	0.66
1:A:2066:LEU:HD11	1:A:2116:VAL:HG11	1.76	0.66
1:A:765:LEU:HB2	1:A:887:MET:HG2	1.78	0.66
1:A:1680:GLN:HG3	1:A:1681:PRO:HD3	1.78	0.66
1:A:1980:THR:HG22	1:A:2020:GLN:HB3	1.78	0.66
1:A:3025:THR:HA	1:A:3064:PRO:HG2	1.79	0.65
1:A:273:GLY:O	1:A:329:ASN:ND2	2.29	0.65
1:A:990:HIS:ND1	1:A:1050:ASP:OD1	2.23	0.65
1:A:1271:ARG:NH2	2:A:3201:ATP:O2G	2.30	0.65
1:A:2058:LEU:HD13	1:A:2078:ILE:HD11	1.79	0.65
1:A:2670:GLU:HB2	1:A:2799:LEU:HD11	1.78	0.64
1:A:2213:GLN:O	1:A:2217:GLN:NE2	2.30	0.64
1:A:2597:HIS:ND1	1:A:2598:ALA:O	2.30	0.64
1:A:406:MET:HE1	1:A:434:TYR:HB3	1.79	0.63
1:A:652:ARG:NH1	1:A:680:GLU:OE2	2.30	0.63
1:A:1998:PHE:HB3	1:A:2002:MET:HB3	1.80	0.63
1:A:3106:THR:HG22	1:A:3107:LYS:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2705:ALA:HB2	1:A:2711:ILE:HD12	1.81	0.62
1:A:775:LYS:N	2:A:3201:ATP:O2B	2.31	0.62
1:A:1261:THR:HB	1:A:2923:THR:HG23	1.82	0.62
1:A:845:TRP:CD2	1:A:887:MET:HE1	2.33	0.62
1:A:1468:ASP:OD1	1:A:1499:ASN:ND2	2.28	0.62
1:A:1118:ASP:OD1	1:A:1121:ARG:NH2	2.32	0.61
1:A:3087:VAL:HG22	1:A:3120:VAL:HB	1.81	0.61
1:A:2650:SER:OG	1:A:2654:ARG:NH2	2.27	0.61
1:A:592:GLN:HA	1:A:615:VAL:HG21	1.82	0.60
1:A:982:LEU:HD21	1:A:996:ARG:HG3	1.82	0.60
1:A:189:SER:HA	1:A:243:ILE:HD11	1.82	0.60
1:A:1329:PHE:HB2	1:A:1339:TYR:HE2	1.67	0.60
1:A:1470:ILE:HD12	1:A:1635:VAL:HG21	1.84	0.60
1:A:418:LEU:O	1:A:421:GLN:NE2	2.35	0.59
1:A:636:ARG:NH2	4:A:3205:VO4:O4	2.31	0.59
1:A:767:MET:HE1	1:A:779:TRP:CD1	2.38	0.59
1:A:2689:ASP:HB3	1:A:2730:TYR:CE1	2.37	0.59
1:A:2028:THR:O	1:A:2032:SER:OG	2.21	0.59
1:A:813:LEU:HD12	1:A:820:TRP:HB2	1.83	0.59
1:A:1966:ARG:HH22	1:A:2224:GLU:CD	2.11	0.59
1:A:1618:GLU:H	1:A:1621:LYS:HZ3	1.51	0.58
1:A:1712:ARG:HH12	1:A:2163:THR:HG23	1.68	0.58
1:A:1723:ASP:OD2	1:A:2063:ARG:NE	2.36	0.58
1:A:1482:GLY:O	1:A:1488:LYS:NZ	2.33	0.58
1:A:1676:ASP:OD1	1:A:1677:LYS:N	2.36	0.58
1:A:1959:SER:HB2	1:A:2251:LEU:HD13	1.85	0.58
1:A:2983:LYS:NZ	1:A:3032:ASP:O	2.27	0.58
1:A:1263:PRO:O	1:A:1265:ARG:NH1	2.37	0.58
1:A:288:ASP:OD2	1:A:349:ARG:NH2	2.32	0.58
1:A:1645:GLU:OE2	1:A:1677:LYS:NZ	2.35	0.58
1:A:1963:GLU:OE1	1:A:1967:TRP:NE1	2.37	0.58
1:A:2360:THR:HG22	1:A:2817:MET:HG3	1.86	0.58
1:A:513:LEU:HD13	1:A:573:LEU:HD23	1.86	0.57
1:A:2201:ASP:OD1	1:A:2202:VAL:N	2.37	0.57
1:A:2505:LEU:HB3	1:A:2536:LEU:HD22	1.87	0.57
1:A:2229:GLN:NE2	1:A:2233:GLU:OE1	2.38	0.57
1:A:602:GLN:OE1	1:A:650:ARG:NH2	2.38	0.57
1:A:2796:PRO:HG2	1:A:2803:ASN:HA	1.87	0.56
1:A:1386:GLU:HG3	1:A:1389:ARG:HH21	1.68	0.56
1:A:262:LEU:HB2	1:A:294:LEU:HD22	1.86	0.56
1:A:1297:ASN:HD22	1:A:1300:MET:HE2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:SER:O	1:A:345:GLN:NE2	2.39	0.56
1:A:612:ASN:O	1:A:3015:GLU:HG3	2.04	0.56
1:A:1488:LYS:HG2	1:A:1639:PHE:CD2	2.41	0.56
1:A:2045:LEU:HD12	1:A:2046:PRO:HD2	1.88	0.56
1:A:2585:MET:SD	1:A:2613:PRO:HB3	2.45	0.56
1:A:171:PHE:CE2	1:A:173:ARG:HB2	2.40	0.56
1:A:279:ASP:OD1	1:A:282:THR:OG1	2.21	0.56
1:A:1305:PRO:HA	1:A:1308:ARG:HD3	1.88	0.56
1:A:398:VAL:O	1:A:401:GLN:NE2	2.39	0.56
1:A:223:SER:OG	1:A:225:GLU:OE1	2.23	0.56
1:A:474:VAL:O	1:A:877:ARG:NH2	2.21	0.56
1:A:2671:ARG:HG3	1:A:2799:LEU:HD12	1.87	0.55
1:A:657:LYS:HB3	1:A:658:ARG:NH2	2.21	0.55
1:A:1168:SER:HA	1:A:1213:LEU:HD23	1.88	0.55
1:A:1026:MET:HG3	1:A:1030:GLN:HB3	1.89	0.55
1:A:2543:GLN:OE1	1:A:2570:ARG:NH2	2.39	0.55
1:A:1126:LEU:HD11	1:A:1138:LEU:HD21	1.89	0.55
1:A:1455:VAL:HG11	1:A:1650:VAL:HG23	1.88	0.55
1:A:2644:VAL:HG13	1:A:2780:ARG:HD3	1.90	0.54
1:A:297:LEU:HD11	1:A:413:TYR:CZ	2.42	0.54
1:A:720:MET:HE1	1:A:756:TYR:CD2	2.42	0.54
1:A:494:CYS:SG	1:A:557:MET:HE3	2.48	0.54
1:A:924:LEU:HD13	1:A:969:GLN:OE1	2.08	0.54
1:A:1133:HIS:CE1	1:A:1203:TRP:CD2	2.96	0.54
1:A:1553:MET:HE2	1:A:1553:MET:HA	1.90	0.54
1:A:1995:ALA:HB1	1:A:2003:ARG:HG2	1.89	0.54
1:A:915:SER:H	1:A:918:MET:HE3	1.71	0.54
1:A:1488:LYS:N	3:A:3203:ADP:O1B	2.40	0.54
1:A:2131:VAL:HB	1:A:2138:VAL:HG13	1.89	0.54
1:A:1509:HIS:H	1:A:1512:TYR:HB2	1.73	0.54
1:A:1683:SER:HB3	1:A:1686:GLU:OE1	2.08	0.54
1:A:1952:ARG:HH21	1:A:2244:ILE:HG23	1.73	0.54
1:A:2053:GLU:HA	1:A:2056:ILE:HD12	1.89	0.54
1:A:244:ASN:OD1	1:A:245:GLU:N	2.41	0.54
1:A:994:LEU:HD11	1:A:999:CYS:SG	2.48	0.53
1:A:2740:GLN:NE2	1:A:2744:ASN:OD1	2.41	0.53
1:A:2533:VAL:HB	1:A:2573:MET:HE1	1.90	0.53
1:A:749:VAL:HA	1:A:752:VAL:HG12	1.90	0.53
1:A:2066:LEU:HD12	1:A:2157:LEU:HB2	1.89	0.53
1:A:2648:CYS:SG	1:A:2655:ALA:HB2	2.49	0.53
1:A:802:LYS:HG3	1:A:851:ASP:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:MET:HG2	2:A:3201:ATP:C2	2.44	0.52
1:A:1166:ASN:ND2	1:A:1559:ASN:OD1	2.34	0.52
1:A:2374:VAL:HG23	1:A:2375:GLY:H	1.73	0.52
1:A:254:MET:O	1:A:258:LEU:HD23	2.10	0.52
1:A:455:THR:N	3:A:3204:ADP:O3B	2.35	0.52
1:A:168:ARG:NH1	1:A:177:VAL:O	2.43	0.52
1:A:790:GLU:OE1	1:A:843:ARG:NH2	2.42	0.52
1:A:2901:LEU:HD21	1:A:2944:HIS:ND1	2.25	0.52
1:A:296:VAL:HG13	1:A:359:GLU:OE1	2.10	0.52
1:A:2248:LEU:HB3	1:A:2252:LYS:NZ	2.24	0.52
1:A:1720:HIS:HB3	1:A:1994:TYR:CE1	2.45	0.51
1:A:1753:ILE:HG22	1:A:1964:ARG:HH11	1.75	0.51
1:A:2416:LEU:HD23	1:A:2425:LEU:HD11	1.92	0.51
1:A:657:LYS:HB3	1:A:658:ARG:HH22	1.74	0.51
1:A:2063:ARG:O	1:A:2175:THR:OG1	2.26	0.51
1:A:746:GLY:O	1:A:749:VAL:HG22	2.10	0.51
1:A:1006:MET:HG2	1:A:1128:THR:HG21	1.92	0.51
1:A:1439:LYS:HG3	1:A:1456:LEU:HD12	1.92	0.51
1:A:918:MET:HG2	2:A:3201:ATP:N1	2.25	0.51
1:A:2578:HIS:HB2	1:A:2609:ASN:HD21	1.75	0.51
1:A:2609:ASN:ND2	1:A:2611:LYS:HE3	2.26	0.51
1:A:2766:VAL:HB	1:A:2798:TRP:CD1	2.45	0.51
1:A:206:VAL:HG13	1:A:221:ILE:HG23	1.92	0.51
1:A:737:THR:HB	1:A:918:MET:HG3	1.93	0.51
1:A:2651:PRO:HB3	1:A:2709:GLN:HA	1.92	0.51
1:A:1339:TYR:HA	1:A:1343:GLU:OE2	2.11	0.51
1:A:2628:PRO:HG3	1:A:2637:ARG:CD	2.40	0.51
1:A:375:ILE:HG12	1:A:382:GLU:HB2	1.93	0.51
1:A:1180:PHE:CE2	1:A:1231:MET:HE1	2.46	0.50
1:A:523:ILE:HD11	1:A:546:LEU:HD11	1.93	0.50
1:A:2116:VAL:HG12	1:A:2159:THR:HB	1.92	0.50
1:A:168:ARG:NH2	1:A:179:ASP:OD1	2.43	0.50
1:A:591:ARG:HG2	1:A:635:LEU:HD13	1.94	0.50
1:A:243:ILE:HD13	1:A:246:TRP:HE1	1.76	0.50
1:A:1483:VAL:HG21	1:A:1641:ASP:HB3	1.94	0.50
1:A:2448:VAL:O	1:A:2467:ARG:NH1	2.45	0.50
1:A:434:TYR:CD1	1:A:464:LEU:HD13	2.47	0.50
1:A:1002:SER:HB3	1:A:1277:PRO:HB3	1.94	0.50
1:A:1333:THR:HG22	1:A:1334:GLN:HG2	1.93	0.50
1:A:1646:ALA:O	1:A:1650:VAL:HG12	2.11	0.50
1:A:1712:ARG:NE	1:A:2165:GLU:OE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2241:ASP:HA	1:A:2244:ILE:HG22	1.92	0.50
1:A:3095:ASP:N	1:A:3095:ASP:OD1	2.44	0.50
1:A:1231:MET:HE2	1:A:1253:PHE:CZ	2.42	0.49
1:A:395:GLN:OE1	1:A:398:VAL:HG12	2.11	0.49
1:A:1613:MET:HE3	1:A:1623:ARG:HH21	1.77	0.49
1:A:2405:LEU:HD23	1:A:2409:GLN:HB3	1.94	0.49
1:A:2635:MET:CE	1:A:2663:TRP:HE3	2.24	0.49
1:A:387:MET:HB2	1:A:406:MET:HE2	1.95	0.49
1:A:3032:ASP:N	1:A:3035:SER:OG	2.44	0.49
1:A:2219:ARG:HG2	1:A:2257:GLU:OE2	2.13	0.49
1:A:2317:VAL:HG21	1:A:2341:LEU:HA	1.94	0.49
1:A:2444:PRO:HD2	1:A:2478:ARG:HG3	1.94	0.49
1:A:1135:PRO:HB2	1:A:1276:VAL:HG12	1.95	0.49
1:A:2891:PHE:CD2	1:A:2982:LEU:HD22	2.48	0.49
1:A:720:MET:HE1	1:A:756:TYR:HD2	1.77	0.48
1:A:1297:ASN:ND2	1:A:1300:MET:HE2	2.28	0.48
1:A:1349:ARG:HG3	1:A:1353:GLU:OE1	2.13	0.48
1:A:192:VAL:HG11	1:A:211:LEU:HD21	1.96	0.48
1:A:2122:VAL:HG12	1:A:2142:LEU:HD22	1.95	0.48
1:A:964:ALA:O	1:A:968:MET:HG3	2.14	0.48
1:A:1448:GLU:HG2	1:A:1497:TRP:NE1	2.28	0.48
1:A:1137:VAL:HG13	1:A:1278:VAL:HG23	1.95	0.48
1:A:2859:HIS:HB2	1:A:2916:CYS:HB3	1.96	0.48
1:A:991:ILE:HD12	1:A:1139:CYS:SG	2.54	0.48
1:A:2313:ILE:HG12	1:A:2348:ARG:HD2	1.95	0.48
1:A:2590:LYS:HE3	1:A:2594:LEU:HD21	1.94	0.48
1:A:2873:LEU:H	1:A:2873:LEU:HD23	1.79	0.48
1:A:2938:LEU:HD12	1:A:2939:PRO:HD2	1.95	0.48
1:A:530:HIS:CE1	1:A:542:ILE:HD12	2.48	0.48
1:A:2286:CYS:SG	1:A:2310:PHE:HZ	2.37	0.48
1:A:776:SER:HA	1:A:779:TRP:CD1	2.49	0.48
1:A:931:PRO:HG3	1:A:958:LEU:HD22	1.95	0.48
1:A:1680:GLN:O	1:A:1682:PRO:HD3	2.14	0.48
1:A:1966:ARG:HA	1:A:1969:LYS:HD2	1.96	0.48
1:A:2385:HIS:CD2	1:A:2416:LEU:HD12	2.48	0.48
1:A:1301:LEU:HD12	1:A:1311:ALA:HA	1.96	0.47
1:A:1755:GLU:HG2	1:A:2237:ARG:HD3	1.96	0.47
1:A:964:ALA:HA	1:A:967:ILE:HD12	1.95	0.47
1:A:1739:LEU:HD23	1:A:1978:MET:HE2	1.95	0.47
1:A:2387:LEU:HB3	1:A:2822:LEU:HD13	1.96	0.47
1:A:694:LEU:HD13	1:A:699:ILE:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1480:LEU:HD23	1:A:1637:ASN:HB2	1.97	0.47
1:A:1966:ARG:NH2	1:A:1967:TRP:HE1	2.12	0.47
1:A:2128:ASN:HB2	1:A:2130:GLU:OE1	2.13	0.47
1:A:380:SER:OG	1:A:382:GLU:OE1	2.29	0.47
1:A:1712:ARG:NH1	1:A:2163:THR:HA	2.28	0.47
1:A:2459:THR:HG23	1:A:2462:GLY:H	1.80	0.47
1:A:1367:ILE:HD12	1:A:1406:ILE:HG12	1.96	0.47
1:A:657:LYS:NZ	1:A:673:ALA:HB3	2.29	0.47
1:A:776:SER:HB2	1:A:889:GLU:OE2	2.14	0.47
1:A:1367:ILE:HG22	1:A:1412:MET:HE3	1.96	0.47
1:A:1719:ARG:NH1	1:A:2128:ASN:OD1	2.47	0.47
1:A:1753:ILE:HD12	1:A:1960:LEU:HD13	1.96	0.47
1:A:986:PHE:HA	1:A:994:LEU:HD23	1.97	0.47
1:A:2258:VAL:HA	1:A:2261:LYS:HG2	1.96	0.47
1:A:2422:PHE:CE1	1:A:2452:TRP:HB3	2.50	0.47
1:A:736:LEU:HD22	2:A:3201:ATP:C5	2.49	0.47
1:A:990:HIS:NE2	1:A:994:LEU:HD22	2.29	0.47
1:A:1344:MET:HE3	1:A:1344:MET:HB3	1.86	0.47
1:A:2220:LEU:O	1:A:2223:LEU:HG	2.15	0.47
1:A:2029:GLU:HG3	1:A:2037:ARG:HH12	1.80	0.46
1:A:2084:ASP:N	1:A:2084:ASP:OD1	2.48	0.46
1:A:692:PRO:HG2	1:A:758:ILE:HD11	1.97	0.46
1:A:1009:GLN:HG2	1:A:1128:THR:HG23	1.97	0.46
1:A:2359:ILE:HG21	1:A:2480:LEU:HD11	1.96	0.46
1:A:1249:GLU:HG2	1:A:1250:ARG:HG3	1.97	0.46
1:A:2577:VAL:O	1:A:2577:VAL:HG13	2.16	0.46
1:A:2634:ASN:O	1:A:2638:THR:HG23	2.15	0.46
1:A:1078:PRO:HB2	1:A:1080:ILE:HG12	1.96	0.46
1:A:406:MET:HG2	1:A:407:ALA:N	2.20	0.46
1:A:582:ARG:NH1	1:A:2728:SER:O	2.42	0.46
1:A:437:MET:SD	1:A:447:GLY:HA3	2.56	0.46
1:A:191:ASN:CG	1:A:194:LYS:HD3	2.41	0.46
1:A:2206:ARG:HG3	1:A:2272:VAL:HG11	1.98	0.46
1:A:2948:PRO:HD3	1:A:3090:ASN:HD22	1.80	0.46
1:A:735:TYR:O	1:A:922:ASN:ND2	2.46	0.45
1:A:152:LEU:HD22	1:A:155:LYS:HD3	1.98	0.45
1:A:2169:ASP:OD1	1:A:2170:LEU:N	2.49	0.45
1:A:1216:MET:HE3	1:A:1266:LYS:HB3	1.99	0.45
1:A:1488:LYS:HG2	1:A:1639:PHE:HD2	1.81	0.45
1:A:1717:THR:HG21	1:A:2172:SER:HB3	1.98	0.45
1:A:1749:GLY:O	1:A:1753:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2075:THR:HG23	1:A:2112:LEU:HD21	1.98	0.45
1:A:2656:ARG:HD2	1:A:2756:PHE:CE2	2.51	0.45
1:A:2394:LEU:HD21	1:A:2397:GLY:H	1.81	0.45
1:A:755:LEU:HD11	1:A:767:MET:SD	2.57	0.45
1:A:1337:TYR:OH	1:A:1387:GLU:OE1	2.33	0.45
1:A:1699:LEU:HD21	1:A:1994:TYR:HB3	1.99	0.45
1:A:722:ALA:O	1:A:725:GLU:HG3	2.17	0.45
1:A:730:VAL:HG22	1:A:788:ARG:NH1	2.32	0.45
1:A:1491:LEU:HD23	1:A:1491:LEU:HA	1.85	0.45
1:A:3043:LEU:HG	1:A:3063:LEU:HD11	1.99	0.45
1:A:2974:ALA:HB2	1:A:2982:LEU:HD21	1.99	0.45
1:A:636:ARG:NH2	3:A:3204:ADP:O1B	2.50	0.45
1:A:644:SER:OG	1:A:685:SER:HB2	2.17	0.45
1:A:2406:THR:HG23	1:A:2409:GLN:H	1.82	0.45
1:A:1044:LEU:HD21	1:A:1060:GLY:HA2	1.98	0.44
1:A:235:VAL:HG23	1:A:253:GLU:OE1	2.17	0.44
1:A:1680:GLN:CG	1:A:1681:PRO:HD3	2.46	0.44
1:A:2090:THR:O	1:A:2113:VAL:HA	2.18	0.44
1:A:3043:LEU:HD12	1:A:3063:LEU:HD21	1.99	0.44
1:A:2128:ASN:HD21	1:A:2173:ARG:HH21	1.64	0.44
1:A:2324:LEU:HD11	1:A:2337:ILE:HG13	1.99	0.44
1:A:2452:TRP:HD1	1:A:2454:GLU:HG2	1.82	0.44
1:A:2584:LEU:HD23	1:A:2613:PRO:HD2	2.00	0.44
1:A:3027:GLN:HG3	1:A:3027:GLN:O	2.17	0.44
1:A:1308:ARG:HH11	1:A:1308:ARG:HG3	1.82	0.44
1:A:2198:GLU:HG2	1:A:2279:TYR:HE2	1.82	0.44
1:A:418:LEU:HD13	1:A:466:HIS:HB3	1.99	0.44
1:A:1133:HIS:ND1	1:A:1203:TRP:CE3	2.85	0.44
1:A:1047:LEU:HB2	1:A:1059:LEU:HD21	2.00	0.44
1:A:1361:LEU:HD23	1:A:1362:PRO:O	2.18	0.44
1:A:3052:LYS:HA	1:A:3103:GLU:O	2.18	0.44
1:A:620:LEU:HD22	1:A:3000:THR:HG23	1.99	0.44
1:A:2168:PRO:HA	1:A:2171:CYS:HB3	1.99	0.44
1:A:1707:ALA:HA	1:A:1711:GLY:HA2	2.00	0.44
1:A:2714:ASP:HB3	1:A:2753:THR:HG21	1.99	0.44
1:A:478:ASP:OD1	1:A:478:ASP:N	2.50	0.43
1:A:1093:TRP:CD1	1:A:1121:ARG:HG2	2.53	0.43
1:A:2351:ARG:HA	1:A:2351:ARG:HD3	1.70	0.43
1:A:864:LEU:HD13	1:A:904:CYS:SG	2.59	0.43
1:A:1037:ARG:NH1	1:A:1070:PRO:HB2	2.33	0.43
1:A:3053:LEU:HD11	1:A:3085:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1594:GLU:HA	1:A:1597:LYS:HE2	2.00	0.43
1:A:2249:GLU:HB2	1:A:2253:ARG:HH21	1.84	0.43
1:A:2515:PRO:HB2	1:A:2596:PRO:HG2	2.00	0.43
1:A:2775:PRO:HB3	1:A:2786:TRP:CD1	2.54	0.43
1:A:858:GLU:OE1	1:A:861:ASN:ND2	2.51	0.43
1:A:1108:ALA:HB1	1:A:1345:THR:HG23	2.00	0.43
1:A:2339:LYS:HE2	1:A:2339:LYS:HB3	1.75	0.43
1:A:92:LEU:HA	1:A:95:ILE:HG12	2.00	0.43
1:A:211:LEU:HA	1:A:218:VAL:HA	2.00	0.43
1:A:434:TYR:HD1	1:A:464:LEU:HD13	1.84	0.43
1:A:2064:TYR:HA	1:A:2065:PRO:HD3	1.92	0.43
1:A:1072:PRO:HG3	1:A:1090:TRP:CG	2.54	0.43
1:A:230:MET:HE3	1:A:230:MET:HB3	1.91	0.43
1:A:406:MET:O	1:A:407:ALA:C	2.61	0.43
1:A:1157:LEU:HD13	1:A:1160:MET:SD	2.59	0.43
1:A:300:GLN:HG3	1:A:359:GLU:CD	2.44	0.42
1:A:344:GLU:HA	1:A:350:ARG:HH22	1.83	0.42
1:A:1048:SER:HB3	1:A:1059:LEU:HD23	2.00	0.42
1:A:561:ILE:O	1:A:561:ILE:HG13	2.19	0.42
1:A:611:ALA:HA	1:A:614:ILE:HG22	2.00	0.42
1:A:1165:LEU:HD21	1:A:1179:THR:OG1	2.19	0.42
1:A:192:VAL:HA	1:A:195:LEU:HD13	2.00	0.42
1:A:616:PRO:HG2	1:A:3015:GLU:HG3	2.01	0.42
1:A:814:ASP:N	1:A:814:ASP:OD1	2.52	0.42
1:A:980:LYS:O	1:A:983:GLU:HG3	2.19	0.42
1:A:1575:MET:HG3	1:A:1592:HIS:ND1	2.33	0.42
1:A:1695:VAL:HG11	1:A:1990:ALA:HB1	2.02	0.42
1:A:1975:LYS:HA	1:A:1975:LYS:HD3	1.59	0.42
1:A:2033:ASN:C	1:A:2037:ARG:HH21	2.26	0.42
1:A:2244:ILE:HA	1:A:2247:THR:HG22	2.01	0.42
1:A:2578:HIS:HD2	1:A:2609:ASN:ND2	2.18	0.42
1:A:2521:MET:HE3	1:A:2603:PHE:HD2	1.83	0.42
1:A:853:ASP:OD1	1:A:853:ASP:N	2.50	0.42
1:A:2738:PHE:CZ	1:A:3086:PRO:HB3	2.55	0.42
1:A:387:MET:HB2	1:A:406:MET:CE	2.49	0.42
1:A:2026:ALA:HB3	1:A:2029:GLU:OE1	2.19	0.42
1:A:1117:LEU:O	1:A:1121:ARG:HG3	2.19	0.42
1:A:210:ILE:O	1:A:219:LEU:N	2.34	0.42
1:A:766:MET:SD	1:A:906:MET:HE1	2.59	0.42
1:A:1992:ILE:HD13	1:A:1992:ILE:HA	1.86	0.42
1:A:1189:THR:N	1:A:1190:PRO:HD3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2779:ARG:NH1	1:A:2780:ARG:HB3	2.34	0.42
1:A:221:ILE:HD13	1:A:221:ILE:HA	1.92	0.42
1:A:813:LEU:HD21	1:A:818:ARG:HA	2.02	0.42
1:A:835:SER:HB3	1:A:840:LEU:HG	2.02	0.42
1:A:1743:GLN:OE1	1:A:1975:LYS:HE2	2.19	0.42
1:A:1988:SER:OG	1:A:2031:LEU:HD11	2.20	0.42
1:A:648:VAL:HG11	1:A:684:GLN:HG2	2.02	0.41
1:A:1375:LEU:HD22	1:A:1379:GLN:OE1	2.19	0.41
1:A:1471:PHE:CD2	1:A:1501:LEU:HD22	2.55	0.41
1:A:1678:LEU:HD12	1:A:1678:LEU:HA	1.89	0.41
1:A:784:LYS:HD2	1:A:784:LYS:HA	1.84	0.41
1:A:958:LEU:HD12	1:A:958:LEU:HA	1.86	0.41
1:A:1746:LEU:HD12	1:A:1746:LEU:HA	1.82	0.41
1:A:2247:THR:HG23	1:A:2248:LEU:HD22	2.01	0.41
1:A:2569:GLY:O	1:A:2570:ARG:HG3	2.20	0.41
1:A:1371:ALA:HB2	1:A:1412:MET:HE1	2.02	0.41
1:A:854:PRO:HD3	1:A:895:TYR:O	2.20	0.41
1:A:1368:ARG:HH12	1:A:1413:SER:HG	1.66	0.41
1:A:1417:LEU:HD22	1:A:1465:LEU:HD12	2.02	0.41
1:A:2638:THR:O	1:A:2641:SER:OG	2.36	0.41
1:A:2674:TYR:HE2	1:A:2806:GLU:HB3	1.85	0.41
1:A:2824:MET:HE3	1:A:2824:MET:HB2	1.76	0.41
1:A:112:ARG:NH2	1:A:155:LYS:HE2	2.36	0.41
1:A:246:TRP:O	1:A:250:VAL:HG13	2.20	0.41
1:A:844:GLN:HB2	1:A:884:VAL:HG22	2.01	0.41
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.92	0.41
1:A:620:LEU:HD12	1:A:3014:LEU:HD13	2.02	0.41
1:A:853:ASP:O	1:A:857:VAL:HG22	2.21	0.41
1:A:2171:CYS:HG	1:A:2176:PHE:HE2	1.69	0.41
1:A:2410:ALA:O	1:A:2413:VAL:HG12	2.20	0.41
1:A:2508:ILE:HA	1:A:2512:GLU:HG3	2.02	0.41
1:A:2533:VAL:CB	1:A:2573:MET:HE1	2.50	0.41
1:A:163:TYR:HD1	1:A:166:ARG:NH2	2.19	0.41
1:A:958:LEU:HG	1:A:962:ARG:HE	1.85	0.41
1:A:1342:ARG:HG2	3:A:3202:ADP:H4'	2.03	0.41
1:A:1706:LEU:HB3	1:A:1713:THR:HG22	2.02	0.41
1:A:2295:SER:O	1:A:2824:MET:HE2	2.21	0.41
1:A:2503:LEU:HD22	1:A:2505:LEU:HG	2.03	0.41
1:A:2749:ARG:HH22	1:A:3115:GLU:HG3	1.86	0.41
1:A:1071:LEU:HD23	1:A:1071:LEU:HA	1.84	0.41
1:A:1958:LYS:HE3	1:A:1958:LYS:HB3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2635:MET:SD	1:A:2787:VAL:HG22	2.60	0.41
1:A:249:LEU:HD23	1:A:249:LEU:HA	1.84	0.40
1:A:1720:HIS:HB3	1:A:1994:TYR:HE1	1.84	0.40
1:A:2701:LEU:HA	1:A:2704:THR:HG22	2.03	0.40
1:A:610:LEU:HD22	1:A:682:LEU:HD12	2.03	0.40
1:A:1097:VAL:O	1:A:1097:VAL:HG23	2.21	0.40
1:A:1296:PHE:HB3	1:A:1348:VAL:HG11	2.02	0.40
1:A:1395:ILE:HD13	1:A:1395:ILE:HA	1.91	0.40
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.83	0.40
1:A:373:SER:HB2	1:A:375:ILE:HD11	2.04	0.40
1:A:527:LEU:HD11	1:A:555:PRO:HA	2.02	0.40
1:A:864:LEU:HB2	1:A:903:ARG:HD3	2.03	0.40
1:A:2385:HIS:HD2	1:A:2416:LEU:HD12	1.83	0.40
1:A:320:ALA:O	1:A:322:PRO:HD3	2.21	0.40
1:A:914:LEU:HD12	1:A:918:MET:SD	2.61	0.40
1:A:1165:LEU:HD23	1:A:1165:LEU:HA	1.91	0.40
1:A:932:LEU:CB	1:A:957:MET:CE	2.85	0.40
1:A:2249:GLU:CB	1:A:2253:ARG:HH21	2.35	0.40
1:A:2387:LEU:HD23	1:A:2387:LEU:HA	1.83	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	2733/3126 (87%)	2628 (96%)	105 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	2437/2766 (88%)	2433 (100%)	4 (0%)	87 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	957	MET
1	A	1544	VAL
1	A	2114	GLN
1	A	2966	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	HIS
1	A	564	ASN
1	A	572	ASN
1	A	1027	GLN
1	A	1379	GLN
1	A	1509	HIS
1	A	1577	GLN
1	A	1614	ASN
1	A	1726	ASN
1	A	1727	HIS
1	A	2004	GLN
1	A	2062	ASN
1	A	2109	ASN
1	A	2114	GLN
1	A	2270	GLN
1	A	2278	GLN
1	A	2315	HIS
1	A	2355	HIS
1	A	2409	GLN
1	A	2576	ASN
1	A	2578	HIS

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Mol	Chain	Res	Type
1	A	2609	ASN
1	A	2740	GLN
1	A	2803	ASN
1	A	2903	GLN
1	A	2966	GLN
1	A	2968	GLN
1	A	3004	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 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\#\|Z\| > 2$
3	ADP	A	3204	5,4	28,29,29	1.39	5 (17%)	43,45,45	1.75	10 (23%)
3	ADP	A	3202	-	28,29,29	1.37	4 (14%)	43,45,45	1.85	8 (18%)
3	ADP	A	3203	-	28,29,29	1.38	5 (17%)	43,45,45	1.82	8 (18%)
2	ATP	A	3201	-	32,33,33	0.61	1 (3%)	48,52,52	0.35	0
4	VO4	A	3205	3,5	0,4,4	-	-	-		

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
3	ADP	A	3202	-	-	5/16/32/32	0/3/3/3
3	ADP	A	3204	5,4	-	2/16/32/32	0/3/3/3
2	ATP	A	3201	-	-	3/22/38/38	0/3/3/3
3	ADP	A	3203	-	-	4/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3202	ADP	C5-C4	4.41	1.47	1.39
3	A	3203	ADP	C5-C4	4.41	1.47	1.39
3	A	3204	ADP	C5-C4	4.32	1.46	1.39
3	A	3202	ADP	C5-N7	-2.65	1.34	1.39
3	A	3203	ADP	C5-N7	-2.64	1.34	1.39
3	A	3204	ADP	C5-N7	-2.54	1.34	1.39
3	A	3203	ADP	C5-C6	2.46	1.47	1.41
3	A	3204	ADP	C5-C6	2.45	1.47	1.41
2	A	3201	ATP	PB-O3B	-2.40	1.56	1.59
3	A	3204	ADP	C4-N9	-2.39	1.32	1.37
3	A	3202	ADP	C5-C6	2.31	1.47	1.41
3	A	3203	ADP	C8-N7	2.12	1.35	1.31
3	A	3204	ADP	C8-N7	2.10	1.35	1.31
3	A	3203	ADP	C4-N9	-2.09	1.33	1.37
3	A	3202	ADP	C8-N7	2.05	1.35	1.31

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	3202	ADP	C5-C4-N3	-5.89	118.60	126.72
3	A	3203	ADP	C5-C4-N3	-5.80	118.73	126.72
3	A	3204	ADP	C5-C4-N3	-5.27	119.46	126.72
3	A	3202	ADP	N3-C4-N9	4.94	135.57	127.17
3	A	3203	ADP	N3-C4-N9	4.67	135.11	127.17
3	A	3204	ADP	N3-C4-N9	4.20	134.31	127.17
3	A	3202	ADP	C2-N3-C4	3.81	121.13	111.83
3	A	3203	ADP	C2-N3-C4	3.63	120.69	111.83
3	A	3202	ADP	N3-C2-N1	-3.51	123.27	128.58
3	A	3204	ADP	C2-N3-C4	3.49	120.35	111.83
3	A	3204	ADP	C4-C5-N7	-3.40	106.69	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	3203	ADP	C4-C5-N7	-3.30	106.81	110.58
3	A	3204	ADP	N3-C2-N1	-3.21	123.73	128.58
3	A	3203	ADP	N3-C2-N1	-3.20	123.74	128.58
3	A	3204	ADP	C4-N9-C8	2.93	108.81	105.74
3	A	3202	ADP	C4-C5-N7	-2.81	107.36	110.58
3	A	3203	ADP	C4-N9-C8	2.67	108.55	105.74
3	A	3202	ADP	C4-N9-C8	2.55	108.42	105.74
3	A	3202	ADP	C3'-C2'-C1'	2.45	106.09	101.46
3	A	3203	ADP	C5-N7-C8	2.42	107.26	103.45
3	A	3204	ADP	C5-N7-C8	2.40	107.22	103.45
3	A	3203	ADP	C3'-C2'-C1'	2.28	105.78	101.46
3	A	3204	ADP	C6-C5-N7	2.24	136.40	132.09
3	A	3202	ADP	C5-N7-C8	2.19	106.89	103.45
3	A	3204	ADP	O3B-PB-O2B	2.14	115.82	107.80
3	A	3204	ADP	N9-C8-N7	-2.03	111.05	113.94

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3202	ADP	C5'-O5'-PA-O2A
3	A	3203	ADP	C5'-O5'-PA-O1A
3	A	3203	ADP	C5'-O5'-PA-O3A
3	A	3203	ADP	O4'-C4'-C5'-O5'
3	A	3204	ADP	C5'-O5'-PA-O3A
3	A	3203	ADP	C3'-C4'-C5'-O5'
2	A	3201	ATP	PB-O3A-PA-O1A
3	A	3202	ADP	PB-O3A-PA-O1A
2	A	3201	ATP	PB-O3A-PA-O5'
3	A	3204	ADP	O4'-C4'-C5'-O5'
3	A	3202	ADP	C5'-O5'-PA-O3A
3	A	3202	ADP	PB-O3A-PA-O2A
2	A	3201	ATP	C4'-C5'-O5'-PA
3	A	3202	ADP	C2'-C1'-N9-C8

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3204	ADP	2	0
3	A	3202	ADP	1	0

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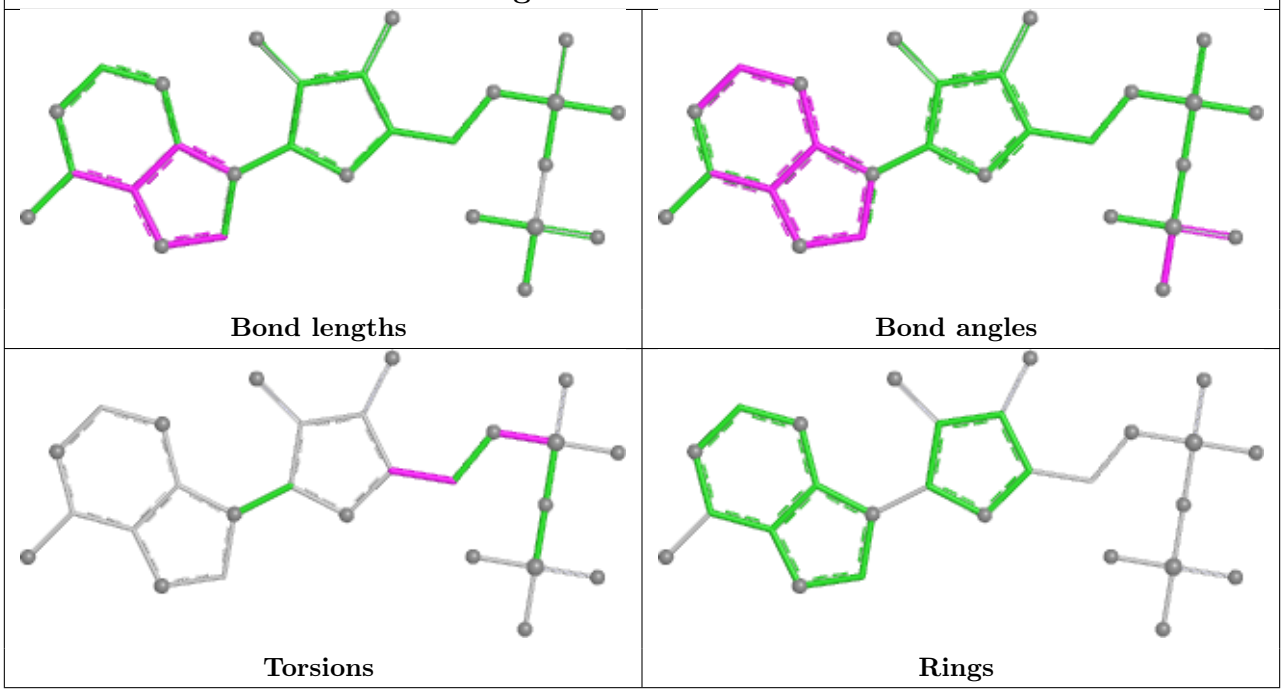
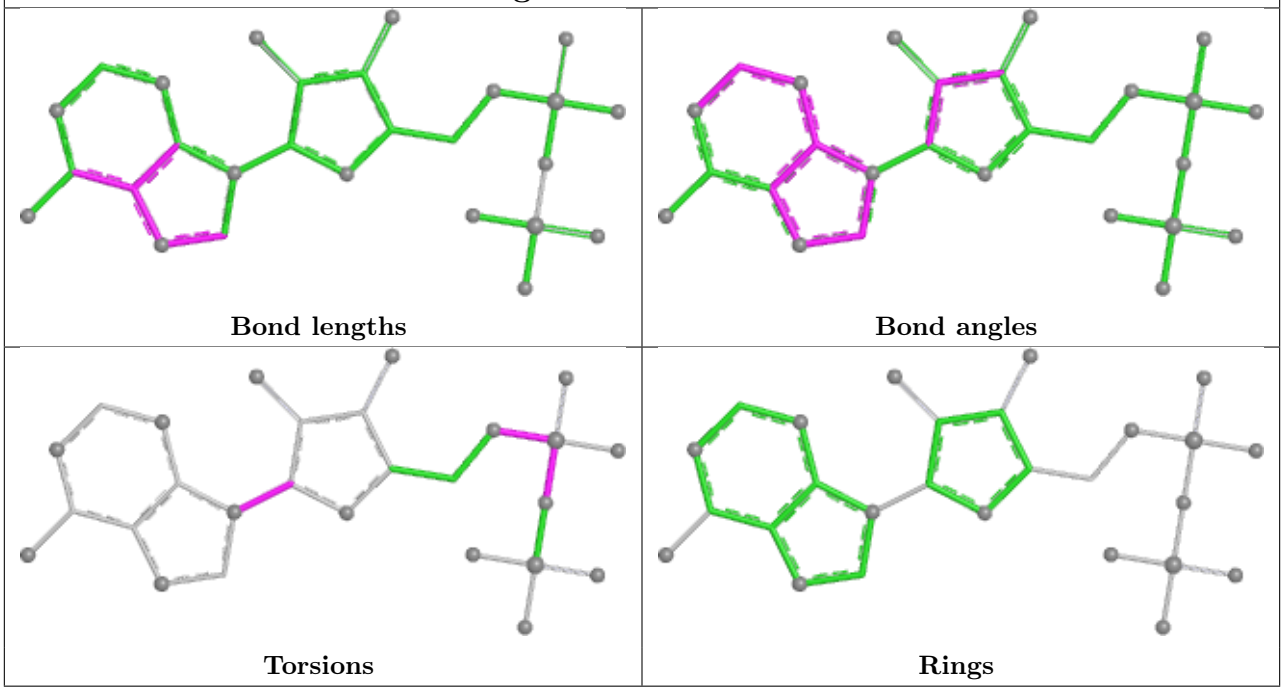
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3203	ADP	1	0
2	A	3201	ATP	5	0
4	A	3205	VO4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

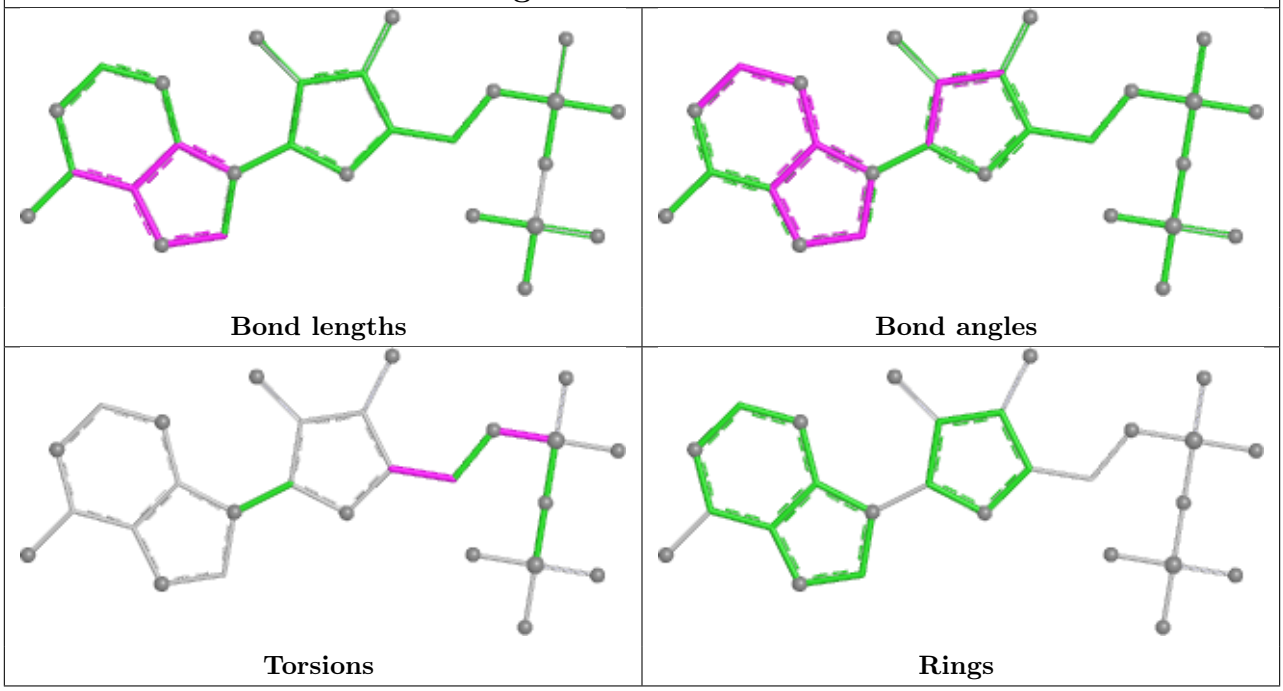
Ligand ADP A 3204



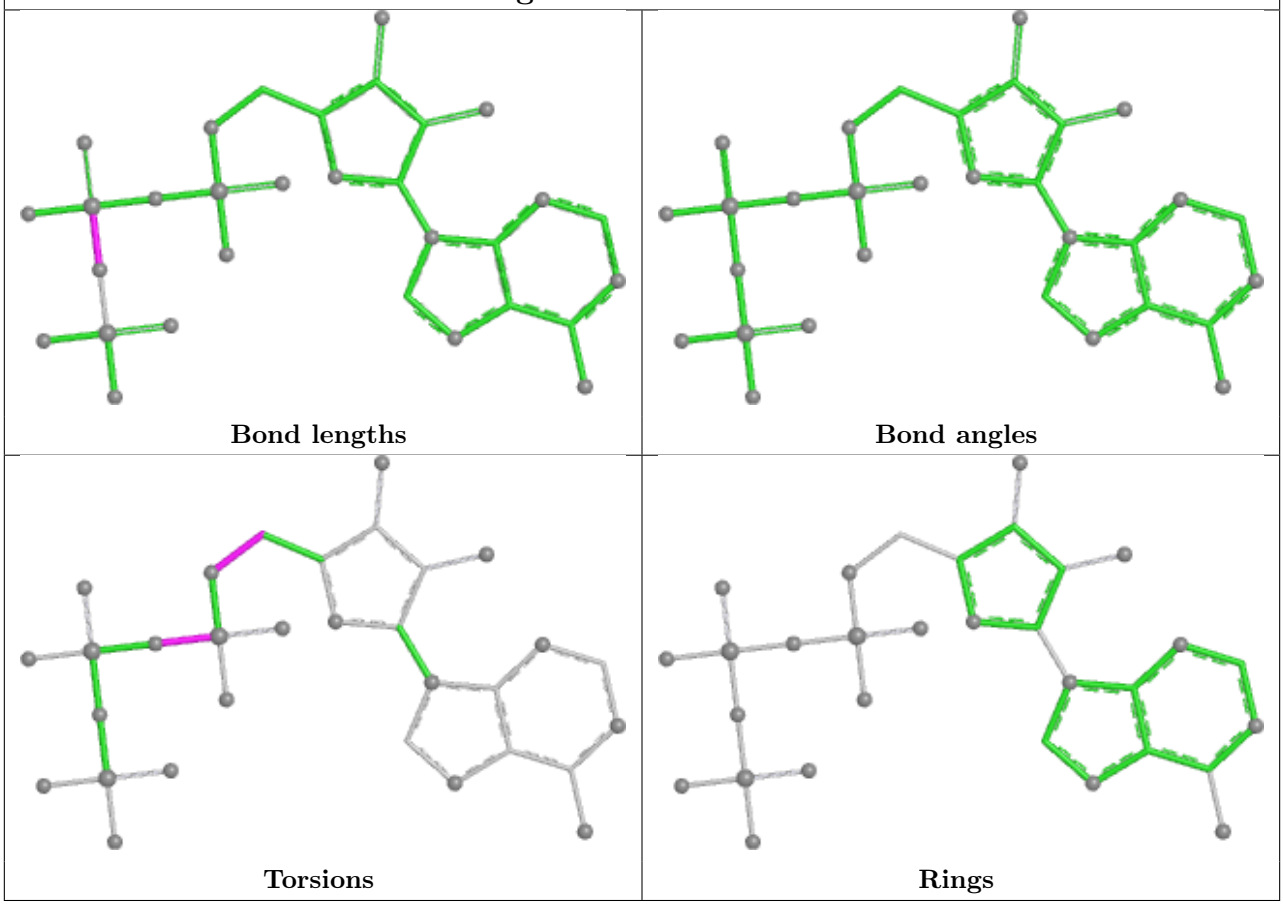
Ligand ADP A 3202

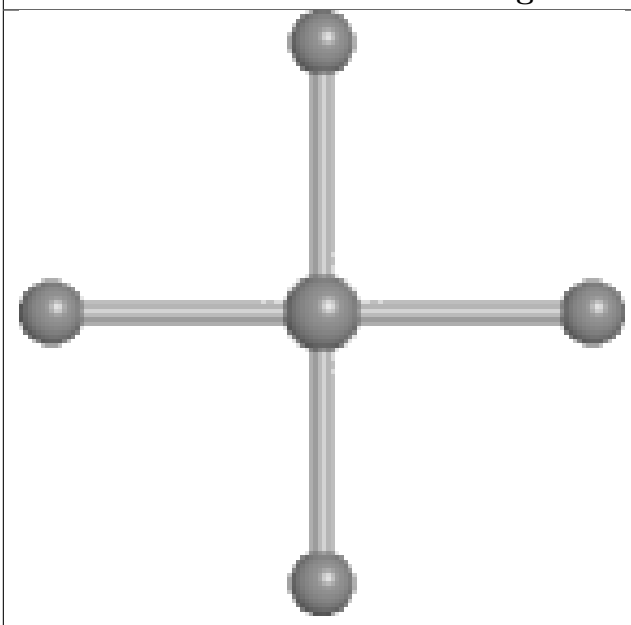
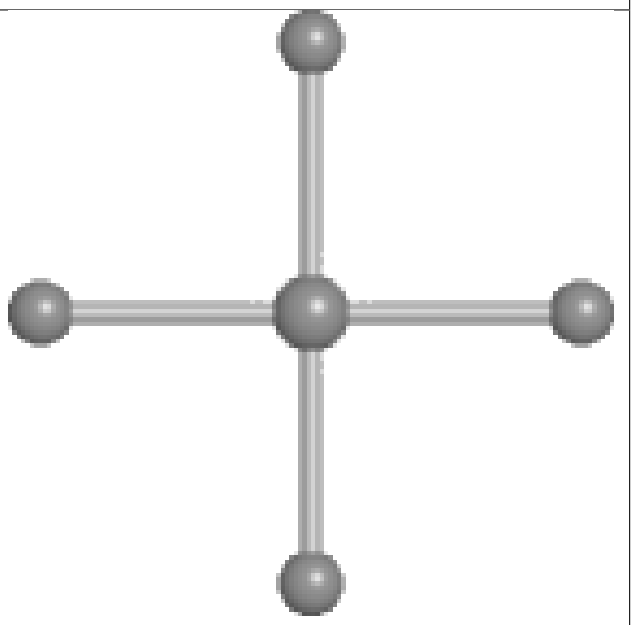
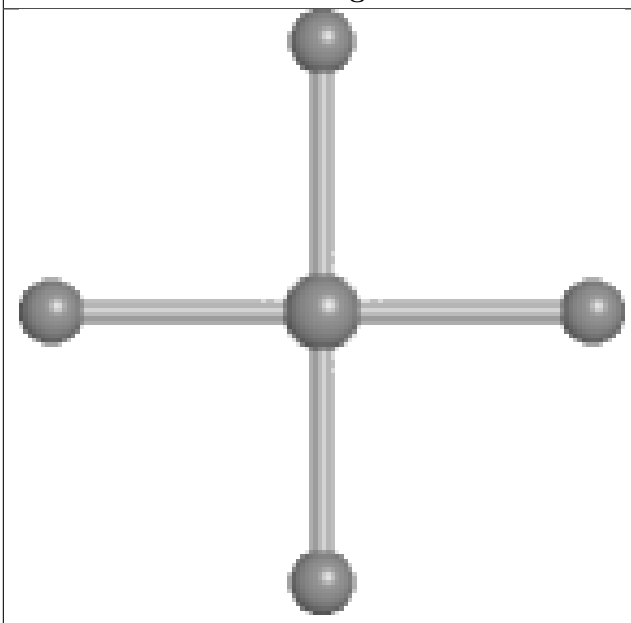
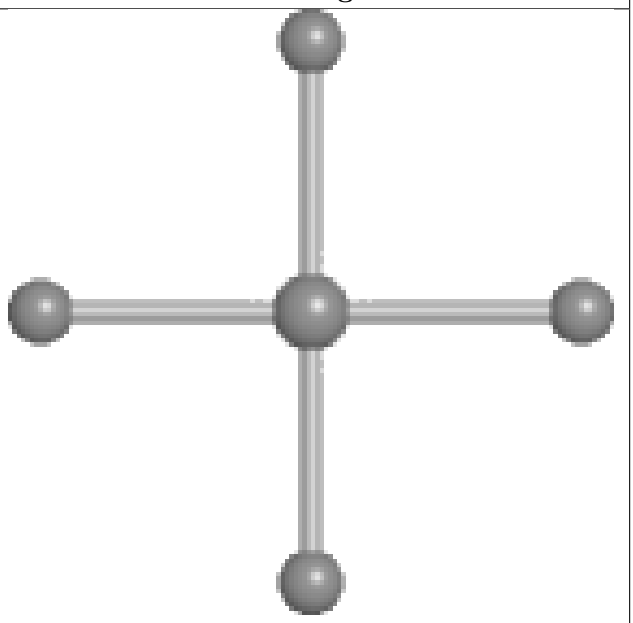


Ligand ADP A 3203



Ligand ATP A 3201



Ligand VO4 A 3205	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

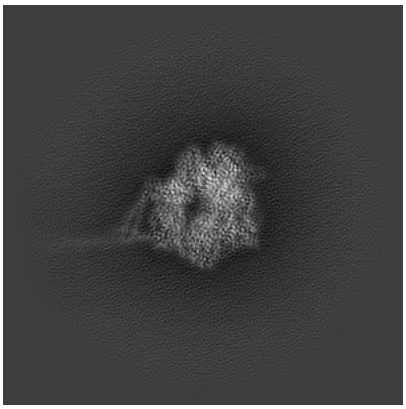
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-29003. These allow visual inspection of the internal detail of the map and identification of artifacts.

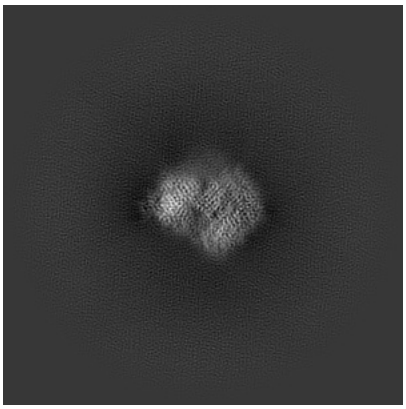
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

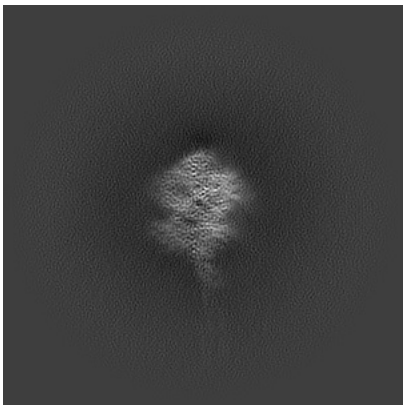
6.1.1 Primary map



X

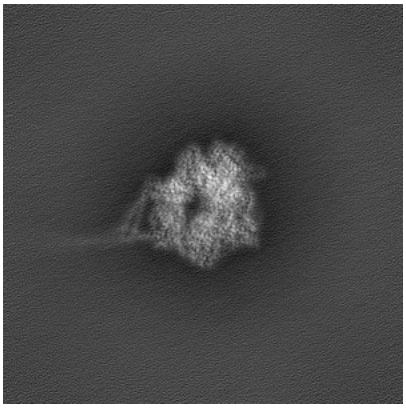


Y

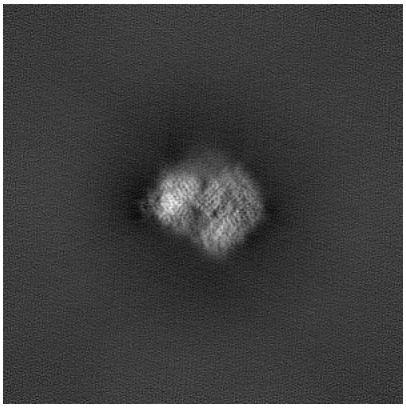


Z

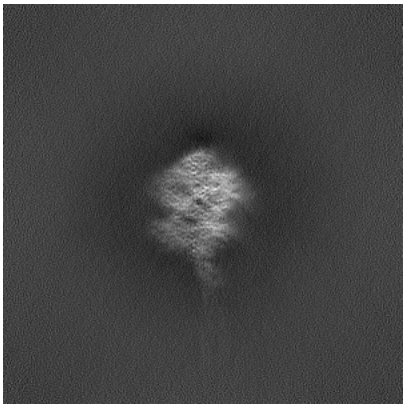
6.1.2 Raw map



X



Y

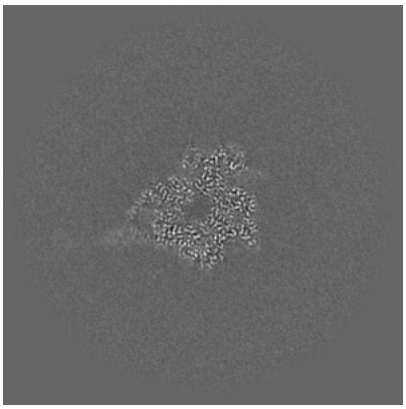


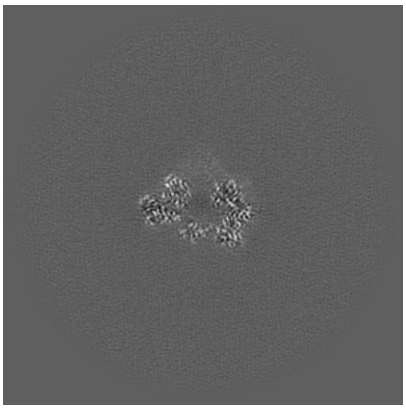
Z

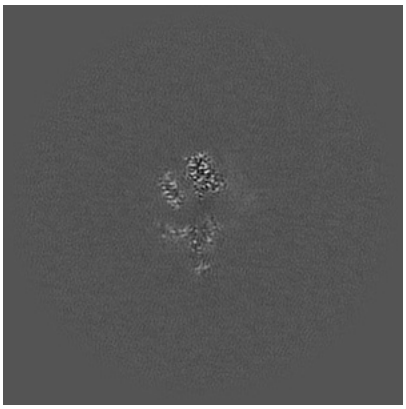
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

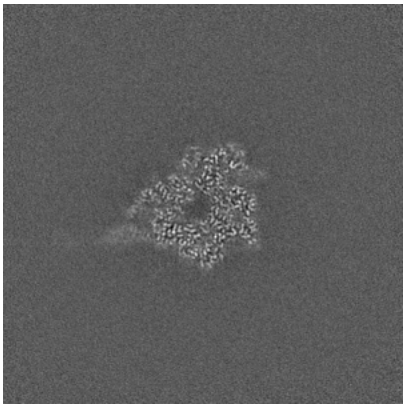
6.2.1 Primary map

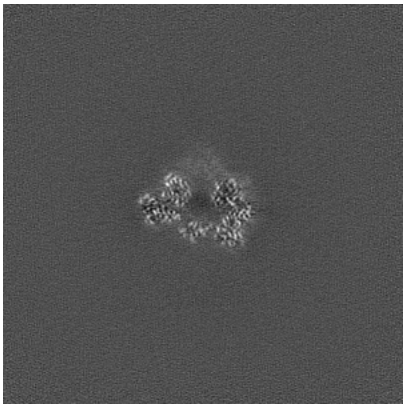

X Index: 180

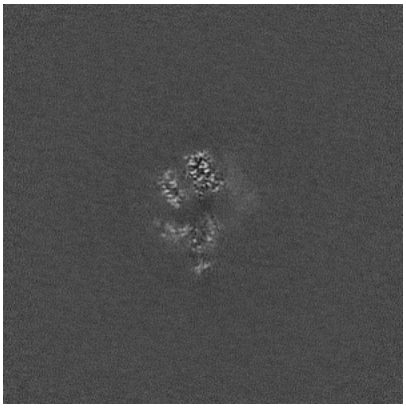

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

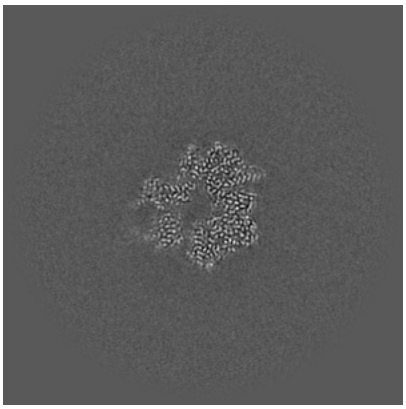

Y Index: 180

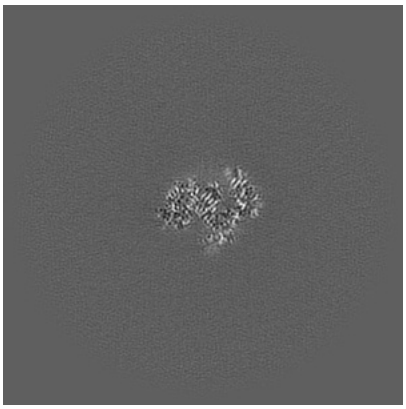

Z Index: 180

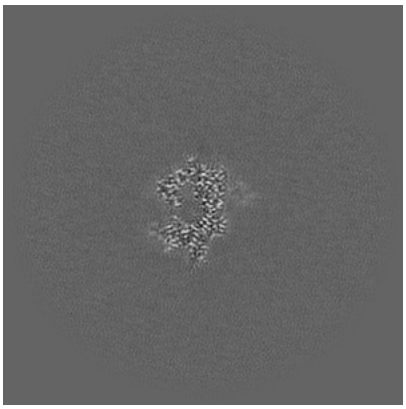
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

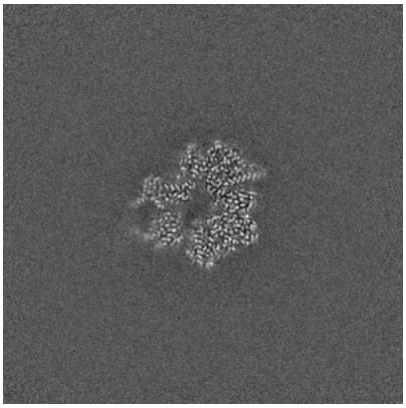
6.3.1 Primary map

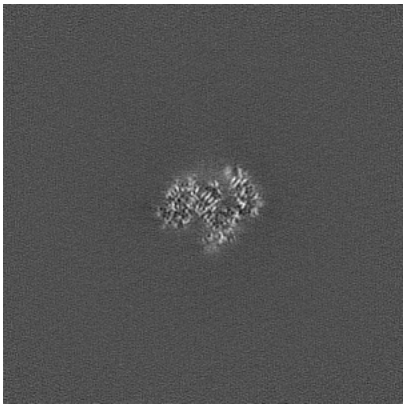

X Index: 174

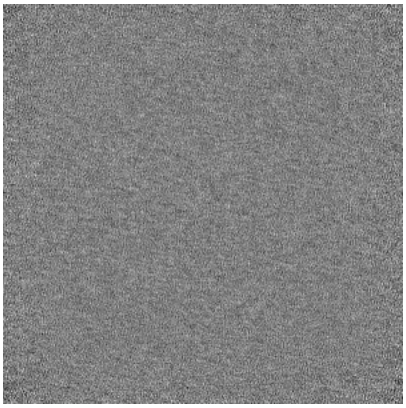

Y Index: 205


Z Index: 193

6.3.2 Raw map


X Index: 174

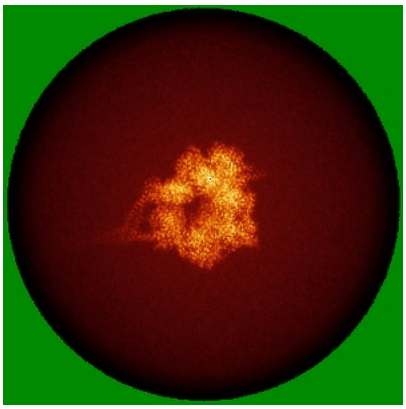

Y Index: 205

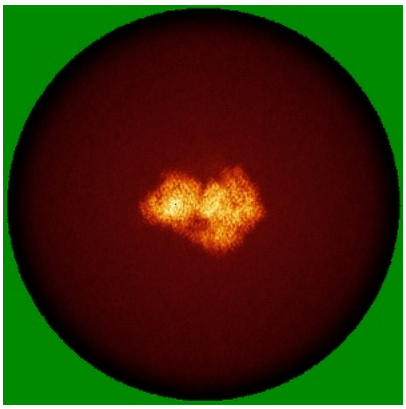

Z Index: 0

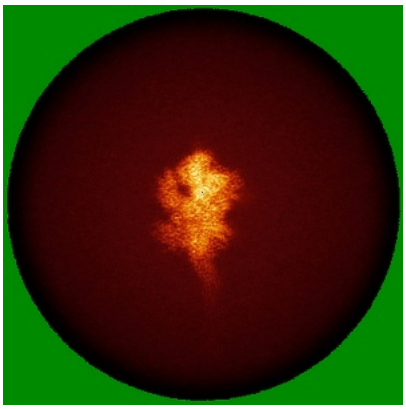
The images above show the largest variance slices of the map in three orthogonal directions.

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

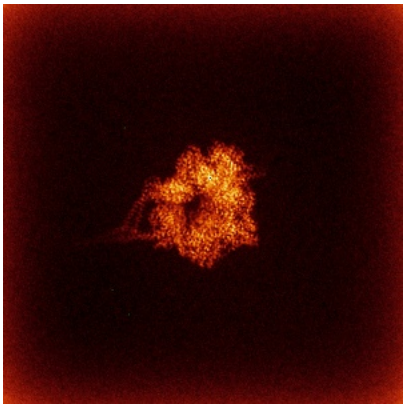
6.4.1 Primary map

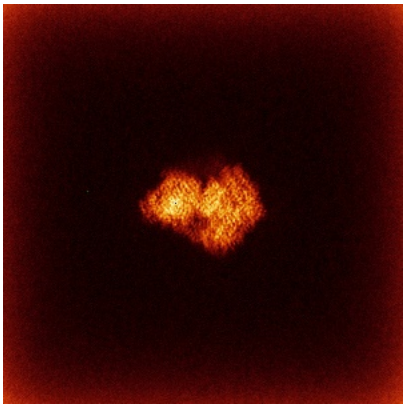

X

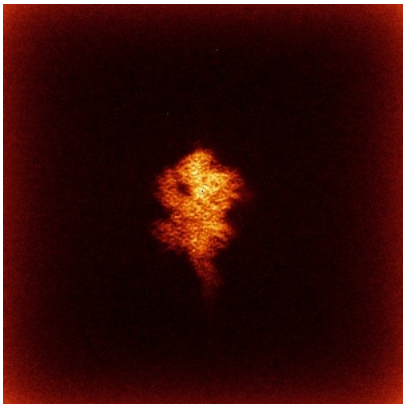

Y


Z

6.4.2 Raw map


X

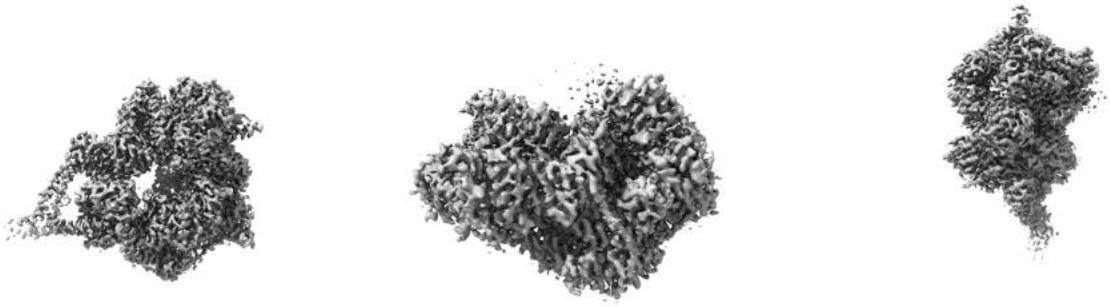

Y


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 0.35. 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.

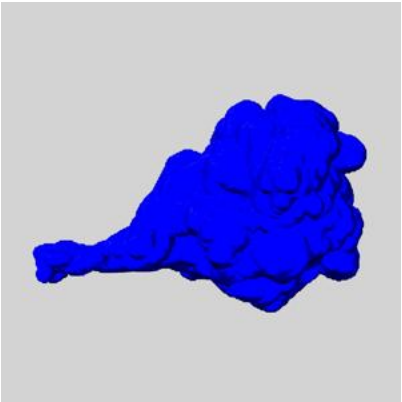
6.6 Mask visualisation (i)

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

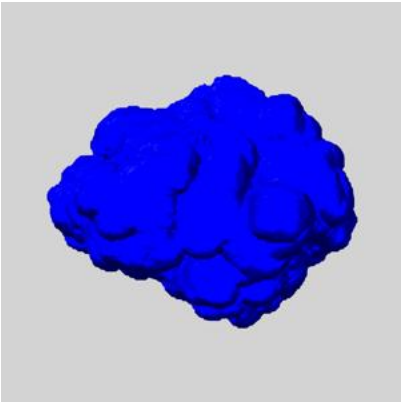
A mask typically either:

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

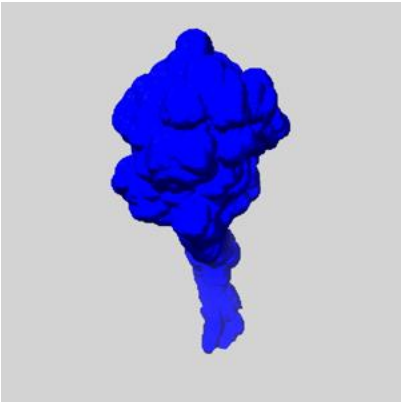
6.6.1 emd_29003_msk_1.map (i)



X



Y

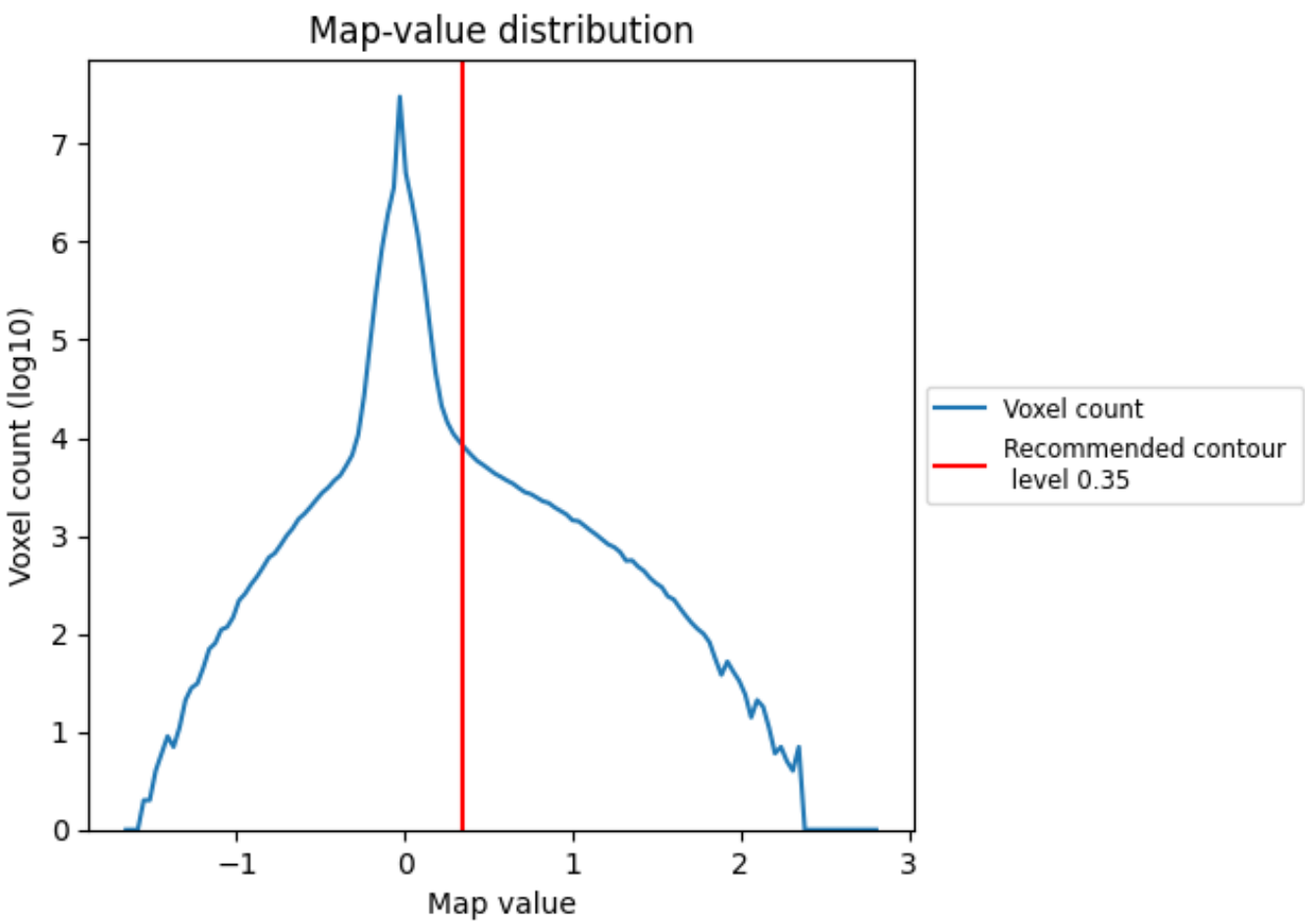


Z

7 Map analysis (i)

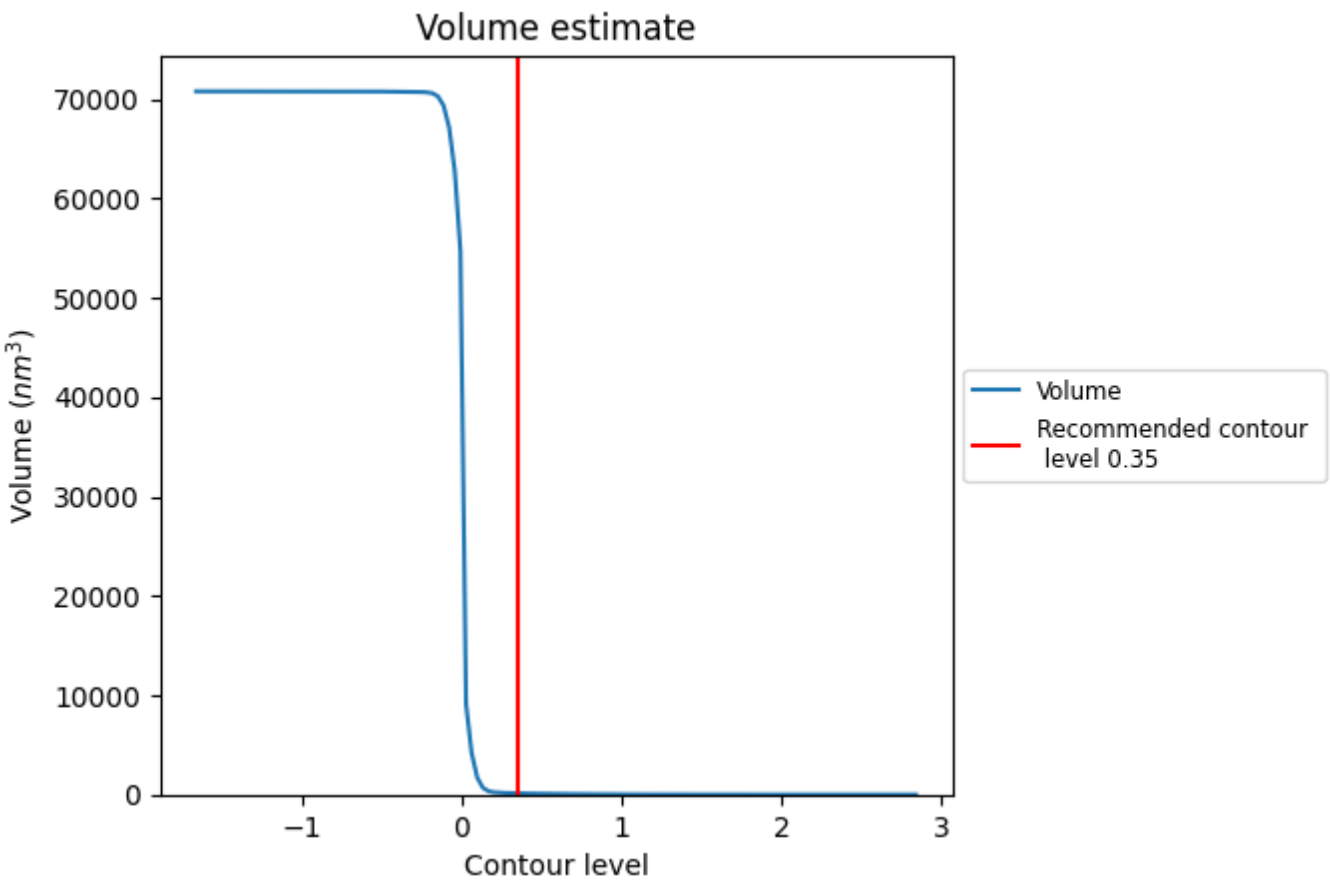
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

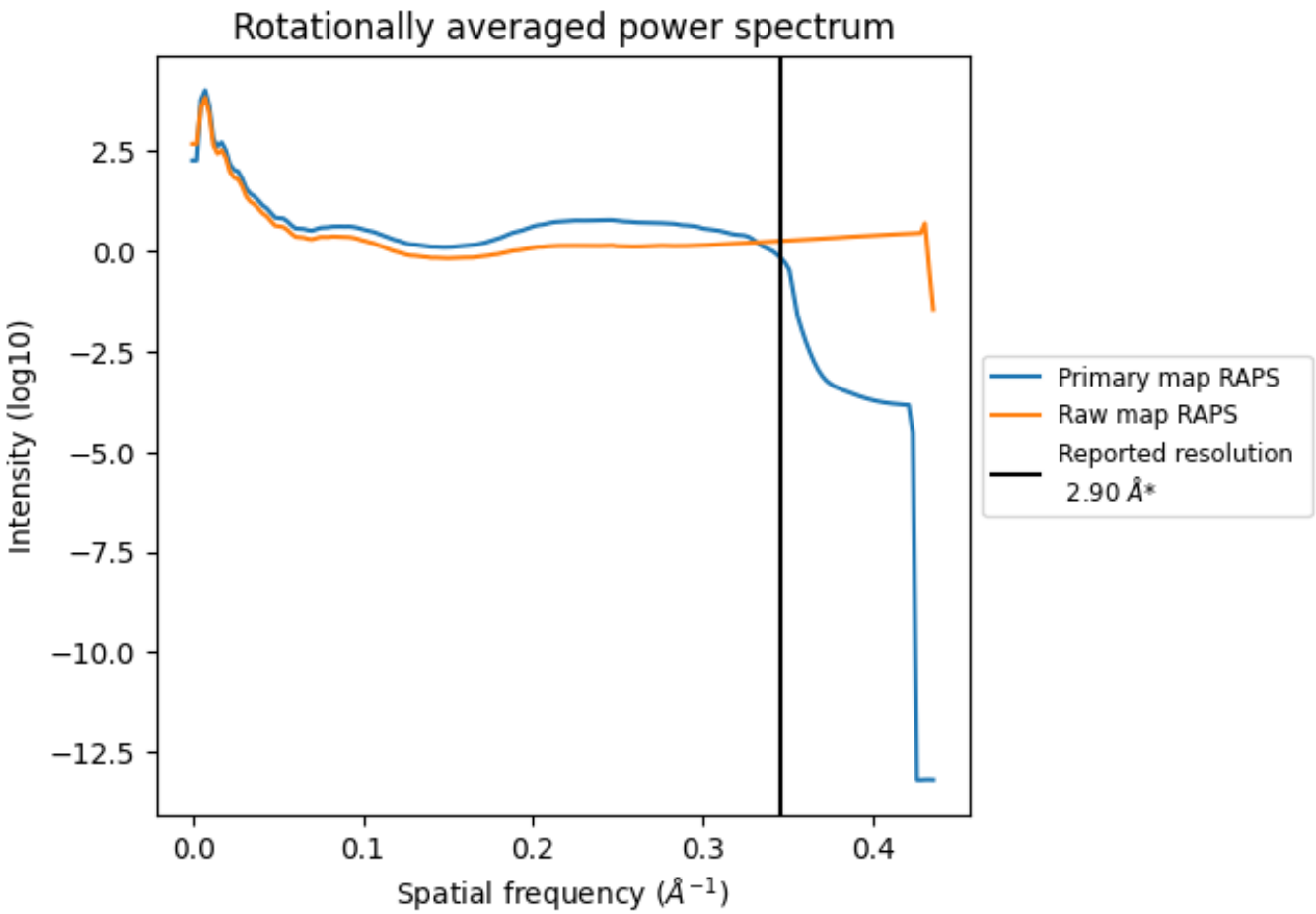
7.2 Volume estimate (i)



The volume at the recommended contour level is 126 nm^3; this corresponds to an approximate mass of 114 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)

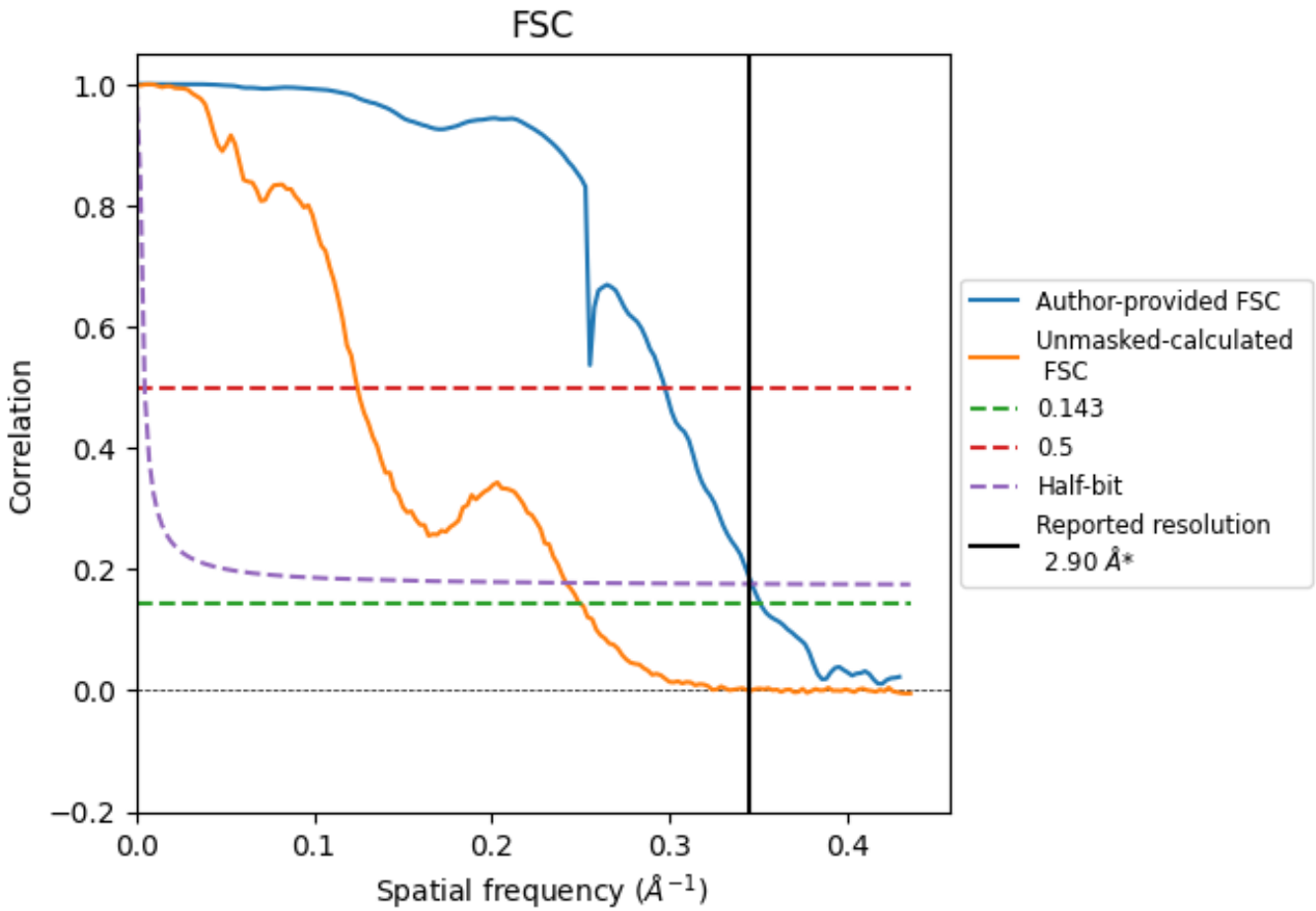


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

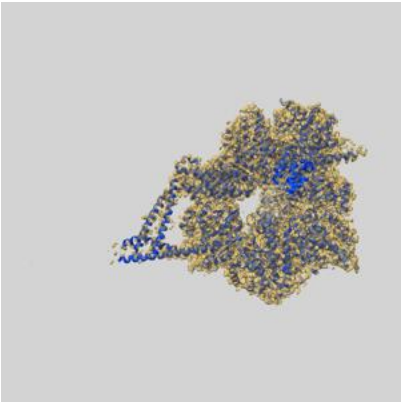
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.85	3.37	2.89
Unmasked-calculated*	4.01	8.05	4.14

*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 4.01 differs from the reported value 2.9 by more than 10 %

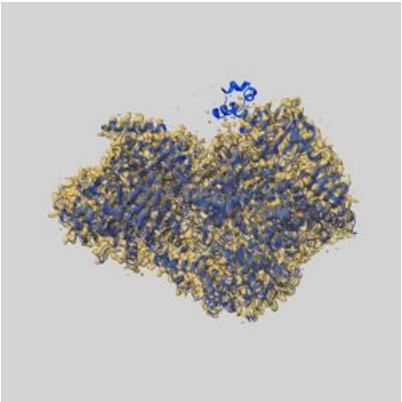
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-29003 and PDB model 8FD6. Per-residue inclusion information can be found in section 3 on page 7.

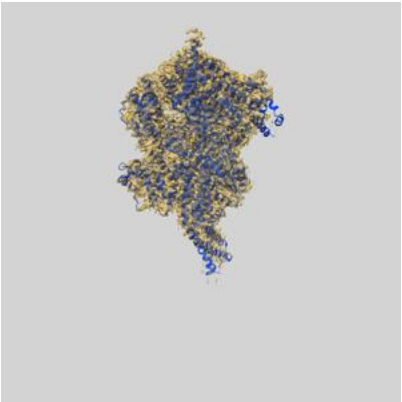
9.1 Map-model overlay (i)



X



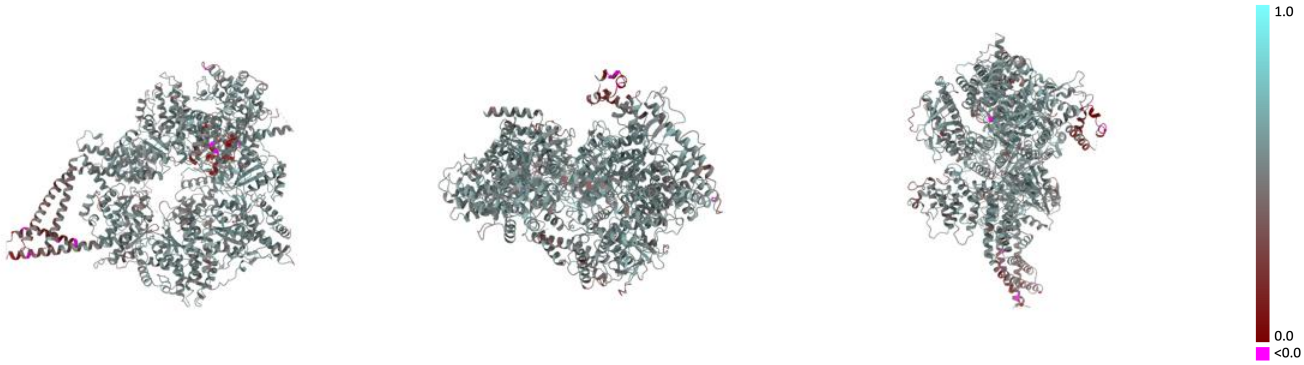
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

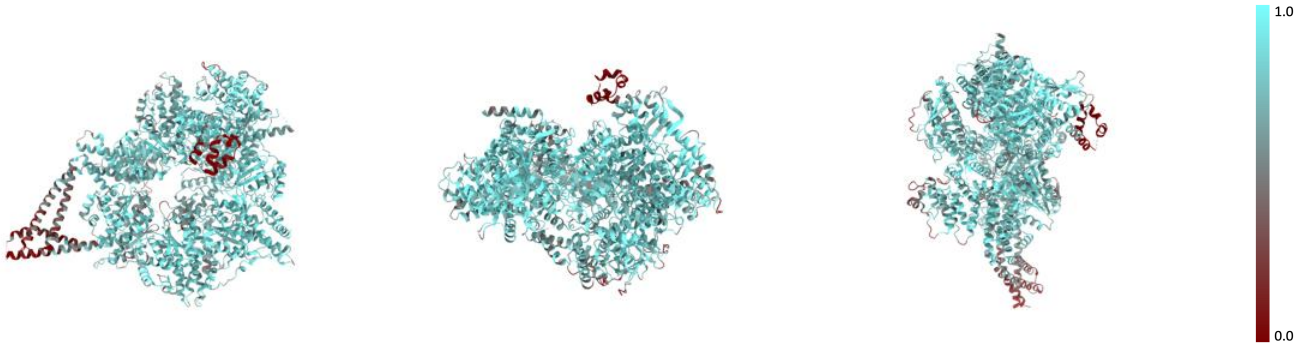
9.2 Q-score mapped to coordinate model (i)



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.

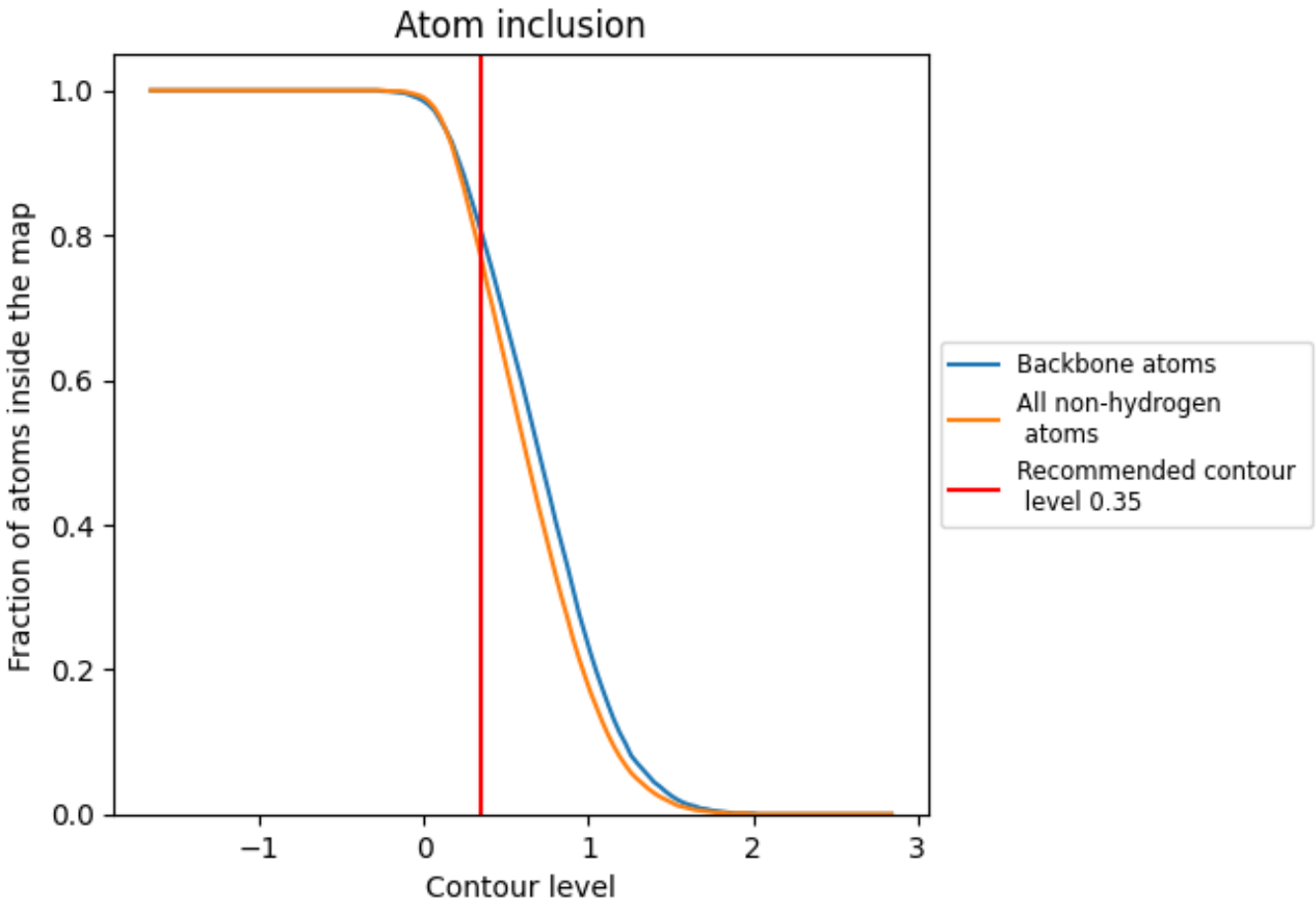
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7670	0.5190
A	0.7670	0.5190