Full wwPDB EM Validation Report

May 25, 2025 – 09:24 PM EDT

PDB ID	:	9BMV / pdb_00009bmv
EMDB ID	:	EMD-44712
Title	:	State-7a-post1 of motor domain from full-length human dynein-1 in 5 mM ADP
Authors	:	Chai, P.; Zhang, K.
Deposited on	:	2024-05-02
Resolution	:	3.70 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:

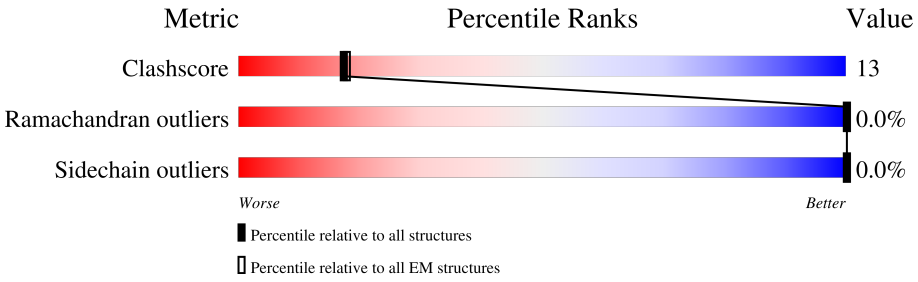
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4646	9% 45% 20% 35%

2 Entry composition

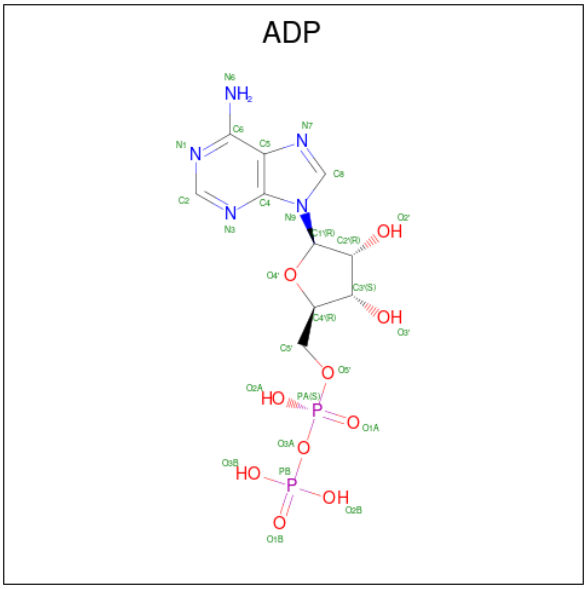
There are 4 unique types of molecules in this entry. The entry contains 24616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

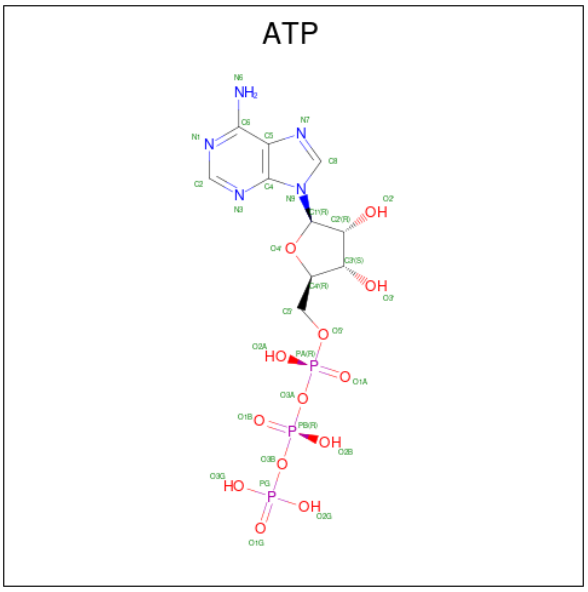
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3043	24503	15606	4234	4541	122	0	0

- 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
			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	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

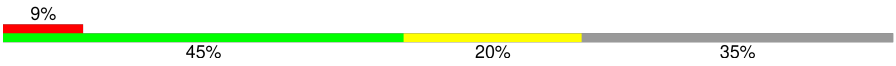
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

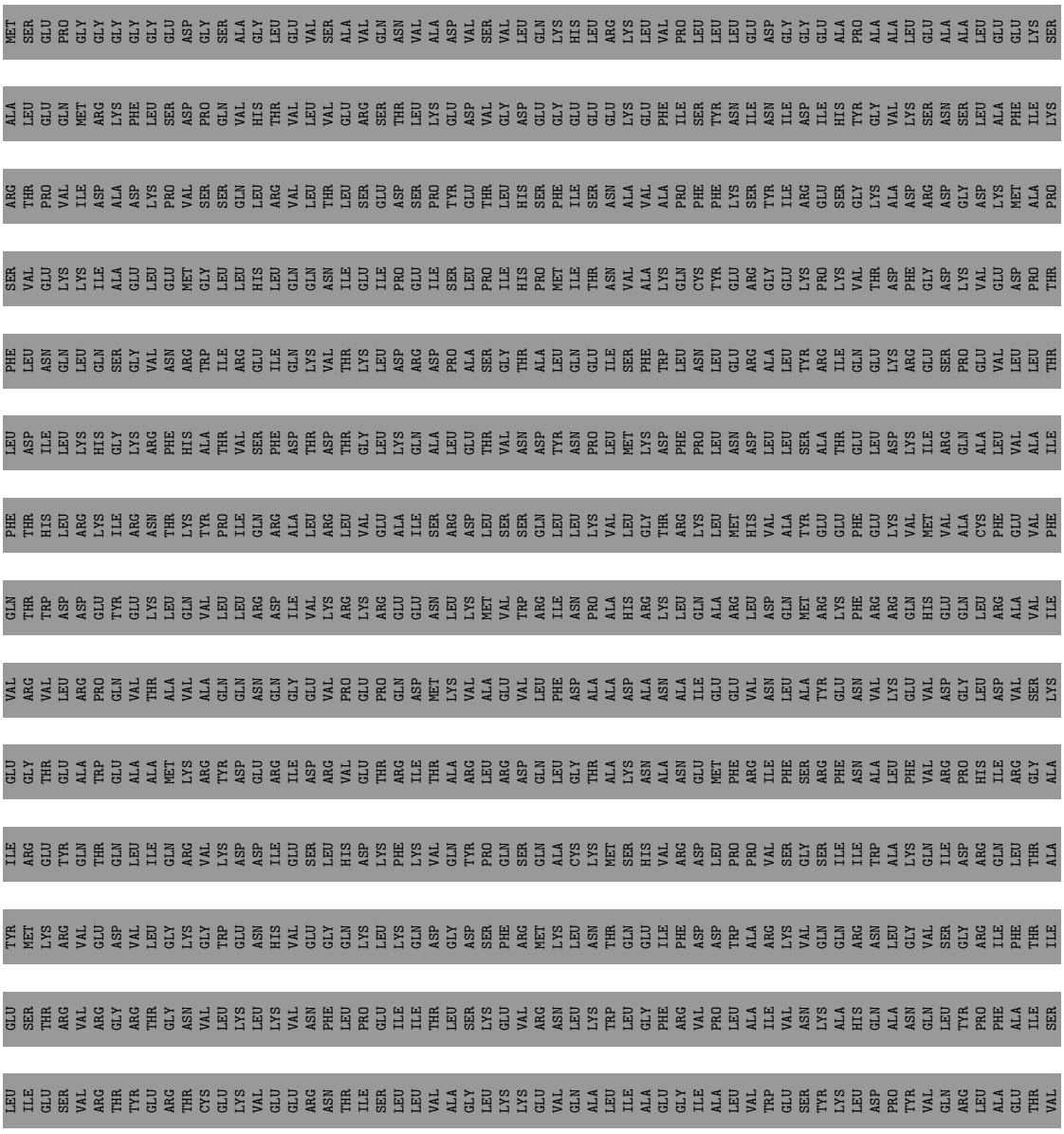
3 Residue-property plots (i)

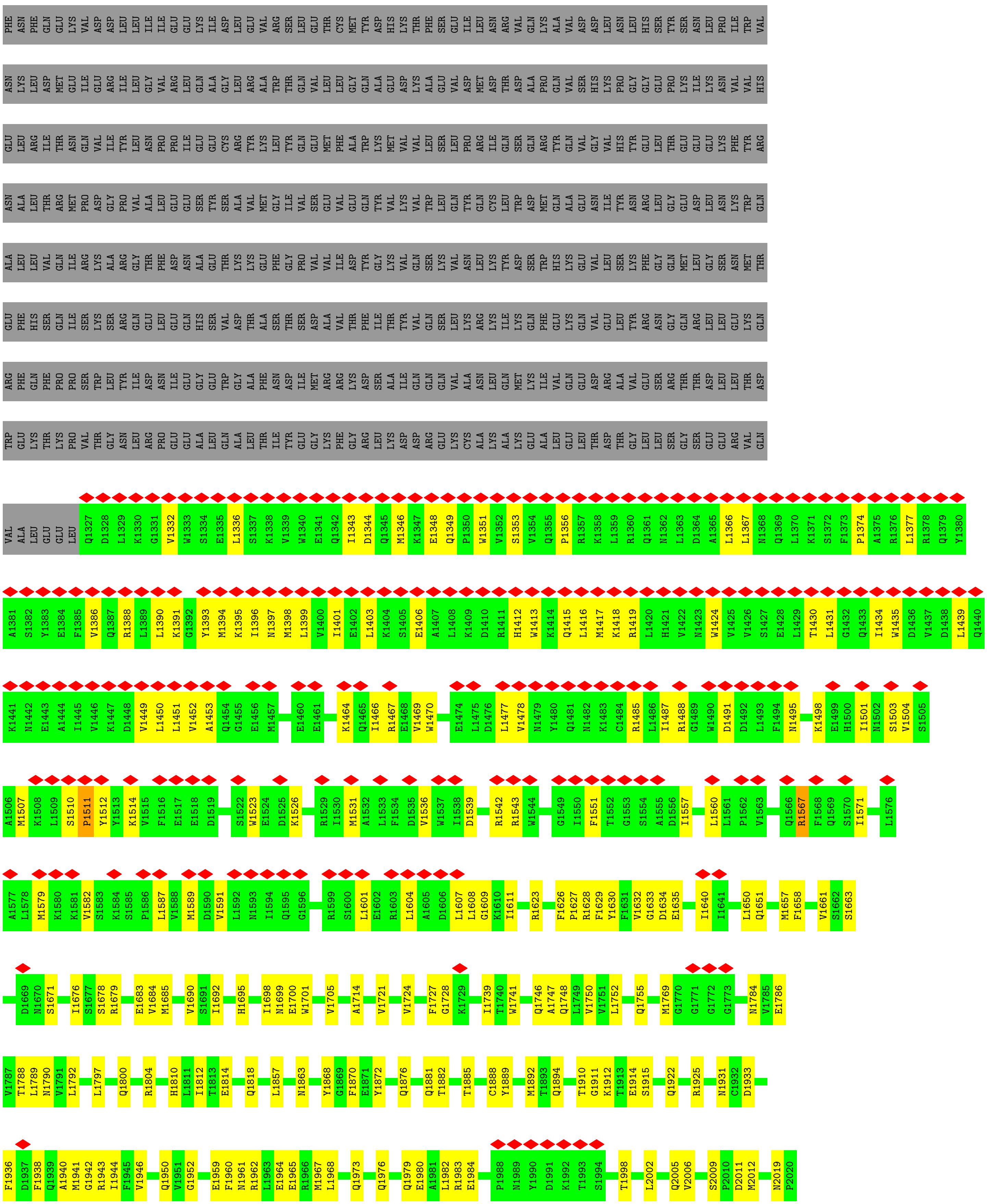
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

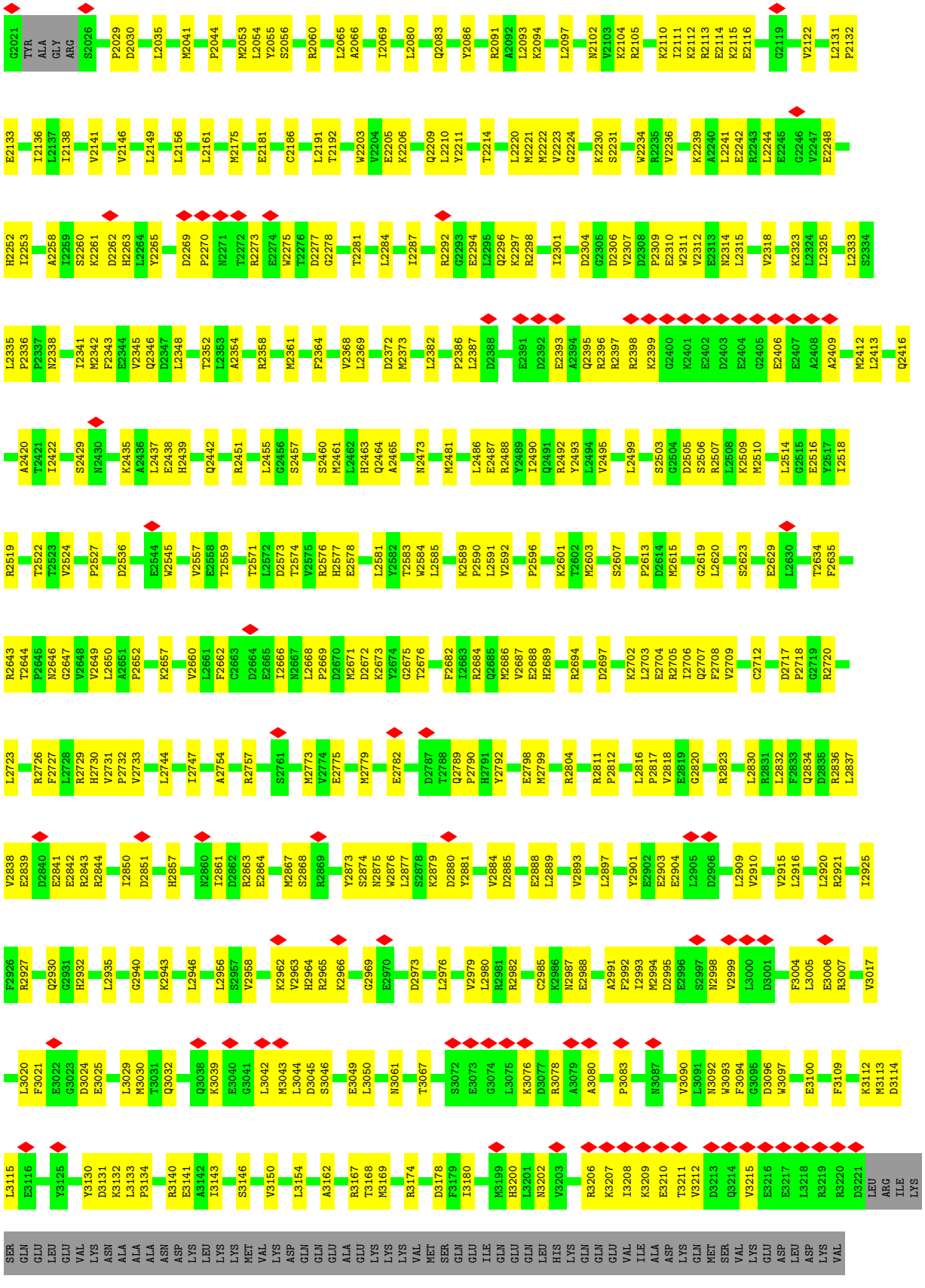
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

Chain A:






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 SER GLY SER GLU GLU ARG VAL GLN
VAL ALA LEU GLU GLU LEU Q1327 D1328 L1329 K1330 G1331 V1332 W1333 S1334 E1335 L1336 S1337 K1338 V1339 W1340 E1341 Q1342 I1343 D1344 Q1345 M1346 K1347 E1348 Q1349 P1350 W1351 V1352 S1353 V1354 Q1355 P1356 R1357 K1358 L1359 R1360 Q1361 N1362 L1363 D1364 A1365 L1366 L1367 N1368 Q1369 L1370 K1371 S1372 F1373 P1374 A1375 R1376 L1377 R1378 Q1379 Y1380
A1381 S1382 Y1383 E1384 F1385 V1386 Q1387 R1388 L1389 L1390 K1391 G1392 Y1393 M1394 K1395 I1396 N1397 M1398 L1399 V1400 I1401 E1402 L1403 K1404 S1405 E1406 A1407 L1408 K1409 D1410 R1411 H1412 W1413 K1414 Q1415 L1416 M1417 K1418 R1419 L1420 H1421 V1422 N1423 W1424 V1425 V1426 S1427 E1428 L1429 T1430 L1431 G1432 Q1433 I1434 W1435 D1436 V1437 D1438 L1439 Q1440
K1441 N1442 E1443 A1444 I1445 V1446 K1447 D1448 V1449 L1450 L1451 V1452 A1453 Q1454 G1455 E1456 M1457 E1460 E1461 K1464 Q1465 I1466 R1467 E1468 V1469 W1470 E1474 L1475 D1476 L1477 V1478 N1479 Y1480 Q1481 N1482 K1483 C1484 R1485 L1486 I1487 R1488 G1489 W1490 D1491 D1492 L1493 F1494 N1495 K1498 E1499 H1500 I1501 N1502 S1503 V1504 S1505
A1506 M1507 K1508 L1509 S1510 P1511 Y1512 Y1513 K1514 V1515 F1516 E1517 E1518 D1519 S1522 W1523 E1524 D1525 K1526 R1529 I1530 M1531 A1532 L1533 F1534 D1535 V1536 W1537 I1538 D1539 R1542 R1543 W1544 G1549 I1550 F1551 T1552 G1553 S1554 A1555 D1556 I1557 L1560 L1561 P1562 V1563 Q1566 R1567 F1568 Q1569 S1570 I1571 L1576
A1577 L1578 M1579 K1580 K1581 V1582 S1583 K1584 S1585 P1586 L1587 V1588 M1589 D1590 V1591 L1592 N1593 I1594 Q1595 G1596 R1599 S1600 L1601 E1602 R1603 L1604 A1605 D1606 L1607 L1608 G1609 K1610 I1611 R1623 F1626 P1627 R1628 F1629 Y1630 F1631 V1632 G1633 D1634 E1635 I1640 I1641 L1650 Q1651 M1657 F1658 V1661 S1662 S1663
D1669 N1670 S1671 I1676 S1677 S1678 R1679 E1683 V1684 M1685 V1690 S1691 I1692 H1695 I1698 N1699 E1700 W1701 V1705 A1714 V1721 V1724 F1727 G1728 K1729 I1739 T1740 W1741 Q1746 A1747 Q1748 L1749 V1750 V1751 L1752 Q1755 M1769 G1770 G1771 G1772 G1773 N1784 V1785 E1786
V1787 T1788 L1789 N1790 V1791 L1792 L1797 Q1800 R1804 H1810 L1811 I1812 T1813 E1814 Q1818 L1857 N1863 Y1868 G1869 F1870 E1871 Y1872 Q1876 Q1881 T1882 T1885 C1888 Y1889 M1892 T1893 Q1894 T1910 G1911 K1912 T1913 E1914 S1915 Q1922 R1925 N1931 C1932 D1933
F1936 D1937 F1938 Q1939 A1940 M1941 G1942 R1943 I1944 F1945 V1946 Q1950 V1951 G1952 E1959 F1960 N1961 R1962 L1963 E1964 E1965 R1966 M1967 L1968 Q1973 Q1976 Q1979 E1980 A1981 L1982 R1983 E1984 P1988 N1989 Y1990 D1991 K1992 T1993 S1994 T1998 L2002 Q2005 V2006 S2009 P2010 D2011 M2012 N2019 P2020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E2133 I2136 L2137 I2138 V2141 V2146 L2149 L2156 L2161 M2175 E2181 C2186 L2191 T2192 W2203 V2204 E2205 K2206 Q2209 L2210 Y2211 T2214 L2220 M2221 M2222 V2223 G2224 K2230 S2231 W2234 R2235 V2236 K2239 A2240 L2241 E2242 R2243 L2244 E2245 G2246 V2247 E2248
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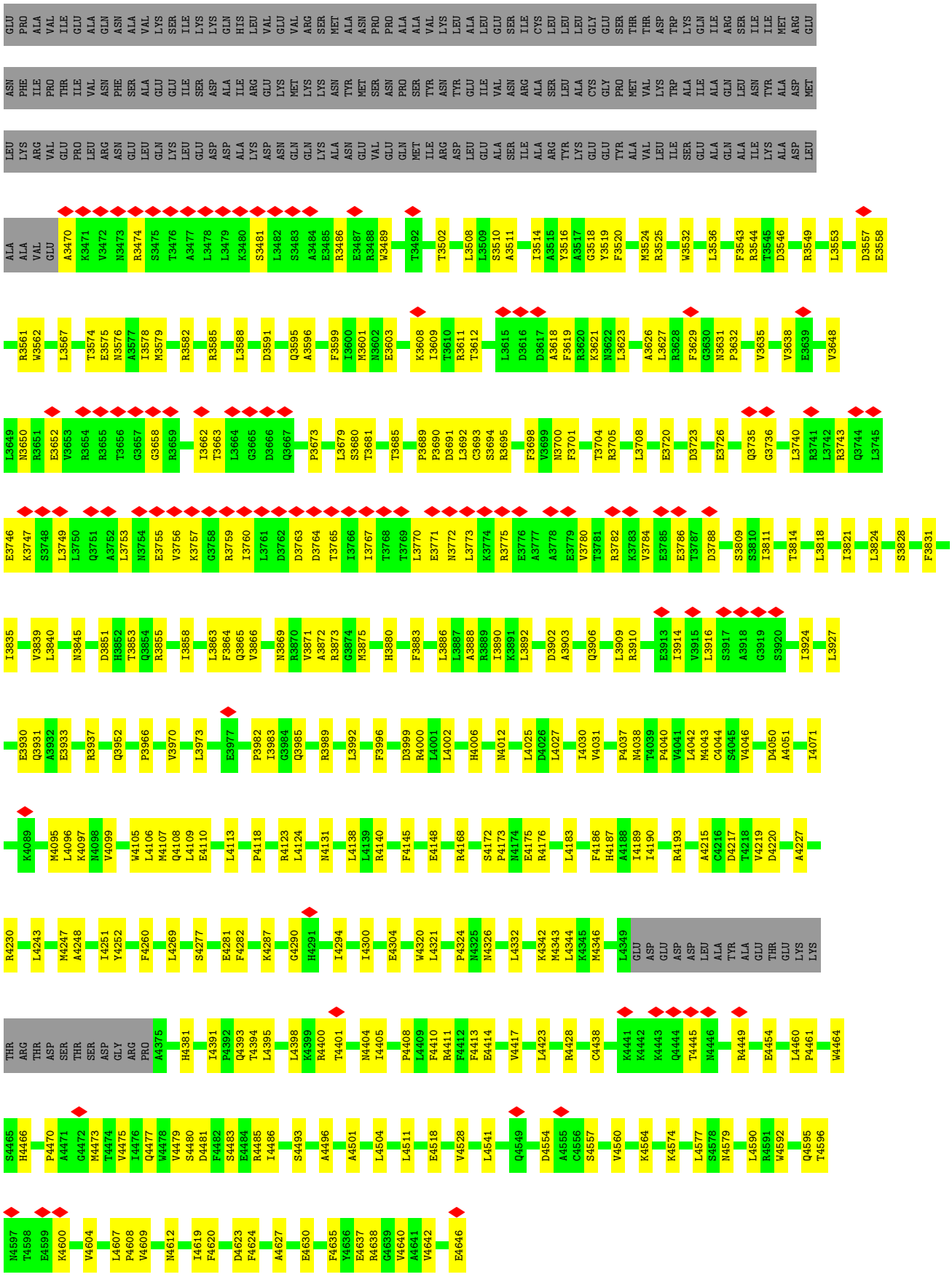
L3020 F3021 E3022 G3023 D3024 E3025 L3029 M3030 T3031 Q3032 Q3038 K3039 E3040 G3041 L3042 M3043 L3044 D3045 S3046 E3049 L3050 N3061 T3067 S3072 E3073 G3074 L3075 K3076 D3077 R3078 A3079 A3080 P3083 N3087 V3090 L3091 N3092 W3093 F3094 G3095 D3096 W3097 E3100 F3109 K3112 M3113 D3114
L3115 E3116 Y3125 Y3130 D3131 K3132 L3133 P3134 R3140 E3141 A3142 I3143 S3146 V3150 L3154 A3162 R3167 T3168 M3169 R3174 D3178 F3179 I3180 M3199 H3200 L3201 N3202 V3203 R3206 K3207 I3208 K3209 E3210 T3211 V3212 D3213 Q3214 V3215 E3216 E3217 L3218 R3219 R3220 D3221 LEU ARG ILE LYS
SER GLN GLU LEU GLU VAL LYS ASN 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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ASN PHE ILE PRO THR ILE VAL ASN PHE SER ALA GLU GLU ILE SER ASP ALA ILE ARG GLU LYS ASP ASN GLN LYS ASN TYR MET SER ASN PRO SER TYR ASN TYR GLU ILE VAL ASN ARG ALA SER LEU ALA CYS GLY PRO MET VAL LYS TRP ALA ILE ALA GLN LEU ASN TYR ALA ASP MET
LEU LYS ARG VAL GLU PRO LEU ARG ASN GLU LEU GLN LYS LEU GLU ASP ASP ALA LYS ASP ASN GLN LYS ALA ASN GLU VAL GLU GLN GLN MET ILE ARG ASP LEU GLU ALA ASN SER ILE ALA ARG TYR LYS GLU GLU TYR ALA VAL LEU ILE SER GLU ALA GLN ALA ALA ILE LYS ALA ALA ASP LEU
ALA ALA VAL GLU A3470 K3471 V3472 N3473 R3474 S3475 T3476 A3477 L3478 L3479 K3480 S3481 L3482 S3483 A3484 E3485 R3486 E3487 R3488 W3489 T3492 T3502 L3508 L3509 S3510 A3511 T3514 A3515 Y3516 A3517 G3518 Y3519 F3520 M3524 R3525 W3532 L3536 F3543 R3544 T3545 D3546 R3549 L3553 D3557 E3558
R3561 W3562 L3567 T3574 E3575 N3576 A3577 I3578 M3579 R3582 R3585 L3588 D3591 Q3595 A3596 F3599 I3600 M3601 N3602 E3603 K3608 I3609 T3610 R3611 T3612 L3615 D3616 D3617 A3618 F3619 R3620 K3621 N3622 L3623 A3626 L3627 R3628 F3629 G3630 N3631 P3632 V3635 V3638 E3639 V3648
L3649 N3650 R3651 E3652 V3653 R3654 R3655 T3656 G3657 G3658 R3659 I3662 T3663 L3664 G3665 D3666 Q3667 P3673 L3679 S3680 T3681 T3685 P3689 P3690 D3691 L3692 C3693 S3694 R3695 F3698 V3699 N3700 F3701 T3704 R3705 L3708 E3720 D3723 E3726 Q3735 G3736 L3740 R3741 L3742 R3743 Q3744 L3745
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I3835 V3839 L3840 N3845 D3851 H3852 T3853 Q3854 R3855 I3858 L3863 F3864 Q3865 V3866 N3869 R3870 V3871 A3872 R3873 G3874 M3875 H3880 F3883 L3886 L3887 A3888 R3889 I3890 K3891 L3892 D3902 A3903 Q3906 L3909 R3910 E3913 I3914 V3915 L3916 S3917 A3918 G3919 S3920 I3924 L3927
E3930 Q3931 A3932 E3933 R3937 Q3952 P3966 V3970 L3973 E3977 P3982 I3983 G3984 Q3985 R3989 L3992 F3996 D3999 R4000 L4001 L4002 H4006 N4012 L4025 D4026 L4027 I4030 V4031 P4037 N4038 T4039 P4040 V4041 L4042 M4043 C4044 S4045 V4046 D4050 A4051 I4071
K4089 M4095 L4096 K4097 N4098 V4099 W4105 L4106 M4107 Q4108 L4109 E4110 L4113 P4118 R4123 L4124 N4131 L4138 L4139 R4140 F4145 E4148 R4168 S4172 P4173 N4174 E4175 R4176 L4183 F4186 H4187 A4188 I4189 I4190 R4193 A4215 C4216 D4217 T4218 V4219 D4220 A4227
R4230 L4243 M4247 A4248 I4251 Y4252 F4260 L4269 S4277 E4281 F4282 K4287 G4290 H4291 I4294 I4300 E4304 W4320 L4321 P4324 N4325 N4326 L4332 K4342 M4343 L4344 K4345 M4346 L4349 GLU ASP GLU ASP LEU ALA TYR ALA GLU THR GLU LYS LYS
THR ARG THR ASP SER THR SER ASP GLY ARG PRO A4375 H4381 I4391 P4392 Q4393 T4394 L4395 L4398 K4399 R4400 T4401 N4404 I4405 P4408 L4409 F4410 R4411 F4412 F4413 E4414 V4417 L4423 R4428 C4438 K4441 K4442 K4443 Q4444 T4445 N4446 R4449 E4454 L4460 P4461 W4464
S4465 H4466 P4470 A4471 G4472 M4473 T4474 V4475 I4476 Q4477 W4478 V4479 S4480 D4481 F4482 S4483 E4484 R4485 I4486 S4493 A4496 A4501 L4504 L4511 E4518 V4528 L4541 Q4549 D4554 A4555 C4556 S4557 V4560 K4564 K4574 L4577 S4578 N4579 L4590 R4591 W4592 Q4595 T4596
N4597 T4598 E4599 K4600 V4604 L4607 P4608 V4609 N4612 I4619 F4620 D4623 F4624 A4627 E4630 F4635 Y4636 E4637 R4638 G4639 V4640 A4641 V4642 E4646

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47280	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.717	Depositor
Minimum map value	-0.337	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	329.984, 329.984, 329.984	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0312, 1.0312, 1.0312	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.16	0/25022	0.34	0/33900

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1567	ARG	Sidechain

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	24503	0	24574	659	0
2	A	81	0	36	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	3	0
4	A	1	0	0	0	0
All	All	24616	0	24622	659	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 13.

All (659) 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:4189:ILE:HD11	1:A:4321:LEU:HA	1.55	0.88
1:A:3818:LEU:HA	1:A:4346:MET:HE1	1.61	0.81
1:A:1551:PHE:HA	1:A:1557:ILE:HD11	1.63	0.80
1:A:3178:ASP:HB2	1:A:3585:ARG:HH21	1.48	0.78
1:A:1632:VAL:HB	1:A:1657:MET:HE1	1.66	0.78
1:A:4609:VAL:HG12	1:A:4642:VAL:HB	1.66	0.75
1:A:3502:THR:HG21	1:A:3544:ARG:HG3	1.67	0.74
1:A:2252:HIS:HB2	1:A:2301:ILE:HG22	1.70	0.73
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.72	0.72
1:A:4398:LEU:HB2	1:A:4414:GLU:HG3	1.70	0.72
1:A:2503:SER:HB3	1:A:2514:LEU:HD13	1.71	0.72
1:A:4193:ARG:NH2	1:A:4637:GLU:O	2.21	0.72
1:A:2851:ASP:HB3	1:A:2867:MET:HE1	1.72	0.70
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.72	0.70
1:A:2413:LEU:HA	1:A:2416:GLN:HE21	1.55	0.70
1:A:1912:LYS:HG2	1:A:2041:MET:HG3	1.75	0.69
1:A:2720:ARG:HH22	1:A:3083:PRO:HG3	1.57	0.69
1:A:2053:MET:HE3	1:A:2094:LYS:HE3	1.75	0.69
1:A:1857:LEU:HD22	1:A:1868:TYR:HB2	1.74	0.69
1:A:2879:LYS:HG3	1:A:2880:ASP:H	1.58	0.68
1:A:1346:MET:HE1	1:A:1366:LEU:HD11	1.75	0.68
1:A:2186:CYS:HA	1:A:2191:LEU:HD12	1.75	0.68
1:A:3588:LEU:HD11	1:A:3638:VAL:HG11	1.75	0.68
1:A:2747:ILE:HD11	2:A:4703:ADP:C6	2.30	0.67
1:A:3100:GLU:HG3	1:A:3130:TYR:HE1	1.58	0.67
1:A:3924:ILE:HB	1:A:3927:LEU:HD23	1.75	0.67
1:A:1925:ARG:HH12	1:A:2011:ASP:HB3	1.60	0.67
1:A:3167:ARG:NH1	1:A:3519:TYR:OH	2.26	0.67
1:A:4187:HIS:ND1	1:A:4252:TYR:OH	2.27	0.66
1:A:2943:LYS:HE2	1:A:3067:THR:HB	1.78	0.66
1:A:2030:ASP:OD2	1:A:4131:ASN:ND2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2935:LEU:HD22	1:A:3094:PHE:HE1	1.61	0.66
1:A:3546:ASP:O	1:A:3735:GLN:NE2	2.24	0.66
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.23	0.65
1:A:2113:ARG:HA	1:A:2116:GLU:HG2	1.78	0.65
1:A:3486:ARG:HA	1:A:3489:TRP:HD1	1.62	0.65
1:A:2261:LYS:NZ	1:A:2310:GLU:O	2.28	0.65
1:A:2581:LEU:HD13	1:A:2591:LEU:HD13	1.79	0.65
1:A:2958:VAL:HA	1:A:2991:ALA:HB3	1.78	0.65
1:A:1728:GLY:O	1:A:1784:ASN:ND2	2.31	0.64
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.31	0.64
1:A:3821:ILE:HG12	1:A:4346:MET:HE2	1.80	0.64
1:A:1406:GLU:HG3	1:A:3658:GLY:HA3	1.77	0.64
1:A:1714:ALA:HA	1:A:1870:PHE:HE2	1.63	0.64
1:A:2348:LEU:HD11	1:A:2361:MET:HE1	1.79	0.64
1:A:2620:LEU:HD11	1:A:2634:THR:HG21	1.79	0.64
1:A:4408:PRO:HA	1:A:4411:ARG:HE	1.63	0.63
1:A:1695:HIS:HB3	1:A:1700:GLU:HG3	1.81	0.63
1:A:3845:ASN:HB3	1:A:3858:ILE:HD11	1.81	0.63
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.31	0.63
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.80	0.63
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.81	0.63
1:A:4031:VAL:O	1:A:4123:ARG:NH1	2.32	0.63
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.32	0.63
1:A:4105:TRP:CD1	1:A:4108:GLN:HE21	2.16	0.63
1:A:2387:LEU:HD13	1:A:2412:MET:HE3	1.81	0.63
1:A:3910:ARG:HE	1:A:4344:LEU:HD11	1.64	0.63
1:A:4600:LYS:NZ	1:A:4604:VAL:O	2.32	0.63
1:A:3209:LYS:HA	1:A:3486:ARG:HH12	1.65	0.62
1:A:4105:TRP:HD1	1:A:4108:GLN:HE21	1.46	0.62
1:A:3005:LEU:HD11	1:A:3078:ARG:HH11	1.65	0.62
1:A:4564:LYS:HG3	1:A:4646:GLU:HG3	1.80	0.62
1:A:2897:LEU:HD21	1:A:2909:LEU:HB2	1.81	0.62
1:A:2258:ALA:HB1	1:A:2682:PHE:HD1	1.65	0.62
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.82	0.62
1:A:4046:VAL:HG21	1:A:4148:GLU:HG3	1.81	0.62
1:A:1797:LEU:HD22	1:A:2060:ARG:HH22	1.64	0.61
1:A:1888:CYS:HB2	1:A:2041:MET:HE1	1.82	0.61
1:A:2629:GLU:N	1:A:2629:GLU:OE1	2.31	0.61
1:A:2603:MET:HE1	2:A:4703:ADP:C4	2.36	0.61
1:A:2823:ARG:HH22	1:A:2868:SER:HB3	1.65	0.61
1:A:2009:SER:HB2	1:A:2012:MET:HE3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2660:VAL:HG22	1:A:2707:GLN:HB2	1.82	0.61
1:A:4040:PRO:HB3	1:A:4124:LEU:HD23	1.83	0.61
1:A:1452:VAL:HG22	1:A:1512:TYR:HE1	1.66	0.61
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.34	0.61
1:A:3914:ILE:H	1:A:3937:ARG:HH12	1.47	0.61
1:A:1941:MET:HG2	1:A:1944:ILE:HD12	1.83	0.61
1:A:3209:LYS:HB2	1:A:3486:ARG:HH22	1.66	0.61
1:A:3743:ARG:NE	1:A:3746:GLU:OE2	2.23	0.60
1:A:4186:PHE:O	1:A:4189:ILE:HG22	2.00	0.60
1:A:3508:LEU:HD23	1:A:3536:LEU:HD21	1.83	0.60
1:A:3567:LEU:HD12	1:A:3595:GLN:HE22	1.66	0.60
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.83	0.60
1:A:2112:LYS:HG3	1:A:2122:VAL:HG11	1.83	0.60
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.67	0.60
1:A:2603:MET:HE1	2:A:4703:ADP:H2'	1.84	0.60
1:A:2915:VAL:HG23	1:A:2946:LEU:HD11	1.83	0.60
1:A:3518:GLY:HA3	1:A:3579:MET:HE1	1.83	0.60
1:A:2717:ASP:HB3	1:A:2720:ARG:HG3	1.84	0.59
1:A:3207:LYS:NZ	1:A:3210:GLU:OE1	2.35	0.59
1:A:3871:VAL:HG12	1:A:3875:MET:HE2	1.85	0.59
1:A:2451:ARG:O	1:A:2455:LEU:HD12	2.02	0.59
1:A:3608:LYS:HE3	1:A:3631:ASN:HB3	1.84	0.59
1:A:1800:GLN:OE1	1:A:1804:ARG:NH1	2.36	0.59
1:A:2495:VAL:HG21	1:A:2524:VAL:HG11	1.84	0.59
1:A:2613:PRO:O	1:A:2657:LYS:NZ	2.35	0.59
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.68	0.59
1:A:1965:GLU:N	1:A:1965:GLU:OE1	2.34	0.59
1:A:2464:GLN:HG2	1:A:2583:THR:HG23	1.85	0.59
1:A:1403:LEU:HD23	1:A:1450:LEU:HD21	1.85	0.58
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.36	0.58
1:A:4454:GLU:OE1	1:A:4461:PRO:HA	2.04	0.58
1:A:2373:MET:HE1	3:A:4702:ATP:C4	2.38	0.58
1:A:2451:ARG:HG2	1:A:2455:LEU:HD11	1.86	0.58
1:A:2790:PRO:HB3	1:A:3076:LYS:HE2	1.86	0.58
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.85	0.58
1:A:2325:LEU:HB3	1:A:2333:LEU:HB2	1.85	0.58
1:A:3208:ILE:O	1:A:3212:VAL:HG23	2.04	0.58
1:A:2386:PRO:HA	1:A:2416:GLN:HE22	1.68	0.57
1:A:2592:VAL:HB	1:A:2733:VAL:HG12	1.85	0.57
1:A:3525:ARG:NH1	1:A:3576:ASN:OD1	2.37	0.57
1:A:4398:LEU:HD21	1:A:4493:SER:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2083:GLN:HB2	1:A:2086:TYR:CD1	2.39	0.57
1:A:2830:LEU:HD22	1:A:2850:ILE:HD13	1.85	0.57
1:A:3154:LEU:HD13	1:A:3516:TYR:CD1	2.40	0.57
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.86	0.57
1:A:2578:GLU:OE2	1:A:2607:SER:OG	2.21	0.57
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.85	0.57
1:A:2287:ILE:HA	1:A:2294:GLU:HG3	1.85	0.57
1:A:2615:MET:SD	1:A:2615:MET:N	2.78	0.57
1:A:2818:VAL:HG11	1:A:2861:ILE:HD12	1.87	0.57
1:A:3553:LEU:O	1:A:3582:ARG:NH1	2.32	0.56
1:A:2744:LEU:HA	1:A:2747:ILE:HG22	1.86	0.56
1:A:1416:LEU:HD23	1:A:1449:VAL:HG11	1.87	0.56
1:A:2175:MET:SD	1:A:2175:MET:N	2.78	0.56
1:A:2694:ARG:HD3	1:A:2697:ASP:HB3	1.87	0.56
1:A:1911:GLY:O	1:A:1915:SER:OG	2.15	0.56
1:A:3763:ASP:OD2	1:A:3765:THR:OG1	2.22	0.56
1:A:1543:ARG:NH1	1:A:1609:GLY:HA2	2.21	0.56
1:A:2623:SER:HA	1:A:2668:LEU:HB3	1.88	0.56
1:A:1960:PHE:HE1	1:A:1968:LEU:HG	1.71	0.56
1:A:3756:VAL:HG13	1:A:3757:LYS:H	1.70	0.56
1:A:2964:HIS:ND1	1:A:2965:ARG:O	2.38	0.56
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.39	0.56
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.88	0.56
1:A:1415:GLN:O	1:A:1419:ARG:HG2	2.06	0.55
1:A:2993:ILE:C	1:A:2994:MET:HE2	2.30	0.55
1:A:2102:ASN:OD1	1:A:2105:ARG:NH2	2.33	0.55
1:A:1396:ILE:HD12	1:A:1439:LEU:HD12	1.86	0.55
1:A:3562:TRP:HB3	1:A:3567:LEU:HD22	1.88	0.55
1:A:3756:VAL:HG23	1:A:3760:ILE:HB	1.89	0.55
1:A:2091:ARG:NH1	2:A:4701:ADP:O3'	2.40	0.55
1:A:2910:VAL:N	2:A:4704:ADP:N1	2.50	0.55
1:A:1982:LEU:HD21	1:A:2012:MET:HB2	1.88	0.55
1:A:2505:ASP:OD1	1:A:2733:VAL:HG23	2.07	0.55
1:A:2965:ARG:O	1:A:2966:LYS:HG2	2.06	0.55
1:A:1979:GLN:HB3	1:A:2035:LEU:HD13	1.89	0.55
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.89	0.55
1:A:1571:ILE:HD11	1:A:1607:LEU:HD12	1.89	0.55
1:A:1501:ILE:HA	1:A:1504:VAL:HG22	1.89	0.55
1:A:1684:VAL:C	1:A:1685:MET:HE2	2.32	0.55
1:A:3902:ASP:OD1	1:A:3903:ALA:N	2.40	0.55
1:A:2270:PRO:HA	1:A:2273:ARG:HH22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2323:LYS:HB3	1:A:2335:LEU:HB3	1.89	0.54
1:A:4480:SER:O	1:A:4483:SER:OG	2.16	0.54
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.89	0.54
1:A:1332:VAL:HB	1:A:1377:LEU:HD22	1.89	0.54
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.88	0.54
1:A:2999:VAL:HG13	1:A:3005:LEU:HD21	1.89	0.54
1:A:3851:ASP:OD2	1:A:3853:THR:OG1	2.25	0.54
1:A:3755:GLU:OE2	1:A:3759:ARG:NH1	2.41	0.54
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.73	0.54
1:A:1925:ARG:NH2	1:A:1952:GLY:O	2.40	0.54
1:A:2925:ILE:HD12	1:A:3090:VAL:HG11	1.88	0.54
1:A:2976:LEU:HA	1:A:2979:VAL:HG12	1.88	0.54
1:A:2325:LEU:HD23	1:A:2333:LEU:HD12	1.90	0.54
1:A:3828:SER:HB3	1:A:4140:ARG:HG2	1.90	0.54
1:A:4414:GLU:HA	1:A:4417:VAL:HG22	1.90	0.54
1:A:1510:SER:O	1:A:1512:TYR:N	2.41	0.53
1:A:4281:GLU:N	1:A:4281:GLU:OE1	2.41	0.53
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.40	0.53
1:A:2422:ILE:HG23	1:A:2487:GLU:HG2	1.90	0.53
1:A:3502:THR:HG23	1:A:3543:PHE:HA	1.90	0.53
1:A:2481:MET:SD	1:A:2481:MET:N	2.81	0.53
1:A:3909:LEU:HD11	1:A:4343:MET:HE3	1.89	0.53
1:A:1658:PHE:HB2	1:A:1661:VAL:HB	1.90	0.53
1:A:2619:GLY:HA2	1:A:2662:PHE:HB3	1.90	0.53
1:A:4511:LEU:HD23	1:A:4560:VAL:HG13	1.89	0.53
1:A:2230:LYS:NZ	3:A:4702:ATP:O2B	2.33	0.53
1:A:2499:LEU:O	1:A:2503:SER:OG	2.22	0.53
1:A:3690:PRO:HA	1:A:3693:CYS:HB3	1.91	0.53
1:A:2684:ARG:HH12	1:A:2726:ARG:HE	1.55	0.53
1:A:2842:GLU:OE1	1:A:2842:GLU:N	2.33	0.53
1:A:3200:HIS:NE2	1:A:3747:LYS:HG3	2.24	0.53
1:A:2838:VAL:HG13	1:A:3093:TRP:CZ2	2.43	0.53
1:A:3474:ARG:HB2	1:A:3764:ASP:HB3	1.89	0.53
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.89	0.53
1:A:1946:VAL:HG13	1:A:2006:VAL:HG21	1.91	0.53
1:A:1968:LEU:HD21	1:A:2029:PRO:HG3	1.91	0.53
1:A:3162:ALA:HB2	1:A:3168:THR:HG21	1.91	0.53
1:A:3208:ILE:HG22	1:A:3486:ARG:NH1	2.23	0.53
1:A:3824:LEU:HD11	1:A:4044:CYS:SG	2.48	0.53
1:A:4470:PRO:HG3	1:A:4612:ASN:HD22	1.74	0.53
1:A:1478:VAL:HG11	1:A:1488:ARG:HE	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.91	0.53
1:A:1398:MET:SD	1:A:1399:LEU:HD22	2.49	0.52
1:A:3635:VAL:HB	1:A:3679:LEU:HD23	1.89	0.52
1:A:3474:ARG:HB3	1:A:3765:THR:HG23	1.91	0.52
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.27	0.52
1:A:3021:PHE:CD2	1:A:3029:LEU:HD22	2.45	0.52
1:A:4183:LEU:HD11	1:A:4215:ALA:HB1	1.91	0.52
1:A:4595:GLN:NE2	1:A:4596:THR:O	2.42	0.52
1:A:1752:LEU:HD11	1:A:1868:TYR:CZ	2.45	0.52
1:A:1959:GLU:OE2	1:A:2019:ASN:ND2	2.35	0.52
1:A:1959:GLU:OE1	1:A:1962:ARG:NH1	2.43	0.52
1:A:1477:LEU:HD23	1:A:1487:ILE:HD13	1.91	0.52
1:A:1579:MET:HA	1:A:1582:VAL:HG12	1.91	0.52
1:A:3131:ASP:OD1	1:A:3132:LYS:HG3	2.10	0.52
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.92	0.52
1:A:1925:ARG:NH1	1:A:2011:ASP:HB3	2.25	0.52
1:A:2843:ARG:HH21	1:A:3093:TRP:HD1	1.58	0.52
1:A:4002:LEU:O	1:A:4006:HIS:ND1	2.41	0.52
1:A:3910:ARG:NE	1:A:4344:LEU:HD11	2.24	0.52
1:A:4577:LEU:HD22	1:A:4638:ARG:HD2	1.92	0.52
1:A:4287:LYS:HD3	1:A:4290:GLY:HA2	1.91	0.51
1:A:1504:VAL:HA	1:A:1507:MET:HG3	1.92	0.51
1:A:2111:ILE:O	1:A:2115:LYS:HG3	2.10	0.51
1:A:2307:VAL:HG23	1:A:2345:VAL:HG11	1.91	0.51
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.43	0.51
1:A:4042:LEU:HD11	1:A:4138:LEU:HG	1.91	0.51
1:A:1418:LYS:HD2	1:A:1419:ARG:HD2	1.92	0.51
1:A:2666:ILE:O	1:A:2669:PRO:HD2	2.10	0.51
1:A:3481:SER:HB2	1:A:3770:LEU:HD11	1.92	0.51
1:A:1881:GLN:HE22	1:A:1889:TYR:HE2	1.59	0.51
1:A:1690:VAL:HG11	1:A:1705:VAL:HG22	1.93	0.51
1:A:2265:TYR:CZ	1:A:2314:ASN:HB2	2.46	0.51
1:A:2666:ILE:HG22	1:A:2723:LEU:HD21	1.91	0.51
1:A:4247:MET:HA	1:A:4251:ILE:HB	1.93	0.51
1:A:1748:GLN:O	1:A:1752:LEU:HG	2.11	0.51
1:A:1938:PHE:CE1	1:A:1967:MET:HG2	2.46	0.51
1:A:3873:ARG:NH1	1:A:4025:LEU:HB3	2.25	0.51
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.28	0.51
1:A:1390:LEU:HD23	1:A:1393:TYR:HD2	1.75	0.51
1:A:1634:ASP:OD1	1:A:1635:GLU:N	2.43	0.51
1:A:2406:GLU:HG2	1:A:2409:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3821:ILE:HD12	1:A:4342:LYS:HG2	1.92	0.51
1:A:2223:VAL:HG21	1:A:2348:LEU:HG	1.93	0.51
1:A:2248:GLU:OE2	1:A:2292:ARG:NH1	2.39	0.51
1:A:2203:TRP:CH2	1:A:2236:VAL:HG11	2.46	0.51
1:A:2473:ASN:HB2	1:A:2481:MET:HE1	1.91	0.51
1:A:3044:LEU:HD13	1:A:3049:GLU:HG3	1.92	0.51
1:A:3549:ARG:NH2	1:A:3575:GLU:OE2	2.33	0.51
1:A:2393:GLU:O	1:A:2397:ARG:NH1	2.44	0.50
1:A:2992:PHE:CE2	1:A:2994:MET:HE3	2.46	0.50
1:A:2192:THR:HB	1:A:2373:MET:HG2	1.93	0.50
1:A:3024:ASP:OD1	1:A:3025:GLU:N	2.43	0.50
1:A:1797:LEU:HD13	1:A:2060:ARG:HH12	1.76	0.50
1:A:2976:LEU:O	1:A:2980:LEU:HD23	2.10	0.50
1:A:2292:ARG:O	1:A:2292:ARG:HD3	2.12	0.50
1:A:2571:THR:H	1:A:2574:THR:HB	1.75	0.50
1:A:4404:ASN:HB3	1:A:4410:PHE:CE2	2.46	0.50
1:A:2596:PRO:O	1:A:2601:LYS:NZ	2.45	0.50
1:A:2973:ASP:OD1	1:A:3007:ARG:NE	2.44	0.50
1:A:4404:ASN:HB3	1:A:4410:PHE:CZ	2.46	0.50
1:A:1557:ILE:HA	1:A:1560:LEU:HB2	1.93	0.50
1:A:1882:THR:O	1:A:1885:THR:OG1	2.27	0.50
1:A:2396:ARG:HG3	1:A:2399:LYS:HE2	1.94	0.50
1:A:1651:GLN:OE1	1:A:1663:SER:HA	2.12	0.50
1:A:1701:TRP:O	1:A:1705:VAL:HG23	2.11	0.50
1:A:1936:PHE:CD2	1:A:1938:PHE:CE1	3.00	0.50
1:A:2559:THR:HG22	1:A:2757:ARG:HB3	1.92	0.50
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.77	0.50
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.45	0.49
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	1.94	0.49
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.93	0.49
1:A:2492:ARG:HD2	1:A:2545:TRP:CE2	2.47	0.49
1:A:2643:ARG:NH1	1:A:2644:THR:O	2.45	0.49
1:A:3561:ARG:NH2	1:A:3603:GLU:OE2	2.44	0.49
1:A:4176:ARG:NH2	1:A:4220:ASP:OD1	2.40	0.49
1:A:1391:LYS:O	1:A:1395:LYS:HG2	2.12	0.49
1:A:1814:GLU:O	1:A:1818:GLN:HG2	2.12	0.49
1:A:2585:LEU:HD21	1:A:2709:VAL:HG11	1.94	0.49
1:A:1698:ILE:HD13	1:A:1701:TRP:HE1	1.77	0.49
1:A:1769:MET:HE3	1:A:1769:MET:HA	1.94	0.49
1:A:2294:GLU:HA	1:A:2297:LYS:HD3	1.95	0.49
1:A:2461:MET:HG3	1:A:2584:TRP:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3756:VAL:HG13	1:A:3757:LYS:N	2.28	0.49
1:A:1424:TRP:CZ3	1:A:1434:ILE:HG12	2.48	0.49
1:A:2789:GLN:HB2	1:A:2792:TYR:CE1	2.48	0.49
1:A:3916:LEU:HD12	1:A:3933:GLU:HG3	1.94	0.49
1:A:3970:VAL:HB	1:A:3989:ARG:HG2	1.93	0.49
1:A:1657:MET:HE2	1:A:1657:MET:N	2.27	0.49
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.94	0.49
1:A:2372:ASP:OD1	1:A:2429:SER:HA	2.12	0.49
1:A:2439:HIS:O	1:A:2442:GLN:HG2	2.12	0.49
1:A:2672:ASP:OD1	1:A:2673:LYS:N	2.41	0.49
1:A:1511:PRO:O	1:A:1514:LYS:HG2	2.12	0.49
1:A:2395:GLN:HB3	1:A:2398:ARG:HH22	1.77	0.49
1:A:3627:LEU:HD23	1:A:3662:ILE:HG21	1.94	0.49
1:A:2296:GLN:N	1:A:2296:GLN:OE1	2.46	0.49
1:A:2811:ARG:HB3	1:A:2812:PRO:HD3	1.93	0.49
1:A:1349:GLN:O	1:A:1430:THR:OG1	2.28	0.48
1:A:2514:LEU:O	1:A:2518:ILE:HG12	2.12	0.48
1:A:3788:ASP:N	1:A:3788:ASP:OD1	2.46	0.48
1:A:1747:ALA:O	1:A:1750:VAL:HG12	2.14	0.48
1:A:2718:PRO:HB2	1:A:3080:ALA:HB2	1.95	0.48
1:A:1466:ILE:HA	1:A:1469:VAL:HG22	1.95	0.48
1:A:1503:SER:O	1:A:1507:MET:HG2	2.14	0.48
1:A:2131:LEU:HD12	1:A:2132:PRO:HD2	1.95	0.48
1:A:3133:LEU:HD12	1:A:3134:PRO:HD2	1.95	0.48
1:A:2488:ARG:O	1:A:2492:ARG:HG2	2.14	0.48
1:A:2965:ARG:HD3	1:A:2966:LYS:H	1.78	0.48
1:A:3609:ILE:HB	1:A:3632:PRO:HG2	1.95	0.48
1:A:3831:PHE:O	1:A:3835:ILE:HD12	2.13	0.48
1:A:1336:LEU:HD11	1:A:1386:VAL:HG21	1.95	0.48
1:A:1868:TYR:HD2	1:A:1870:PHE:CD1	2.32	0.48
1:A:2993:ILE:O	1:A:2994:MET:HE2	2.13	0.48
1:A:3635:VAL:O	1:A:3680:SER:N	2.47	0.48
1:A:2671:MET:HG2	1:A:2675:GLY:HA2	1.95	0.48
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.40	0.48
1:A:3818:LEU:HD23	1:A:4346:MET:HE3	1.96	0.48
1:A:4324:PRO:HB3	1:A:4638:ARG:HH11	1.79	0.48
1:A:1571:ILE:HG23	1:A:1604:LEU:HD22	1.96	0.48
1:A:1933:ASP:OD2	1:A:1962:ARG:NH1	2.47	0.48
1:A:2080:LEU:HD23	1:A:2156:LEU:HD22	1.95	0.48
1:A:2963:VAL:HB	1:A:2998:ASN:HB3	1.96	0.48
1:A:3767:ILE:O	1:A:3771:GLU:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.28	0.47
1:A:4395:LEU:HD11	1:A:4486:ILE:HD12	1.96	0.47
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.19	0.47
1:A:3588:LEU:HD23	1:A:3698:PHE:CE1	2.50	0.47
1:A:3982:PRO:HA	1:A:3985:GLN:HG2	1.96	0.47
1:A:3992:LEU:HD22	1:A:3996:PHE:HE2	1.79	0.47
1:A:1498:LYS:HA	1:A:1501:ILE:HG12	1.96	0.47
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.49	0.47
1:A:2879:LYS:HG3	1:A:2880:ASP:N	2.28	0.47
1:A:2373:MET:HE1	3:A:4702:ATP:C5	2.50	0.47
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.96	0.47
1:A:2834:GLN:HA	1:A:2837:LEU:HD13	1.95	0.47
1:A:1356:PRO:HB3	1:A:1401:ILE:HG12	1.95	0.47
1:A:1748:GLN:HE22	1:A:1872:TYR:HA	1.79	0.47
1:A:2284:LEU:HA	1:A:2287:ILE:HG12	1.97	0.47
1:A:2301:ILE:HD11	1:A:2341:ILE:HG12	1.95	0.47
1:A:2649:VAL:HG22	1:A:2702:LYS:HB3	1.95	0.47
1:A:2841:GLU:CD	1:A:2844:ARG:HH21	2.22	0.47
1:A:1507:MET:HE3	1:A:1507:MET:HB3	1.81	0.47
1:A:1964:GLU:OE1	1:A:1967:MET:N	2.38	0.47
1:A:2104:LYS:HB2	1:A:2136:ILE:HG21	1.96	0.47
1:A:2110:LYS:O	1:A:2114:GLU:HG2	2.14	0.47
1:A:2635:PHE:CZ	1:A:2650:LEU:HD22	2.49	0.47
1:A:2956:LEU:HG	1:A:2991:ALA:HB2	1.96	0.47
1:A:3865:GLN:NE2	1:A:3869:ASN:OD1	2.47	0.47
1:A:3892:LEU:HD13	1:A:3983:ILE:HG12	1.96	0.47
1:A:4401:THR:O	1:A:4405:ILE:HG12	2.15	0.47
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.97	0.47
1:A:4473:MET:SD	1:A:4477:GLN:HB2	2.55	0.47
1:A:2987:ASN:OD1	1:A:3061:ASN:ND2	2.47	0.47
1:A:4391:ILE:HD11	1:A:4479:VAL:HG23	1.95	0.47
1:A:1789:LEU:HD11	1:A:2055:TYR:HE2	1.80	0.47
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.50	0.47
1:A:2239:LYS:O	1:A:2242:GLU:HG3	2.14	0.47
1:A:2652:PRO:HD2	1:A:2705:ARG:HH11	1.79	0.47
1:A:2903:GLU:HG3	1:A:2904:GLU:OE1	2.15	0.47
1:A:2506:SER:OG	1:A:2507:ARG:N	2.47	0.47
1:A:2557:VAL:HG13	1:A:2754:ALA:HB2	1.97	0.47
1:A:4219:VAL:HG22	1:A:4243:LEU:HD22	1.96	0.47
1:A:4393:GLN:OE1	1:A:4393:GLN:N	2.39	0.47
1:A:1683:GLU:O	1:A:1746:GLN:NE2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3140:ARG:HA	1:A:3143:ILE:HG22	1.97	0.46
1:A:3872:ALA:O	1:A:3880:HIS:NE2	2.47	0.46
1:A:1998:THR:HG21	1:A:2005:GLN:HB3	1.97	0.46
1:A:2940:GLY:HA3	1:A:3174:ARG:HG3	1.97	0.46
1:A:3039:LYS:HA	1:A:3039:LYS:HD3	1.71	0.46
1:A:1812:ILE:HD13	1:A:2056:SER:HA	1.96	0.46
1:A:2220:LEU:O	1:A:2342:MET:HA	2.15	0.46
1:A:4324:PRO:HD3	1:A:4638:ARG:HG3	1.96	0.46
1:A:1343:ILE:HA	1:A:1346:MET:HE2	1.98	0.46
1:A:2083:GLN:HB2	1:A:2086:TYR:HD1	1.81	0.46
1:A:3618:ALA:HA	1:A:3621:LYS:NZ	2.31	0.46
1:A:3772:ASN:HA	1:A:3775:ARG:HE	1.79	0.46
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.49	0.46
1:A:1941:MET:HA	1:A:1944:ILE:HB	1.96	0.46
1:A:3601:MET:HG3	1:A:3611:ARG:HH21	1.80	0.46
1:A:4095:MET:HE1	1:A:4097:LYS:NZ	2.30	0.46
1:A:1451:LEU:HG	1:A:3673:PRO:HG2	1.97	0.46
1:A:2465:ALA:HB2	1:A:2493:TYR:CD2	2.51	0.46
1:A:2507:ARG:HE	1:A:2509:LYS:NZ	2.13	0.46
1:A:3650:ASN:OD1	1:A:3695:ARG:NH1	2.49	0.46
1:A:4609:VAL:HG23	1:A:4619:ILE:HB	1.98	0.46
1:A:3115:LEU:HD13	1:A:3143:ILE:HG21	1.97	0.46
1:A:3511:ALA:HA	1:A:3514:ILE:HG22	1.97	0.46
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.98	0.46
1:A:4577:LEU:HG	1:A:4630:GLU:OE1	2.15	0.46
1:A:1633:GLY:HA2	1:A:1943:ARG:NH1	2.30	0.46
1:A:1661:VAL:HG22	1:A:1676:ILE:HG21	1.98	0.46
1:A:1910:THR:HG22	1:A:2044:PRO:HD3	1.98	0.46
1:A:1942:GLY:HA3	1:A:2002:LEU:HD21	1.98	0.46
1:A:1351:TRP:H	1:A:1430:THR:HA	1.81	0.46
1:A:1630:TYR:O	1:A:1943:ARG:NE	2.34	0.46
1:A:1964:GLU:O	1:A:1968:LEU:N	2.28	0.46
1:A:2262:ASP:OD2	1:A:2263:HIS:N	2.49	0.46
1:A:2307:VAL:HA	1:A:2311:TRP:CZ2	2.51	0.46
1:A:2686:MET:SD	1:A:2703:LEU:HD11	2.56	0.46
1:A:3591:ASP:N	1:A:3591:ASP:OD1	2.48	0.46
1:A:3557:ASP:OD1	1:A:3558:GLU:N	2.49	0.46
1:A:3704:THR:HG22	1:A:3705:ARG:H	1.81	0.46
1:A:4405:ILE:O	1:A:4411:ARG:NH2	2.49	0.46
1:A:1388:ARG:HA	1:A:1391:LYS:HE2	1.98	0.45
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2584:TRP:CH2	1:A:2732:PRO:HB2	2.51	0.45
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.49	0.45
1:A:4186:PHE:O	1:A:4190:ILE:HD12	2.16	0.45
1:A:4413:PHE:CD2	1:A:4504:LEU:HD22	2.50	0.45
1:A:3567:LEU:HB2	1:A:3599:PHE:CD1	2.51	0.45
1:A:1582:VAL:HG23	1:A:1591:VAL:HG22	1.98	0.45
1:A:2577:HIS:O	1:A:2581:LEU:HD23	2.17	0.45
1:A:2804:ARG:HH12	1:A:2811:ARG:HH22	1.64	0.45
1:A:2982:ARG:NH2	1:A:2988:GLU:OE2	2.40	0.45
1:A:3174:ARG:HH12	1:A:3695:ARG:CZ	2.28	0.45
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.98	0.45
1:A:4037:PRO:HB2	1:A:4118:PRO:HB2	1.97	0.45
1:A:4401:THR:OG1	1:A:4404:ASN:OD1	2.34	0.45
1:A:4410:PHE:O	1:A:4414:GLU:OE1	2.35	0.45
1:A:4518:GLU:HG3	1:A:4619:ILE:HG23	1.99	0.45
1:A:1507:MET:SD	1:A:3629:PHE:HE1	2.39	0.45
1:A:1510:SER:N	1:A:3608:LYS:HZ3	2.14	0.45
1:A:1881:GLN:NE2	1:A:1889:TYR:HE2	2.14	0.45
1:A:2839:GLU:N	1:A:2839:GLU:OE1	2.49	0.45
1:A:3619:PHE:CE2	1:A:3623:LEU:HD11	2.52	0.45
1:A:1498:LYS:HE2	1:A:1531:MET:HE1	1.97	0.45
1:A:2224:GLY:H	1:A:2230:LYS:HD3	1.80	0.45
1:A:1755:GLN:OE1	1:A:1922:GLN:NE2	2.50	0.45
1:A:2260:SER:OG	1:A:2262:ASP:OD2	2.28	0.45
1:A:2837:LEU:HD23	1:A:2842:GLU:HG2	1.98	0.45
1:A:3167:ARG:HH11	1:A:3519:TYR:HH	1.60	0.45
1:A:3174:ARG:NH2	2:A:4704:ADP:O3A	2.49	0.45
1:A:3574:THR:O	1:A:3578:ILE:HG12	2.15	0.45
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	1.98	0.45
1:A:3909:LEU:HD23	1:A:4344:LEU:HA	1.98	0.45
1:A:4227:ALA:O	1:A:4230:ARG:HG3	2.17	0.45
1:A:4445:THR:O	1:A:4449:ARG:HG3	2.16	0.45
1:A:4609:VAL:HG22	1:A:4620:PHE:O	2.17	0.45
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.98	0.45
1:A:3043:MET:SD	1:A:3043:MET:N	2.87	0.45
1:A:2451:ARG:HG2	1:A:2455:LEU:CD1	2.46	0.45
1:A:2921:ARG:O	1:A:2925:ILE:HG12	2.16	0.45
1:A:3154:LEU:HD13	1:A:3516:TYR:HD1	1.79	0.44
1:A:4027:LEU:HD21	1:A:4043:MET:HE2	1.98	0.44
1:A:4395:LEU:HD21	1:A:4486:ILE:HG23	1.99	0.44
1:A:1397:ASN:O	1:A:1401:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1523:TRP:HA	1:A:1526:LYS:HG2	1.98	0.44
1:A:2210:LEU:O	1:A:2214:THR:HG23	2.17	0.44
1:A:2875:ASN:HD21	1:A:2927:ARG:NH1	2.15	0.44
1:A:4248:ALA:HB2	1:A:4269:LEU:HD12	1.99	0.44
1:A:4600:LYS:HE2	1:A:4604:VAL:HG12	2.00	0.44
1:A:2704:GLU:O	1:A:2706:ILE:HG12	2.16	0.44
1:A:2798:GLU:OE1	1:A:2836:ARG:NH2	2.50	0.44
1:A:3510:SER:HB2	1:A:3553:LEU:HD11	1.98	0.44
1:A:4391:ILE:O	1:A:4428:ARG:NH2	2.50	0.44
1:A:1868:TYR:HB3	1:A:1870:PHE:CD1	2.52	0.44
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	2.00	0.44
1:A:2506:SER:OG	1:A:2510:MET:HB3	2.18	0.44
1:A:2516:GLU:O	1:A:2519:ARG:HG2	2.17	0.44
1:A:3596:ALA:HB2	1:A:3701:PHE:CE2	2.52	0.44
1:A:3906:GLN:OE1	1:A:3910:ARG:HG3	2.17	0.44
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	2.00	0.44
1:A:1367:LEU:HD21	1:A:1394:MET:HE1	2.00	0.44
1:A:1727:PHE:HE2	1:A:1741:TRP:CG	2.36	0.44
1:A:1863:ASN:OD1	1:A:1894:GLN:NE2	2.39	0.44
1:A:1888:CYS:O	1:A:1892:MET:HG2	2.17	0.44
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.32	0.44
1:A:2527:PRO:HD3	1:A:2545:TRP:CD1	2.53	0.44
1:A:2744:LEU:O	1:A:2747:ILE:HG22	2.18	0.44
1:A:2874:SER:HB2	1:A:2920:LEU:HD11	2.00	0.44
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.51	0.44
1:A:3612:THR:O	1:A:3635:VAL:HA	2.18	0.44
1:A:3720:GLU:OE2	1:A:3855:ARG:HD3	2.17	0.44
1:A:4635:PHE:CD2	1:A:4640:VAL:HG11	2.53	0.44
1:A:1374:PRO:HD2	1:A:1377:LEU:HD12	2.00	0.44
1:A:1417:MET:HE1	1:A:1424:TRP:CE3	2.53	0.44
1:A:1608:LEU:O	1:A:1611:ILE:HG22	2.18	0.44
1:A:2253:ILE:HG21	1:A:2689:HIS:CE1	2.53	0.44
1:A:3626:ALA:HA	1:A:3631:ASN:OD1	2.17	0.44
1:A:4481:ASP:OD2	1:A:4485:ARG:NE	2.36	0.44
1:A:3109:PHE:HD2	1:A:3180:ILE:HG21	1.83	0.43
1:A:3973:LEU:HB2	1:A:3992:LEU:HD11	1.99	0.43
1:A:2094:LYS:HD3	2:A:4701:ADP:O2'	2.18	0.43
1:A:2368:VAL:HG12	1:A:2369:LEU:HD22	2.00	0.43
1:A:4332:LEU:HD23	1:A:4332:LEU:HA	1.85	0.43
1:A:1536:VAL:HG12	1:A:1601:LEU:HG	2.00	0.43
1:A:1626:PHE:CE2	1:A:1628:ARG:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2146:VAL:HA	1:A:2149:LEU:HD23	1.99	0.43
1:A:3689:PRO:HB2	1:A:3691:ASP:OD1	2.18	0.43
1:A:1413:TRP:O	1:A:1417:MET:HG2	2.18	0.43
1:A:1417:MET:HE1	1:A:1424:TRP:CZ3	2.53	0.43
1:A:1491:ASP:OD1	1:A:1495:ASN:ND2	2.48	0.43
1:A:1504:VAL:HA	1:A:1507:MET:CG	2.48	0.43
1:A:1714:ALA:HA	1:A:1870:PHE:CE2	2.49	0.43
1:A:2306:ASP:HB2	1:A:2676:THR:HG21	1.99	0.43
1:A:4393:GLN:HG2	1:A:4394:THR:N	2.33	0.43
1:A:1349:GLN:NE2	1:A:1353:SER:O	2.52	0.43
1:A:1678:SER:HB2	1:A:1872:TYR:HE2	1.84	0.43
1:A:2893:VAL:HG11	1:A:2916:LEU:HD13	2.01	0.43
1:A:3886:LEU:O	1:A:3890:ILE:HG12	2.19	0.43
1:A:3916:LEU:HD23	1:A:3916:LEU:HA	1.88	0.43
1:A:4172:SER:O	1:A:4176:ARG:NH1	2.50	0.43
1:A:1699:ASN:C	1:A:1699:ASN:HD22	2.26	0.43
1:A:2110:LYS:HA	1:A:2113:ARG:CZ	2.48	0.43
1:A:2206:LYS:HB3	1:A:2364:PHE:CE2	2.53	0.43
1:A:2435:LYS:O	1:A:2438:GLU:HG3	2.18	0.43
1:A:2465:ALA:HB2	1:A:2493:TYR:CE2	2.54	0.43
1:A:2590:PRO:HG2	1:A:2687:VAL:HG21	2.00	0.43
1:A:2241:LEU:HB3	1:A:2298:ARG:NH2	2.34	0.43
1:A:3202:ASN:O	1:A:3206:ARG:HG3	2.18	0.43
1:A:3576:ASN:CB	1:A:3701:PHE:HE1	2.31	0.43
1:A:3888:ALA:HB1	1:A:4012:ASN:HD22	1.83	0.43
1:A:4050:ASP:OD1	1:A:4051:ALA:N	2.49	0.43
1:A:4423:LEU:HD21	1:A:4466:HIS:ND1	2.33	0.43
1:A:1914:GLU:OE1	2:A:4701:ADP:H3'	2.19	0.43
1:A:2354:ALA:HB1	1:A:2358:ARG:HH21	1.83	0.43
1:A:2995:ASP:OD1	1:A:3067:THR:OG1	2.35	0.43
1:A:3030:MET:SD	1:A:3050:LEU:HD11	2.59	0.43
1:A:3723:ASP:O	1:A:3726:GLU:HG3	2.17	0.43
1:A:1671:SER:O	1:A:1692:ILE:HG22	2.19	0.43
1:A:2309:PRO:HB3	1:A:2352:THR:HG23	2.01	0.43
1:A:2522:THR:OG1	1:A:2524:VAL:HG12	2.19	0.43
1:A:2727:PHE:O	1:A:2731:VAL:HG22	2.18	0.43
1:A:4109:LEU:HD23	1:A:4113:LEU:HD23	2.01	0.43
1:A:1367:LEU:HD11	1:A:1394:MET:SD	2.58	0.42
1:A:1412:HIS:CE1	1:A:1453:ALA:HA	2.54	0.42
1:A:1587:LEU:HD23	1:A:1589:MET:H	1.83	0.42
1:A:2222:MET:HE2	1:A:2222:MET:HB2	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2457:SER:OG	1:A:2584:TRP:HZ2	2.01	0.42
1:A:2985:CYS:SG	1:A:3032:GLN:HB3	2.58	0.42
1:A:3650:ASN:HB3	1:A:3652:GLU:HG2	1.99	0.42
1:A:1467:ARG:HA	1:A:1523:TRP:CH2	2.55	0.42
1:A:2309:PRO:HA	1:A:2312:VAL:HG12	2.01	0.42
1:A:3169:MET:HB3	1:A:3693:CYS:SG	2.60	0.42
1:A:1882:THR:HG23	1:A:1885:THR:H	1.84	0.42
1:A:1940:ALA:HB1	1:A:1943:ARG:CZ	2.49	0.42
1:A:1961:ASN:ND2	1:A:2019:ASN:O	2.51	0.42
1:A:2885:ASP:HB3	1:A:2888:GLU:OE1	2.19	0.42
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.54	0.42
1:A:3999:ASP:OD1	1:A:4000:ARG:HG2	2.19	0.42
1:A:1626:PHE:HB3	1:A:1629:PHE:CD2	2.54	0.42
1:A:1629:PHE:HE1	1:A:1640:ILE:HG21	1.84	0.42
1:A:2666:ILE:HB	1:A:2712:CYS:SG	2.59	0.42
1:A:1608:LEU:HA	1:A:1611:ILE:HG22	2.01	0.42
1:A:1931:ASN:O	1:A:1936:PHE:HD1	2.03	0.42
1:A:2138:ILE:HG13	1:A:2161:LEU:HD21	2.01	0.42
1:A:2863:ARG:NH2	1:A:2864:GLU:OE2	2.52	0.42
1:A:3930:GLU:HG2	1:A:3931:GLN:N	2.34	0.42
1:A:2823:ARG:HH12	1:A:2868:SER:N	2.18	0.42
1:A:2843:ARG:HH21	1:A:3093:TRP:CD1	2.37	0.42
1:A:3211:THR:HG21	1:A:3753:LEU:HD21	2.01	0.42
1:A:3840:LEU:HD23	1:A:3840:LEU:HA	1.85	0.42
1:A:1983:ARG:HB3	1:A:1983:ARG:NH1	2.35	0.42
1:A:2138:ILE:HA	1:A:2141:VAL:HG12	2.01	0.42
1:A:2412:MET:O	1:A:2416:GLN:HG2	2.19	0.42
1:A:2779:MET:HA	1:A:2782:GLU:HG3	2.02	0.42
1:A:3112:LYS:HE3	1:A:3113:MET:HE3	2.02	0.42
1:A:3150:VAL:HG13	1:A:3532:TRP:CE2	2.54	0.42
1:A:3780:VAL:O	1:A:3784:VAL:HG23	2.20	0.42
1:A:3782:ARG:O	1:A:3786:GLU:HG2	2.19	0.42
1:A:3814:THR:O	1:A:3818:LEU:HG	2.20	0.42
1:A:2486:LEU:O	1:A:2490:ILE:HG12	2.20	0.42
1:A:2686:MET:HE1	1:A:2708:PHE:CZ	2.55	0.42
1:A:2962:LYS:HE3	1:A:3663:THR:HG21	2.00	0.42
1:A:3146:SER:O	1:A:3150:VAL:HG23	2.20	0.42
1:A:3596:ALA:HB2	1:A:3701:PHE:CD2	2.55	0.42
1:A:3736:GLY:O	1:A:3740:LEU:N	2.40	0.42
1:A:4173:PRO:HB2	1:A:4175:GLU:OE1	2.20	0.42
1:A:4294:ILE:HD11	1:A:4320:TRP:NE1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4623:ASP:OD2	1:A:4624:PHE:N	2.53	0.42
1:A:1416:LEU:HD12	1:A:1417:MET:HE2	2.01	0.42
1:A:1539:ASP:HA	1:A:1542:ARG:HD3	2.00	0.42
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	2.01	0.42
1:A:3212:VAL:HA	1:A:3215:VAL:HG12	2.02	0.42
1:A:3704:THR:HG22	1:A:3705:ARG:N	2.35	0.42
1:A:1390:LEU:O	1:A:1394:MET:HE3	2.20	0.41
1:A:1623:ARG:HB3	1:A:1630:TYR:CZ	2.55	0.41
1:A:2460:SER:OG	1:A:2589:LYS:HD2	2.20	0.41
1:A:3209:LYS:HE2	1:A:3486:ARG:NH2	2.34	0.41
1:A:2278:GLY:N	1:A:2281:THR:OG1	2.52	0.41
1:A:2387:LEU:HD21	1:A:2463:HIS:ND1	2.35	0.41
1:A:4461:PRO:HG2	1:A:4464:TRP:CE3	2.55	0.41
1:A:4607:LEU:HD22	1:A:4640:VAL:HG13	2.02	0.41
1:A:2205:GLU:O	1:A:2209:GLN:HG3	2.19	0.41
1:A:2211:TYR:CE1	1:A:2241:LEU:HD21	2.54	0.41
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.52	0.41
1:A:4107:MET:O	1:A:4110:GLU:HG2	2.21	0.41
1:A:1678:SER:OG	1:A:1679:ARG:N	2.53	0.41
1:A:2723:LEU:HD23	1:A:2723:LEU:HA	1.84	0.41
1:A:3470:ALA:O	1:A:3474:ARG:HG3	2.20	0.41
1:A:1464:LYS:HE2	1:A:1464:LYS:HB2	1.89	0.41
1:A:2269:ASP:O	1:A:2273:ARG:NH2	2.54	0.41
1:A:2684:ARG:O	1:A:2688:GLU:HG3	2.20	0.41
1:A:3209:LYS:HB2	1:A:3486:ARG:NH2	2.35	0.41
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.56	0.41
1:A:1650:LEU:HD23	1:A:1650:LEU:HA	1.90	0.41
1:A:2729:ARG:HE	1:A:2730:HIS:CD2	2.38	0.41
1:A:2773:MET:HB3	1:A:2799:MET:HE3	2.01	0.41
1:A:2832:LEU:HD23	1:A:2832:LEU:HA	1.92	0.41
1:A:2884:VAL:HG21	1:A:2889:LEU:HD12	2.01	0.41
1:A:4038:ASN:HB3	1:A:4118:PRO:HG2	2.02	0.41
1:A:4554:ASP:N	1:A:4557:SER:OG	2.53	0.41
1:A:1431:LEU:HD21	1:A:1435:TRP:CZ2	2.56	0.41
1:A:1940:ALA:HB1	1:A:1943:ARG:NH2	2.35	0.41
1:A:1980:GLU:O	1:A:1984:GLU:HG3	2.21	0.41
1:A:2094:LYS:HE2	1:A:2094:LYS:HB3	1.80	0.41
1:A:2413:LEU:HD13	1:A:2416:GLN:NE2	2.35	0.41
1:A:3017:VAL:O	1:A:3020:LEU:HD22	2.21	0.41
1:A:4277:SER:HA	1:A:4282:PHE:CD2	2.56	0.41
1:A:1661:VAL:HG13	1:A:1676:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1788:THR:O	1:A:1792:LEU:HD23	2.21	0.41
1:A:1973:GLN:HA	1:A:1976:GLN:HE21	1.86	0.41
1:A:3042:LEU:O	1:A:3044:LEU:HG	2.20	0.41
1:A:3167:ARG:NH2	1:A:3685:THR:HA	2.36	0.41
1:A:1390:LEU:C	1:A:1394:MET:HE3	2.45	0.41
1:A:1470:TRP:CE3	1:A:1470:TRP:HA	2.56	0.41
1:A:1786:GLU:OE2	1:A:1790:ASN:ND2	2.54	0.41
1:A:2054:LEU:HG	1:A:2097:LEU:HD12	2.03	0.41
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	2.02	0.41
1:A:2253:ILE:HG21	1:A:2689:HIS:NE2	2.36	0.41
1:A:2265:TYR:OH	1:A:2315:LEU:HG	2.21	0.41
1:A:2335:LEU:HD23	1:A:2336:PRO:O	2.21	0.41
1:A:2873:TYR:HB3	1:A:2881:TYR:CE2	2.56	0.41
1:A:2876:TRP:HA	1:A:2876:TRP:CE3	2.56	0.41
1:A:2909:LEU:HA	2:A:4704:ADP:C2	2.56	0.41
1:A:2927:ARG:O	1:A:2927:ARG:HG3	2.21	0.41
1:A:2930:GLN:HG3	1:A:2932:HIS:CD2	2.55	0.41
1:A:3481:SER:HB2	1:A:3770:LEU:CD1	2.51	0.41
1:A:4400:ARG:HB3	1:A:4405:ILE:HD11	2.03	0.41
1:A:4404:ASN:ND2	1:A:4501:ALA:HB2	2.36	0.41
1:A:1351:TRP:CE3	1:A:1434:ILE:HD12	2.56	0.41
1:A:1931:ASN:O	1:A:1936:PHE:CD1	2.74	0.41
1:A:2009:SER:O	1:A:2012:MET:HG2	2.21	0.41
1:A:2395:GLN:HB3	1:A:2398:ARG:NH2	2.36	0.41
1:A:2591:LEU:H	1:A:2709:VAL:HG12	1.86	0.41
1:A:2916:LEU:HD12	1:A:2916:LEU:HA	1.91	0.41
1:A:3045:ASP:OD1	1:A:3046:SER:N	2.53	0.41
1:A:3924:ILE:HG23	1:A:3952:GLN:OE1	2.21	0.41
1:A:2206:LYS:HD3	1:A:2206:LYS:HA	1.89	0.40
1:A:2646:ASN:OD1	1:A:2647:GLY:N	2.54	0.40
1:A:2935:LEU:HD23	1:A:3092:ASN:HB3	2.03	0.40
1:A:3174:ARG:HD2	1:A:3694:SER:OG	2.21	0.40
1:A:3811:ILE:HD11	1:A:3864:PHE:CE1	2.55	0.40
1:A:1344:ASP:O	1:A:1348:GLU:HG2	2.21	0.40
1:A:2093:LEU:O	1:A:2097:LEU:HD23	2.22	0.40
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	2.04	0.40
1:A:4300:ILE:N	1:A:4304:GLU:OE2	2.45	0.40
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	2.02	0.40
1:A:2224:GLY:N	1:A:2230:LYS:HD3	2.36	0.40
1:A:2789:GLN:HB2	1:A:2792:TYR:HE1	1.87	0.40
1:A:2888:GLU:OE1	1:A:2888:GLU:N	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3627:LEU:HD21	1:A:3648:VAL:HG22	2.03	0.40
1:A:3749:LEU:HD13	1:A:3773:LEU:HD22	2.02	0.40
1:A:3835:ILE:HG23	1:A:3866:VAL:HG12	2.04	0.40
1:A:1477:LEU:HB3	1:A:1485:ARG:HG2	2.04	0.40
1:A:1739:ILE:HD13	1:A:1739:ILE:HA	1.91	0.40
1:A:2315:LEU:HA	1:A:2318:VAL:HG22	2.02	0.40
1:A:3209:LYS:CA	1:A:3486:ARG:HH12	2.33	0.40
1:A:3772:ASN:O	1:A:3775:ARG:HG2	2.21	0.40
1:A:4277:SER:HA	1:A:4282:PHE:CG	2.56	0.40
1:A:1523:TRP:CE3	1:A:1526:LYS:HD2	2.56	0.40
1:A:2877:LEU:HD12	1:A:2884:VAL:HB	2.02	0.40
1:A:3746:GLU:HA	1:A:3773:LEU:HD21	2.04	0.40
1:A:4186:PHE:CE1	1:A:4190:ILE:HD11	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	3035/4646 (65%)	2956 (97%)	78 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1511	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2706/4125 (66%)	2705 (100%)	1 (0%)	100 100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1567	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1566	GLN
1	A	1755	GLN
1	A	1876	GLN
1	A	1922	GLN
1	A	1950	GLN
1	A	2051	GLN
1	A	2263	HIS
1	A	2282	HIS
1	A	2299	GLN
1	A	2377	ASN
1	A	2414	GLN
1	A	2416	GLN
1	A	2439	HIS
1	A	2442	GLN
1	A	2475	ASN
1	A	2677	GLN
1	A	2698	GLN
1	A	2786	GLN
1	A	3032	GLN
1	A	3038	GLN
1	A	3202	ASN
1	A	3535	HIS
1	A	3646	ASN
1	A	4156	ASN
1	A	4191	GLN
1	A	4262	GLN
1	A	4446	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	ATP	A	4702	4	28,33,33	0.75	0	34,52,52	0.61	1 (2%)
2	ADP	A	4701	-	24,29,29	0.87	0	29,45,45	1.26	3 (10%)
2	ADP	A	4704	-	24,29,29	0.85	0	29,45,45	1.24	2 (6%)
2	ADP	A	4703	-	24,29,29	0.87	0	29,45,45	1.29	3 (10%)

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	4	-	5/18/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	2/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4703	ADP	N3-C2-N1	-3.62	123.76	128.67
2	A	4704	ADP	N3-C2-N1	-3.57	123.83	128.67
2	A	4701	ADP	N3-C2-N1	-3.54	123.86	128.67
2	A	4704	ADP	C4-C5-N7	-2.53	106.67	109.34
2	A	4701	ADP	C4-C5-N7	-2.48	106.72	109.34
2	A	4703	ADP	C4-C5-N7	-2.45	106.75	109.34
3	A	4702	ATP	C5-C6-N6	2.41	123.98	120.31
2	A	4701	ADP	C4'-O4'-C1'	2.34	112.07	109.92
2	A	4703	ADP	C4'-O4'-C1'	2.26	112.00	109.92

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
3	A	4702	ATP	PB-O3B-PG-O3G
2	A	4703	ADP	O4'-C4'-C5'-O5'
2	A	4703	ADP	C3'-C4'-C5'-O5'
3	A	4702	ATP	PB-O3B-PG-O1G
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4701	ADP	PB-O3A-PA-O2A
3	A	4702	ATP	PA-O3A-PB-O1B
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	O4'-C4'-C5'-O5'
2	A	4701	ADP	PB-O3A-PA-O1A

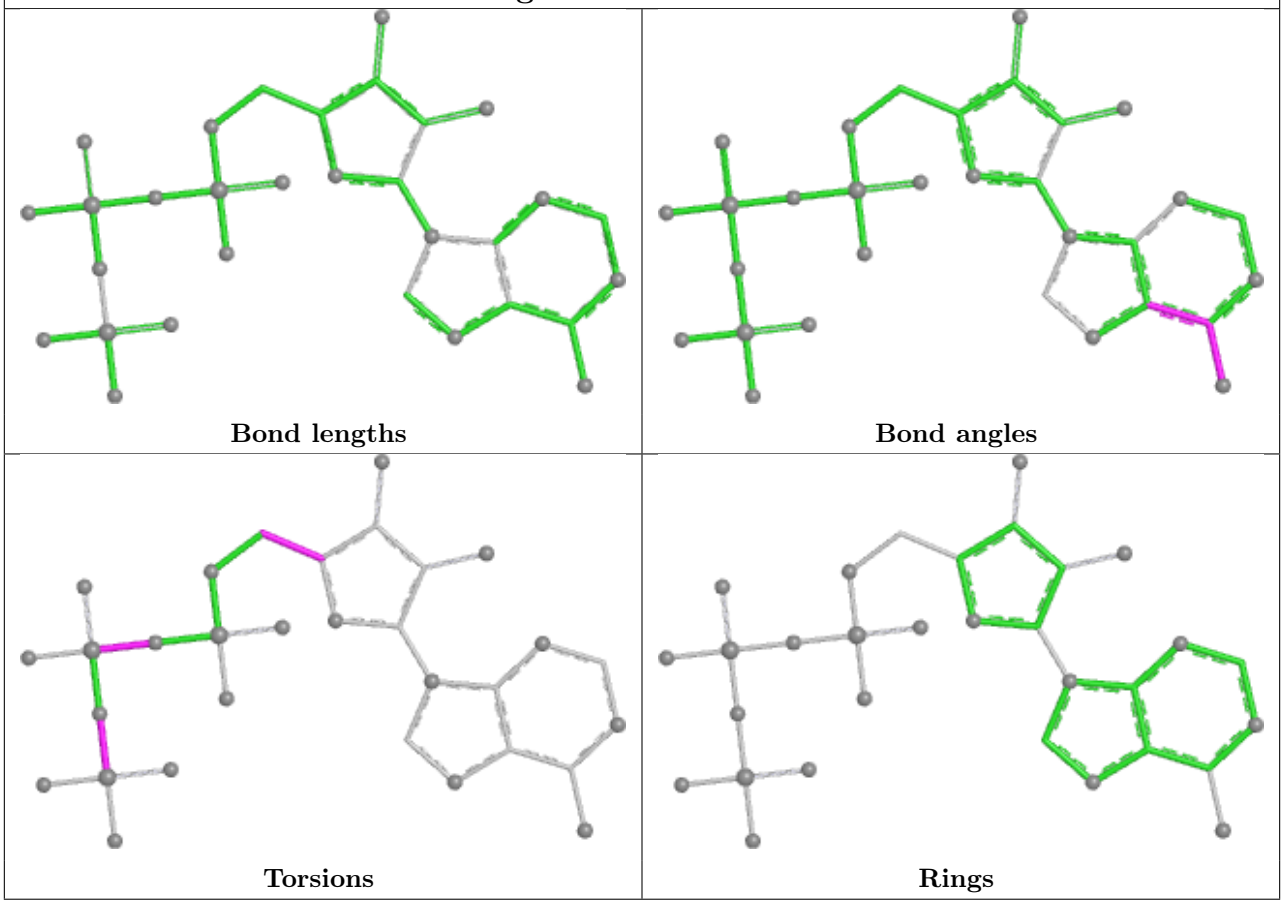
There are no ring outliers.

4 monomers are involved in 12 short contacts:

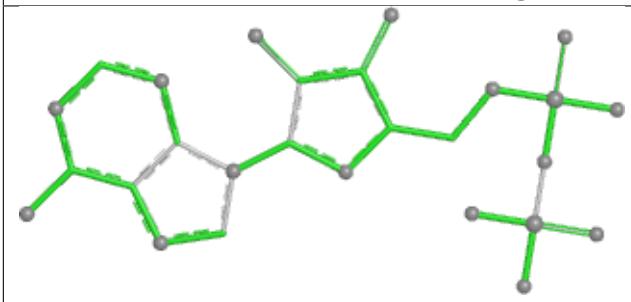
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	3	0
2	A	4701	ADP	3	0
2	A	4704	ADP	3	0
2	A	4703	ADP	3	0

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.

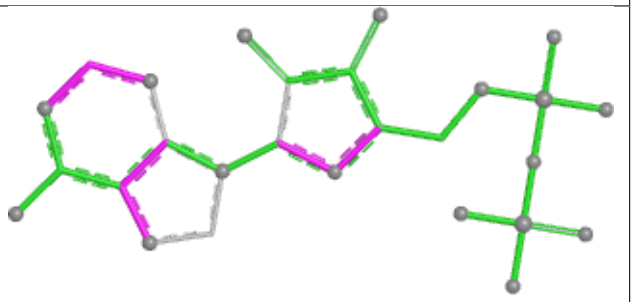
Ligand ATP A 4702



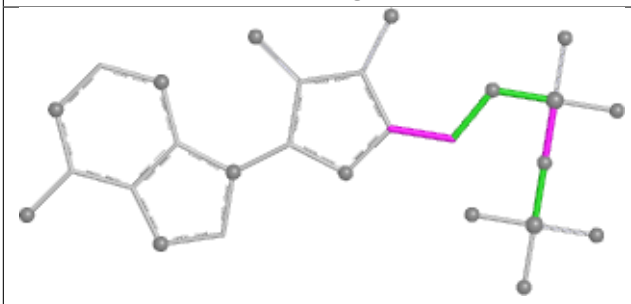
Ligand ADP A 4701



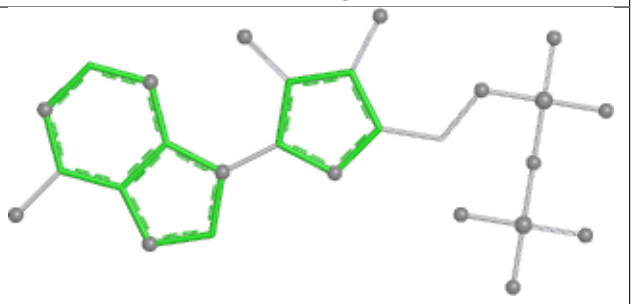
Bond lengths



Bond angles

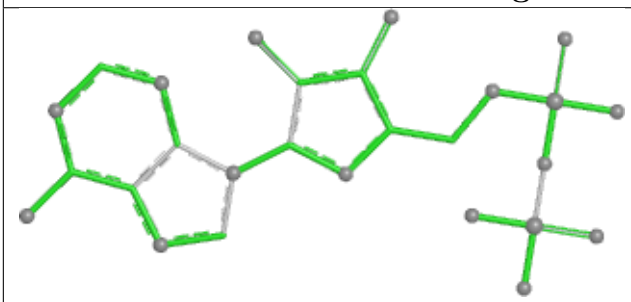


Torsions

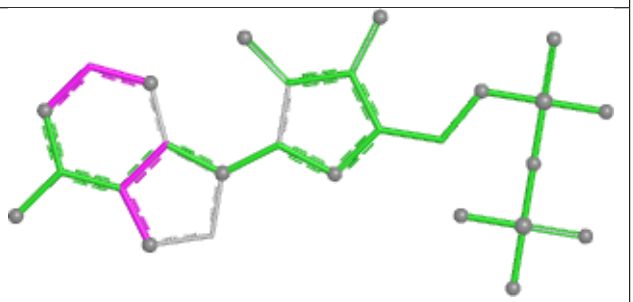


Rings

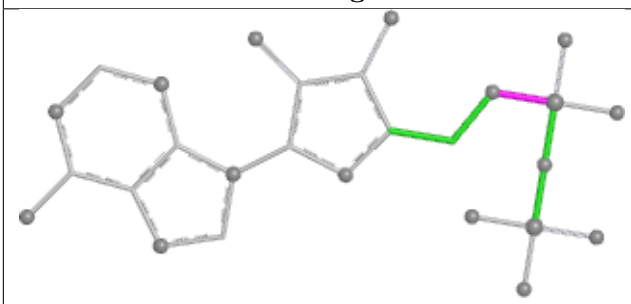
Ligand ADP A 4704



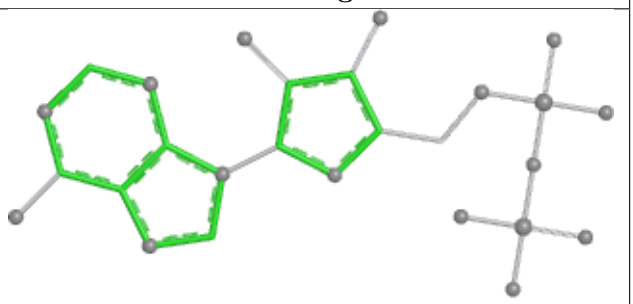
Bond lengths



Bond angles

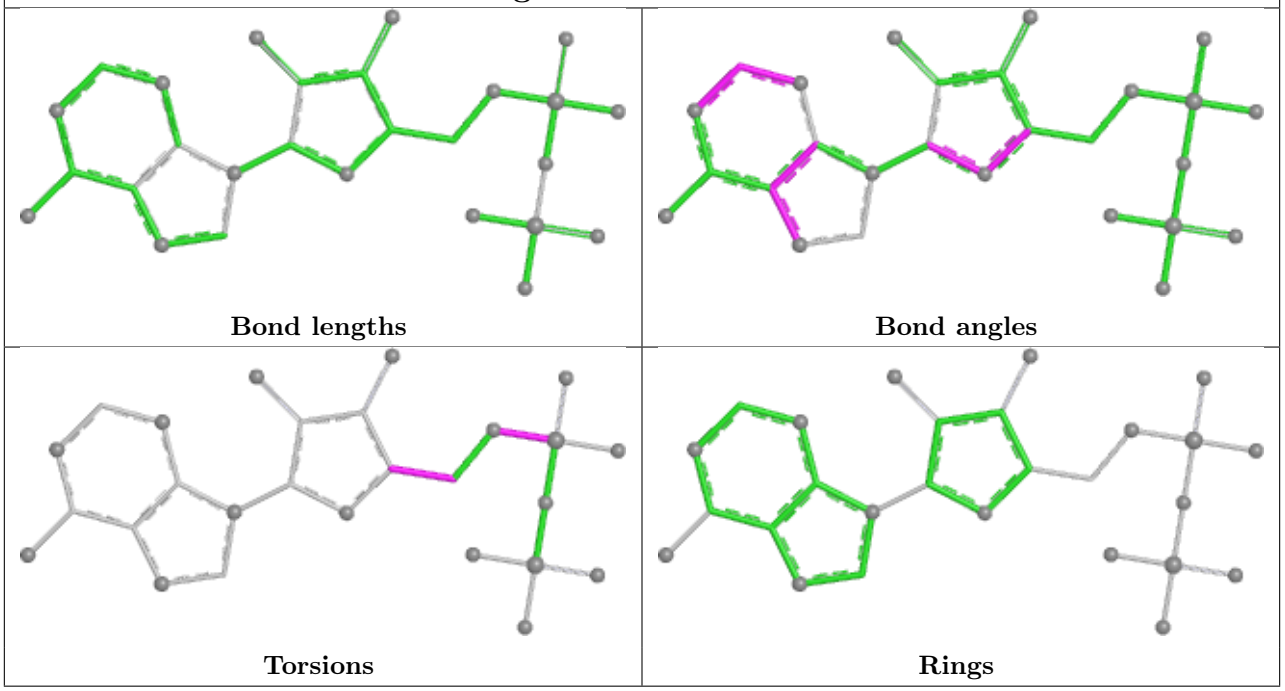


Torsions



Rings

Ligand ADP A 4703



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

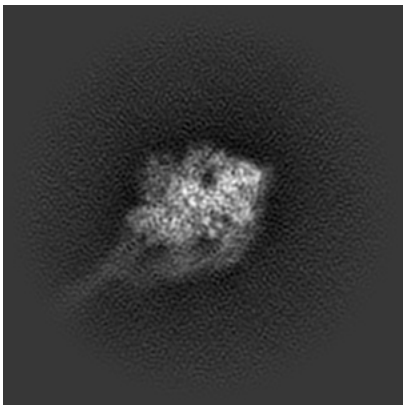
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44712. These allow visual inspection of the internal detail of the map and identification of artifacts.

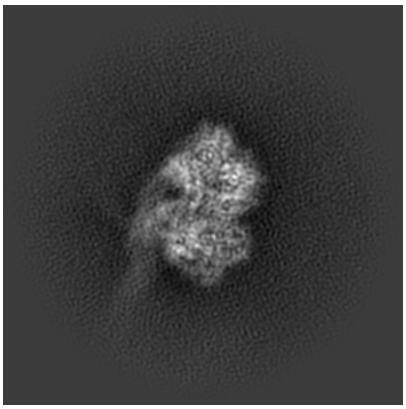
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

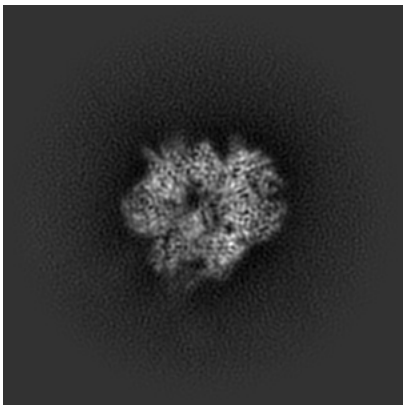
6.1.1 Primary map



X

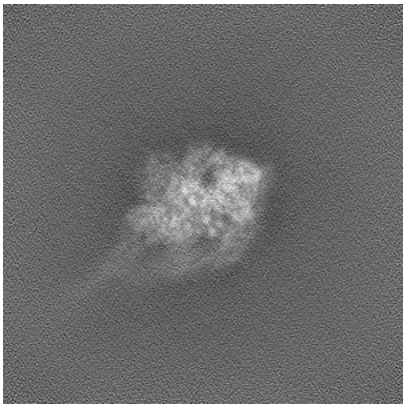


Y

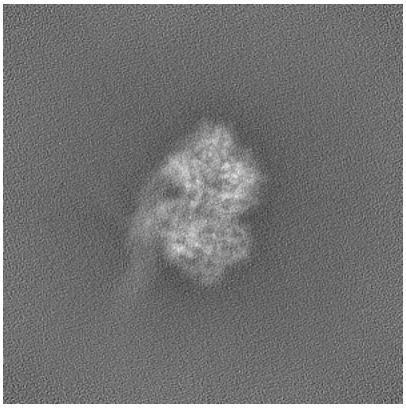


Z

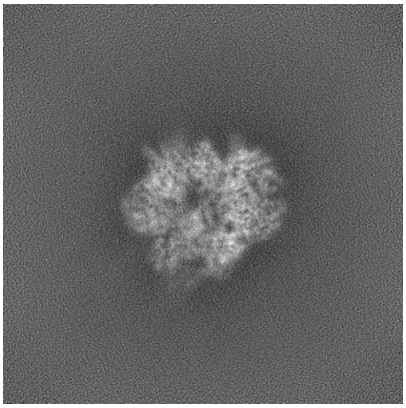
6.1.2 Raw map



X



Y

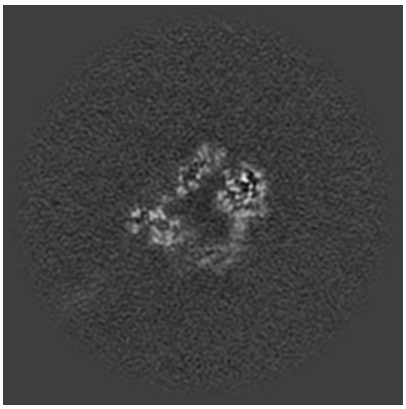


Z

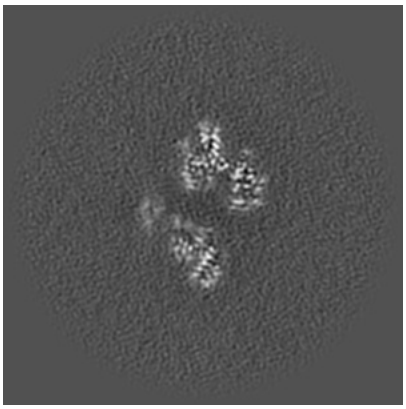
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

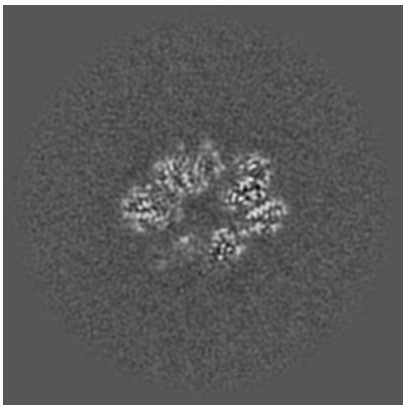
6.2.1 Primary map



X Index: 160

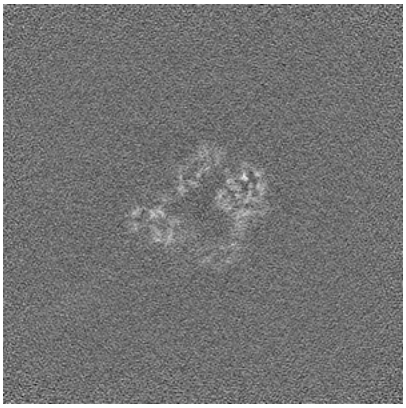


Y Index: 160

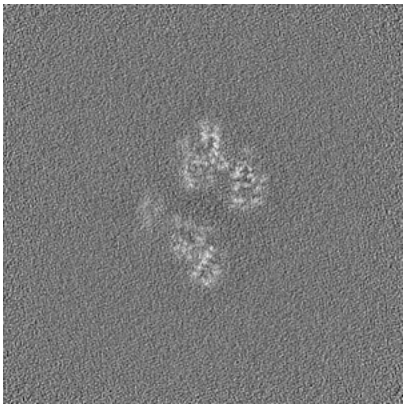


Z Index: 160

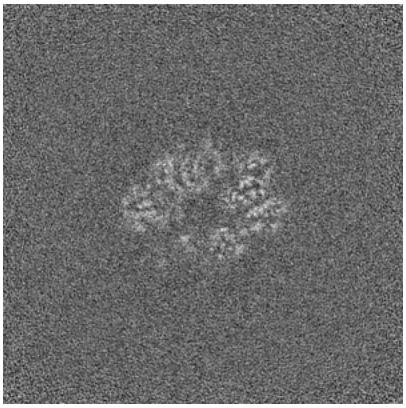
6.2.2 Raw map



X Index: 160



Y Index: 160

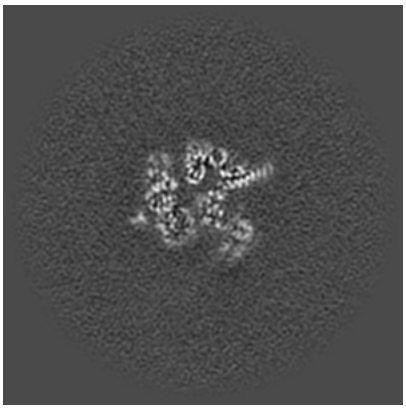


Z Index: 160

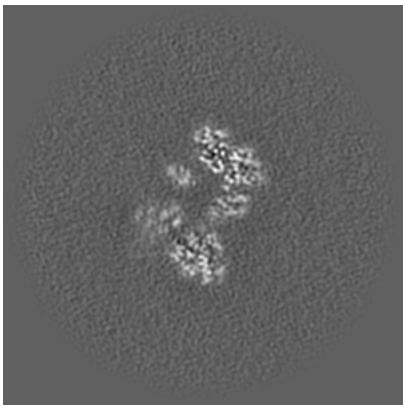
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

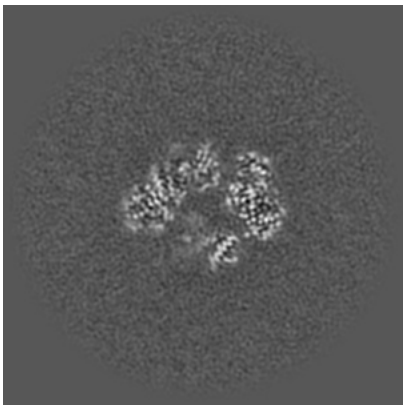
6.3.1 Primary map



X Index: 182

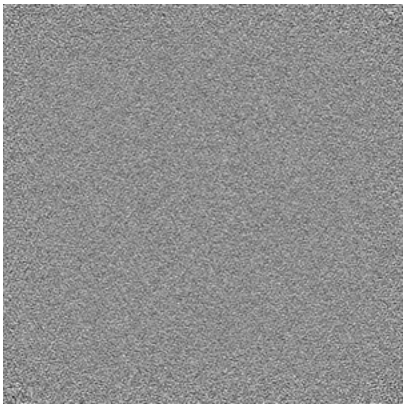


Y Index: 150

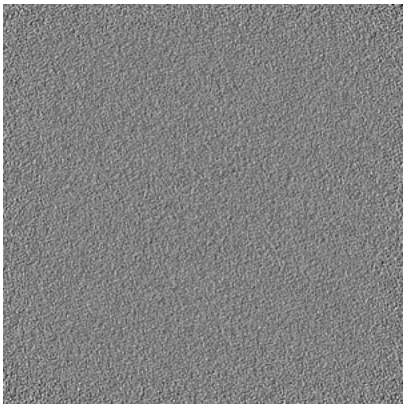


Z Index: 165

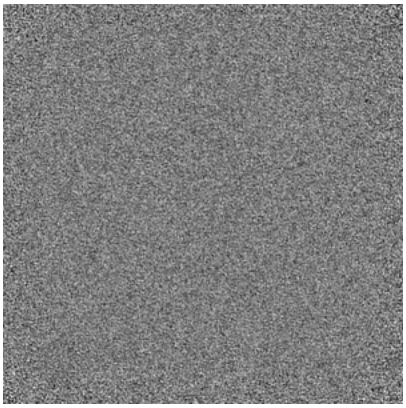
6.3.2 Raw map



X Index: 0



Y Index: 0

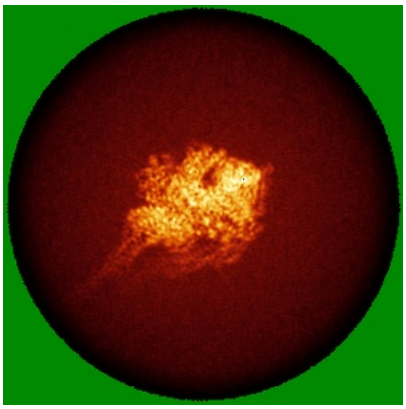


Z Index: 0

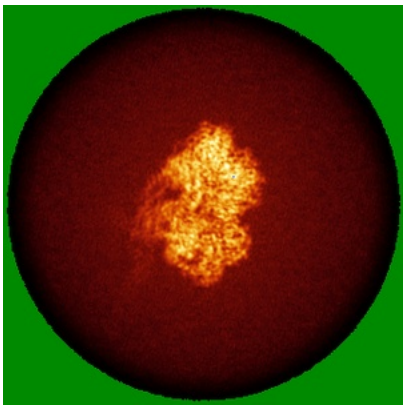
The images above show the largest variance slices of the map in three orthogonal directions.

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

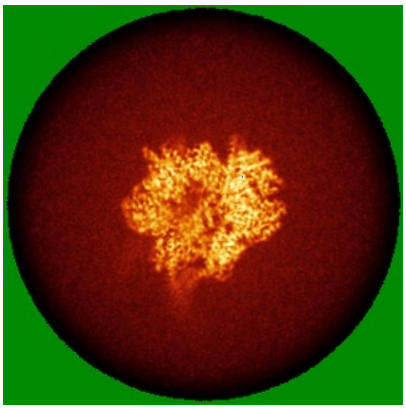
6.4.1 Primary map



X

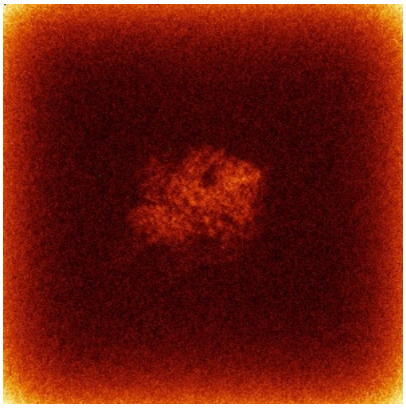


Y

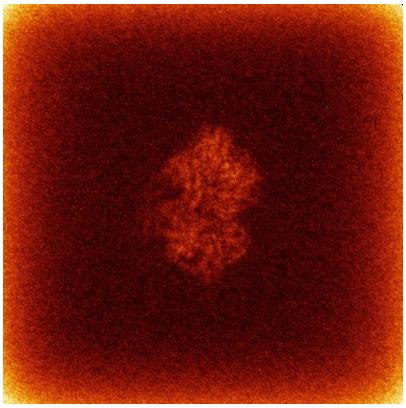


Z

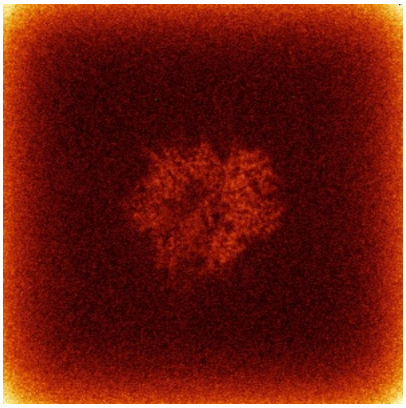
6.4.2 Raw map



X



Y

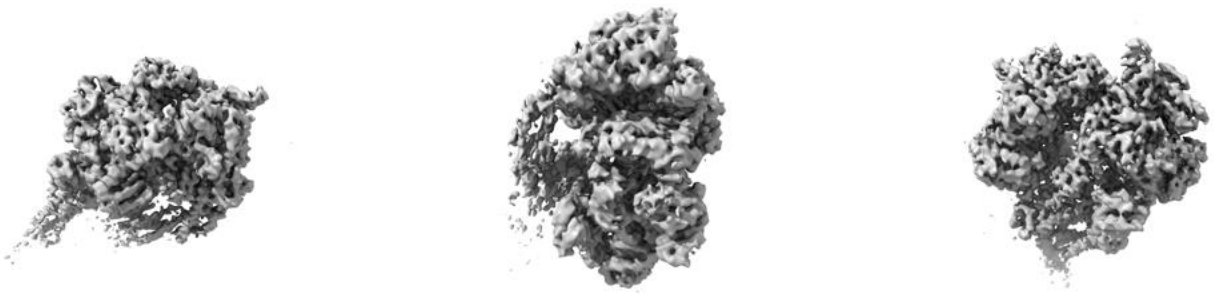


Z

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)

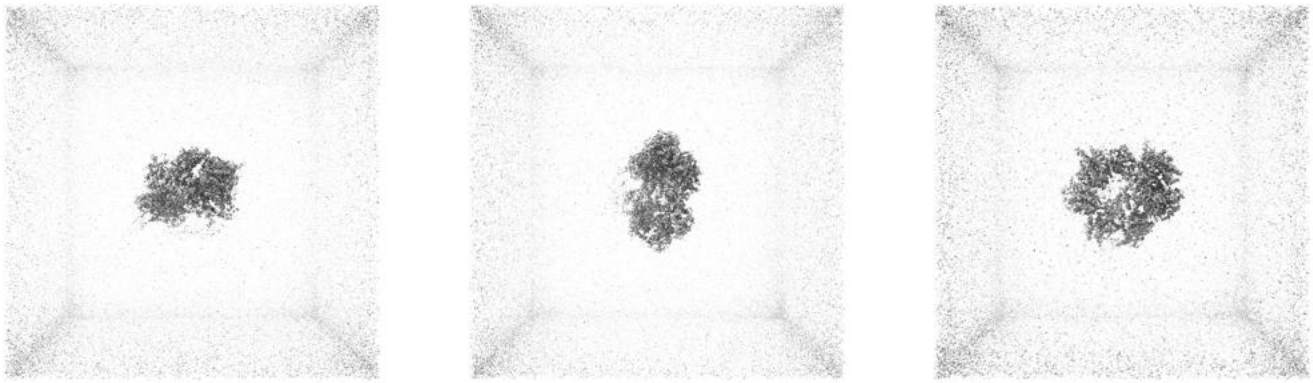
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

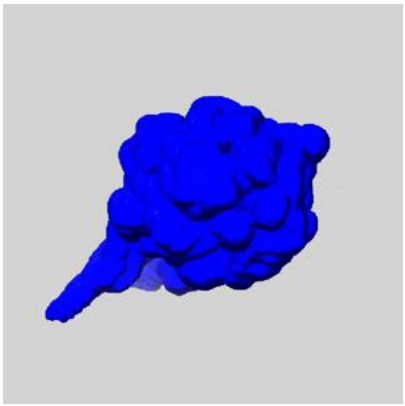
6.6 Mask visualisation (i)

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

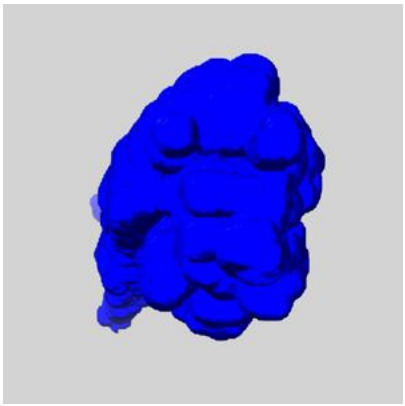
A mask typically either:

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

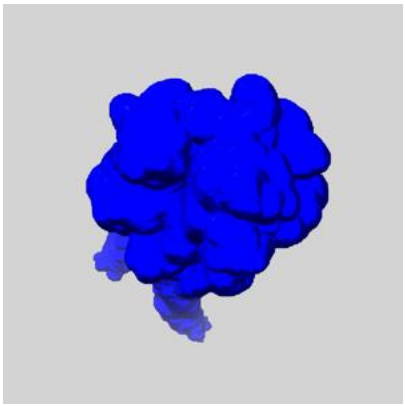
6.6.1 emd_44712_msk_1.map (i)



X



Y

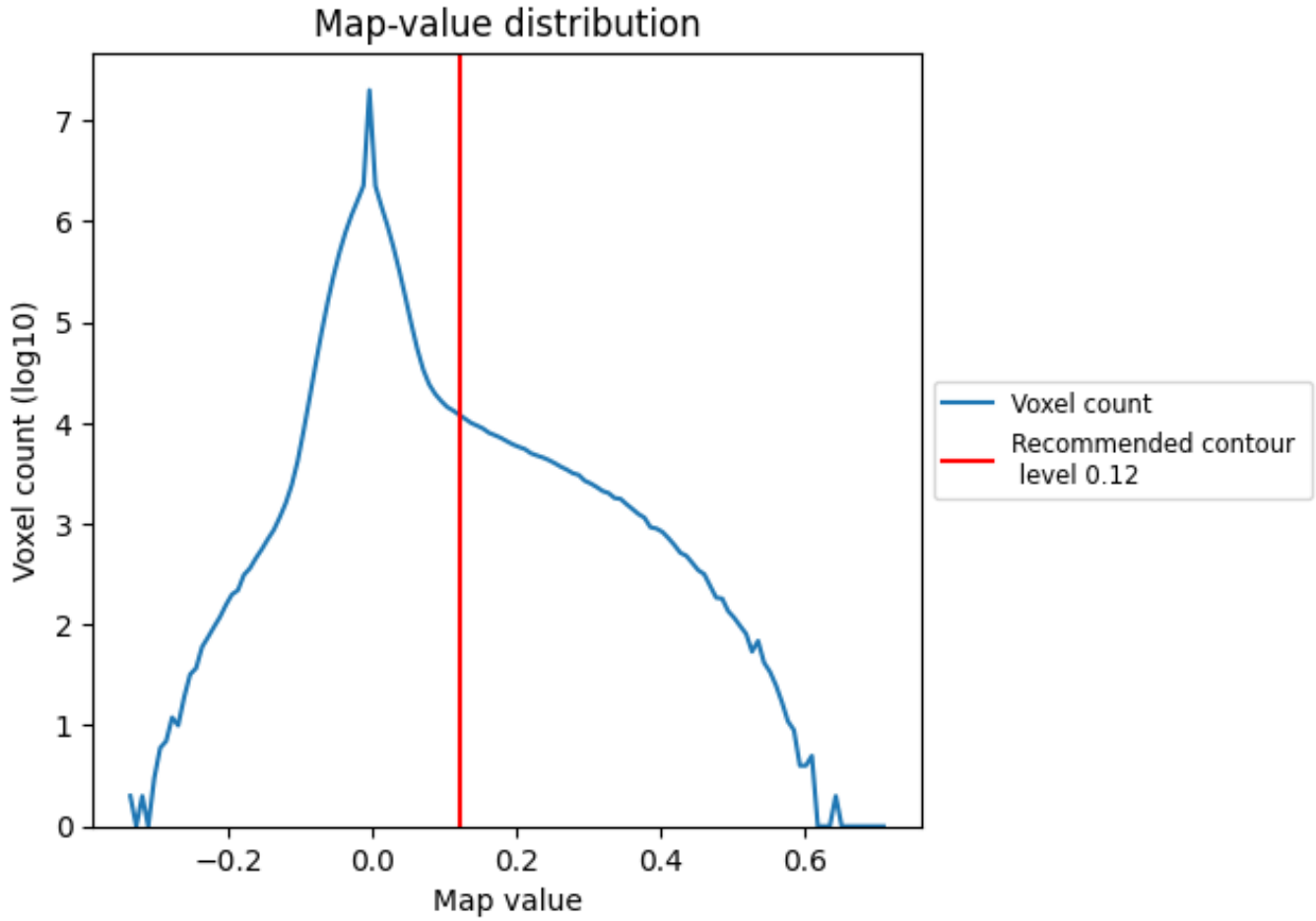


Z

7 Map analysis

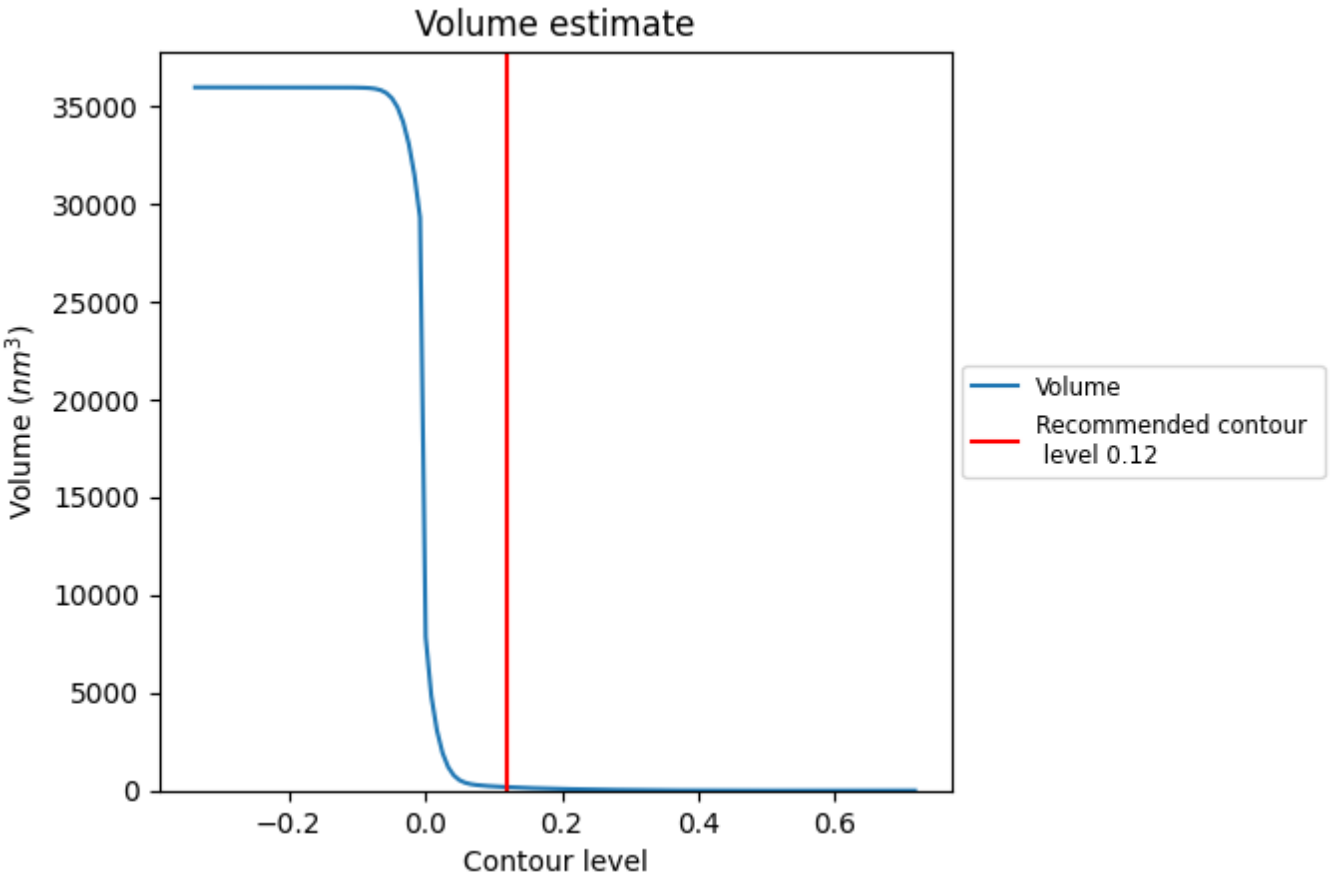
This section contains the results of statistical analysis of the map.

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.

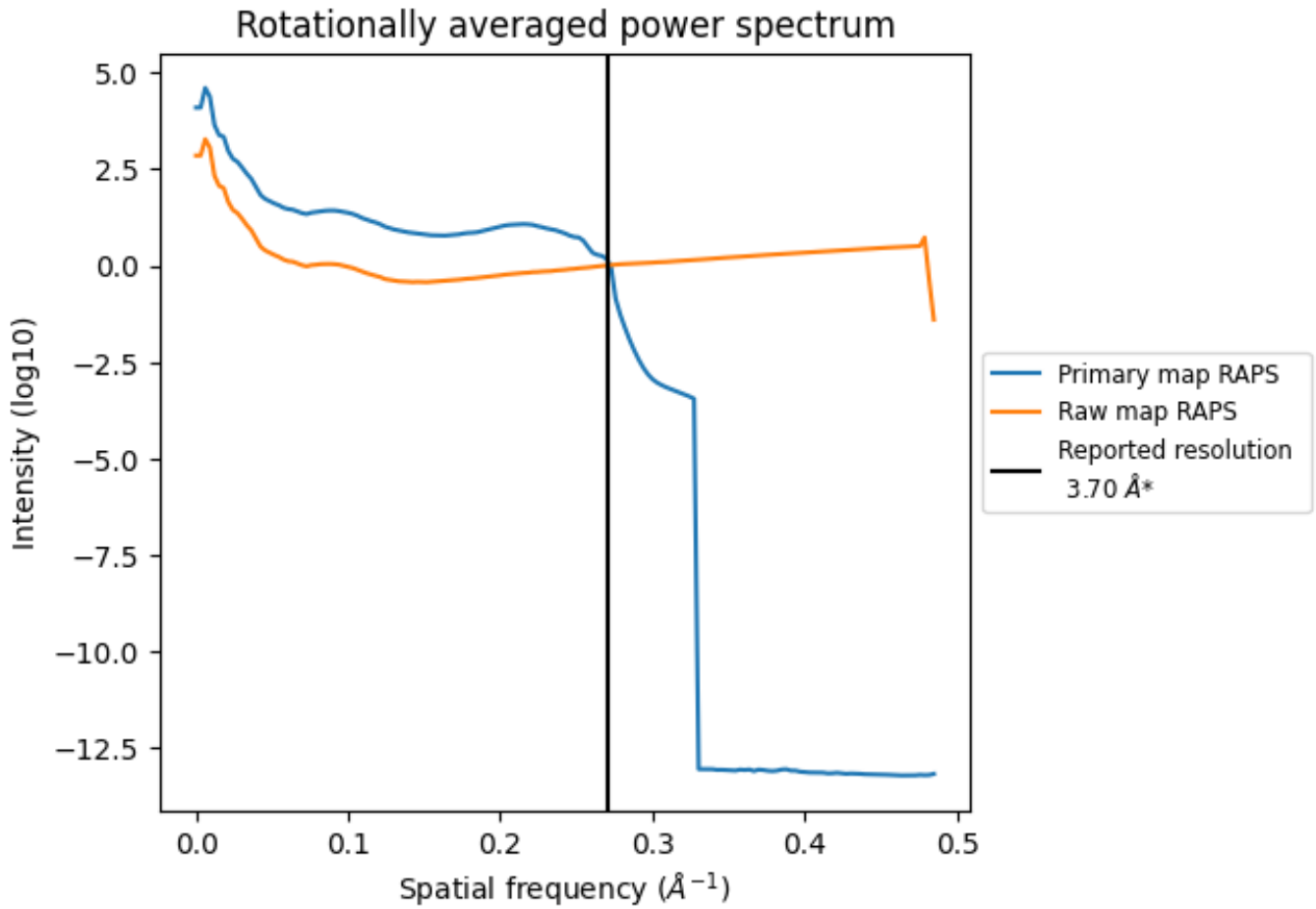
7.2 Volume estimate (i)



The volume at the recommended contour level is 177 nm^3; this corresponds to an approximate mass of 159 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

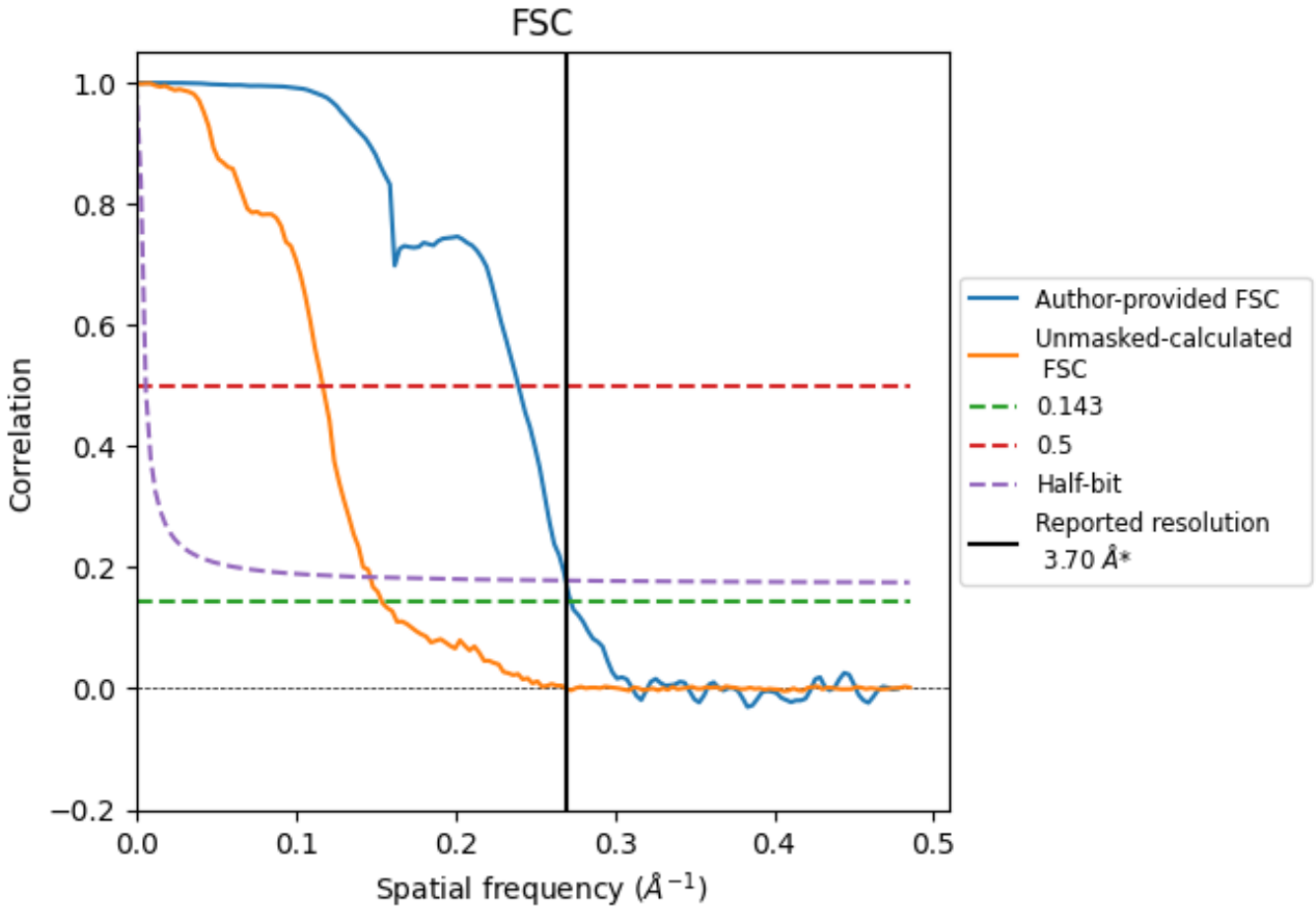


*Reported resolution corresponds to spatial frequency of 0.270 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

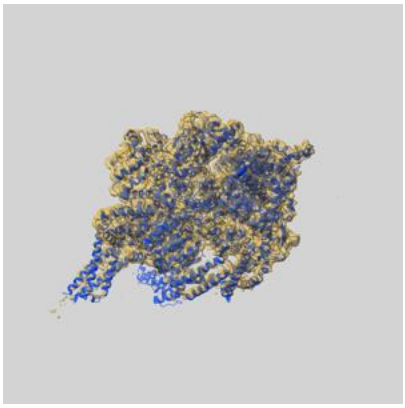
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.67	4.17	3.71
Unmasked-calculated*	6.49	8.55	6.81

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

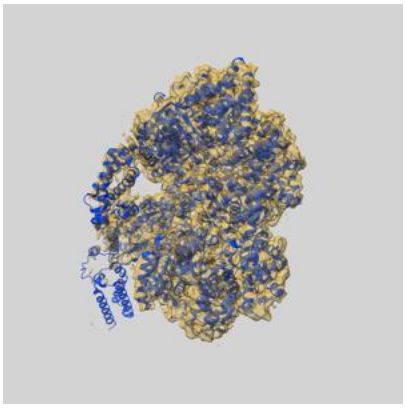
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44712 and PDB model 9BMV. Per-residue inclusion information can be found in section 3 on page 5.

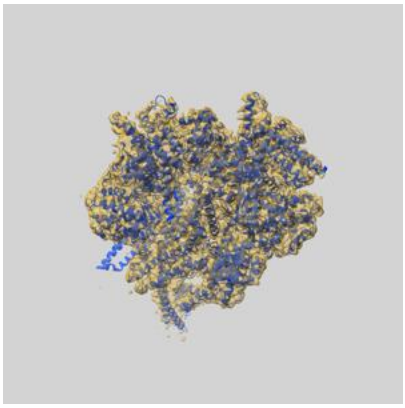
9.1 Map-model overlay



X



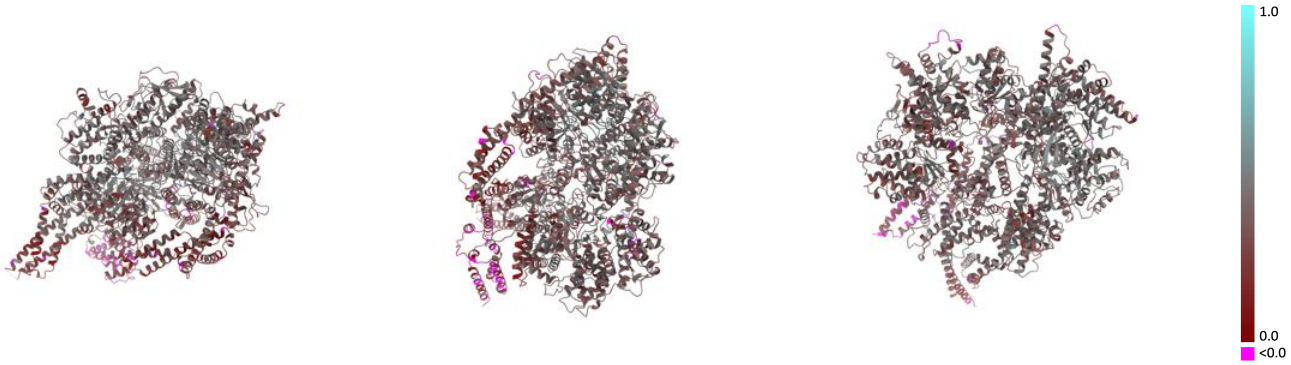
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

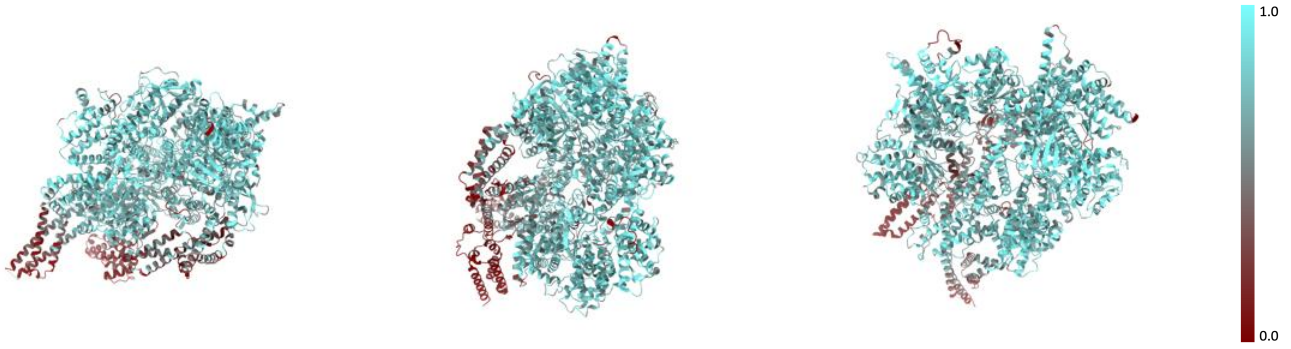
9.2 Q-score mapped to coordinate model (i)



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.

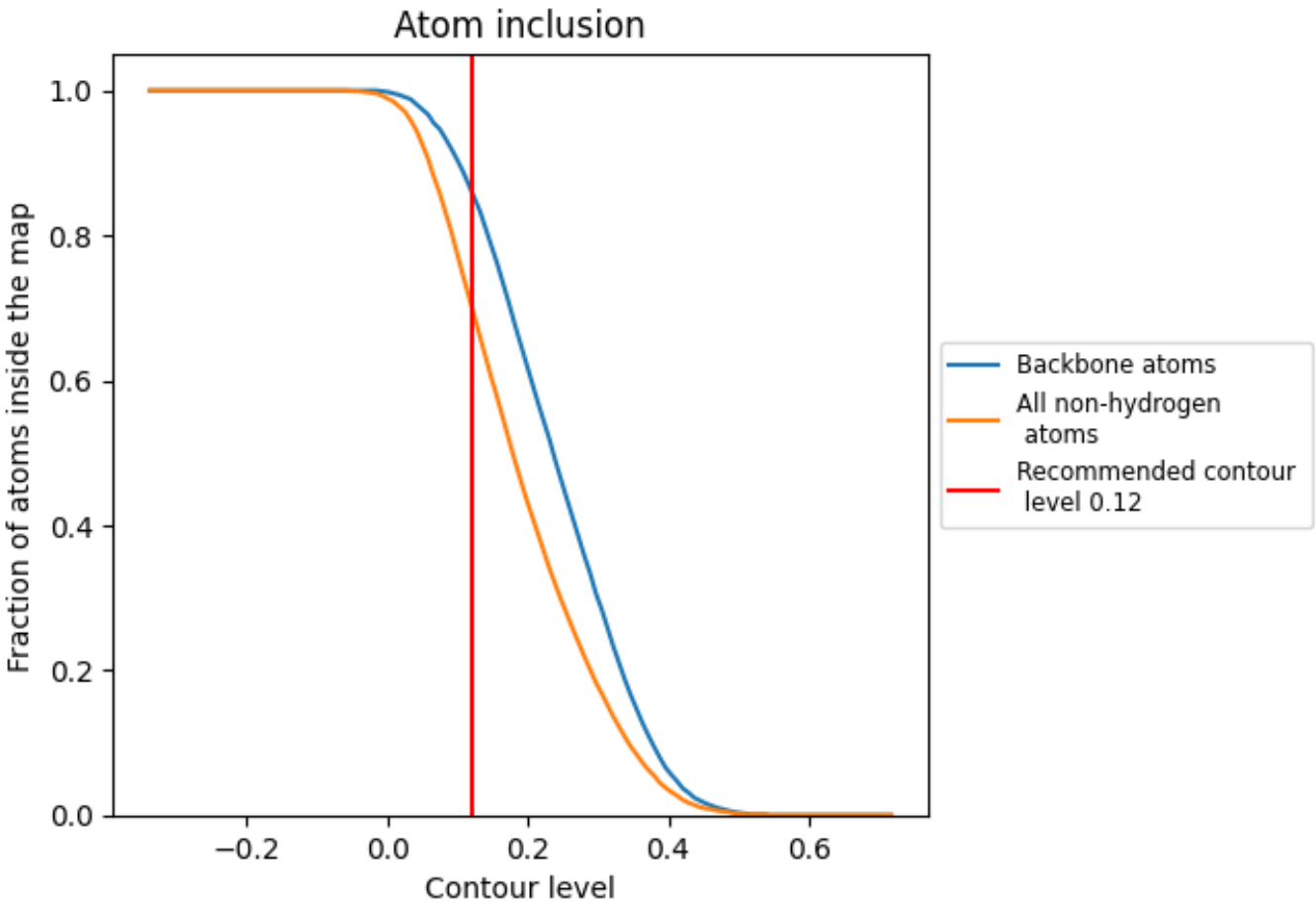
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 70% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7030	0.3600
A	0.7030	0.3600