Full wwPDB EM Validation Report

May 25, 2025 – 10:43 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:

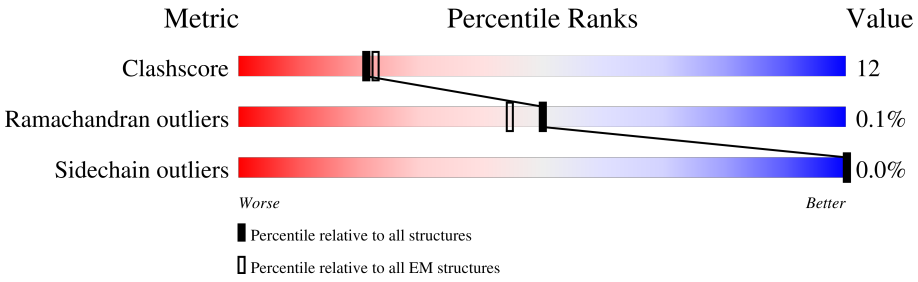
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 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% 17% 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.

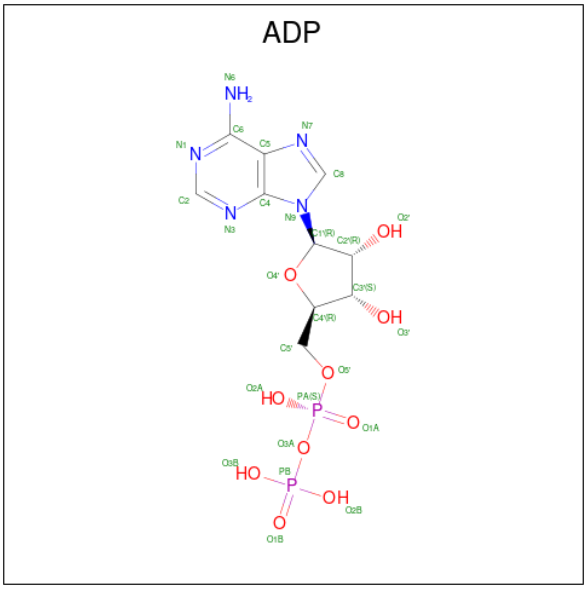
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

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

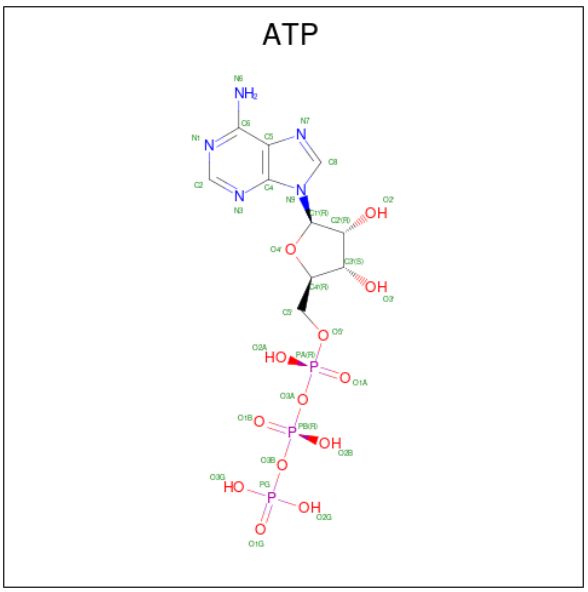
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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).

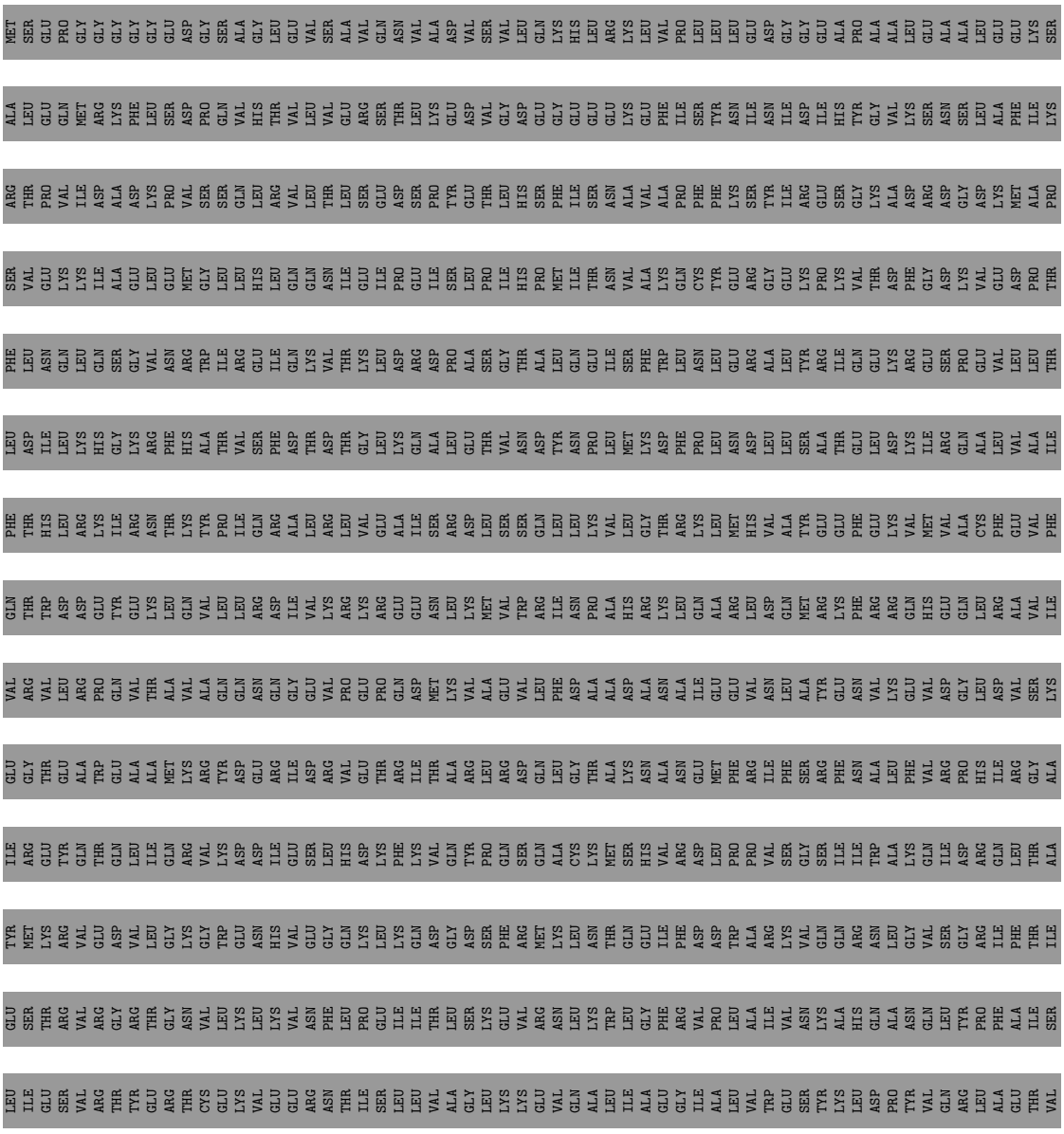


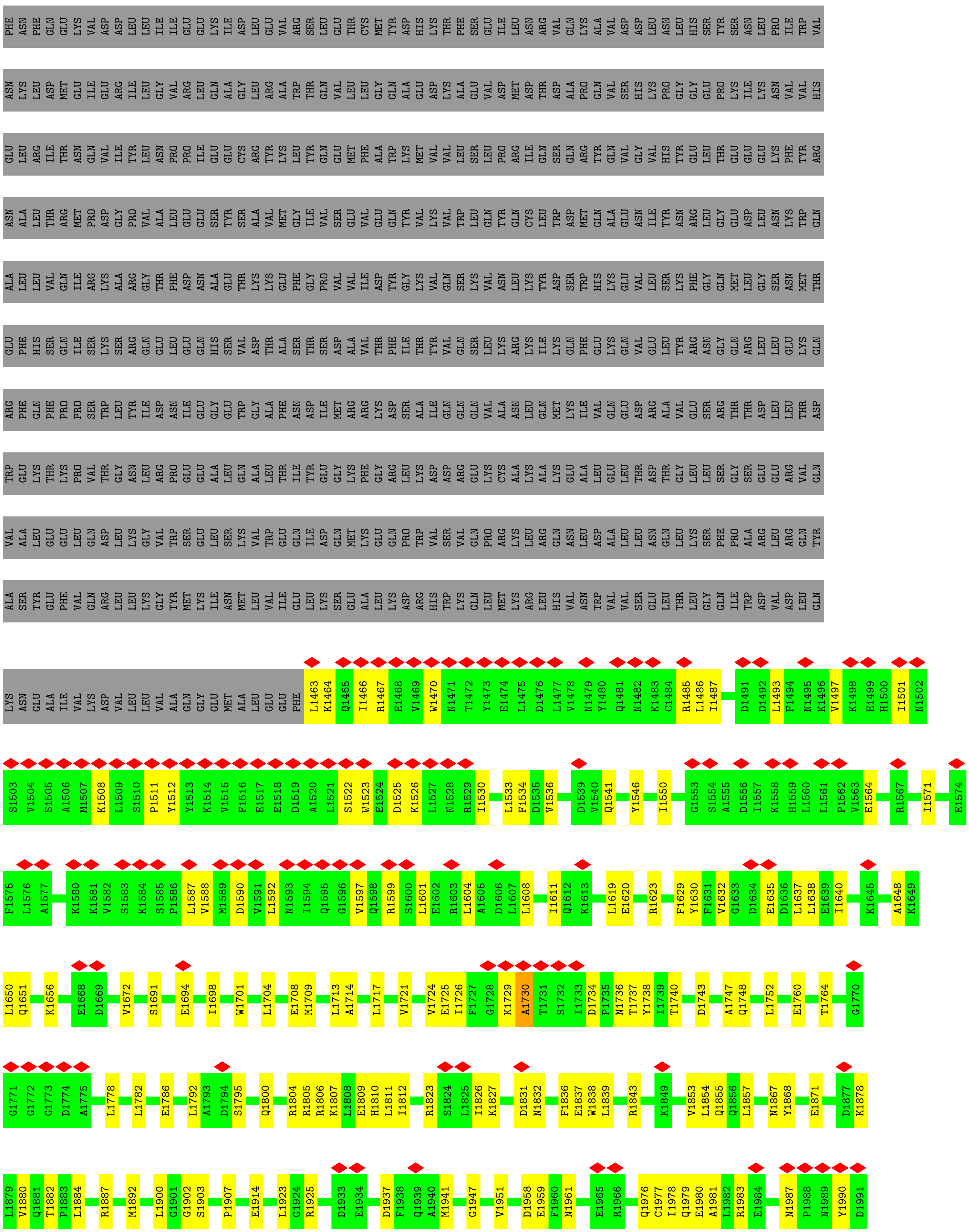
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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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
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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
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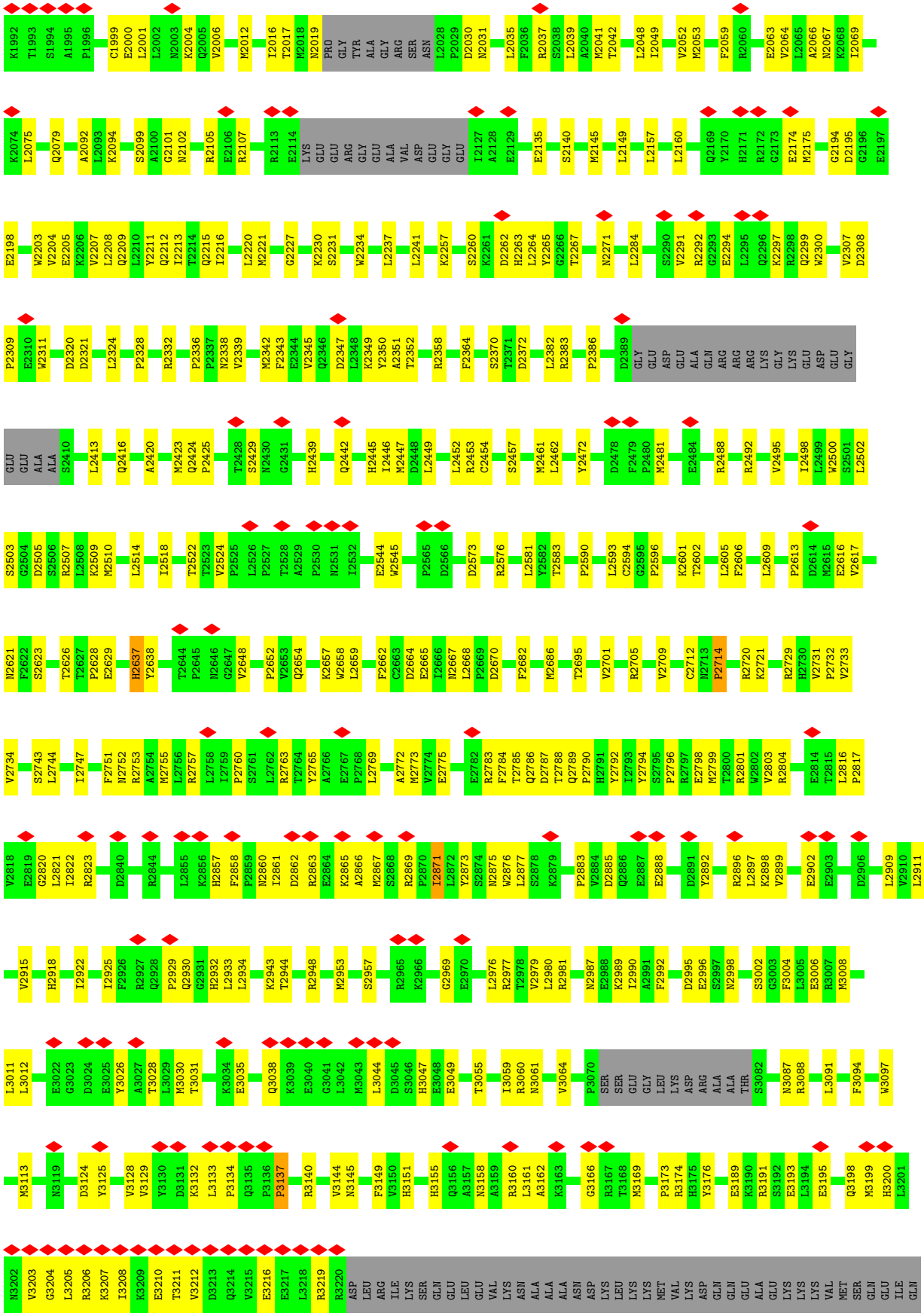
G1771 G1772 G1773 D1774 A1775 L1778 L1782 E1786 L1792 A1793 D1794 S1795 Q1800 R1804 R1805 R1806 K1807 L1808 E1809 H1810 L1811 I1812 R1823 S1824 L1825 I1826 K1827 D1831 N1832 F1836 E1837 W1838 L1839 R1843 K1849 V1853 L1854 Q1855 Q1856 L1857 N1867 Y1868 E1871 D1877 K1878
L1879 V1880 Q1881 T1882 P1883 L1884 R1887 M1892 L1900 G1901 G1902 S1903 P1907 E1914 L1923 G1924 R1925 D1933 E1934 D1937 F1938 Q1939 A1940 M1941 G1947 V1951 D1958 E1959 F1960 N1961 E1965 R1966 Q1976 C1977 I1978 Q1979 E1980 A1981 L1982 R1983 E1984 N1987 P1988 N1989 Y1990 D1991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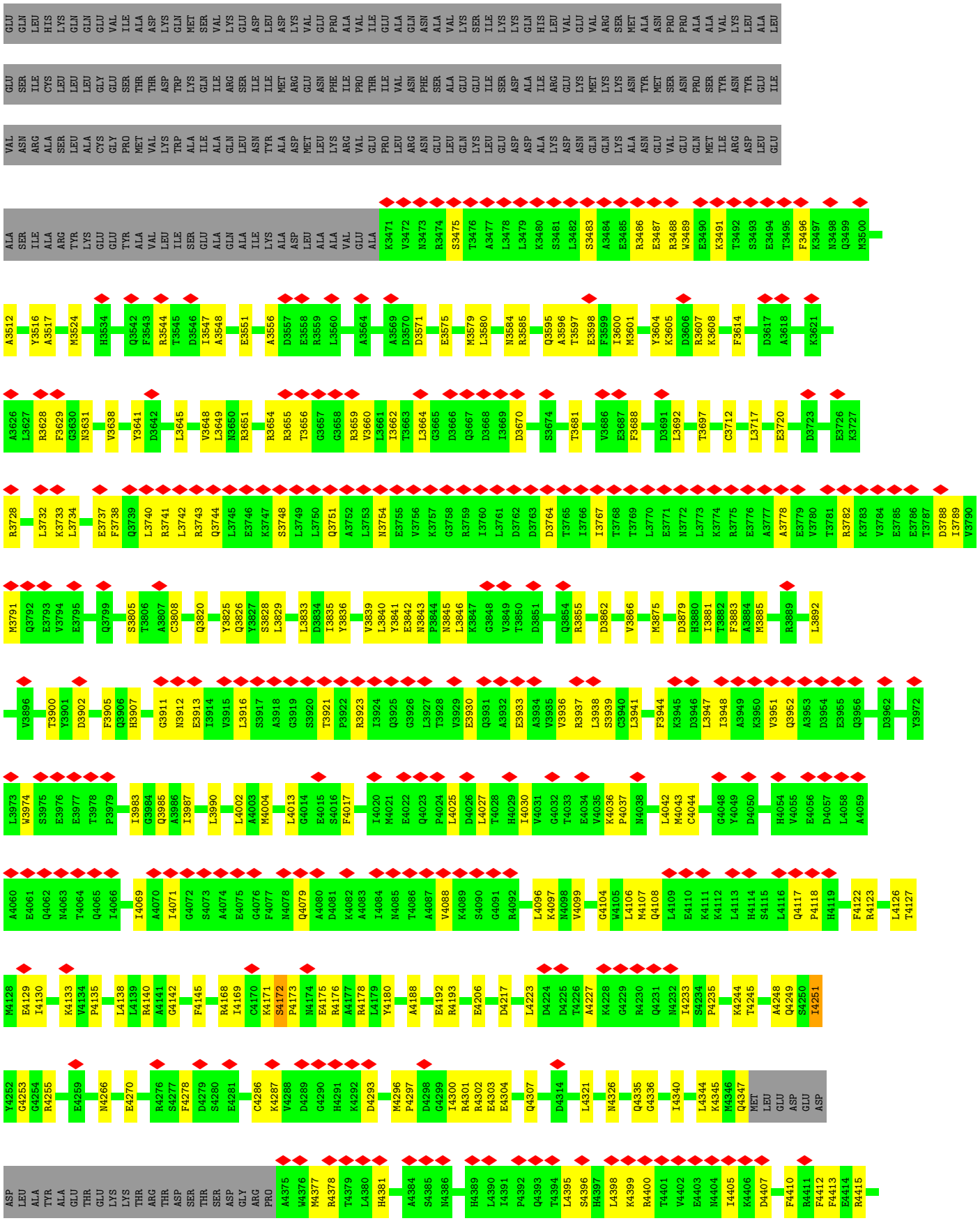
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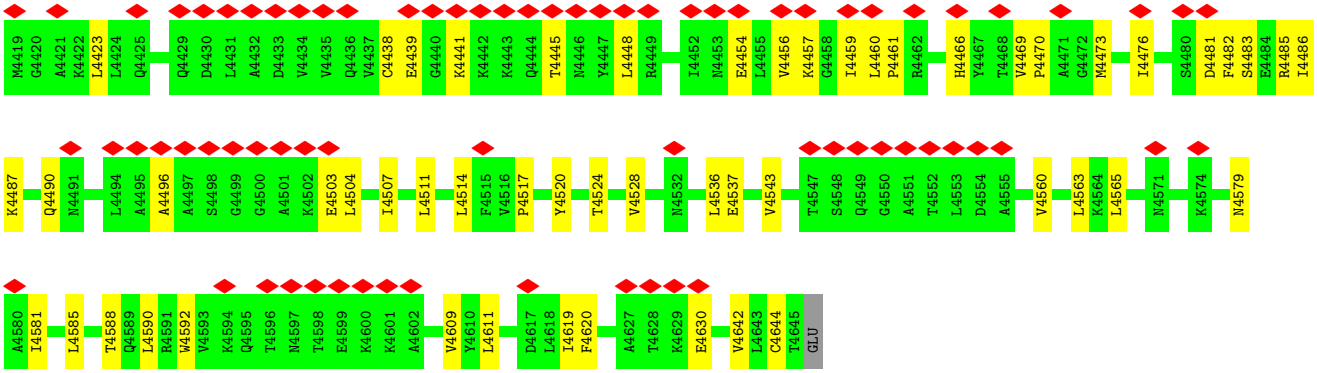
ASP LEU ALA TYR ALA GLU THR GLU LYS LYS THR ARG THR ASP SER THR SER ASP GLY ARG PRO A4375 W4376 M4377 R4378 T4379 L4380 H4381 A4384 S4385 N4386 H4389 L4390 I4391 P4392 Q4393 T4394 L4395 S4396 H4397 L4398 K4399 R4400 T4401 V4402 E4403 M4404 I4405 K4406 D4407 F4410 R4411 F4412 F4413 E4414 R4415


M4419 G4420 A4421 K4422 L4423 L4424 Q4425 Q4429 D4430 L4431 A4432 D4433 V4434 V4435 Q4436 V4437 C4438 E4439 G4440 K4441 K4442 K4443 Q4444 T4445 N4446 Y4447 L4448 R4449 I4452 N4453 E4454 L4455 V4456 K4457 G4458 I4459 L4460 P4461 R4462 H4466 Y4467 T4468 V4469 P4470 A4471 G4472 M4473 I4476 S4480 D4481 F4482 S4483 E4484 R4485 I4486
K4487 Q4490 N4491 L4494 A4495 A4496 A4497 S4498 G4499 G4500 A4501 K4502 E4503 L4504 I4507 L4511 L4514 F4515 V4516 P4517 Y4520 T4524 V4528 N4532 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: ADP, ATP

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	0.17	1/23454 (0.0%)	0.39	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	-6.02	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	-10.21	97.70	112.00
1	A	2714	PRO	N-CD-CG	-8.44	90.54	103.20
1	A	2714	PRO	CA-CB-CG	-7.95	89.40	104.50
1	A	2714	PRO	CA-N-CD	-7.19	101.93	112.00
1	A	2328	PRO	CA-CB-CG	-6.72	91.72	104.50
1	A	3137	PRO	N-CD-CG	-5.89	94.36	103.20
1	A	4300	ILE	N-CA-C	-5.70	107.72	113.47

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	537	0
2	A	54	0	24	2	0
3	A	62	0	24	0	0
All	All	23078	0	23078	537	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (537) 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:4469:VAL:HG13	1:A:4473:MET:HE2	1.65	0.76
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:4377:MET:HE3	1:A:4438:CYS:HA	1.73	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:3488:ARG:HH11	1:A:3489:TRP:CD1	2.18	0.62
1:A:3948:ILE:HG22	1:A:3952:GLN:HE22	1.65	0.62
1:A:2507:ARG:HH21	1:A:2510:MET:HE2	1.64	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2934:LEU:HD23	1:A:3091:LEU:HG	1.85	0.59
1:A:2773:MET:HE1	1:A:2803:VAL:HG22	1.85	0.59
1:A:3151:HIS:NE2	1:A:3155:HIS:HE1	1.99	0.59
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:3008:MET:HA	1:A:3008:MET:HE2	1.85	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:1709:MET:HE3	1:A:1871:GLU:HA	1.86	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:3030:MET:HA	1:A:3030:MET:HE3	1.86	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:4027:LEU:HD11	1:A:4043:MET:HE1	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:2823:ARG:HD2	1:A:2867:MET:HE3	1.90	0.52
1:A:1493:LEU:HD21	1:A:1534:PHE:CG	2.44	0.52
1:A:2876:TRP:CD1	1:A:2892:TYR:HH	2.28	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:3875:MET:HE1	1:A:3883:PHE:HB2	1.91	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:2823:ARG:HB2	1:A:2867:MET:HE3	1.91	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:2175:MET:HE3	1:A:2208:LEU:HD13	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3161:LEU:HD13	1:A:3524:MET:HE3	1.92	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
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:2752:ASN:HD22	1:A:2755:MET:HE2	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:2092:ALA:HB1	1:A:2145:MET:HE1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2107:ARG:NH1	1:A:2135:GLU:OE2	2.47	0.48
1:A:3748:SER:HA	1:A:3751:GLN:CD	2.39	0.48
1:A:4069:ILE:HG23	1:A:4079:GLN:HE21	1.79	0.48
1:A:2876:TRP:CZ2	1:A:2953:MET:HE3	2.49	0.48
1:A:3517:ALA:O	1:A:3579:MET:HE1	2.12	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:3204:GLY:C	1:A:3489:TRP:HZ3	2.22	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
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:3160:ARG:NH2	1:A:3524:MET:HE1	2.30	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:1941:MET:HE3	1:A:1941:MET:HA	1.96	0.47
1:A:2262:ASP:OD1	1:A:2267:THR:OG1	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2099:SER:OG	1:A:2140:SER:OG	2.19	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:3907:HIS:HE2	1:A:3938:LEU:HG	1.80	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
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:2220:LEU:HD21	1:A:2342:MET:HE2	1.98	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:2423:MET:HE1	1:A:2462:LEU:HD12	1.98	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3733:LYS:HE2	1:A:3738:PHE:CE1	2.51	0.45
1:A:3907:HIS:HE2	1:A:3938:LEU:HA	1.80	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:1620:GLU:OE2	1:A:2004:LYS:NZ	2.43	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:1837:GLU:H	1:A:1837:GLU:CD	2.24	0.45
1:A:1914:GLU:HG3	2:A:4701:ADP:H3'	1.99	0.45
1:A:2053:MET:HB3	1:A:2053:MET:HE2	1.78	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1978:ILE:HG23	1:A:2012:MET:HE1	1.98	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:2472:TYR:CD2	1:A:2481:MET:HE2	2.54	0.42
1:A:2896:ARG:HA	1:A:2899:VAL:HG12	2.01	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2307:VAL:HA	1:A:2311:TRP:CZ2	2.55	0.42
1:A:2773:MET:HB3	1:A:2799:MET:HE3	2.02	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
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:3169:MET:HE1	1:A:3688:PHE:H	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4004:MET:HE2	1:A:4004:MET:HA	2.03	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:2461:MET:HE1	1:A:2500:TRP:HB2	2.02	0.41
1:A:2799:MET:HE2	1:A:2799:MET:HB3	1.98	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
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:3556:ALA:HB2	1:A:3737:GLU:CD	2.45	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:2682:PHE:CE2	1:A:2686:MET:HE2	2.56	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	2539 (100%)	1 (0%)	100 100

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

Mol	Chain	Res	Type
1	A	2637	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1541	GLN
1	A	1595	GLN
1	A	1612	GLN
1	A	1832	ASN
1	A	1867	ASN
1	A	1881	GLN
1	A	1979	GLN
1	A	2445	HIS
1	A	2464	GLN
1	A	2485	GLN
1	A	2621	ASN
1	A	2677	GLN
1	A	2689	HIS
1	A	2713	ASN
1	A	2725	HIS
1	A	3069	ASN
1	A	3087	ASN
1	A	3104	GLN
1	A	3155	HIS
1	A	3526	GLN
1	A	3631	ASN
1	A	3667	GLN
1	A	3744	GLN
1	A	3754	ASN

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Mol	Chain	Res	Type
1	A	3830	GLN
1	A	3843	ASN
1	A	3952	GLN
1	A	3956	GLN
1	A	4079	GLN
1	A	4262	GLN
1	A	4335	GLN
1	A	4595	GLN
1	A	4612	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)

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	$\#\|Z\| > 2$
2	ADP	A	4701	-	24,29,29	0.88	0	29,45,45	1.24	2 (6%)
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%)
3	ATP	A	4702	-	28,33,33	0.65	0	34,52,52	0.59	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4701	-	-	3/12/32/32	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
3	ATP	A	4702	-	-	7/18/38/38	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

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Mol	Chain	Res	Type	Atoms
3	A	4702	ATP	PB-O3A-PA-O2A

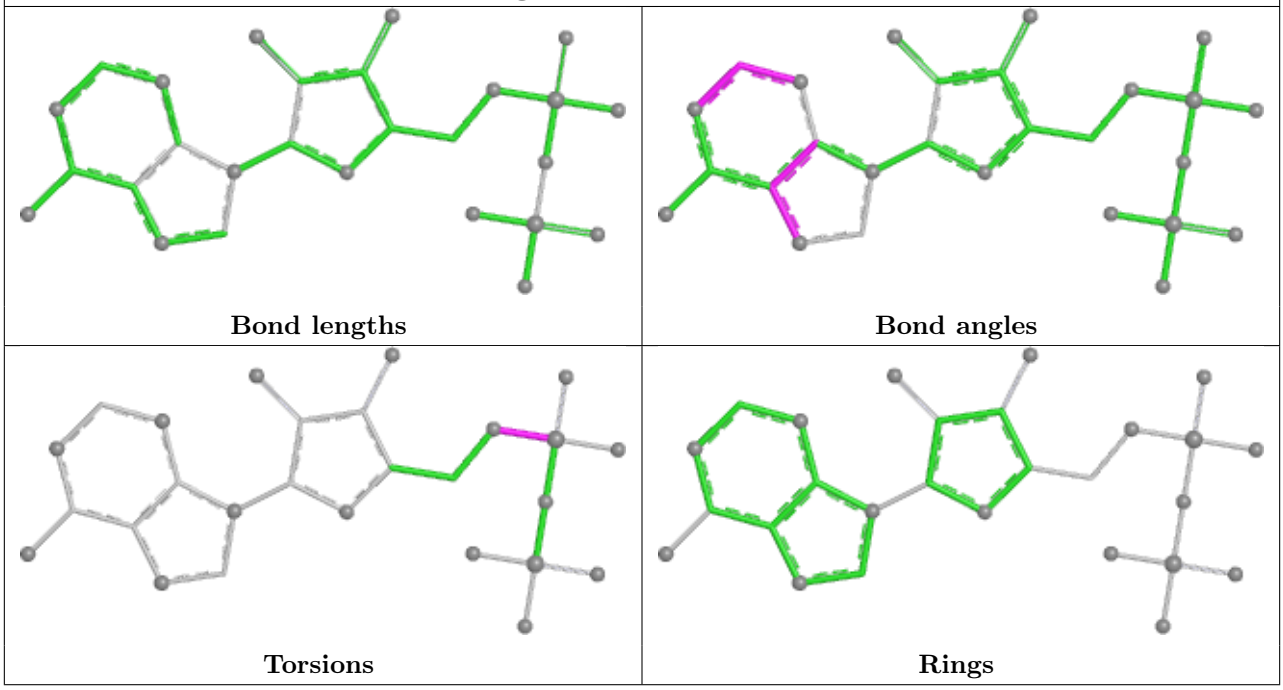
There are no ring outliers.

2 monomers are involved in 2 short contacts:

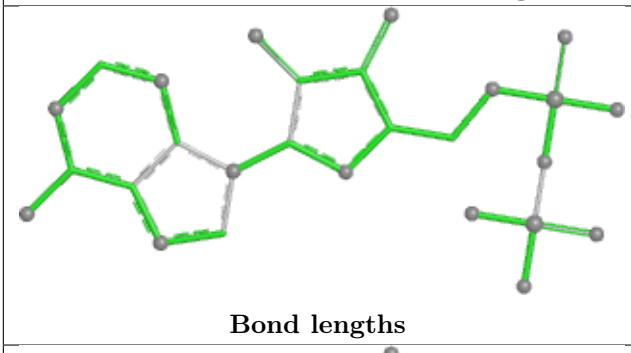
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	1	0
2	A	4704	ADP	1	0

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.

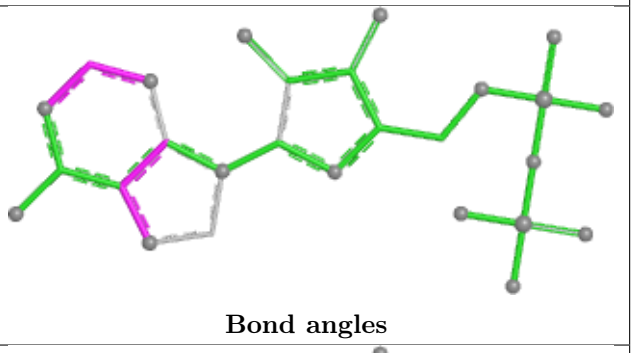
Ligand ADP A 4701



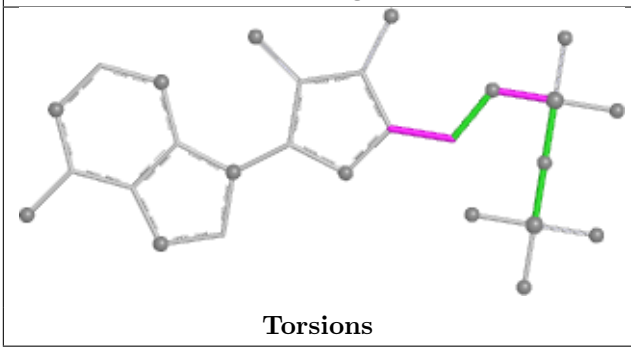
Ligand ADP A 4704



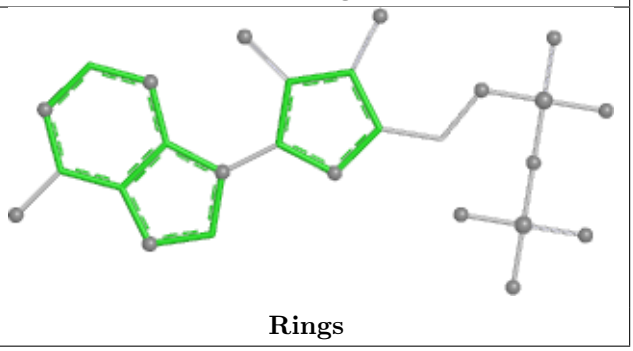
Bond lengths



Bond angles

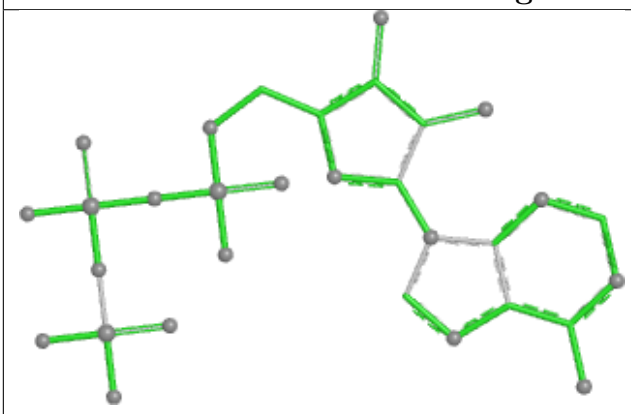


Torsions

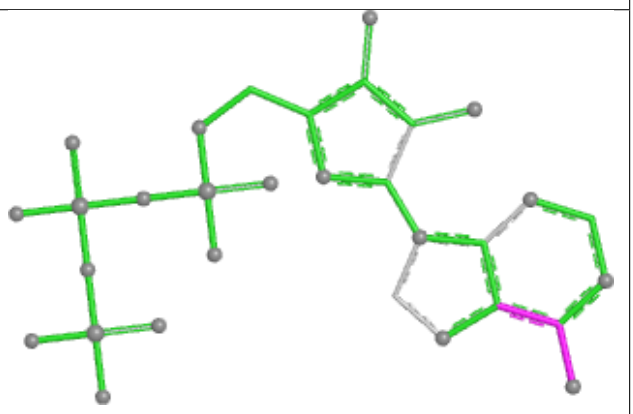


Rings

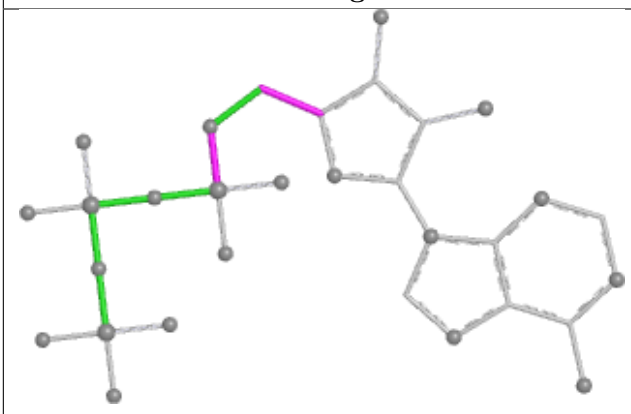
Ligand ATP A 4703



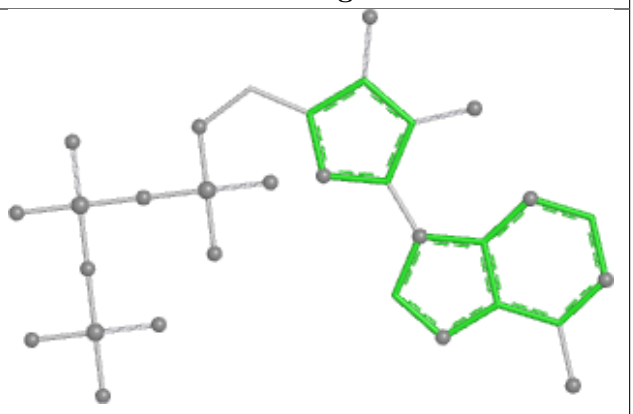
Bond lengths



Bond angles

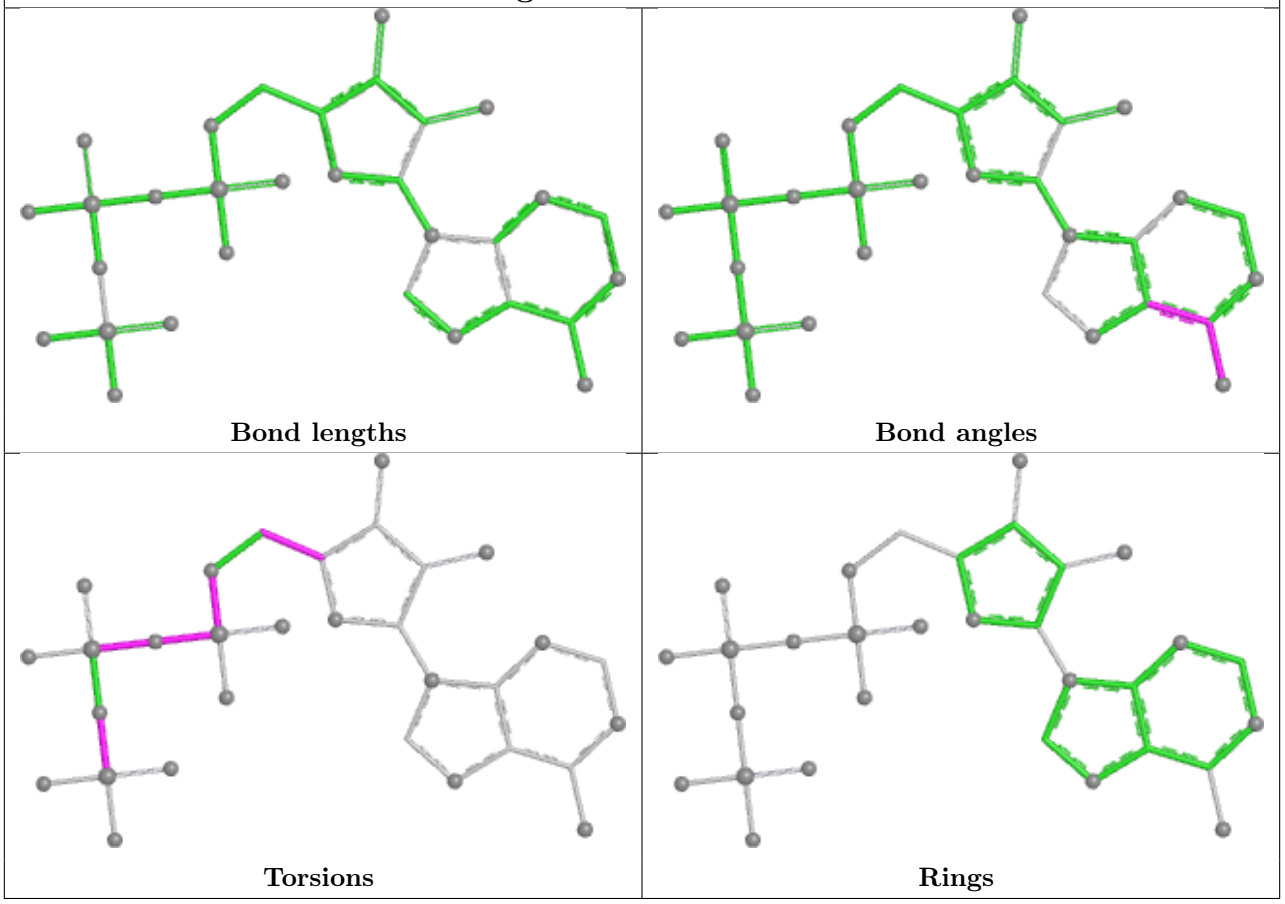


Torsions



Rings

Ligand ATP A 4702



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.

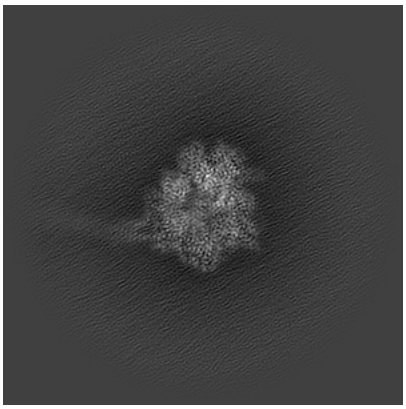
6 Map visualisation

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

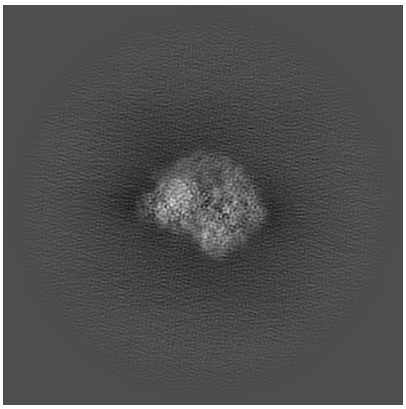
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

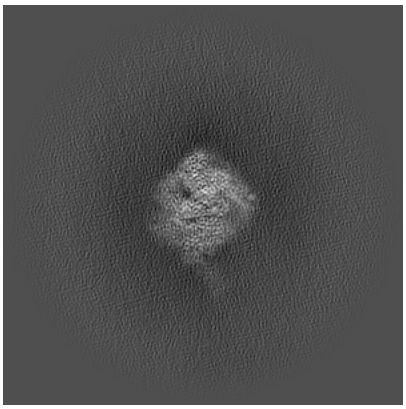
6.1.1 Primary map



X

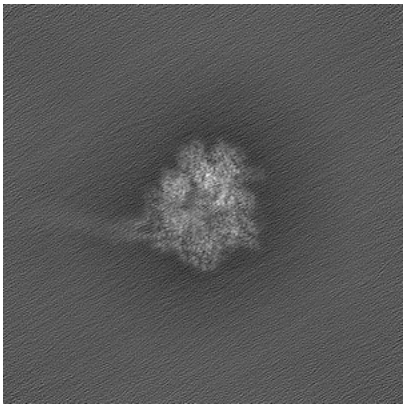


Y

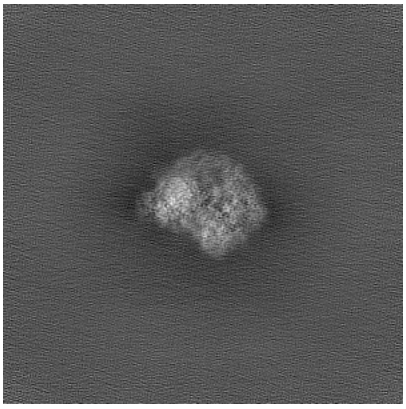


Z

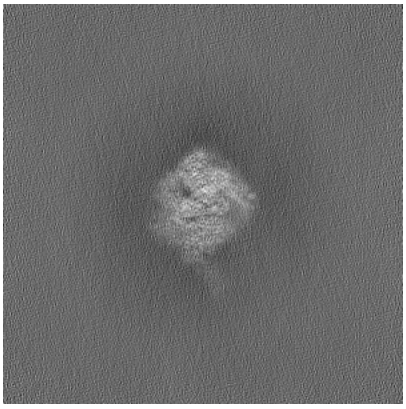
6.1.2 Raw map



X



Y

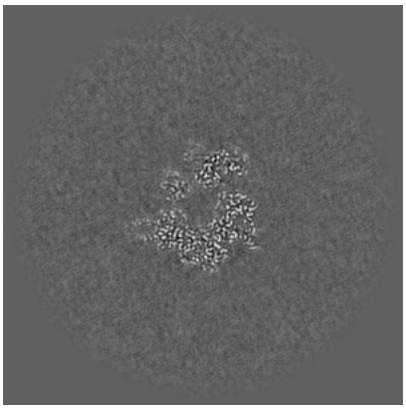


Z

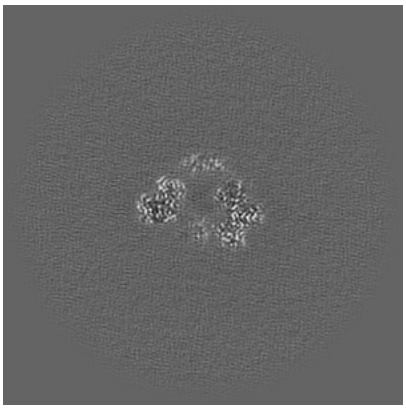
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

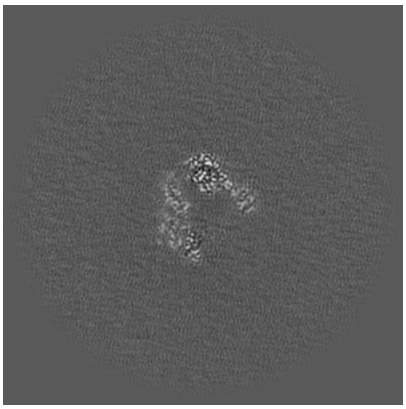
6.2.1 Primary map



X Index: 180

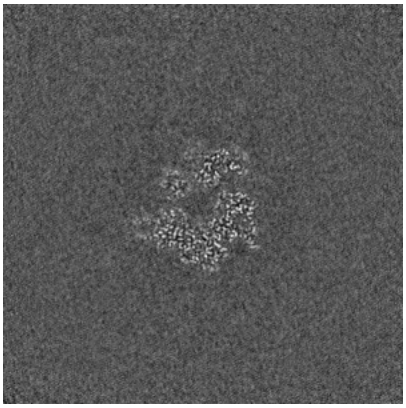


Y Index: 180

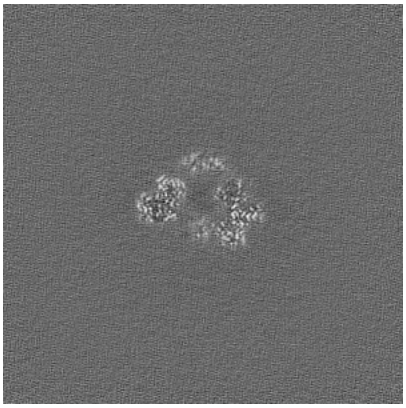


Z Index: 180

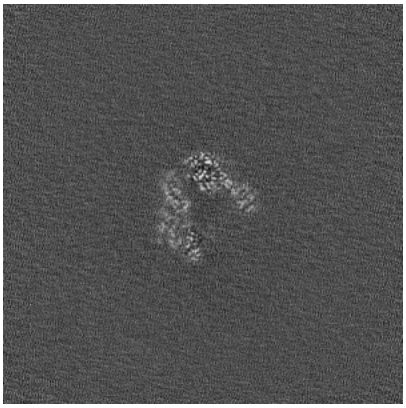
6.2.2 Raw map



X Index: 180



Y Index: 180

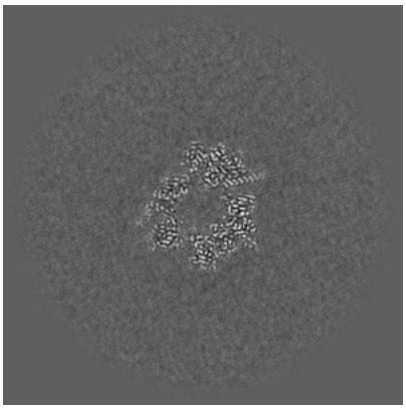


Z Index: 180

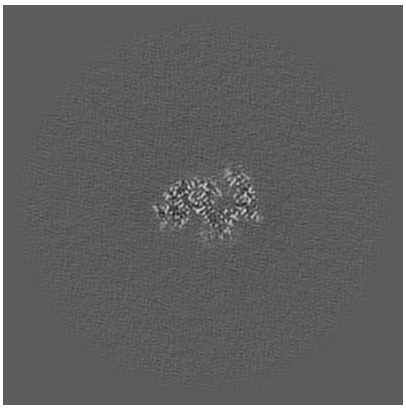
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

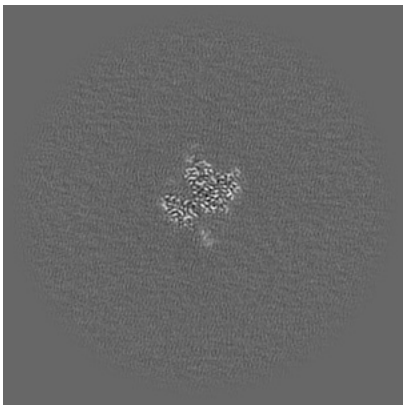
6.3.1 Primary map



X Index: 175

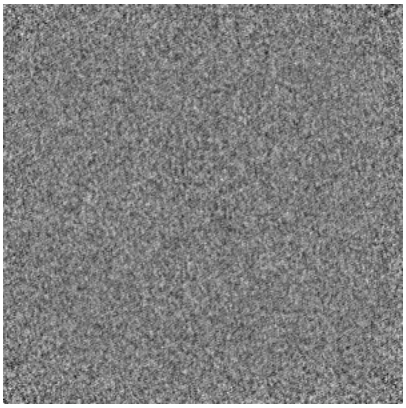


Y Index: 203

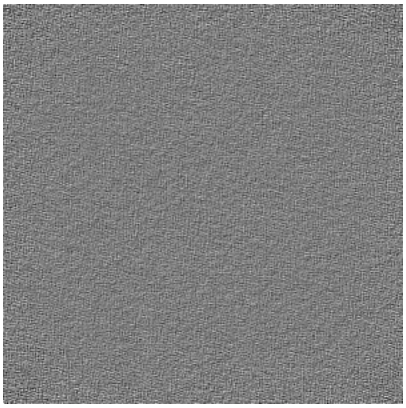


Z Index: 209

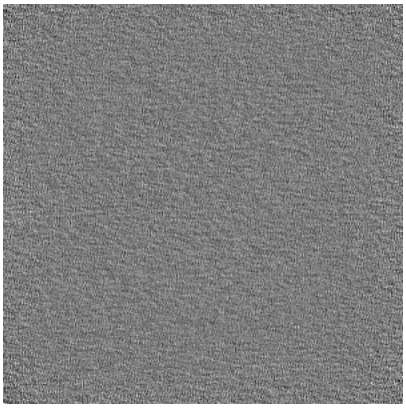
6.3.2 Raw map



X Index: 0



Y Index: 0

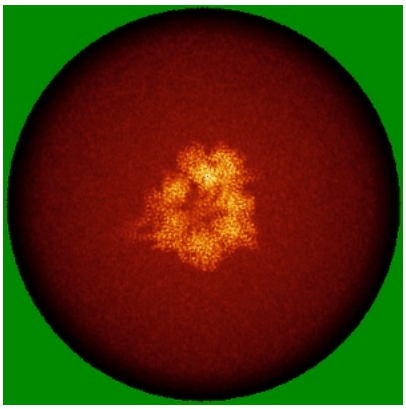


Z Index: 0

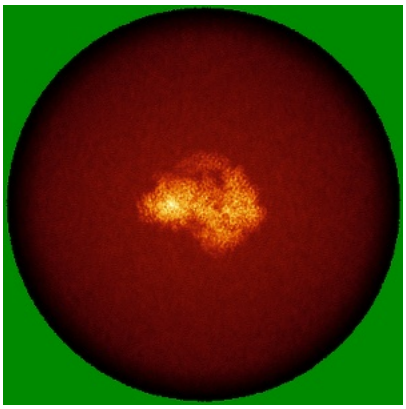
The images above show the largest variance slices of the map in three orthogonal directions.

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

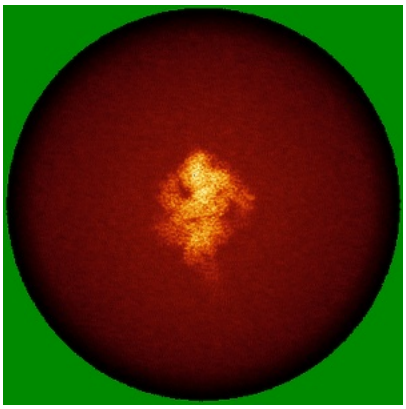
6.4.1 Primary map



X

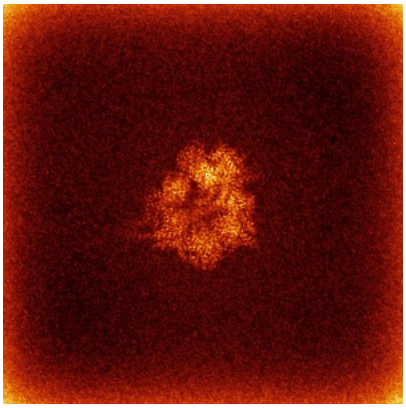


Y

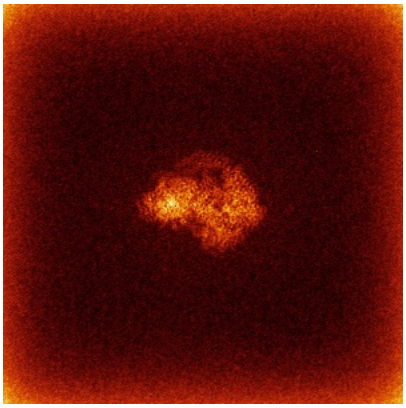


Z

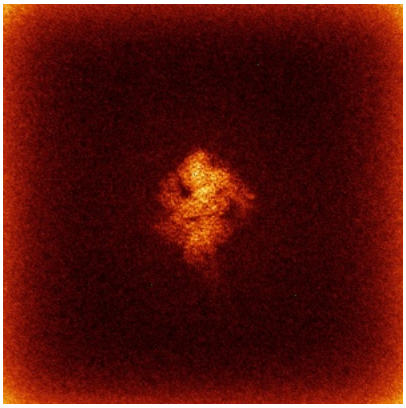
6.4.2 Raw map



X



Y

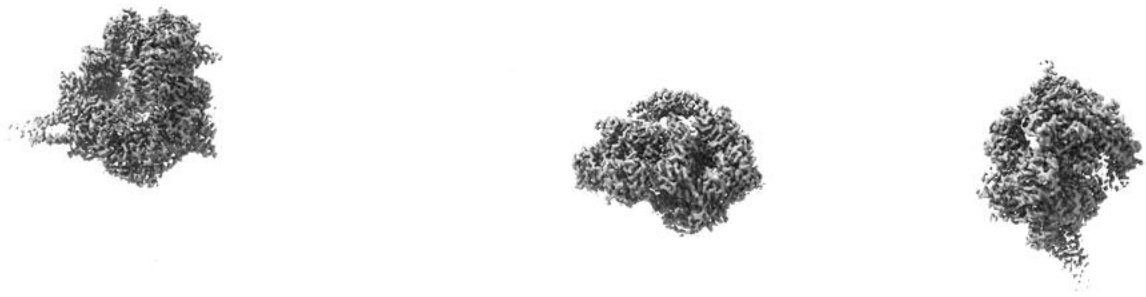


Z

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)

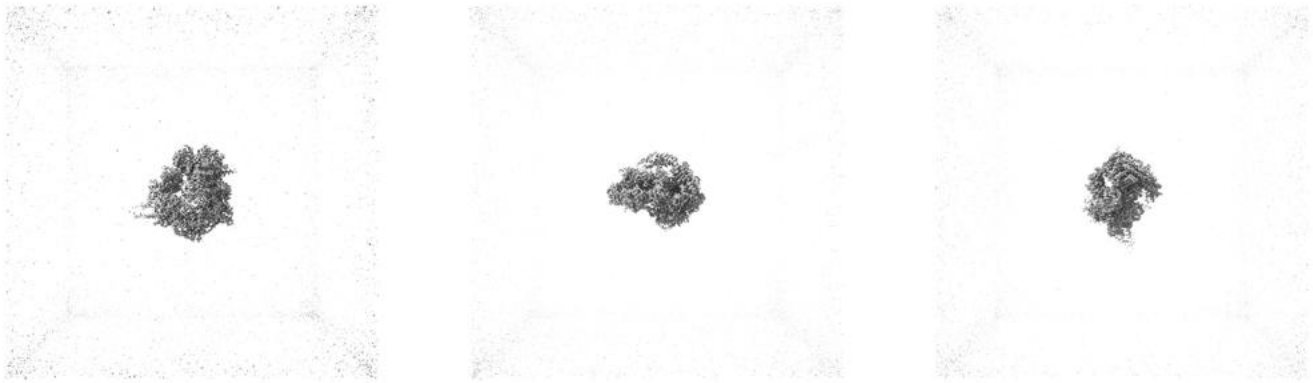
6.5.1 Primary map



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.

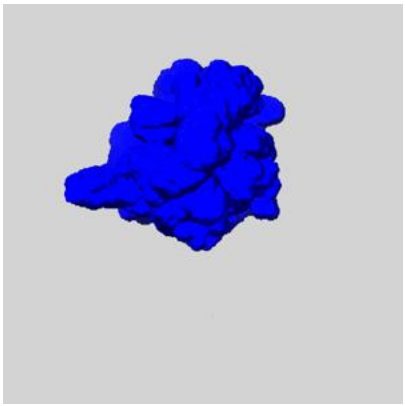
6.6 Mask visualisation

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

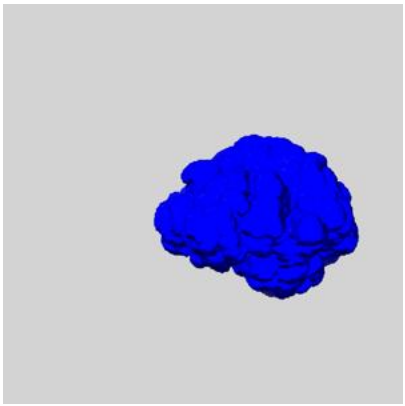
A mask typically either:

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

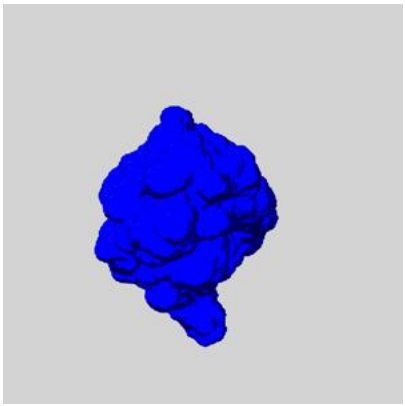
6.6.1 emd_44721_msk_1.map



X



Y

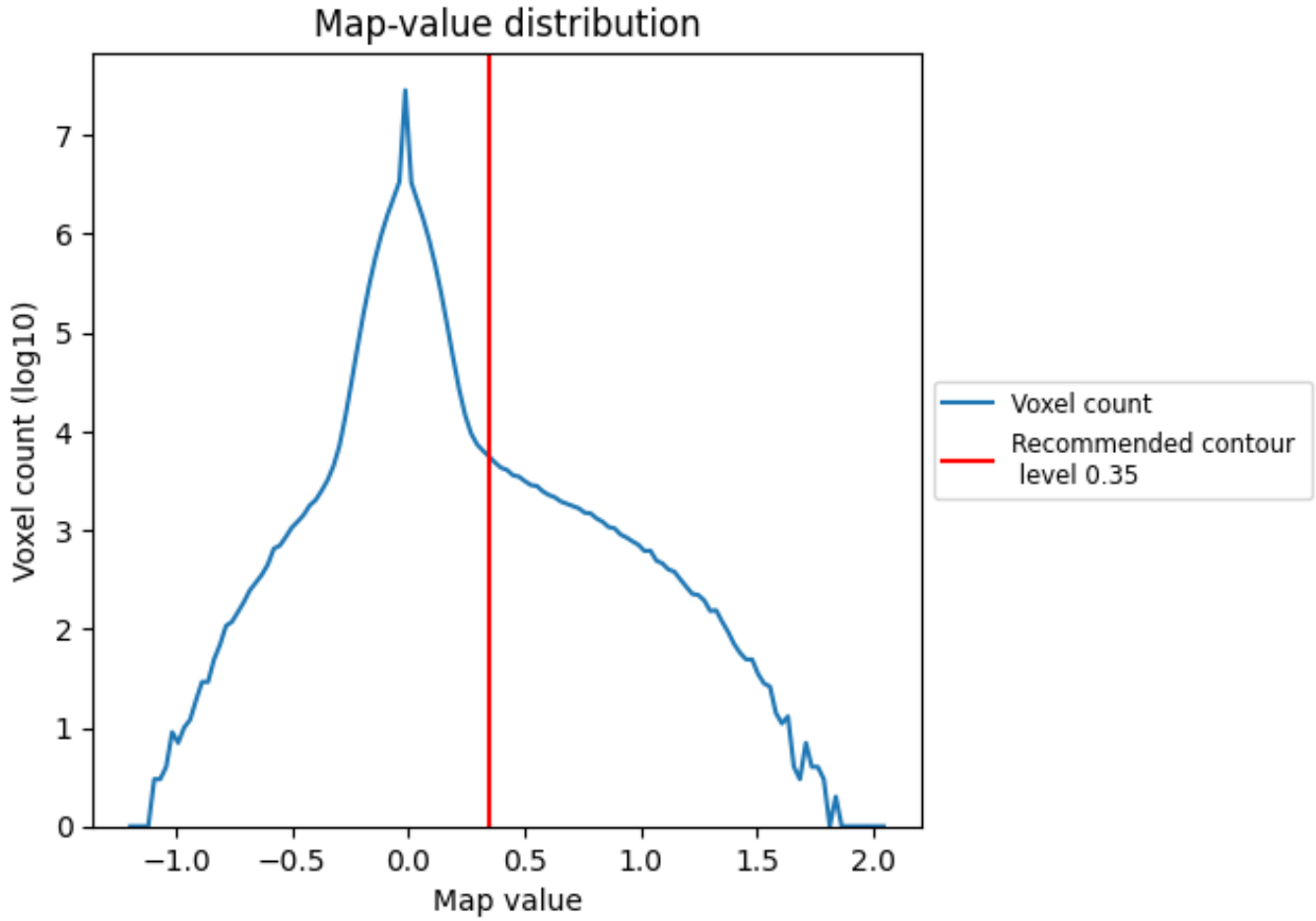


Z

7 Map analysis

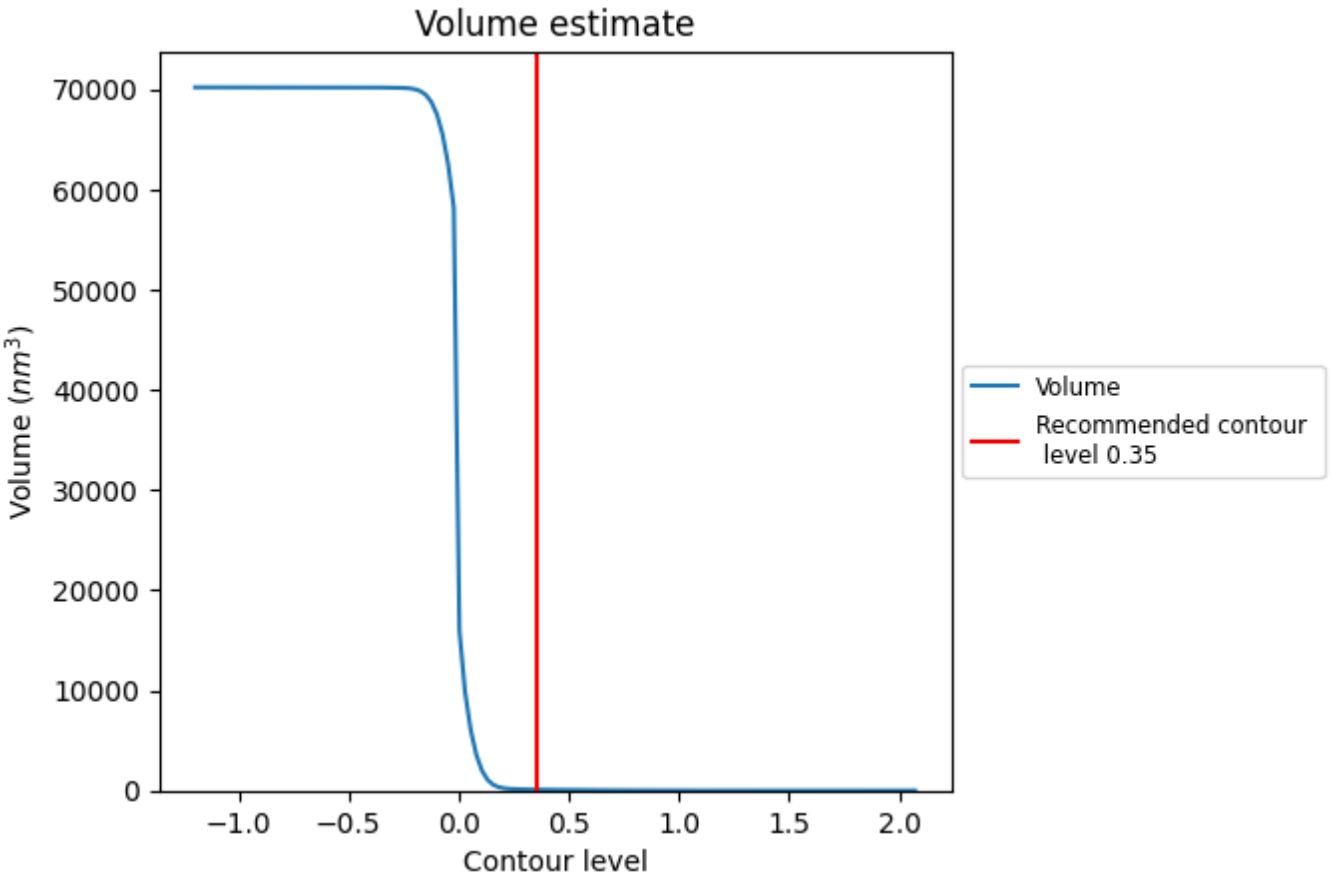
This section contains the results of statistical analysis of the map.

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.

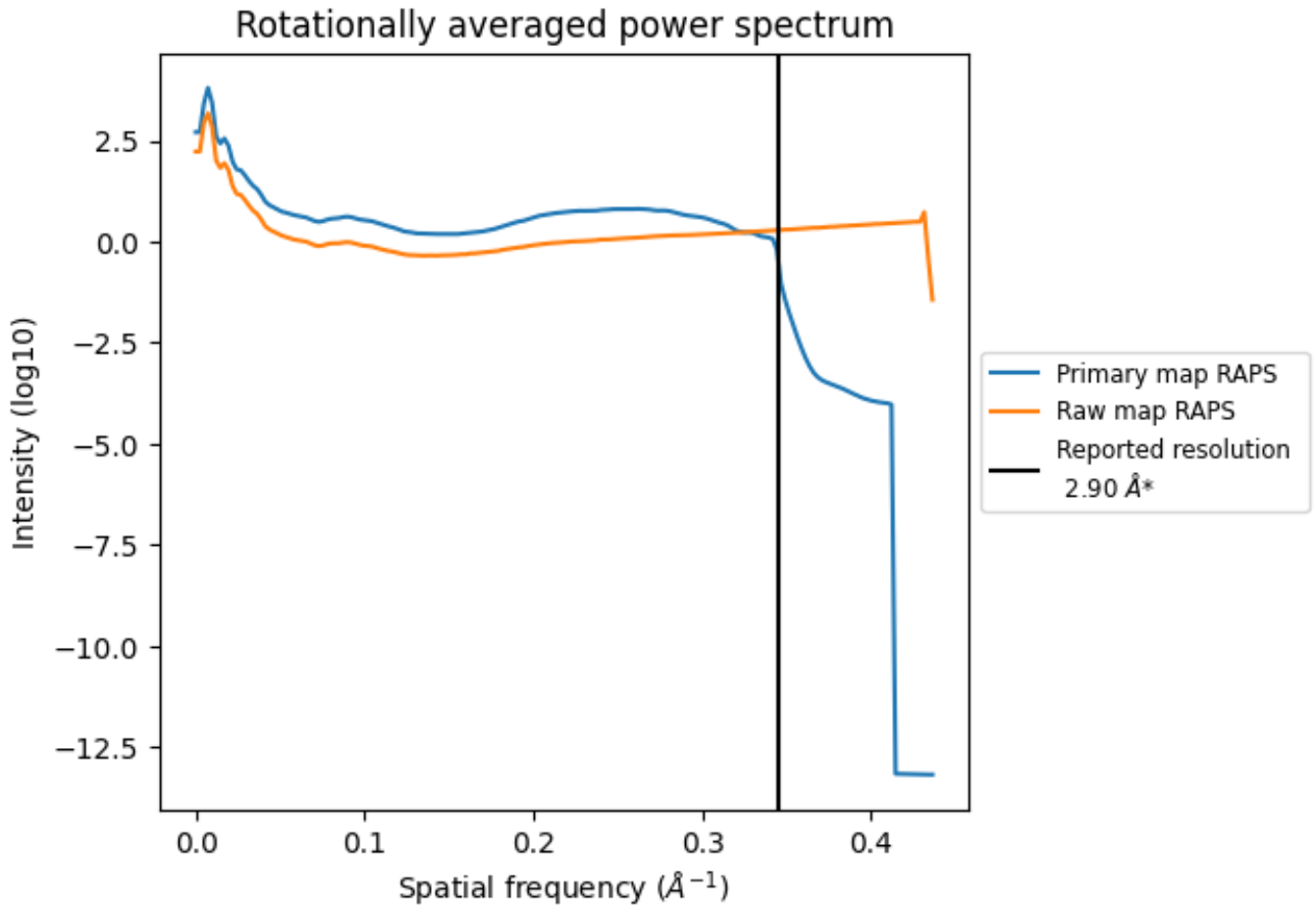
7.2 Volume estimate



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)

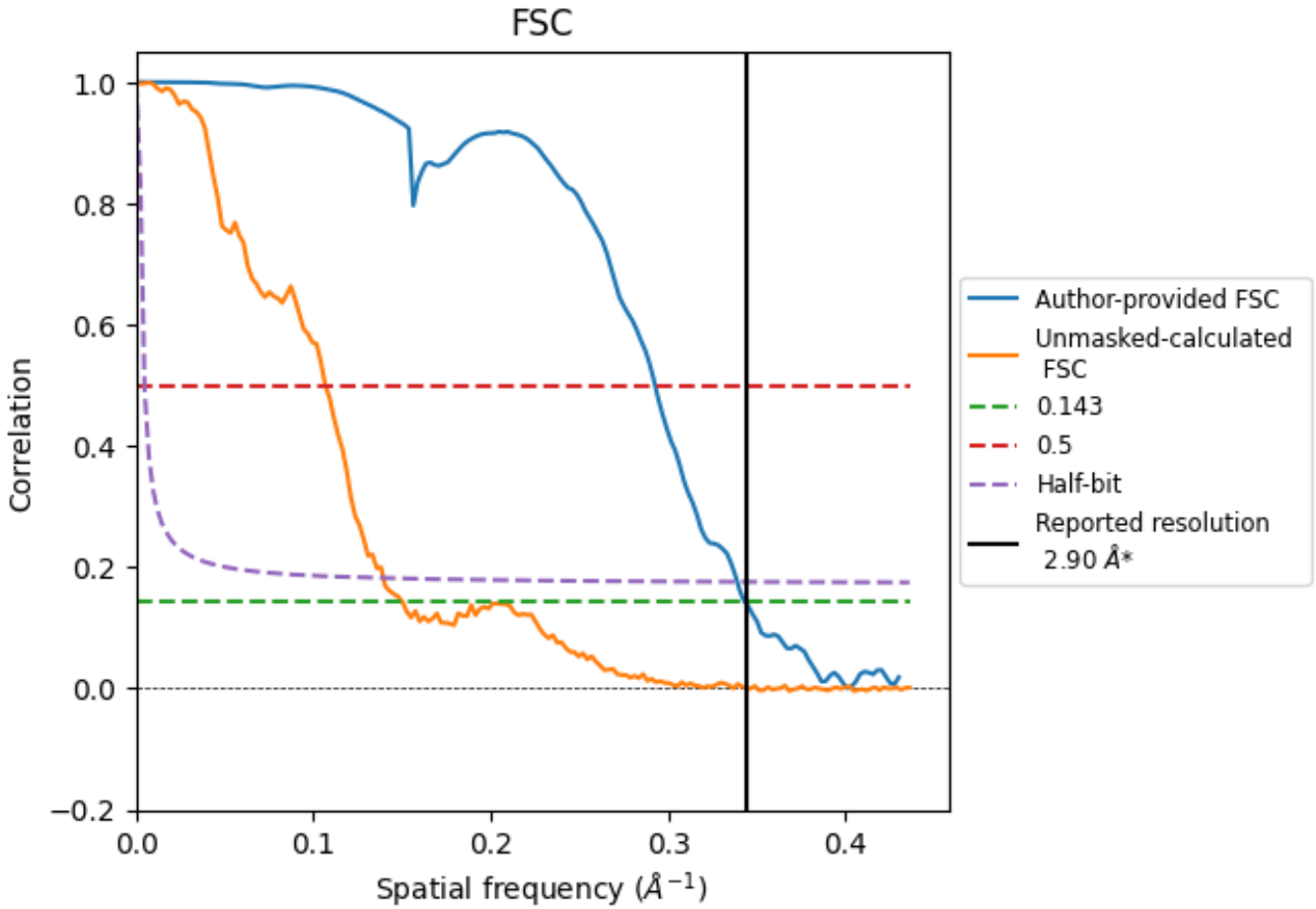


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

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)

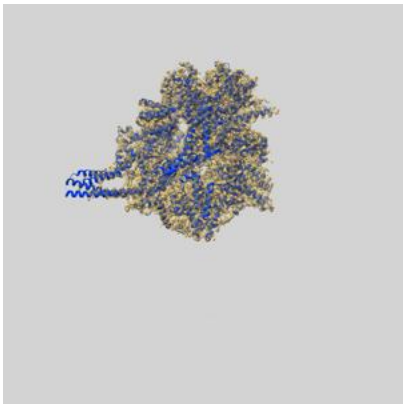
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.91	3.42	2.95
Unmasked-calculated*	6.66	9.37	7.16

*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 %

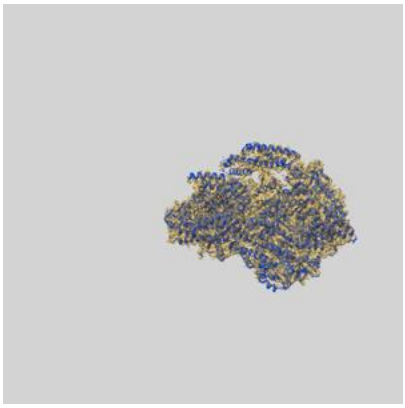
9 Map-model fit

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.

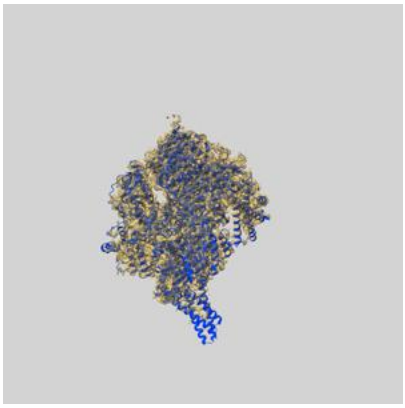
9.1 Map-model overlay



X



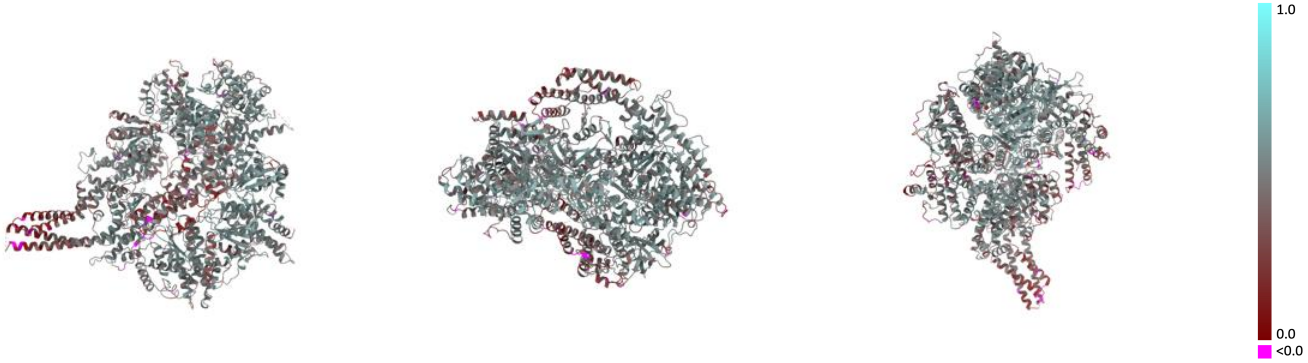
Y



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.

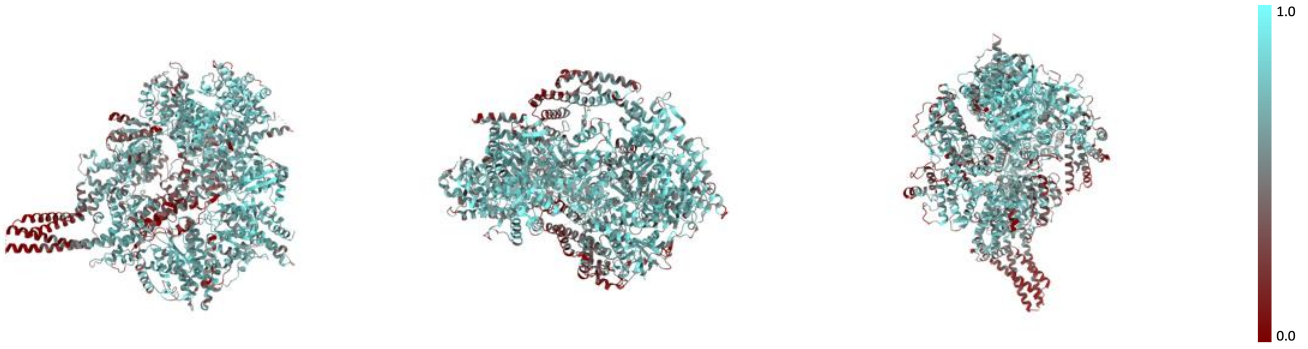
9.2 Q-score mapped to coordinate model (i)



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.

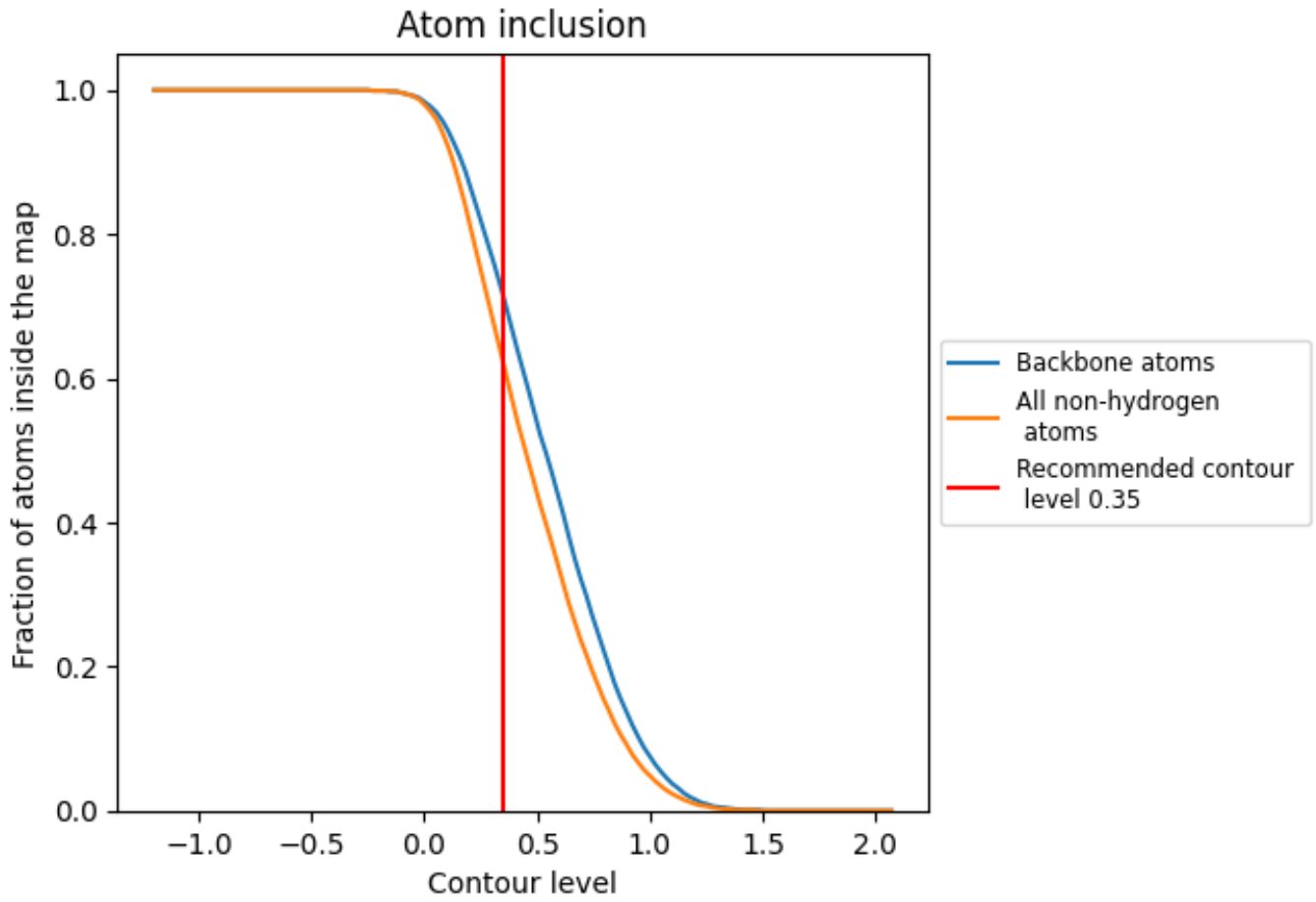
9.3 Atom inclusion mapped to coordinate model (i)



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