Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 01:26 PM EDT

PDB ID	:	9BMP / pdb_00009bmp
EMDB ID	:	EMD-44706
Title	:	State-7 of the motor domain from full-length human dynein-1 in 5mM AMPPNP
Authors	:	Chai, P.; Zhang, K.
Deposited on	:	2024-05-02
Resolution	:	3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

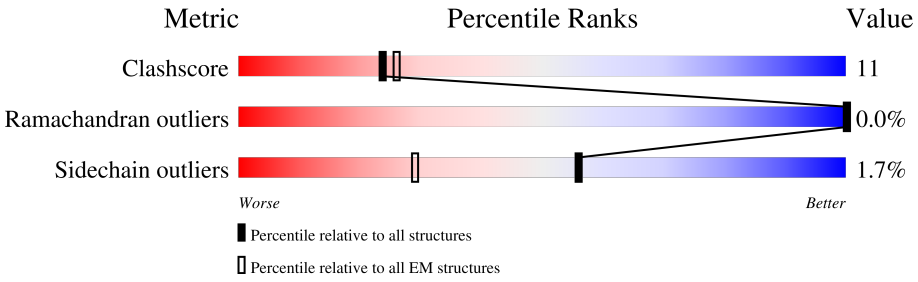
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	6% 46% 15% • 38%

2 Entry composition

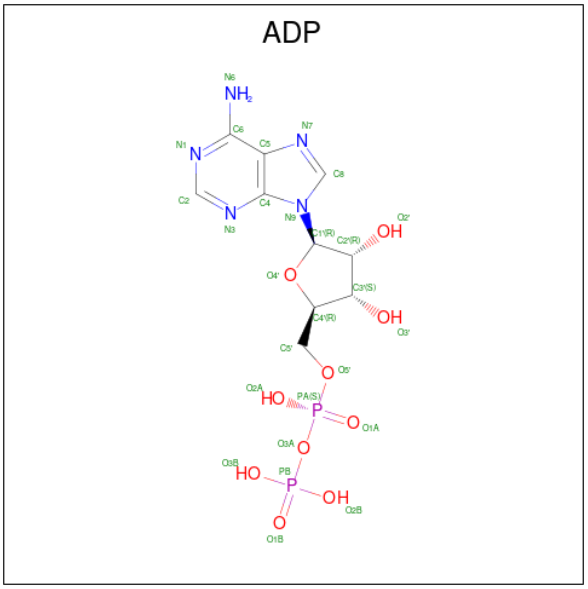
There are 4 unique types of molecules in this entry. The entry contains 23110 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

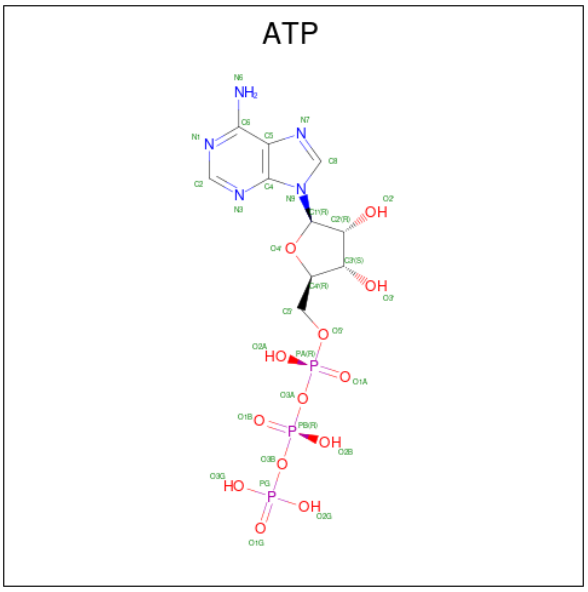
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2858	22994	14663	3967	4249	115	0	0

- 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).



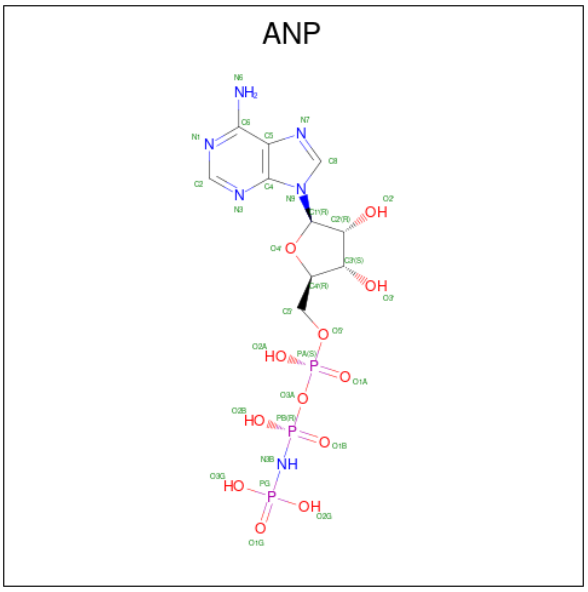
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0

- 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 PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



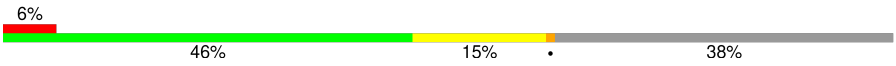
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

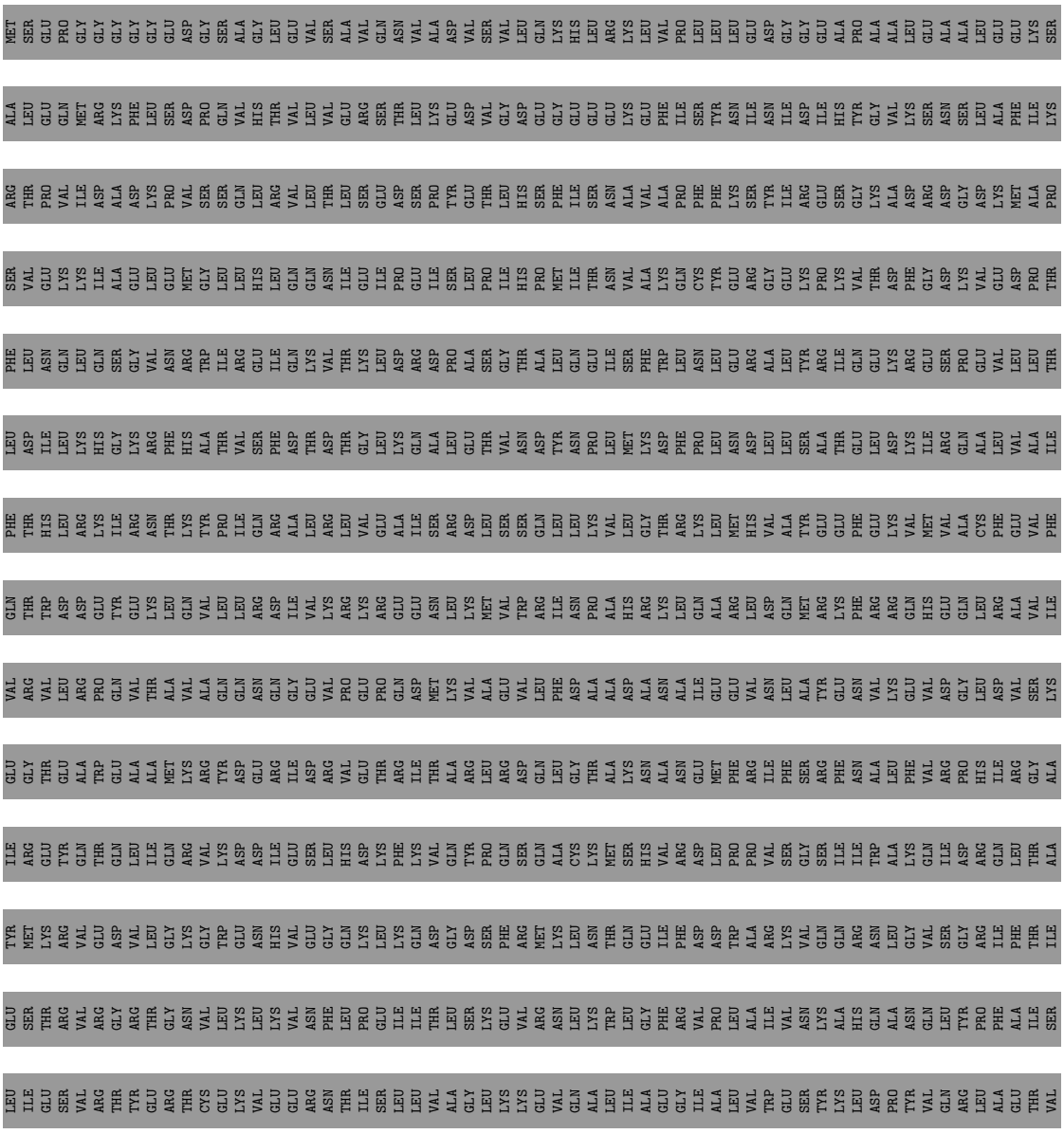
3 Residue-property plots (i)

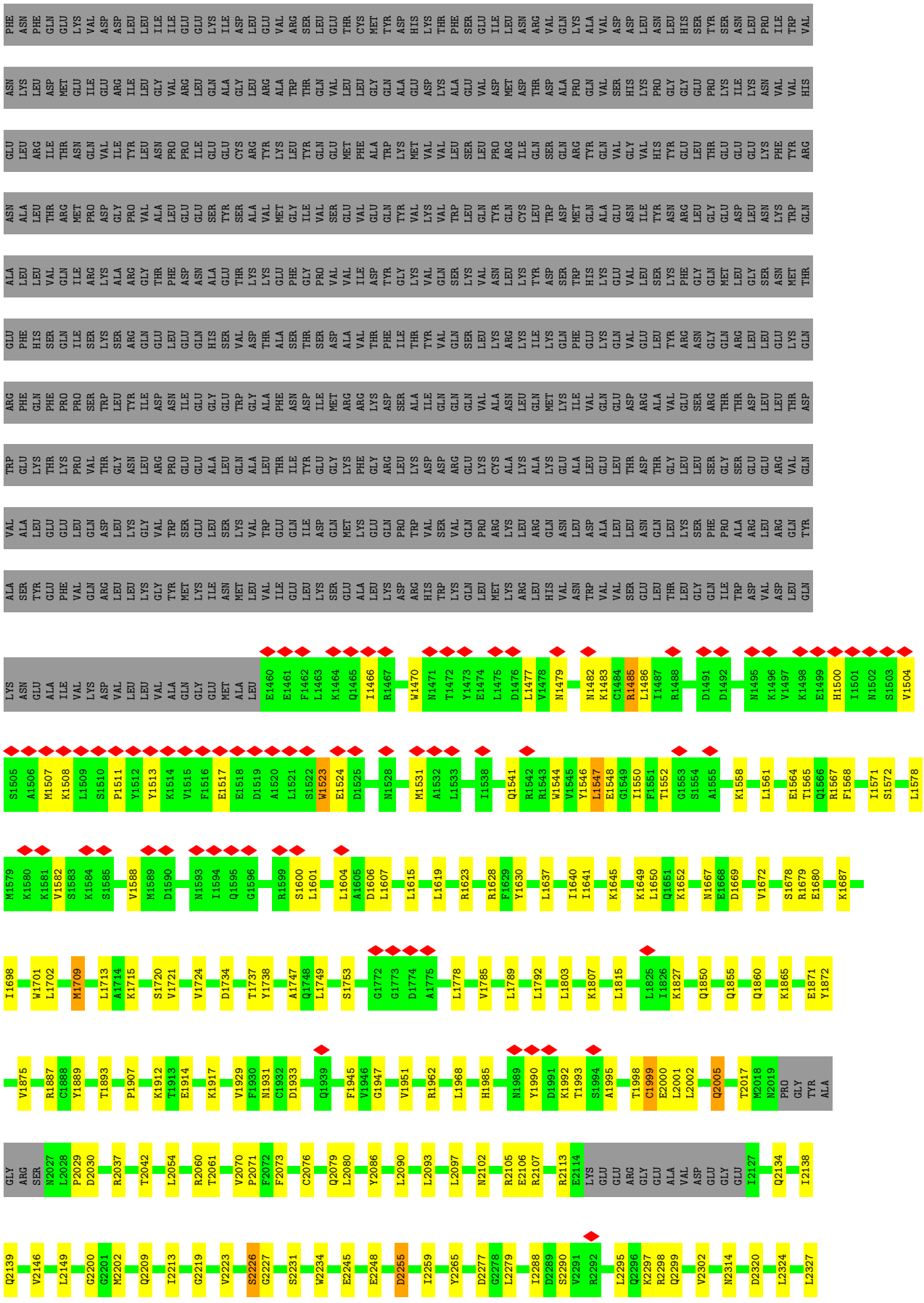
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

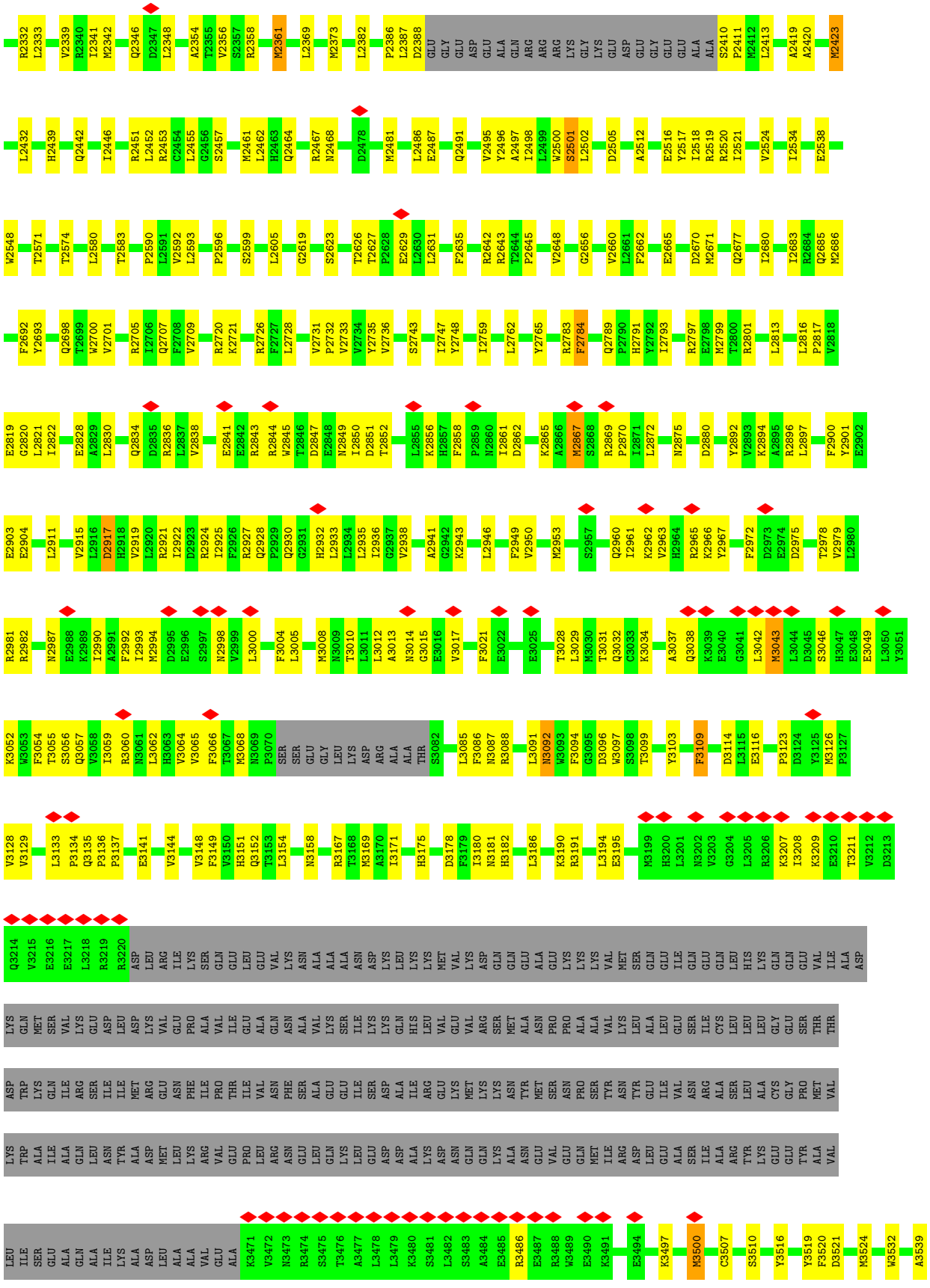
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

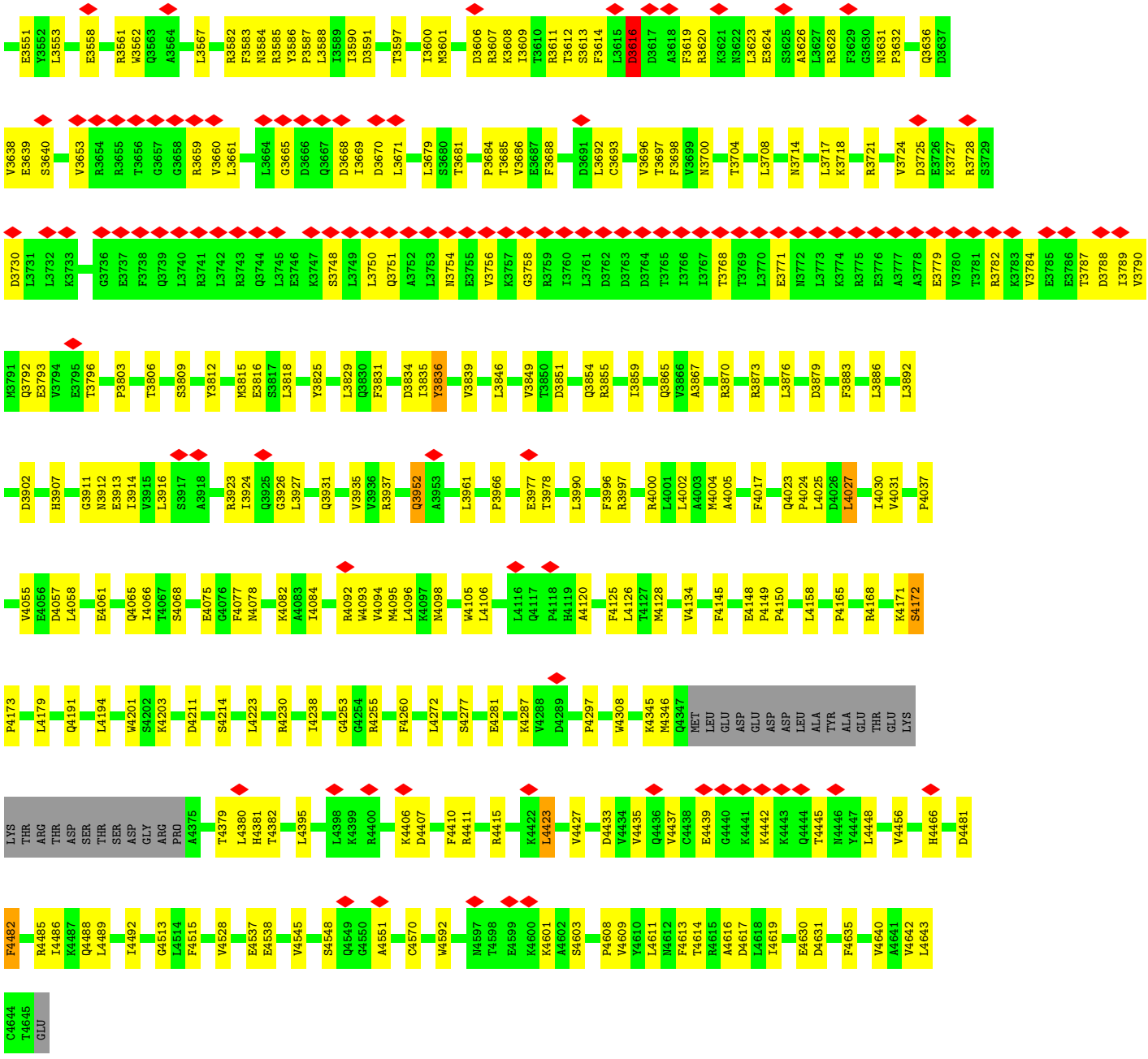
Chain A:










E3551 Y3552 L3553 E3558 R3561 W3562 Q3563 A3564 L3567 R3582 F3583 N3584 R3585 Y3586 P3587 L3588 I3589 I3590 D3591 T3597 I3600 M3601 D3606 R3607 K3608 I3609 T3610 R3611 T3612 S3613 F3614 L3615 D3616 D3617 A3618 F3619 R3620 K3621 N3622 L3623 E3624 S3625 A3626 L3627 R3628 F3629 G3630 N3631 P3632 Q3636 D3637
V3638 E3639 S3640 V3653 R3654 R3655 T3656 G3657 G3658 R3659 V3660 L3661 L3664 G3665 D3666 Q3667 D3668 I3669 D3670 L3671 L3679 S3680 T3681 P3684 T3685 V3686 E3687 F3688 D3691 L3692 C3693 V3696 T3697 F3698 V3699 N3700 T3704 L3708 N3714 L3717 K3718 R3721 V3724 D3725 E3726 K3727 R3728 S3729
D3730 L3731 L3732 K3733 G3736 E3737 F3738 Q3739 L3740 R3741 L3742 R3743 Q3744 L3745 E3746 K3747 S3748 L3749 L3750 Q3751 A3752 L3753 N3754 E3755 V3756 K3757 G3758 R3759 I3760 L3761 D3762 D3763 D3764 T3765 I3766 I3767 T3768 T3769 L3770 E3771 N3772 L3773 K3774 R3775 E3776 A3777 A3778 E3779 V3780 T3781 R3782 K3783 V3784 E3785 E3786 T3787 D3788 I3789 V3790
M3791 Q3792 E3793 V3794 E3795 T3796 P3803 T3806 S3809 Y3812 M3815 E3816 S3817 L3818 Y3825 L3829 Q3830 F3831 D3834 I3835 Y3836 V3839 L3846 V3849 T3850 D3851 Q3854 R3855 I3859 Q3865 V3866 A3867 R3870 R3873 L3876 D3879 F3883 L3886 L3892
D3902 H3907 G3911 N3912 E3913 I3914 V3915 L3916 S3917 A3918 R3923 I3924 Q3925 G3926 L3927 Q3931 V3935 V3936 R3937 Q3952 A3953 L3961 P3966 E3977 T3978 L3990 F3996 R3997 R4000 L4001 L4002 A4003 M4004 A4005 F4017 Q4023 P4024 L4025 D4026 L4027 I4030 V4031 P4037
V4055 E4056 D4057 L4058 E4061 Q4065 I4066 T4067 S4068 E4075 G4076 F4077 N4078 K4082 A4083 I4084 R4092 W4093 V4094 M4095 L4096 K4097 N4098 W4105 L4106 L4116 Q4117 P4118 H4119 A4120 F4125 L4126 T4127 M4128 V4134 F4145 E4148 P4149 P4150 L4158 P4165 R4168 K4171 S4172
P4173 L4179 Q4191 L4194 W4201 S4202 K4203 D4211 S4214 L4223 R4230 I4238 G4253 G4254 R4255 F4260 L4272 S4277 E4281 K4287 V4288 D4289 P4297 W4308 K4345 M4346 Q4347 MET LEU GLU ASP GLU ASP ASP LEU ALA TYR ALA GLU THR GLU LYS
LYS THR ARG THR ASP SER THR SER ASP GLY ARG PRO A4375 T4379 L4380 H4381 T4382 L4395 L4398 K4399 R4400 K4406 D4407 F4410 R4411 R4415 K4422 L4423 V4427 D4433 V4434 V4435 Q4436 V4437 C4438 E4439 G4440 K4441 K4442 K4443 Q4444 T4445 N4446 Y4447 L4448 V4456 H4466 D4481
F4482 R4485 I4486 K4487 Q4488 L4489 I4492 G4513 L4514 F4515 V4528 E4537 E4538 V4545 S4548 Q4549 G4550 A4551 C4570 W4592 N4597 T4598 E4599 K4600 K4601 A4602 S4603 P4608 V4609 Y4610 L4611 N4612 F4613 T4614 R4615 A4616 D4617 L4618 I4619 E4630 D4631 F4635 V4640 A4641 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	47831	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.499	Depositor
Minimum map value	-0.825	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	333.312, 333.312, 333.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.302, 1.302, 1.302	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, ANP, 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	0.26	0/23487	0.51	4/31835 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3616	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	4423	LEU	CA-CB-CG	5.20	127.27	115.30
1	A	4027	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	1547	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	22994	0	23055	493	0
2	A	54	0	24	2	0
3	A	31	0	12	1	0
4	A	31	0	13	0	0
All	All	23110	0	23104	493	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 11.

All (493) 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:3151:HIS:HD1	1:A:3516:TYR:HH	1.18	0.86
1:A:2836:ARG:HG3	1:A:3091:LEU:HB2	1.58	0.84
1:A:1698:ILE:HD12	1:A:1701:TRP:HE1	1.50	0.77
1:A:2762:LEU:HD13	1:A:2821:LEU:HD12	1.67	0.77
1:A:3727:LYS:HE2	1:A:3790:VAL:HG13	1.68	0.76
1:A:4423:LEU:HD12	1:A:4466:HIS:HB2	1.68	0.75
1:A:2979:VAL:HG13	1:A:2990:ILE:HG21	1.70	0.73
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.70	0.73
1:A:2819:GLU:HG3	1:A:2865:LYS:HD2	1.69	0.73
1:A:3883:PHE:HA	1:A:3886:LEU:HD12	1.70	0.73
1:A:3638:VAL:HG12	1:A:3679:LEU:HD22	1.71	0.72
1:A:2519:ARG:HH21	1:A:2534:ILE:HD11	1.57	0.70
1:A:1933:ASP:HA	1:A:1962:ARG:HH22	1.57	0.70
1:A:2922:ILE:HD13	1:A:2933:LEU:HD21	1.75	0.69
1:A:3043:MET:N	1:A:3043:MET:SD	2.65	0.69
1:A:2919:VAL:HG23	1:A:2950:VAL:HG22	1.74	0.68
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.58	0.68
1:A:2847:ASP:HA	1:A:2850:ILE:HD12	1.76	0.68
1:A:4084:ILE:HG22	1:A:4094:VAL:HG21	1.76	0.67
1:A:3626:ALA:HA	1:A:3631:ASN:HB2	1.76	0.67
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.77	0.66
1:A:1548:GLU:O	1:A:1552:THR:OG1	2.11	0.66
1:A:4065:GLN:HE21	1:A:4092:ARG:HD3	1.61	0.66
1:A:2227:GLY:HA2	1:A:2452:LEU:HD12	1.77	0.65
1:A:2828:GLU:OE1	1:A:2924:ARG:NH2	2.28	0.65
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.79	0.65
1:A:3990:LEU:HD12	1:A:4004:MET:HG3	1.78	0.65
1:A:4066:ILE:HG13	1:A:4093:TRP:HB2	1.78	0.65
1:A:3600:ILE:HG23	1:A:3601:MET:HE3	1.79	0.64
1:A:2915:VAL:HG23	1:A:2946:LEU:HD11	1.79	0.63
1:A:3521:ASP:HB2	1:A:3704:THR:HG21	1.80	0.63
1:A:2925:ILE:HB	1:A:2933:LEU:HD22	1.81	0.63
1:A:3154:LEU:HB3	1:A:3171:ILE:HD13	1.80	0.63
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.81	0.63
1:A:2845:TRP:O	1:A:2849:ASN:ND2	2.30	0.63
1:A:2643:ARG:O	1:A:2643:ARG:NH1	2.32	0.62
1:A:3167:ARG:NH2	1:A:3684:PRO:O	2.32	0.62
1:A:3181:ASN:OD1	1:A:3584:ASN:ND2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2320:ASP:HB3	1:A:2358:ARG:HD3	1.83	0.61
1:A:2665:GLU:OE1	1:A:2720:ARG:NH1	2.30	0.61
1:A:1606:ASP:OD1	1:A:1607:LEU:N	2.34	0.61
1:A:3128:VAL:HG21	1:A:3149:PHE:HB2	1.82	0.61
1:A:2801:ARG:NH2	1:A:3087:ASN:O	2.32	0.61
1:A:3609:ILE:HA	1:A:3632:PRO:HG2	1.83	0.61
1:A:3727:LYS:NZ	1:A:3793:GLU:OE1	2.33	0.61
1:A:3923:ARG:HH11	1:A:3952:GLN:HG3	1.65	0.61
1:A:3005:LEU:HD11	1:A:3085:LEU:HD22	1.83	0.60
1:A:3653:VAL:HG13	1:A:3660:VAL:HG23	1.83	0.60
1:A:1477:LEU:HB3	1:A:1485:ARG:HB3	1.82	0.60
1:A:2512:ALA:O	1:A:2516:GLU:HG3	2.01	0.60
1:A:2950:VAL:HA	1:A:2953:MET:HG3	1.84	0.60
1:A:2102:ASN:OD1	1:A:2105:ARG:NH2	2.33	0.60
1:A:2248:GLU:HB2	1:A:2297:LYS:HG2	1.84	0.60
1:A:2487:GLU:O	1:A:2491:GLN:HG3	2.01	0.60
1:A:2836:ARG:HE	1:A:3091:LEU:HD23	1.67	0.60
1:A:2965:ARG:HH22	1:A:3614:PHE:HB3	1.67	0.60
1:A:2259:ILE:HD13	1:A:2279:LEU:HD12	1.81	0.59
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.82	0.59
1:A:3607:ARG:HG2	1:A:3632:PRO:HD3	1.85	0.59
1:A:1568:PHE:HA	1:A:1571:ILE:HG22	1.84	0.59
1:A:2813:LEU:HD21	1:A:2816:LEU:HB2	1.84	0.59
1:A:3779:GLU:OE2	1:A:3782:ARG:NH1	2.35	0.59
1:A:2302:VAL:HG12	1:A:2342:MET:HB2	1.83	0.59
1:A:2498:ILE:HG23	1:A:2502:LEU:HD13	1.84	0.59
1:A:3134:PRO:HG2	1:A:3137:PRO:HA	1.85	0.59
1:A:2419:ALA:O	1:A:2423:MET:HG3	2.03	0.59
1:A:4437:VAL:HG21	1:A:4448:LEU:HD21	1.84	0.59
1:A:2660:VAL:HG22	1:A:2707:GLN:HB2	1.83	0.59
1:A:3000:LEU:H	1:A:3004:PHE:HD1	1.51	0.59
1:A:3924:ILE:HG23	1:A:3926:GLY:H	1.68	0.59
1:A:2965:ARG:NH2	1:A:3640:SER:O	2.36	0.58
1:A:2921:ARG:HD3	1:A:3092:ASN:HD21	1.68	0.58
1:A:1889:TYR:O	1:A:1893:THR:HG23	2.03	0.58
1:A:3913:GLU:OE2	1:A:3913:GLU:N	2.37	0.58
1:A:3037:ALA:HB1	1:A:3042:LEU:HB2	1.85	0.58
1:A:1561:LEU:O	1:A:1565:THR:OG1	2.14	0.58
1:A:3907:HIS:HA	1:A:3911:GLY:HA3	1.84	0.57
1:A:2851:ASP:OD1	1:A:2852:THR:N	2.38	0.57
1:A:3013:ALA:HB2	1:A:3088:ARG:HH11	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3029:LEU:HD22	1:A:3032:GLN:HE21	1.70	0.57
1:A:1483:LYS:NZ	1:A:1548:GLU:OE2	2.38	0.57
1:A:2054:LEU:HG	1:A:2097:LEU:HD13	1.87	0.57
1:A:2231:SER:OG	3:A:4702:ATP:O1B	2.19	0.57
1:A:2623:SER:N	1:A:2626:THR:OG1	2.38	0.56
1:A:1720:SER:O	1:A:1724:VAL:HG12	2.05	0.56
1:A:2670:ASP:HA	1:A:2721:LYS:HE3	1.86	0.56
1:A:2992:PHE:HD2	1:A:3064:VAL:HG12	1.69	0.56
1:A:1558:LYS:HD2	1:A:1565:THR:HG21	1.88	0.56
1:A:3608:LYS:HD2	1:A:3631:ASN:HD21	1.70	0.56
1:A:3768:THR:O	1:A:3771:GLU:HG3	2.04	0.56
1:A:4128:MET:HE3	1:A:4134:VAL:HG11	1.86	0.56
1:A:2354:ALA:HB1	1:A:2358:ARG:HH21	1.70	0.56
1:A:2290:SER:HB3	1:A:2295:LEU:HD13	1.88	0.56
1:A:2481:MET:HG3	1:A:2486:LEU:HB2	1.88	0.56
1:A:2759:ILE:HD12	1:A:2762:LEU:HD12	1.87	0.56
1:A:2299:GLN:HB2	1:A:2339:VAL:HG22	1.87	0.56
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.87	0.56
1:A:4172:SER:HB3	1:A:4173:PRO:HD2	1.87	0.55
1:A:2880:ASP:OD1	1:A:2880:ASP:N	2.38	0.55
1:A:4407:ASP:OD2	1:A:4410:PHE:N	2.36	0.55
1:A:2356:VAL:HG13	1:A:2361:MET:HE1	1.88	0.55
1:A:3815:MET:O	1:A:3818:LEU:HB2	2.07	0.55
1:A:1486:LEU:HD13	1:A:1541:GLN:HE22	1.72	0.55
1:A:2517:TYR:CE2	1:A:2521:ILE:HD11	2.41	0.55
1:A:2961:ILE:HD11	1:A:2967:TYR:HE2	1.71	0.55
1:A:2852:THR:O	1:A:2856:LYS:HG2	2.07	0.55
1:A:1724:VAL:HG11	1:A:1753:SER:HB3	1.89	0.55
1:A:2932:HIS:NE2	1:A:3066:PHE:HB3	2.22	0.55
1:A:4096:LEU:HB2	1:A:4126:LEU:HD23	1.88	0.54
1:A:1470:TRP:HB2	1:A:1523:TRP:HH2	1.72	0.54
1:A:3558:GLU:HA	1:A:3561:ARG:NH1	2.22	0.54
1:A:3977:GLU:HG3	1:A:3978:THR:HG23	1.89	0.54
1:A:3784:VAL:HA	1:A:3787:THR:HG23	1.88	0.54
1:A:4411:ARG:O	1:A:4415:ARG:HG3	2.07	0.54
1:A:1470:TRP:CE3	1:A:1588:VAL:HG11	2.42	0.54
1:A:1887:ARG:NH2	1:A:4253:GLY:O	2.41	0.54
1:A:1667:ASN:ND2	1:A:1669:ASP:OD1	2.32	0.54
1:A:2791:HIS:HD2	1:A:2836:ARG:HG2	1.73	0.54
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.37	0.54
1:A:3836:TYR:HA	1:A:3839:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4201:TRP:O	1:A:4203:LYS:N	2.41	0.54
1:A:1985:HIS:O	1:A:1985:HIS:ND1	2.38	0.54
1:A:2134:GLN:O	1:A:2138:ILE:HG22	2.08	0.54
1:A:4380:LEU:HD21	1:A:4456:VAL:HG12	1.90	0.54
1:A:4281:GLU:OE2	1:A:4281:GLU:N	2.41	0.54
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.90	0.53
1:A:2605:LEU:HD11	1:A:2709:VAL:HG11	1.90	0.53
1:A:2993:ILE:HG12	1:A:3065:VAL:CG2	2.39	0.53
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.09	0.53
1:A:1667:ASN:HB2	1:A:1672:VAL:HG22	1.91	0.53
1:A:2327:LEU:HD11	1:A:2333:LEU:HD23	1.91	0.53
1:A:1479:ASN:HD21	1:A:1482:ASN:HA	1.74	0.53
1:A:4272:LEU:O	1:A:4277:SER:OG	2.27	0.53
1:A:2897:LEU:HD13	1:A:2901:TYR:HE1	1.74	0.53
1:A:2079:GLN:OE1	1:A:4411:ARG:NH2	2.39	0.52
1:A:2209:GLN:O	1:A:2213:ILE:HG12	2.09	0.52
1:A:3924:ILE:HG22	1:A:3927:LEU:HD23	1.90	0.52
1:A:1504:VAL:HG11	1:A:1524:GLU:HB2	1.91	0.52
1:A:2073:PHE:HE2	1:A:2093:LEU:HA	1.75	0.52
1:A:2841:GLU:OE2	1:A:2844:ARG:NH1	2.40	0.52
1:A:4023:GLN:HG2	1:A:4024:PRO:HD2	1.91	0.52
1:A:2279:LEU:HD11	1:A:2693:TYR:HB3	1.90	0.52
1:A:3597:THR:O	1:A:3601:MET:HG2	2.09	0.52
1:A:1803:LEU:HD11	1:A:1875:VAL:HG21	1.92	0.52
1:A:2605:LEU:HD21	1:A:2709:VAL:HG12	1.91	0.52
1:A:3835:ILE:HD13	1:A:3867:ALA:HA	1.90	0.52
1:A:3037:ALA:O	1:A:3042:LEU:N	2.41	0.52
1:A:1513:TYR:CZ	1:A:1517:GLU:HG2	2.45	0.52
1:A:1601:LEU:HA	1:A:1604:LEU:HD12	1.91	0.52
1:A:3012:LEU:HD13	1:A:3088:ARG:HB3	1.92	0.51
1:A:3055:THR:O	1:A:3059:ILE:HG23	2.10	0.51
1:A:2619:GLY:HA2	1:A:2662:PHE:HB3	1.92	0.51
1:A:3167:ARG:NH2	1:A:3685:THR:HA	2.26	0.51
1:A:3865:GLN:HA	1:A:4017:PHE:HE2	1.76	0.51
1:A:4057:ASP:OD2	1:A:4058:LEU:N	2.42	0.51
1:A:2245:GLU:OE1	1:A:2298:ARG:NH2	2.34	0.51
1:A:2592:VAL:HB	1:A:2733:VAL:HG12	1.92	0.51
1:A:3133:LEU:HB3	1:A:3134:PRO:HD3	1.91	0.51
1:A:4128:MET:CE	1:A:4134:VAL:HG11	2.40	0.51
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.91	0.51
1:A:4601:LYS:HE2	1:A:4603:SER:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2202:MET:SD	1:A:2202:MET:N	2.84	0.51
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.45	0.51
1:A:3606:ASP:OD2	1:A:3607:ARG:N	2.44	0.51
1:A:2925:ILE:HG13	1:A:2933:LEU:HD13	1.92	0.50
1:A:3031:THR:O	1:A:3034:LYS:HG2	2.11	0.50
1:A:3611:ARG:NH2	1:A:3636:GLN:OE1	2.44	0.50
1:A:1931:ASN:ND2	1:A:1933:ASP:OD2	2.43	0.50
1:A:1968:LEU:HD21	1:A:2029:PRO:HG3	1.93	0.50
1:A:3590:ILE:HA	1:A:3681:THR:HG22	1.93	0.50
1:A:4084:ILE:HA	1:A:4094:VAL:HG11	1.92	0.50
1:A:2113:ARG:HG2	1:A:2113:ARG:O	2.11	0.50
1:A:2830:LEU:HD22	1:A:2850:ILE:HD13	1.93	0.50
1:A:3612:THR:OG1	1:A:3613:SER:N	2.44	0.50
1:A:4171:LYS:NZ	1:A:4172:SER:OG	2.42	0.50
1:A:1547:LEU:HD13	1:A:1550:ILE:HD11	1.93	0.50
1:A:3659:ARG:NH1	1:A:3661:LEU:HD21	2.26	0.50
1:A:2933:LEU:HB3	1:A:3065:VAL:HG12	1.93	0.50
1:A:1999:CYS:SG	1:A:2001:LEU:HD13	2.52	0.50
1:A:2446:ILE:HG22	1:A:2505:ASP:O	2.12	0.50
1:A:2972:PHE:CD1	1:A:3004:PHE:HD2	2.30	0.50
1:A:3015:GLY:HA3	1:A:3059:ILE:HG22	1.94	0.50
1:A:3186:LEU:HD23	1:A:3190:LYS:HG2	1.94	0.50
1:A:1628:ARG:NH1	1:A:1871:GLU:OE2	2.45	0.49
1:A:3519:TYR:HA	1:A:3700:ASN:HB2	1.94	0.49
1:A:3661:LEU:HD12	1:A:3668:ASP:OD1	2.12	0.49
1:A:3624:GLU:O	1:A:3628:ARG:HG2	2.11	0.49
1:A:2060:ARG:HG3	1:A:2061:THR:HG23	1.92	0.49
1:A:4635:PHE:HD2	1:A:4640:VAL:HG11	1.76	0.49
1:A:1640:ILE:HG23	1:A:1650:LEU:HD21	1.93	0.49
1:A:2960:GLN:HB3	1:A:2962:LYS:HE3	1.93	0.49
1:A:2961:ILE:HD11	1:A:2967:TYR:CE2	2.47	0.49
1:A:1564:GLU:HG3	1:A:1567:ARG:HH21	1.76	0.49
1:A:1619:LEU:HD22	1:A:1637:LEU:HD23	1.94	0.49
1:A:1734:ASP:HB3	1:A:1737:THR:HG22	1.94	0.49
1:A:2497:ALA:O	1:A:2501:SER:HB2	2.12	0.49
1:A:2656:GLY:H	1:A:2705:ARG:HH11	1.60	0.49
1:A:3178:ASP:OD2	1:A:3182:HIS:HD2	1.95	0.49
1:A:2593:LEU:HD11	1:A:2605:LEU:HD13	1.94	0.48
1:A:3607:ARG:HG2	1:A:3607:ARG:O	2.13	0.48
1:A:4002:LEU:O	1:A:4005:ALA:HB3	2.13	0.48
1:A:2037:ARG:NH2	1:A:4214:SER:OG	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.95	0.48
1:A:2960:GLN:OE1	1:A:2993:ILE:HB	2.13	0.48
1:A:3748:SER:O	1:A:3751:GLN:HG2	2.13	0.48
1:A:1850:GLN:HG2	1:A:1855:GLN:HB2	1.95	0.48
1:A:2870:PRO:O	1:A:2872:LEU:HD13	2.13	0.48
1:A:2875:ASN:OD1	1:A:2927:ARG:NH2	2.47	0.48
1:A:3109:PHE:HB3	1:A:3180:ILE:HG21	1.95	0.48
1:A:3551:GLU:OE1	1:A:3551:GLU:N	2.42	0.48
1:A:2387:LEU:O	1:A:2467:ARG:NH2	2.47	0.48
1:A:2677:GLN:HB2	1:A:2680:ILE:HB	1.96	0.48
1:A:3167:ARG:HG3	1:A:3519:TYR:OH	2.14	0.48
1:A:3688:PHE:HB2	1:A:3693:CYS:SG	2.53	0.48
1:A:4548:SER:HB3	1:A:4551:ALA:HB2	1.96	0.48
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.47	0.48
1:A:2783:ARG:HG2	1:A:2784:PHE:N	2.29	0.48
1:A:2935:LEU:HD13	1:A:2943:LYS:HB3	1.95	0.48
1:A:2516:GLU:O	1:A:2520:ARG:HG3	2.13	0.48
1:A:4395:LEU:HD23	1:A:4486:ILE:HG23	1.96	0.47
1:A:1645:LYS:HA	1:A:1645:LYS:HD3	1.69	0.47
1:A:1713:LEU:HD13	1:A:1749:LEU:HD21	1.96	0.47
1:A:2789:GLN:NE2	1:A:2838:VAL:HG21	2.29	0.47
1:A:2963:VAL:HG21	1:A:2998:ASN:HA	1.96	0.47
1:A:3558:GLU:HA	1:A:3561:ARG:HH12	1.78	0.47
1:A:2223:VAL:HG21	1:A:2348:LEU:HD12	1.95	0.47
1:A:3062:LEU:HD21	1:A:3064:VAL:HG13	1.96	0.47
1:A:3591:ASP:N	1:A:3591:ASP:OD1	2.47	0.47
1:A:4078:ASN:O	1:A:4082:LYS:HG2	2.14	0.47
1:A:1600:SER:O	1:A:1604:LEU:HG	2.14	0.47
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.15	0.47
1:A:2386:PRO:HG3	1:A:2413:LEU:HD13	1.95	0.47
1:A:2631:LEU:HD11	1:A:2683:ILE:HD11	1.97	0.47
1:A:3010:THR:HG23	1:A:3017:VAL:HG22	1.95	0.47
1:A:3714:ASN:OD1	1:A:3728:ARG:NH2	2.47	0.47
1:A:2797:ARG:O	1:A:2801:ARG:HG3	2.14	0.47
1:A:2892:TYR:O	1:A:2896:ARG:HG2	2.15	0.47
1:A:2915:VAL:O	1:A:2919:VAL:HG12	2.14	0.47
1:A:3208:ILE:HG22	1:A:3486:ARG:HH22	1.78	0.47
1:A:4381:HIS:CE1	1:A:4435:VAL:HG13	2.49	0.47
1:A:4037:PRO:HG3	1:A:4120:ALA:HA	1.96	0.47
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	1.95	0.47
1:A:4058:LEU:O	1:A:4061:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4211:ASP:OD1	1:A:4255:ARG:NH1	2.48	0.47
1:A:2219:GLY:HA2	1:A:2341:ILE:HG23	1.97	0.47
1:A:1615:LEU:O	1:A:1619:LEU:HG	2.15	0.46
1:A:2925:ILE:HG21	1:A:2933:LEU:HB2	1.97	0.46
1:A:3660:VAL:HG22	1:A:3671:LEU:HB3	1.97	0.46
1:A:3825:TYR:OH	1:A:3876:LEU:HB2	2.16	0.46
1:A:2938:VAL:HG23	1:A:2941:ALA:HB2	1.96	0.46
1:A:3751:GLN:HA	1:A:3754:ASN:HD21	1.80	0.46
1:A:1546:TYR:O	1:A:1550:ILE:HG12	2.14	0.46
1:A:2461:MET:HG2	1:A:2583:THR:CG2	2.42	0.46
1:A:3034:LYS:O	1:A:3038:GLN:HG2	2.15	0.46
1:A:3849:VAL:HG12	1:A:3855:ARG:HG2	1.97	0.46
1:A:1649:LYS:HA	1:A:1652:LYS:HE2	1.97	0.46
1:A:2966:LYS:HG2	1:A:3620:ARG:HH21	1.79	0.46
1:A:1998:THR:HB	1:A:2005:GLN:HG2	1.98	0.46
1:A:3167:ARG:NH1	1:A:3519:TYR:OH	2.49	0.46
1:A:1917:LYS:HD2	1:A:1929:VAL:HG21	1.97	0.46
1:A:2648:VAL:HB	1:A:2701:VAL:HG12	1.98	0.46
1:A:2932:HIS:CD2	1:A:2933:LEU:N	2.83	0.46
1:A:3616:ASP:OD1	1:A:3619:PHE:N	2.48	0.46
1:A:4609:VAL:HG13	1:A:4642:VAL:HG12	1.96	0.46
1:A:1785:VAL:HG13	1:A:1815:LEU:HD12	1.97	0.46
1:A:2086:TYR:CE2	1:A:2149:LEU:HD23	2.51	0.46
1:A:2255:ASP:OD1	1:A:2685:GLN:HB2	2.15	0.46
1:A:1544:TRP:HE1	1:A:1572:SER:HA	1.81	0.46
1:A:1623:ARG:HB3	1:A:1630:TYR:CZ	2.51	0.46
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.97	0.46
1:A:2743:SER:O	1:A:2747:ILE:HG22	2.16	0.46
1:A:2728:LEU:HD23	1:A:2728:LEU:HA	1.82	0.46
1:A:2862:ASP:OD1	1:A:2862:ASP:N	2.47	0.46
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.48	0.46
1:A:4537:GLU:HG2	1:A:4538:GLU:HG3	1.97	0.46
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.51	0.45
1:A:3914:ILE:O	1:A:3937:ARG:NE	2.50	0.45
1:A:4191:GLN:O	1:A:4194:LEU:HB2	2.15	0.45
1:A:1778:LEU:HB3	1:A:1827:LYS:NZ	2.31	0.45
1:A:2279:LEU:HD11	1:A:2693:TYR:CB	2.46	0.45
1:A:2834:GLN:NE2	1:A:2843:ARG:HD3	2.31	0.45
1:A:4489:LEU:HD11	1:A:4515:PHE:HE2	1.82	0.45
1:A:1508:LYS:HA	1:A:1513:TYR:CD1	2.52	0.45
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2102:ASN:O	1:A:2106:GLU:HG2	2.16	0.45
1:A:2748:TYR:CZ	1:A:2799:MET:HB2	2.51	0.45
1:A:3194:LEU:HD22	1:A:3500:MET:SD	2.56	0.45
1:A:4106:LEU:HD23	1:A:4106:LEU:HA	1.84	0.45
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.99	0.45
1:A:3028:THR:O	1:A:3032:GLN:HG2	2.17	0.45
1:A:4423:LEU:CD1	1:A:4466:HIS:HB2	2.43	0.45
1:A:4437:VAL:HG21	1:A:4448:LEU:CD2	2.47	0.45
1:A:2452:LEU:HD23	1:A:2452:LEU:HA	1.83	0.45
1:A:3103:TYR:HB2	1:A:3129:VAL:HG21	1.99	0.45
1:A:4287:LYS:HG2	1:A:4287:LYS:O	2.16	0.45
1:A:2936:ILE:HD12	1:A:3068:MET:HB2	1.97	0.45
1:A:3141:GLU:HA	1:A:3144:VAL:HG22	1.99	0.45
1:A:4381:HIS:NE2	1:A:4439:GLU:OE2	2.50	0.45
1:A:2439:HIS:O	1:A:2442:GLN:HG2	2.16	0.45
1:A:2369:LEU:O	1:A:2451:ARG:NH1	2.47	0.45
1:A:2671:MET:HG3	1:A:2721:LYS:HG2	1.99	0.45
1:A:2894:LYS:HA	1:A:2897:LEU:HG	1.99	0.45
1:A:3519:TYR:HB2	1:A:3698:PHE:HB3	1.98	0.45
1:A:1912:LYS:HD2	1:A:2017:THR:HG23	1.99	0.45
1:A:2861:ILE:HD12	1:A:2865:LYS:HZ1	1.82	0.45
1:A:3029:LEU:HD22	1:A:3032:GLN:NE2	2.30	0.45
1:A:3169:MET:SD	1:A:3169:MET:N	2.90	0.45
1:A:3923:ARG:HA	1:A:3923:ARG:NE	2.30	0.45
1:A:1547:LEU:HA	1:A:1550:ILE:HG12	1.99	0.44
1:A:1914:GLU:HG3	2:A:4701:ADP:H3'	1.99	0.44
1:A:3588:LEU:HD22	1:A:3698:PHE:CD2	2.52	0.44
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.17	0.44
1:A:1637:LEU:O	1:A:1641:ILE:HG12	2.17	0.44
1:A:2226:SER:HB2	1:A:2726:ARG:HG2	2.00	0.44
1:A:3792:GLN:O	1:A:3796:THR:HG23	2.17	0.44
1:A:2500:TRP:CD2	1:A:2580:LEU:HD11	2.51	0.44
1:A:2596:PRO:HD3	1:A:2735:TYR:CE1	2.53	0.44
1:A:1912:LYS:N	2:A:4701:ADP:O1B	2.50	0.44
1:A:2000:GLU:O	1:A:2001:LEU:HD12	2.17	0.44
1:A:2922:ILE:HG22	1:A:2950:VAL:HG11	1.99	0.44
1:A:2369:LEU:HD12	1:A:2373:MET:SD	2.57	0.44
1:A:3086:PHE:O	1:A:3091:LEU:HD21	2.18	0.44
1:A:3497:LYS:HE2	1:A:3497:LYS:HB2	1.81	0.44
1:A:3876:LEU:HD22	1:A:4148:GLU:OE2	2.18	0.44
1:A:4031:VAL:HG21	1:A:4125:PHE:HZ	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.51	0.44
1:A:4297:PRO:HB3	1:A:4308:TRP:CD1	2.53	0.44
1:A:3803:PRO:O	1:A:3806:THR:OG1	2.28	0.44
1:A:4223:LEU:HD12	1:A:4223:LEU:HA	1.76	0.44
1:A:3175:HIS:HD2	1:A:3585:ARG:HH22	1.64	0.44
1:A:3209:LYS:HG2	1:A:3486:ARG:HH21	1.81	0.44
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.82	0.44
1:A:2495:VAL:HG21	1:A:2524:VAL:HG11	2.00	0.44
1:A:4631:ASP:OD1	1:A:4631:ASP:N	2.51	0.44
1:A:2793:ILE:HG21	1:A:3087:ASN:HB2	2.00	0.44
1:A:4545:VAL:HG11	1:A:4570:CYS:SG	2.58	0.44
1:A:2324:LEU:HD21	1:A:2332:ARG:HE	1.82	0.43
1:A:3116:GLU:N	1:A:3116:GLU:OE2	2.51	0.43
1:A:1860:GLN:HG2	1:A:1865:LYS:HG2	1.99	0.43
1:A:3626:ALA:HB1	1:A:3631:ASN:O	2.19	0.43
1:A:1571:ILE:HD11	1:A:1604:LEU:HD23	2.00	0.43
1:A:1578:LEU:O	1:A:1582:VAL:HG12	2.18	0.43
1:A:2571:THR:H	1:A:2574:THR:HB	1.82	0.43
1:A:2978:THR:HG22	1:A:2982:ARG:HD3	2.01	0.43
1:A:3851:ASP:O	1:A:3855:ARG:HG3	2.18	0.43
1:A:2994:MET:SD	1:A:3066:PHE:CD1	3.11	0.43
1:A:4025:LEU:HD11	1:A:4027:LEU:HB3	2.01	0.43
1:A:4488:GLN:O	1:A:4492:ILE:HG12	2.19	0.43
1:A:1992:LYS:HA	1:A:1992:LYS:HD2	1.90	0.43
1:A:2903:GLU:O	1:A:2904:GLU:HB3	2.18	0.43
1:A:3141:GLU:CD	1:A:3141:GLU:H	2.21	0.43
1:A:3718:LYS:HE3	1:A:3718:LYS:HB2	1.72	0.43
1:A:3812:TYR:CZ	1:A:3829:LEU:HD13	2.54	0.43
1:A:1511:PRO:HB3	1:A:3659:ARG:HH22	1.83	0.43
1:A:2277:ASP:O	1:A:2698:GLN:NE2	2.52	0.43
1:A:2439:HIS:HB2	1:A:2517:TYR:CE2	2.54	0.43
1:A:2789:GLN:HE21	1:A:2838:VAL:HG21	1.83	0.43
1:A:3052:LYS:HE3	1:A:3052:LYS:HB3	1.84	0.43
1:A:2288:ILE:HD12	1:A:2288:ILE:HA	1.82	0.43
1:A:2932:HIS:HE1	1:A:3008:MET:SD	2.42	0.43
1:A:3659:ARG:NH2	1:A:3670:ASP:OD2	2.52	0.43
1:A:3835:ILE:HG12	1:A:3870:ARG:HD3	2.00	0.43
1:A:4179:LEU:HD23	1:A:4179:LEU:HA	1.85	0.43
1:A:4379:THR:HA	1:A:4382:THR:HG22	2.00	0.43
1:A:3148:VAL:O	1:A:3152:GLN:HG2	2.18	0.43
1:A:1486:LEU:HD22	1:A:1541:GLN:CD	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2897:LEU:HD21	1:A:2911:LEU:HD23	2.01	0.42
1:A:3851:ASP:HB3	1:A:3854:GLN:HB3	1.99	0.42
1:A:1547:LEU:HA	1:A:1550:ILE:CG1	2.50	0.42
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.34	0.42
1:A:3056:SER:HB2	1:A:3060:ARG:NH2	2.35	0.42
1:A:3661:LEU:HD13	1:A:3669:ILE:O	2.19	0.42
1:A:3725:ASP:OD1	1:A:3728:ARG:NH1	2.52	0.42
1:A:1715:LYS:HD3	1:A:1715:LYS:HA	1.81	0.42
1:A:2822:ILE:HD11	1:A:2858:PHE:CD2	2.53	0.42
1:A:2919:VAL:HG21	1:A:2949:PHE:HE2	1.85	0.42
1:A:2922:ILE:HD11	1:A:2935:LEU:HD11	2.01	0.42
1:A:1990:TYR:OH	1:A:1995:ALA:N	2.52	0.42
1:A:2869:ARG:N	1:A:2870:PRO:HD2	2.34	0.42
1:A:3021:PHE:CD1	1:A:3029:LEU:HG	2.55	0.42
1:A:3912:ASN:O	1:A:3937:ARG:HD2	2.20	0.42
1:A:4613:PHE:HA	1:A:4643:LEU:HD13	2.00	0.42
1:A:2200:GLY:HA2	1:A:2373:MET:CE	2.49	0.42
1:A:2921:ARG:O	1:A:2925:ILE:HG12	2.18	0.42
1:A:3012:LEU:HB3	1:A:3088:ARG:CG	2.49	0.42
1:A:3114:ASP:HB3	1:A:3191:ARG:HH12	1.84	0.42
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.90	0.42
1:A:1789:LEU:HG	1:A:1815:LEU:HB3	2.01	0.42
1:A:1993:THR:O	1:A:1993:THR:OG1	2.38	0.42
1:A:1747:ALA:HB2	1:A:1807:LYS:HG2	2.01	0.42
1:A:2911:LEU:HA	1:A:2915:VAL:HG11	2.02	0.42
1:A:3046:SER:HB3	1:A:3049:GLU:HB2	2.02	0.42
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.53	0.42
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.53	0.42
1:A:3154:LEU:HD21	1:A:3532:TRP:HZ2	1.85	0.42
1:A:3916:LEU:HD23	1:A:3916:LEU:HA	1.91	0.42
1:A:3927:LEU:HD11	1:A:3996:PHE:HE1	1.84	0.42
1:A:1466:ILE:HG12	1:A:1500:HIS:CE1	2.55	0.42
1:A:2686:MET:HG2	1:A:2692:PHE:HB3	2.02	0.42
1:A:3961:LEU:O	1:A:3997:ARG:NH1	2.45	0.42
1:A:4158:LEU:HD12	1:A:4158:LEU:HA	1.93	0.42
1:A:4345:LYS:HB2	1:A:4345:LYS:HE3	1.77	0.42
1:A:1571:ILE:HD11	1:A:1604:LEU:HA	2.01	0.41
1:A:2453:ARG:HD3	1:A:2728:LEU:O	2.19	0.41
1:A:2642:ARG:HG2	1:A:2645:PRO:HD3	2.00	0.41
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	2.01	0.41
1:A:2900:PHE:CD2	1:A:2949:PHE:HD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2993:ILE:HG12	1:A:3065:VAL:HG23	2.02	0.41
1:A:3012:LEU:HD23	1:A:3012:LEU:HA	1.75	0.41
1:A:2538:GLU:HB3	1:A:2548:TRP:NE1	2.35	0.41
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	2.02	0.41
1:A:3558:GLU:H	1:A:3558:GLU:CD	2.22	0.41
1:A:3717:LEU:HD23	1:A:3717:LEU:HA	1.91	0.41
1:A:4223:LEU:HD11	1:A:4238:ILE:HD12	2.01	0.41
1:A:4406:LYS:H	1:A:4406:LYS:HD2	1.85	0.41
1:A:1568:PHE:O	1:A:1571:ILE:HG22	2.21	0.41
1:A:2146:VAL:HA	1:A:2149:LEU:HD12	2.03	0.41
1:A:3123:PRO:HG3	1:A:3539:ALA:C	2.41	0.41
1:A:4077:PHE:HD2	1:A:4105:TRP:CD1	2.39	0.41
1:A:4630:GLU:OE1	1:A:4630:GLU:N	2.52	0.41
1:A:2090:LEU:HD12	1:A:2090:LEU:HA	1.78	0.41
1:A:2455:LEU:HD23	1:A:2455:LEU:HA	1.89	0.41
1:A:3553:LEU:O	1:A:3582:ARG:NH1	2.54	0.41
1:A:3812:TYR:OH	1:A:3816:GLU:OE1	2.27	0.41
1:A:3846:LEU:HD11	1:A:3859:ILE:HG13	2.02	0.41
1:A:4055:VAL:O	1:A:4058:LEU:HG	2.20	0.41
1:A:2386:PRO:C	1:A:2388:ASP:H	2.24	0.41
1:A:3750:LEU:O	1:A:3754:ASN:ND2	2.53	0.41
1:A:3825:TYR:OH	1:A:3879:ASP:OD2	2.30	0.41
1:A:1687:LYS:H	1:A:1687:LYS:HG2	1.73	0.41
1:A:2432:LEU:HD11	1:A:2518:ILE:HG13	2.03	0.41
1:A:2464:GLN:NE2	1:A:2468:ASN:OD1	2.53	0.41
1:A:3178:ASP:OD1	1:A:3585:ARG:NH2	2.51	0.41
1:A:1678:SER:OG	1:A:1679:ARG:N	2.54	0.41
1:A:2076:CYS:O	1:A:2080:LEU:HB2	2.20	0.41
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.35	0.41
1:A:2265:TYR:CE1	1:A:2314:ASN:HB2	2.55	0.41
1:A:2962:LYS:HB2	1:A:3665:GLY:HA2	2.01	0.41
1:A:2975:ASP:O	1:A:2979:VAL:HG23	2.21	0.41
1:A:3135:GLN:HB2	1:A:3136:PRO:HD3	2.03	0.41
1:A:3207:LYS:O	1:A:3211:THR:HG23	2.21	0.41
1:A:4481:ASP:O	1:A:4485:ARG:HG3	2.19	0.41
1:A:2981:ARG:HD2	1:A:3032:GLN:HE22	1.86	0.41
1:A:3186:LEU:HD22	1:A:3507:CYS:SG	2.60	0.41
1:A:3195:GLU:OE2	1:A:3195:GLU:HA	2.21	0.41
1:A:1907:PRO:HD2	1:A:2042:THR:HA	2.03	0.41
1:A:2227:GLY:O	1:A:2369:LEU:HD23	2.21	0.41
1:A:2324:LEU:HD11	1:A:2332:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.20	0.41
1:A:2599:SER:OG	1:A:2736:VAL:HG12	2.21	0.41
1:A:2627:THR:HG23	1:A:2629:GLU:HB2	2.03	0.41
1:A:2932:HIS:CD2	1:A:2933:LEU:H	2.38	0.41
1:A:2963:VAL:HG11	1:A:2998:ASN:HA	2.03	0.41
1:A:3056:SER:HB2	1:A:3060:ARG:CZ	2.50	0.41
1:A:3099:THR:HG22	1:A:3129:VAL:HG22	2.02	0.41
1:A:3209:LYS:HD2	1:A:3209:LYS:HA	1.88	0.41
1:A:3562:TRP:HB3	1:A:3567:LEU:HD22	2.02	0.41
1:A:3583:PHE:CD2	1:A:3587:PRO:HD3	2.56	0.41
1:A:3608:LYS:HG3	1:A:3608:LYS:O	2.21	0.41
1:A:3756:VAL:HG23	1:A:3758:GLY:H	1.84	0.41
1:A:3831:PHE:HZ	1:A:3870:ARG:HB3	1.86	0.41
1:A:2631:LEU:HD23	1:A:2631:LEU:HA	1.86	0.41
1:A:3639:GLU:HG3	1:A:3686:VAL:HG21	2.03	0.41
1:A:4165:PRO:HD2	1:A:4168:ARG:HD3	2.03	0.41
1:A:4442:LYS:HE3	1:A:4442:LYS:HB2	1.88	0.41
1:A:4614:THR:O	1:A:4616:ALA:N	2.54	0.41
1:A:1680:GLU:OE2	1:A:1875:VAL:HB	2.21	0.40
1:A:1721:VAL:HA	1:A:1724:VAL:CG1	2.52	0.40
1:A:2086:TYR:HE2	1:A:2149:LEU:HD23	1.86	0.40
1:A:2496:TYR:CE1	1:A:2500:TRP:HD1	2.39	0.40
1:A:2693:TYR:CE1	1:A:2700:TRP:HB2	2.56	0.40
1:A:2927:ARG:CZ	1:A:2927:ARG:HB2	2.51	0.40
1:A:3585:ARG:HB2	1:A:3697:THR:HG23	2.03	0.40
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.57	0.40
1:A:2783:ARG:HD2	1:A:2845:TRP:CZ3	2.56	0.40
1:A:2867:MET:HA	1:A:2869:ARG:HH21	1.86	0.40
1:A:2928:GLN:HB3	1:A:2930:GLN:OE1	2.21	0.40
1:A:3892:LEU:HD12	1:A:3892:LEU:HA	1.85	0.40
1:A:4149:PRO:HA	1:A:4150:PRO:HD3	1.96	0.40
1:A:2410:SER:N	1:A:2411:PRO:HD2	2.36	0.40
1:A:2462:LEU:HD13	1:A:2462:LEU:HA	1.87	0.40
1:A:3721:ARG:HE	1:A:3724:VAL:HG21	1.87	0.40
1:A:3788:ASP:OD1	1:A:3789:ILE:N	2.52	0.40
1:A:4427:VAL:HG21	1:A:4482:PHE:HE2	1.87	0.40
1:A:1709:MET:CE	1:A:1872:TYR:H	2.34	0.40
1:A:2872:LEU:HD21	1:A:2917:ASP:OD1	2.22	0.40
1:A:3586:TYR:HA	1:A:3587:PRO:HD3	1.95	0.40
1:A:3751:GLN:HA	1:A:3754:ASN:ND2	2.36	0.40
1:A:4066:ILE:HG21	1:A:4095:MET:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4445:THR:HG23	1:A:4448:LEU:H	1.86	0.40
1:A:2500:TRP:CE3	1:A:2580:LEU:HD11	2.57	0.40
1:A:3619:PHE:O	1:A:3623:LEU:HB2	2.21	0.40
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	2.03	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	2844/4646 (61%)	2762 (97%)	81 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	SER

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	2544/4125 (62%)	2502 (98%)	42 (2%)	56	75

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1485	ARG
1	A	1507	MET
1	A	1523	TRP
1	A	1531	MET
1	A	1709	MET
1	A	1945	PHE
1	A	1999	CYS
1	A	2002	LEU
1	A	2005	GLN
1	A	2030	ASP
1	A	2226	SER
1	A	2255	ASP
1	A	2361	MET
1	A	2423	MET
1	A	2457	SER
1	A	2501	SER
1	A	2635	PHE
1	A	2765	TYR
1	A	2784	PHE
1	A	2867	MET
1	A	2917	ASP
1	A	3014	ASN
1	A	3043	MET
1	A	3054	PHE
1	A	3092	ASN
1	A	3094	PHE
1	A	3109	PHE
1	A	3126	MET
1	A	3500	MET
1	A	3616	ASP
1	A	3730	ASP
1	A	3834	ASP
1	A	3836	TYR
1	A	3902	ASP
1	A	3952	GLN
1	A	4075	GLU
1	A	4098	ASN
1	A	4230	ARG
1	A	4346	MET
1	A	4433	ASP
1	A	4482	PHE
1	A	4617	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	1748	GLN
1	A	1755	GLN
1	A	2834	GLN
1	A	2932	HIS
1	A	3057	GLN
1	A	3092	ASN
1	A	3754	ASN
1	A	4065	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	A	4702	-	28,33,33	0.70	0	34,52,52	0.59	1 (2%)
4	ANP	A	4703	-	29,33,33	1.13	4 (13%)	31,52,52	0.88	1 (3%)
2	ADP	A	4701	-	24,29,29	0.89	0	29,45,45	1.24	2 (6%)
2	ADP	A	4704	-	24,29,29	0.90	0	29,45,45	1.36	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	-	-	7/18/38/38	0/3/3/3
4	ANP	A	4703	-	-	4/14/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	5/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4703	ANP	PG-O1G	2.53	1.50	1.46
4	A	4703	ANP	PB-O3A	-2.42	1.56	1.59
4	A	4703	ANP	PG-N3B	2.42	1.69	1.63
4	A	4703	ANP	PB-O1B	2.36	1.49	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4701	ADP	N3-C2-N1	-3.76	123.57	128.67
2	A	4704	ADP	N3-C2-N1	-3.69	123.67	128.67
2	A	4704	ADP	O4'-C1'-N9	3.03	112.76	108.75
2	A	4704	ADP	C4-C5-N7	-2.68	106.51	109.34
2	A	4701	ADP	C4-C5-N7	-2.49	106.71	109.34
3	A	4702	ATP	C5-C6-N6	2.30	123.81	120.31
4	A	4703	ANP	C5-C6-N6	2.29	123.80	120.31

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C5'-O5'-PA-O2A
3	A	4702	ATP	C5'-O5'-PA-O3A
4	A	4703	ANP	PB-N3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
4	A	4703	ANP	PG-N3B-PB-O1B
4	A	4703	ANP	PG-N3B-PB-O3A
2	A	4704	ADP	C3'-C4'-C5'-O5'
4	A	4703	ANP	PB-O3A-PA-O1A
3	A	4702	ATP	PB-O3B-PG-O1G
2	A	4701	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
3	A	4702	ATP	PG-O3B-PB-O1B
3	A	4702	ATP	PG-O3B-PB-O2B

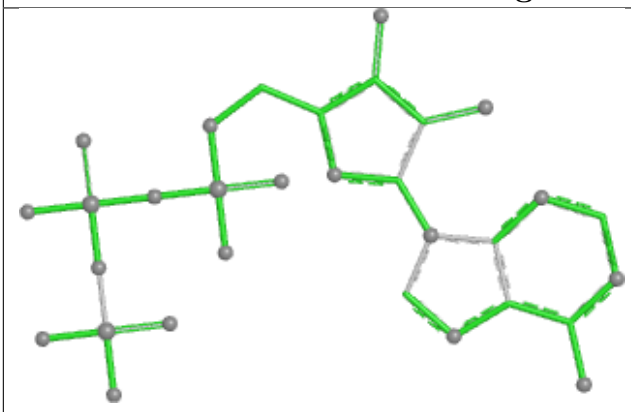
There are no ring outliers.

2 monomers are involved in 3 short contacts:

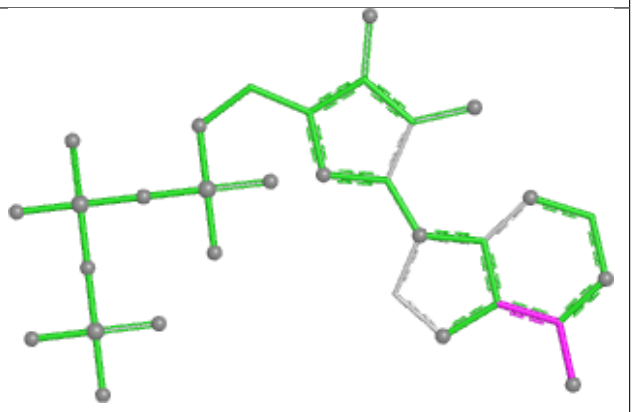
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	1	0
2	A	4701	ADP	2	0

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

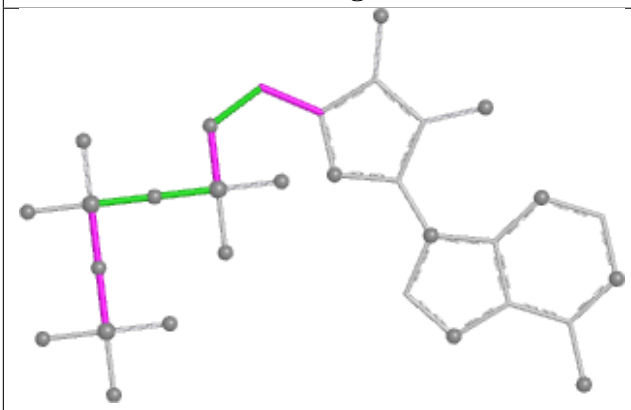
Ligand ATP A 4702



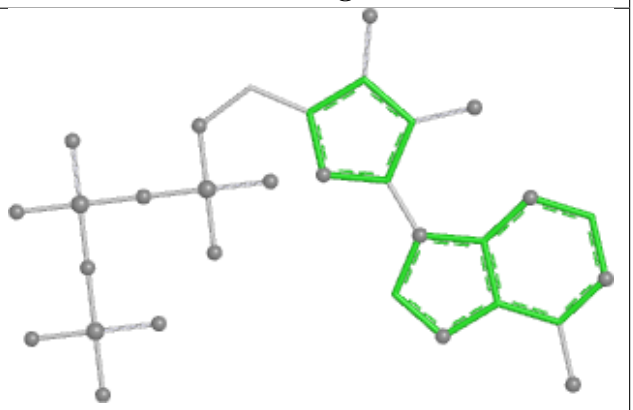
Bond lengths



Bond angles

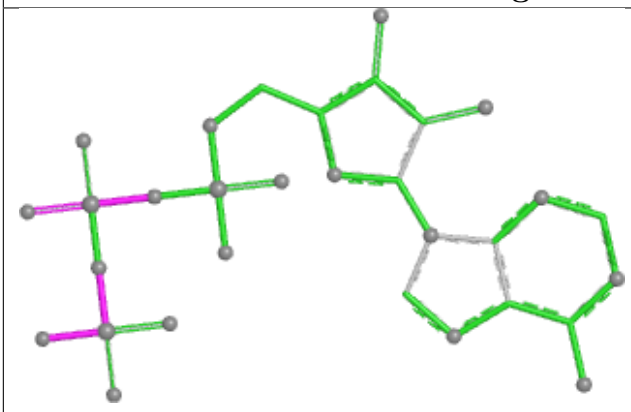


Torsions

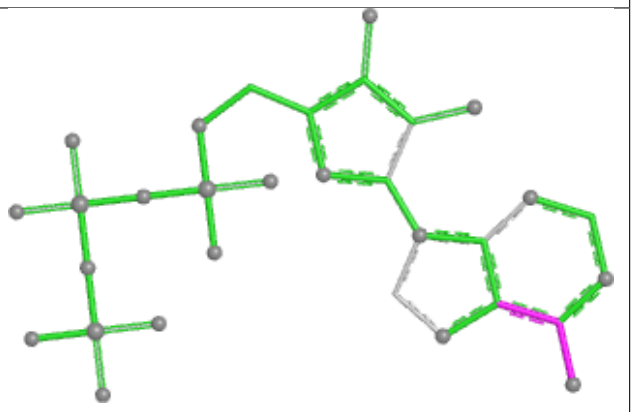


Rings

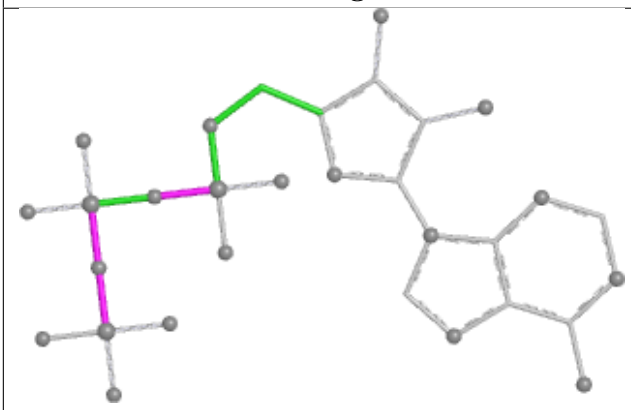
Ligand ANP A 4703



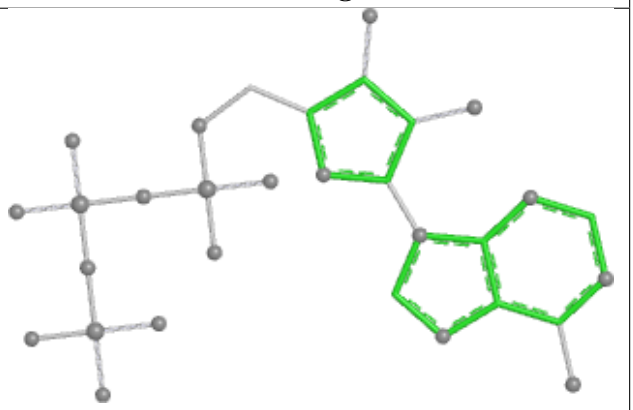
Bond lengths



Bond angles

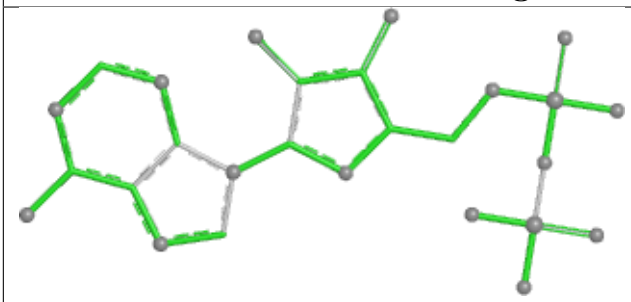


Torsions

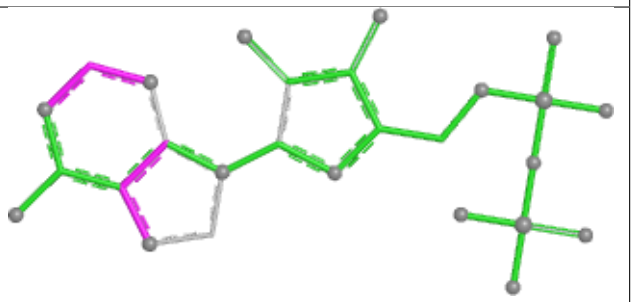


Rings

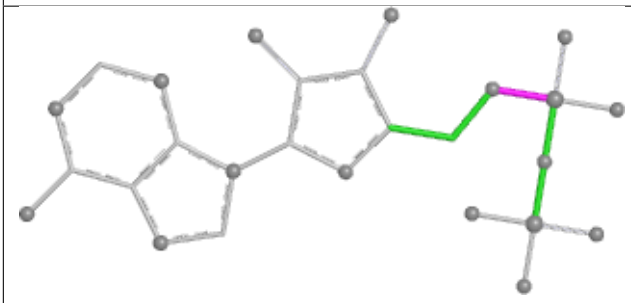
Ligand ADP A 4701



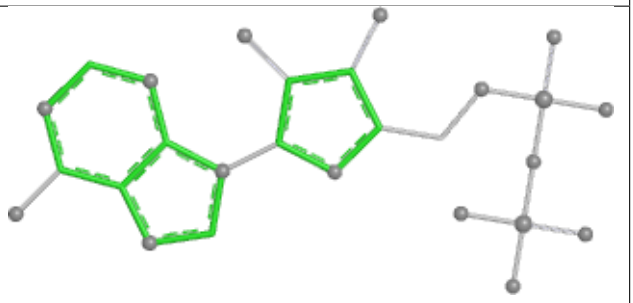
Bond lengths



Bond angles

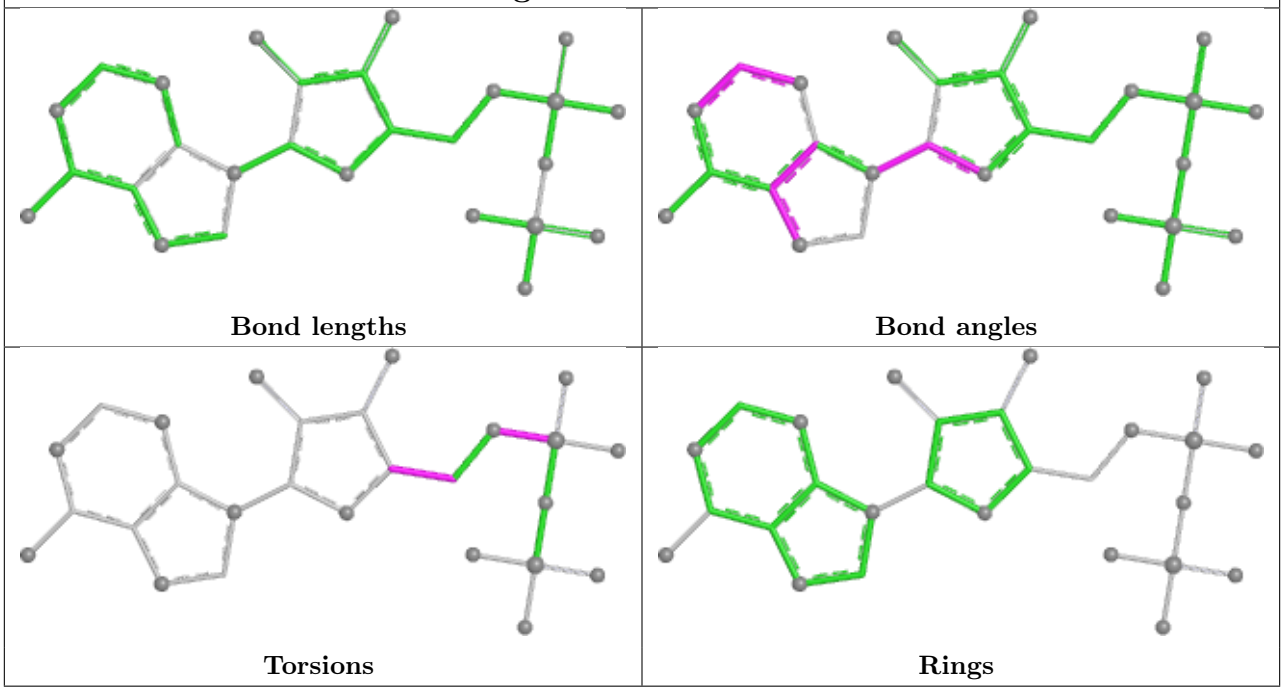


Torsions



Rings

Ligand ADP A 4704



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.

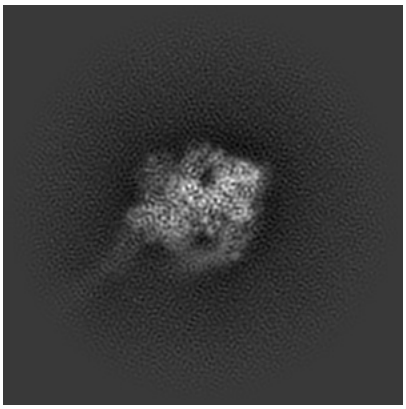
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44706. These allow visual inspection of the internal detail of the map and identification of artifacts.

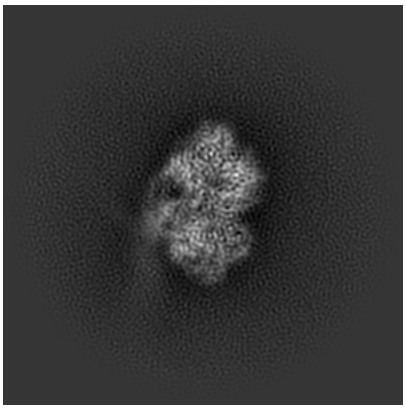
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

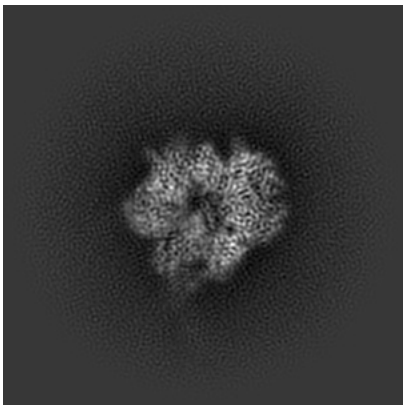
6.1.1 Primary map



X

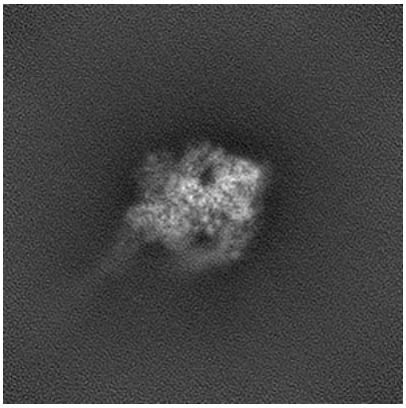


Y

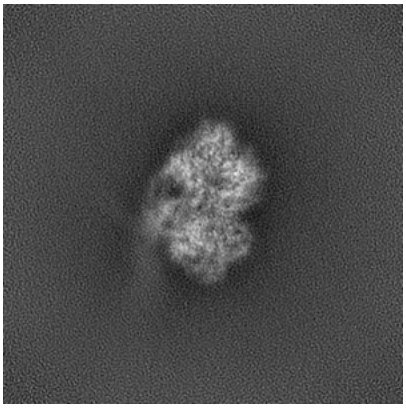


Z

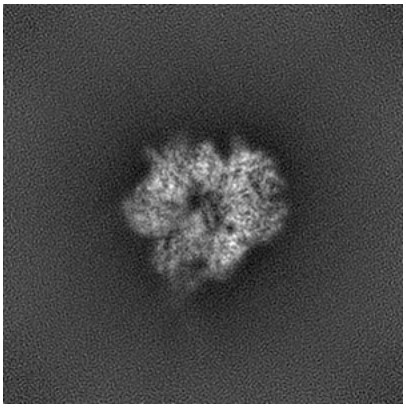
6.1.2 Raw map



X



Y

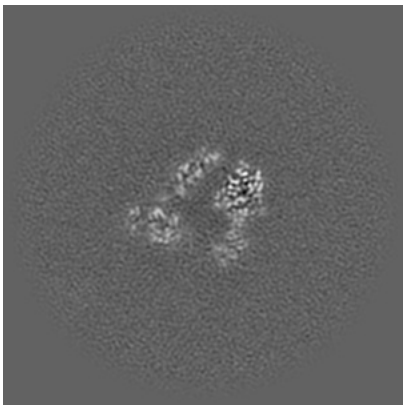


Z

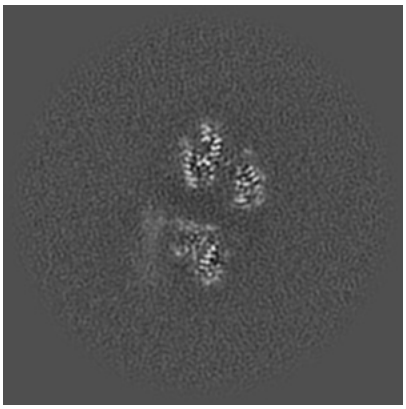
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

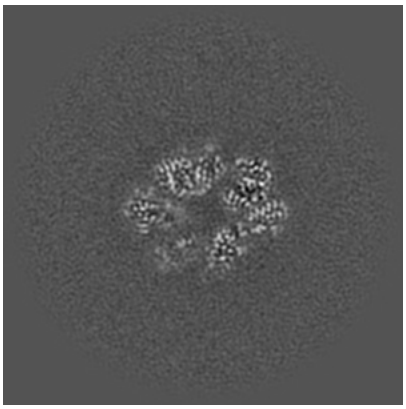
6.2.1 Primary map



X Index: 128

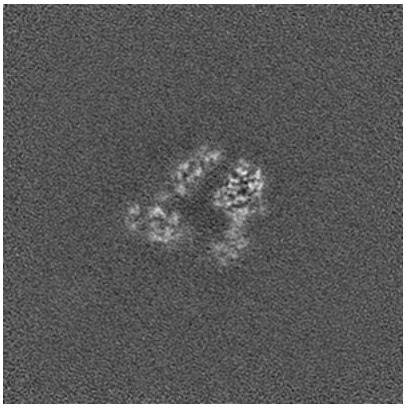


Y Index: 128

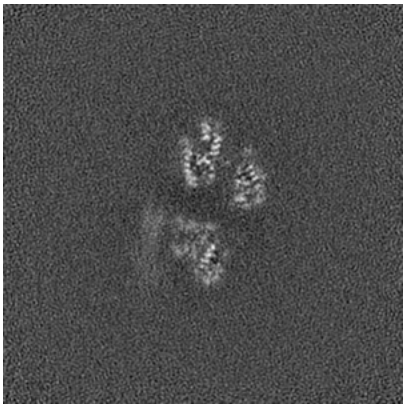


Z Index: 128

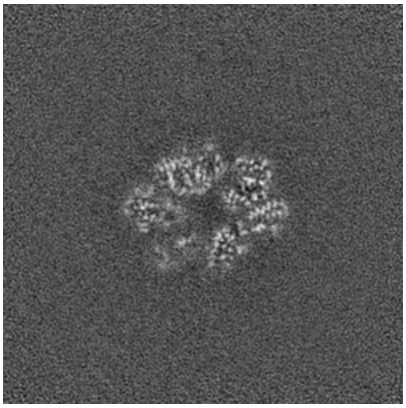
6.2.2 Raw map



X Index: 128



Y Index: 128

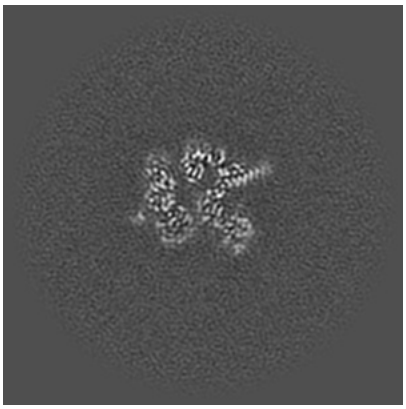


Z Index: 128

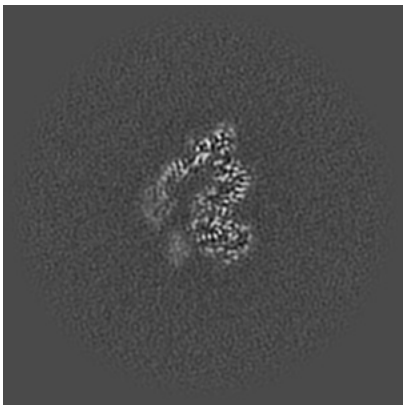
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

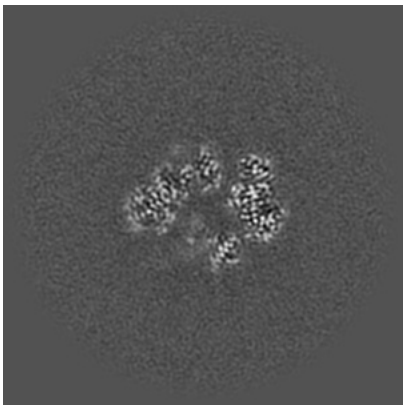
6.3.1 Primary map



X Index: 147

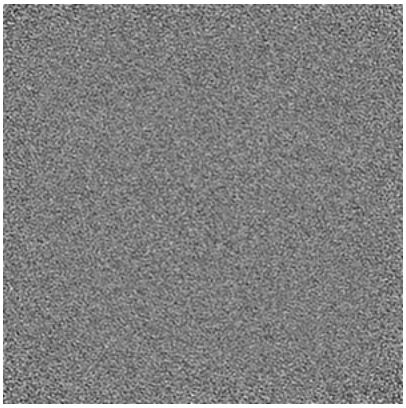


Y Index: 143

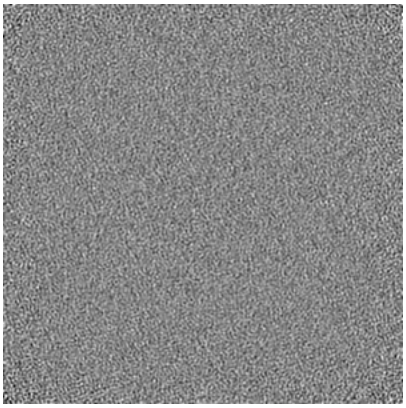


Z Index: 133

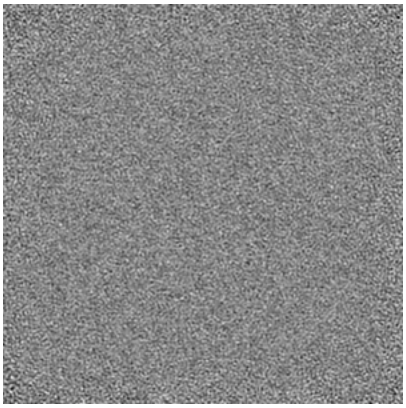
6.3.2 Raw map



X Index: 0



Y Index: 0

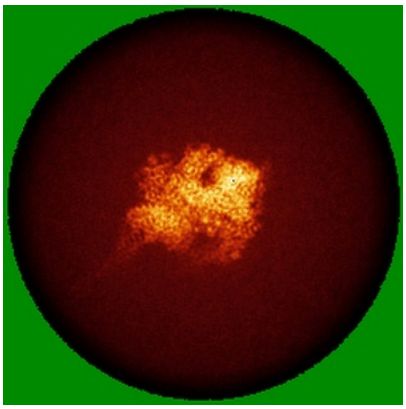


Z Index: 0

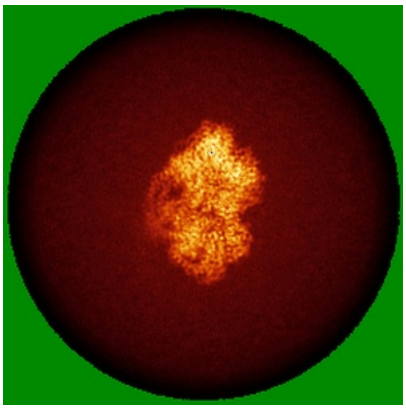
The images above show the largest variance slices of the map in three orthogonal directions.

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

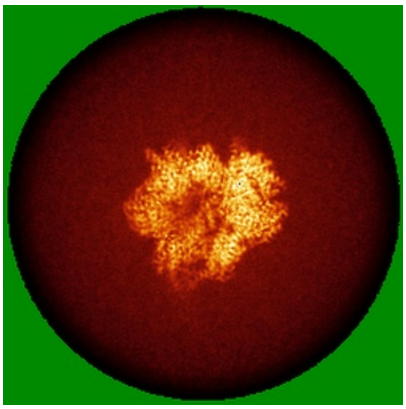
6.4.1 Primary map



X

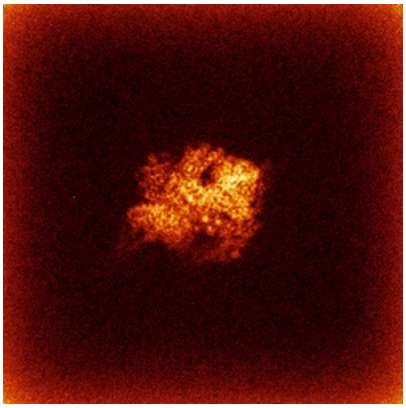


Y

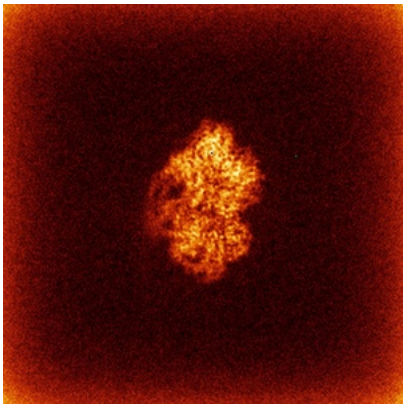


Z

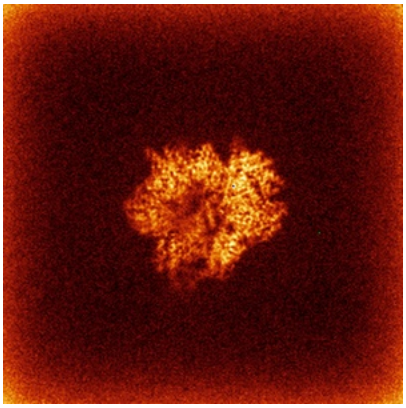
6.4.2 Raw map



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 0.2. 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.

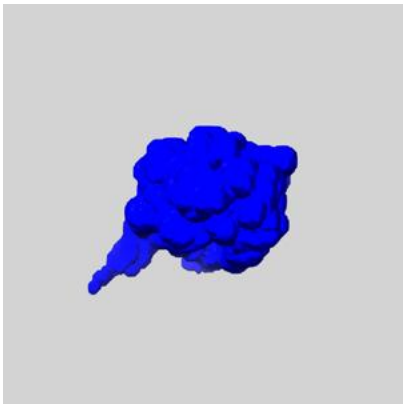
6.6 Mask visualisation (i)

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

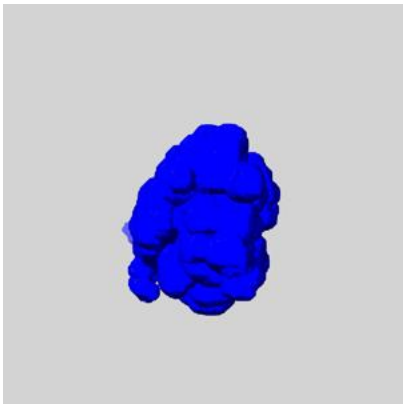
A mask typically either:

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

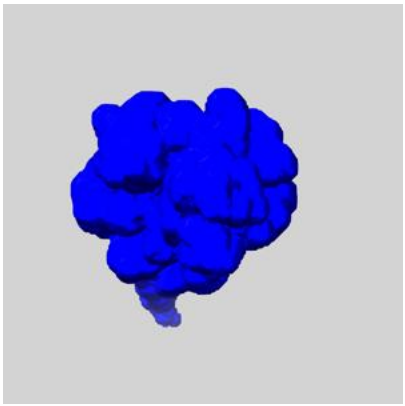
6.6.1 emd_44706_msk_1.map (i)



X



Y

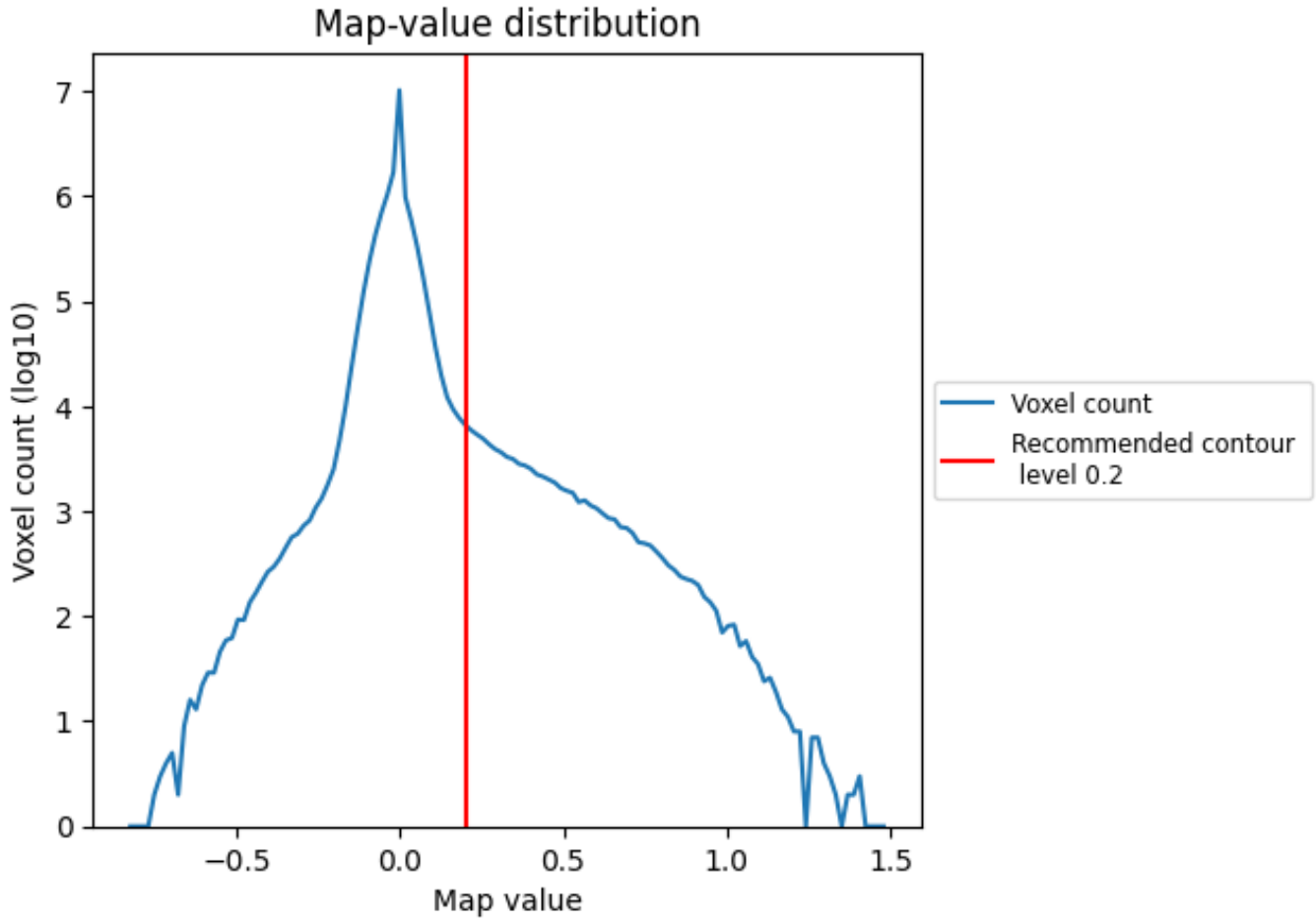


Z

7 Map analysis

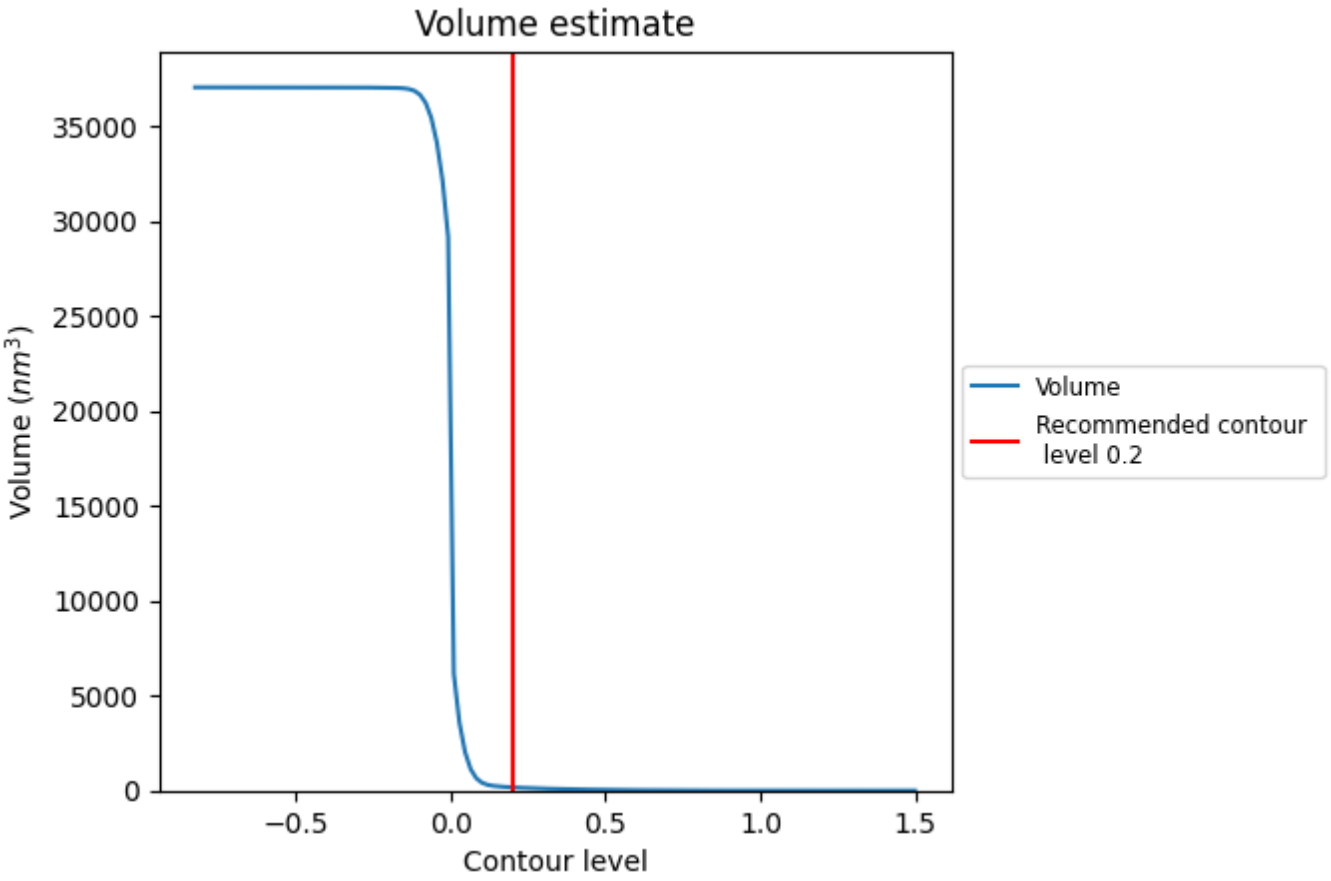
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

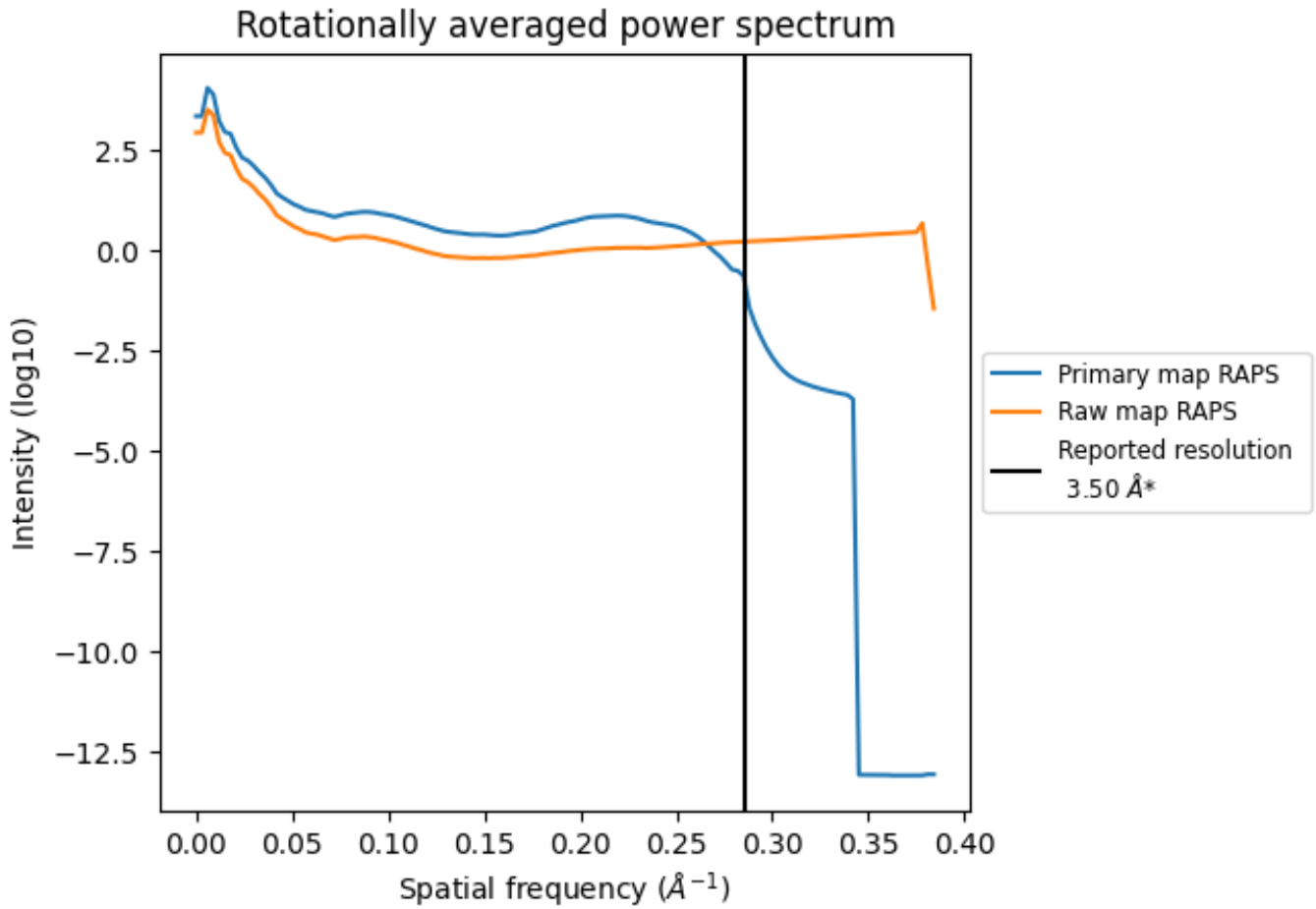
7.2 Volume estimate



The volume at the recommended contour level is 168 nm^3; this corresponds to an approximate mass of 152 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)

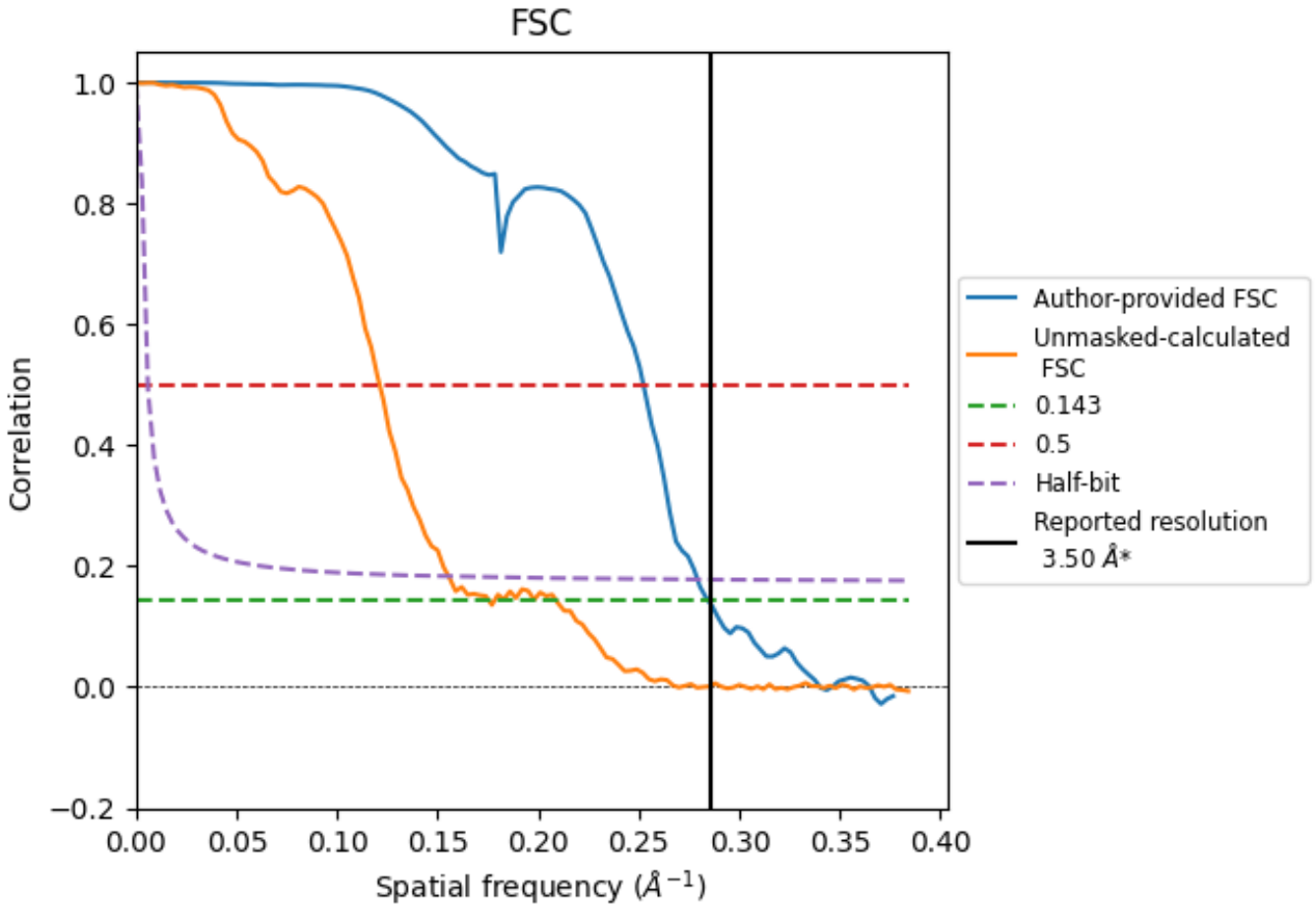


*Reported resolution corresponds to spatial frequency of 0.286 $Å^{-1}$

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

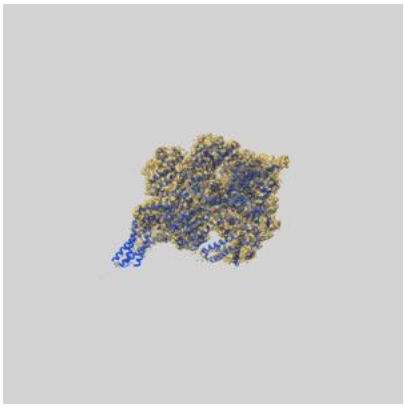
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	3.96	3.58
Unmasked-calculated*	5.70	8.25	6.43

*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 5.70 differs from the reported value 3.5 by more than 10 %

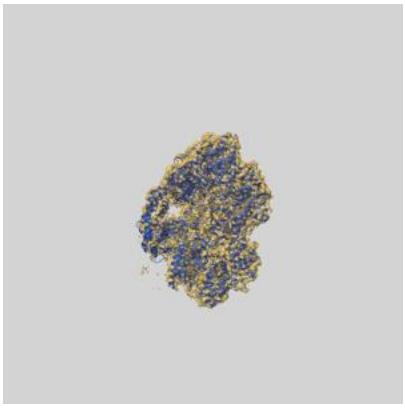
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44706 and PDB model 9BMP. Per-residue inclusion information can be found in section 3 on page 5.

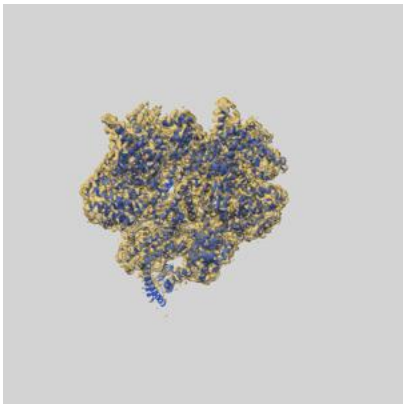
9.1 Map-model overlay



X



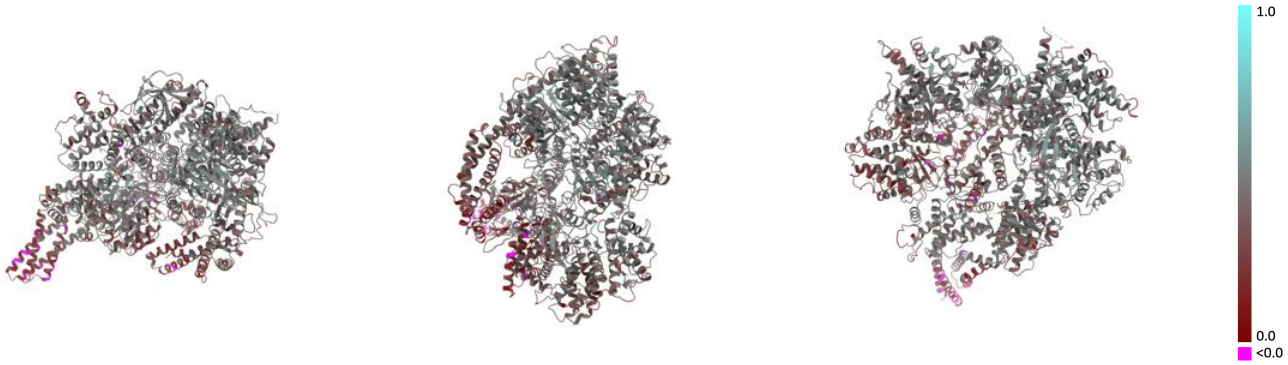
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

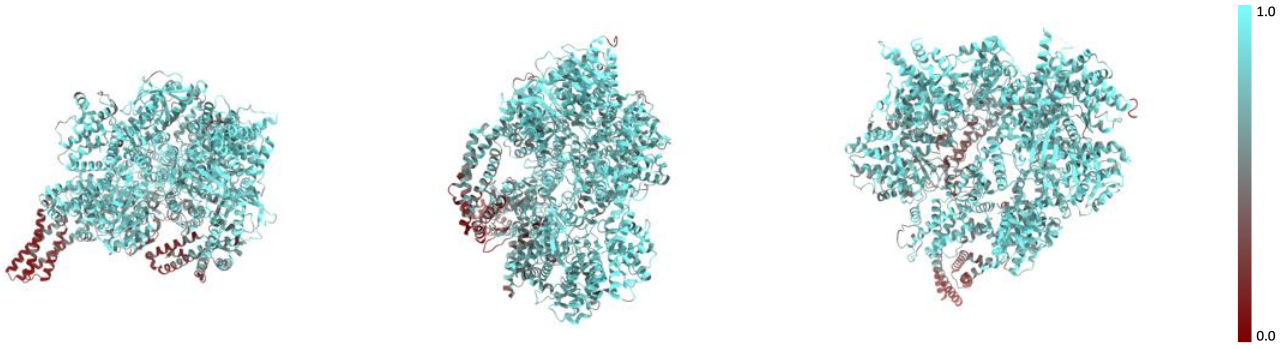
9.2 Q-score mapped to coordinate model (i)



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.

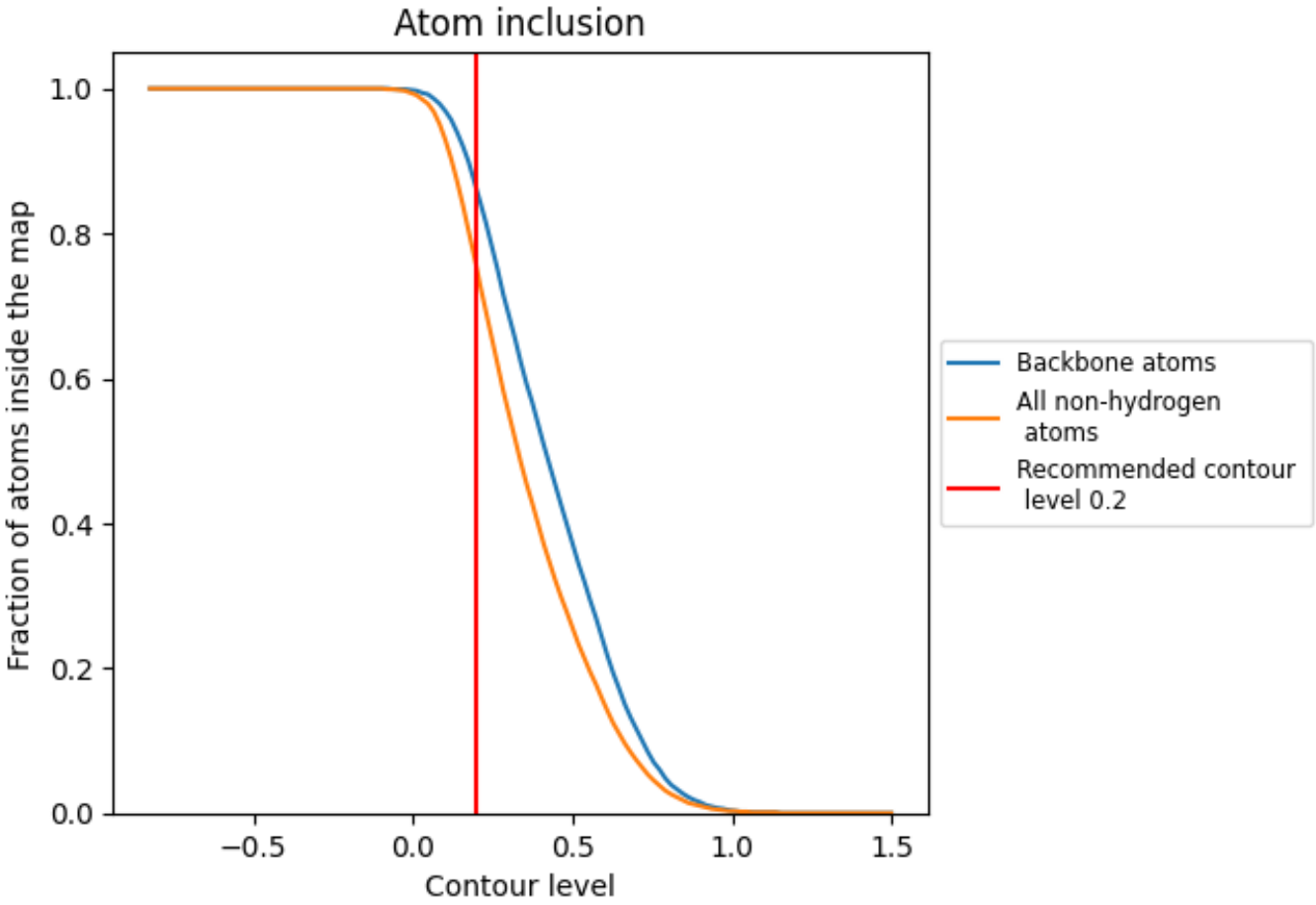
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7510	0.4100
A	0.7510	0.4100