



## Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 01:01 PM EDT

PDB ID : 9BMR / pdb\_00009bmr  
EMDB ID : EMD-44708  
Title : State-1 of motor domain from full-length human phi dynein-1 in 5 mM ADP  
Authors : Chai, P.; Zhang, K.  
Deposited on : 2024-05-02  
Resolution : 2.60 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](mailto: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>.

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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

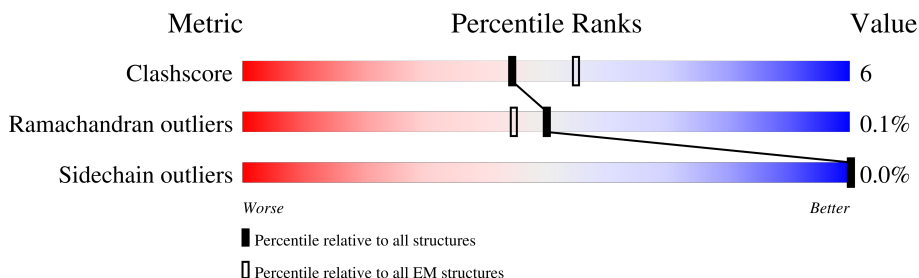
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.60 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  $\geq 3$ , 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  $\leq 5\%$ . 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	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23707 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	2937	23593	15028	4070	4378	117	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
2	A	1	27	10	5	10	2	0
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 31	C 10	N 5	O 13	P 3	0

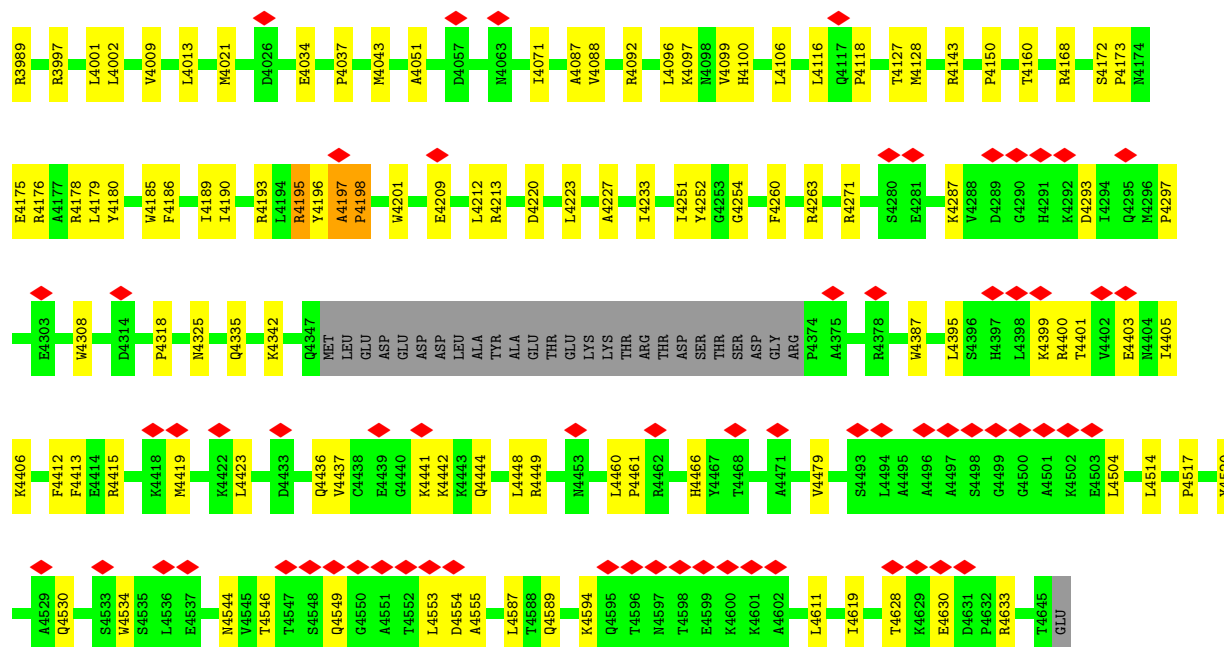
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total 2	Mg 2	0





G3897	R3741	M5579	Y3451	PRO	SER	ILE	E3210	I3059	H2867	V2887	E2513	GLU
E3898	L3742	L3580	A3452	MET	THR	ALA	T3211	S3072	N2860	E2868	E2530	ASP
F3908	R3743	R3581	V3453	VAL	THR	ASP	D3212	E3073	I2861	H2889	P2530	ALA
L3909	Q3744	R3582	L3454	LYS	TRP	GLN	D3213	K3076	D2862	R2694	N2531	GLN
R3910	L3745	F3583	I3455	ALA	LYS	MET	E3216	D3077	R2863	D2697	D2536	ARG
G3911	L3750	N3584	S3456	ILE	GLN	SER	E3217	R3077	E2864	Q2698	Y2537	ARG
N3912	N3754	R3585	E3457	ALA	ILE	VAL	L3218	N3092	R2869	C2712	E2538	LYS
E3913	K3757	L3588	A3458	GLN	SER	GLU	E3219	N3096	R2869	GLY	W2548	LYS
L3914	G3758	T3597	I3459	ASN	ILE	ASP	R3220	D3096	R2869	GLU	W2548	GLU
V3915	R3759	A3600	Q3460	ASP	ASP	ASP	D3221	W3097	I2882	ASP	V2557	ASP
L3916	L3760	M3601	I3461	LYS	ARG	LYS	L3222	P3097	P2883	GLU	V2557	GLU
S3917	D3761	D3606	K3462	MET	GLU	VAL	R3223	T3110	L2905	H2730	V2562	GLY
A3918	D3762	R3607	A3463	LEU	ASP	GLU	PHE	M3113	D2906	V2731	A2563	GLU
G3919	D3763	K3608	I3464	LYS	ILE	ALA	K3226	D3114	F2912	P2732	A2564	GLU
S3920	D3764	R3608	L3465	ARG	THR	VAL	S3226	L3116	F2912	ALA	V2567	ALA
S3921	D3765	R3611	A3466	VAL	THR	ILE	Q3227	E3116	E2914	ALA	V2567	ALA
F3922	T3766	R3617	E3469	GLU	VAL	ALA	E3228	K3117	D2917	ALA	S2410	ALA
R3923	I3767	D3617	A3470	ASN	ASN	GLN	L3229	D3124	D2917	ALA	S2410	ALA
I3924	E3776	E3624	K3471	ASP	PHE	ASN	E3230	Y3125	R2921	ALA	S2410	ALA
Q3925	A3777	L3634	V3472	GLU	SER	ALA	V3231	Q3135	Q2930	ALA	S2410	ALA
G3926	R3782	V3638	N3473	LYS	GLU	VAL	K3232	H3139	E2775	ALA	S2410	ALA
E3930	E3785	P3643	S3475	LEU	ALA	VAL	N3233	R3140	E2776	ALA	S2410	ALA
E3933	D3788	R3651	E3485	ASP	ALA	GLN	A3234	I3143	F2784	ALA	S2410	ALA
R3937	I3789	E3652	R3486	ALA	ILE	GLN	N3237	Q3152	D2787	ALA	S2410	ALA
F3942	V3790	R3655	E3487	ASP	ARG	LEU	D3238	T3153	T2788	ALA	S2410	ALA
A3943	K3791	V3660	R3488	ASP	GLU	VAL	K3239	L3154	Q2789	ALA	S2410	ALA
K3945	Q3792	L3661	K3491	ASN	LYS	GLU	L3240	V3148	H2791	ALA	S2410	ALA
D3946	E3793	L3661	E3494	ALA	MET	VAL	K3241	Q3152	Y2792	ALA	S2410	ALA
L3947	I3821	D3666	E3494	ASN	TYR	ALA	MET	R3160	V2792	ALA	S2410	ALA
K3950	L3829	Q3667	K3497	GLU	MET	ASN	VAL	K3163	F2807	ALA	S2410	ALA
V3951	I3835	D3668	N3498	VAL	SER	PRO	LYS	R3164	L2630	ALA	S2410	ALA
Q3952	Y3836	I3669	Q3499	GLU	ASN	PRO	ASP	N2998	L2631	ALA	S2410	ALA
A3953	T3835	T3681	K3500	GLN	PRO	ALA	GLN	D3001	L2632	ALA	S2410	ALA
D3954	V3839	D3691	S3510	MET	TYR	ALA	GLU	S3002	K2633	ALA	S2410	ALA
E3955	K3847	L3692	I3514	ILE	TYR	VAL	LYS	R3007	Y2638	ALA	S2410	ALA
Q3956	D3862	C3693	A3515	ASP	GLU	ALA	LYS	N3014	D2835	ALA	S2410	ALA
D3962	L3863	S3694	Y3516	LEU	ILE	LEU	VAL	H3175	W2825	ALA	S2410	ALA
P3966	V3866	V3703	F3520	SER	ASN	GLU	LYS	H3182	D2839	ALA	S2410	ALA
L3973	R3870	V3716	K3524	ILE	ARG	ILE	VAL	H3188	E2840	ALA	S2410	ALA
W3974	H3880	L3731	D3546	ALA	ALA	CYS	GLN	R3191	E2841	ALA	S2410	ALA
S3975	K3891	E3737	I3547	TYR	SER	LEU	LEU	L3044	R2844	ALA	S2410	ALA
E3976	L3892	L3740	L3553	LYS	LEU	LEU	ILE	L3044	T2846	ALA	S2410	ALA
T3977	P3979	L3740	D3557	GLY	GLY	GLU	GLN	D3045	A2854	ALA	S2410	ALA
P3979	L3983	L3740	E3558	GLU	GLY	GLU	GLN	E3049		ALA	S2410	ALA
I3983	G3984	L3740	W3562	GLU	GLY	GLU	GLN			ALA	S2410	ALA
Q3985		L3740	I3578	GLU	GLY	GLU	GLN			ALA	S2410	ALA





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	174680	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.973	Depositor
Minimum map value	-1.420	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.38	Depositor
Map size ( $\text{\AA}$ )	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	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: ADP, MG, 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	0.27	0/24093	0.48	2/32651 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1669	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	2308	ASP	CB-CG-OD1	5.14	122.93	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4195	ARG	Sidechain

### 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	23593	0	23657	294	0
2	A	81	0	36	3	0
3	A	31	0	12	4	0
4	A	2	0	0	0	0
All	All	23707	0	23705	296	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 6.

All (296) 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:2221:MET:HG2	1:A:2343:PHE:HB2	1.55	0.89
1:A:2629:GLU:OE2	1:A:2633:LYS:NZ	2.12	0.83
1:A:4271:ARG:HD3	1:A:4633:ARG:HH12	1.43	0.83
1:A:1490:TRP:HH2	1:A:1537:TRP:HD1	1.29	0.80
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.67	0.76
1:A:2562:VAL:O	1:A:2804:ARG:NH1	2.21	0.74
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.68	0.74
1:A:1571:ILE:HD13	1:A:1607:LEU:HB3	1.69	0.73
1:A:1490:TRP:CH2	1:A:1537:TRP:HD1	2.08	0.72
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.71	0.72
1:A:2788:THR:HG22	1:A:2789:GLN:HG2	1.72	0.72
1:A:2930:GLN:HG3	1:A:3059:ILE:HG23	1.73	0.71
1:A:4190:ILE:HD12	1:A:4201:TRP:HZ2	1.56	0.70
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.72	0.70
1:A:4549:GLN:HG3	1:A:4587:LEU:HB2	1.73	0.70
1:A:1466:ILE:HG12	1:A:1500:HIS:HD1	1.57	0.69
1:A:4197:ALA:HB3	1:A:4198:PRO:HD3	1.76	0.68
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.24	0.67
1:A:4176:ARG:NH1	1:A:4220:ASP:OD2	2.27	0.66
1:A:3661:LEU:HD12	1:A:3668:ASP:HB2	1.76	0.66
1:A:2906:ASP:OD2	1:A:3655:ARG:NH1	2.29	0.65
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.79	0.64
1:A:2452:LEU:HD13	1:A:2729:ARG:HH21	1.63	0.64
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.31	0.64
1:A:1487:ILE:HD12	1:A:1537:TRP:NE1	2.14	0.63
1:A:1908:ALA:HB3	1:A:2353:LEU:HD22	1.81	0.63
1:A:3557:ASP:OD1	1:A:3743:ARG:NH1	2.32	0.62
1:A:2138:ILE:HD12	1:A:2161:LEU:HD22	1.79	0.62
3:A:4702:ATP:C8	3:A:4702:ATP:H5'1	2.35	0.62
1:A:4097:LYS:HA	1:A:4127:THR:HB	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2080:LEU:O	1:A:4415:ARG:NH1	2.33	0.62
3:A:4702:ATP:H5'1	3:A:4702:ATP:H8	1.64	0.62
1:A:2226:SER:HA	3:A:4702:ATP:O1G	2.00	0.61
1:A:1751:VAL:HG21	1:A:1878:LYS:HE3	1.83	0.61
1:A:2457:SER:HB2	1:A:2732:PRO:HB3	1.82	0.61
1:A:2905:LEU:HD11	1:A:3652:GLU:HB3	1.82	0.61
1:A:3761:LEU:HA	1:A:3767:ILE:HD11	1.82	0.60
1:A:4436:GLN:HG3	1:A:4441:LYS:HB2	1.84	0.60
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	1.84	0.60
1:A:2488:ARG:HG3	1:A:2492:ARG:HH12	1.65	0.60
1:A:1466:ILE:HG12	1:A:1500:HIS:ND1	2.17	0.59
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.85	0.59
1:A:1623:ARG:HD3	1:A:1630:TYR:HA	1.84	0.59
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.85	0.59
1:A:2562:VAL:HG11	1:A:2755:MET:HB2	1.85	0.58
1:A:4287:LYS:H	1:A:4293:ASP:HB3	1.68	0.58
1:A:2279:LEU:HA	1:A:2698:GLN:HG3	1.86	0.58
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	1.85	0.58
1:A:2841:GLU:OE1	1:A:2844:ARG:NH1	2.36	0.58
1:A:3951:VAL:CG2	1:A:3973:LEU:HD21	2.33	0.58
1:A:4071:ILE:HD11	1:A:4096:LEU:HB3	1.86	0.57
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.85	0.57
1:A:4544:ASN:HD22	1:A:4589:GLN:HG3	1.70	0.57
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.38	0.57
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.86	0.57
1:A:4209:GLU:OE2	1:A:4213:ARG:NE	2.36	0.57
1:A:1567:ARG:O	1:A:1571:ILE:HG13	2.05	0.57
1:A:1931:ASN:HD22	1:A:2317:SER:H	1.51	0.57
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.86	0.56
1:A:4444:GLN:O	1:A:4449:ARG:NH1	2.38	0.56
1:A:2319:LEU:HD13	1:A:2359:CYS:SG	2.45	0.56
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	1.87	0.56
1:A:3601:MET:HG3	1:A:3611:ARG:NH2	2.21	0.56
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.46	0.56
1:A:1490:TRP:HH2	1:A:1537:TRP:CD1	2.17	0.56
1:A:4168:ARG:NE	1:A:4220:ASP:OD1	2.30	0.56
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	1.87	0.55
1:A:3951:VAL:HG22	1:A:3973:LEU:HD21	1.87	0.55
1:A:4554:ASP:OD1	1:A:4555:ALA:N	2.37	0.55
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.87	0.55
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1537:TRP:CE3	1:A:1601:LEU:HD11	2.41	0.55
1:A:1985:HIS:CD2	1:A:1997:ILE:HD13	2.41	0.55
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.40	0.55
1:A:1998:THR:HG21	1:A:2005:GLN:HB3	1.88	0.55
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.89	0.55
1:A:2294:GLU:OE1	1:A:2294:GLU:N	2.39	0.55
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.89	0.54
1:A:2694:ARG:NH1	1:A:2697:ASP:OD2	2.40	0.54
1:A:1571:ILE:HD12	1:A:1611:ILE:HD11	1.90	0.54
1:A:2596:PRO:HB2	1:A:2738:TYR:CZ	2.43	0.54
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	1.90	0.53
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.40	0.53
1:A:1543:ARG:NH1	1:A:1612:GLN:OE1	2.41	0.53
1:A:3914:ILE:O	1:A:3937:ARG:NH1	2.42	0.53
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.42	0.53
1:A:1887:ARG:HE	1:A:2039:LEU:HD11	1.74	0.53
1:A:3916:LEU:HD11	1:A:3937:ARG:HG3	1.91	0.52
1:A:2621:ASN:OD1	1:A:3014:ASN:ND2	2.43	0.52
1:A:3750:LEU:O	1:A:3754:ASN:ND2	2.42	0.52
1:A:1832:ASN:HD21	1:A:1834:LYS:HB2	1.72	0.52
1:A:1687:LYS:HD3	1:A:1712:THR:HG23	1.91	0.52
1:A:2620:LEU:HD22	1:A:2631:LEU:HD23	1.91	0.52
1:A:3044:LEU:HD22	1:A:3049:GLU:HB3	1.90	0.52
1:A:1965:GLU:HG2	1:A:2026:SER:HB3	1.91	0.52
1:A:2973:ASP:OD2	1:A:3007:ARG:NH2	2.43	0.51
1:A:1487:ILE:HD12	1:A:1537:TRP:HE1	1.73	0.51
1:A:1929:VAL:H	1:A:2332:ARG:NH2	2.09	0.51
1:A:2835:ASP:HB3	1:A:3092:ASN:HD22	1.74	0.51
1:A:1467:ARG:HE	1:A:1523:TRP:HZ2	1.56	0.51
1:A:3624:GLU:HG3	1:A:3669:ILE:HD13	1.93	0.51
1:A:3194:LEU:HD23	1:A:3500:MET:SD	2.51	0.51
1:A:4179:LEU:HD12	1:A:4223:LEU:HD22	1.92	0.51
1:A:4413:PHE:HD2	1:A:4504:LEU:HD13	1.75	0.51
1:A:1860:GLN:HG2	1:A:1865:LYS:HG2	1.93	0.51
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.44	0.51
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.91	0.50
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.12	0.50
1:A:4517:PRO:HG3	1:A:4611:LEU:HD13	1.93	0.50
1:A:2144:THR:HG22	1:A:2145:MET:HE2	1.94	0.50
1:A:3750:LEU:HG	1:A:3754:ASN:HD21	1.76	0.50
1:A:1671:SER:HB2	1:A:1693:THR:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2487:GLU:O	1:A:2491:GLN:HG3	2.11	0.50
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.93	0.50
1:A:1929:VAL:H	1:A:2332:ARG:HH21	1.59	0.50
1:A:2807:PHE:CE2	1:A:2811:ARG:HD3	2.46	0.50
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.92	0.50
1:A:2638:TYR:HB3	1:A:2659:LEU:HD11	1.93	0.50
1:A:3211:THR:HG23	1:A:3761:LEU:HD11	1.93	0.50
1:A:1575:PHE:O	1:A:1579:MET:HG2	2.12	0.49
1:A:2917:ASP:OD2	1:A:2921:ARG:NH2	2.45	0.49
1:A:2374:ILE:HD13	1:A:2452:LEU:HD21	1.95	0.49
1:A:2564:ALA:HB3	1:A:2567:VAL:HG23	1.94	0.49
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.48	0.49
1:A:1929:VAL:HG13	1:A:1958:ASP:OD2	2.12	0.49
1:A:1914:GLU:HG2	2:A:4701:ADP:O1A	2.13	0.49
1:A:2869:ARG:HA	1:A:2869:ARG:NE	2.28	0.49
1:A:4403:GLU:HA	1:A:4406:LYS:HE2	1.95	0.49
1:A:4436:GLN:HG2	1:A:4442:LYS:HG2	1.95	0.49
1:A:3944:PHE:CE1	1:A:3974:TRP:HB3	2.48	0.49
1:A:4043:MET:HB3	1:A:4051:ALA:HB3	1.95	0.49
1:A:2174:GLU:OE1	1:A:2176:THR:OG1	2.30	0.48
1:A:4400:ARG:HE	1:A:4405:ILE:HD11	1.77	0.48
1:A:1647:VAL:HG21	1:A:1670:ASN:HB3	1.95	0.48
1:A:4387:TRP:CD1	1:A:4479:VAL:HG11	2.47	0.48
1:A:2069:ILE:HB	1:A:2137:LEU:HD21	1.96	0.48
1:A:1959:GLU:HB3	1:A:1962:ARG:HG3	1.96	0.48
1:A:4180:TYR:OH	1:A:4220:ASP:OD1	2.30	0.48
1:A:2211:TYR:O	1:A:2214:THR:OG1	2.29	0.48
1:A:2751:PHE:HB3	1:A:2803:VAL:HG11	1.96	0.48
1:A:3950:LYS:HB3	1:A:3973:LEU:CD1	2.43	0.48
1:A:4251:ILE:HG22	1:A:4252:TYR:CD2	2.49	0.48
1:A:1556:ASP:OD2	1:A:1621:ARG:NH2	2.43	0.47
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.28	0.47
1:A:1761:ASN:HB3	1:A:1781:VAL:HG22	1.96	0.47
1:A:2443:LEU:HD21	1:A:2513:GLU:OE1	2.14	0.47
1:A:4196:TYR:O	1:A:4197:ALA:C	2.52	0.47
1:A:3731:LEU:HD11	1:A:3790:VAL:HG12	1.97	0.47
1:A:1931:ASN:HD21	1:A:2316:ASN:HB2	1.79	0.47
1:A:3175:HIS:CD2	1:A:3585:ARG:HH22	2.32	0.47
1:A:2061:THR:OG1	1:A:2133:GLU:OE1	2.28	0.47
1:A:2386:PRO:HG3	1:A:2413:LEU:HD13	1.97	0.47
1:A:1623:ARG:NH1	1:A:1632:VAL:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4628:THR:OG1	1:A:4630:GLU:HG2	2.15	0.47
1:A:2134:GLN:O	1:A:2138:ILE:HG12	2.15	0.47
1:A:2138:ILE:HD11	1:A:2165:PHE:CG	2.50	0.47
1:A:3703:VAL:HG21	1:A:3829:LEU:HD22	1.97	0.47
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	1.95	0.46
1:A:3966:PRO:HG3	1:A:3997:ARG:HG3	1.97	0.46
1:A:2592:VAL:HG23	1:A:2731:VAL:HG11	1.97	0.46
1:A:4423:LEU:HD13	1:A:4466:HIS:ND1	2.31	0.46
1:A:4175:GLU:OE1	1:A:4175:GLU:N	2.48	0.46
1:A:2179:ARG:NH2	1:A:2195:ASP:OD1	2.43	0.46
1:A:1623:ARG:NH1	1:A:1629:PHE:O	2.47	0.46
1:A:2445:HIS:HB3	1:A:2505:ASP:OD2	2.15	0.46
1:A:3553:LEU:HB2	1:A:3578:ILE:HD13	1.97	0.46
1:A:1931:ASN:ND2	1:A:2316:ASN:HB2	2.31	0.46
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.15	0.46
1:A:2790:PRO:HB3	1:A:3076:LYS:HG2	1.98	0.46
1:A:3175:HIS:HB3	1:A:3516:TYR:CE1	2.50	0.46
1:A:4172:SER:HB2	1:A:4173:PRO:HD3	1.98	0.45
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.49	0.45
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.98	0.45
1:A:1937:ASP:HA	1:A:1967:MET:HG3	1.98	0.45
1:A:2688:GLU:OE1	1:A:2689:HIS:CE1	2.69	0.45
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.98	0.45
1:A:3117:LYS:HE2	1:A:3139:HIS:CD2	2.51	0.45
1:A:3921:THR:HG21	1:A:3933:GLU:HG2	1.98	0.45
1:A:4087:ALA:HA	1:A:4092:ARG:HB3	1.98	0.45
1:A:3217:GLU:HB2	1:A:3220:ARG:HH21	1.82	0.45
1:A:1879:LEU:HD22	2:A:4701:ADP:C4	2.51	0.45
1:A:4401:THR:O	1:A:4405:ILE:HG12	2.17	0.45
1:A:2668:LEU:HD21	1:A:2720:ARG:CZ	2.47	0.45
1:A:4412:PHE:HZ	1:A:4514:LEU:HD13	1.82	0.45
1:A:4190:ILE:HD12	1:A:4201:TRP:CZ2	2.45	0.45
1:A:4517:PRO:HG2	1:A:4619:ILE:HD12	1.98	0.45
1:A:2963:VAL:HG23	1:A:3643:PRO:HB2	1.99	0.44
1:A:1635:GLU:HA	1:A:1638:LEU:HD12	1.98	0.44
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.99	0.44
1:A:4100:HIS:HB3	1:A:4128:MET:HB2	1.99	0.44
1:A:1697:LYS:HB3	1:A:1700:GLU:OE1	2.18	0.44
1:A:2912:PHE:CE2	1:A:2914:GLU:HB2	2.52	0.44
1:A:3485:GLU:HG3	1:A:3488:ARG:HH22	1.83	0.44
1:A:4185:TRP:O	1:A:4189:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4189:ILE:O	1:A:4193:ARG:HG3	2.17	0.44
1:A:4034:GLU:OE1	1:A:4143:ARG:NH1	2.41	0.44
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.99	0.44
1:A:4186:PHE:O	1:A:4190:ILE:HG12	2.18	0.44
1:A:1980:GLU:OE2	1:A:1983:ARG:NH1	2.51	0.44
1:A:2548:TRP:CD1	1:A:2576:ARG:HG2	2.53	0.44
1:A:1625:SER:HB2	1:A:1699:ASN:ND2	2.33	0.44
1:A:3601:MET:HG3	1:A:3611:ARG:HH21	1.80	0.44
1:A:2776:PHE:HZ	1:A:2846:THR:HG23	1.83	0.43
1:A:1763:GLU:OE2	1:A:1838:TRP:NE1	2.37	0.43
1:A:3160:ARG:O	1:A:3163:LYS:HG2	2.17	0.43
1:A:3880:HIS:ND1	1:A:4021:MET:HG3	2.33	0.43
1:A:1666:LEU:HD23	1:A:1673:VAL:HA	2.00	0.43
1:A:1724:VAL:HG11	1:A:1753:SER:HB3	2.00	0.43
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	2.00	0.43
1:A:2557:VAL:O	1:A:2757:ARG:NH2	2.52	0.43
1:A:2994:MET:HG3	1:A:2998:ASN:HD22	1.84	0.43
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	2.01	0.43
1:A:4415:ARG:HE	1:A:4415:ARG:HB3	1.54	0.43
1:A:2028:LEU:HG	1:A:2032:LEU:HD23	1.99	0.43
1:A:2457:SER:O	1:A:2461:MET:HG3	2.18	0.43
1:A:4437:VAL:HG21	1:A:4448:LEU:HD13	2.00	0.43
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.54	0.43
1:A:2538:GLU:HB3	1:A:2548:TRP:CZ2	2.54	0.43
1:A:3148:VAL:O	1:A:3152:GLN:HG3	2.19	0.43
1:A:3240:LEU:HD23	1:A:3240:LEU:HA	1.93	0.43
1:A:2882:ILE:HB	1:A:2883:PRO:HD2	2.01	0.43
1:A:2975:ASP:O	1:A:2979:VAL:HG23	2.18	0.43
1:A:3514:ILE:HD11	1:A:3553:LEU:HD13	2.00	0.43
1:A:4297:PRO:HB3	1:A:4308:TRP:CD1	2.54	0.43
1:A:4415:ARG:O	1:A:4419:MET:HG2	2.19	0.43
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	2.00	0.43
1:A:1997:ILE:H	1:A:1997:ILE:HD12	1.83	0.42
1:A:2230:LYS:HG2	1:A:2364:PHE:CG	2.54	0.42
1:A:3232:LYS:HA	1:A:3232:LYS:HD3	1.76	0.42
1:A:3745:LEU:HD13	1:A:3777:ALA:HA	2.01	0.42
1:A:2825:TRP:CZ3	1:A:2854:ALA:HB2	2.55	0.42
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.50	0.42
1:A:3110:THR:O	1:A:3113:MET:HB2	2.19	0.42
1:A:4173:PRO:HD2	1:A:4176:ARG:HH21	1.84	0.42
1:A:4395:LEU:HD12	1:A:4395:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3558:GLU:HG2	1:A:3562:TRP:CE2	2.54	0.42
1:A:2079:GLN:HB2	1:A:2160:LEU:HD11	2.00	0.42
1:A:4196:TYR:CZ	1:A:4318:PRO:HB3	2.55	0.42
1:A:3194:LEU:HD21	1:A:3499:GLN:HB2	2.01	0.42
1:A:2784:PHE:HB3	1:A:2792:TYR:CD2	2.54	0.42
1:A:2488:ARG:CG	1:A:2492:ARG:HH12	2.32	0.42
1:A:1475:LEU:HD12	1:A:1591:VAL:HG21	2.02	0.41
1:A:1899:ARG:N	1:A:1899:ARG:HD2	2.34	0.41
1:A:2163:ASP:OD1	1:A:4530:GLN:NE2	2.53	0.41
1:A:2581:LEU:HD12	1:A:2604:THR:HG22	2.02	0.41
1:A:2961:ILE:HG13	1:A:2963:VAL:HG13	2.00	0.41
1:A:3862:ASP:OD1	1:A:3866:VAL:HG23	2.20	0.41
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.55	0.41
1:A:4423:LEU:HD22	1:A:4466:HIS:HB2	2.01	0.41
1:A:1526:LYS:O	1:A:1530:ILE:HG13	2.20	0.41
1:A:3741:ARG:NH2	1:A:3776:GLU:OE1	2.53	0.41
1:A:4546:THR:HG21	1:A:4589:GLN:HE21	1.85	0.41
1:A:1490:TRP:HZ3	1:A:1534:PHE:HB3	1.83	0.41
1:A:3209:LYS:HB2	1:A:3209:LYS:HE2	1.77	0.41
1:A:3908:PHE:HE1	1:A:4001:LEU:HD11	1.86	0.41
1:A:4260:PHE:HD1	1:A:4263:ARG:NH2	2.19	0.41
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.54	0.41
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	2.01	0.41
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	2.02	0.41
1:A:2631:LEU:HD13	1:A:2686:MET:HE1	2.02	0.41
1:A:3115:LEU:HD13	1:A:3143:ILE:HG21	2.01	0.41
1:A:2107:ARG:HD2	1:A:2136:ILE:HG12	2.03	0.41
1:A:3740:LEU:O	1:A:3744:GLN:HG3	2.20	0.41
1:A:1895:ALA:HB2	1:A:2037:ARG:HB2	2.02	0.41
1:A:3951:VAL:HG23	1:A:3973:LEU:HD21	2.01	0.41
1:A:2091:ARG:NH1	2:A:4701:ADP:H5'2	2.36	0.41
1:A:3584:ASN:O	1:A:3651:ARG:NH2	2.53	0.41
1:A:4150:PRO:O	1:A:4195:ARG:NH2	2.53	0.41
1:A:1834:LYS:HA	1:A:1834:LYS:HD3	1.88	0.41
1:A:2226:SER:OG	1:A:2729:ARG:HD2	2.21	0.41
1:A:2912:PHE:HE2	1:A:2914:GLU:HB2	1.86	0.41
1:A:3017:VAL:HB	1:A:3020:LEU:HB2	2.03	0.41
1:A:3985:GLN:HB3	1:A:3989:ARG:NH1	2.36	0.41
1:A:4099:VAL:HG23	1:A:4106:LEU:HD11	2.02	0.41
1:A:4553:LEU:HD23	1:A:4553:LEU:HA	1.87	0.41
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2132:PRO:HB2	1:A:2135:GLU:HB3	2.02	0.41
1:A:2582:TYR:CE2	1:A:2612:LEU:HD13	2.56	0.41
1:A:2667:ASN:OD1	1:A:2712:CYS:HB2	2.20	0.41
1:A:3588:LEU:HD21	1:A:3638:VAL:HG11	2.02	0.41
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.20	0.41
1:A:1508:LYS:HG2	1:A:1513:TYR:CZ	2.56	0.41
1:A:3229:LEU:HD12	1:A:3465:LEU:HD13	2.03	0.40
1:A:3912:ASN:O	1:A:3937:ARG:NH1	2.54	0.40
1:A:4002:LEU:HD11	1:A:4335:GLN:HB3	2.04	0.40
1:A:4399:LYS:HE2	1:A:4399:LYS:HB3	1.95	0.40
1:A:3001:ASP:OD1	1:A:3002:SER:N	2.54	0.40
1:A:3821:ILE:HB	1:A:4342:LYS:HG2	2.04	0.40
1:A:1744:LYS:HD3	1:A:1745:TYR:CE2	2.55	0.40
1:A:2059:PHE:CZ	1:A:2104:LYS:HD3	2.55	0.40
1:A:2290:SER:HA	1:A:2294:GLU:OE1	2.21	0.40
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	2.03	0.40
1:A:1612:GLN:HG3	1:A:1638:LEU:HD13	2.04	0.40
1:A:2229:GLY:HA2	3:A:4702:ATP:O2A	2.21	0.40
1:A:2839:GLU:OE1	1:A:2839:GLU:HA	2.22	0.40
1:A:4534:TRP:CD2	1:A:4594:LYS:HD3	2.56	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	2929/4646 (63%)	2882 (98%)	45 (2%)	2 (0%)	48 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4197	ALA

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Mol	Chain	Res	Type
1	A	4198	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2605/4125 (63%)	2604 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	A	2471	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1643	ASN
1	A	1931	ASN
1	A	2554	GLN
1	A	2713	ASN
1	A	3092	ASN
1	A	3200	HIS
1	A	3602	ASN
1	A	3735	GLN
1	A	3754	ASN
1	A	4335	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	A	4704	-	24,29,29	0.75	0	29,45,45	0.74	1 (3%)
2	ADP	A	4703	-	24,29,29	0.75	0	29,45,45	0.73	1 (3%)
3	ATP	A	4702	4	28,33,33	0.76	0	34,52,52	0.79	1 (2%)
2	ADP	A	4701	4	24,29,29	0.74	0	29,45,45	0.75	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4704	-	-	2/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	1/12/32/32	0/3/3/3
3	ATP	A	4702	4	-	2/18/38/38	0/3/3/3
2	ADP	A	4701	4	-	0/12/32/32	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	C5-C6-N6	2.34	123.87	120.31
2	A	4704	ADP	C5-C6-N6	2.31	123.83	120.31
2	A	4703	ADP	C5-C6-N6	2.26	123.75	120.31
3	A	4702	ATP	C5-C6-N6	2.22	123.70	120.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

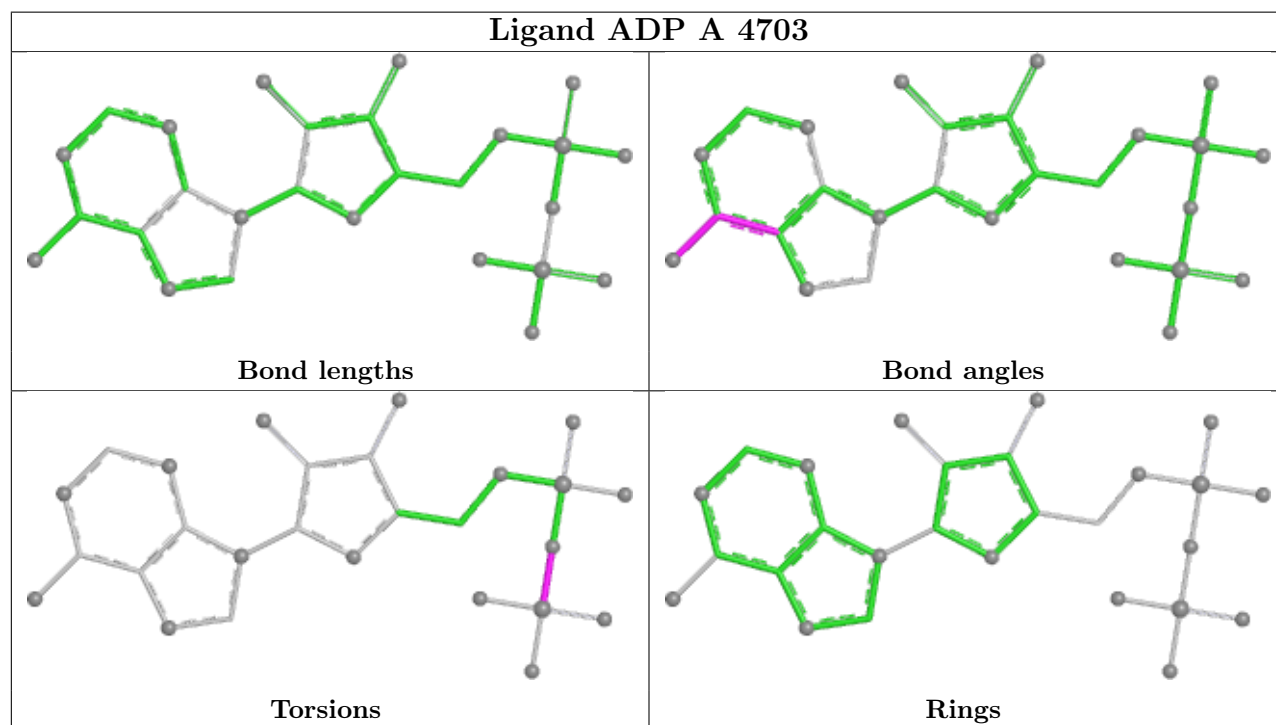
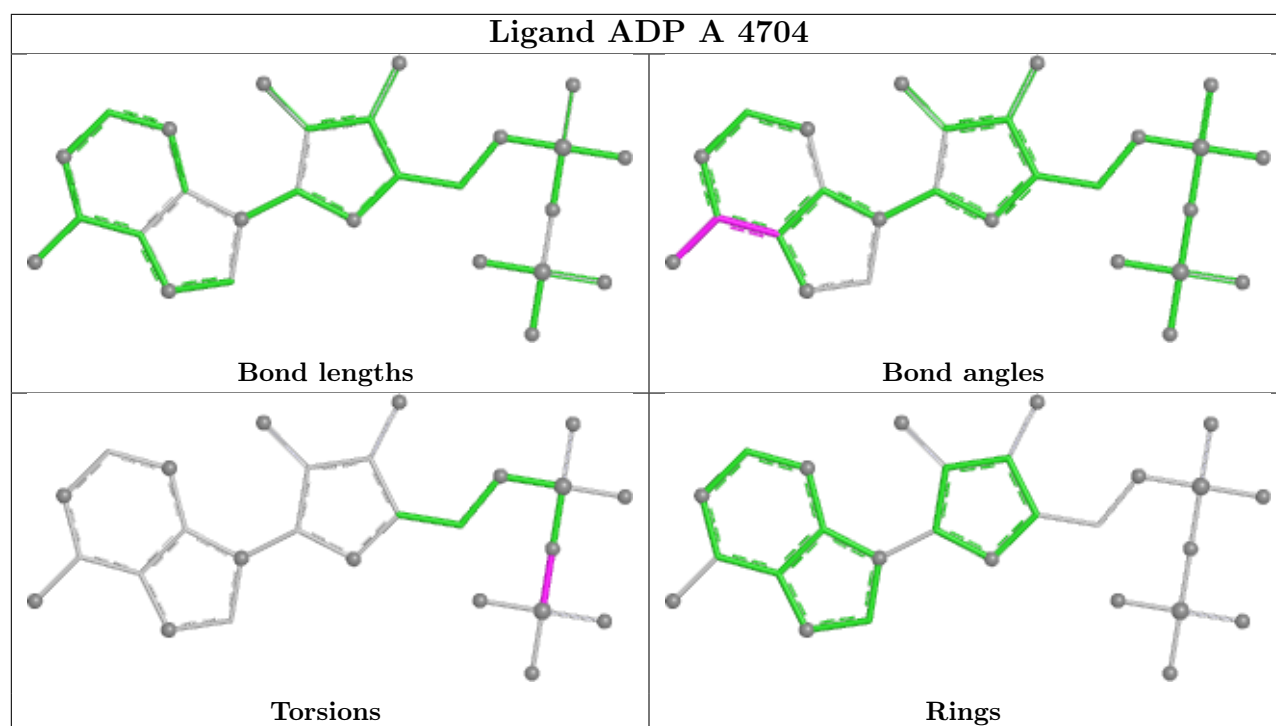
Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	PA-O3A-PB-O2B
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4704	ADP	PA-O3A-PB-O1B
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4703	ADP	PA-O3A-PB-O3B

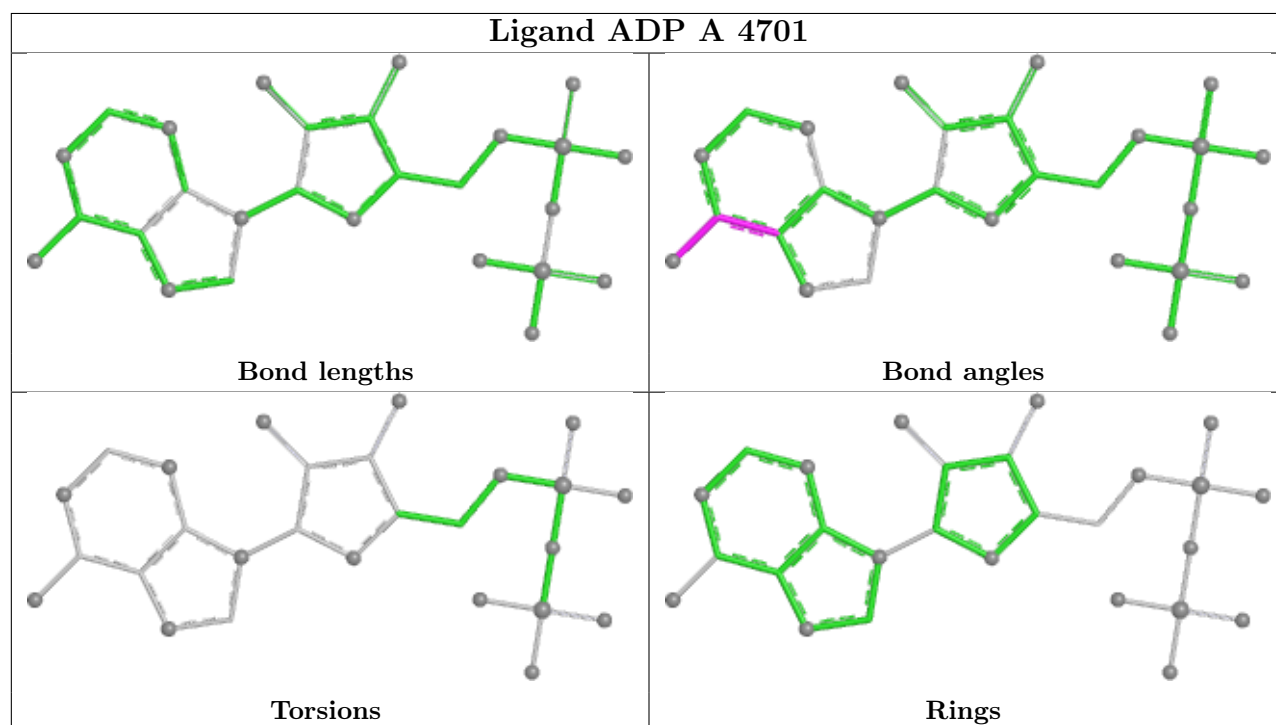
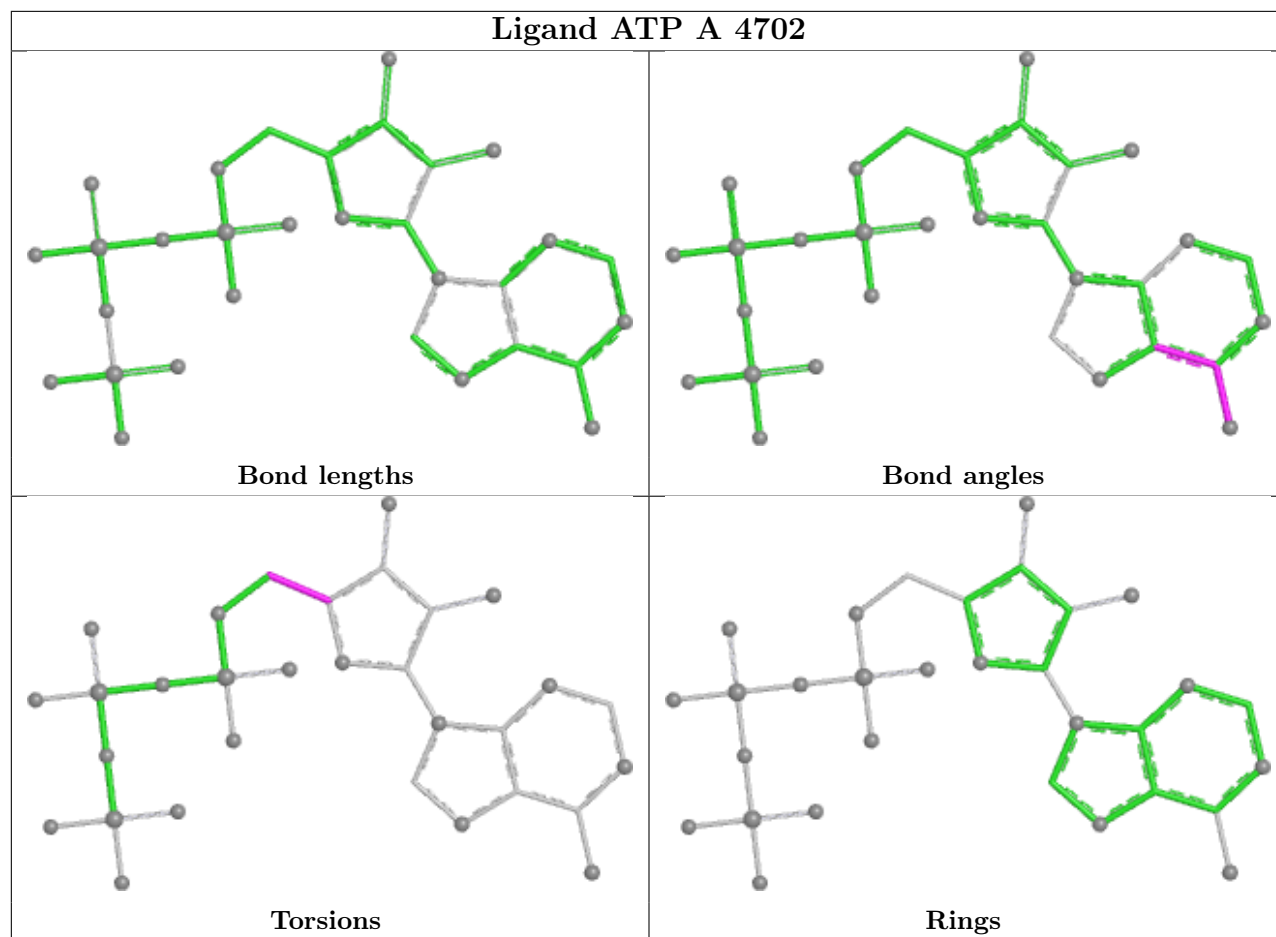
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	4	0
2	A	4701	ADP	3	0

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





## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



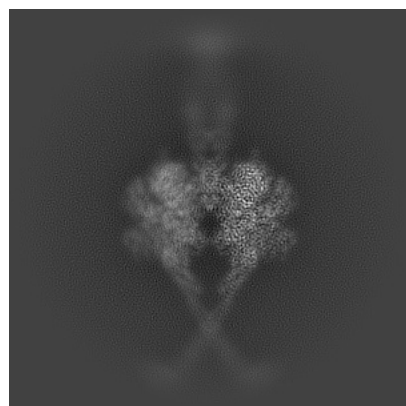
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44708. These allow visual inspection of the internal detail of the map and identification of artifacts.

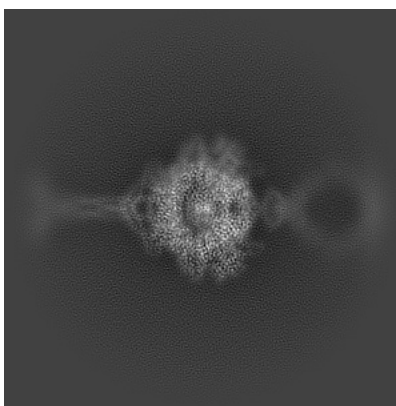
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

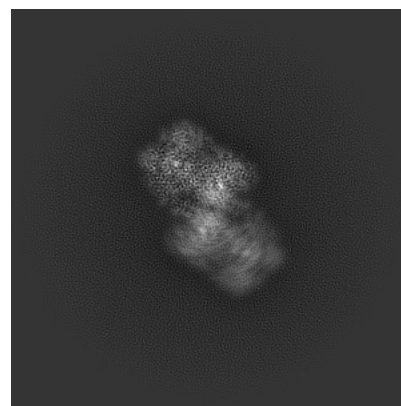
#### 6.1.1 Primary map



X

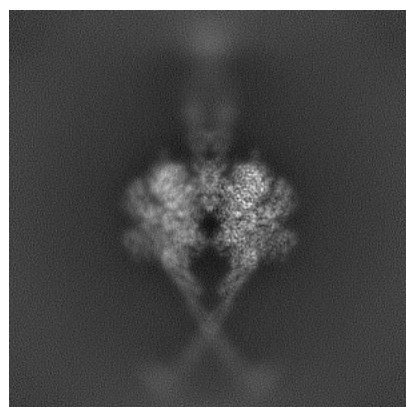


Y

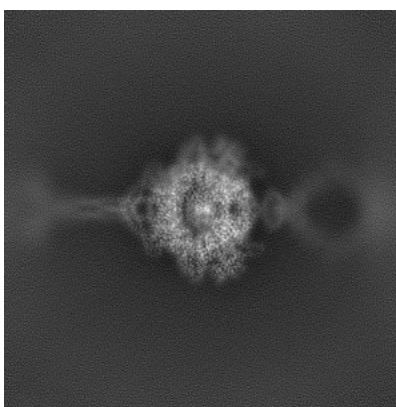


Z

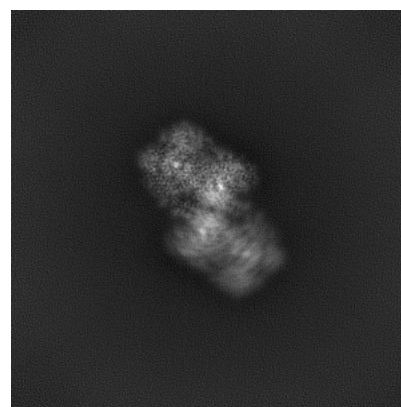
#### 6.1.2 Raw map



X



Y

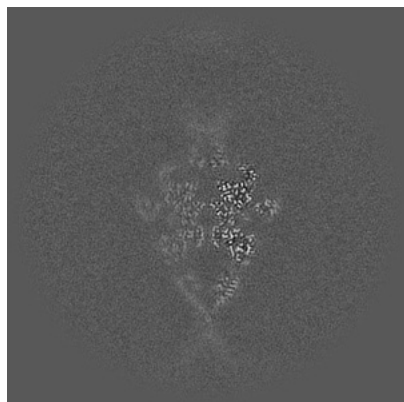


Z

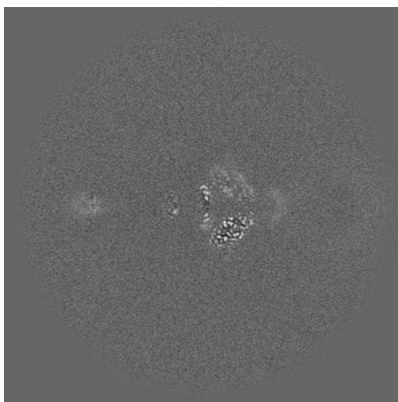
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

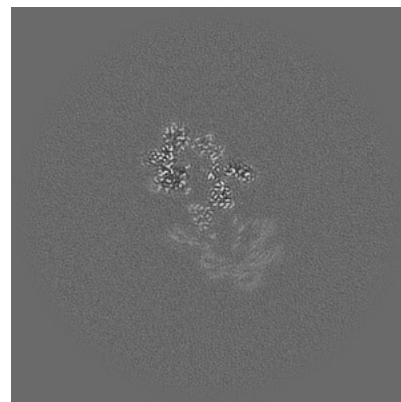
### 6.2.1 Primary map



X Index: 192

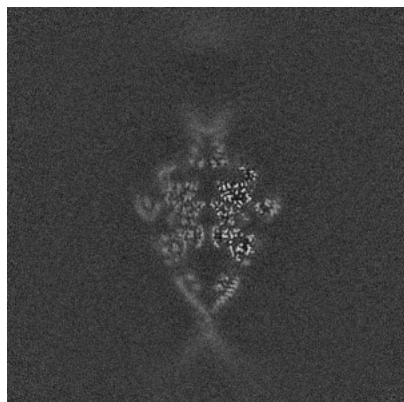


Y Index: 192

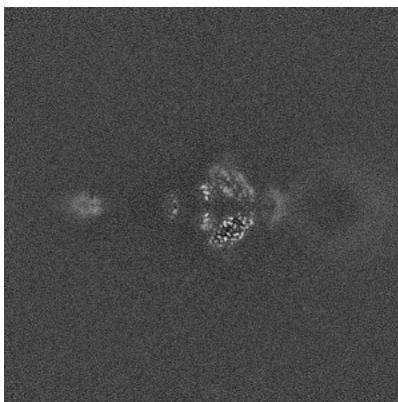


Z Index: 192

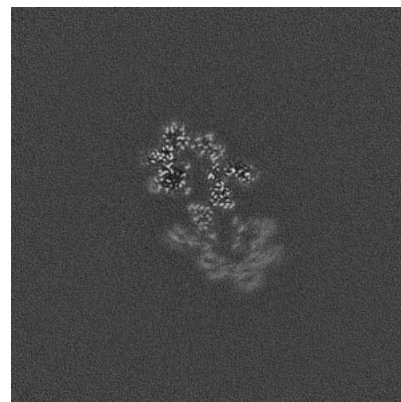
### 6.2.2 Raw map



X Index: 192



Y Index: 192

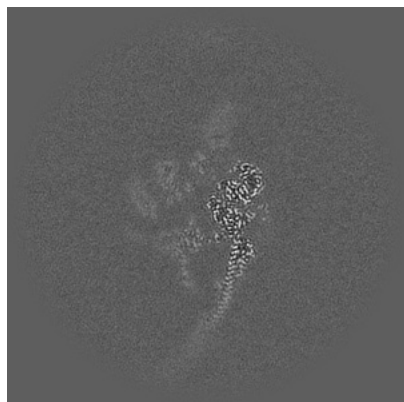


Z Index: 192

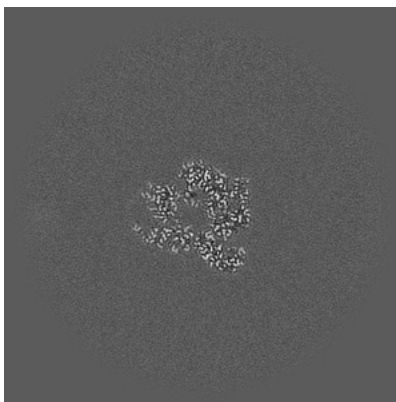
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

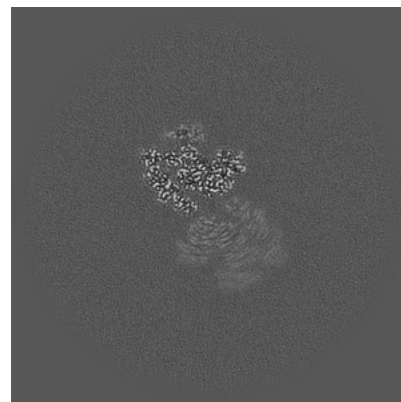
### 6.3.1 Primary map



X Index: 201



Y Index: 226

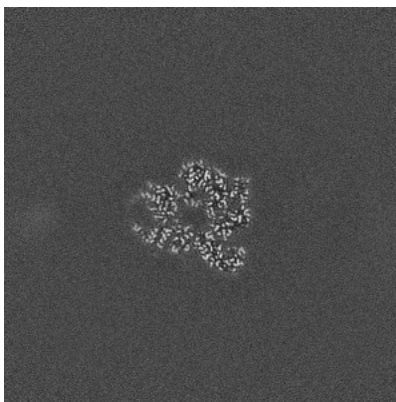


Z Index: 211

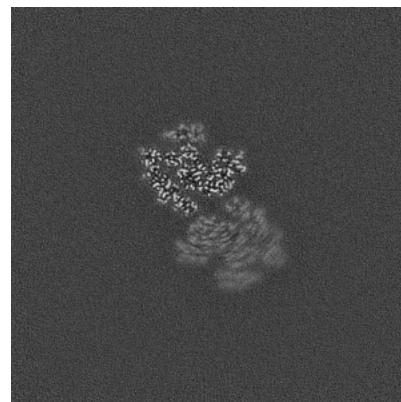
### 6.3.2 Raw map



X Index: 201



Y Index: 226



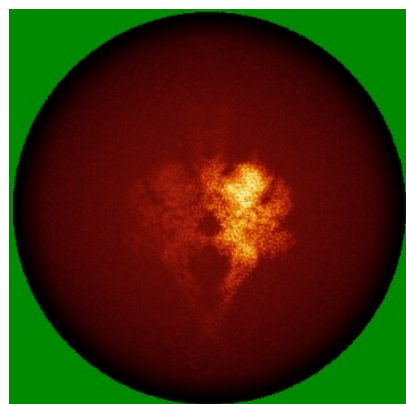
Z Index: 211

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

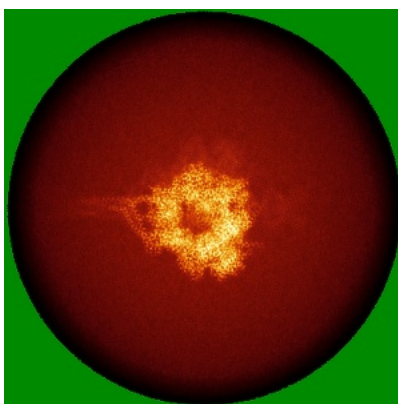


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

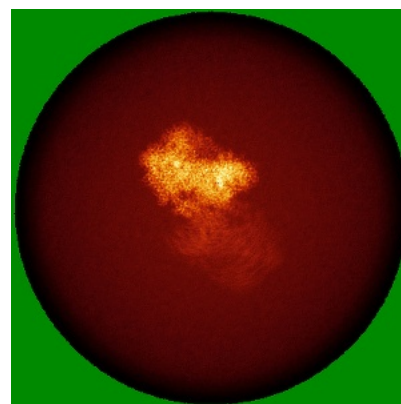
### 6.4.1 Primary map



X

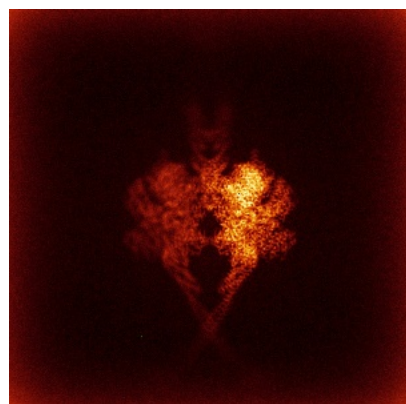


Y

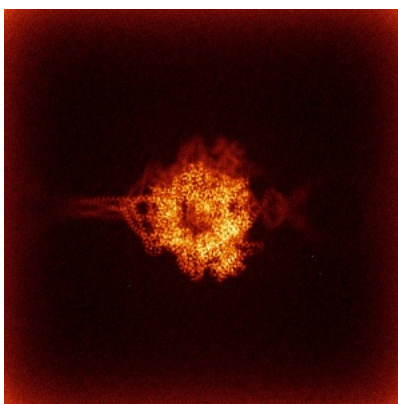


Z

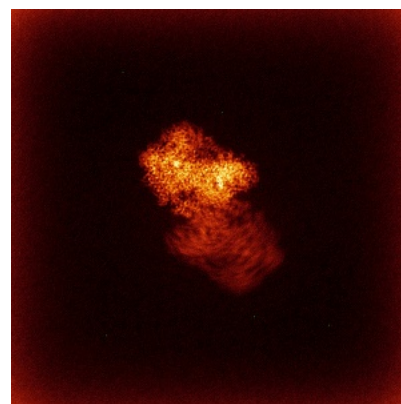
### 6.4.2 Raw map



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 0.38. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

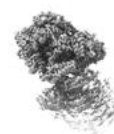
### 6.5.2 Raw map



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.

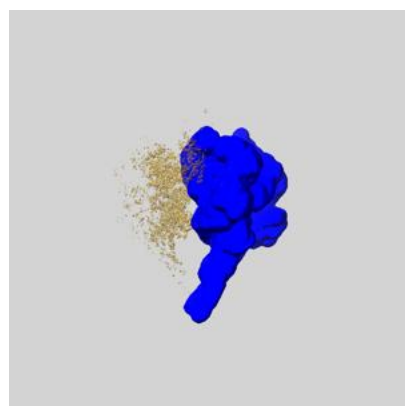
## 6.6 Mask visualisation [i](#)

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

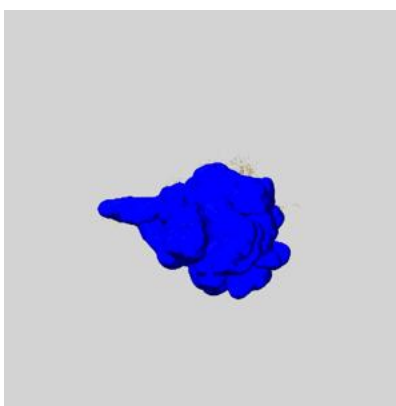
A mask typically either:

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

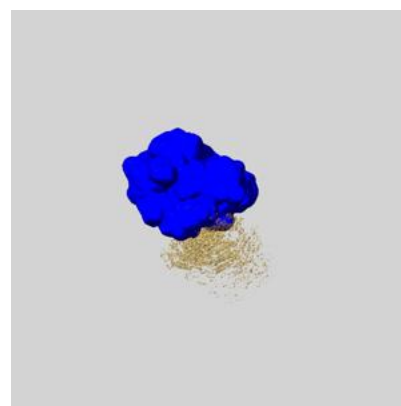
### 6.6.1 emd\_44708\_msk\_1.map [i](#)



X



Y

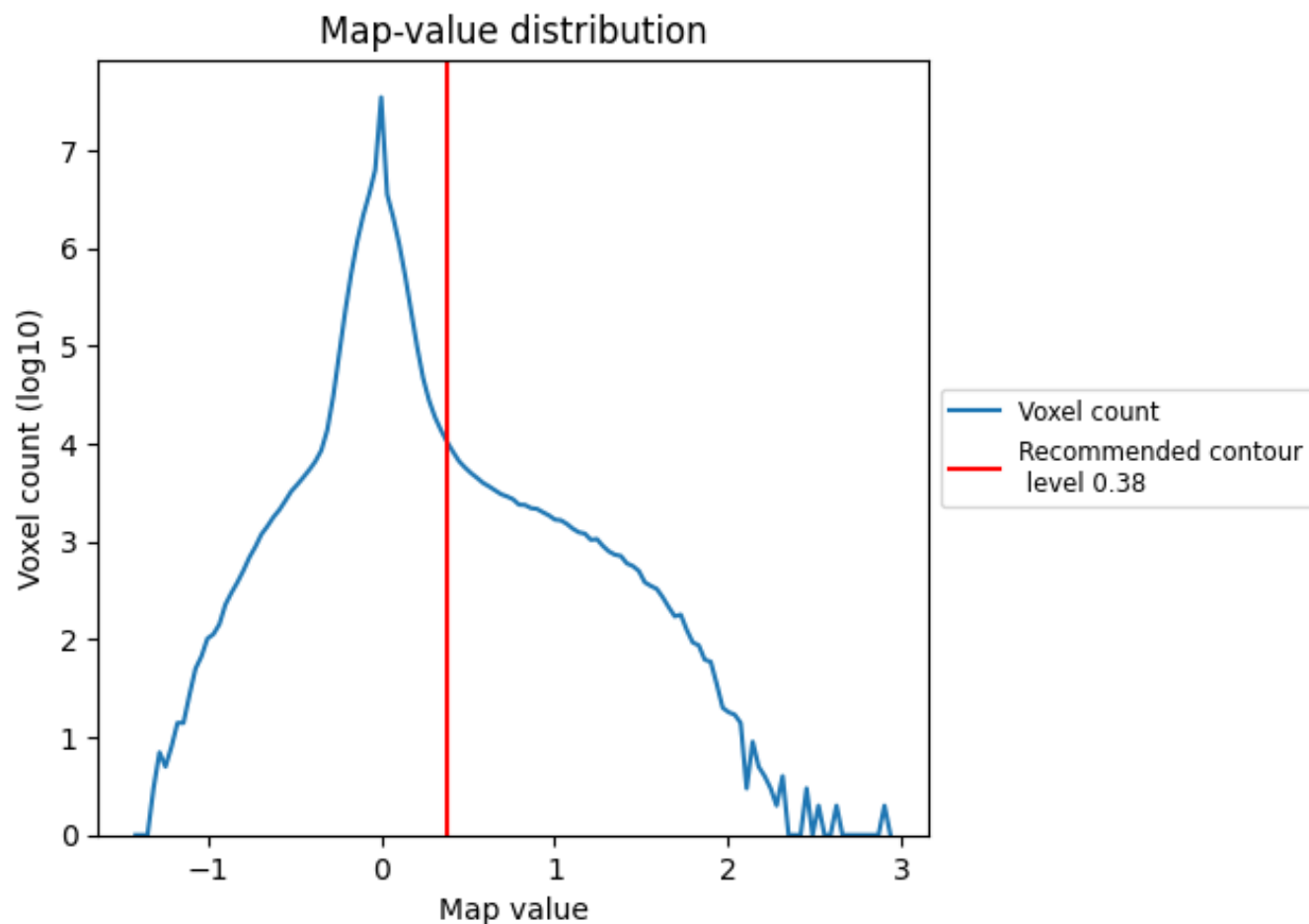


Z

## 7 Map analysis [i](#)

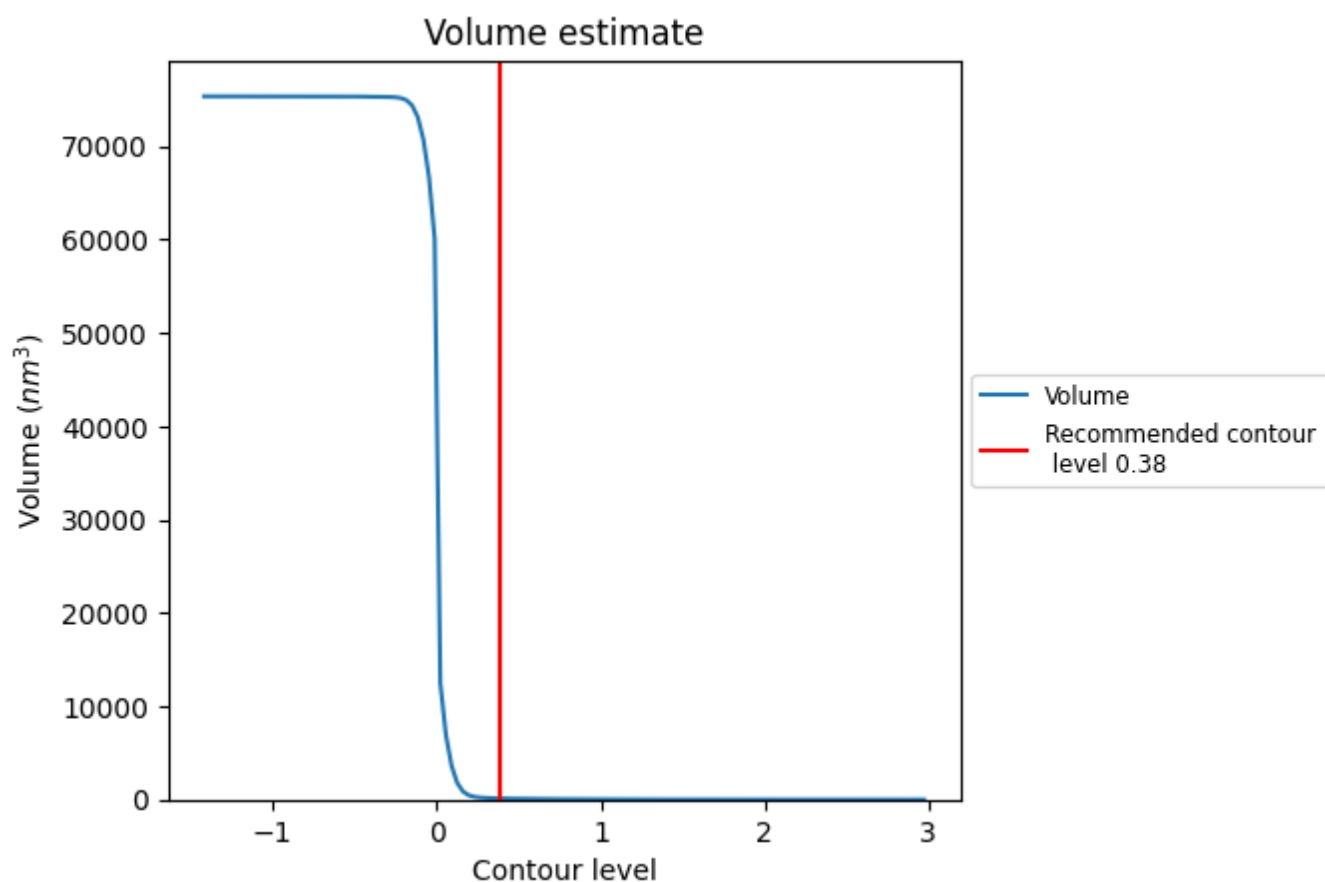
This section contains the results of statistical analysis of the map.

### 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](#)

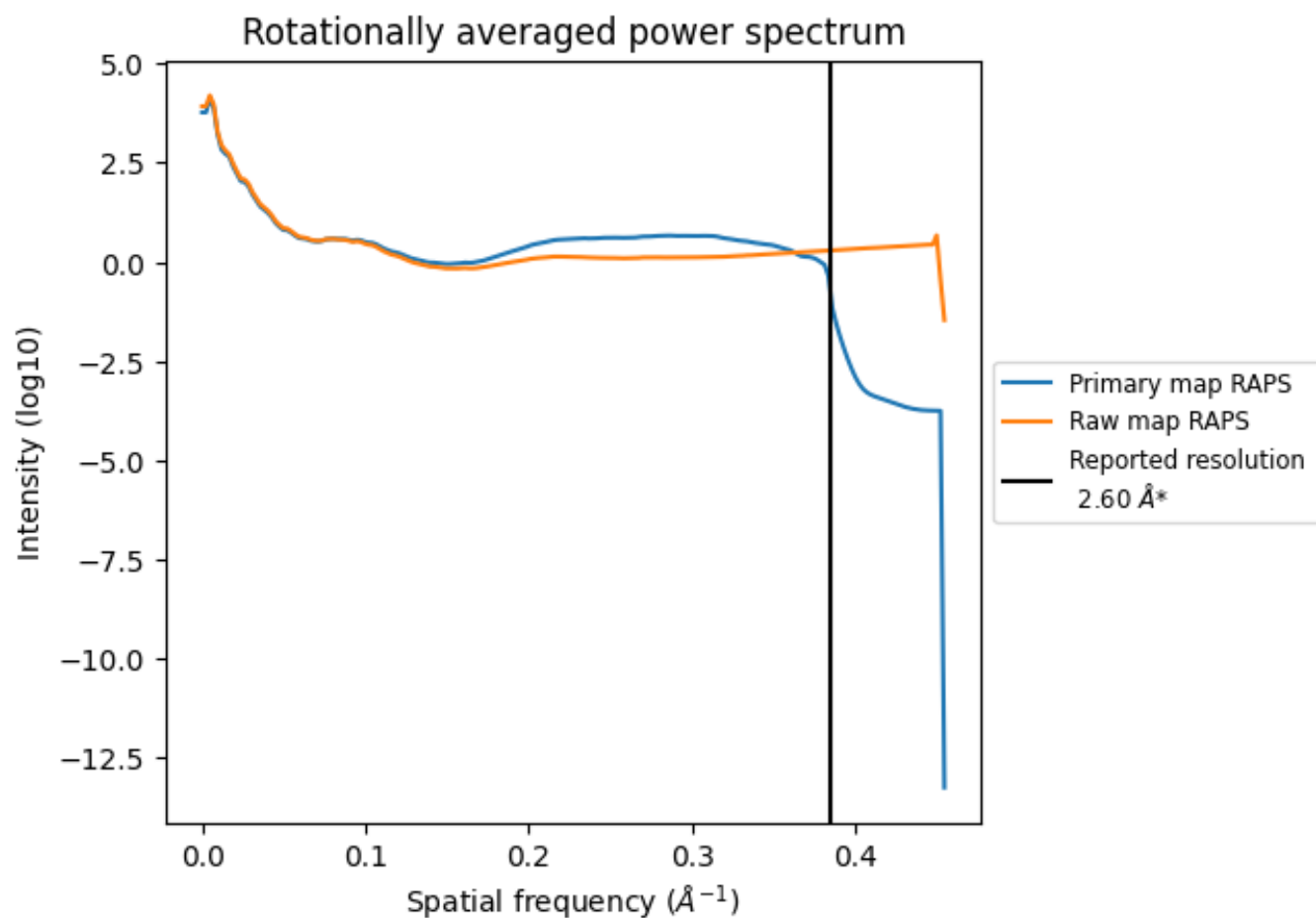


The volume at the recommended contour level is 121 nm<sup>3</sup>; this corresponds to an approximate mass of 109 kDa.

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 ⓘ

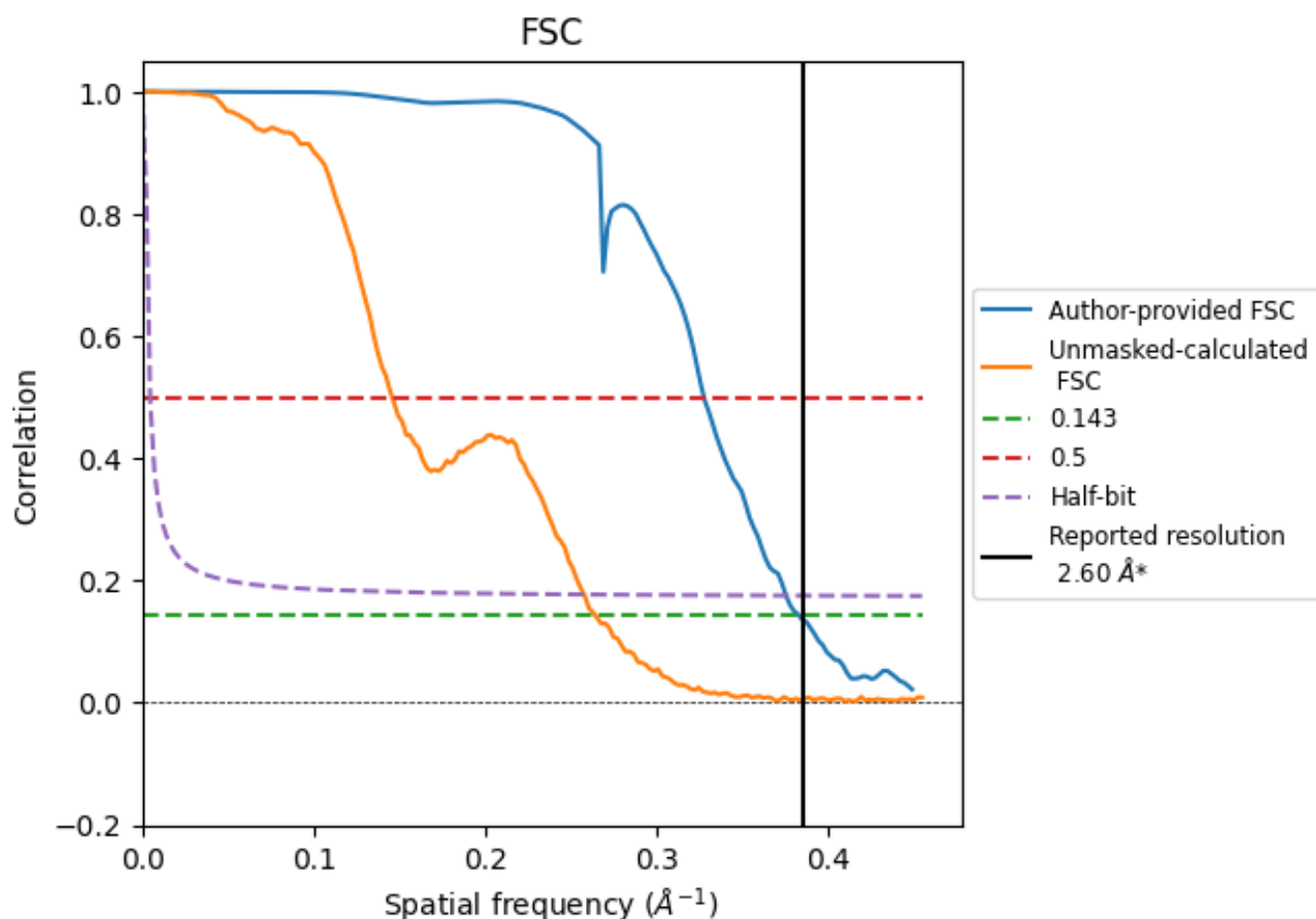


\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>

## 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 0.385  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

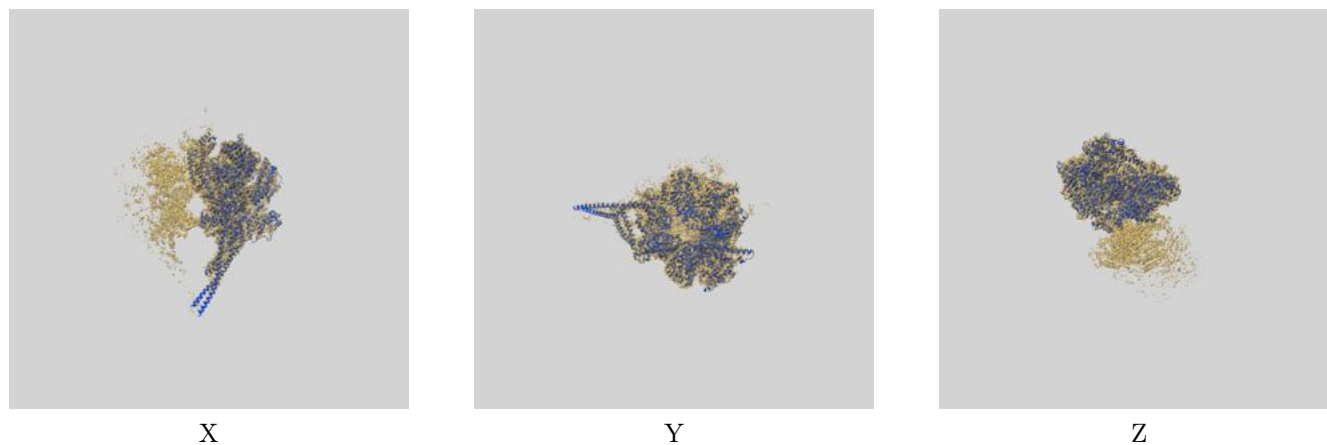
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.61	3.05	2.67
Unmasked-calculated*	3.79	6.86	3.88

\*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 3.79 differs from the reported value 2.6 by more than 10 %

## 9 Map-model fit [i](#)

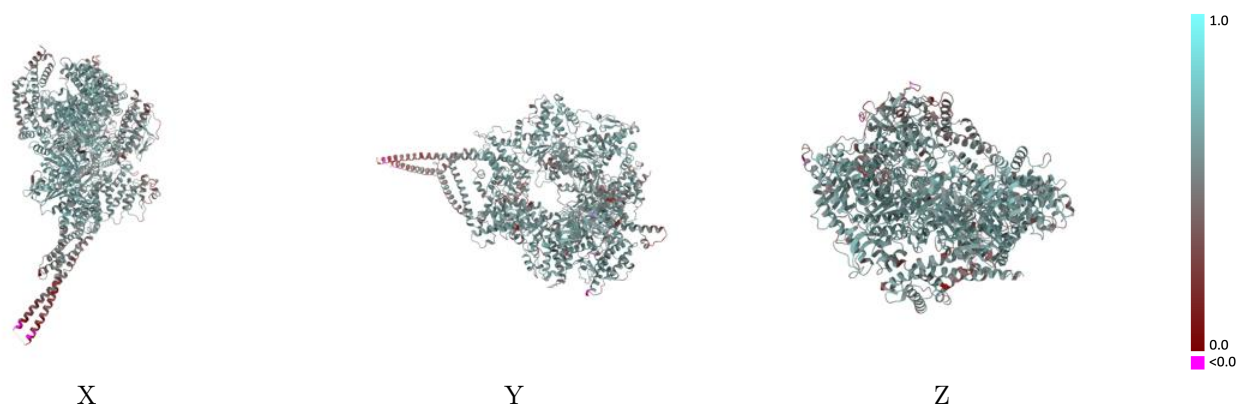
This section contains information regarding the fit between EMDB map EMD-44708 and PDB model 9BMR. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

### 9.1 Map-model overlay [i](#)



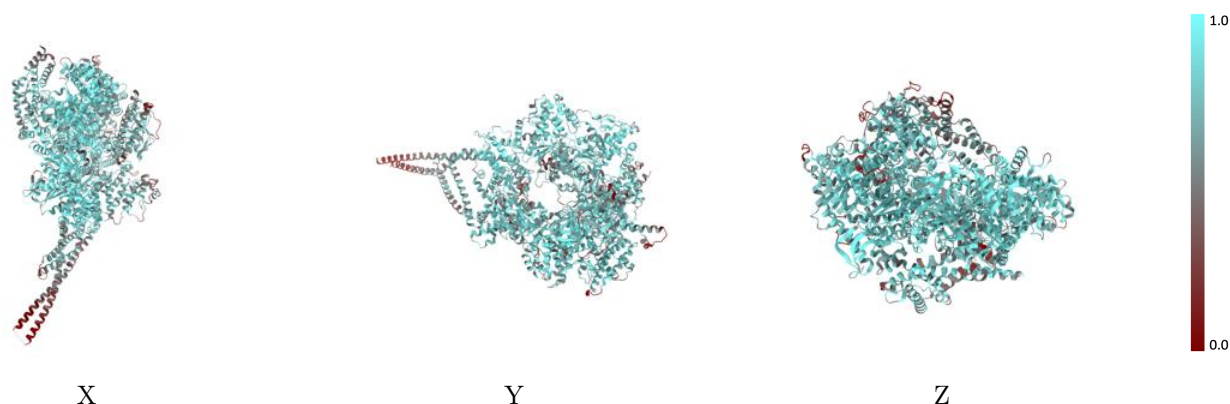
The images above show the 3D surface view of the map at the recommended contour level 0.38 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



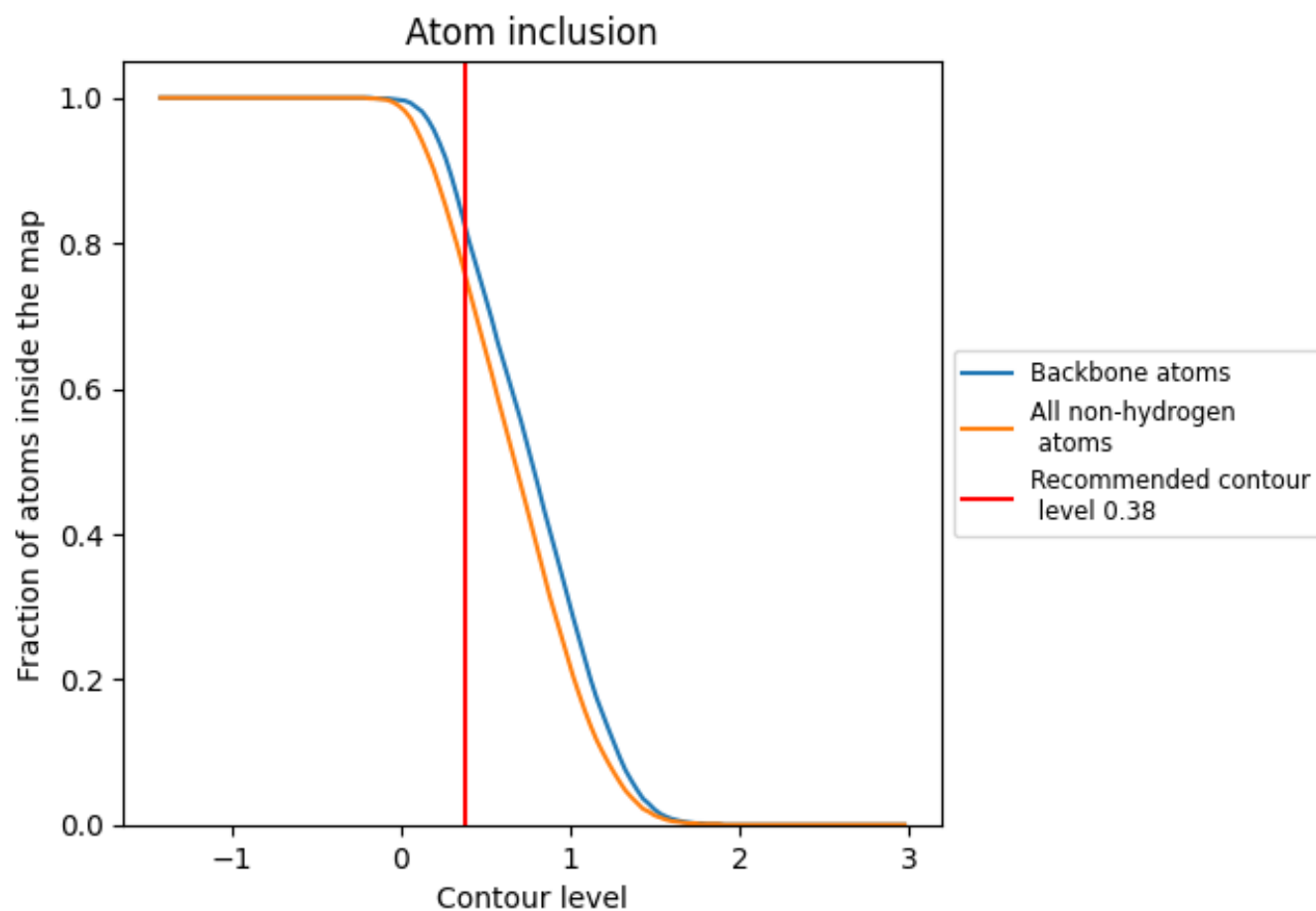
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.38).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7550	<div></div> 0.5630
A	<div></div> 0.7550	<div></div> 0.5630

