Full wwPDB EM Validation Report ⓘ

Apr 17, 2025 – 03:34 PM EDT

PDB ID	:	9BN4 / pdb_00009bn4
EMDB ID	:	EMD-44721
Title	:	The alpha registry-locked dynein motor domain mutant in 5mM ATP condition, class2
Authors	:	Chai, P.; Zhang, K.
Deposited on	:	2024-05-02
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 ⓘ 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:

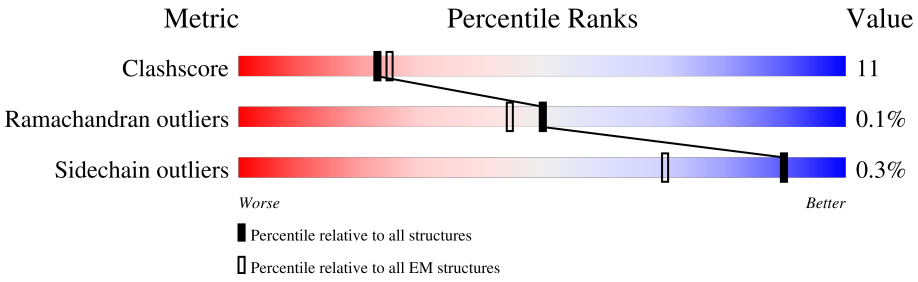
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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)
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	4646	13% 45% 16% 39%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23078 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.

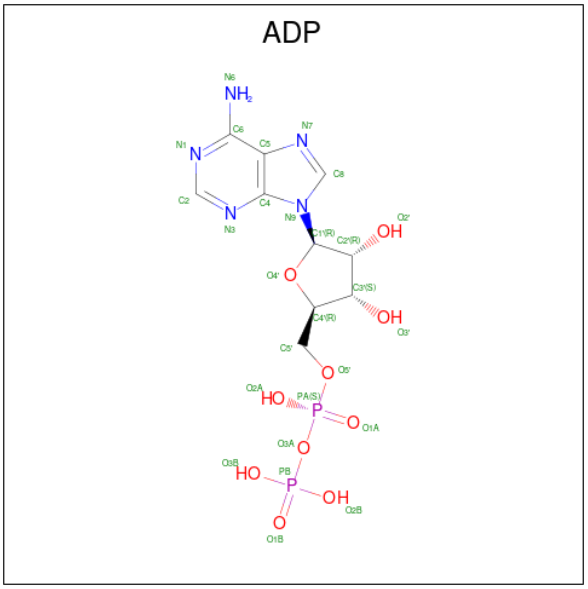
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2855	22962	14643	3963	4241	115	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2389	ASP	GLU	conflict	UNP Q14204

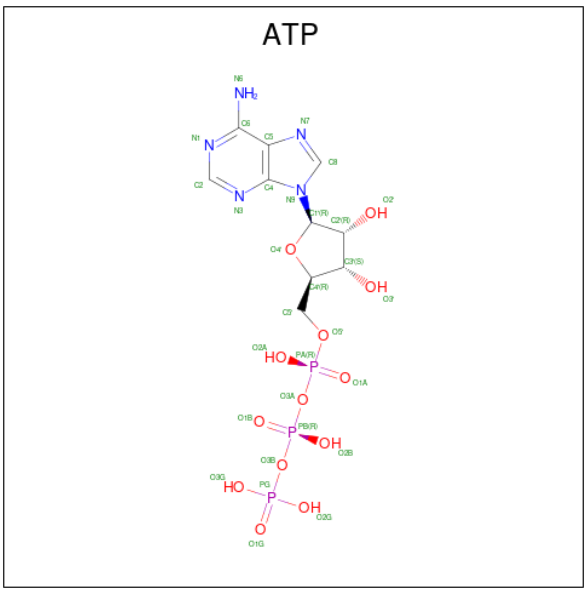
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$)

(labeled as "Ligand of Interest" by depositor).

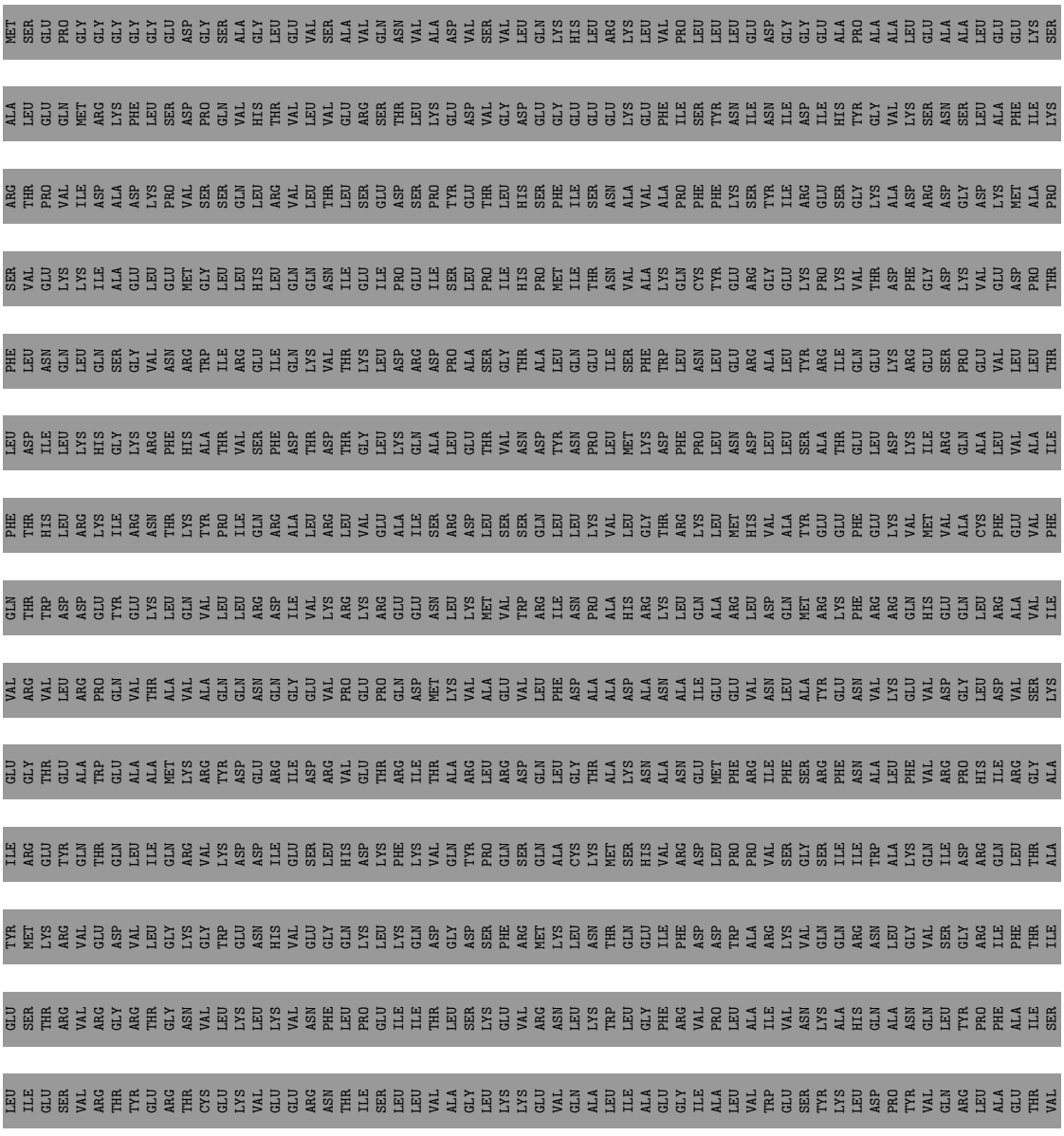


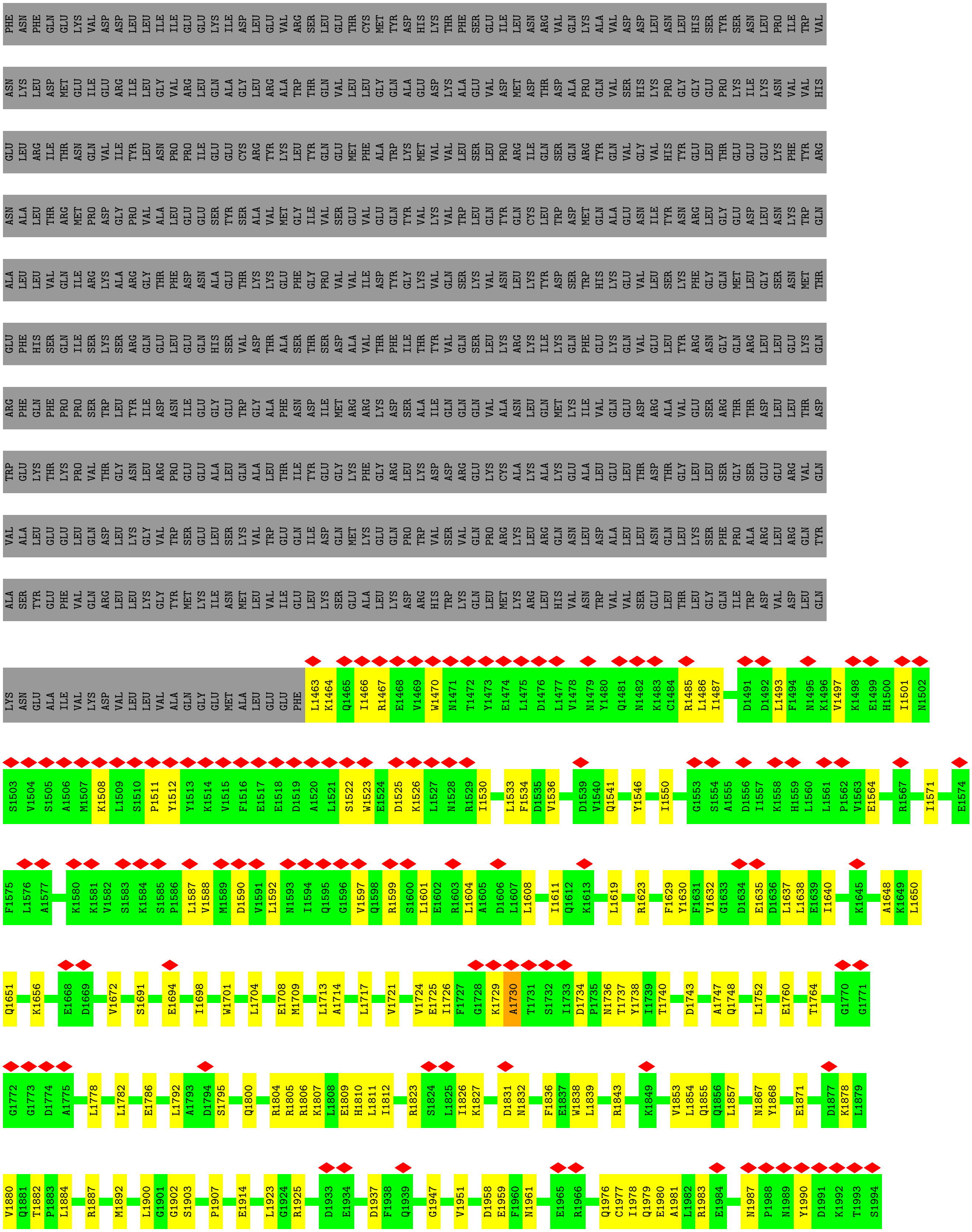
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

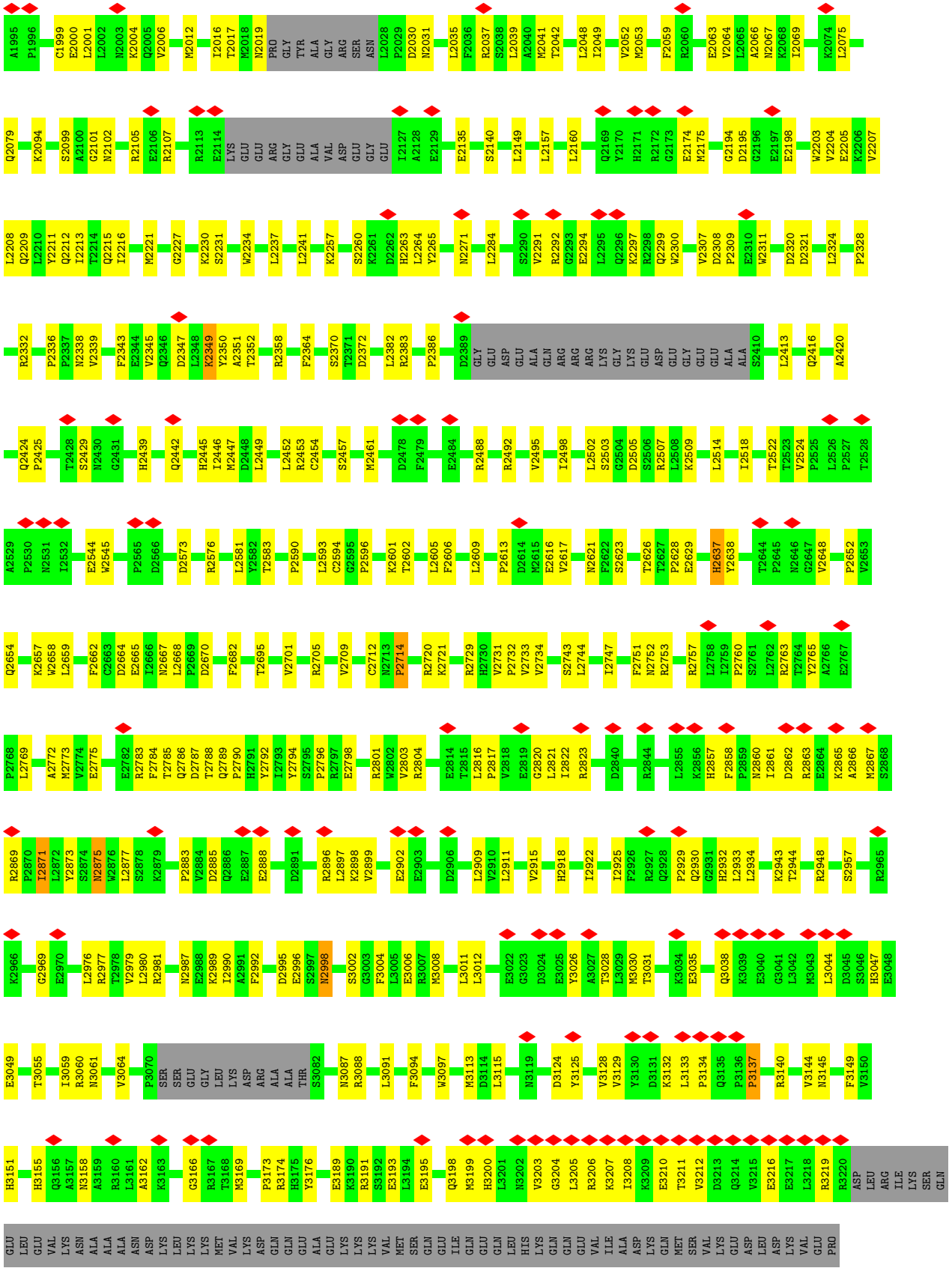
3 Residue-property plots (i)

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




PHE ASN PHE GLN GLU LYS VAL ASP ASP LEU LEU ILE ILE GLU GLU LYS ILE ASP LEU GLU VAL ARG SER LEU GLU THR CYS MET TYR ASP HIS LYS THR PHE SER GLU ILE LEU ASN ARG VAL GLN LYS ALA VAL ASP ASP LEU ASN LEU HIS SER TYR SER ASN LEU PRO ILE TRP VAL
ASN LYS LEU ASP MET GLU ILE GLU ARG ILE LEU GLY VAL ARG LEU GLN ALA GLY LEU ARG ALA TRP THR GLN VAL LEU LEU GLY GLN ALA GLU ASP LYS ALA GLU VAL ASP MET ASP THR ASP ALA PRO GLN VAL SER HIS LYS PRO GLY GLY GLU PRO LYS ILE LYS ASN VAL VAL HIS
GLU LEU ARG ILE THR ASN GLN VAL ILE TYR LEU ASN PRO PRO ILE GLU GLU CYS ARG TYR LYS LEU TYR GLN GLU MET PHE ALA TRP LYS MET VAL VAL LEU SER LEU PRO ARG ILE GLN SER GLN ARG TYR GLN VAL GLY VAL HIS TYR GLU LEU THR GLU GLU GLU LYS PHE TYR ARG
ASN ALA LEU THR ARG MET PRO ASP GLY PRO VAL ALA LEU GLU GLU SER TYR SER ALA VAL MET GLY ILE VAL SER GLU VAL GLU GLN TYR VAL LYS VAL TRP LEU GLN TYR GLN CYS LEU TRP ASP MET GLN ALA GLU ASN ILE TYR ASN ARG LEU GLY GLU ASP LEU ASN LYS TRP GLN
ALA LEU LEU VAL GLN ILE ARG LYS ALA ARG GLY THR PHE ASP ASN ALA GLU THR LYS LYS GLU PHE GLY PRO VAL VAL ILE ASP TYR GLY LYS VAL GLN SER LYS VAL ASN LEU LYS TYR ASP SER TRP HIS LYS GLU VAL LEU SER LYS PHE GLY GLN MET LEU GLY SER ASN MET THR
GLU PHE HIS SER GLN ILE SER LYS SER ARG GLN GLU LEU GLU GLN HIS SER VAL ASP THR ALA SER THR SER ASP ALA VAL THR PHE ILE THR TYR VAL GLN SER LEU LYS ARG LYS ILE LYS GLN PHE GLU LYS GLN VAL GLU LEU TYR ARG ASN GLY GLN ARG LEU LEU GLU LYS GLN
ARG PHE GLN PHE PRO PRO SER TRP LEU TYR ILE ASP ASN ILE GLU GLY GLU TRP GLY ALA PHE ASN ASP ILE MET ARG ARG LYS ASP SER ALA ILE GLN GLN GLN VAL ALA ASN LEU GLN MET LYS ILE VAL GLN GLU ASP ARG ALA VAL GLU SER ARG THR THR ASP LEU LEU THR ASP
TRP GLU LYS THR LYS PRO VAL THR GLY ASN LEU ARG PRO GLU GLU ALA LEU GLN ALA LEU THR ILE TYR GLU GLY LYS PHE GLY ARG LEU LYS ASP ASP ARG GLU LYS CYS ALA LYS ALA LYS GLU ALA LEU GLU LEU THR ASP THR GLY LEU LEU SER GLY SER GLU GLU ARG VAL GLN
VAL ALA LEU GLU GLU LEU GLN ASP LEU LYS GLY VAL TRP SER GLU LEU SER LYS VAL TRP GLU GLN ILE ASP GLN MET LYS GLU GLN PRO TRP VAL SER VAL GLN PRO ARG LYS LEU ARG GLN ASN LEU ASP ALA LEU LEU ASN GLN LEU LYS SER PHE PRO ALA ARG LEU ARG GLN TYR
ALA SER TYR GLU PHE VAL GLN ARG LEU LEU LYS GLY TYR MET LYS ILE ASN MET LEU VAL ILE GLU LEU LYS SER GLU ALA LEU LYS ASP ARG HIS TRP LYS GLN LEU MET LYS ARG LEU HIS VAL ASN TRP VAL VAL SER GLU LEU THR LEU GLY GLY GLN ILE TRP ASP VAL ASP LEU GLN
LYS ASN GLU ALA ILE VAL LYS ASP VAL LEU LEU VAL ALA GLN GLY GLU MET ALA LEU GLU GLU PHE L1463 K1464 Q1465 I1466 R1467 E1468 V1469 W1470 N1471 T1472 Y1473 E1474 L1475 D1476 L1477 V1478 N1479 Y1480 Q1481 N1482 K1483 C1484 R1485 L1486 I1487 D1491 D1492 L1493 F1494 N1495 K1496 V1497 K1498 E1499 H1500 I1501 N1502
S1503 V1504 S1505 A1506 M1507 K1508 L1509 S1510 P1511 Y1512 Y1513 K1514 V1515 F1516 E1517 E1518 D1519 A1520 L1521 S1522 W1523 E1524 D1525 K1526 L1527 N1528 R1529 I1530 L1533 F1534 D1535 V1536 D1539 V1540 Q1541 Y1546 I1550 G1553 S1554 A1555 D1556 I1557 K1558 H1559 L1560 L1561 P1562 V1563 E1564 R1567 I1571 E1574
F1575 L1576 A1577 K1580 K1581 V1582 S1583 K1584 S1585 P1586 L1587 V1588 M1589 D1590 V1591 L1592 N1593 I1594 Q1595 G1596 V1597 Q1598 R1599 S1600 L1601 E1602 R1603 L1604 A1605 D1606 L1607 L1608 I1611 Q1612 K1613 L1619 R1623 F1629 Y1630 F1631 V1632 G1633 D1634 E1635 D1636 L1637 L1638 E1639 I1640 K1645 A1648 K1649 L1650
Q1651 K1656 E1668 D1669 V1672 S1691 E1694 I1698 W1701 L1704 E1708 M1709 L1713 A1714 L1717 V1721 V1724 E1725 I1726 F1727 G1728 K1729 A1730 T1731 S1732 I1733 D1734 P1735 N1736 T1737 Y1738 I1739 T1740 D1743 A1747 Q1748 L1752 E1760 T1764 G1770 G1771
G1772 G1773 D1774 A1775 L1778 L1782 E1786 L1792 A1793 D1794 S1795 Q1800 R1804 R1805 R1806 K1807 L1808 E1809 H1810 L1811 I1812 R1823 S1824 L1825 I1826 K1827 D1831 N1832 F1836 E1837 W1838 L1839 R1843 K1849 V1853 L1854 Q1855 Q1856 L1857 N1867 Y1868 E1871 D1877 K1878 L1879
V1880 Q1881 T1882 P1883 L1884 R1887 M1892 L1900 G1901 G1902 S1903 P1907 E1914 L1923 G1924 R1925 D1933 E1934 D1937 F1938 Q1939 G1947 V1951 D1958 E1959 F1960 N1961 E1965 R1966 Q1976 C1977 I1978 Q1979 E1980 A1981 L1982 R1983 E1984 N1987 P1988 N1989 Y1990 D1991 K1992 T1993 S1994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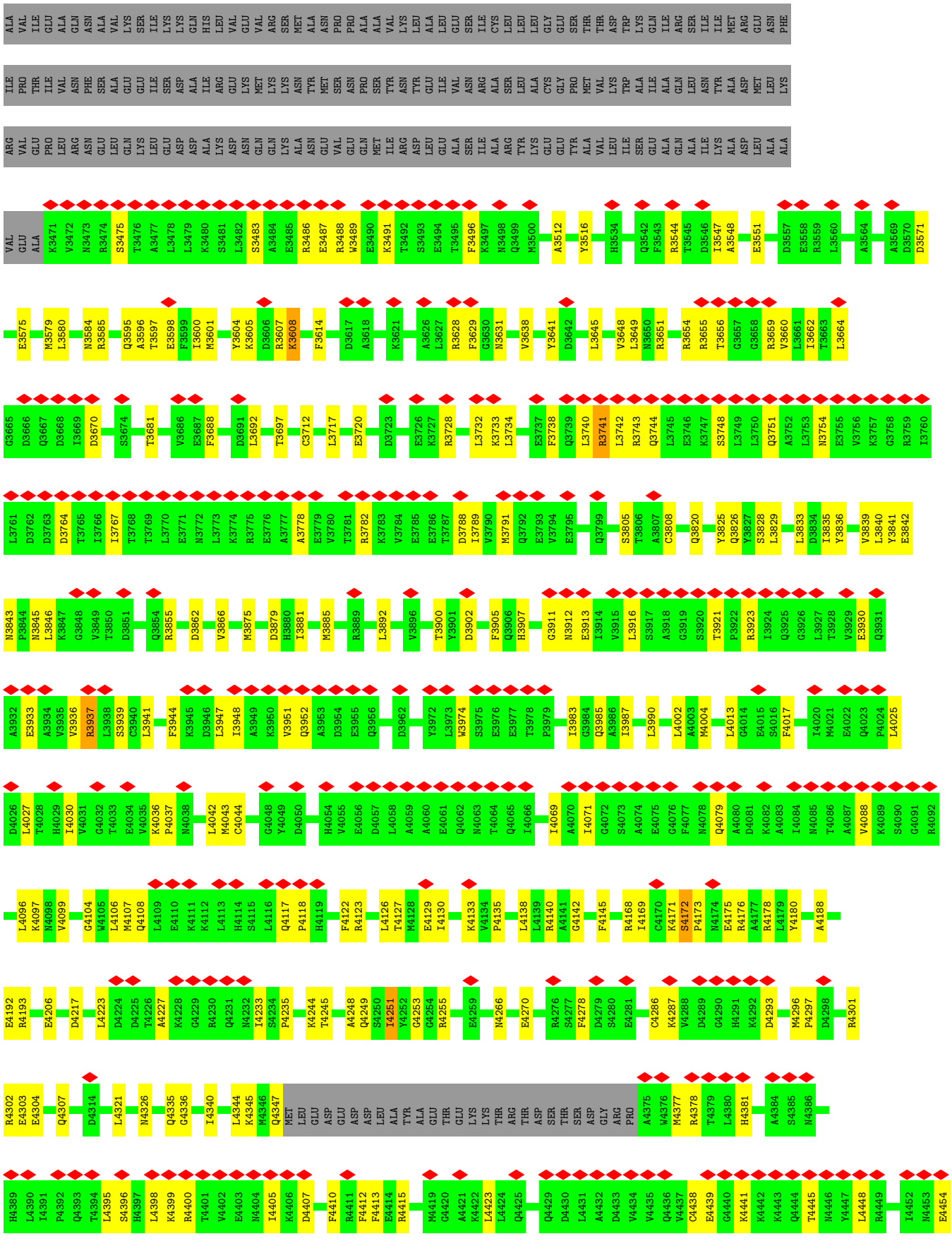
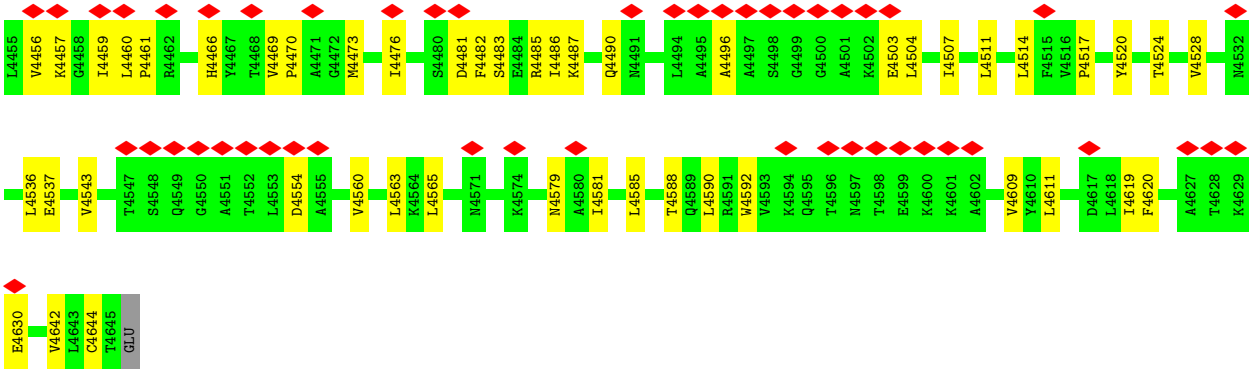
Q2079 K2094 S2099 A2100 G2101 N2102 R2105 E2106 R2107 R2113 E2114 LYS GLU GLU ARG GLY GLU ALA VAL ASP GLU GLY GLU I2127 A2128 E2129 E2135 S2140 L2149 L2157 L2160 Q2169 Y2170 H2171 R2172 G2173 E2174 M2175 G2194 D2195 G2196 E2197 E2198 W2203 V2204 E2205 K2206 V2207
L2208 Q2209 L2210 Y2211 Q2212 I2213 T2214 Q2215 I2216 M2221 G2227 K2230 S2231 W2234 L2237 L2241 K2257 S2260 K2261 D2262 H2263 L2264 Y2265 N2271 L2284 S2290 V2291 R2292 G2293 E2294 L2295 Q2296 K2297 R2298 Q2299 W2300 V2307 D2308 P2309 E2310 W2311 D2320 D2321 L2324 P2328
R2332 P2336 P2337 N2338 V2339 F2343 E2344 V2345 Q2346 D2347 L2348 K2349 Y2350 A2351 T2352 R2358 F2364 S2370 T2371 D2372 L2382 R2383 P2386 D2389 GLY GLU ASP GLU ALA GLN ARG ARG LYS GLY LYS GLU ASP GLU GLY GLU GLU ALA ALA S2410 L2413 Q2416 A2420
Q2424 P2425 T2428 S2429 N2430 G2431 H2439 Q2442 H2445 I2446 M2447 D2448 L2449 L2452 R2453 C2454 S2457 M2461 D2478 F2479 E2484 R2488 R2492 V2495 I2498 L2502 S2503 G2504 D2505 S2506 R2507 L2508 K2509 L2514 I2518 T2522 T2523 V2524 P2525 L2526 P2527 T2528
A2529 P2530 N2531 I2532 E2544 W2545 P2565 D2566 D2573 R2576 L2581 Y2582 T2583 P2590 L2593 C2594 G2595 P2596 K2601 T2602 L2605 F2606 L2609 P2613 D2614 M2615 E2616 V2617 N2621 F2622 S2623 T2626 T2627 P2628 E2629 H2637 Y2638 T2644 P2645 N2646 G2647 V2648 P2652 V2653
Q2654 K2657 W2658 L2659 F2662 C2663 D2664 E2665 I2666 N2667 L2668 P2669 D2670 F2682 T2695 V2701 R2705 V2709 C2712 N2713 P2714 R2720 K2721 R2729 H2730 V2731 P2732 V2733 V2734 S2743 L2744 I2747 F2751 N2752 R2753 R2757 L2758 I2759 P2760 S2761 L2762 R2763 T2764 Y2765 A2766 E2767
P2768 L2769 A2772 M2773 Y2774 E2775 E2782 R2783 F2784 T2785 Q2786 D2787 T2788 Q2789 P2790 H2791 Y2792 I2793 Y2794 S2795 P2796 R2797 E2798 R2801 W2802 Y2803 R2804 E2814 T2815 L2816 P2817 V2818 E2819 G2820 L2821 I2822 R2823 D2840 R2844 L2855 K2856 H2857 F2858 P2859 N2860 I2861 D2862 R2863 E2864 K2865 A2866 M2867 S2868
R2869 P2870 I2871 L2872 Y2873 S2874 N2875 W2876 L2877 S2878 K2879 P2883 V2884 D2885 Q2886 E2887 E2888 D2891 R2896 L2897 K2898 V2899 E2902 E2903 D2906 L2909 V2910 L2911 V2915 H2918 I2922 I2925 F2926 R2927 Q2928 P2929 Q2930 G2931 H2932 L2933 L2934 K2943 T2944 R2948 S2957 R2965
K2966 G2969 E2970 L2976 R2977 T2978 V2979 L2980 R2981 N2987 E2988 K2989 I2990 A2991 F2992 D2995 E2996 S2997 N2998 S3002 G3003 F3004 L3005 E3006 R3007 M3008 L3011 L3012 E3022 G3023 D3024 E3025 Y3026 A3027 T3028 L3029 M3030 T3031 K3034 E3035 Q3038 K3039 E3040 G3041 L3042 M3043 L3044 D3045 S3046 H3047 E3048
E3049 T3055 I3059 R3060 N3061 V3064 P3070 SER SER GLU GLY LEU LYS ASP ARG ALA ALA THR S3082 N3087 R3088 L3091 F3094 W3097 M3113 D3114 L3115 N3119 D3124 Y3125 V3128 V3129 Y3130 D3131 K3132 L3133 P3134 Q3135 P3136 P3137 R3140 V3144 N3145 F3149 V3150
H3151 H3155 Q3156 A3157 N3158 A3159 R3160 L3161 A3162 K3163 G3166 R3167 T3168 M3169 P3173 R3174 H3175 Y3176 E3189 K3190 R3191 S3192 E3193 L3194 E3195 Q3198 M3199 H3200 L3201 H3202 V3203 G3204 L3205 R3206 K3207 I3208 K3209 E3210 T3211 V3212 D3213 Q3214 V3215 E3216 E3217 L3218 R3219 R3220 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 VAL LYS GLU ASP LEU ASP LYS VAL GLU PRO

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L4536 E4537 V4543 T4547 S4548 Q4549 G4550 A4551 T4552 L4553 D4554 A4555 V4560 L4563 K4564 L4565 N4571 K4574 N4579 A4580 I4581 L4585 T4588 Q4589 L4590 R4591 W4592 V4593 K4594 Q4595 T4596 N4597 T4598 E4599 K4600 K4601 A4602 V4609 Y4610 L4611 D4617 L4618 I4619 F4620 A4627 T4628 K4629
E4630 V4642 L4643 C4644 T4645 GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91718	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)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.072	Depositor
Minimum map value	-1.197	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	412.488, 412.488, 412.488	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1458, 1.1458, 1.1458	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.27	1/23454 (0.0%)	0.53	8/31791 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2328	PRO	CG-CD	-6.17	1.30	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2328	PRO	N-CD-CG	-11.60	85.79	103.20
1	A	2328	PRO	CA-N-CD	-9.86	97.70	111.50
1	A	2714	PRO	N-CD-CG	-8.44	90.54	103.20
1	A	2714	PRO	CA-CB-CG	-7.68	89.40	104.00
1	A	2714	PRO	CA-N-CD	-6.83	101.93	111.50
1	A	2328	PRO	CA-CB-CG	-6.46	91.72	104.00
1	A	3137	PRO	N-CD-CG	-5.89	94.36	103.20
1	A	4554	ASP	CB-CG-OD2	5.45	123.20	118.30

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	22962	0	23030	507	0
2	A	54	0	24	2	0
3	A	62	0	24	0	0
All	All	23078	0	23078	507	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 11.

All (507) 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:2925:ILE:HG13	1:A:2933:LEU:HD13	1.59	0.85
1:A:2929:PRO:HB3	1:A:3060:ARG:HA	1.56	0.85
1:A:2987:ASN:OD1	1:A:3061:ASN:ND2	2.10	0.85
1:A:2324:LEU:HD11	1:A:2332:ARG:HB3	1.61	0.82
1:A:2453:ARG:HB2	1:A:2729:ARG:HA	1.59	0.82
1:A:4037:PRO:HG2	1:A:4117:GLN:HE21	1.48	0.79
1:A:4511:LEU:HD23	1:A:4563:LEU:HD21	1.66	0.77
1:A:2930:GLN:HE21	1:A:3059:ILE:HA	1.51	0.75
1:A:3948:ILE:O	1:A:3952:GLN:NE2	2.19	0.74
1:A:1466:ILE:HG22	1:A:1523:TRP:HE1	1.53	0.73
1:A:4099:VAL:HG22	1:A:4106:LEU:HD21	1.70	0.73
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.22	0.73
1:A:4071:ILE:HG21	1:A:4099:VAL:HA	1.69	0.72
1:A:3044:LEU:HD12	1:A:3049:GLU:HG3	1.70	0.72
1:A:3788:ASP:OD1	1:A:3789:ILE:HD12	1.90	0.72
1:A:2347:ASP:OD2	1:A:2349:LYS:NZ	2.23	0.72
1:A:2804:ARG:HH22	1:A:2929:PRO:HB2	1.55	0.71
1:A:1487:ILE:O	1:A:2271:ASN:ND2	2.24	0.71
1:A:1978:ILE:HD11	1:A:2001:LEU:HD11	1.73	0.70
1:A:2488:ARG:HB3	1:A:2492:ARG:HH12	1.53	0.70
1:A:1526:LYS:O	1:A:1530:ILE:HD12	1.91	0.70
1:A:4611:LEU:HD12	1:A:4644:CYS:HB2	1.74	0.69
1:A:4106:LEU:HD12	1:A:4138:LEU:HD22	1.74	0.69
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.11	0.69
1:A:4396:SER:HB2	1:A:4398:LEU:HD23	1.75	0.69
1:A:1857:LEU:HD22	1:A:1868:TYR:HB2	1.75	0.67
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.59	0.67
1:A:2507:ARG:HH22	1:A:2509:LYS:HD2	1.60	0.67
1:A:2775:GLU:OE2	1:A:2857:HIS:NE2	2.25	0.67
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.60	0.66
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3734:LEU:HD23	1:A:3738:PHE:HD2	1.61	0.65
1:A:4169:ILE:HG21	1:A:4302:ARG:HD2	1.78	0.65
1:A:2593:LEU:HD12	1:A:2605:LEU:HD22	1.77	0.65
1:A:3203:VAL:HA	1:A:3206:ARG:HE	1.61	0.65
1:A:1900:LEU:HD21	1:A:1983:ARG:HH21	1.62	0.65
1:A:2205:GLU:O	1:A:2209:GLN:HG3	1.97	0.64
1:A:3907:HIS:HA	1:A:3911:GLY:HA3	1.79	0.64
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.79	0.64
1:A:3585:ARG:HB2	1:A:3697:THR:HG23	1.79	0.64
1:A:2308:ASP:OD1	1:A:2311:TRP:NE1	2.31	0.63
1:A:4176:ARG:HE	1:A:4223:LEU:HD23	1.63	0.63
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.80	0.63
1:A:4206:GLU:O	1:A:4255:ARG:NH1	2.31	0.63
1:A:1786:GLU:OE2	1:A:1823:ARG:NH2	2.31	0.62
1:A:2823:ARG:HD2	1:A:2867:MET:HE3	1.80	0.62
1:A:2977:ARG:O	1:A:2981:ARG:HG3	1.99	0.62
1:A:1976:GLN:O	1:A:1980:GLU:HG3	1.98	0.62
1:A:2783:ARG:HG2	1:A:2784:PHE:H	1.65	0.62
1:A:3608:LYS:HD2	1:A:3608:LYS:O	1.99	0.62
1:A:3544:ARG:HD2	1:A:3547:ILE:HD12	1.81	0.62
1:A:3948:ILE:HG22	1:A:3952:GLN:HE22	1.65	0.62
1:A:2822:ILE:HG13	1:A:2861:ILE:HG12	1.80	0.62
1:A:1981:ALA:HB2	1:A:1999:CYS:HB3	1.81	0.61
1:A:1882:THR:HG22	1:A:2048:LEU:HD23	1.82	0.61
1:A:3826:GLN:OE1	1:A:4140:ARG:NH2	2.34	0.61
1:A:3921:THR:OG1	1:A:3923:ARG:NH1	2.34	0.61
1:A:4454:GLU:HG2	1:A:4461:PRO:HA	1.82	0.60
1:A:2495:VAL:HG21	1:A:2524:VAL:HG21	1.83	0.60
1:A:1721:VAL:O	1:A:1725:GLU:HG2	2.02	0.60
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.83	0.60
1:A:1640:ILE:HG23	1:A:1650:LEU:HD13	1.84	0.60
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	1.83	0.60
1:A:3208:ILE:O	1:A:3212:VAL:HG23	2.02	0.60
1:A:1792:LEU:HD21	1:A:1811:LEU:HB3	1.82	0.60
1:A:4377:MET:HE2	1:A:4438:CYS:HA	1.84	0.60
1:A:2488:ARG:HB3	1:A:2492:ARG:NH1	2.16	0.60
1:A:2823:ARG:HA	1:A:2866:ALA:HB1	1.84	0.60
1:A:2862:ASP:OD2	1:A:2863:ARG:N	2.35	0.59
1:A:2897:LEU:HD21	1:A:2909:LEU:HB2	1.84	0.59
1:A:2934:LEU:HD23	1:A:3091:LEU:HG	1.85	0.59
1:A:3151:HIS:NE2	1:A:3155:HIS:HE1	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1564:GLU:HG3	1:A:1611:ILE:HG13	1.85	0.59
1:A:1748:GLN:NE2	1:A:1868:TYR:OH	2.32	0.58
1:A:2875:ASN:ND2	1:A:2875:ASN:O	2.36	0.58
1:A:1635:GLU:OE1	1:A:1635:GLU:N	2.30	0.58
1:A:1958:ASP:O	1:A:2017:THR:OG1	2.20	0.58
1:A:2211:TYR:HB2	1:A:2237:LEU:HD11	1.85	0.58
1:A:2386:PRO:HG3	1:A:2413:LEU:HD21	1.84	0.58
1:A:3124:ASP:OD1	1:A:3125:TYR:N	2.36	0.58
1:A:2370:SER:OG	1:A:2372:ASP:OD2	2.19	0.58
1:A:3608:LYS:HE3	1:A:3631:ASN:HD22	1.69	0.58
1:A:1752:LEU:HD11	1:A:1868:TYR:CZ	2.38	0.58
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.36	0.58
1:A:2382:LEU:O	1:A:2416:GLN:NE2	2.37	0.57
1:A:2865:LYS:HD2	1:A:2869:ARG:HA	1.84	0.57
1:A:3151:HIS:CE1	1:A:3176:TYR:HB2	2.39	0.57
1:A:2804:ARG:NH1	1:A:2929:PRO:O	2.36	0.57
1:A:3198:GLN:HG3	1:A:3496:PHE:HD1	1.68	0.57
1:A:1587:LEU:HB2	1:A:1590:ASP:HB2	1.86	0.57
1:A:1760:GLU:O	1:A:1764:THR:HG23	2.04	0.57
1:A:1747:ALA:HB2	1:A:1807:LYS:HG2	1.86	0.56
1:A:2593:LEU:HD23	1:A:2734:VAL:HB	1.87	0.56
1:A:3035:GLU:OE1	1:A:3038:GLN:NE2	2.38	0.56
1:A:4395:LEU:HA	1:A:4490:GLN:HE22	1.70	0.56
1:A:4563:LEU:HD12	1:A:4588:THR:HG21	1.87	0.56
1:A:2175:MET:HE3	1:A:2208:LEU:HD13	1.87	0.56
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.88	0.56
1:A:3151:HIS:CD2	1:A:3155:HIS:HE1	2.23	0.56
1:A:3199:MET:SD	1:A:3200:HIS:ND1	2.77	0.56
1:A:3916:LEU:HD13	1:A:3936:VAL:HG12	1.86	0.56
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.39	0.56
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.87	0.56
1:A:2291:VAL:N	1:A:2294:GLU:OE2	2.38	0.56
1:A:1805:ARG:O	1:A:1809:GLU:HG3	2.06	0.56
1:A:2445:HIS:HE2	1:A:2449:LEU:HD22	1.70	0.56
1:A:2823:ARG:NH1	1:A:2873:TYR:OH	2.39	0.56
1:A:3628:ARG:HH12	1:A:3629:PHE:HB2	1.70	0.56
1:A:2079:GLN:HG3	1:A:2160:LEU:HD21	1.88	0.55
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.89	0.55
1:A:3133:LEU:HB3	1:A:3134:PRO:HD3	1.88	0.55
1:A:2079:GLN:HB2	1:A:2160:LEU:HD11	1.88	0.55
1:A:3208:ILE:HG23	1:A:3486:ARG:HH22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4106:LEU:HB3	1:A:4135:PRO:HG2	1.89	0.55
1:A:2957:SER:HB2	1:A:2990:ILE:HD13	1.88	0.55
1:A:3584:ASN:O	1:A:3651:ARG:NH2	2.40	0.55
1:A:3628:ARG:NH1	1:A:3629:PHE:HB2	2.21	0.55
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.41	0.55
1:A:2445:HIS:HD2	1:A:2449:LEU:HB2	1.72	0.55
1:A:2099:SER:OG	1:A:2140:SER:OG	2.19	0.55
1:A:4169:ILE:HG13	1:A:4180:TYR:CD2	2.42	0.55
1:A:4326:ASN:HD21	1:A:4581:ILE:HG23	1.72	0.55
1:A:4445:THR:HG22	1:A:4448:LEU:HD23	1.87	0.55
1:A:2382:LEU:HD22	1:A:2420:ALA:HB2	1.90	0.54
1:A:2425:PRO:O	1:A:2429:SER:OG	2.25	0.54
1:A:2457:SER:HB3	1:A:2732:PRO:HB3	1.89	0.54
1:A:2877:LEU:HD21	1:A:2888:GLU:HG3	1.90	0.54
1:A:3751:GLN:HA	1:A:3754:ASN:ND2	2.22	0.54
1:A:4454:GLU:HG3	1:A:4459:ILE:HG23	1.89	0.54
1:A:1987:ASN:HB2	1:A:1990:TYR:HB3	1.88	0.54
1:A:3571:ASP:O	1:A:3575:GLU:HG3	2.08	0.54
1:A:1907:PRO:HD2	1:A:2042:THR:HA	1.89	0.54
1:A:2492:ARG:HG3	1:A:2492:ARG:HH11	1.73	0.54
1:A:3845:ASN:ND2	1:A:3862:ASP:OD1	2.40	0.54
1:A:2602:THR:O	1:A:2606:PHE:HB2	2.07	0.54
1:A:2976:LEU:O	1:A:2980:LEU:HD23	2.08	0.54
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.41	0.54
1:A:1855:GLN:OE1	1:A:1867:ASN:ND2	2.41	0.54
1:A:2629:GLU:OE2	1:A:2629:GLU:N	2.37	0.54
1:A:2102:ASN:OD1	1:A:2105:ARG:NH2	2.41	0.54
1:A:4399:LYS:HE2	1:A:4413:PHE:HB3	1.90	0.54
1:A:4043:MET:HB2	1:A:4127:THR:HA	1.89	0.53
1:A:1738:TYR:HE2	1:A:1792:LEU:HD11	1.73	0.53
1:A:2981:ARG:NH2	1:A:3028:THR:OG1	2.41	0.53
1:A:2063:GLU:OE2	1:A:2064:VAL:HG23	2.09	0.53
1:A:3655:ARG:HG3	1:A:3660:VAL:HG12	1.90	0.53
1:A:1880:VAL:HG11	1:A:2049:ILE:HA	1.89	0.53
1:A:2221:MET:HB3	1:A:2343:PHE:HB2	1.90	0.53
1:A:3788:ASP:HA	1:A:3791:MET:HG2	1.90	0.53
1:A:3843:ASN:HD22	1:A:3846:LEU:HG	1.73	0.53
1:A:4483:SER:O	1:A:4487:LYS:HG3	2.09	0.53
1:A:1782:LEU:O	1:A:1786:GLU:HG2	2.09	0.53
1:A:2785:THR:OG1	1:A:2787:ASP:OD1	2.27	0.53
1:A:3905:PHE:HE1	1:A:3987:ILE:HD12	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1493:LEU:HD21	1:A:1534:PHE:CG	2.44	0.52
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.91	0.52
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.42	0.52
1:A:2714:PRO:O	1:A:2714:PRO:HG2	2.10	0.52
1:A:3900:THR:HG23	1:A:3902:ASP:H	1.75	0.52
1:A:2581:LEU:HD11	1:A:2605:LEU:HD13	1.92	0.52
1:A:3128:VAL:HG21	1:A:3149:PHE:HB2	1.90	0.52
1:A:2308:ASP:OD1	1:A:2308:ASP:N	2.43	0.52
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.10	0.52
1:A:2786:GLN:N	1:A:2786:GLN:OE1	2.43	0.52
1:A:4287:LYS:O	1:A:4287:LYS:HG3	2.10	0.52
1:A:1806:ARG:HG3	1:A:1806:ARG:HH11	1.75	0.51
1:A:3738:PHE:O	1:A:3741:ARG:HD3	2.10	0.51
1:A:3825:TYR:CZ	1:A:3875:MET:HG3	2.44	0.51
1:A:1880:VAL:HG21	1:A:2052:VAL:HG21	1.91	0.51
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.43	0.51
1:A:2596:PRO:O	1:A:2601:LYS:NZ	2.43	0.51
1:A:3645:LEU:HG	1:A:3649:LEU:HD13	1.91	0.51
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.10	0.51
1:A:3087:ASN:O	1:A:3088:ARG:HG2	2.11	0.51
1:A:1619:LEU:HD11	1:A:1637:LEU:HB3	1.93	0.51
1:A:2581:LEU:HD11	1:A:2605:LEU:CD1	2.40	0.51
1:A:3002:SER:O	1:A:3006:GLU:HG2	2.11	0.51
1:A:4266:ASN:O	1:A:4270:GLU:HG3	2.11	0.51
1:A:2213:ILE:HA	1:A:2216:ILE:HG22	1.91	0.51
1:A:2665:GLU:OE1	1:A:2720:ARG:NH1	2.44	0.51
1:A:3151:HIS:CD2	1:A:3155:HIS:CE1	2.99	0.51
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.92	0.51
1:A:2753:ARG:O	1:A:2757:ARG:HG3	2.11	0.51
1:A:2820:GLY:HA2	1:A:2823:ARG:HG2	1.93	0.51
1:A:4037:PRO:HB2	1:A:4117:GLN:HG3	1.91	0.51
1:A:4303:GLU:O	1:A:4307:GLN:HG2	2.11	0.51
1:A:4511:LEU:HD11	1:A:4517:PRO:HB3	1.93	0.51
1:A:1623:ARG:NH1	1:A:1632:VAL:O	2.44	0.50
1:A:2998:ASN:O	1:A:2998:ASN:ND2	2.44	0.50
1:A:3216:GLU:OE2	1:A:3219:ARG:NH2	2.43	0.50
1:A:3912:ASN:O	1:A:3937:ARG:NH1	2.43	0.50
1:A:3512:ALA:O	1:A:3516:TYR:HB2	2.10	0.50
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.93	0.50
1:A:2658:TRP:CE3	1:A:2705:ARG:HA	2.47	0.50
1:A:1463:LEU:HD22	1:A:1467:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2751:PHE:HB3	1:A:2803:VAL:HG11	1.92	0.50
1:A:2934:LEU:HB3	1:A:3091:LEU:HA	1.94	0.50
1:A:2518:ILE:O	1:A:2522:THR:HG22	2.12	0.50
1:A:2609:LEU:HD23	1:A:2617:VAL:HG13	1.93	0.50
1:A:2867:MET:SD	1:A:2871:ILE:HA	2.52	0.50
1:A:3923:ARG:HE	1:A:3948:ILE:HG12	1.77	0.50
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.92	0.49
1:A:2209:GLN:O	1:A:2213:ILE:HG12	2.12	0.49
1:A:2918:HIS:O	1:A:2922:ILE:HG13	2.12	0.49
1:A:3203:VAL:HG13	1:A:3206:ARG:HH21	1.77	0.49
1:A:3751:GLN:HA	1:A:3754:ASN:HD21	1.77	0.49
1:A:2789:GLN:HB2	1:A:2792:TYR:CD2	2.47	0.49
1:A:2911:LEU:HD12	1:A:2915:VAL:HG12	1.93	0.49
1:A:4172:SER:HB2	1:A:4173:PRO:HD2	1.94	0.49
1:A:4175:GLU:O	1:A:4175:GLU:HG3	2.13	0.49
1:A:3044:LEU:HD12	1:A:3049:GLU:CG	2.41	0.49
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.94	0.49
1:A:2260:SER:O	1:A:2264:LEU:N	2.45	0.49
1:A:2744:LEU:HD21	1:A:2796:PRO:HB3	1.95	0.49
1:A:4301:ARG:NH1	1:A:4304:GLU:OE1	2.44	0.49
1:A:1672:VAL:HA	1:A:1691:SER:HA	1.95	0.49
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.94	0.49
1:A:1979:GLN:HB3	1:A:2035:LEU:HD13	1.95	0.49
1:A:3208:ILE:HD12	1:A:3211:THR:OG1	2.12	0.49
1:A:1961:ASN:HD21	1:A:2019:ASN:HB3	1.77	0.48
1:A:4097:LYS:HA	1:A:4127:THR:HB	1.95	0.48
1:A:2263:HIS:ND1	1:A:2695:THR:HG21	2.27	0.48
1:A:1486:LEU:HD13	1:A:1541:GLN:HE21	1.77	0.48
1:A:2107:ARG:NH1	1:A:2135:GLU:OE2	2.47	0.48
1:A:4069:ILE:HG23	1:A:4079:GLN:HE21	1.79	0.48
1:A:3828:SER:HB3	1:A:4140:ARG:HG2	1.96	0.48
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.96	0.48
1:A:3808:CYS:HG	1:A:3836:TYR:HE1	1.61	0.48
1:A:2227:GLY:HA2	1:A:2452:LEU:HD12	1.95	0.48
1:A:2665:GLU:HB3	1:A:2668:LEU:HB2	1.96	0.48
1:A:2769:LEU:HD22	1:A:2821:LEU:HD11	1.96	0.48
1:A:3031:THR:O	1:A:3035:GLU:HG2	2.14	0.48
1:A:3488:ARG:HH21	1:A:3742:LEU:HG	1.78	0.48
1:A:1485:ARG:O	1:A:1486:LEU:HD23	2.14	0.48
1:A:3487:GLU:HB2	1:A:3491:LYS:NZ	2.28	0.48
1:A:4042:LEU:HD21	1:A:4138:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4044:CYS:HB3	1:A:4130:ILE:HG12	1.95	0.48
1:A:1533:LEU:HD11	1:A:1597:VAL:HG12	1.96	0.47
1:A:1648:ALA:HA	1:A:1651:GLN:HG3	1.96	0.47
1:A:3820:GLN:HB3	1:A:4345:LYS:HE2	1.95	0.47
1:A:2621:ASN:HA	1:A:2664:ASP:HB2	1.95	0.47
1:A:2858:PHE:CE2	1:A:2860:ASN:HB2	2.49	0.47
1:A:3597:THR:O	1:A:3601:MET:HG2	2.14	0.47
1:A:1923:LEU:HB3	1:A:1925:ARG:NH1	2.30	0.47
1:A:2605:LEU:HD11	1:A:2709:VAL:HG21	1.95	0.47
1:A:2760:PRO:HA	1:A:2763:ARG:HE	1.78	0.47
1:A:2498:ILE:HG23	1:A:2502:LEU:HD22	1.96	0.47
1:A:3132:LYS:HG3	1:A:3134:PRO:HD2	1.96	0.47
1:A:1536:VAL:HG12	1:A:1601:LEU:HG	1.96	0.47
1:A:1629:PHE:CG	1:A:1637:LEU:HD11	2.49	0.47
1:A:3983:ILE:O	1:A:3987:ILE:HG12	2.15	0.47
1:A:4036:LYS:HE3	1:A:4036:LYS:HB2	1.66	0.47
1:A:1903:SER:HA	1:A:2016:ILE:O	2.14	0.47
1:A:2309:PRO:HG3	1:A:2352:THR:HG23	1.96	0.47
1:A:2623:SER:N	1:A:2626:THR:OG1	2.48	0.47
1:A:2783:ARG:HG2	1:A:2784:PHE:N	2.27	0.47
1:A:2979:VAL:HG23	1:A:2990:ILE:HG21	1.96	0.47
1:A:2989:LYS:HD3	1:A:2989:LYS:N	2.29	0.47
1:A:2067:ASN:O	1:A:4537:GLU:HG2	2.15	0.47
1:A:2194:GLY:O	1:A:2204:VAL:HG11	2.15	0.47
1:A:2544:GLU:OE2	1:A:2545:TRP:N	2.43	0.47
1:A:3488:ARG:NH2	1:A:3742:LEU:HG	2.30	0.47
1:A:4002:LEU:HD11	1:A:4335:GLN:HB2	1.96	0.47
1:A:4104:GLY:O	1:A:4108:GLN:HG2	2.15	0.47
1:A:4412:PHE:O	1:A:4415:ARG:HG2	2.14	0.47
1:A:2320:ASP:OD2	1:A:2358:ARG:NH1	2.48	0.47
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.97	0.47
1:A:1470:TRP:CH2	1:A:1497:VAL:HG22	2.50	0.46
1:A:4235:PRO:HB3	1:A:4278:PHE:CD1	2.50	0.46
1:A:4287:LYS:N	1:A:4293:ASP:OD1	2.49	0.46
1:A:4520:TYR:O	1:A:4524:THR:HG23	2.15	0.46
1:A:1522:SER:HA	1:A:1525:ASP:OD2	2.16	0.46
1:A:1623:ARG:HD3	1:A:1630:TYR:HA	1.95	0.46
1:A:3788:ASP:OD1	1:A:3789:ILE:N	2.47	0.46
1:A:3829:LEU:HG	1:A:3833:LEU:HD13	1.97	0.46
1:A:2772:ALA:HA	1:A:2857:HIS:CD2	2.51	0.46
1:A:4096:LEU:HB2	1:A:4126:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1511:PRO:HG2	1:A:3670:ASP:HB3	1.97	0.46
1:A:2944:THR:O	1:A:2948:ARG:HG3	2.14	0.46
1:A:3207:LYS:HE2	1:A:3754:ASN:HB3	1.96	0.46
1:A:1497:VAL:O	1:A:1501:ILE:HG13	2.14	0.46
1:A:2237:LEU:HD22	1:A:2300:TRP:HH2	1.79	0.46
1:A:4122:PHE:O	1:A:4123:ARG:NH1	2.49	0.46
1:A:4188:ALA:O	1:A:4192:GLU:HG2	2.15	0.46
1:A:4469:VAL:HG12	1:A:4470:PRO:O	2.15	0.46
1:A:1599:ARG:HD2	1:A:1599:ARG:O	2.16	0.46
1:A:2174:GLU:HG2	1:A:2175:MET:N	2.31	0.46
1:A:2203:TRP:O	1:A:2207:VAL:HG23	2.15	0.46
1:A:4482:PHE:O	1:A:4486:ILE:HG12	2.16	0.46
1:A:3648:VAL:HA	1:A:3662:ILE:HD11	1.97	0.46
1:A:4104:GLY:O	1:A:4107:MET:HB2	2.15	0.46
1:A:4470:PRO:HD2	1:A:4473:MET:HE1	1.97	0.46
1:A:1937:ASP:OD1	1:A:1937:ASP:N	2.48	0.45
1:A:1976:GLN:OE1	1:A:2031:ASN:HB3	2.16	0.45
1:A:2257:LYS:HD2	1:A:2257:LYS:HA	1.78	0.45
1:A:3733:LYS:HE2	1:A:3738:PHE:CE1	2.51	0.45
1:A:4456:VAL:HG23	1:A:4457:LYS:HD3	1.98	0.45
1:A:1726:ILE:O	1:A:1729:LYS:HG2	2.17	0.45
1:A:1778:LEU:HD21	1:A:1826:ILE:HG22	1.98	0.45
1:A:2446:ILE:HG23	1:A:2447:MET:HG3	1.98	0.45
1:A:2628:PRO:HB3	1:A:2682:PHE:CD2	2.51	0.45
1:A:2865:LYS:HG3	1:A:2866:ALA:H	1.80	0.45
1:A:3575:GLU:O	1:A:3579:MET:HG3	2.16	0.45
1:A:2000:GLU:O	1:A:2001:LEU:HD23	2.16	0.45
1:A:2053:MET:SD	1:A:2094:LYS:HD2	2.57	0.45
1:A:4543:VAL:HG12	1:A:4590:LEU:HD23	1.98	0.45
1:A:1550:ILE:HD12	1:A:1638:LEU:HD13	1.97	0.45
1:A:2602:THR:O	1:A:2606:PHE:CB	2.64	0.45
1:A:2789:GLN:OE1	1:A:2790:PRO:HD2	2.16	0.45
1:A:3208:ILE:HG21	1:A:3486:ARG:HH12	1.81	0.45
1:A:1914:GLU:HG3	2:A:4701:ADP:H3'	1.99	0.45
1:A:2820:GLY:HA2	1:A:2823:ARG:NE	2.31	0.45
1:A:3748:SER:HA	1:A:3751:GLN:NE2	2.32	0.45
1:A:4395:LEU:HA	1:A:4490:GLN:NE2	2.30	0.45
1:A:4439:GLU:HB3	1:A:4441:LYS:NZ	2.31	0.45
1:A:1588:VAL:O	1:A:1592:LEU:HD23	2.17	0.45
1:A:4244:LYS:HD3	1:A:4270:GLU:HA	1.98	0.45
1:A:2059:PHE:HE1	1:A:2101:GLY:HA2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2383:ARG:NH2	1:A:2424:GLN:OE1	2.49	0.45
1:A:3055:THR:O	1:A:3059:ILE:HG12	2.16	0.45
1:A:3601:MET:O	1:A:3605:LYS:HG3	2.17	0.45
1:A:1608:LEU:HA	1:A:1611:ILE:HG22	1.99	0.45
1:A:2992:PHE:HB3	1:A:3064:VAL:HA	1.98	0.45
1:A:3174:ARG:NH2	2:A:4704:ADP:H5'1	2.31	0.45
1:A:4301:ARG:HG2	1:A:4304:GLU:OE2	2.17	0.45
1:A:1704:LEU:HD23	1:A:1704:LEU:HA	1.81	0.44
1:A:1892:MET:SD	1:A:1902:GLY:HA3	2.58	0.44
1:A:2980:LEU:HD21	1:A:3011:LEU:HD11	1.99	0.44
1:A:3835:ILE:HG23	1:A:3866:VAL:HG12	1.98	0.44
1:A:3030:MET:HG3	1:A:3047:HIS:CE1	2.53	0.44
1:A:3641:TYR:HE1	1:A:3645:LEU:HD23	1.81	0.44
1:A:2898:LYS:NZ	1:A:2902:GLU:HB3	2.32	0.44
1:A:3825:TYR:OH	1:A:3879:ASP:OD2	2.29	0.44
1:A:4245:THR:O	1:A:4249:GLN:HG2	2.17	0.44
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.82	0.44
1:A:3808:CYS:SG	1:A:3836:TYR:HE1	2.40	0.44
1:A:3836:TYR:CE2	1:A:3840:LEU:HD11	2.52	0.44
1:A:1512:TYR:N	1:A:3659:ARG:HH22	2.16	0.44
1:A:4400:ARG:HH22	1:A:4405:ILE:HD11	1.82	0.44
1:A:1887:ARG:HG3	1:A:2039:LEU:HD21	2.00	0.44
1:A:3204:GLY:O	1:A:3208:ILE:HG22	2.17	0.44
1:A:3608:LYS:HE3	1:A:3631:ASN:ND2	2.32	0.44
1:A:3892:LEU:HD23	1:A:3905:PHE:HZ	1.82	0.44
1:A:1571:ILE:HG23	1:A:1604:LEU:HD22	1.99	0.44
1:A:3974:TRP:HZ2	1:A:3985:GLN:HG3	1.82	0.44
1:A:4336:GLY:O	1:A:4340:ILE:HG12	2.18	0.44
1:A:4511:LEU:CD1	1:A:4517:PRO:HB3	2.47	0.44
1:A:1827:LYS:HA	1:A:1827:LYS:HD3	1.81	0.44
1:A:1959:GLU:OE2	1:A:2019:ASN:ND2	2.46	0.44
1:A:2307:VAL:HG23	1:A:2351:ALA:HB2	2.00	0.44
1:A:3548:ALA:HB3	1:A:3551:GLU:OE2	2.17	0.44
1:A:4378:ARG:HA	1:A:4378:ARG:HD3	1.77	0.44
1:A:1795:SER:O	1:A:1800:GLN:NE2	2.43	0.43
1:A:1838:TRP:CZ2	1:A:1843:ARG:HG2	2.53	0.43
1:A:2030:ASP:OD2	1:A:4133:LYS:NZ	2.50	0.43
1:A:2637:HIS:NE2	1:A:2638:TYR:HE1	2.16	0.43
1:A:2784:PHE:O	1:A:2792:TYR:HB3	2.18	0.43
1:A:2037:ARG:HH22	1:A:4251:ILE:HA	1.83	0.43
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2452:LEU:HD23	1:A:2452:LEU:HA	1.75	0.43
1:A:2637:HIS:CD2	1:A:2638:TYR:CE1	3.07	0.43
1:A:2652:PRO:HG3	1:A:2659:LEU:HB2	2.00	0.43
1:A:3595:GLN:O	1:A:3598:GLU:HG2	2.19	0.43
1:A:4171:LYS:HE2	1:A:4176:ARG:NH1	2.32	0.43
1:A:1709:MET:HE3	1:A:1871:GLU:HA	2.00	0.43
1:A:1743:ASP:OD2	1:A:1804:ARG:NH2	2.50	0.43
1:A:1792:LEU:HB3	1:A:1812:ILE:HG12	2.00	0.43
1:A:4565:LEU:HB2	1:A:4585:LEU:HD11	1.99	0.43
1:A:3659:ARG:NH2	1:A:3670:ASP:HB2	2.33	0.43
1:A:3941:LEU:HD23	1:A:3944:PHE:HD2	1.83	0.43
1:A:4400:ARG:NH2	1:A:4405:ILE:HD11	2.33	0.43
1:A:2794:TYR:HA	1:A:2798:GLU:OE2	2.18	0.43
1:A:3191:ARG:O	1:A:3195:GLU:HG2	2.19	0.43
1:A:3728:ARG:O	1:A:3732:LEU:HD23	2.19	0.43
1:A:4088:VAL:O	1:A:4118:PRO:HG2	2.18	0.43
1:A:1637:LEU:HA	1:A:1637:LEU:HD12	1.82	0.43
1:A:1709:MET:O	1:A:1713:LEU:HD23	2.19	0.43
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.50	0.43
1:A:2932:HIS:CG	1:A:3012:LEU:HD22	2.53	0.43
1:A:2995:ASP:OD2	1:A:2996:GLU:N	2.51	0.43
1:A:3748:SER:HA	1:A:3751:GLN:CD	2.39	0.43
1:A:2230:LYS:HG2	1:A:2364:PHE:CD2	2.53	0.43
1:A:2609:LEU:HB3	1:A:2617:VAL:CG2	2.48	0.43
1:A:3204:GLY:C	1:A:3489:TRP:HZ3	2.22	0.43
1:A:4296:MET:SD	1:A:4297:PRO:HD2	2.59	0.43
1:A:2349:LYS:HG3	1:A:2350:TYR:CD2	2.54	0.43
1:A:2616:GLU:OE2	1:A:2654:GLN:HG3	2.18	0.43
1:A:2765:TYR:HE2	1:A:2858:PHE:CZ	2.36	0.43
1:A:3488:ARG:NH2	1:A:3743:ARG:HH21	2.17	0.43
1:A:4025:LEU:CD2	1:A:4027:LEU:HB2	2.48	0.43
1:A:2221:MET:CB	1:A:2343:PHE:HB2	2.49	0.43
1:A:3162:ALA:HA	1:A:3166:GLY:HA2	2.00	0.43
1:A:3604:TYR:HD1	1:A:3607:ARG:HD3	1.84	0.43
1:A:1717:LEU:HD21	1:A:1857:LEU:HD12	2.00	0.43
1:A:2439:HIS:HA	1:A:2442:GLN:HG2	2.01	0.43
1:A:2445:HIS:CD2	1:A:2449:LEU:HB2	2.53	0.43
1:A:3764:ASP:HA	1:A:3767:ILE:HB	2.01	0.43
1:A:1811:LEU:HD23	1:A:1811:LEU:HA	1.91	0.42
1:A:2896:ARG:HA	1:A:2899:VAL:HG12	2.01	0.42
1:A:3113:MET:HE2	1:A:3115:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3933:GLU:O	1:A:3937:ARG:NE	2.49	0.42
1:A:2209:GLN:O	1:A:2212:GLN:HG2	2.19	0.42
1:A:3134:PRO:HG2	1:A:3137:PRO:HA	2.01	0.42
1:A:4511:LEU:HB2	1:A:4560:VAL:HG21	2.01	0.42
1:A:1729:LYS:HG3	1:A:1730:ALA:N	2.33	0.42
1:A:2049:ILE:O	1:A:2053:MET:HG3	2.19	0.42
1:A:2743:SER:O	1:A:2747:ILE:HG12	2.19	0.42
1:A:2885:ASP:OD1	1:A:2888:GLU:HG2	2.18	0.42
1:A:4286:CYS:SG	1:A:4287:LYS:N	2.92	0.42
1:A:1508:LYS:HA	1:A:1508:LYS:HD2	1.73	0.42
1:A:2291:VAL:HG12	1:A:2292:ARG:HG3	2.02	0.42
1:A:2505:ASP:HB3	1:A:2733:VAL:HG23	2.00	0.42
1:A:3947:LEU:O	1:A:3951:VAL:HG13	2.19	0.42
1:A:1978:ILE:HG23	1:A:2012:MET:HE1	2.01	0.42
1:A:3189:GLU:O	1:A:3193:GLU:HG2	2.19	0.42
1:A:3712:CYS:SG	1:A:3805:SER:HA	2.59	0.42
1:A:1691:SER:OG	1:A:1694:GLU:OE1	2.36	0.42
1:A:2307:VAL:HA	1:A:2311:TRP:CZ2	2.55	0.42
1:A:1736:ASN:O	1:A:1740:THR:HG23	2.19	0.42
1:A:2195:ASP:N	1:A:2198:GLU:OE2	2.52	0.42
1:A:3916:LEU:HD12	1:A:3937:ARG:HG3	2.02	0.42
1:A:2299:GLN:O	1:A:2339:VAL:HA	2.20	0.42
1:A:1734:ASP:HB3	1:A:1737:THR:HG22	2.01	0.42
1:A:2284:LEU:HD12	1:A:2284:LEU:HA	1.91	0.42
1:A:2454:CYS:SG	1:A:2502:LEU:HG	2.60	0.42
1:A:3662:ILE:HG23	1:A:3664:LEU:HG	2.02	0.42
1:A:4514:LEU:HD23	1:A:4514:LEU:HA	1.85	0.42
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	2.01	0.42
1:A:1530:ILE:HG23	1:A:1534:PHE:CD2	2.55	0.42
1:A:1708:GLU:HA	1:A:1708:GLU:OE1	2.20	0.42
1:A:1714:ALA:HB2	1:A:1853:VAL:HG23	2.01	0.42
1:A:1806:ARG:HG3	1:A:1806:ARG:NH1	2.35	0.42
1:A:1884:LEU:HD21	1:A:2041:MET:HB3	2.01	0.42
1:A:2667:ASN:OD1	1:A:2712:CYS:HB2	2.20	0.42
1:A:2798:GLU:HG2	1:A:2801:ARG:HH12	1.85	0.42
1:A:3614:PHE:CD1	1:A:3638:VAL:HA	2.55	0.42
1:A:3841:TYR:HB2	1:A:3842:GLU:OE2	2.20	0.42
1:A:4193:ARG:HG3	1:A:4321:LEU:HB3	2.00	0.42
1:A:2648:VAL:HB	1:A:2701:VAL:HG12	2.02	0.41
1:A:2787:ASP:OD1	1:A:2788:THR:N	2.53	0.41
1:A:3717:LEU:HD23	1:A:3717:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.55	0.41
1:A:4486:ILE:O	1:A:4490:GLN:HG2	2.20	0.41
1:A:2823:ARG:NH1	1:A:2883:PRO:HG3	2.34	0.41
1:A:3198:GLN:HG3	1:A:3496:PHE:CD1	2.52	0.41
1:A:3913:GLU:HB3	1:A:4476:ILE:HD12	2.02	0.41
1:A:4407:ASP:HB3	1:A:4410:PHE:HB3	2.01	0.41
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.36	0.41
1:A:1810:HIS:HD2	1:A:1878:LYS:HB2	1.85	0.41
1:A:2075:LEU:HD11	1:A:4536:LEU:HD22	2.02	0.41
1:A:2594:CYS:HA	1:A:2712:CYS:O	2.20	0.41
1:A:3008:MET:O	1:A:3012:LEU:HG	2.20	0.41
1:A:3026:TYR:O	1:A:3030:MET:HG2	2.20	0.41
1:A:3720:GLU:OE1	1:A:3855:ARG:NH1	2.40	0.41
1:A:1782:LEU:HD22	1:A:1827:LYS:HE3	2.03	0.41
1:A:3035:GLU:O	1:A:3038:GLN:HG2	2.20	0.41
1:A:3990:LEU:HD13	1:A:4004:MET:HG3	2.02	0.41
1:A:4423:LEU:HD21	1:A:4466:HIS:CG	2.56	0.41
1:A:1831:ASP:OD1	1:A:1832:ASN:N	2.54	0.41
1:A:2670:ASP:HA	1:A:2721:LYS:HD3	2.01	0.41
1:A:4344:LEU:O	1:A:4347:GLN:HG2	2.21	0.41
1:A:4503:GLU:O	1:A:4507:ILE:HG23	2.20	0.41
1:A:1853:VAL:HG13	1:A:1854:LEU:HG	2.02	0.41
1:A:2321:ASP:OD2	1:A:2321:ASP:N	2.54	0.41
1:A:3140:ARG:O	1:A:3144:VAL:HG23	2.19	0.41
1:A:2004:LYS:HE3	1:A:2006:VAL:HG12	2.02	0.41
1:A:2307:VAL:HG13	1:A:2345:VAL:HG11	2.03	0.41
1:A:2605:LEU:HD23	1:A:2662:PHE:CE2	2.56	0.41
1:A:3740:LEU:O	1:A:3744:GLN:HG2	2.20	0.41
1:A:3881:ILE:O	1:A:3885:MET:HG2	2.20	0.41
1:A:1464:LYS:HG3	1:A:1467:ARG:NH1	2.36	0.41
1:A:1546:TYR:O	1:A:1550:ILE:HG12	2.20	0.41
1:A:3129:VAL:HG12	1:A:3145:ASN:OD1	2.21	0.41
1:A:3219:ARG:HD3	1:A:3475:SER:HB3	2.03	0.41
1:A:3483:SER:O	1:A:3486:ARG:HB2	2.20	0.41
1:A:3596:ALA:O	1:A:3600:ILE:HG12	2.20	0.41
1:A:3654:ARG:HG2	1:A:3656:THR:OG1	2.21	0.41
1:A:3836:TYR:HA	1:A:3839:VAL:HG12	2.02	0.41
1:A:4248:ALA:O	1:A:4253:GLY:HA3	2.21	0.41
1:A:4630:GLU:OE1	1:A:4630:GLU:HA	2.21	0.41
1:A:1632:VAL:HG12	1:A:1656:LYS:HE2	2.02	0.41
1:A:2211:TYR:CE1	1:A:2241:LEU:HD21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2503:SER:HB2	1:A:2514:LEU:HD22	2.03	0.41
1:A:2744:LEU:HA	1:A:2747:ILE:HG12	2.03	0.41
1:A:3930:GLU:HA	1:A:3933:GLU:HG2	2.03	0.41
1:A:3948:ILE:CG2	1:A:3952:GLN:HE22	2.30	0.41
1:A:3128:VAL:HB	1:A:3145:ASN:OD1	2.21	0.40
1:A:3205:LEU:N	1:A:3489:TRP:HZ3	2.18	0.40
1:A:4129:GLU:HG2	1:A:4130:ILE:N	2.36	0.40
1:A:4481:ASP:O	1:A:4485:ARG:HG3	2.21	0.40
1:A:1463:LEU:HD23	1:A:1467:ARG:HE	1.85	0.40
1:A:1977:CYS:SG	1:A:1999:CYS:HB2	2.61	0.40
1:A:2943:LYS:HG2	1:A:3094:PHE:CD2	2.56	0.40
1:A:3974:TRP:CZ2	1:A:3985:GLN:HG3	2.56	0.40
1:A:4013:LEU:HD13	1:A:4017:PHE:CE2	2.57	0.40
1:A:4117:GLN:OE1	1:A:4117:GLN:N	2.54	0.40
1:A:1979:GLN:HG2	1:A:2035:LEU:HB3	2.04	0.40
1:A:3778:ALA:O	1:A:3782:ARG:HD3	2.21	0.40
1:A:2215:GLN:OE1	1:A:2215:GLN:HA	2.21	0.40
1:A:2336:PRO:HG2	1:A:2339:VAL:HG23	2.01	0.40
1:A:3939:SER:HA	1:A:3944:PHE:O	2.21	0.40
1:A:4042:LEU:HD13	1:A:4142:GLY:HA3	2.04	0.40
1:A:2613:PRO:O	1:A:2657:LYS:NZ	2.55	0.40
1:A:2752:ASN:HD21	1:A:2773:MET:HE1	1.86	0.40
1:A:3097:TRP:CE3	1:A:3173:PRO:HB3	2.56	0.40
1:A:3206:ARG:O	1:A:3210:GLU:HG2	2.22	0.40
1:A:3688:PHE:CD1	1:A:3692:LEU:HD23	2.57	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	2841/4646 (61%)	2765 (97%)	72 (2%)	4 (0%)	48 77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	SER
1	A	4251	ILE
1	A	1730	ALA
1	A	2871	ILE

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	2540/4125 (62%)	2533 (100%)	7 (0%)	91 97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2349	LYS
1	A	2637	HIS
1	A	2875	ASN
1	A	2998	ASN
1	A	3608	LYS
1	A	3741	ARG
1	A	3937	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1541	GLN
1	A	1867	ASN
1	A	2677	GLN
1	A	3155	HIS
1	A	3631	ASN
1	A	3952	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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	ATP	A	4702	-	28,33,33	0.65	0	34,52,52	0.59	1 (2%)
2	ADP	A	4704	-	24,29,29	0.87	0	29,45,45	1.24	2 (6%)
3	ATP	A	4703	-	28,33,33	0.67	0	34,52,52	0.60	1 (2%)
2	ADP	A	4701	-	24,29,29	0.88	0	29,45,45	1.24	2 (6%)

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	ATP	A	4702	-	-	7/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	3/12/32/32	0/3/3/3
3	ATP	A	4703	-	-	5/18/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4701	ADP	N3-C2-N1	-3.68	123.68	128.67
2	A	4704	ADP	N3-C2-N1	-3.58	123.81	128.67
2	A	4704	ADP	C4-C5-N7	-2.63	106.56	109.34
2	A	4701	ADP	C4-C5-N7	-2.55	106.64	109.34
3	A	4702	ATP	C5-C6-N6	2.31	123.83	120.31
3	A	4703	ATP	C5-C6-N6	2.30	123.81	120.31

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	O4'-C4'-C5'-O5'
2	A	4704	ADP	C3'-C4'-C5'-O5'
3	A	4702	ATP	PB-O3B-PG-O2G
3	A	4702	ATP	C5'-O5'-PA-O2A
3	A	4702	ATP	C5'-O5'-PA-O3A
3	A	4703	ATP	C5'-O5'-PA-O1A
3	A	4703	ATP	C5'-O5'-PA-O2A
3	A	4703	ATP	C5'-O5'-PA-O3A
3	A	4703	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	PB-O3B-PG-O1G
3	A	4703	ATP	C3'-C4'-C5'-O5'
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	PA-O3A-PB-O2B
3	A	4702	ATP	PB-O3A-PA-O2A

There are no ring outliers.

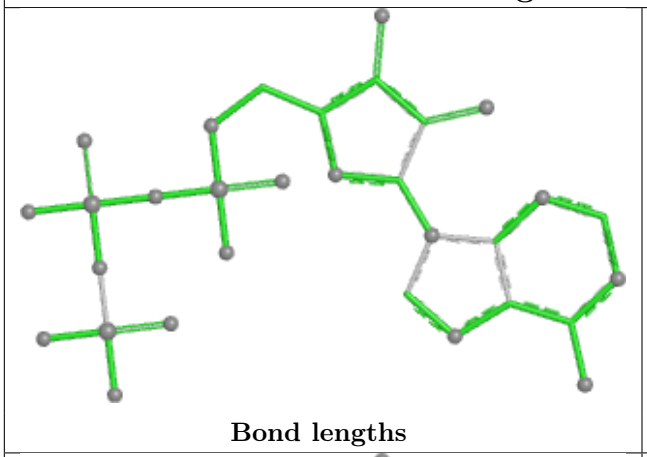
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4704	ADP	1	0
2	A	4701	ADP	1	0

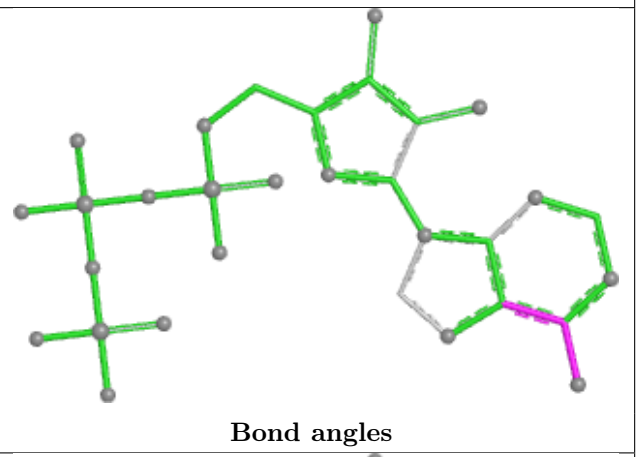
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

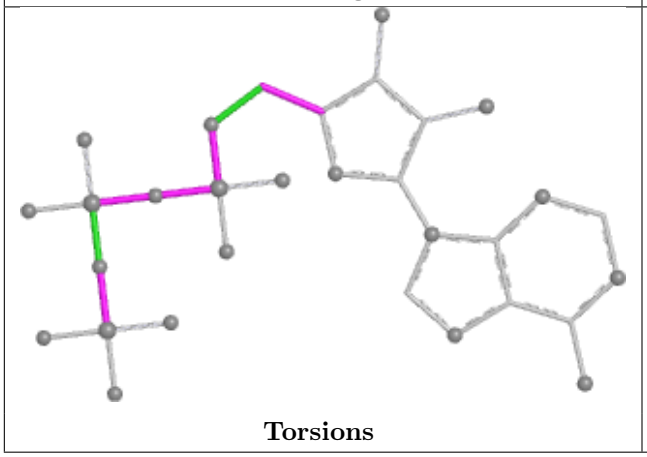
Ligand ATP A 4702



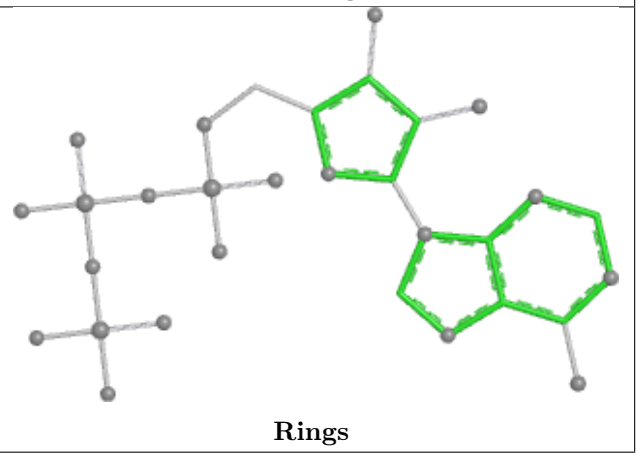
Bond lengths



Bond angles

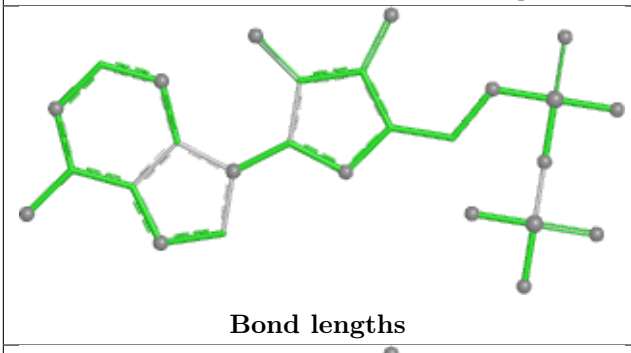


Torsions

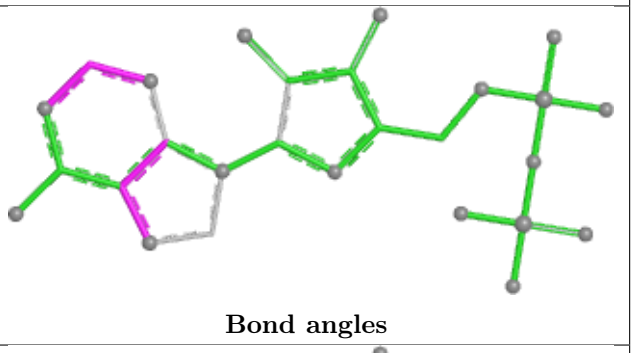


Rings

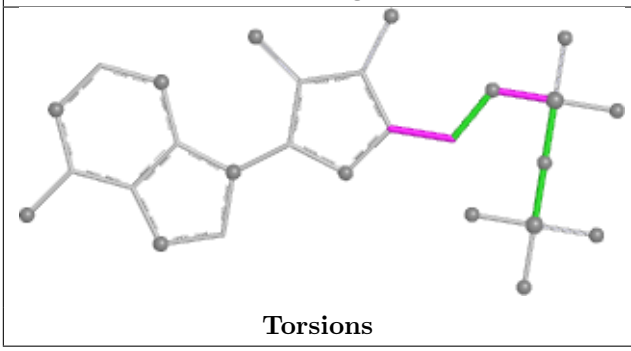
Ligand ADP A 4704



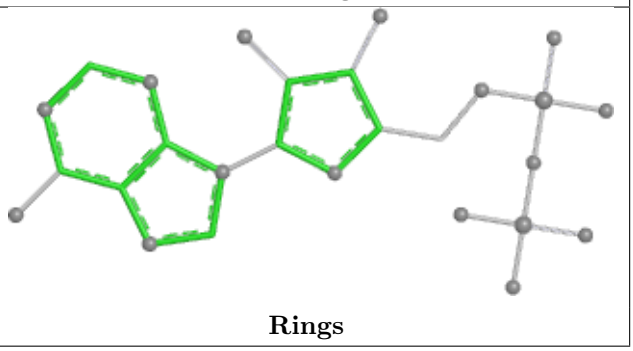
Bond lengths



Bond angles

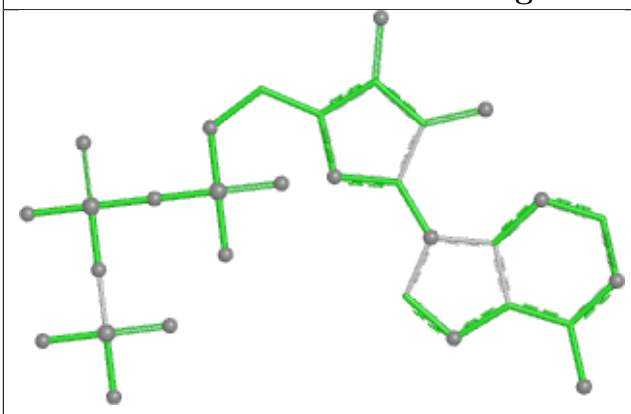


Torsions

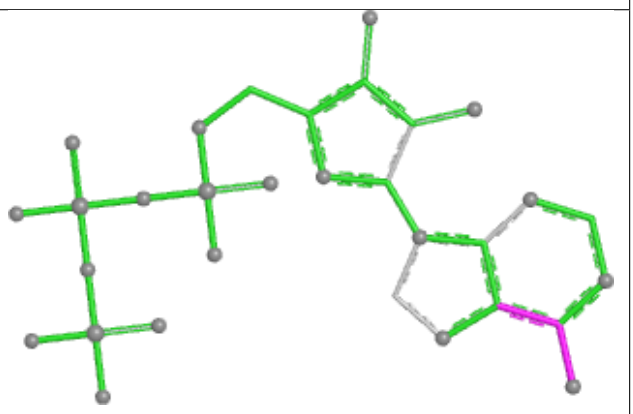


Rings

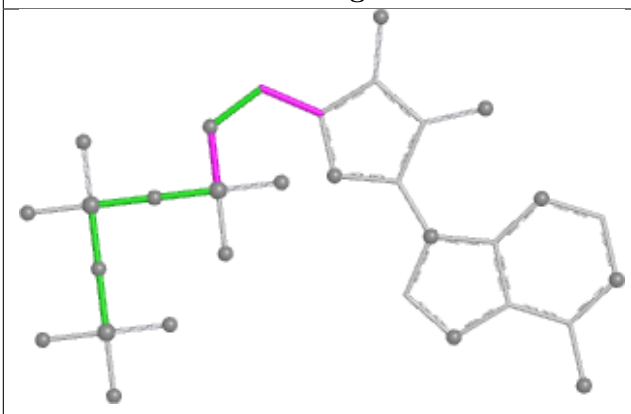
Ligand ATP A 4703



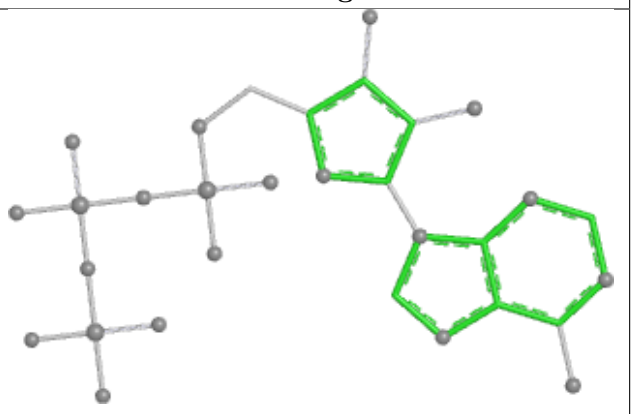
Bond lengths



Bond angles

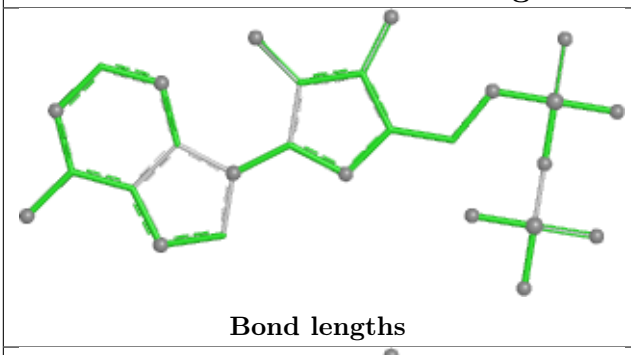


Torsions

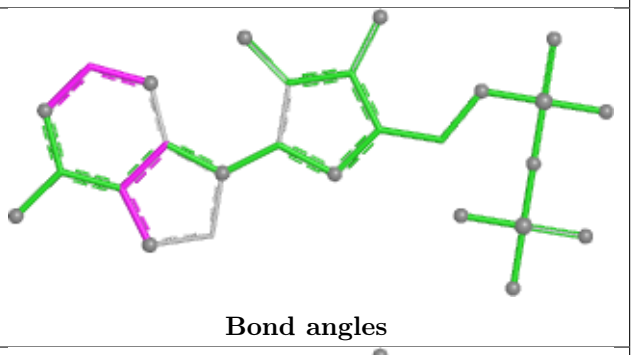


Rings

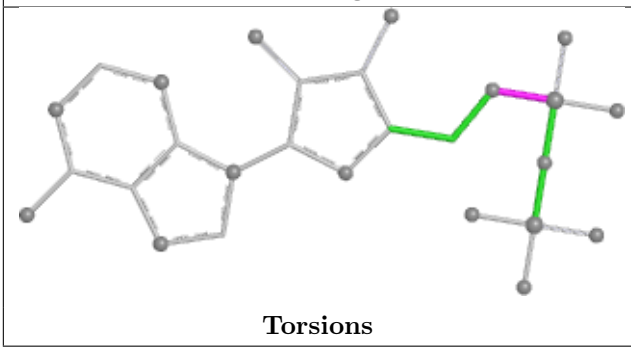
Ligand ADP A 4701



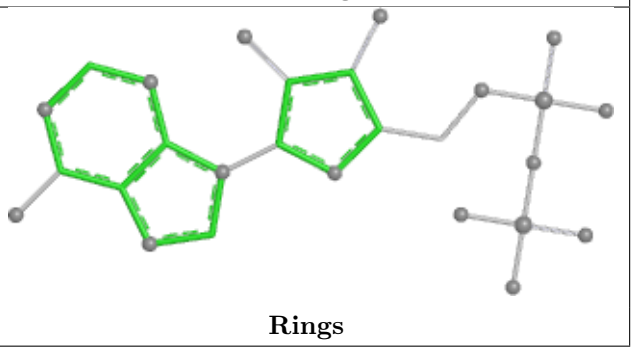
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

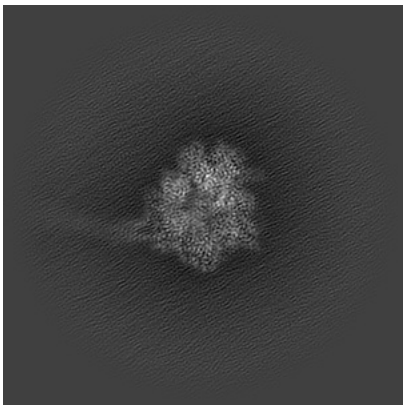
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44721. These allow visual inspection of the internal detail of the map and identification of artifacts.

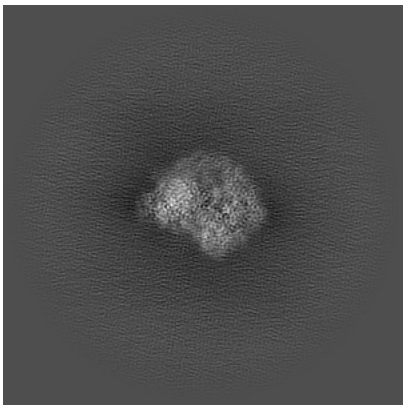
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

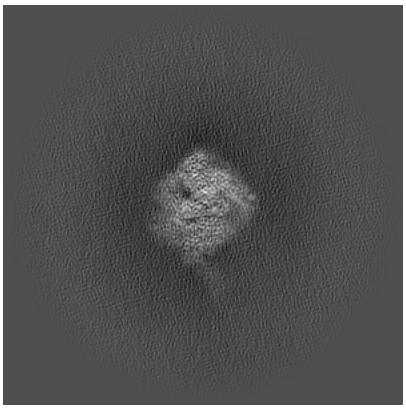
6.1.1 Primary map



X

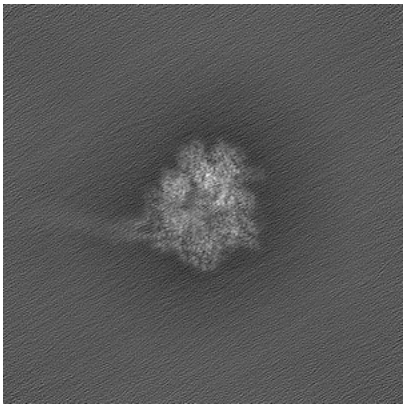


Y

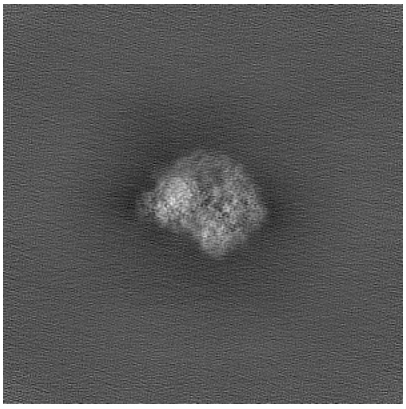


Z

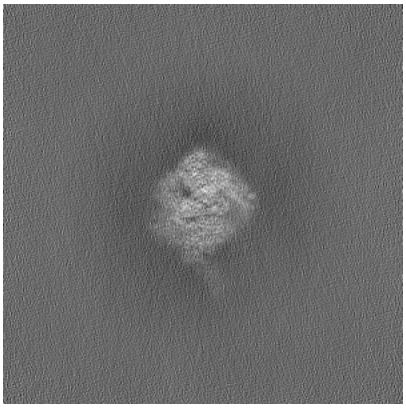
6.1.2 Raw map



X



Y

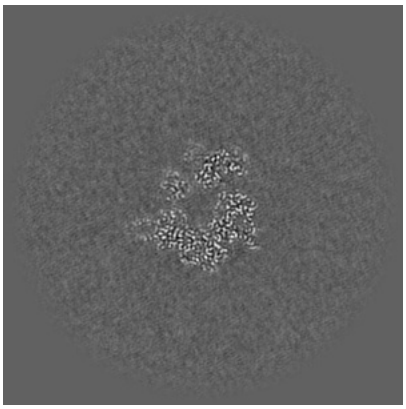


Z

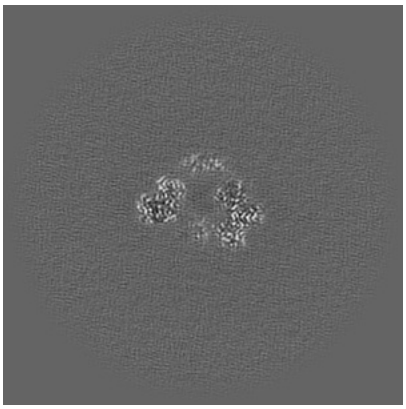
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

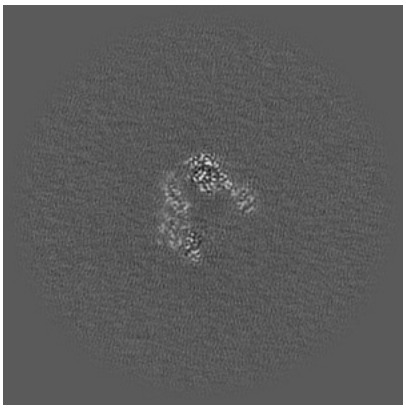
6.2.1 Primary map



X Index: 180

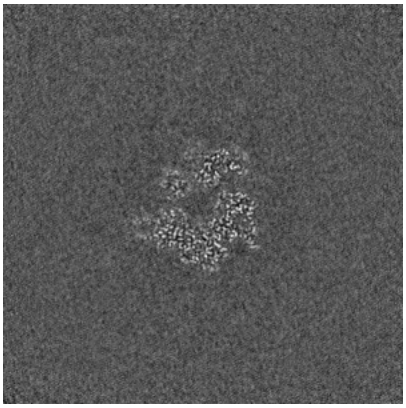


Y Index: 180

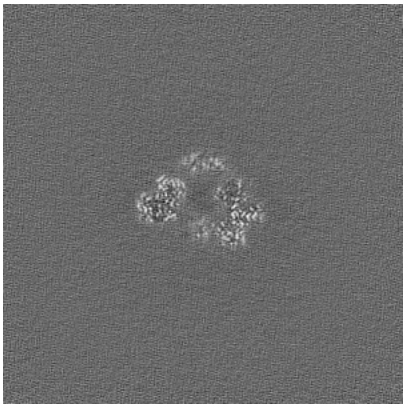


Z Index: 180

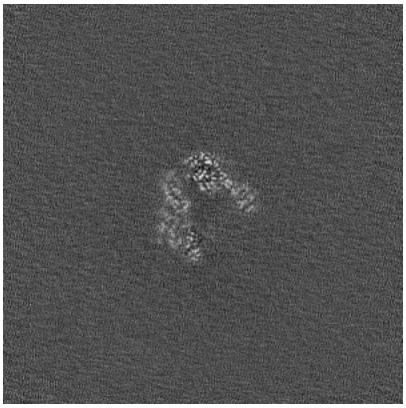
6.2.2 Raw map



X Index: 180



Y Index: 180

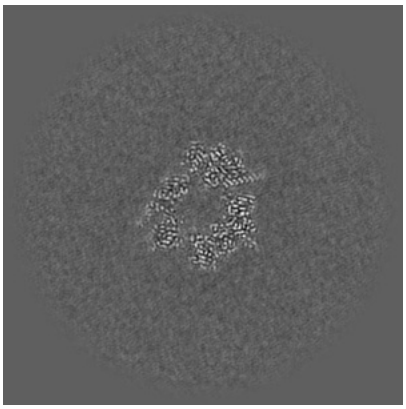


Z Index: 180

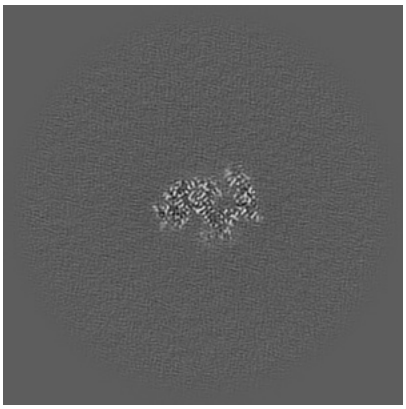
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

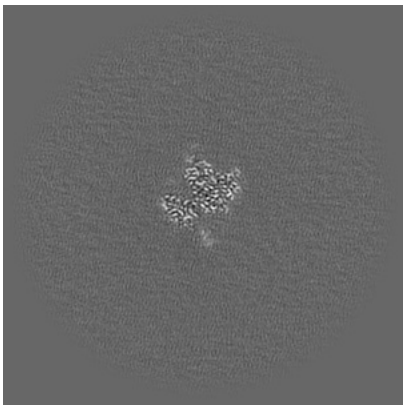
6.3.1 Primary map



X Index: 175

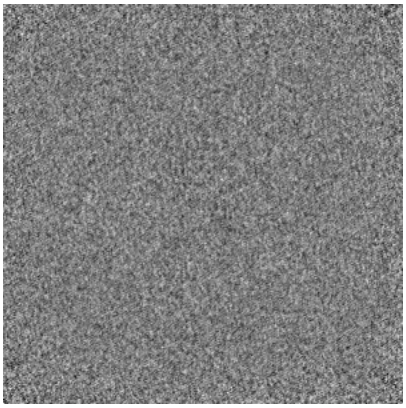


Y Index: 203

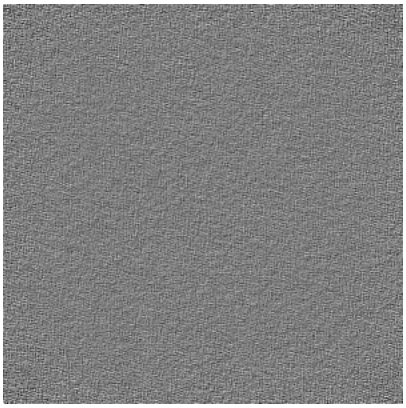


Z Index: 209

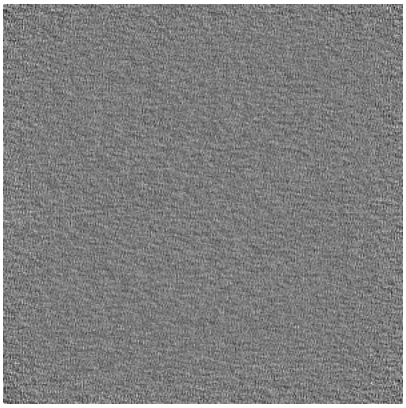
6.3.2 Raw map



X Index: 0



Y Index: 0

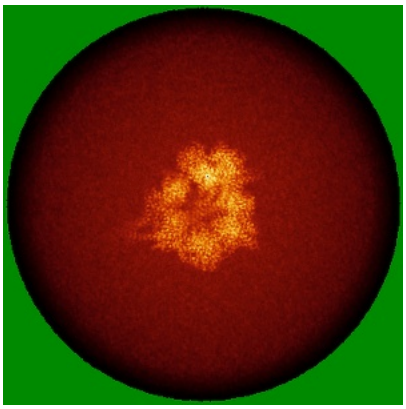


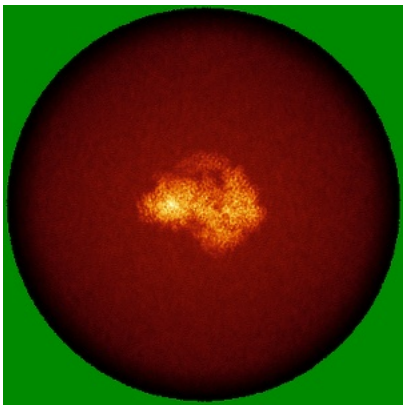
Z Index: 0

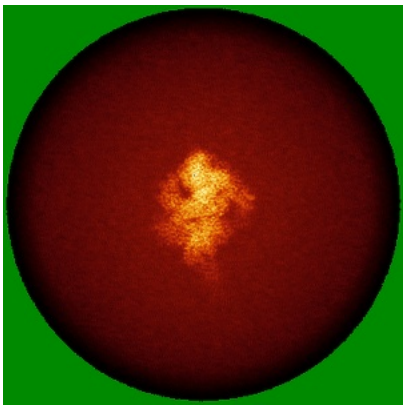
The images above show the largest variance slices of the map in three orthogonal directions.

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

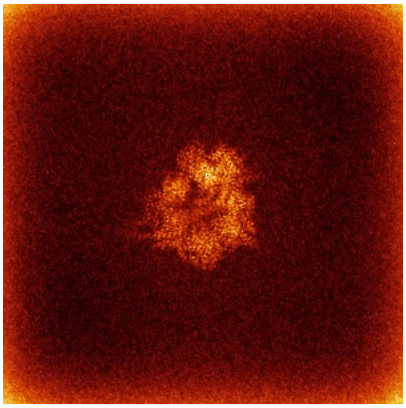
6.4.1 Primary map

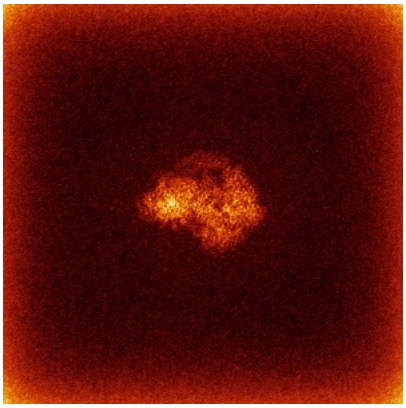

X

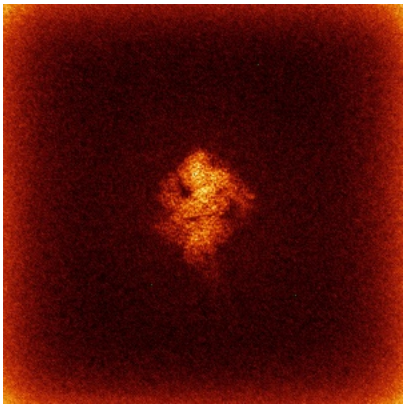

Y


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.

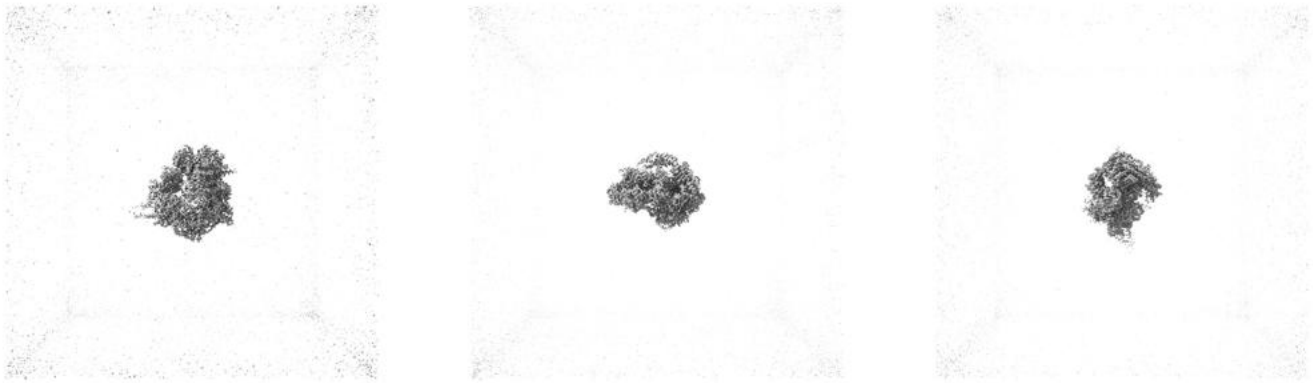
6.5 Orthogonal surface views (i)

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.

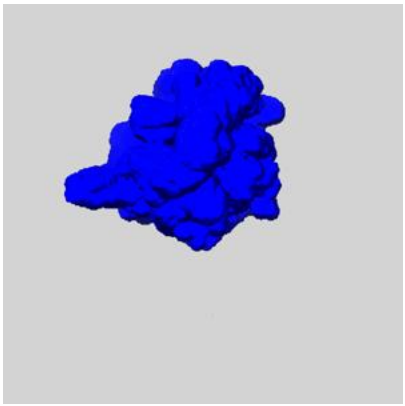
6.6 Mask visualisation (i)

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

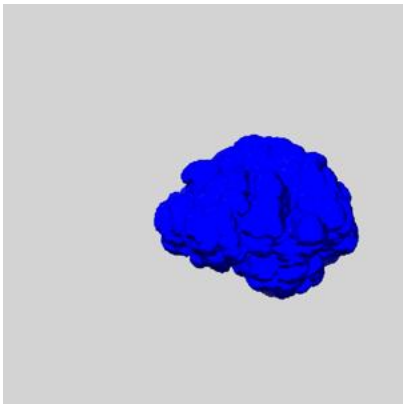
A mask typically either:

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

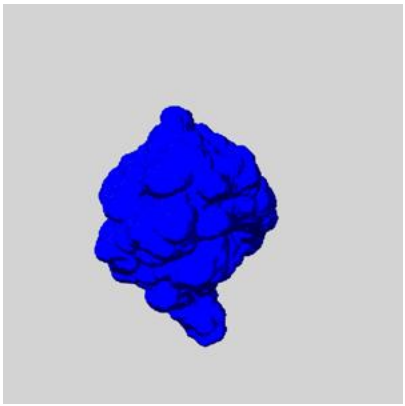
6.6.1 emd_44721_msk_1.map (i)



X



Y

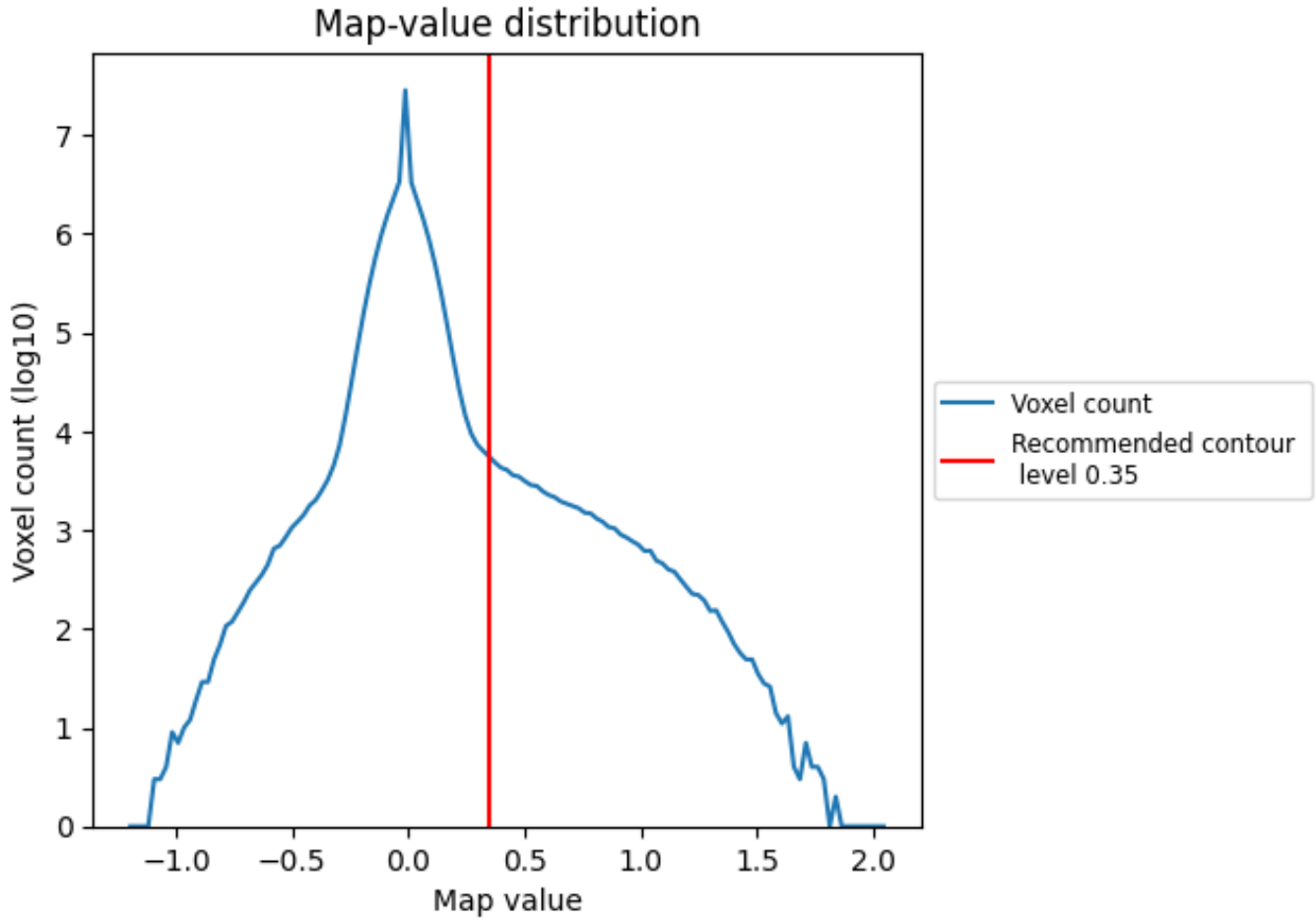


Z

7 Map analysis

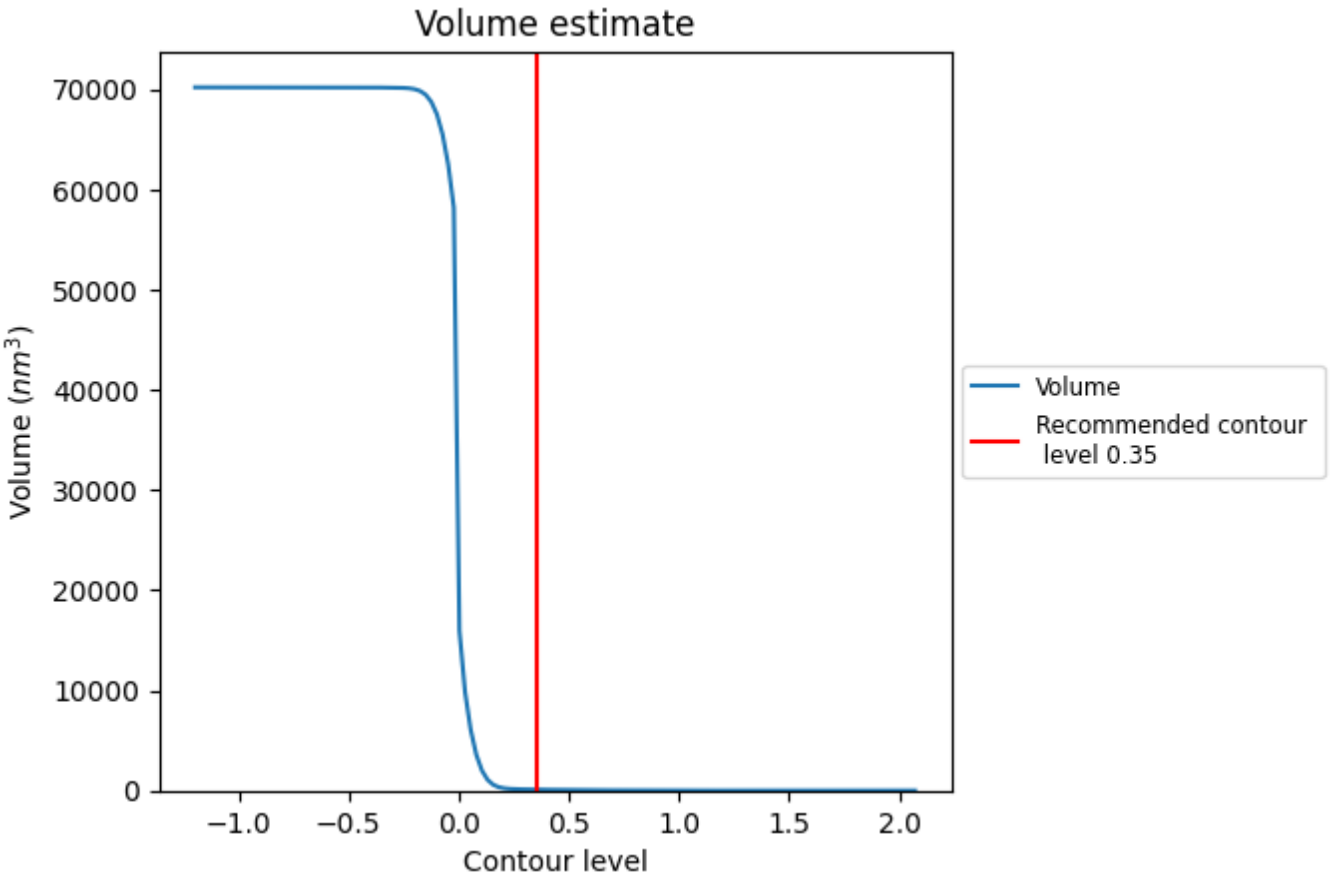
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

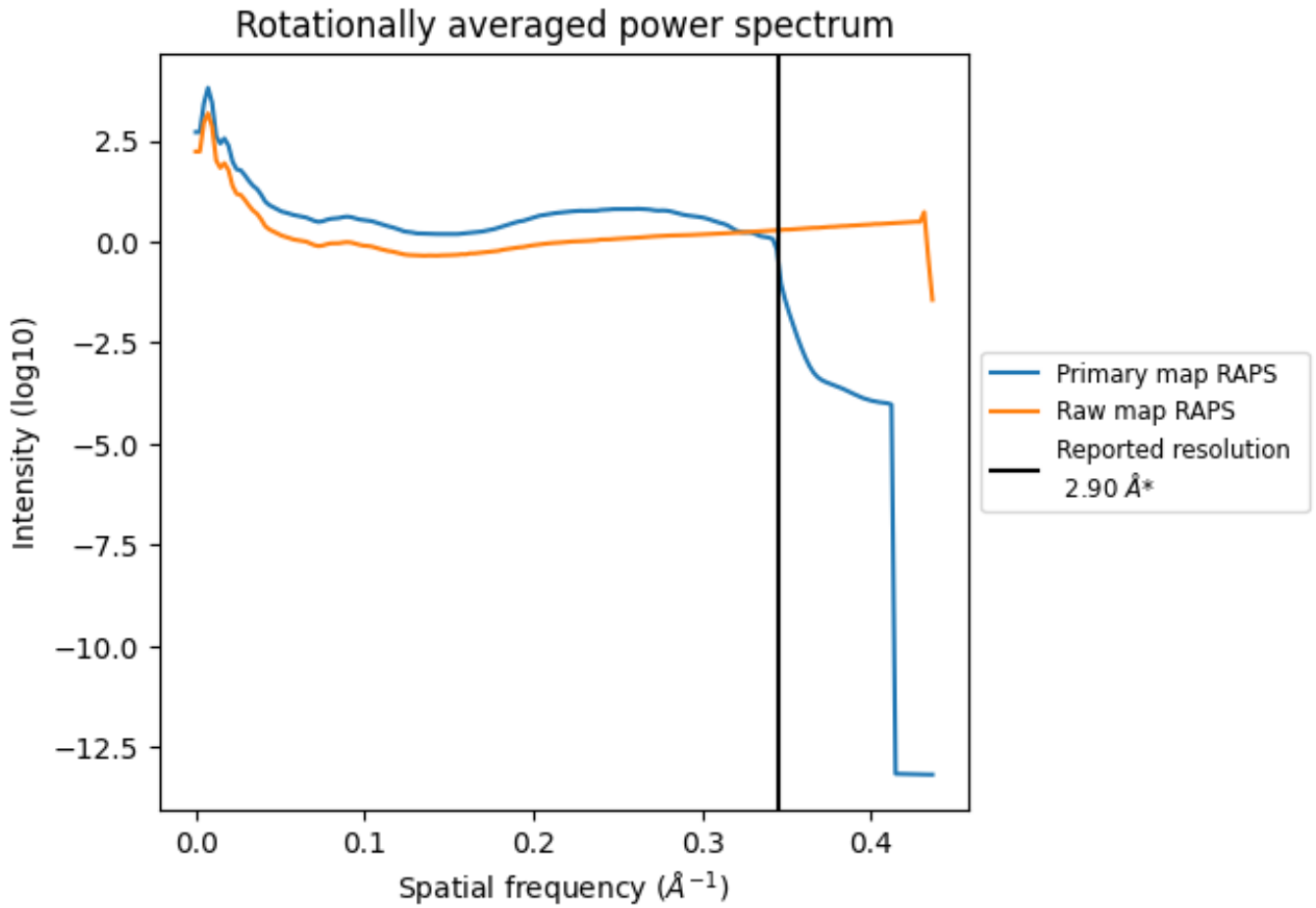
7.2 Volume estimate



The volume at the recommended contour level is 96 nm^3; this corresponds to an approximate mass of 87 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)

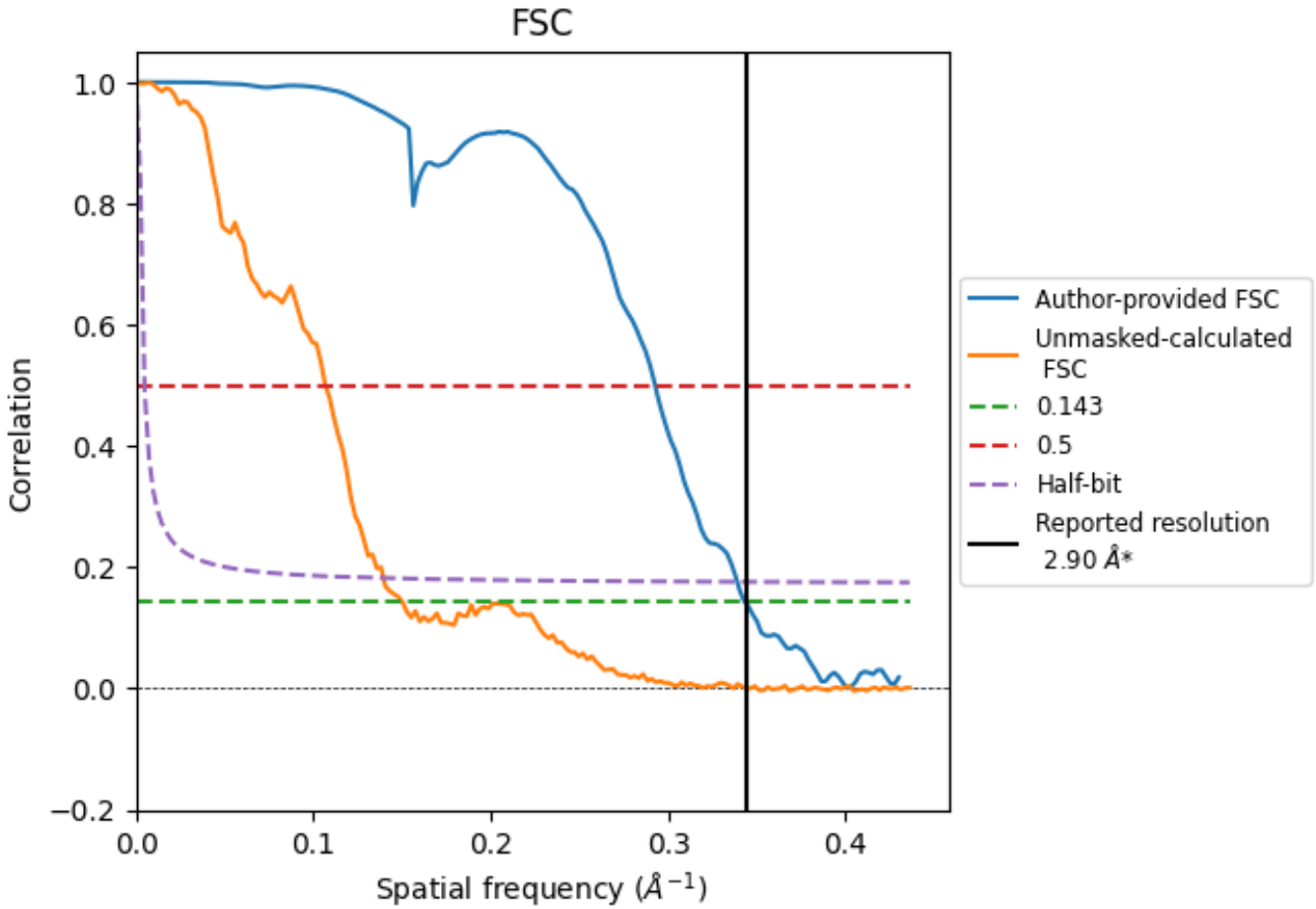


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

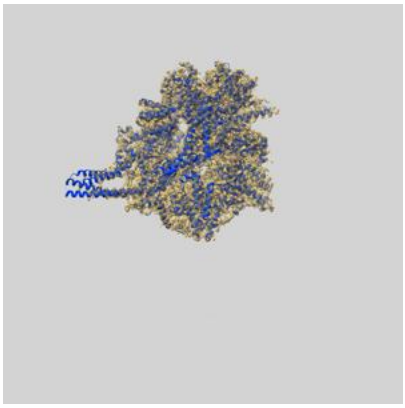
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.91	3.42	2.95
Unmasked-calculated*	6.66	9.37	7.16

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

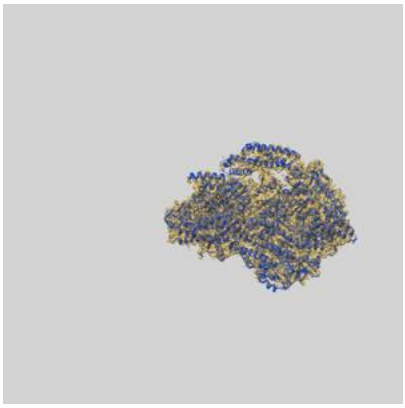
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44721 and PDB model 9BN4. Per-residue inclusion information can be found in section 3 on page 5.

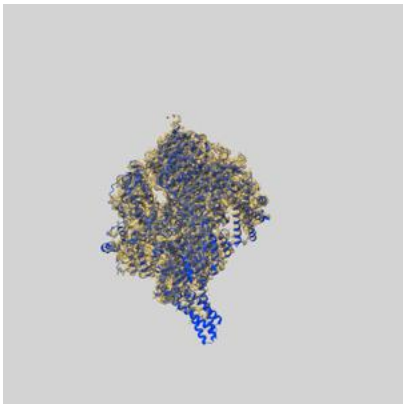
9.1 Map-model overlay



X



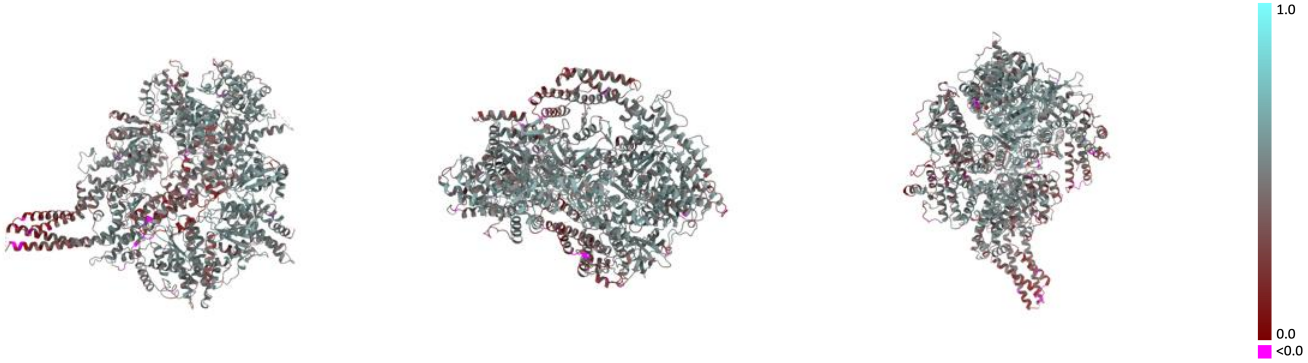
Y



Z

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

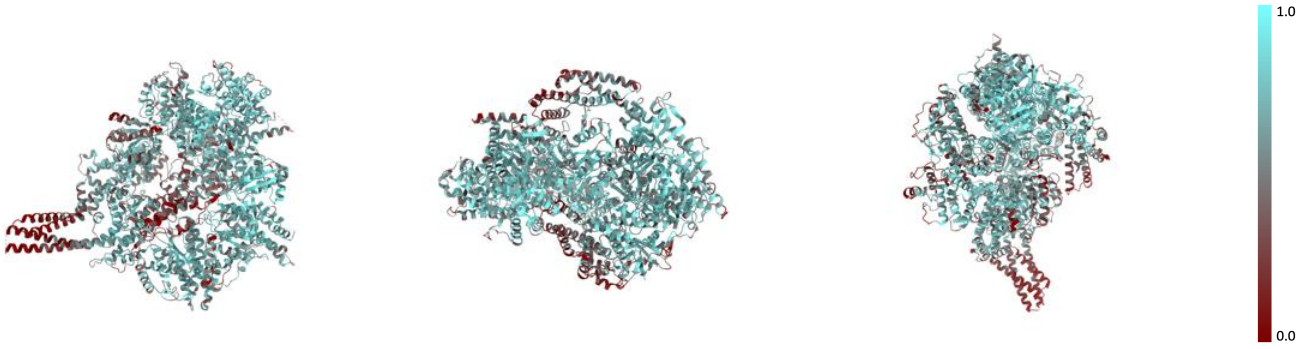
9.2 Q-score mapped to coordinate model (i)



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.

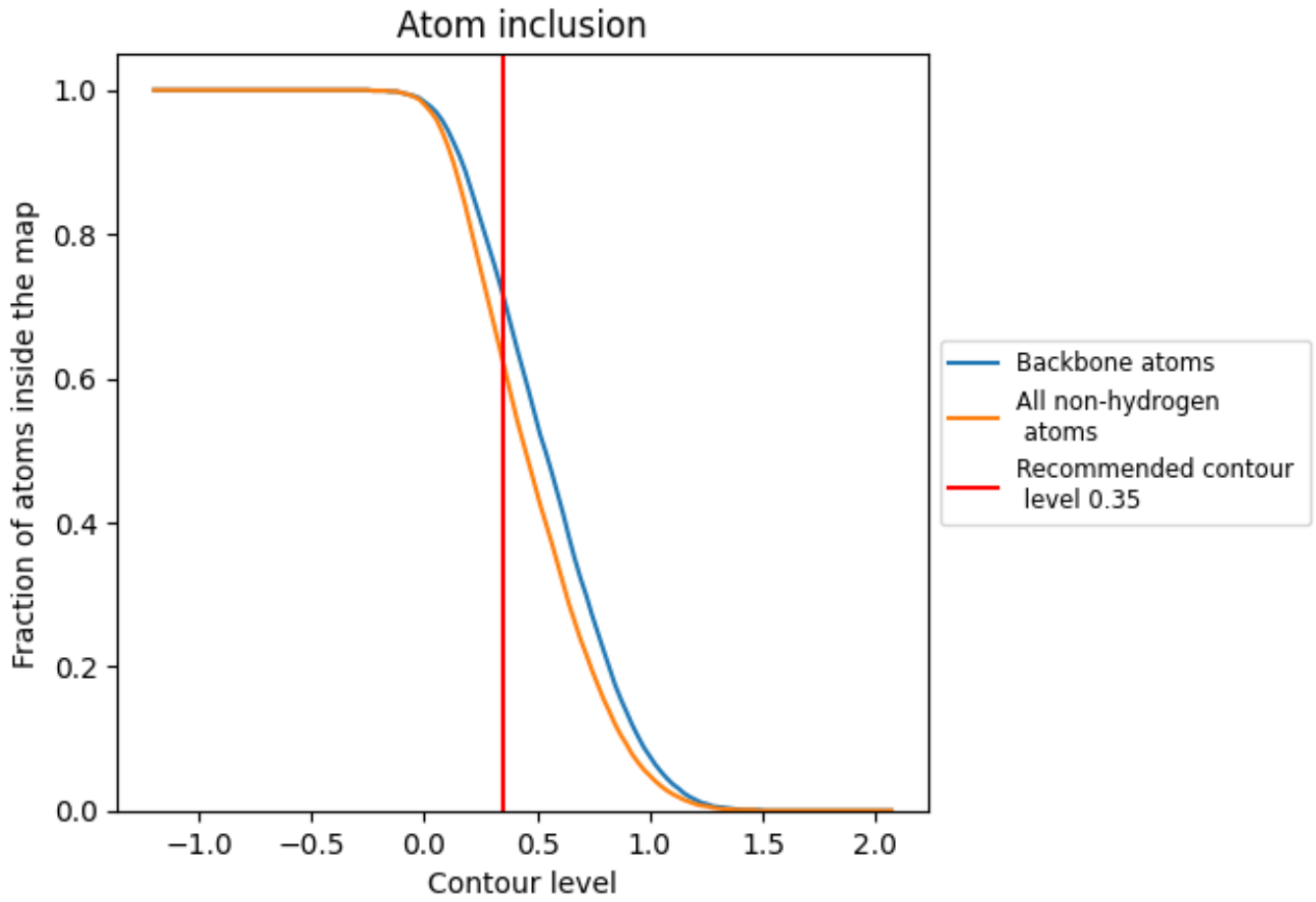
9.3 Atom inclusion mapped to coordinate model (i)



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, 72% of all backbone atoms, 62% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6220	0.4680
A	0.6220	0.4680