Full wwPDB EM Validation Report (i)

May 19, 2024 – 09:49 AM EDT

PDB ID	:	7MI3
EMDB ID	:	EMD-23838
Title	:	Signal subtracted reconstruction of AAA2, AAA3, and AAA4 domains of dynein in the presence of a pyrazolo-pyrimidinone-based compound, Model 4
Authors	:	Santarossa, C.C.; Coudray, N.; Urnavicius, L.; Ekiert, D.C.; Bhabha, G.; Kapoor, T.M.
Deposited on	:	2021-04-16
Resolution	:	3.50 Å(reported)
Based on initial model	:	7MI1

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

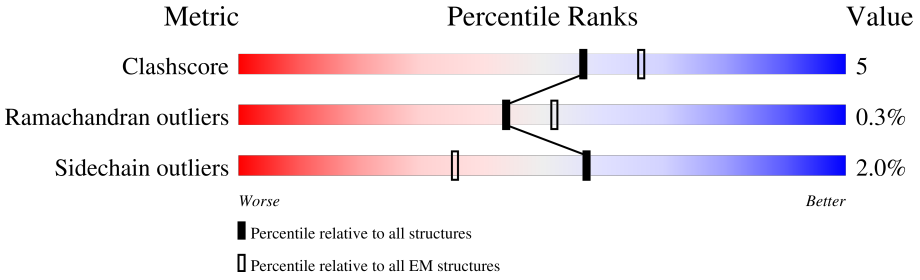
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2661	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9682 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 Fusion protein of Dynein and Endolysin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1192	9590	6143	1611	1787	49	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1363	GLY	-	expression tag	UNP P36022
A	1849	GLN	GLU	conflict	UNP P36022
A	3120	GLY	-	linker	UNP P36022
A	3121	SER	-	linker	UNP P36022
A	3122	GLY	-	linker	UNP P36022
A	3123	SER	-	linker	UNP P36022
A	3124	GLY	-	linker	UNP P36022
A	3125	SER	-	linker	UNP P36022
A	3136	GLY	ARG	conflict	UNP P00720
A	3178	THR	CYS	conflict	UNP P00720
A	3221	ALA	CYS	conflict	UNP P00720
A	3261	ARG	ILE	conflict	UNP P00720
A	3286	GLY	-	linker	UNP P00720
A	3287	SER	-	linker	UNP P00720
A	3288	GLY	-	linker	UNP P00720
A	3289	SER	-	linker	UNP P00720
A	3290	GLY	-	linker	UNP P00720
A	3291	SER	-	linker	UNP P00720
A	3742	ASP	ASN	conflict	UNP P36022
A	3895	VAL	PHE	conflict	UNP P36022
A	4072	ASP	ASN	conflict	UNP P36022
A	4093	GLY	-	expression tag	UNP P36022
A	4094	SER	-	expression tag	UNP P36022
A	4095	GLY	-	expression tag	UNP P36022
A	4096	SER	-	expression tag	UNP P36022
A	4097	GLY	-	expression tag	UNP P36022
A	4098	SER	-	expression tag	UNP P36022
A	4099	HIS	-	expression tag	UNP P36022

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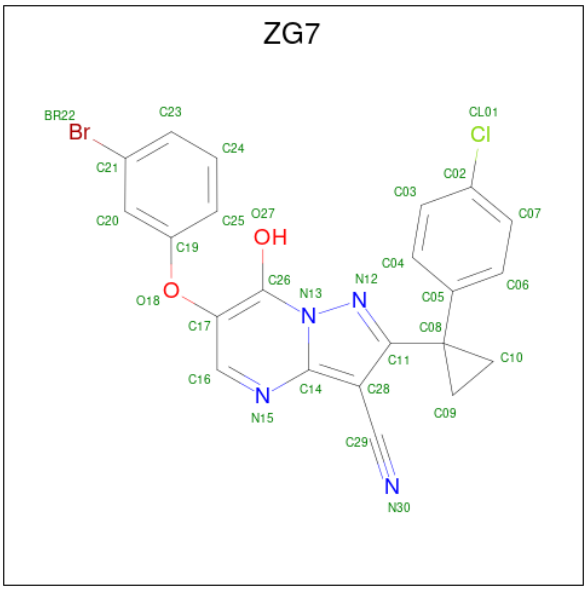
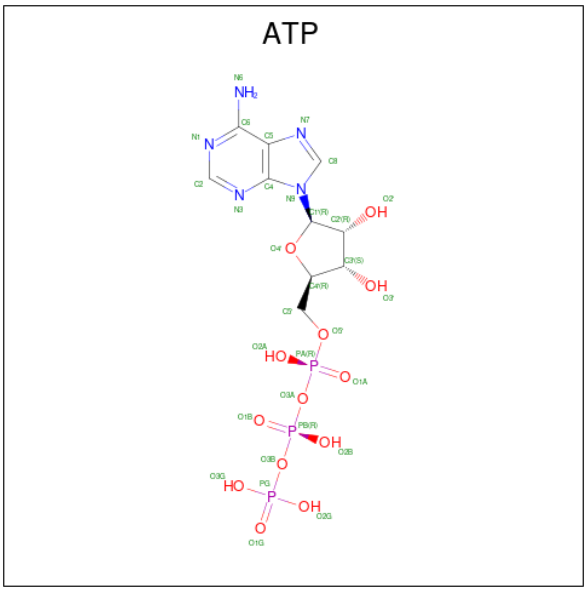
Chain	Residue	Modelled	Actual	Comment	Reference
A	4100	HIS	-	expression tag	UNP P36022
A	4101	HIS	-	expression tag	UNP P36022
A	4102	HIS	-	expression tag	UNP P36022
A	4103	HIS	-	expression tag	UNP P36022
A	4104	HIS	-	expression tag	UNP P36022

- Molecule 2 is (8S)-6-(3-bromophenoxy)-2-[1-(4-chlorophenyl)cyclopropyl]-7-hydroxypyrazolo[1,5-a]pyrimidine-3-carbonitrile (three-letter code: ZG7) (formula: $C_{22}H_{14}BrClN_4O_2$).



Mol	Chain	Residues	Atoms						AltConf
			Total	Br	C	Cl	N	O	
2	A	1	30	1	22	1	4	2	0
			Total	Br	C	Cl	N	O	
2	A	1	30	1	22	1	4	2	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

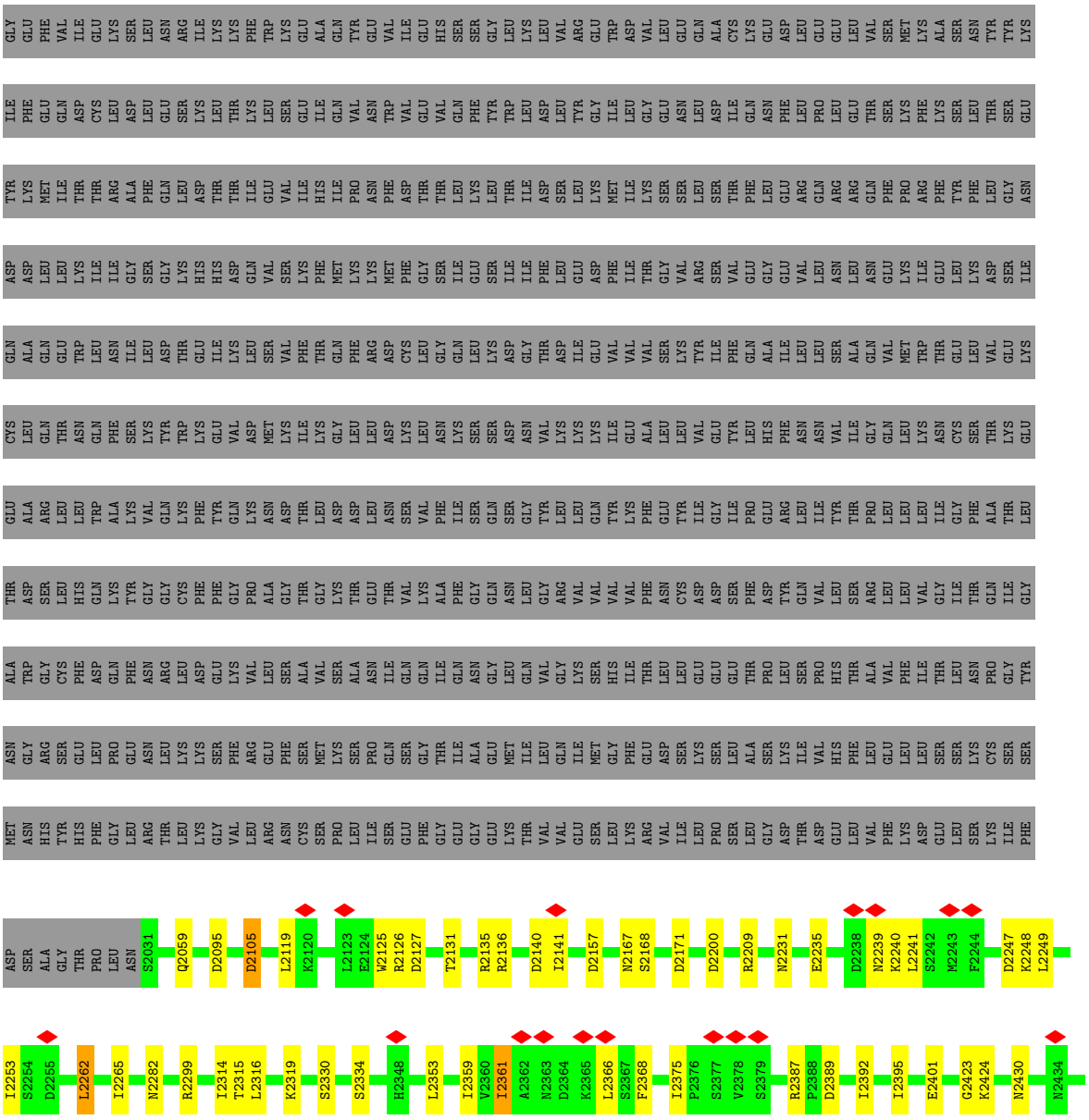
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0

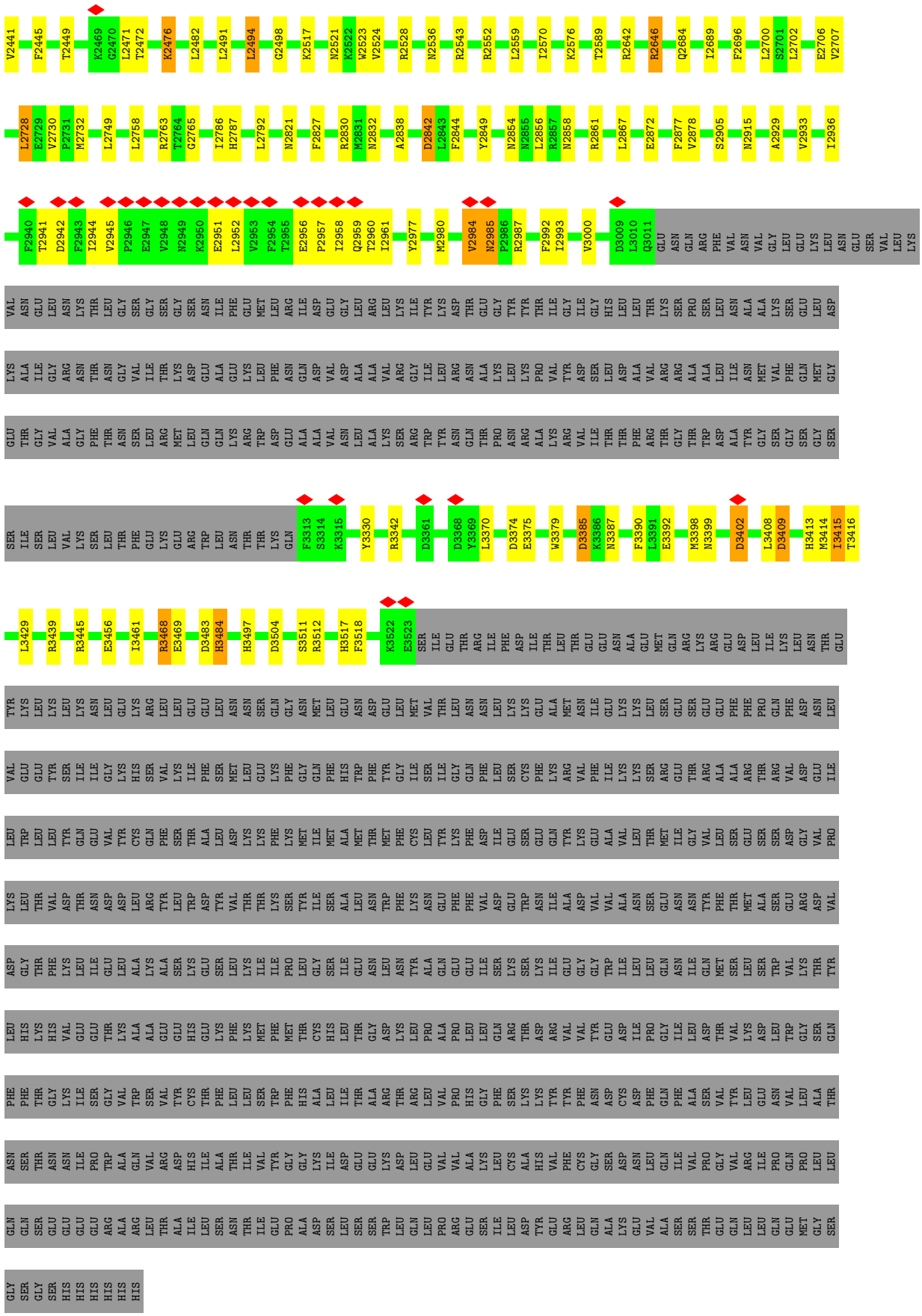
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fusion protein of Dynein and Endolysin

Chain A:




V2441 F2445 T2449 K2469 G2470 L2471 T2472 K2476 L2482 L2491 L2494 G2498 K2517 N2521 K2522 W2523 V2524 R2528 N2536 R2543 R2552 L2559 I2570 K2576 T2589 R2642 R2646 Q2684 I2689 F2696 L2700 S2701 L2702 E2706 V2707
L2728 E2729 V2730 P2731 M2732 L2749 L2758 R2763 T2764 G2765 I2786 H2787 L2792 N2821 F2827 R2830 M2831 N2832 A2838 D2842 L2843 F2844 Y2849 N2854 N2855 L2856 R2857 N2858 R2861 L2867 E2872 F2877 V2878 S2905 N2915 A2929 V2933 I2936
F2940 T2941 D2942 F2943 I2944 V2945 P2946 E2947 V2948 N2949 K2950 E2951 L2952 V2953 F2954 T2955 E2956 P2957 I2958 Q2959 T2960 I2961 Y2977 M2980 V2984 N2985 P2986 R2987 F2992 I2993 V3000 D3009 L3010 Q3011 GLU ASN GLN ARG PHE VAL ASN VAL GLY LEU GLU LYS LEU ASN GLU SER VAL LEU LYS
VAL ASN GLU LEU ASN LYS THR LEU GLY SER GLY SER GLY SER ASN ILE PHE GLU MET LEU ARG ILE ASP GLU GLY LEU ARG LEU LYS ILE TYR LYS ASP THR GLU GLY TYR TYR THR ILE GLY ILE ILE GLY HIS LEU LEU THR LYS SER PRO SER LEU ASN ALA ALA LYS SER GLU ASP
LYS ALA ILE GLY ARG ASN THR ASN GLY VAL ILE THR LYS ASP GLU ALA GLU LYS LEU PHE ASN GLN ASP VAL ASP ALA ALA VAL ARG GLY ILE LEU ARG ASN ALA LYS LEU LYS PRO VAL TYR ASP SER LEU ASP ALA VAL ARG ARG ALA ALA LEU ILE ASN MET VAL PHE GLN MET GLY
GLU THR GLY VAL ALA GLY PHE THR ASN SER LEU ARG MET LEU GLN GLN LYS ARG TRP ASP GLU ALA ALA VAL ASN LEU ALA LYS SER ARG TRP TYR ASN GLN THR PRO ASN ARG ALA LYS ARG VAL ILE THR THR PHE ARG THR GLY TYR TRP ASP ALA TYR GLY SER GLY GLY SER
SER ILE SER LEU VAL LYS SER LEU THR PHE GLU LYS GLU ARG TRP LEU ASN THR THR LYS GLN F3313 S3314 K3315 Y3330 R3342 D3361 D3368 Y3369 L3370 D3374 E3375 W3379 D3385 K3386 N3387 F3390 L3391 E3392 M3398 N3399 D3402 L3408 D3409 H3413 M3414 I3415 T3416
L3429 R3439 R3445 E3456 I3461 R3468 E3469 D3483 H3484 H3497 D3504 S3511 R3512 H3517 F3518 K3522 E3523 SER ILE GLU THR ARG ILE PHE ASP ILE THR LEU THR GLU GLU ASN ALA GLU MET GLN ARG LYS ARG GLU ASP ILE LEU ILE LYS LEU ASN THR GLU
TYR LYS LEU LYS LEU LYS ASN LEU GLU LYS ARG LEU LEU GLU GLU GLN GLY ASN MET LEU GLU ASN ASP GLU LEU MET VAL THR LEU ASN ASN LEU LYS LYS GLU ALA MET ASN ILE GLU LYS LYS LEU SER GLU GLU GLU PHE PHE PRO GLN PHE ASP ASN LEU
VAL GLU GLU TYR SER ILE ILE GLY LYS HIS SER VAL LYS ILE PHE SER MET LEU GLU LYS PHE GLY GLN PHE HIS TRP PHE TYR GLY ILE SER ILE GLY GLN PHE LEU SER CYS PHE LYS ARG VAL PHE ILE LYS LYS SER ARG GLU THR ARG ARG GLU GLU ALA ALA ARG THR ARG VAL ASP GLU ILE
LEU TRP LEU LEU TYR GLN GLU VAL TYR CYS GLN PHE SER THR ALA LEU ASP LYS LYS PHE MET LEU GLN ALA MET THR MET PHE CYS LEU TYR LYS PHE ASP ILE GLU SER GLU GLN TYR LYS GLU ALA VAL LEU THR MET ILE GLY VAL LEU SER GLU SER SER ASP GLY VAL PRO
LYS LEU THR VAL ASP THR ASN ASP TYR LEU TYR TYR ASP ASP ASP LEU ARG TYR LEU TRP VAL THR THR LYS SER TYR ILE SER ALA LEU ASN TRP PHE LYS ASN GLU PHE PHE VAL ASP GLU TRP ASN ILE ALA ASP VAL VAL ALA ASN SER GLU ASN TYR PHE THR MET ALA ASN GLU ASP VAL
ASP GLY THR PHE LYS LEU ILE ILE GLU LEU SER LYS ALA ALA SER ILE SER GLU ILE PRO LEU GLY SER ILE GLU ASN LEU ASN TYR ALA GLN GLU ILE SER LYS SER LYS ILE GLU GLY GLY TRP ILE LEU LEU GLN ASN ILE GLN MET SER THR MET ILE GLY VAL LEU SER LEU SER ASP GLY VAL
LEU HIS LYS HIS VAL GLU GLU THR LEU LYS ALA ALA GLU GLU HIS GLU LYS PHE LYS MET PHE MET THR CYS HIS LEU THR GLY ASP LYS LEU PRO ALA PRO LEU LEU GLN ARG THR ASP ARG VAL VAL TYR GLU ASP ILE PRO GLY ILE LEU ASP ASN THR VAL VAL LYS ASP LEU WRG GLY SER GLN
PHE PHE THR GLY LYS ILE SER GLY VAL TRP SER VAL TYR CYS THR PHE LEU LEU SER TRP PHE HIS ALA LEU ILE THR ALA ARG THR ARG LEU VAL PRO HIS GLY PHE SER LYS LYS TYR TYR PHE ASN ASP CYS ASP PHE GLN PHE ALA SER VAL TYR LEU GLU ASN VAL TYR THR GLY
ASN SER THR ASN ASN ILE PRO TRP ALA GLN VAL ARG ASP HIS ILE ALA THR ILE VAL TYR GLY GLY HIS ALA LYS ILE ASP GLU GLU LYS ASP LEU GLU VAL VAL ALA LYS LEU CYS ALA HIS VAL PHE CYS GLY SER ASP ASN LEU GLN ILE VAL PRO GLY VAL ARG ILE PRO GLN PRO LEU LEU
GLN GLN SER GLU GLU GLU ARG LEU THR ALA ILE LEU SER SER LEU SER SER SER TRP LEU GLN LEU PRO ARG GLU SER ILE LEU ASP TYR GLU ARG LEU GLN ALA LYS GLU VAL ALA SER SER THR GLU GLN LEU LEU GLN MET GLY
GLY SER GLY SER HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	131702	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.020	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	190.62401, 190.62401, 190.62401	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.518, 0.518, 0.518	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ZG7

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	0.49	0/9788	0.75	8/13249 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3402	ASP	CB-CG-OD1	9.88	127.19	118.30
1	A	2952	LEU	CA-CB-CG	7.92	133.52	115.30
1	A	2646	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	3456	GLU	C-N-CA	5.81	136.22	121.70
1	A	3330	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	A	2262	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	3415	ILE	CG1-CB-CG2	-5.09	100.19	111.40
1	A	2141	ILE	CG1-CB-CG2	-5.03	100.34	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9590	0	9637	98	0
2	A	60	0	0	3	0
3	A	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
All	All	9682	0	9649	98	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 5.

All (98) 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:2476:LYS:HE3	1:A:2528:ARG:HD2	1.59	0.85
1:A:2838:ALA:HB3	1:A:2878:VAL:HG13	1.76	0.65
1:A:2763:ARG:NH1	1:A:3511:SER:O	2.30	0.64
1:A:2517:LYS:O	1:A:2521:ASN:N	2.32	0.60
1:A:2366:LEU:HD23	1:A:2368:PHE:HE2	1.67	0.59
1:A:2395:ILE:HD12	1:A:2395:ILE:H	1.68	0.58
1:A:2696:PHE:HA	1:A:2706:GLU:HA	1.86	0.57
1:A:2786:ILE:HD11	1:A:2821:ASN:HA	1.86	0.57
1:A:2316:LEU:HD23	1:A:2359:ILE:HD11	1.87	0.57
1:A:3342:ARG:NH1	1:A:3392:GLU:OE1	2.37	0.56
1:A:3504:ASP:N	1:A:3504:ASP:OD1	2.40	0.55
1:A:3409:ASP:HB3	1:A:3518:PHE:HB2	1.89	0.54
1:A:2136:ARG:O	1:A:2140:ASP:HB2	2.09	0.53
1:A:3408:LEU:HD23	1:A:3517:HIS:CE1	2.43	0.52
1:A:2476:LYS:HD3	1:A:2476:LYS:H	1.74	0.52
1:A:2728:LEU:HD13	1:A:2730:VAL:HG23	1.92	0.52
1:A:3385:ASP:OD1	1:A:3385:ASP:N	2.43	0.52
1:A:2642:ARG:O	1:A:2646:ARG:HG2	2.11	0.51
1:A:2984:VAL:O	1:A:2987:ARG:NH1	2.44	0.51
1:A:2984:VAL:HG13	1:A:2985:ASN:H	1.75	0.51
1:A:2832:ASN:OD1	1:A:2905:SER:OG	2.26	0.51
1:A:2241:LEU:HD13	1:A:2299:ARG:HH11	1.76	0.50
1:A:2765:GLY:H	2:A:4201:ZG7:C26	2.24	0.50
1:A:2936:ILE:HD12	1:A:3000:VAL:HA	1.93	0.50
1:A:2157:ASP:N	1:A:2157:ASP:OD1	2.43	0.50
1:A:2401:GLU:OE2	1:A:2430:ASN:ND2	2.32	0.50
1:A:2758:LEU:HD23	1:A:2915:ASN:HB3	1.93	0.50
1:A:2262:LEU:HA	1:A:2265:ILE:HD12	1.93	0.49
1:A:2944:ILE:HG21	1:A:2961:ILE:HG12	1.94	0.49
1:A:2387:ARG:NH2	1:A:2389:ASP:OD2	2.33	0.49
1:A:2494:LEU:HD22	1:A:2498:GLY:HA2	1.94	0.49
1:A:2552:ARG:NH1	3:A:4203:ATP:O1G	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2330:SER:HB3	1:A:2334:SER:HB2	1.93	0.49
1:A:3387:ASN:HB3	1:A:3390:PHE:HD1	1.77	0.49
1:A:2646:ARG:NH1	1:A:2706:GLU:OE1	2.46	0.48
1:A:2842:ASP:OD1	1:A:2842:ASP:N	2.38	0.48
1:A:2471:LEU:HD12	1:A:2523:TRP:HB3	1.95	0.48
1:A:2646:ARG:HH11	1:A:2646:ARG:HG3	1.79	0.47
1:A:2171:ASP:OD1	1:A:2209:ARG:NH1	2.46	0.47
1:A:2951:GLU:OE1	1:A:2951:GLU:N	2.39	0.47
1:A:2441:VAL:HG23	1:A:2482:LEU:HD11	1.96	0.47
1:A:2929:ALA:HB2	1:A:2992:PHE:HZ	1.80	0.47
1:A:2472:THR:O	1:A:2524:VAL:HA	2.14	0.46
1:A:2933:VAL:O	1:A:2936:ILE:HG22	2.14	0.46
1:A:2941:THR:O	1:A:2944:ILE:HG12	2.14	0.46
1:A:3379:TRP:NE1	1:A:3398:MET:SD	2.88	0.46
1:A:2491:LEU:HD21	1:A:2543:ARG:NH1	2.29	0.46
1:A:2792:LEU:HA	1:A:2827:PHE:HE1	1.79	0.46
1:A:2105:ASP:N	1:A:2105:ASP:OD1	2.48	0.46
1:A:2730:VAL:HG12	1:A:2732:MET:HG3	1.98	0.46
1:A:2728:LEU:HD22	1:A:3469:GLU:HG2	1.98	0.46
1:A:2424:LYS:HG2	1:A:2559:LEU:HD12	1.97	0.46
1:A:2700:LEU:HD22	1:A:2707:VAL:HG11	1.97	0.46
1:A:3468:ARG:HA	1:A:3468:ARG:HD3	1.80	0.46
1:A:3483:ASP:OD1	1:A:3484:HIS:ND1	2.47	0.46
1:A:2445:PHE:HA	1:A:2449:THR:HG21	1.97	0.45
1:A:2856:LEU:HD21	1:A:2877:PHE:HB2	1.97	0.45
1:A:2319:LYS:HB3	1:A:2353:LEU:HD22	1.98	0.45
1:A:2536:ASN:HB2	1:A:2543:ARG:HE	1.81	0.45
1:A:2253:ILE:HD11	1:A:2314:ILE:HD12	1.99	0.45
1:A:2375:ILE:HD11	1:A:2395:ILE:HG13	1.98	0.45
1:A:2247:ASP:OD1	1:A:2248:LYS:N	2.50	0.45
1:A:2249:LEU:O	1:A:2253:ILE:HG12	2.17	0.45
1:A:2241:LEU:HD13	1:A:2299:ARG:HD2	1.99	0.45
1:A:2095:ASP:N	1:A:2095:ASP:OD1	2.51	0.44
1:A:2200:ASP:N	1:A:2200:ASP:OD1	2.50	0.44
1:A:3414:MET:C	1:A:3416:THR:H	2.20	0.44
1:A:3370:LEU:HD21	1:A:3399:ASN:HD22	1.83	0.44
1:A:3512:ARG:HH22	2:A:4201:ZG7:C25	2.31	0.44
1:A:2792:LEU:HD11	1:A:2830:ARG:HE	1.84	0.43
1:A:2977:TYR:CE2	1:A:2987:ARG:HB2	2.53	0.43
1:A:2282:ASN:HB3	1:A:2552:ARG:HG3	1.99	0.43
1:A:2576:LYS:HA	1:A:2589:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2844:PHE:O	1:A:2849:TYR:HB2	2.18	0.43
1:A:2392:ILE:HG13	1:A:2570:ILE:HG23	2.01	0.43
1:A:2787:HIS:HB3	1:A:3461:ILE:HG23	2.01	0.43
1:A:2858:ASN:OD1	1:A:2861:ARG:NH2	2.53	0.42
1:A:2992:PHE:HD2	1:A:2993:ILE:HD12	1.84	0.42
1:A:2315:THR:O	1:A:2319:LYS:HG3	2.20	0.42
1:A:2389:ASP:OD1	1:A:2389:ASP:N	2.52	0.42
1:A:2239:ASN:OD1	1:A:2240:LYS:N	2.53	0.42
1:A:2684:GLN:N	1:A:2684:GLN:OE1	2.54	0.41
1:A:2689:ILE:HD12	1:A:2689:ILE:HG23	1.76	0.41
1:A:2423:GLY:N	2:A:4202:ZG7:O27	2.48	0.41
1:A:2125:TRP:CZ3	1:A:2127:ASP:HA	2.56	0.41
1:A:3415:ILE:HD11	1:A:3497:HIS:ND1	2.36	0.41
1:A:2956:GLU:HG3	1:A:2957:PRO:HD2	2.02	0.41
1:A:2240:LYS:NZ	1:A:2299:ARG:HH22	2.18	0.41
1:A:2786:ILE:HG13	1:A:2821:ASN:HD22	1.85	0.41
1:A:3374:ASP:OD1	1:A:3375:GLU:N	2.52	0.41
1:A:2361:ILE:HG22	1:A:2368:PHE:CE1	2.56	0.40
1:A:2749:LEU:HD23	1:A:2749:LEU:HA	1.91	0.40
1:A:3408:LEU:HD23	1:A:3517:HIS:ND1	2.36	0.40
1:A:2119:LEU:HD21	1:A:2126:ARG:NE	2.37	0.40
1:A:2167:ASN:OD1	1:A:2168:SER:N	2.55	0.40
1:A:2867:LEU:HD22	1:A:2872:GLU:HB3	2.03	0.40
1:A:2231:ASN:O	1:A:2235:GLU:HG3	2.22	0.40
1:A:3429:LEU:HD21	1:A:3439:ARG:HD2	2.02	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	1188/2661 (45%)	1103 (93%)	81 (7%)	4 (0%)	41 75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3413	HIS
1	A	2984	VAL
1	A	2959	GLN
1	A	2985	ASN

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	1084/2406 (45%)	1062 (98%)	22 (2%)	55 79

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2059	GLN
1	A	2105	ASP
1	A	2131	THR
1	A	2135	ARG
1	A	2361	ILE
1	A	2476	LYS
1	A	2494	LEU
1	A	2702	LEU
1	A	2728	LEU
1	A	2842	ASP
1	A	2854	ASN
1	A	2942	ASP
1	A	2945	VAL
1	A	2958	ILE
1	A	2960	THR
1	A	2980	MET
1	A	3385	ASP
1	A	3402	ASP
1	A	3409	ASP
1	A	3445	ARG
1	A	3468	ARG

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Mol	Chain	Res	Type
1	A	3484	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2363	ASN
1	A	2481	ASN
1	A	2508	GLN
1	A	2714	ASN
1	A	2854	ASN
1	A	2959	GLN
1	A	3517	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ZG7	A	4201	-	29,34,34	3.44	8 (27%)	33,51,51	2.55	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ZG7	A	4202	-	29,34,34	3.64	8 (27%)	33,51,51	2.38	10 (30%)
3	ATP	A	4203	4	26,33,33	0.96	0	31,52,52	1.64	5 (16%)

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	ZG7	A	4201	-	-	1/10/22/22	0/5/5/5
2	ZG7	A	4202	-	-	0/10/22/22	0/5/5/5
3	ATP	A	4203	4	-	6/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4202	ZG7	C14-N15	12.99	1.53	1.35
2	A	4201	ZG7	C14-N15	12.17	1.52	1.35
2	A	4202	ZG7	C16-N15	8.39	1.45	1.31
2	A	4201	ZG7	C28-C29	8.10	1.53	1.44
2	A	4202	ZG7	C28-C29	7.91	1.53	1.44
2	A	4201	ZG7	C16-N15	7.78	1.44	1.31
2	A	4202	ZG7	O27-C26	-5.26	1.17	1.32
2	A	4202	ZG7	C16-C17	5.10	1.46	1.38
2	A	4201	ZG7	C16-C17	4.66	1.46	1.38
2	A	4201	ZG7	O27-C26	-4.56	1.19	1.32
2	A	4202	ZG7	C17-C26	2.54	1.46	1.40
2	A	4201	ZG7	C17-C26	2.48	1.46	1.40
2	A	4201	ZG7	C11-N12	2.39	1.37	1.34
2	A	4202	ZG7	BR22-C21	2.31	1.94	1.90
2	A	4202	ZG7	C11-N12	2.26	1.37	1.34
2	A	4201	ZG7	BR22-C21	2.14	1.94	1.90

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4201	ZG7	C09-C08-C11	10.57	137.00	117.43
2	A	4202	ZG7	C09-C08-C11	8.05	132.33	117.43
2	A	4201	ZG7	C05-C08-C11	-7.16	95.55	113.07
2	A	4202	ZG7	C05-C08-C11	-5.36	99.96	113.07
2	A	4202	ZG7	C10-C08-C11	4.92	126.55	117.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4202	ZG7	C16-N15-C14	3.98	121.81	116.73
3	A	4203	ATP	C3'-C2'-C1'	3.75	106.62	100.98
3	A	4203	ATP	C4-C5-N7	-3.51	105.74	109.40
3	A	4203	ATP	PA-O3A-PB	-3.30	121.50	132.83
2	A	4202	ZG7	O18-C17-C16	3.22	129.91	118.65
3	A	4203	ATP	N3-C2-N1	-3.18	123.70	128.68
2	A	4201	ZG7	C16-N15-C14	2.97	120.53	116.73
2	A	4201	ZG7	C11-C28-C29	-2.94	123.11	127.33
3	A	4203	ATP	O5'-C5'-C4'	2.58	117.89	108.99
2	A	4202	ZG7	C17-C16-N15	-2.45	118.90	122.66
2	A	4202	ZG7	C09-C08-C10	2.35	60.15	58.70
2	A	4202	ZG7	C06-C05-C04	2.32	121.43	117.97
2	A	4201	ZG7	C08-C11-N12	2.26	123.19	120.61
2	A	4202	ZG7	O18-C17-C26	-2.25	113.14	117.84
2	A	4202	ZG7	C03-C04-C05	-2.05	118.48	121.22

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4203	ATP	PB-O3B-PG-O3G
3	A	4203	ATP	PB-O3B-PG-O1G
3	A	4203	ATP	PG-O3B-PB-O1B
3	A	4203	ATP	PB-O3A-PA-O1A
2	A	4201	ZG7	C06-C05-C08-C10
3	A	4203	ATP	PB-O3A-PA-O2A
3	A	4203	ATP	C4'-C5'-O5'-PA

There are no ring outliers.

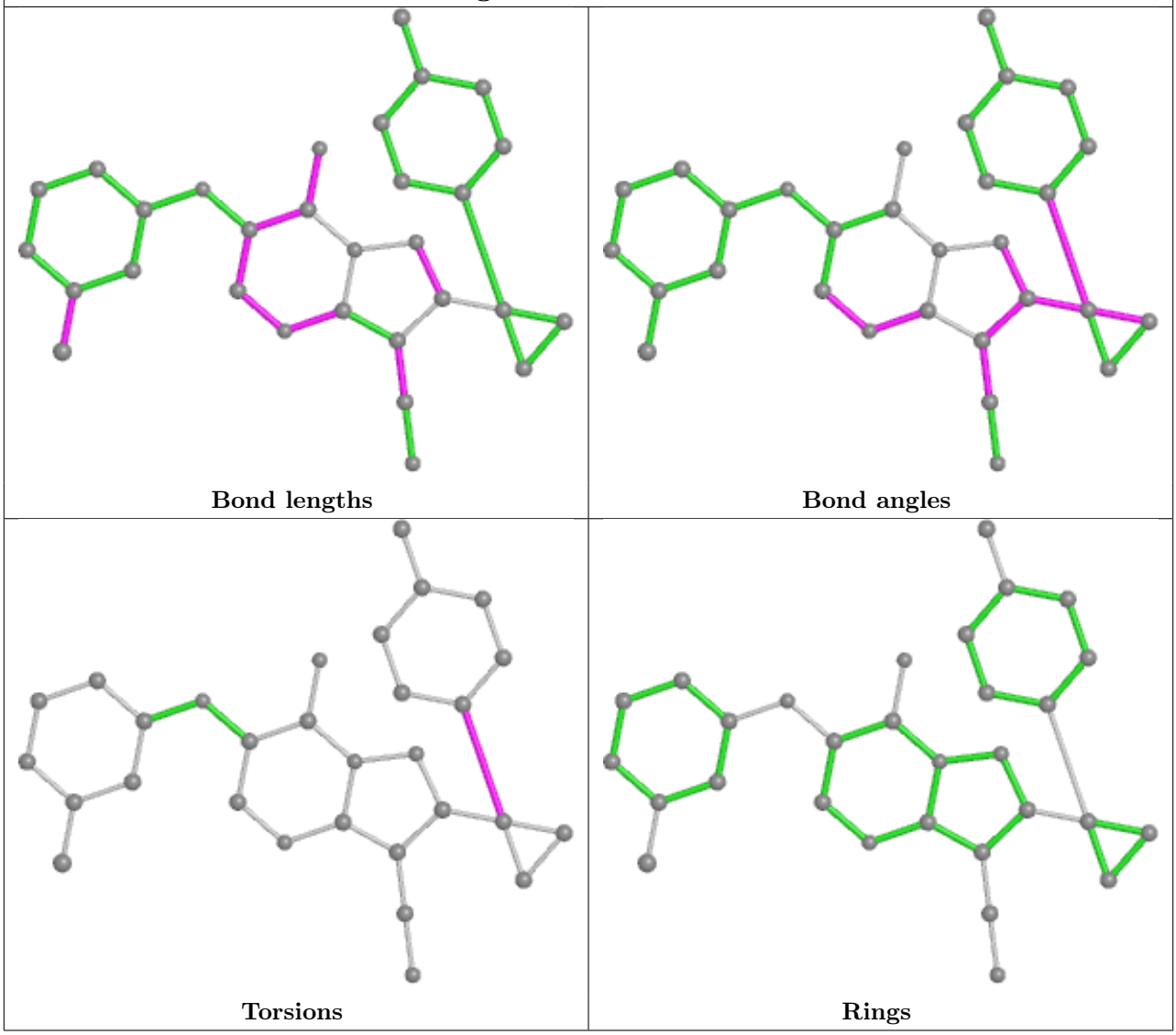
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4201	ZG7	2	0
2	A	4202	ZG7	1	0
3	A	4203	ATP	1	0

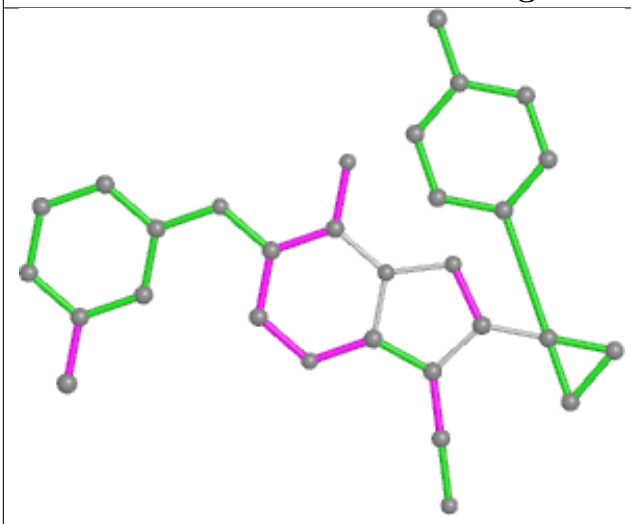
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

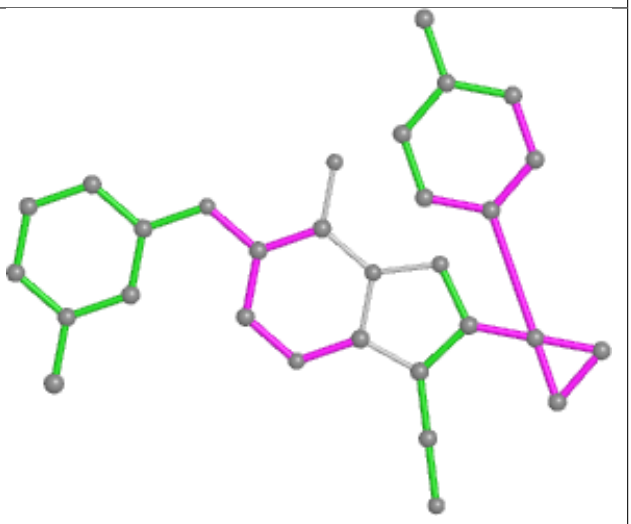
Ligand ZG7 A 4201



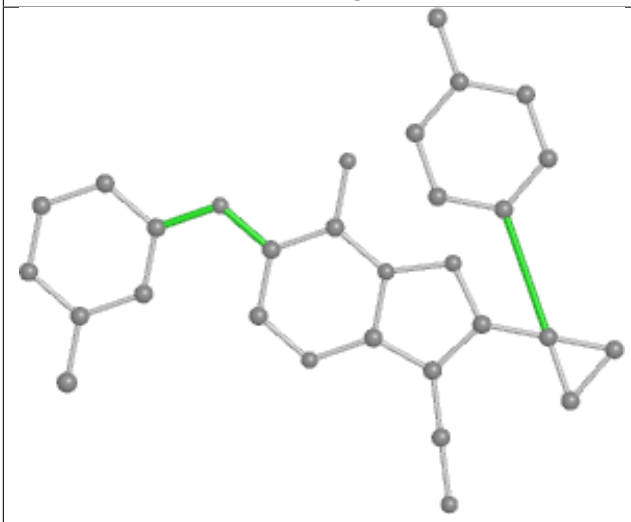
Ligand ZG7 A 4202



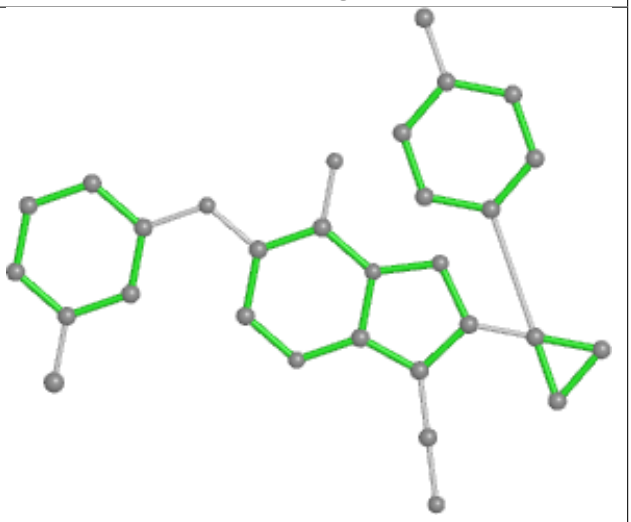
Bond lengths



Bond angles

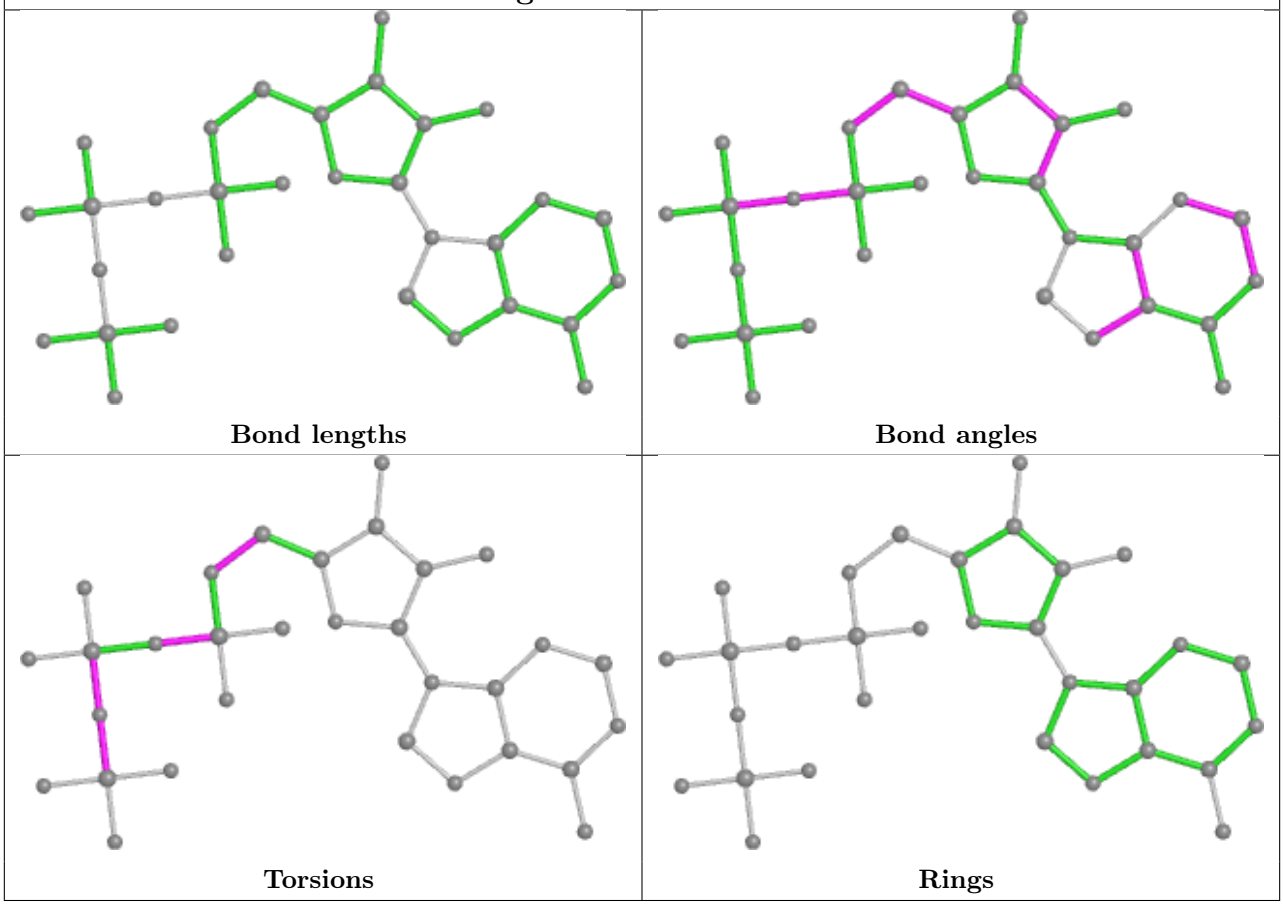


Torsions



Rings

Ligand ATP A 4203



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

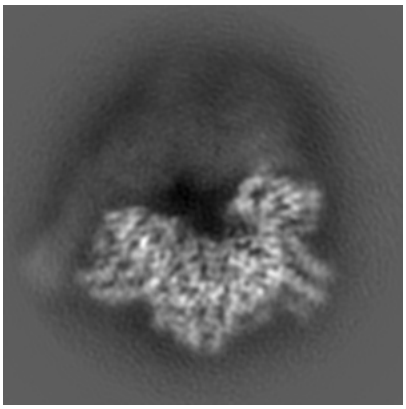
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23838. These allow visual inspection of the internal detail of the map and identification of artifacts.

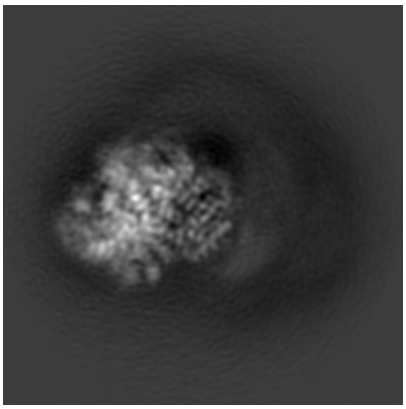
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

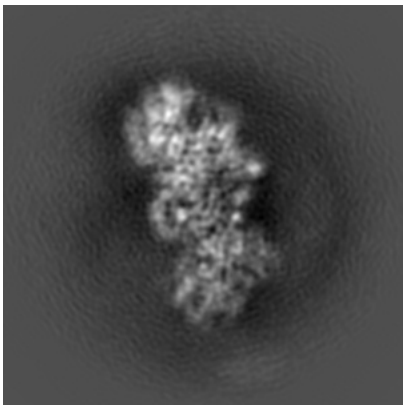
6.1.1 Primary map



X

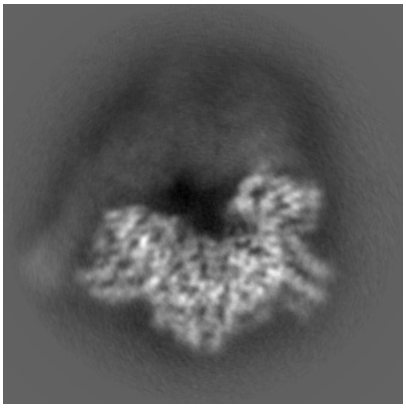


Y

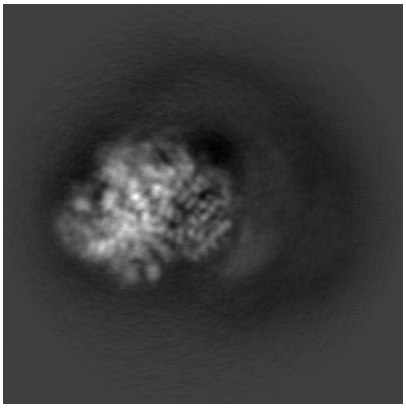


Z

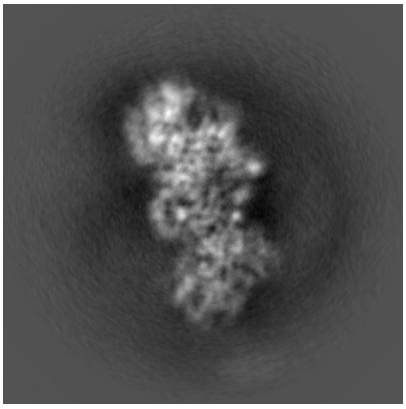
6.1.2 Raw map



X



Y

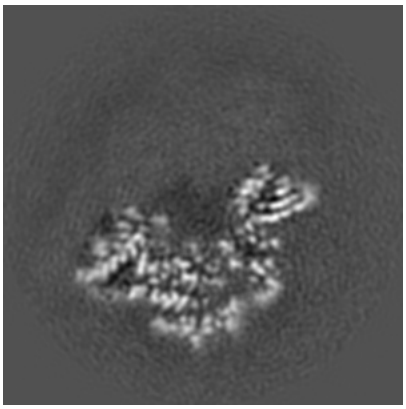


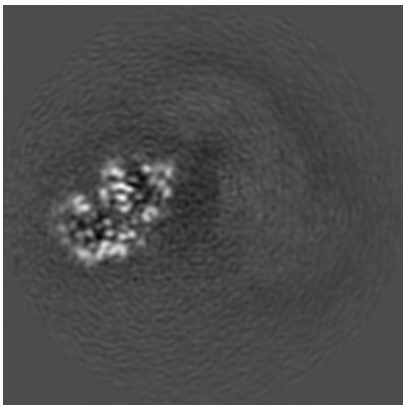
Z

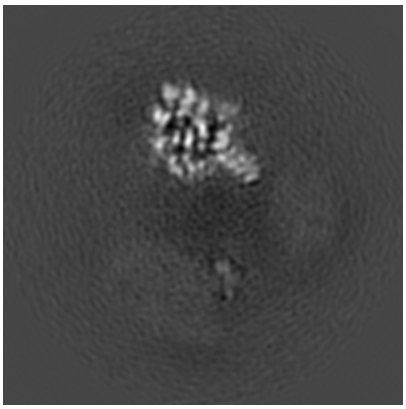
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

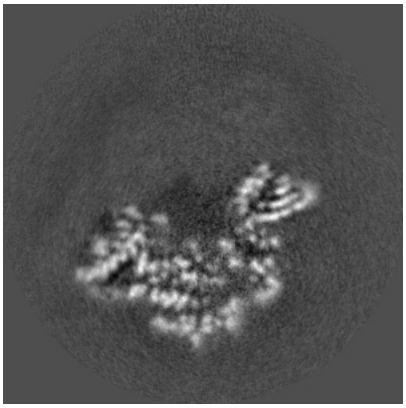
6.2.1 Primary map

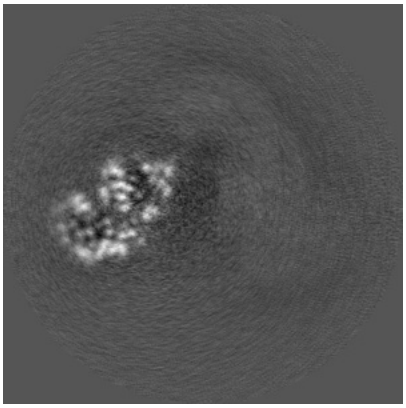

X Index: 184

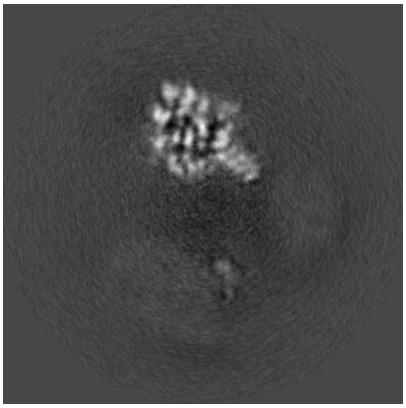

Y Index: 184


Z Index: 184

6.2.2 Raw map


X Index: 184

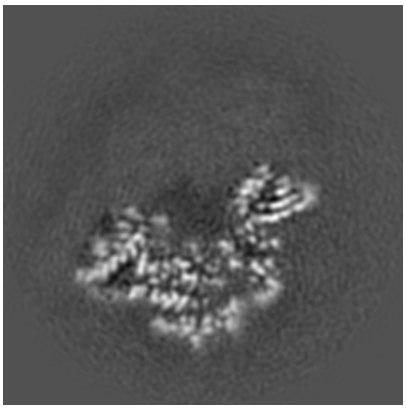

Y Index: 184

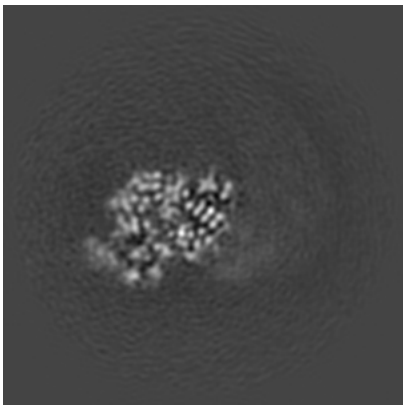

Z Index: 184

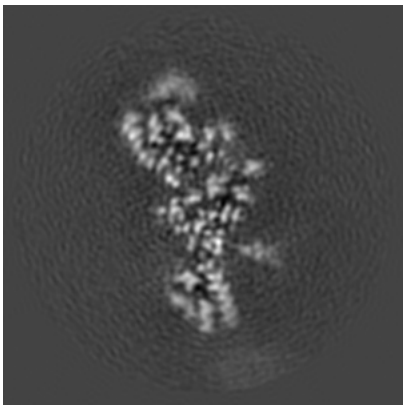
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

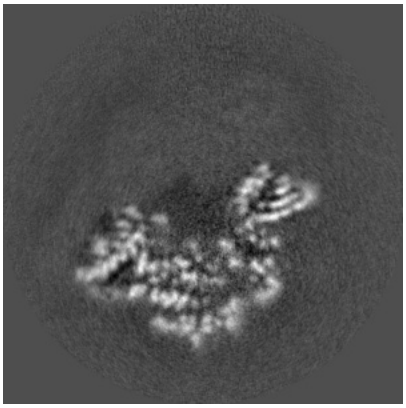
6.3.1 Primary map

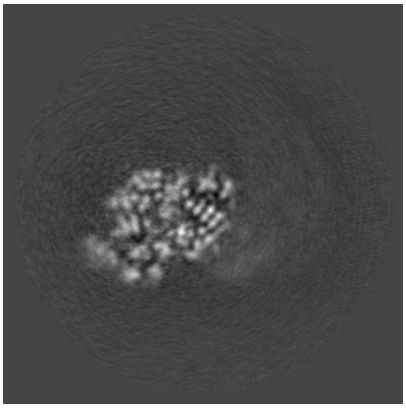

X Index: 184

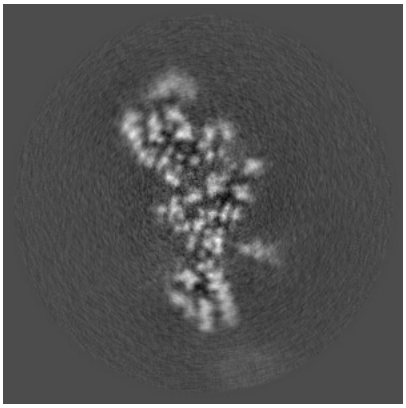

Y Index: 247


Z Index: 120

6.3.2 Raw map


X Index: 184

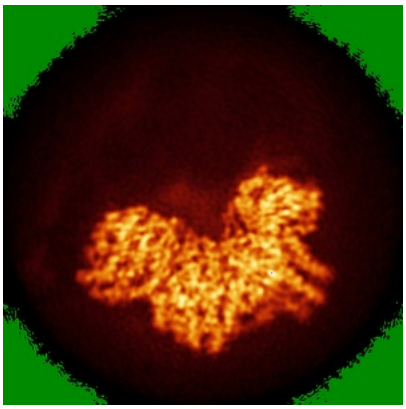

Y Index: 246

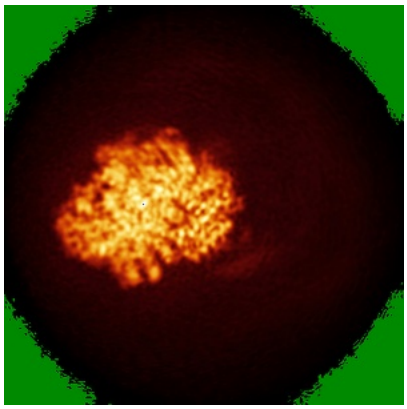

Z Index: 120

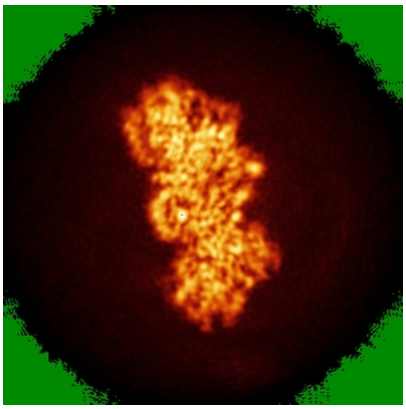
The images above show the largest variance slices of the map in three orthogonal directions.

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

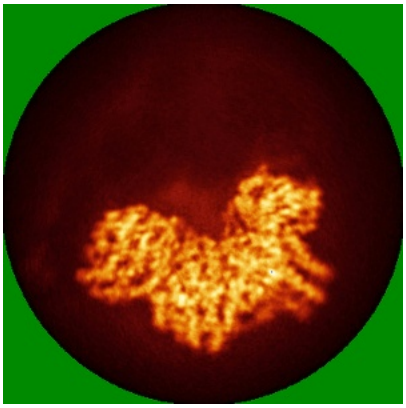
6.4.1 Primary map

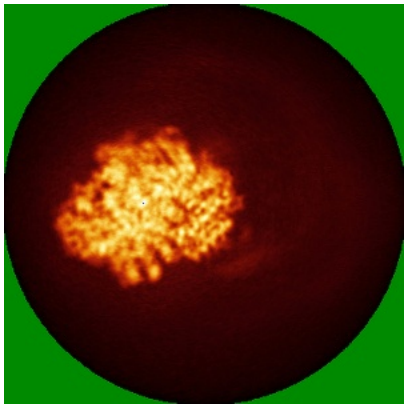

X

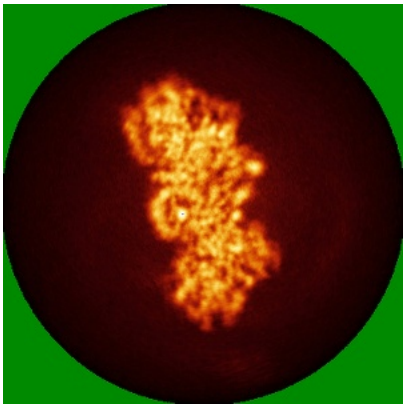

Y


Z

6.4.2 Raw map


X

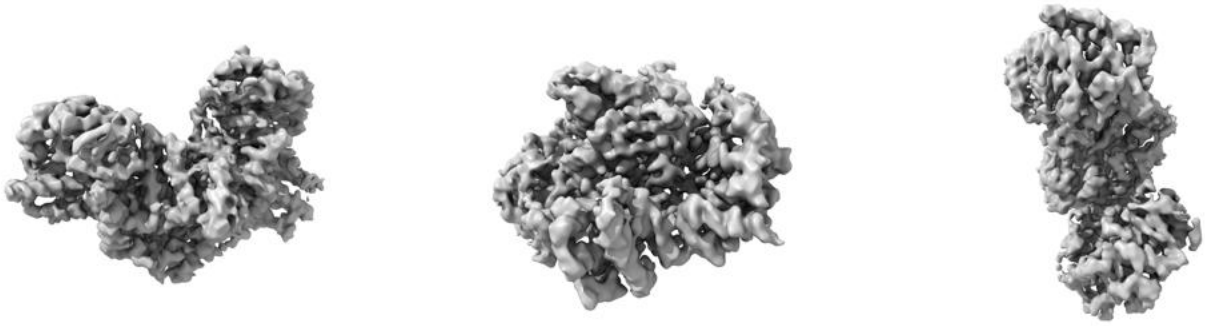

Y


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)

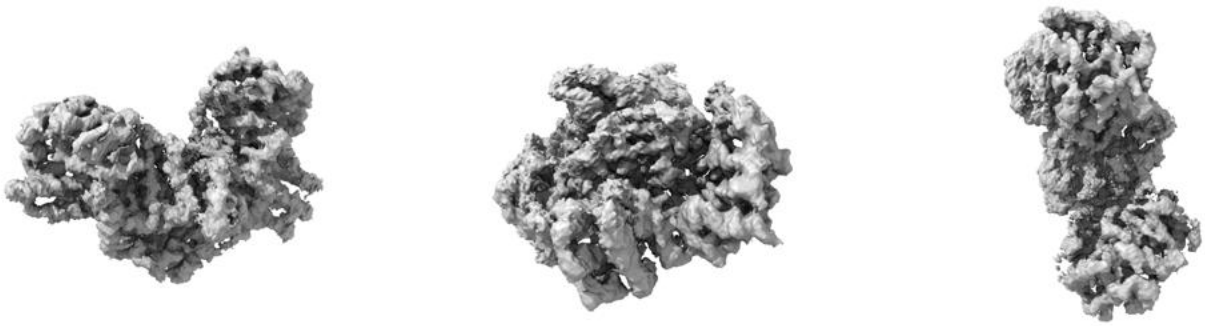
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. 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.

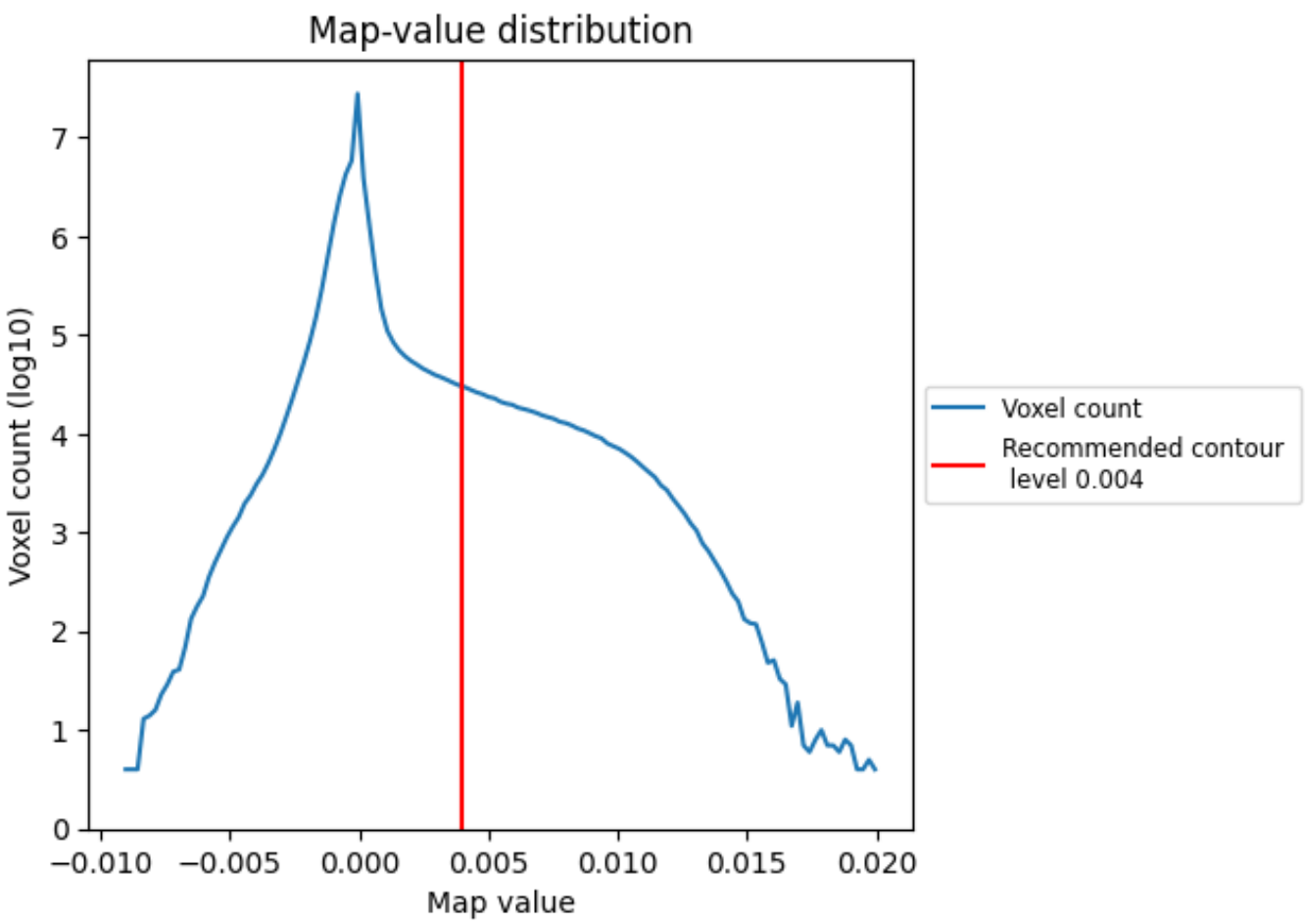
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

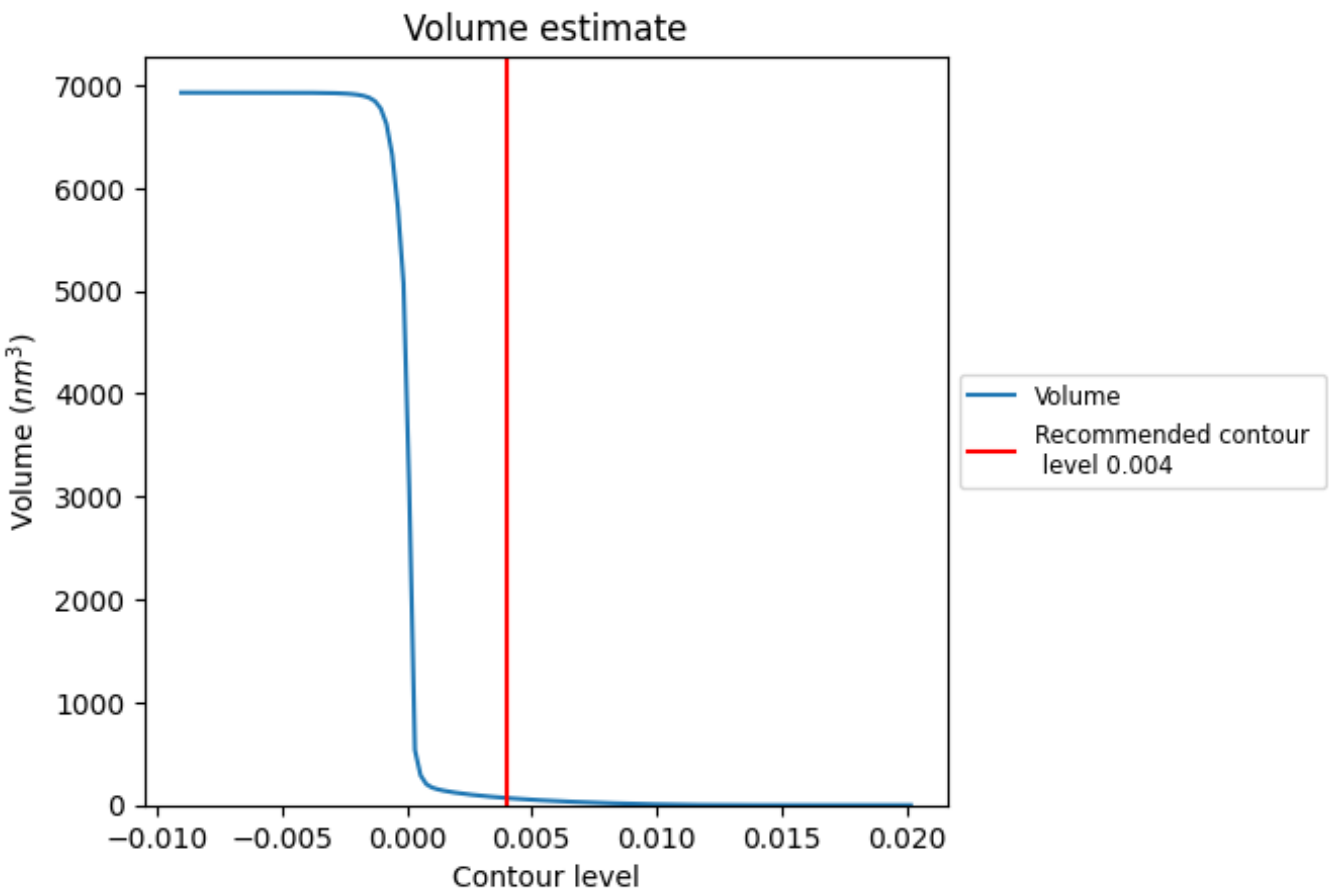
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

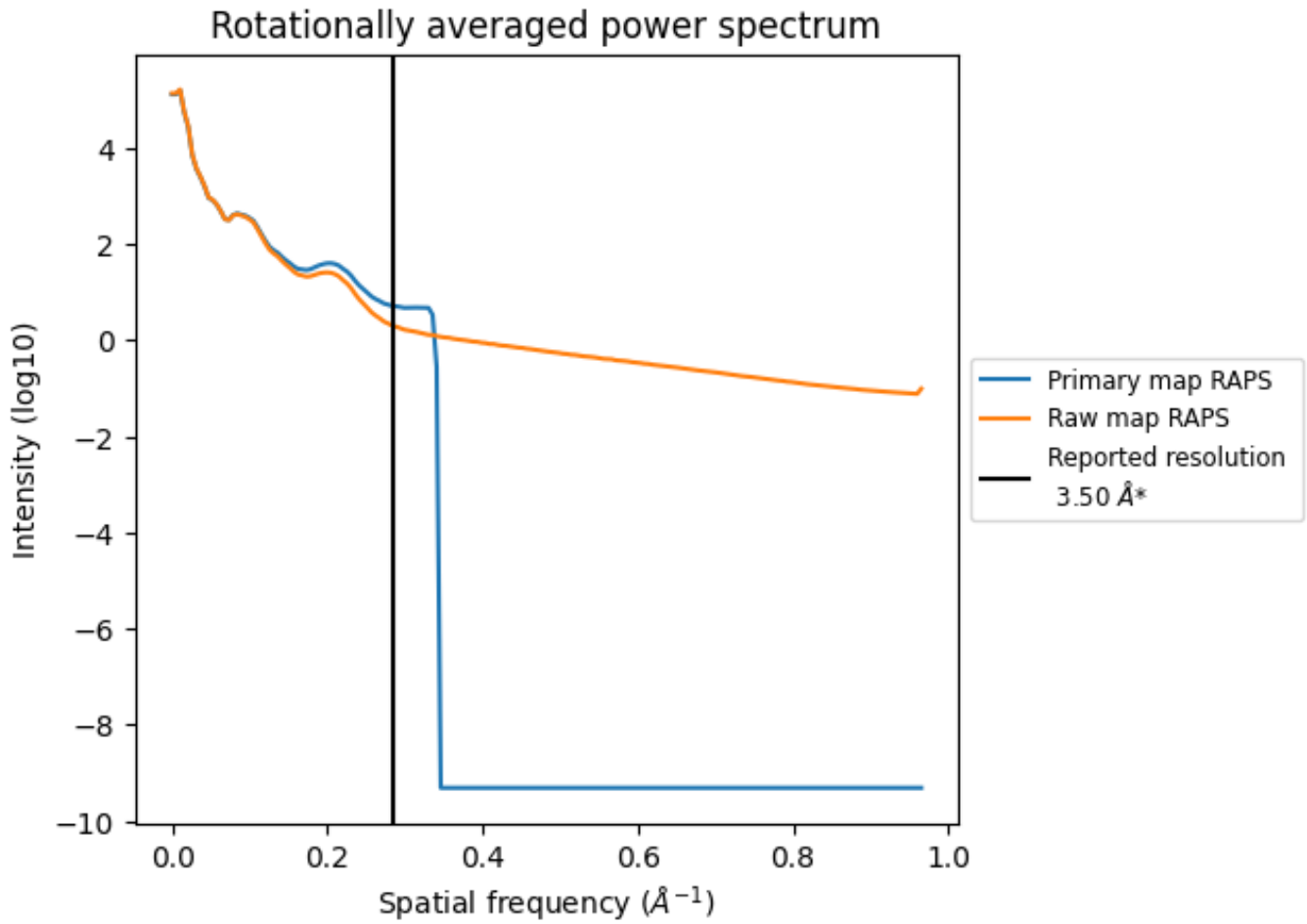
7.2 Volume estimate (i)



The volume at the recommended contour level is 69 nm^3; this corresponds to an approximate mass of 63 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)

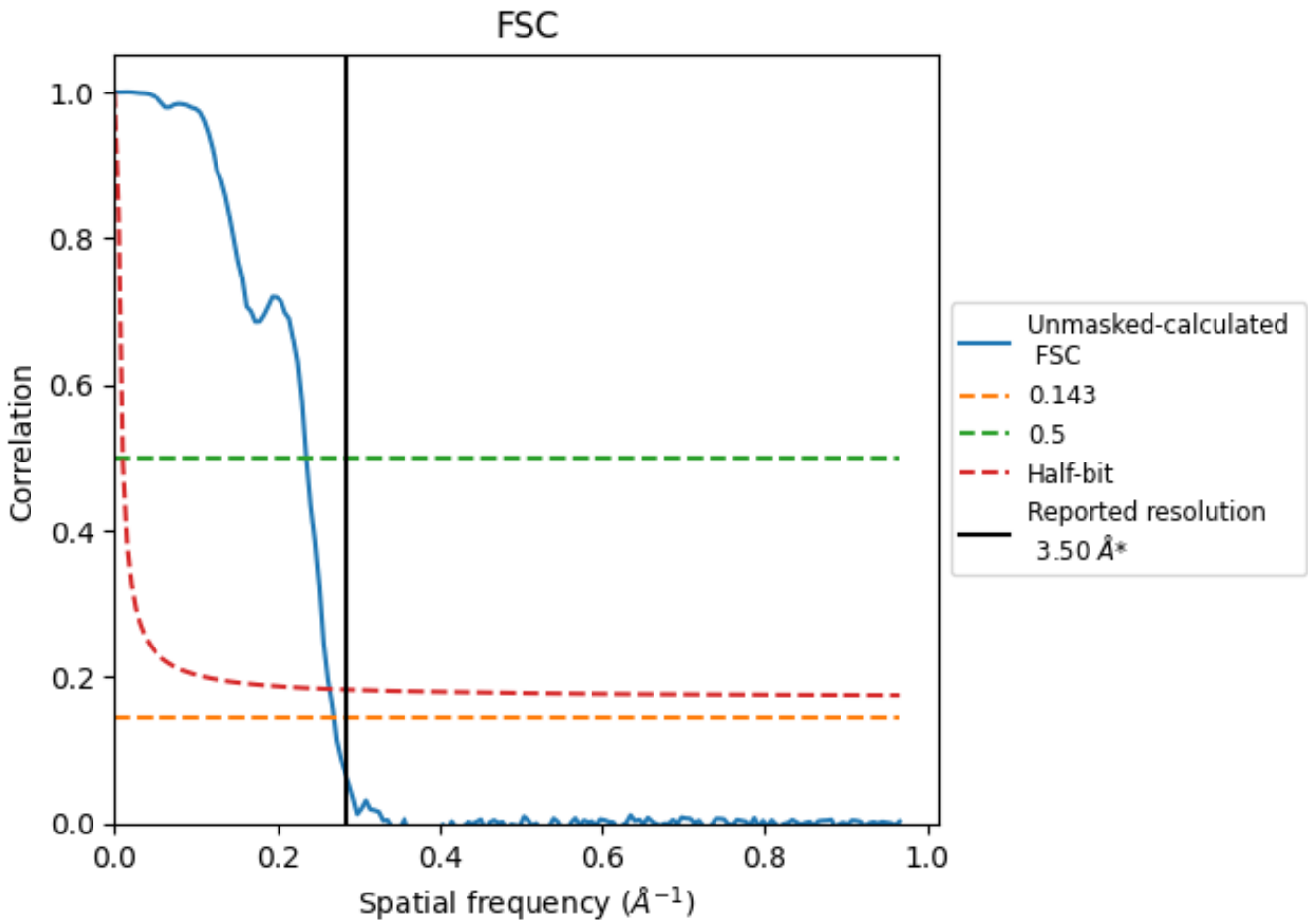


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



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

8.2 Resolution estimates (i)

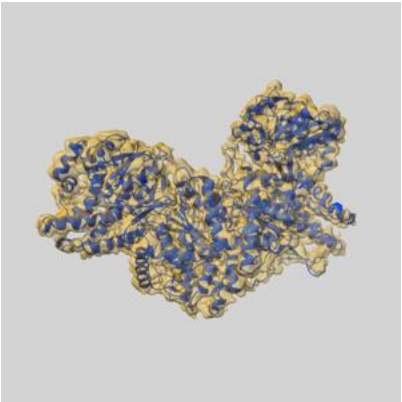
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.71	4.24	3.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

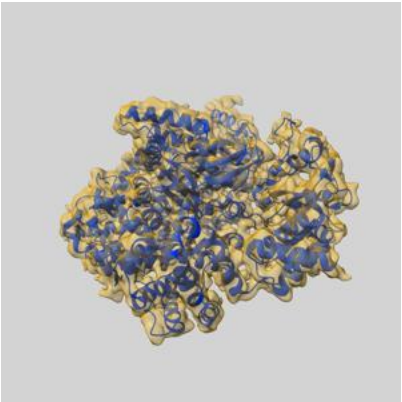
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23838 and PDB model 7MI3. Per-residue inclusion information can be found in section 3 on page 6.

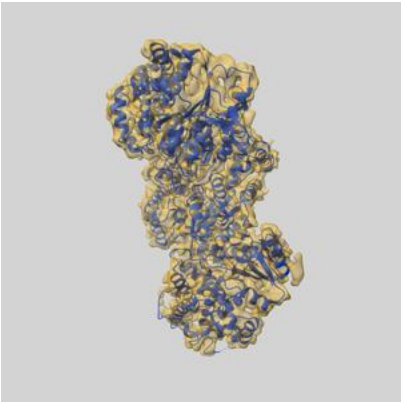
9.1 Map-model overlay (i)



X



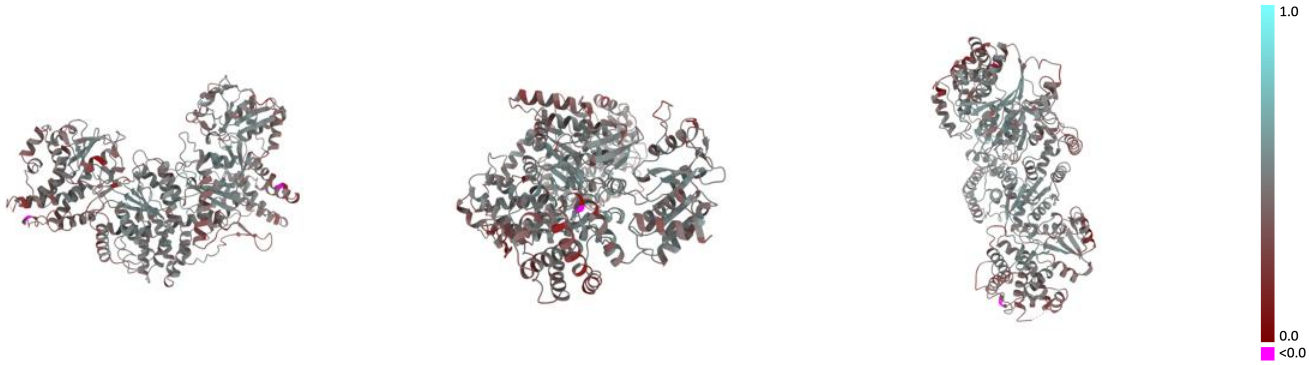
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 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.

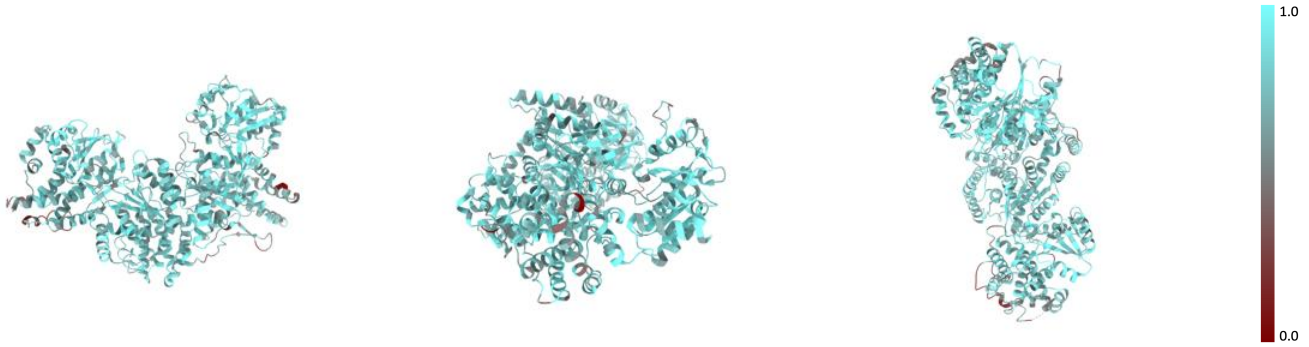
9.2 Q-score mapped to coordinate model (i)



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.

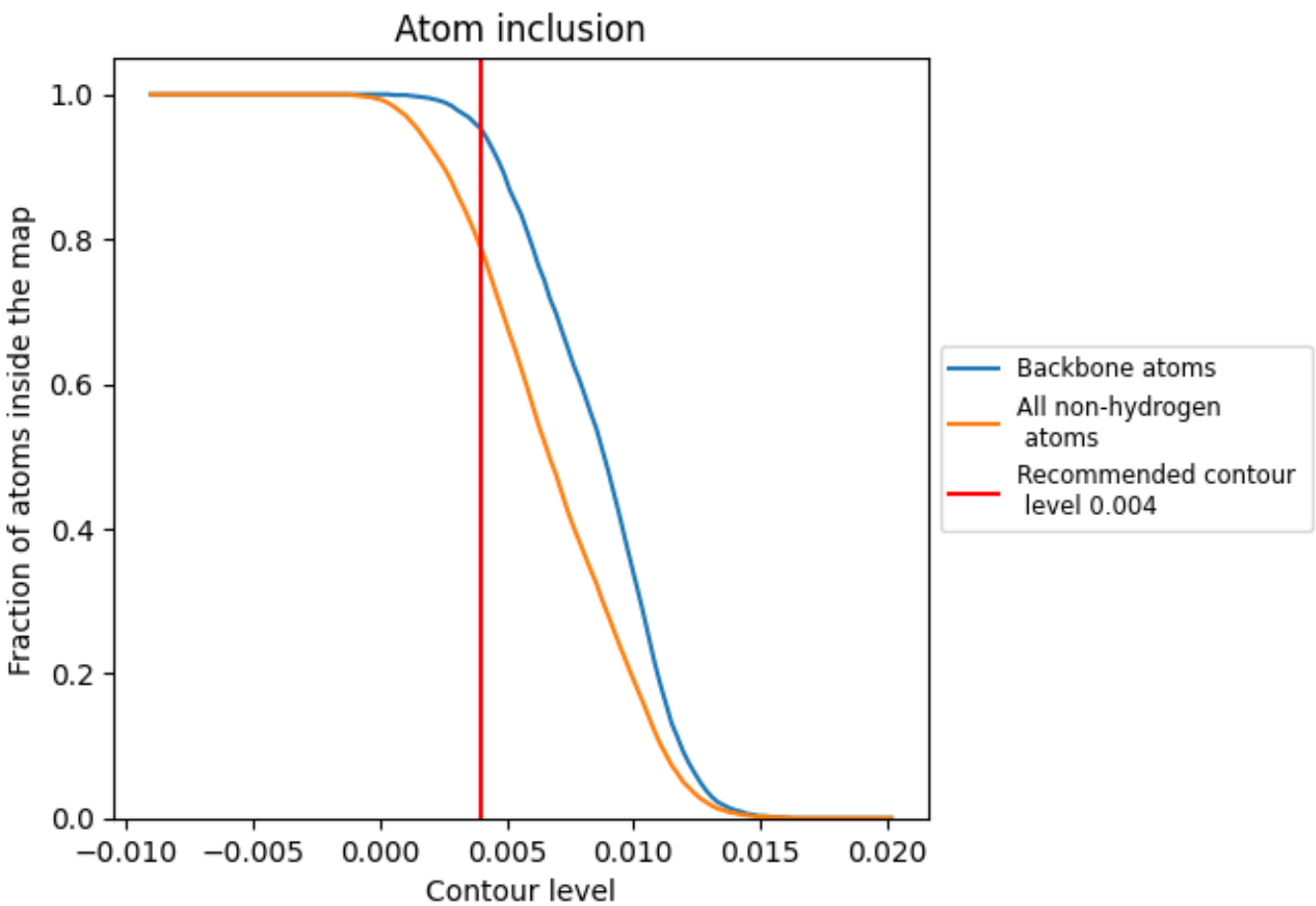
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.004).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 79% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7860	0.4410
A	0.7860	0.4410