



## Full wwPDB EM Validation Report ⓘ

Sep 2, 2025 – 02:18 PM EDT

PDB ID : 9DGP / pdb\_00009dgp  
EMDB ID : EMD-46843  
Title : Motor domain of dynein-1 complex on microtubules  
Authors : Rao, Q.; Chai, P.; Zhang, K.  
Deposited on : 2024-09-03  
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](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.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

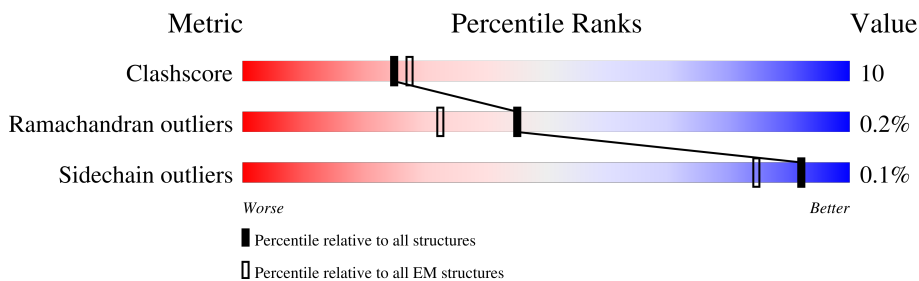
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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  $\geq 3$ , 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 5 unique types of molecules in this entry. The entry contains 24585 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	3037	24461	15582	4227	4533	119	1	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).



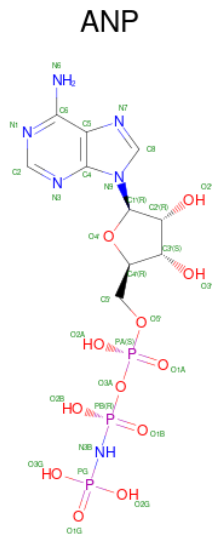
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0

- 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:  $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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





R3607	K3491	LEU	ALA	VAL	ALA	P3127	D3024	V2915	E2775	T2694	Y2493	A2408	D2321
R3620	Q3499	GLU	ASN	LYS	ASN	D3131	T3028	H2918	F2776	L2605	L2494	A2409	R2322
E3624	M3500	ILE	LYS	LEU	LYS	L3133	C3033	R2921	T2777	L2620	L2498	L2413	R2323
R3628	L3503	ASP	LYS	LYS	LYS	P3137	L3042	L2922	E2782	T2634	L2499	Q2414	R2332
F3629	L3508	ALA	HIS	GLN	MET	R3140	M3043	R2923	D2787	R2643	L2502	I2415	L2333
V3638	L3509	ARG	LEU	VAL	VAL	R3141	L3044	R2924	T2788	T2644	S2503	Q2416	S2334
D3642	S3510	LYS	GLU	VAL	GLN	A3142	L3044	F2925	G2504	G2504	G2504	R2417	L2335
P3643	G3518	ASN	ASN	VAL	GLN	I3143	E3048	R2927	R2797	G2647	D2505	A2419	N2338
P3644	Y3519	GLN	ARG	VAL	GLN	V3144	E3049	Q2928	E2798	V2648	S2506	A2420	V2339
L3645	F3520	LYS	SER	SER	GLU	V3148	W3053	L2933	K2799	F2682	N2510	Q2424	R2340
N3646	P3523	ASN	MET	ALA	ALA	A3157	Q3057	L2934	T2800	I2666	R2511	P2425	R2342
V3648	M3524	PRO	ASN	PRO	LYS	N3158	Q3057	L2935	W2802	N2667	L2514	T2428	F2343
L3649	L3536	ASN	PRO	PRO	LYS	T3168	N3061	G2936	E2808	L2668	I2518	P2429	V2345
R3659	Q3537	PRO	ALA	ALA	VAL	T3172	V3064	V2938	R2811	M2671	L2514	L2432	Q2346
V3660	Q3538	SER	ALA	ALA	MET	D3178	V3064	K2943	R2823	D2672	T2522	V2433	R2347
I3661	A3539	VAL	VAL	VAL	SER	A3184	V3065	L2946	E2828	Y2674	W2524	T2434	L2348
I3662	N3540	TYR	GLN	LEU	GLN	E3196	F3066	S2947	A2829	K2673	T2524	L2437	C2359
T3663	I3541	ILE	ILE	ALA	ILE	E3199	M3068	R2948	R2836	Y2675	T2524	H2439	W2360
L3664	E3551	GLU	GLN	LEU	GLN	R3206	M3069	F2949	R2836	G2675	P2527	A2440	R2361
D3668	Y3552	VAL	GLU	GLU	GLU	K3207	P3070	V2950	E2864	M2684	A2529	F2441	W2363
L3671	L3553	ALA	ILE	ALA	ILE	E3210	S3082	E2970	E2867	V2701	L2532	L2442	T2352
L3679	R3559	ALA	ALA	ALA	ALA	E3211	R3088	D2973	S2868	F2708	P2532	L2443	L2369
S3680	L3560	LEU	THR	THR	THR	E3217	V3089	R2982	R2869	C2712	P2533	E2444	S2370
T3681	R3561	LEU	THR	THR	THR	E3217	V3090	R2986	E2867	H2445	L2534	H2445	S2370
R3682	P3568	GLY	GLY	GLY	GLY	E3217	L3091	K2986	E2867	I2446	L2535	I2446	T2371
D3691	C3573	PRO	PRO	PRO	PRO	E3217	N3092	K2989	E2867	M2447	L2541	D2446	D2372
L3692	T3574	THR	THR	THR	THR	E3217	W3093	K2989	E2867	L2449	G2543	L2449	M2373
C3693	E3575	ASP	ASP	ASP	ASP	E3217	T3081	D2973	E2867	R2720	W2545	R2451	I2374
S3694	I3578	LEU	ASP	ASP	ASP	E3217	R3088	E2970	E2867	L2723	T2559	L2452	L2382
R3695	M3579	LEU	ASP	ASP	ASP	E3217	C3089	E2970	E2867	R2726	L2561	R2453	T2385
V3696	L3580	ALA	ASP	ASP	ASP	E3217	V3090	E2970	E2867	F2727	K2561	C2454	P2386
N3700	K3581	ALA	ASP	ASP	ASP	E3217	L3091	E2970	E2867	L2728	T2571	S2460	D2388
S3706	R3582	ALA	ASP	ASP	ASP	E3217	N3092	E2970	E2867	V2731	T2574	A2465	E2389
F3707	N3584	ALA	ASP	ASP	ASP	E3217	W3093	E2970	E2867	P2732	T2574	C2466	D2392
L3708	D3591	ALA	ASP	ASP	ASP	E3217	T3099	E2970	E2867	V2733	L2581	N2468	E2393
V3716	P3592	ALA	ASP	ASP	ASP	E3217	Y3103	E2970	E2867	V2734	L2581	Q2471	R2396
V3724	S3593	ALA	ASP	ASP	ASP	E3217	Y3103	E2970	E2867	I2747	E2587	Y2472	R2397
Q3739	A3596	ALA	ASP	ASP	ASP	E3217	E3108	E2970	E2867	Y2748	H2588	N2473	R2398
L3740	T3597	ALA	ASP	ASP	ASP	E3217	M3113	E2970	E2867	G2749	P2590	M2481	R2399
R3743	L3600	ALA	ASP	ASP	ASP	E3217	D3114	E2970	E2867	T2750	L2591	L2486	G2400
L3749	M3601	ALA	ASP	ASP	ASP	E3217	L3115	E2970	E2867	R2757	L2593	L2486	R2401
	E3603	ALA	ASP	ASP	ASP	E3217	P3123	E2970	E2867	L2762	L2593	E2487	E2402
		ALA	ASP	ASP	ASP	E3217	M3126	E2970	E2867	Y2765	M2603	Y2489	D2403
		ALA	ASP	ASP	ASP	E3217		E2970	E2867				E2405
		ALA	ASP	ASP	ASP	E3217		E2970	E2867				E2406
		ALA	ASP	ASP	ASP	E3217		E2970	E2867				E2407



A3752	L3753	N3754	E3755	V3756	K3757	K3758	K3759	I3760	L3761	D3762	D3763	D3764	T3765	I3766	I3767	T3768	T3769	L3770	E3771	N3772	L3773	K3774	T3787	K3791	V3794	V3797	V3801	S3809	S3817	Q3820	I3821	L3829	I3835	Y3836	V3839	V3849	L3856	C3857	I3858	I3859	L3863	V3866	R3870				
V3871	M3875	L3876	H3877	Q3878	D3879	A3884	M3885	L3886	L3887	A3888	R3889	I3890	K3891	T3900	Y3901	E3902	L3909	K3912	E3913	I3914	V3915	L3916	S3917	A3918	P3922	K3923	I3924	Q3931	A3932	E3933	A3934	V3935	V3936	F3944	P3966	W3974	T3983	F3996	R4000	V4009	N4012	L4013	L4027				
T4028	H4029	I4030	M4043	C4044	S4045	Y4049	V4055	L4058	S4068	I4069	A4070	I4071	Q4079	A4080	D4081	K4082	M4085	T4086	A4087	V4088	K4089	S4090	G4091	R4092	W4093	V4094	M4095	L4096	K4097	W4098	V4099	H4100	W4105	L4106	P4118	R4123	L4124	F4125	L4126	T4127	W4128	E4129	I4130	M4137	L4138	F4145	V4146
F4147	T4160	R4168	I4169	S4172	E4175	R4176	A4177	R4178	Q4191	E4192	R4193	L4194	E4209	L4212	R4213	S4214	D4217	D4224	P4239	A4242	A4248	I4251	Y4252	G4253	T4267	R4271	R4276	S4277	F4278	D4279	F4282	K4283	L4284	V4288	K4292	D4293	I4294	G4299	I4300								
R4301	R4302	Q4307	L4311	P4324	W4325	N4326	V4330	T4333	K4342	M4343	L4344	K4345	M4346	L4349	E4350	D4351	E4352	D4353	ASP	LEU	ALA	TYR	ALA	GLU	THR	GLU	LYS	THR	ARG	THR	ASP	SER	THR	ALA	ASP	GLY	ARG	PRO	A4375	H4381	M4386	W4387	L4390	L4398	T4401		
N4404	I4405	P4408	R4411	F4412	V4417	L4423	L4424	Q4429	D4433	C4438	K4442	L4448	L4460	S4463	W4464	S4465	H4466	V4475	I4476	Q4477	W4478	V4479	R4485	I4486	S4493	A4496	L4504	K4505	G4513	P4517	Y4520	I4521	T4524	R4525	Q4526	Y4527	L4536	E4537									
E4538	L4539	C4540	L4541	V4543	S4548	Q4549	S4550	A4551	D4554	S4557	F4558	K4564	T4569	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	N4597	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	E4646									

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106660	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.813	Depositor
Minimum map value	-1.093	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.15	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: ANP, MG, ADP, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.37	0/24982	0.49	0/33848

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	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1360	ARG	Sidechain
1	A	2292	ARG	Sidechain
1	A	2757	ARG	Sidechain
1	A	4123	ARG	Sidechain
1	A	4302	ARG	Sidechain

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	24461	0	24528	508	0
2	A	27	0	12	2	0
3	A	31	0	12	2	0
4	A	62	0	26	4	0
5	A	4	0	0	0	0
All	All	24585	0	24578	508	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 10.

All (508) 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:2598:GLY:H	4:A:4703:ANP:HNB1	1.23	0.85
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.64	0.79
1:A:1370:LEU:HD11	1:A:1390:LEU:HD12	1.66	0.77
1:A:2581:LEU:HD21	1:A:2605:LEU:HD23	1.68	0.75
1:A:2506:SER:HB3	1:A:2510:MET:HB2	1.71	0.70
1:A:4569:THR:HG22	1:A:4583:THR:HG21	1.73	0.70
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.75	0.69
1:A:4079:GLN:HA	1:A:4082:LYS:HE3	1.73	0.68
1:A:1898:ALA:O	1:A:1983:ARG:NH1	2.26	0.67
1:A:3474:ARG:HE	1:A:3764:ASP:HB3	1.59	0.67
1:A:3691:ASP:OD1	1:A:3695:ARG:NH1	2.27	0.67
1:A:4408:PRO:HA	1:A:4411:ARG:HE	1.59	0.67
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.75	0.66
1:A:1374:PRO:HD2	1:A:1377:LEU:HD12	1.77	0.66
1:A:3194:LEU:HD22	1:A:3500:MET:HE3	1.75	0.66
1:A:2179:ARG:NH2	1:A:2195:ASP:OD1	2.28	0.66
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.76	0.66
1:A:1336:LEU:HA	1:A:1339:ILE:HD12	1.77	0.66
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.77	0.66
1:A:1462:PHE:HB2	1:A:3628:ARG:HD2	1.78	0.65
1:A:4276:ARG:NH2	1:A:4279:ASP:OD2	2.30	0.65
1:A:2148:LYS:HG2	1:A:2361:MET:HB3	1.78	0.65
1:A:2925:ILE:HG21	1:A:2933:LEU:HB2	1.78	0.65
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.79	0.65
1:A:3113:MET:HE2	1:A:3184:ALA:HA	1.78	0.65
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.78	0.64
1:A:4564:LYS:HG3	1:A:4646:GLU:HB2	1.79	0.64
1:A:2221:MET:HE3	1:A:2343:PHE:HD2	1.61	0.64
1:A:2324:LEU:HD11	1:A:2332:ARG:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2320:ASP:OD1	1:A:2321:ASP:N	2.31	0.63
1:A:2428:THR:HB	1:A:2429:PRO:HD2	1.81	0.63
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.31	0.63
1:A:1666:LEU:HB3	1:A:1670:ASN:HA	1.80	0.63
1:A:2925:ILE:HG13	1:A:2933:LEU:HD13	1.79	0.63
1:A:4543:VAL:HG21	1:A:4622:VAL:HG12	1.79	0.63
1:A:1571:ILE:HG23	1:A:1604:LEU:HD22	1.80	0.62
1:A:3871:VAL:HG12	1:A:3875:MET:HE2	1.80	0.62
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.82	0.62
1:A:3820:GLN:HE21	1:A:4345:LYS:HG2	1.63	0.62
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.32	0.62
1:A:3113:MET:HB3	1:A:3115:LEU:HG	1.82	0.62
1:A:1417:MET:HE1	1:A:1423:ASN:HA	1.82	0.61
1:A:4193:ARG:NH2	1:A:4637:GLU:O	2.25	0.61
1:A:2453:ARG:NH1	1:A:2505:ASP:OD2	2.33	0.61
1:A:2889:LEU:HD13	1:A:2920:LEU:HD11	1.82	0.61
1:A:2385:ILE:O	1:A:2416:GLN:NE2	2.32	0.61
1:A:2138:ILE:HG13	1:A:2161:LEU:HD21	1.82	0.60
1:A:4172:SER:O	1:A:4176:ARG:NH1	2.33	0.60
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.82	0.59
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.85	0.59
1:A:2728:LEU:HA	1:A:2731:VAL:HG22	1.84	0.59
1:A:2605:LEU:HD13	1:A:2662:PHE:HE1	1.67	0.59
1:A:3749:LEU:HD11	1:A:3770:LEU:HG	1.83	0.59
1:A:2230:LYS:NZ	1:A:2345:VAL:O	2.35	0.59
1:A:3488:ARG:HA	1:A:3491:LYS:HE2	1.85	0.58
1:A:3553:LEU:HB2	1:A:3578:ILE:HD13	1.85	0.58
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.86	0.58
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	1.84	0.58
1:A:2447:MET:HG3	1:A:2733:VAL:HG11	1.86	0.58
1:A:4300:ILE:HG13	1:A:4301:ARG:HD3	1.85	0.58
1:A:1961:ASN:ND2	1:A:2019:ASN:O	2.37	0.57
1:A:2386:PRO:HG3	1:A:2413:LEU:HD22	1.85	0.57
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.33	0.57
1:A:3624:GLU:HG2	1:A:3664:LEU:HD23	1.87	0.57
1:A:1964:GLU:HG2	1:A:1967:MET:HE2	1.85	0.57
1:A:2968:THR:HG22	1:A:2970:GLU:H	1.70	0.57
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.70	0.57
1:A:2593:LEU:HD23	1:A:2734:VAL:HB	1.86	0.57
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.87	0.57
1:A:2559:THR:HG22	1:A:2757:ARG:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2776:PHE:HZ	1:A:2846:THR:HG23	1.68	0.57
1:A:1687:LYS:HG3	1:A:1715:LYS:HD2	1.86	0.56
1:A:2324:LEU:HD21	1:A:2332:ARG:HG2	1.87	0.56
1:A:4175:GLU:OE1	1:A:4175:GLU:N	2.38	0.56
1:A:3211:THR:HG21	1:A:3753:LEU:HD11	1.86	0.56
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.86	0.56
1:A:1688:THR:OG1	1:A:1708:GLU:OE2	2.16	0.56
1:A:2472:TYR:CD1	1:A:2541:ILE:HG21	2.40	0.56
1:A:3008:MET:HG2	1:A:3066:PHE:HZ	1.69	0.56
1:A:2396:ARG:NH1	1:A:2406:GLU:OE2	2.39	0.56
1:A:2511:ARG:HD3	1:A:2535:ILE:HD13	1.87	0.56
1:A:3661:LEU:HD12	1:A:3668:ASP:HB3	1.86	0.56
1:A:1397:ASN:O	1:A:1401:ILE:HD12	2.05	0.56
1:A:1510:SER:HB2	1:A:3629:PHE:HB3	1.87	0.56
1:A:2188:GLU:OE1	1:A:2243:ARG:NH1	2.39	0.56
1:A:1545:VAL:O	1:A:1548:GLU:HG3	2.06	0.56
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.87	0.56
1:A:4543:VAL:HG13	1:A:4588:THR:HG23	1.88	0.55
1:A:2694:ARG:HG3	1:A:2701:VAL:HG21	1.87	0.55
1:A:3889:ARG:HH12	1:A:3909:LEU:HD11	1.71	0.55
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.06	0.55
1:A:3620:ARG:NH2	1:A:3642:ASP:OD2	2.39	0.55
1:A:2965:ARG:HG3	1:A:2966:LYS:HD2	1.88	0.55
1:A:4088:VAL:HG23	1:A:4118:PRO:HA	1.88	0.55
1:A:4386:ASN:O	1:A:4390:LEU:HG	2.05	0.55
1:A:2192:THR:HB	1:A:2373:MET:HG2	1.89	0.55
1:A:2075:LEU:HD11	1:A:4536:LEU:CD2	2.38	0.54
1:A:3716:VAL:HG23	1:A:3836:TYR:OH	2.06	0.54
1:A:3879:ASP:OD1	1:A:4342:LYS:NZ	2.35	0.54
1:A:4465:SER:OG	1:A:4478:TRP:NE1	2.41	0.54
1:A:3194:LEU:HD11	1:A:3499:GLN:HB2	1.89	0.54
1:A:3835:ILE:HG23	1:A:3866:VAL:HG12	1.90	0.54
1:A:2075:LEU:HD11	1:A:4536:LEU:HD22	1.88	0.54
1:A:2104:LYS:HA	1:A:2136:ILE:HD13	1.89	0.54
1:A:2374:ILE:HD13	1:A:2452:LEU:HD21	1.89	0.54
1:A:2914:GLU:O	1:A:2918:HIS:ND1	2.28	0.54
1:A:1368:ASN:HA	1:A:1371:LYS:HD2	1.89	0.54
1:A:4398:LEU:HD21	1:A:4493:SER:HA	1.90	0.54
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.89	0.54
1:A:4527:TYR:CD2	1:A:4558:PHE:HZ	2.25	0.54
1:A:4398:LEU:HG	1:A:4417:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1632:VAL:HG12	1:A:1656:LYS:HD2	1.90	0.53
1:A:3499:GLN:O	1:A:3503:ILE:HG13	2.08	0.53
1:A:3551:GLU:HG3	1:A:3559:ARG:NH1	2.23	0.53
1:A:1457:MET:HE2	1:A:3659:ARG:HB3	1.90	0.53
1:A:2081:SER:O	1:A:2083:GLN:HG2	2.08	0.53
1:A:2797:ARG:NH1	4:A:4703:ANP:O1G	2.36	0.53
1:A:1925:ARG:HG2	1:A:1954:TRP:CD1	2.42	0.53
1:A:2910:VAL:HG22	1:A:3108:GLU:HG2	1.90	0.53
1:A:2936:ILE:HG23	1:A:3093:TRP:HE3	1.73	0.53
1:A:3123:PRO:HG3	1:A:3539:ALA:HA	1.89	0.53
1:A:4093:TRP:CD1	1:A:4123:ARG:HB2	2.43	0.53
1:A:2156:LEU:O	1:A:2160:LEU:HG	2.09	0.53
1:A:2309:PRO:HB3	1:A:2352:THR:HG23	1.90	0.53
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.40	0.53
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	1.91	0.53
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	1.91	0.53
1:A:2718:PRO:HG2	1:A:3082:SER:HA	1.90	0.53
1:A:3659:ARG:HG3	1:A:3661:LEU:HD21	1.90	0.53
1:A:4525:ARG:HE	1:A:4539:LEU:HB2	1.73	0.53
1:A:3581:LYS:NZ	1:A:3582:ARG:HH11	2.06	0.53
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.08	0.53
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.89	0.53
1:A:2248:GLU:HG2	1:A:2297:LYS:NZ	2.23	0.53
1:A:2591:LEU:HA	1:A:2732:PRO:HD2	1.91	0.53
1:A:3644:VAL:HG22	1:A:3664:LEU:HD12	1.91	0.53
1:A:2060:ARG:HG3	1:A:2061:THR:HG23	1.91	0.52
1:A:2488:ARG:HH21	1:A:2543:GLY:H	1.57	0.52
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.26	0.52
1:A:3835:ILE:HG12	1:A:3870:ARG:HG3	1.91	0.52
1:A:2218:HIS:HA	1:A:2340:ARG:HD3	1.90	0.52
1:A:3901:TYR:HE2	1:A:3983:ILE:HG23	1.75	0.52
1:A:2080:LEU:HD12	1:A:2088:PHE:CZ	2.44	0.52
1:A:2154:ILE:N	1:A:2155:PRO:HD2	2.24	0.52
1:A:3088:ARG:NH1	4:A:4703:ANP:O1G	2.42	0.52
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.91	0.52
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.49	0.52
1:A:2896:ARG:HG3	1:A:2953:MET:HE3	1.92	0.52
1:A:1882:THR:HG22	1:A:2048:LEU:HD23	1.92	0.52
1:A:3593:SER:O	1:A:3682:ARG:NH2	2.43	0.52
1:A:1755:GLN:HG3	1:A:1814:GLU:OE2	2.09	0.52
1:A:2808:GLU:OE1	1:A:2811:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2440:ALA:HB2	1:A:2502:LEU:HB3	1.90	0.51
1:A:3762:ASP:OD1	1:A:3763:ASP:N	2.43	0.51
1:A:1513:TYR:CZ	1:A:1517:GLU:HG2	2.45	0.51
1:A:4271:ARG:NH1	1:A:4284:LEU:O	2.38	0.51
1:A:1419:ARG:HD2	1:A:1445:VAL:HG13	1.91	0.51
1:A:2481:MET:HE2	1:A:2486:LEU:HA	1.92	0.51
1:A:4071:ILE:HD11	1:A:4096:LEU:HD22	1.93	0.51
1:A:4520:TYR:O	1:A:4524:THR:HG23	2.10	0.51
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.93	0.51
1:A:2072:PHE:HE2	1:A:2141:VAL:HG11	1.76	0.51
1:A:2295:LEU:HA	1:A:2338:ASN:ND2	2.26	0.51
1:A:2424:GLN:HB3	1:A:2425:PRO:HD3	1.92	0.51
1:A:3133:LEU:HD21	1:A:3137:PRO:HB3	1.93	0.51
1:A:4086:THR:O	1:A:4090:SER:OG	2.26	0.51
1:A:2053:MET:HE1	1:A:2094:LYS:HB3	1.92	0.51
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.92	0.51
1:A:3679:LEU:HD12	1:A:3696:VAL:HG11	1.93	0.51
1:A:4543:VAL:HG21	1:A:4622:VAL:CG1	2.40	0.51
1:A:2499:LEU:O	1:A:2503:SER:OG	2.25	0.50
1:A:1964:GLU:OE2	1:A:1966:ARG:NH1	2.45	0.50
1:A:3131:ASP:OD1	1:A:3132:LYS:N	2.44	0.50
1:A:2747:ILE:O	1:A:2750:THR:OG1	2.27	0.50
1:A:3561:ARG:NH1	1:A:3603:GLU:OE1	2.44	0.50
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.93	0.50
1:A:4288:VAL:HG21	1:A:4294:ILE:HG13	1.94	0.50
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.46	0.50
1:A:3044:LEU:HD22	1:A:3049:GLU:HG2	1.93	0.50
1:A:3551:GLU:HG3	1:A:3559:ARG:HH12	1.77	0.50
1:A:2919:VAL:HG13	1:A:2950:VAL:HG22	1.94	0.50
1:A:3194:LEU:HD13	1:A:3500:MET:HE2	1.94	0.50
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	1.93	0.50
1:A:2666:ILE:HB	1:A:2712:CYS:SG	2.52	0.50
1:A:3143:ILE:HD13	1:A:3541:ILE:HD13	1.93	0.50
1:A:4342:LYS:O	1:A:4346:MET:HG2	2.12	0.50
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	1.94	0.49
1:A:3191:ARG:O	1:A:3195:GLU:HG3	2.12	0.49
1:A:4099:VAL:HG21	1:A:4126:LEU:HB3	1.94	0.49
1:A:3912:LYS:HB2	1:A:4476:ILE:HG21	1.94	0.49
1:A:1399:LEU:HD12	1:A:1446:VAL:HG11	1.94	0.49
1:A:2787:ASP:OD1	1:A:2788:THR:N	2.45	0.49
1:A:3591:ASP:OD2	1:A:3596:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1332:VAL:HB	1:A:1377:LEU:HD22	1.94	0.49
1:A:3024:ASP:O	1:A:3028:THR:HG23	2.12	0.49
1:A:3771:GLU:OE1	1:A:3774:LYS:NZ	2.34	0.49
1:A:4442:LYS:HE2	1:A:4448:LEU:HD11	1.94	0.49
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	1.93	0.49
1:A:3767:ILE:HA	1:A:3770:LEU:HD13	1.94	0.49
1:A:2872:LEU:HD13	1:A:2889:LEU:HD12	1.95	0.49
1:A:3888:ALA:O	1:A:4012:ASN:ND2	2.46	0.49
1:A:1425:VAL:HB	1:A:1428:GLU:HB2	1.94	0.49
1:A:2179:ARG:HD3	1:A:2208:LEU:HD11	1.94	0.49
1:A:2232:MET:HG3	3:A:4702:ATP:C8	2.48	0.49
1:A:4045:SER:HB3	1:A:4049:TYR:HB3	1.93	0.49
1:A:1751:VAL:HG11	1:A:1878:LYS:HD2	1.94	0.49
1:A:2495:VAL:HG21	1:A:2524:VAL:HG11	1.95	0.49
1:A:1540:VAL:HG13	1:A:1608:LEU:HD12	1.94	0.49
1:A:2209:GLN:O	1:A:2212:GLN:HG2	2.12	0.49
1:A:3127:PRO:HG3	1:A:3538:GLN:HB3	1.94	0.49
1:A:2053:MET:SD	1:A:2094:LYS:HG2	2.53	0.48
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.48	0.48
1:A:2666:ILE:HG22	1:A:2723:LEU:HD21	1.94	0.48
1:A:2223:VAL:HG11	1:A:2348:LEU:HG	1.94	0.48
1:A:2472:TYR:HB2	1:A:2541:ILE:HD12	1.95	0.48
1:A:4069:ILE:HD13	1:A:4079:GLN:HG2	1.95	0.48
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.49	0.48
1:A:3193:GLU:O	1:A:3196:GLU:HG3	2.13	0.48
1:A:3597:THR:O	1:A:3601:MET:HG2	2.13	0.48
1:A:2415:ILE:HD11	1:A:2473:ASN:HD22	1.79	0.48
1:A:2965:ARG:HE	1:A:2966:LYS:HD2	1.79	0.48
1:A:4081:ASP:OD1	1:A:4082:LYS:N	2.47	0.48
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.94	0.48
1:A:2918:HIS:O	1:A:2922:ILE:HG13	2.13	0.48
1:A:4178:ARG:NH2	1:A:4299:GLY:O	2.46	0.48
1:A:2446:ILE:HG23	1:A:2447:MET:HG2	1.95	0.48
1:A:3659:ARG:HG3	1:A:3661:LEU:CD2	2.44	0.48
1:A:1403:LEU:HD21	1:A:1446:VAL:HG13	1.94	0.48
1:A:1556:ASP:O	1:A:1560:LEU:HG	2.13	0.48
1:A:3766:ILE:O	1:A:3769:THR:HG22	2.14	0.48
1:A:3801:TYR:HD1	1:A:3856:LEU:HD13	1.79	0.48
1:A:3157:ALA:HB1	1:A:3524:MET:HE2	1.96	0.48
1:A:2757:ARG:HG3	1:A:2757:ARG:HH11	1.79	0.47
1:A:3488:ARG:HH12	1:A:3773:LEU:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3575:GLU:O	1:A:3579:MET:HG3	2.14	0.47
1:A:1769:ILE:HD11	1:A:1778:LEU:HB2	1.96	0.47
1:A:3123:PRO:HG2	1:A:3126:MET:HG3	1.96	0.47
1:A:1403:LEU:HD23	1:A:1450:LEU:HD11	1.96	0.47
1:A:1987:SER:HB3	1:A:1990:HIS:CD2	2.49	0.47
1:A:2534:ILE:HD12	1:A:2534:ILE:H	1.79	0.47
1:A:1628:ARG:NH2	1:A:1871:GLU:OE1	2.47	0.47
1:A:3194:LEU:HD13	1:A:3500:MET:CE	2.44	0.47
1:A:4424:LEU:HD13	1:A:4486:ILE:HG13	1.95	0.47
1:A:2439:HIS:HA	1:A:2442:LYS:HD2	1.97	0.47
1:A:3817:SER:C	1:A:4346:MET:HE1	2.39	0.47
1:A:1397:ASN:O	1:A:1400:VAL:HB	2.14	0.47
1:A:1469:VAL:HG11	1:A:1500:HIS:CE1	2.50	0.47
1:A:2268:LEU:HB3	1:A:2275:TRP:HE3	1.79	0.47
1:A:2371:THR:HG22	1:A:2451:ARG:HD2	1.97	0.47
1:A:3849:VAL:HG11	1:A:3858:ILE:HD12	1.96	0.47
1:A:4044:CYS:HB3	1:A:4130:ILE:HG12	1.96	0.47
1:A:1511:PRO:O	1:A:1514:LYS:NZ	2.37	0.47
1:A:2956:LEU:HG	1:A:2989:LYS:HB3	1.97	0.47
1:A:3935:VAL:HG22	1:A:3996:PHE:HE1	1.79	0.47
1:A:1456:GLU:HG2	1:A:1512:TYR:HB3	1.97	0.47
1:A:3724:VAL:HG13	1:A:3794:VAL:HG12	1.96	0.47
1:A:4137:ASN:OD1	1:A:4138:LEU:N	2.48	0.47
1:A:1850:GLN:HB2	1:A:1856:GLN:HG2	1.97	0.46
1:A:2726:ARG:NH1	3:A:4702:ATP:O3G	2.48	0.46
1:A:4055:VAL:HB	1:A:4095:MET:HE1	1.96	0.46
1:A:1701:TRP:O	1:A:1705:VAL:HG23	2.15	0.46
1:A:2094:LYS:NZ	2:A:4701:ADP:O2'	2.32	0.46
1:A:2080:LEU:HD22	1:A:2153:ASP:HB3	1.97	0.46
1:A:2454:CYS:HB3	1:A:2502:LEU:HD23	1.97	0.46
1:A:3909:LEU:HB3	1:A:4344:LEU:HD21	1.97	0.46
1:A:3591:ASP:O	1:A:3682:ARG:HA	2.15	0.46
1:A:3915:VAL:HG21	1:A:4390:LEU:HD22	1.97	0.46
1:A:1571:ILE:HD11	1:A:1607:LEU:HB3	1.97	0.46
1:A:1619:LEU:HD22	1:A:1637:LEU:HD23	1.97	0.46
1:A:1847:ASP:OD1	1:A:1849:LYS:HG2	2.15	0.46
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.16	0.46
1:A:4027:LEU:HD11	1:A:4043:MET:HE1	1.96	0.46
1:A:4405:ILE:HD12	1:A:4411:ARG:HG2	1.97	0.46
1:A:1763:GLU:CD	1:A:1838:TRP:HE1	2.23	0.46
1:A:2206:LYS:NZ	1:A:2363:TRP:O	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2227:GLY:HA3	1:A:2452:LEU:HD12	1.97	0.46
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.31	0.46
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.98	0.46
1:A:4094:VAL:HB	1:A:4124:LEU:HD12	1.98	0.46
1:A:1793:ALA:HA	1:A:1796:VAL:HG12	1.98	0.46
1:A:2453:ARG:HD3	1:A:2728:LEU:O	2.16	0.46
1:A:2748:TYR:CD2	1:A:2799:MET:HE3	2.51	0.46
1:A:3044:LEU:HD13	1:A:3049:GLU:HG3	1.97	0.46
1:A:2934:LEU:HD23	1:A:3091:LEU:CD2	2.46	0.46
1:A:1859:ILE:HD11	1:A:1868:TYR:HD1	1.80	0.45
1:A:4267:THR:HG21	1:A:4636:TYR:HD2	1.79	0.45
1:A:2135:GLU:HG2	1:A:2168:VAL:HG13	1.97	0.45
1:A:2135:GLU:HA	1:A:2138:ILE:HG22	1.97	0.45
1:A:2419:ALA:HA	1:A:2490:ILE:HD13	1.98	0.45
1:A:2935:LEU:HD23	1:A:3092:ASN:HB3	1.99	0.45
1:A:3568:PRO:HG2	1:A:3573:CYS:SG	2.56	0.45
1:A:4554:ASP:H	1:A:4557:SER:HB2	1.81	0.45
1:A:2643:ARG:HE	1:A:2648:VAL:HG22	1.80	0.45
1:A:2936:ILE:HA	1:A:3068:MET:O	2.16	0.45
1:A:2996:GLU:HA	1:A:2999:VAL:HB	1.99	0.45
1:A:4214:SER:HB2	1:A:4251:ILE:HG23	1.98	0.45
1:A:1468:GLU:O	1:A:1472:THR:HG22	2.17	0.45
1:A:2775:GLU:O	1:A:2778:THR:OG1	2.35	0.45
1:A:3207:LYS:HZ1	1:A:3754:ASN:HA	1.81	0.45
1:A:3821:ILE:HD12	1:A:4342:LYS:HG2	1.97	0.45
1:A:3839:VAL:HG12	1:A:3859:ILE:HG23	1.98	0.45
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.98	0.45
1:A:2905:LEU:HD23	1:A:2948:ARG:HH22	1.82	0.45
1:A:1480:TYR:OH	1:A:1548:GLU:OE2	2.27	0.45
1:A:1635:GLU:HG2	1:A:1636:ASP:N	2.32	0.45
1:A:2369:LEU:HD12	1:A:2373:MET:HE2	1.99	0.45
1:A:3196:GLU:HA	1:A:3199:MET:HG3	1.97	0.45
1:A:2134:GLN:HE21	1:A:2168:VAL:HG21	1.82	0.45
1:A:2288:ILE:CD1	1:A:2333:LEU:HD22	2.47	0.45
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.98	0.45
1:A:2468:ASN:HA	1:A:2471:GLN:HG2	1.99	0.45
1:A:2560:HIS:O	1:A:2561:LYS:HG2	2.17	0.45
1:A:2884:VAL:HG13	1:A:2889:LEU:HD11	1.98	0.45
1:A:2924:ARG:O	1:A:2928:GLN:HG2	2.16	0.45
1:A:3057:GLN:O	1:A:3061:ASN:HB2	2.16	0.45
1:A:3178:ASP:OD1	1:A:3584:ASN:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2072:PHE:CE2	1:A:2141:VAL:HG11	2.52	0.45
1:A:2191:LEU:HD12	1:A:2236:VAL:HG21	1.98	0.45
1:A:3900:THR:HB	1:A:3902:GLU:HG3	1.98	0.45
1:A:3944:PHE:CE1	1:A:3974:TRP:HB3	2.52	0.45
1:A:4277:SER:HA	1:A:4282:PHE:CG	2.52	0.45
1:A:2065:LEU:HD21	1:A:2134:GLN:HG2	1.99	0.45
1:A:2452:LEU:HD23	1:A:2452:LEU:HA	1.79	0.45
1:A:2093:LEU:O	1:A:2097:LEU:HG	2.17	0.45
1:A:1459:LEU:HD22	1:A:1507:MET:HG3	1.99	0.44
1:A:1561:LEU:HB3	1:A:1564:GLU:HB2	2.00	0.44
1:A:1721:VAL:O	1:A:1725:GLU:HG3	2.17	0.44
1:A:2202:MET:O	1:A:2205:GLU:HG2	2.18	0.44
1:A:2823:ARG:HH12	1:A:2868:SER:H	1.64	0.44
1:A:3901:TYR:CE2	1:A:3983:ILE:HG23	2.52	0.44
1:A:4401:THR:H	1:A:4404:ASN:HB2	1.82	0.44
1:A:4517:PRO:O	1:A:4521:ILE:HG12	2.18	0.44
1:A:1778:LEU:HD23	1:A:1778:LEU:HA	1.89	0.44
1:A:2323:LYS:HB3	1:A:2335:LEU:HB3	1.98	0.44
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.98	0.44
1:A:2884:VAL:HG11	1:A:2889:LEU:HD21	1.99	0.44
1:A:3643:PRO:O	1:A:3646:ASN:ND2	2.50	0.44
1:A:3724:VAL:HG21	1:A:3797:VAL:HG21	1.98	0.44
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.50	0.44
1:A:3922:PRO:HD2	1:A:3936:VAL:HG21	1.98	0.44
1:A:1334:SER:O	1:A:1338:LYS:HD3	2.17	0.44
1:A:1337:SER:O	1:A:1341:GLU:HG2	2.17	0.44
1:A:1394:LEU:HD23	1:A:1394:LEU:HA	1.85	0.44
1:A:2443:LEU:HD11	1:A:2514:LEU:HB2	2.00	0.44
1:A:2905:LEU:HD23	1:A:2948:ARG:NH2	2.32	0.44
1:A:3878:GLN:HG3	1:A:3879:ASP:OD1	2.17	0.44
1:A:4423:LEU:HD13	1:A:4466:HIS:ND1	2.33	0.44
1:A:1464:LYS:HE3	1:A:1464:LYS:HB2	1.78	0.44
1:A:1599:ARG:HG3	1:A:1599:ARG:HH11	1.81	0.44
1:A:2204:VAL:O	1:A:2207:VAL:HG12	2.18	0.44
1:A:2798:GLU:HG3	1:A:2801:ARG:HH21	1.81	0.44
1:A:2938:VAL:O	1:A:2943:LYS:NZ	2.51	0.44
1:A:2439:HIS:HD2	1:A:2514:LEU:HD12	1.82	0.44
1:A:2778:THR:O	1:A:2782:GLU:HG3	2.17	0.44
1:A:4191:GLN:O	1:A:4194:LEU:HB2	2.18	0.44
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.51	0.44
1:A:1968:LEU:O	1:A:1972:SER:OG	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2460:SER:OG	1:A:2589:LYS:HD2	2.18	0.44
1:A:2915:VAL:HG13	1:A:2946:LEU:HD21	2.00	0.44
1:A:2620:LEU:HD11	1:A:2634:THR:HG21	2.00	0.44
1:A:4086:THR:HG23	1:A:4089:LYS:HZ3	1.83	0.44
1:A:4087:ALA:O	1:A:4091:GLY:N	2.51	0.44
1:A:4330:VAL:O	1:A:4333:THR:HG22	2.18	0.44
1:A:1974:GLN:O	1:A:1978:ILE:HG13	2.18	0.43
1:A:1350:PRO:O	1:A:1354:VAL:HG23	2.18	0.43
1:A:1409:LYS:O	1:A:1413:TRP:HD1	2.01	0.43
1:A:2288:ILE:HD13	1:A:2333:LEU:HD22	2.00	0.43
1:A:2895:ALA:O	1:A:2899:VAL:HG23	2.19	0.43
1:A:1646:ASN:ND2	1:A:1649:LYS:HE2	2.33	0.43
1:A:2309:PRO:HB3	1:A:2352:THR:CG2	2.49	0.43
1:A:3708:LEU:HD13	1:A:3829:LEU:HD11	1.99	0.43
1:A:2671:MET:HB3	1:A:2675:GLY:HA2	1.99	0.43
1:A:2828:GLU:OE1	1:A:2924:ARG:NH1	2.51	0.43
1:A:3008:MET:HE3	1:A:3011:LEU:HD23	2.01	0.43
1:A:2319:LEU:HD13	1:A:2359:CYS:SG	2.58	0.43
1:A:2923:ASP:OD1	1:A:2927:ARG:NH2	2.50	0.43
1:A:1408:LEU:O	1:A:1412:HIS:HB2	2.19	0.43
1:A:2221:MET:HE3	1:A:2343:PHE:CD2	2.48	0.43
1:A:2388:ASP:OD1	1:A:2389:GLU:N	2.52	0.43
1:A:3008:MET:HE2	1:A:3064:VAL:HG21	2.00	0.43
1:A:3884:ALA:HB1	1:A:4009:VAL:HG11	2.01	0.43
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.84	0.43
1:A:4324:PRO:HB2	1:A:4326:ASN:OD1	2.18	0.43
1:A:2762:LEU:HA	1:A:2765:TYR:HD2	1.83	0.43
1:A:3500:MET:HE2	1:A:3503:ILE:HD12	2.01	0.43
1:A:4097:LYS:HA	1:A:4127:THR:OG1	2.18	0.43
1:A:2175:MET:HE1	1:A:2211:TYR:HD2	1.84	0.43
1:A:4087:ALA:HB1	1:A:4092:ARG:O	2.18	0.43
1:A:1547:LEU:HD22	1:A:1608:LEU:HD22	2.00	0.43
1:A:2049:ILE:HD13	1:A:2090:LEU:HD21	2.00	0.43
1:A:2936:ILE:HG23	1:A:3093:TRP:CE3	2.54	0.43
1:A:3767:ILE:O	1:A:3771:GLU:HG2	2.19	0.43
1:A:3913:GLU:O	1:A:3914:ILE:C	2.62	0.43
1:A:4429:GLN:NE2	1:A:4433:ASP:OD1	2.48	0.43
1:A:1339:ILE:HG21	1:A:1386:VAL:HG11	2.01	0.43
1:A:1873:LEU:HD13	1:A:1921:HIS:HB3	2.00	0.43
1:A:2086:TYR:OH	1:A:2153:ASP:OD2	2.32	0.43
1:A:2232:MET:HE2	1:A:2232:MET:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2413:LEU:HG	1:A:2417:ARG:HE	1.84	0.43
1:A:2864:GLU:CD	1:A:2864:GLU:H	2.26	0.43
1:A:1878:LYS:HE3	1:A:1878:LYS:HB3	1.84	0.42
1:A:1927:VAL:HG22	1:A:1954:TRP:HB2	2.01	0.42
1:A:1980:GLU:O	1:A:1984:GLU:HG3	2.19	0.42
1:A:2071:PRO:O	1:A:2075:LEU:HG	2.20	0.42
1:A:3787:THR:O	1:A:3791:MET:HG3	2.19	0.42
1:A:2514:LEU:O	1:A:2518:ILE:HG12	2.19	0.42
1:A:2925:ILE:HD11	1:A:3090:VAL:HG11	2.00	0.42
1:A:4209:GLU:O	1:A:4213:ARG:HG3	2.19	0.42
1:A:1741:TRP:CH2	1:A:1750:VAL:HG13	2.54	0.42
1:A:2467:ARG:NH1	1:A:2587:GLU:OE2	2.51	0.42
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	2.00	0.42
1:A:4605:VAL:HB	1:A:4626:ILE:HD11	2.00	0.42
1:A:2219:GLY:HA2	1:A:2341:ILE:O	2.19	0.42
1:A:4169:ILE:HD12	1:A:4302:ARG:HE	1.85	0.42
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.52	0.42
1:A:1411:ARG:O	1:A:1415:GLN:HG3	2.18	0.42
1:A:2278:GLY:N	1:A:2281:THR:OG1	2.53	0.42
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.50	0.42
1:A:3518:GLY:O	1:A:3700:ASN:N	2.50	0.42
1:A:1952:GLY:HA2	1:A:2012:MET:HB3	2.01	0.42
1:A:4043:MET:HE2	1:A:4147:PHE:CE1	2.54	0.42
1:A:1838:TRP:CZ2	1:A:1843:ARG:HG2	2.55	0.42
1:A:1911:GLY:N	2:A:4701:ADP:O1B	2.47	0.42
1:A:2982:ARG:HA	1:A:2986:LYS:HD2	2.00	0.42
1:A:2999:VAL:HG13	1:A:3005:LEU:HD21	2.02	0.42
1:A:3581:LYS:HZ2	1:A:3582:ARG:HH11	1.65	0.42
1:A:4100:HIS:CD2	1:A:4129:GLU:HG2	2.54	0.42
1:A:4123:ARG:HD3	1:A:4123:ARG:HA	1.90	0.42
1:A:4346:MET:HE3	1:A:4346:MET:HB3	1.90	0.42
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	2.01	0.42
1:A:1414:LYS:O	1:A:1417:MET:HB3	2.20	0.42
1:A:1425:VAL:O	1:A:1429:LEU:N	2.53	0.42
1:A:1912:LYS:HE3	1:A:1912:LYS:HB2	1.84	0.42
1:A:4028:THR:HA	1:A:4058:LEU:HD11	2.02	0.42
1:A:3103:TYR:OH	1:A:3141:GLU:HG2	2.20	0.41
1:A:3645:LEU:HG	1:A:3649:LEU:HG	2.02	0.41
1:A:3648:VAL:HA	1:A:3662:ILE:HD11	2.01	0.41
1:A:4476:ILE:HD12	1:A:4476:ILE:H	1.85	0.41
1:A:2836:ARG:NH1	1:A:3091:LEU:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3607:ARG:HE	1:A:3607:ARG:HB3	1.67	0.41
1:A:4387:TRP:NE1	1:A:4479:VAL:HG21	2.35	0.41
1:A:4569:THR:HG23	1:A:4578:SER:HB2	2.02	0.41
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.84	0.41
1:A:1356:PRO:CB	1:A:1401:ILE:HG13	2.49	0.41
1:A:2333:LEU:HD23	1:A:2333:LEU:HA	1.95	0.41
1:A:2529:ALA:HB1	1:A:2532:ILE:HB	2.02	0.41
1:A:2593:LEU:HD12	1:A:2605:LEU:HG	2.02	0.41
1:A:3474:ARG:NE	1:A:3764:ASP:HB3	2.32	0.41
1:A:3740:LEU:O	1:A:3743:ARG:HG2	2.20	0.41
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	2.02	0.41
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.86	0.41
1:A:1795:SER:O	1:A:1800:GLN:NE2	2.35	0.41
1:A:2673:LYS:NZ	1:A:2674:TYR:OH	2.53	0.41
1:A:3620:ARG:O	1:A:3624:GLU:HG3	2.20	0.41
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	2.03	0.41
1:A:1461:GLU:O	1:A:1465:GLN:HG3	2.21	0.41
1:A:2863:LYS:O	1:A:2867:MET:N	2.54	0.41
1:A:3033:CYS:HG	1:A:3053:TRP:HE3	1.68	0.41
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	2.03	0.41
1:A:1698:ILE:O	1:A:1702:LEU:HB2	2.20	0.41
1:A:2667:ASN:HB3	1:A:2720:ARG:HB3	2.02	0.41
1:A:2668:LEU:HD21	1:A:2720:ARG:HH11	1.85	0.41
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.55	0.41
1:A:3013:ALA:HB2	1:A:3088:ARG:NE	2.36	0.41
1:A:3158:ASN:OD1	1:A:3168:THR:HB	2.21	0.41
1:A:3508:LEU:HD22	1:A:3536:LEU:HD11	2.02	0.41
1:A:4248:ALA:O	1:A:4253:GLY:HA3	2.21	0.41
1:A:4601:LYS:HB2	1:A:4604:VAL:HG23	2.01	0.41
1:A:1493:LEU:HD21	1:A:1534:PHE:CD2	2.56	0.41
1:A:1910:THR:HG22	1:A:2044:PRO:HD3	2.02	0.41
1:A:2445:HIS:CD2	1:A:2449:LEU:HD22	2.56	0.41
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.56	0.41
1:A:1339:ILE:HD11	1:A:1373:PHE:CE2	2.56	0.41
1:A:1899:ARG:HD3	1:A:1899:ARG:HA	1.86	0.41
1:A:2068:LYS:HG2	1:A:4537:GLU:OE2	2.20	0.41
1:A:2175:MET:O	1:A:2179:ARG:HG2	2.21	0.41
1:A:2518:ILE:O	1:A:2522:THR:HG22	2.21	0.41
1:A:2893:VAL:HG22	1:A:2953:MET:HE1	2.02	0.41
1:A:3523:GLN:HG2	1:A:3706:SER:CB	2.50	0.41
1:A:3983:ILE:HD12	1:A:3983:ILE:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4085:ASN:HA	1:A:4088:VAL:HG12	2.03	0.41
1:A:4626:ILE:HG21	1:A:4630:GLU:O	2.21	0.41
1:A:1481:GLN:N	1:A:2271:ASN:O	2.51	0.41
1:A:2432:LEU:HD11	1:A:2518:ILE:HD12	2.03	0.41
1:A:3140:ARG:O	1:A:3144:VAL:HG23	2.20	0.41
1:A:3739:GLN:HB3	1:A:3743:ARG:HH21	1.85	0.41
1:A:1408:LEU:HD12	1:A:1408:LEU:HA	1.87	0.40
1:A:2214:THR:HG22	1:A:2220:LEU:HD21	2.03	0.40
1:A:2603:MET:SD	4:A:4703:ANP:H2'	2.62	0.40
1:A:3113:MET:HE2	1:A:3184:ALA:CA	2.48	0.40
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.54	0.40
1:A:3756:VAL:HG12	1:A:3760:ILE:HD13	2.03	0.40
1:A:4460:LEU:HD21	1:A:4465:SER:OG	2.20	0.40
1:A:4463:SER:O	1:A:4466:HIS:NE2	2.54	0.40
1:A:1776:ALA:HB3	1:A:1777:PRO:HD3	2.02	0.40
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	2.03	0.40
1:A:2248:GLU:HG2	1:A:2297:LYS:HZ2	1.85	0.40
1:A:2571:THR:H	1:A:2574:THR:HB	1.85	0.40
1:A:1554:SER:HB3	1:A:1557:ILE:HG12	2.04	0.40
1:A:1629:PHE:HE2	1:A:1699:ASN:ND2	2.19	0.40
1:A:1876:GLN:HG2	1:A:1921:HIS:CD2	2.57	0.40
1:A:2434:THR:O	1:A:2438:GLU:HG2	2.21	0.40
1:A:2590:PRO:HA	1:A:2708:PHE:O	2.21	0.40
1:A:4307:GLN:O	1:A:4311:LEU:HG	2.21	0.40
1:A:2174:GLU:HG3	1:A:2176:THR:HG23	2.03	0.40
1:A:1354:VAL:HG21	1:A:1431:LEU:HB2	2.03	0.40
1:A:1454:GLN:NE2	1:A:3671:LEU:O	2.41	0.40
1:A:2115:LYS:HE2	1:A:2127: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	3026/4646 (65%)	2968 (98%)	53 (2%)	5 (0%)	44 75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3914	ILE
1	A	4586	PRO
1	A	4028	THR
1	A	4292	LYS
1	A	4130	ILE

### 5.3.2 Protein sidechains ⓘ

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	2704/4122 (66%)	2702 (100%)	2 (0%)	92 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2295	LEU
1	A	2855	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1442	ASN
1	A	1482	ASN
1	A	1528	ASN
1	A	1646	ASN
1	A	1670	ASN
1	A	1817	HIS
1	A	1863	ASN
1	A	1876	GLN
1	A	1894	GLN

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Mol	Chain	Res	Type
1	A	1990	HIS
1	A	2051	GLN
1	A	2263	HIS
1	A	2282	HIS
1	A	2377	ASN
1	A	2482	GLN
1	A	2685	GLN
1	A	2752	ASN
1	A	2786	GLN
1	A	2834	GLN
1	A	2849	ASN
1	A	2886	GLN
1	A	3057	GLN
1	A	3139	HIS
1	A	3584	ASN
1	A	3799	GLN
1	A	3820	GLN
1	A	4012	ASN
1	A	4054	HIS
1	A	4078	ASN
1	A	4100	HIS
1	A	4174	ASN
1	A	4490	GLN
1	A	4506	ASN
1	A	4579	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 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
4	ANP	A	4704	5	29,33,33	2.51	6 (20%)	31,52,52	1.50	4 (12%)
4	ANP	A	4703	5	29,33,33	2.49	6 (20%)	31,52,52	1.45	3 (9%)
2	ADP	A	4701	-	24,29,29	0.88	0	29,45,45	1.22	2 (6%)
3	ATP	A	4702	5	28,33,33	0.72	0	34,52,52	0.58	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	A	4704	5	-	8/14/38/38	0/3/3/3
4	ANP	A	4703	5	-	4/14/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/12/32/32	0/3/3/3
3	ATP	A	4702	5	-	3/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4704	ANP	PB-O3A	8.86	1.70	1.59
4	A	4703	ANP	PB-O3A	8.83	1.70	1.59
4	A	4703	ANP	PG-N3B	6.22	1.79	1.63
4	A	4704	ANP	PG-N3B	6.17	1.79	1.63
4	A	4704	ANP	PG-O1G	4.69	1.53	1.46
4	A	4703	ANP	PG-O1G	4.66	1.53	1.46
4	A	4704	ANP	PB-O1B	2.64	1.50	1.46
4	A	4703	ANP	PB-O1B	2.61	1.50	1.46
4	A	4703	ANP	C8-N7	-2.32	1.30	1.34
4	A	4704	ANP	C8-N7	-2.29	1.30	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4703	ANP	PB-O2B	-2.23	1.50	1.56
4	A	4704	ANP	PB-O2B	-2.20	1.51	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4703	ANP	O2B-PB-O1B	4.90	120.38	109.87
4	A	4704	ANP	O2B-PB-O1B	4.81	120.18	109.87
4	A	4704	ANP	O1G-PG-N3B	-4.09	105.75	111.77
4	A	4703	ANP	O1G-PG-N3B	-3.84	106.12	111.77
2	A	4701	ADP	N3-C2-N1	-3.69	123.67	128.67
2	A	4701	ADP	C4-C5-N7	-2.57	106.62	109.34
4	A	4704	ANP	O2G-PG-O3G	2.54	114.41	107.59
4	A	4703	ANP	O2G-PG-O3G	2.47	114.23	107.59
3	A	4702	ATP	C5-C6-N6	2.32	123.85	120.31
4	A	4704	ANP	C4'-O4'-C1'	-2.09	108.01	109.92

There are no chirality outliers.

All (18) torsion outliers are listed below:

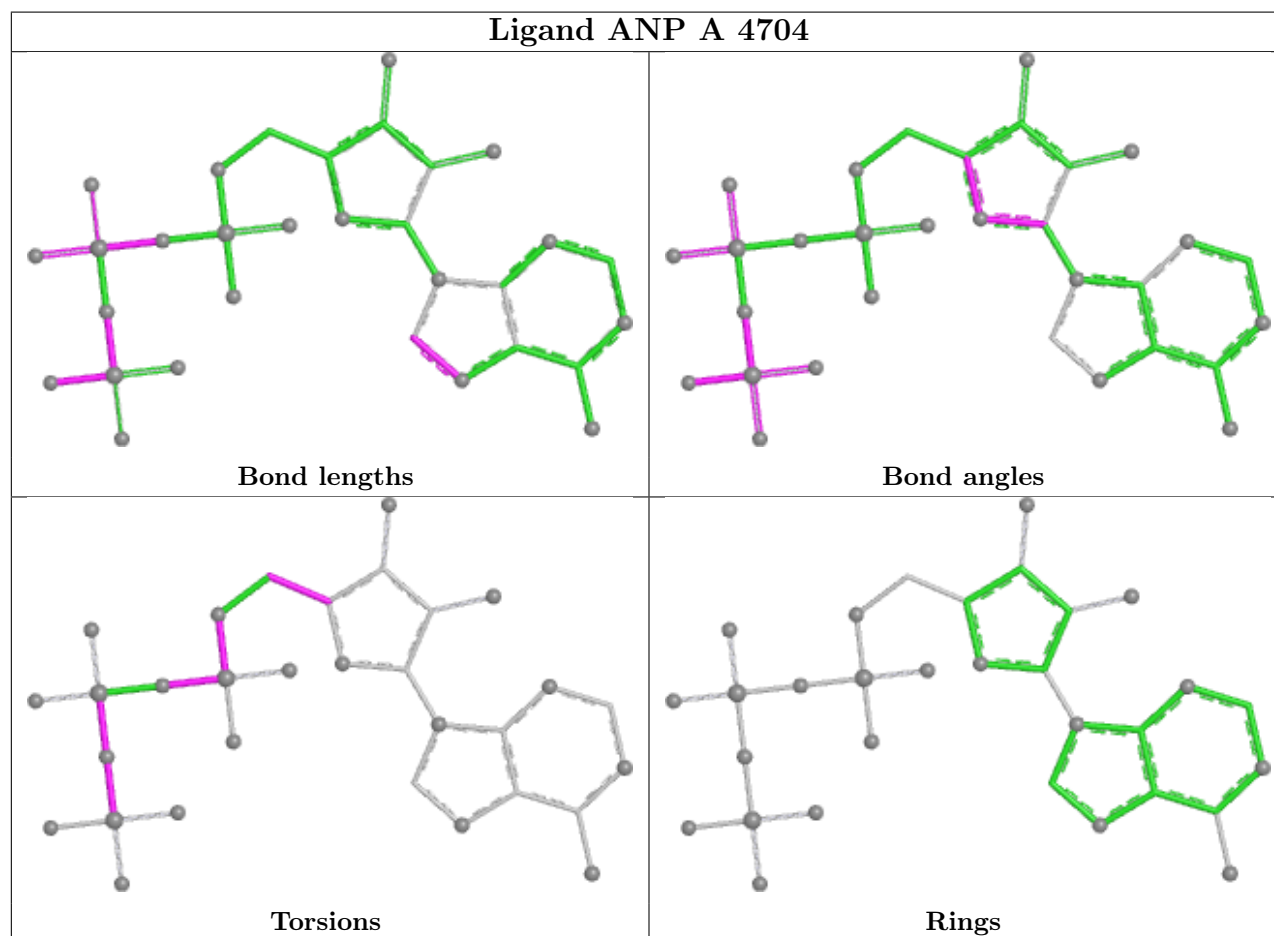
Mol	Chain	Res	Type	Atoms
4	A	4703	ANP	PB-N3B-PG-O1G
4	A	4703	ANP	PA-O3A-PB-O2B
4	A	4704	ANP	PB-N3B-PG-O1G
4	A	4704	ANP	PG-N3B-PB-O1B
4	A	4704	ANP	C5'-O5'-PA-O2A
4	A	4704	ANP	C5'-O5'-PA-O3A
4	A	4704	ANP	O4'-C4'-C5'-O5'
4	A	4704	ANP	C3'-C4'-C5'-O5'
2	A	4701	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	PB-O3B-PG-O1G
3	A	4702	ATP	PB-O3B-PG-O2G
2	A	4701	ADP	PB-O3A-PA-O2A
2	A	4701	ADP	PB-O3A-PA-O1A
4	A	4703	ANP	O4'-C4'-C5'-O5'
4	A	4704	ANP	PB-O3A-PA-O2A
4	A	4703	ANP	PA-O3A-PB-O1B
4	A	4704	ANP	PG-N3B-PB-O3A
3	A	4702	ATP	PG-O3B-PB-O2B

There are no ring outliers.

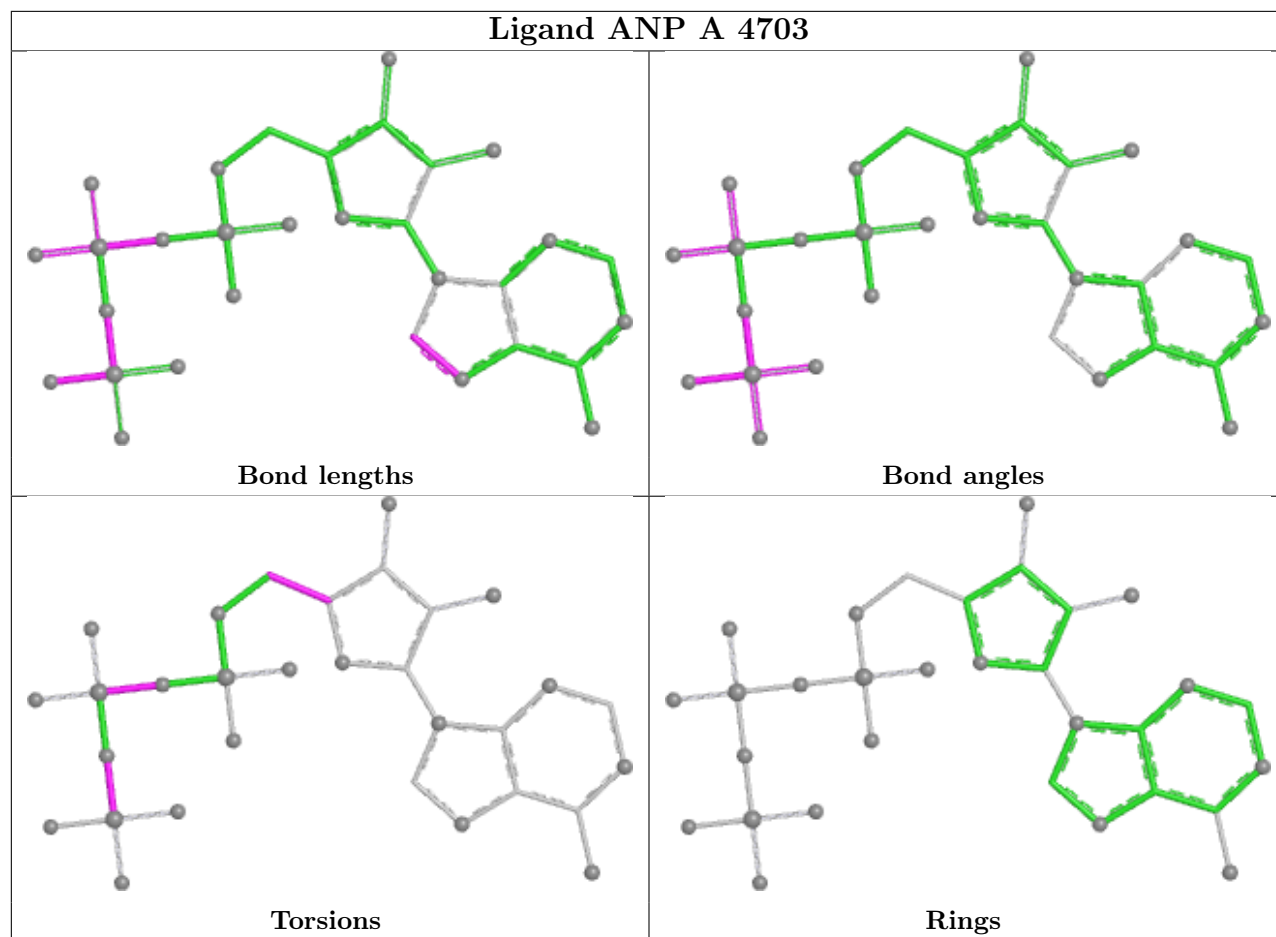
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4703	ANP	4	0
2	A	4701	ADP	2	0
3	A	4702	ATP	2	0

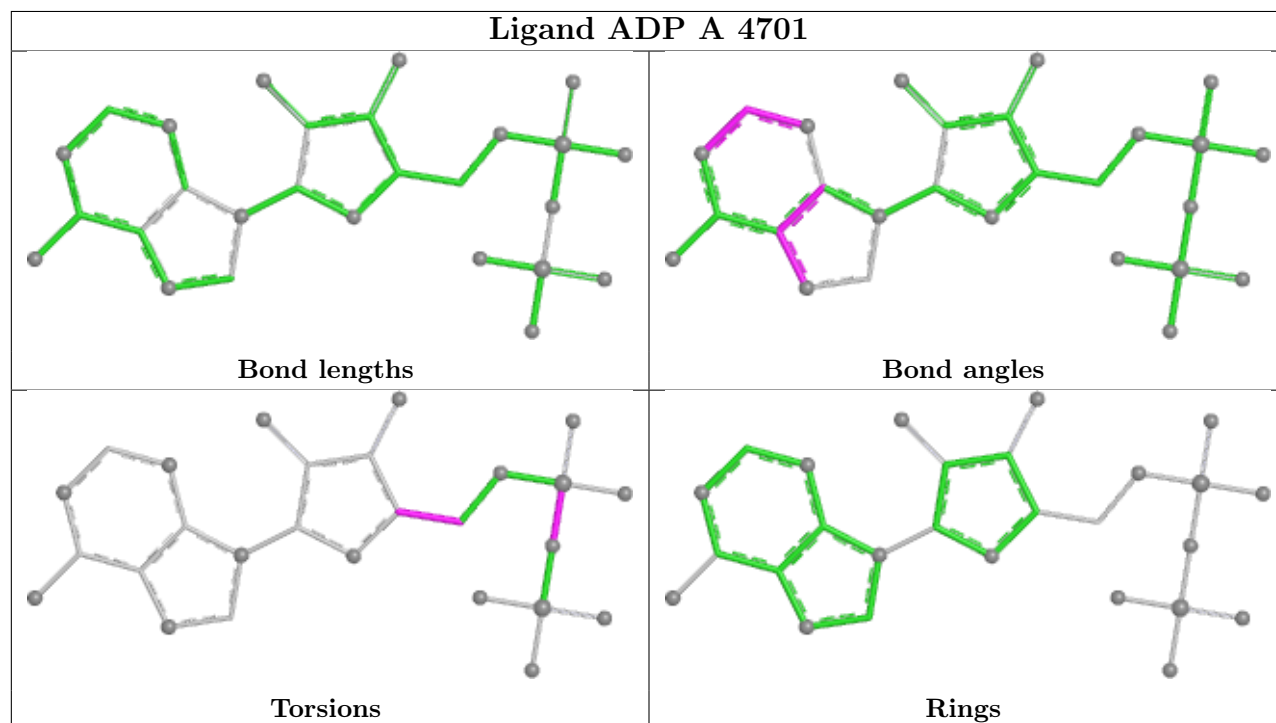
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

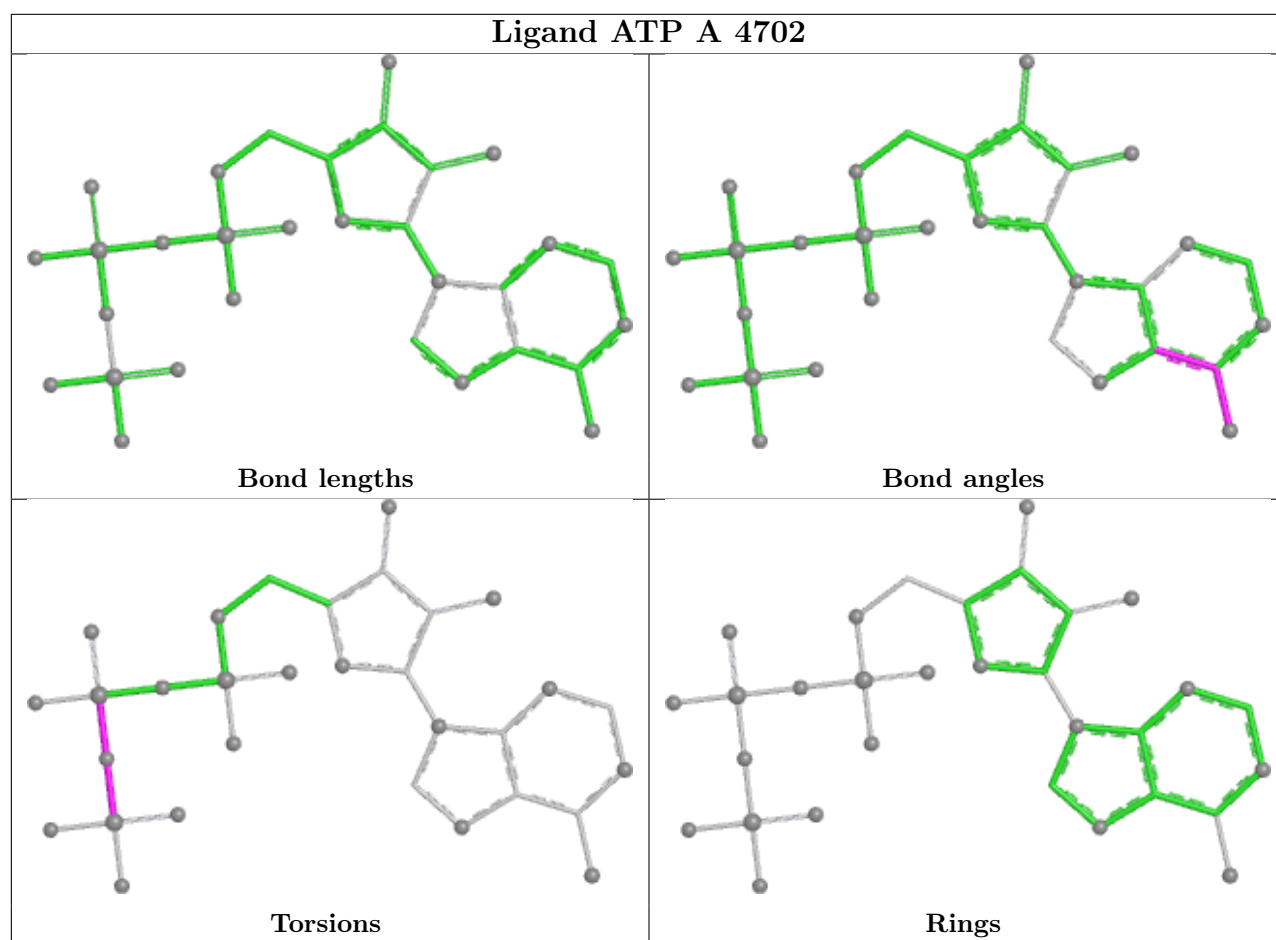


## Ligand ANP A 4703



## Ligand ADP A 4701





## 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.

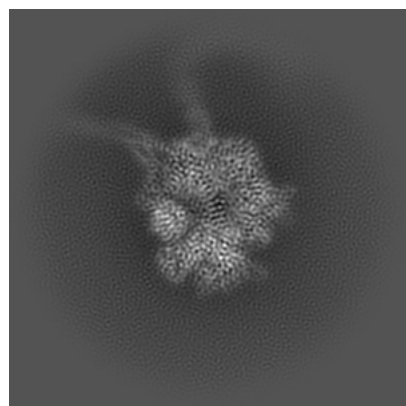
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46843. These allow visual inspection of the internal detail of the map and identification of artifacts.

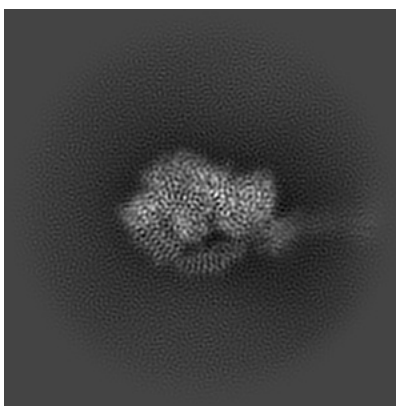
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

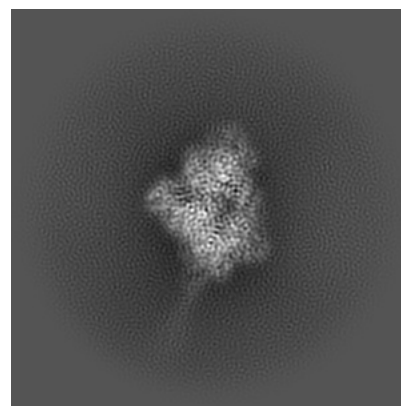
#### 6.1.1 Primary map



X

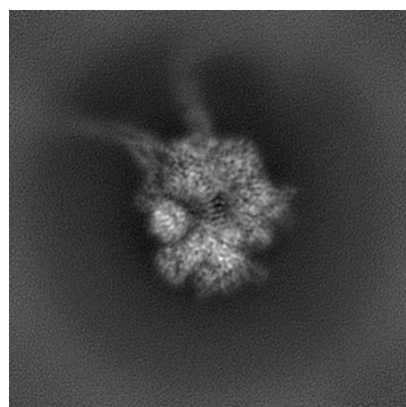


Y

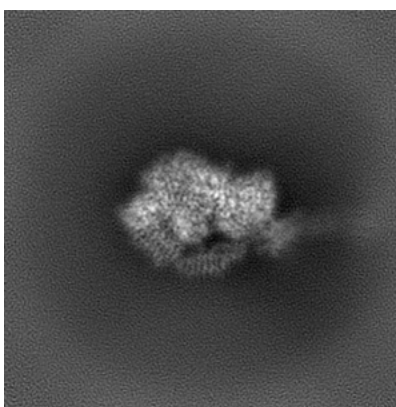


Z

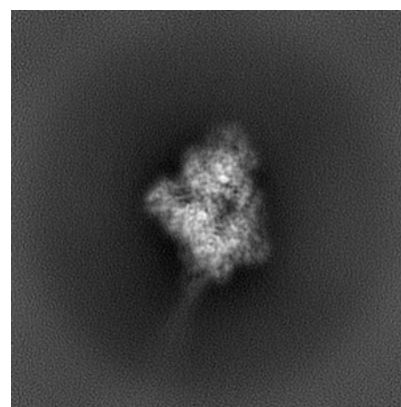
#### 6.1.2 Raw map



X



Y



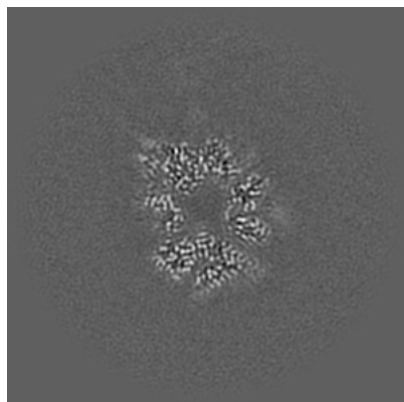
Z

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

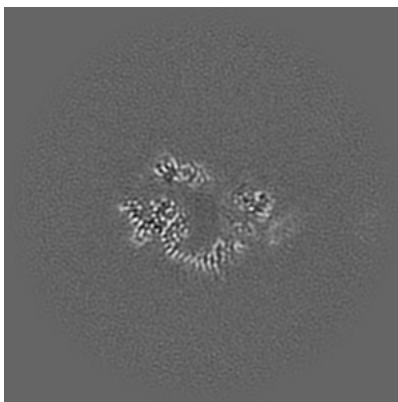


## 6.2 Central slices [i](#)

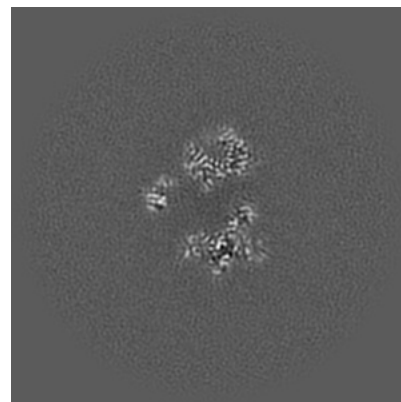
### 6.2.1 Primary map



X Index: 128

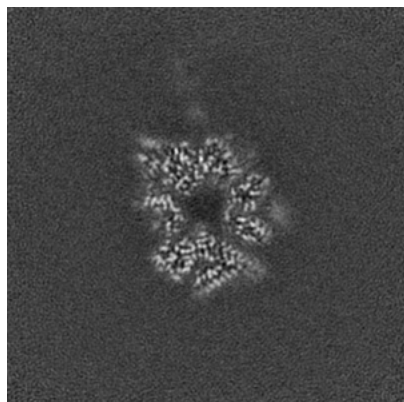


Y Index: 128

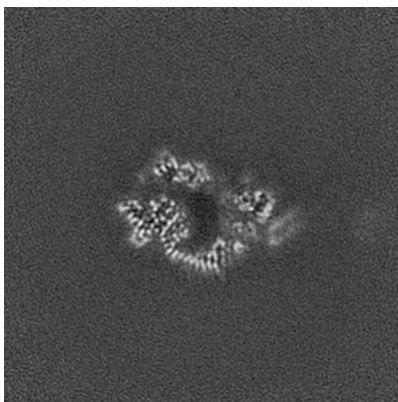


Z Index: 128

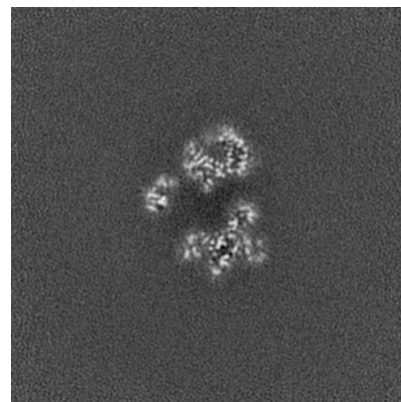
### 6.2.2 Raw map



X Index: 128



Y Index: 128

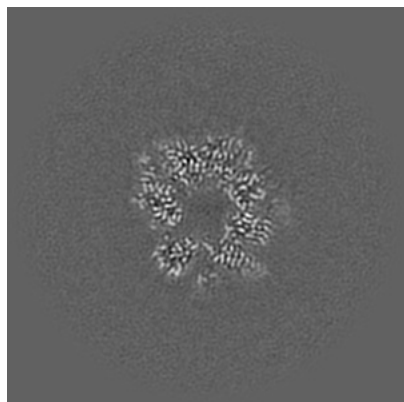


Z Index: 128

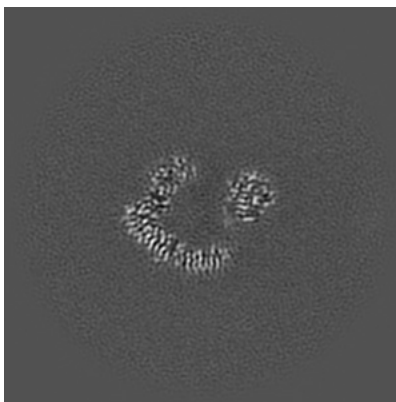
The images above show central slices of the map in three orthogonal directions.

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

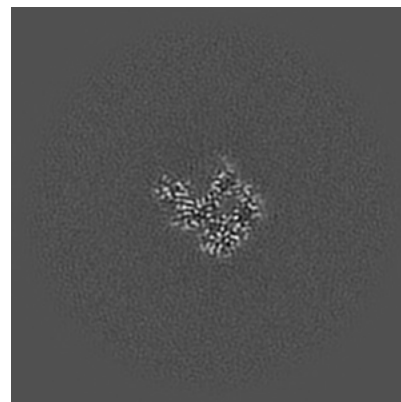
### 6.3.1 Primary map



X Index: 132

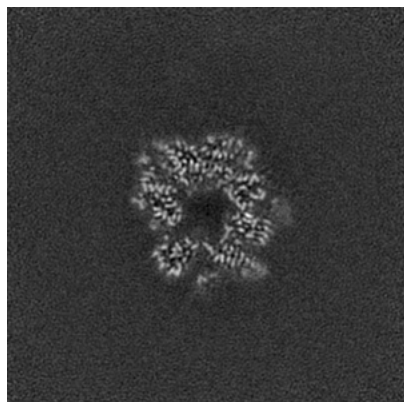


Y Index: 136

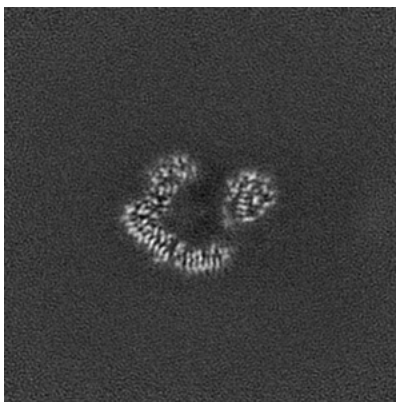


Z Index: 101

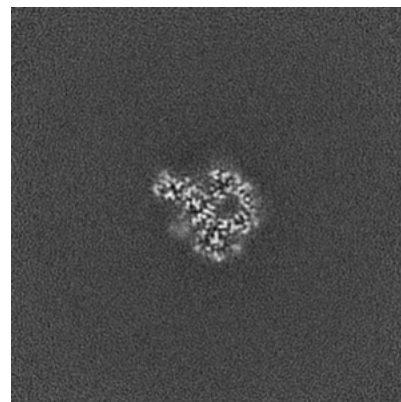
### 6.3.2 Raw map



X Index: 132



Y Index: 136

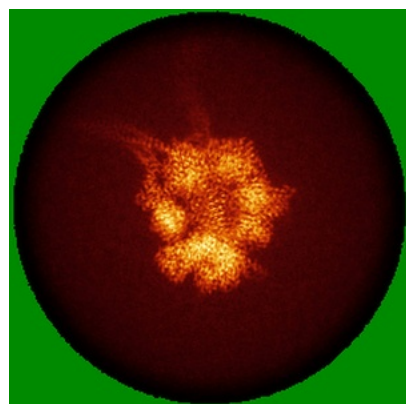


Z Index: 97

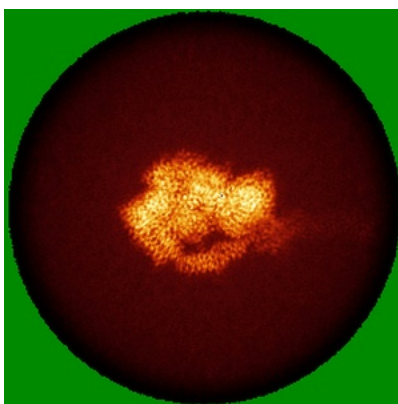
The images above show the largest variance slices of the map in three orthogonal directions.

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

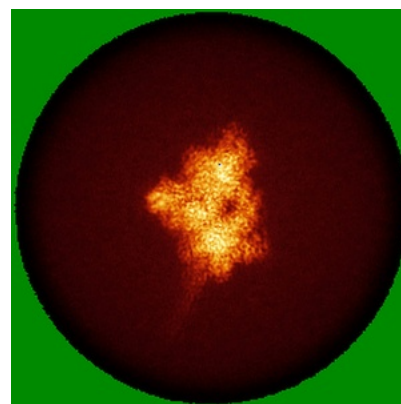
### 6.4.1 Primary map



X

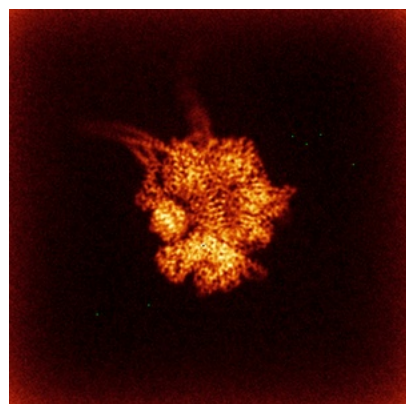


Y

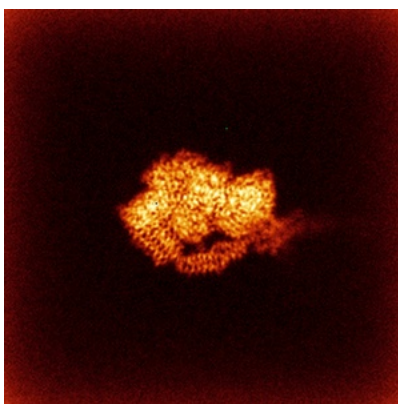


Z

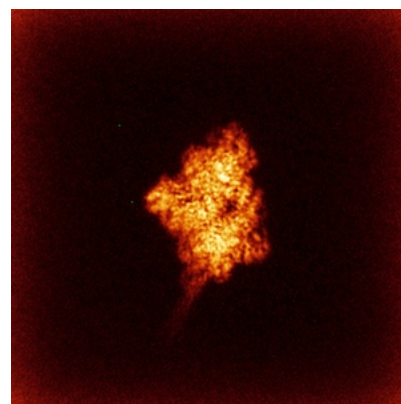
### 6.4.2 Raw map



X



Y

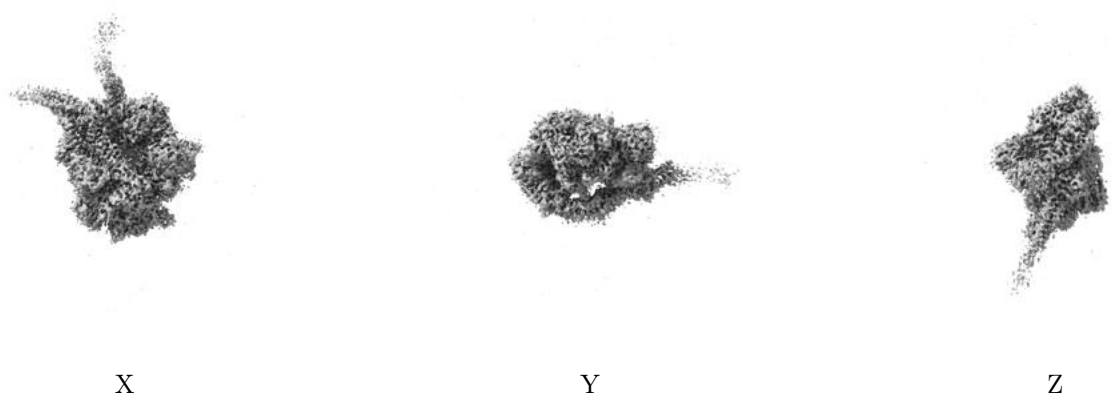


Z

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.

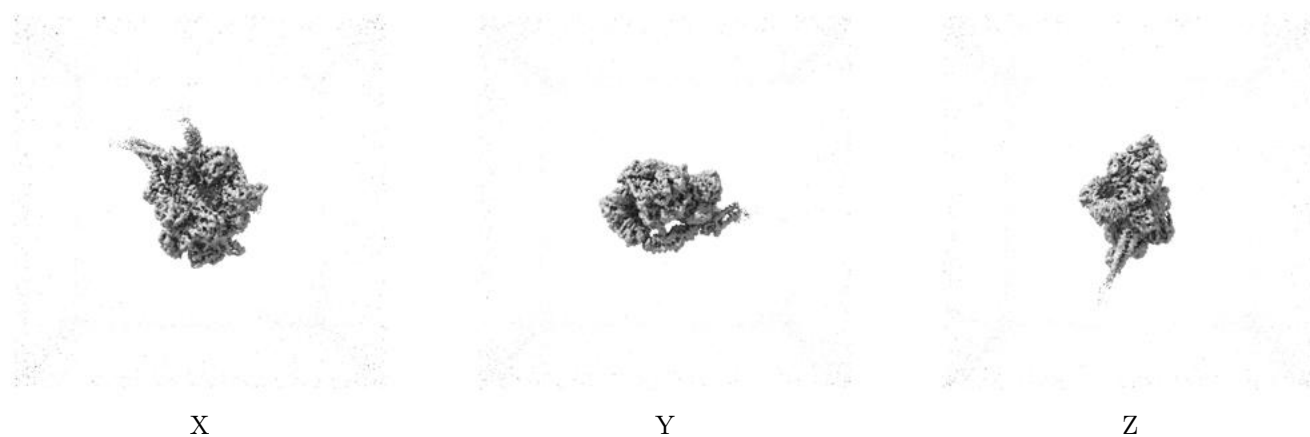
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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



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.

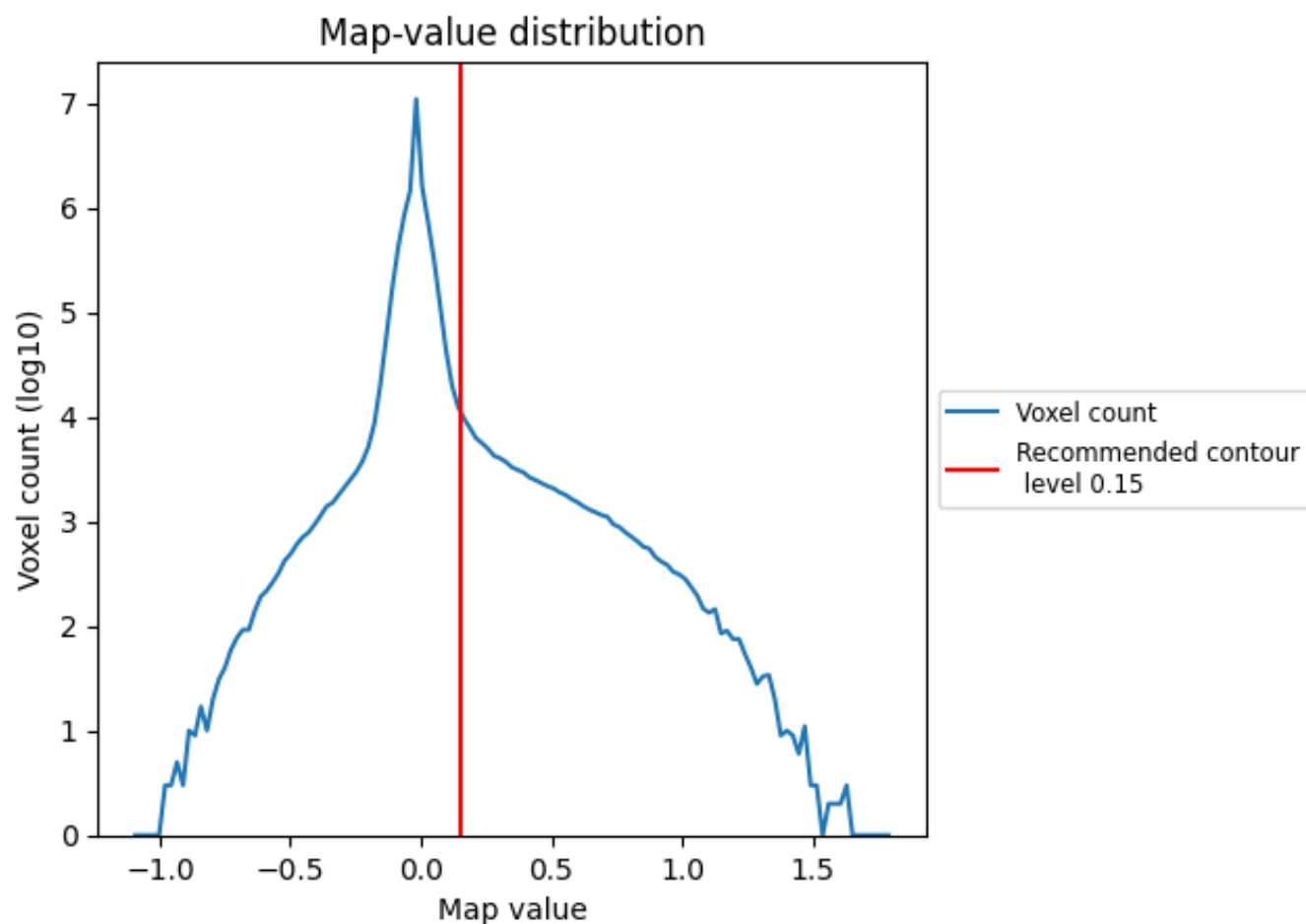
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

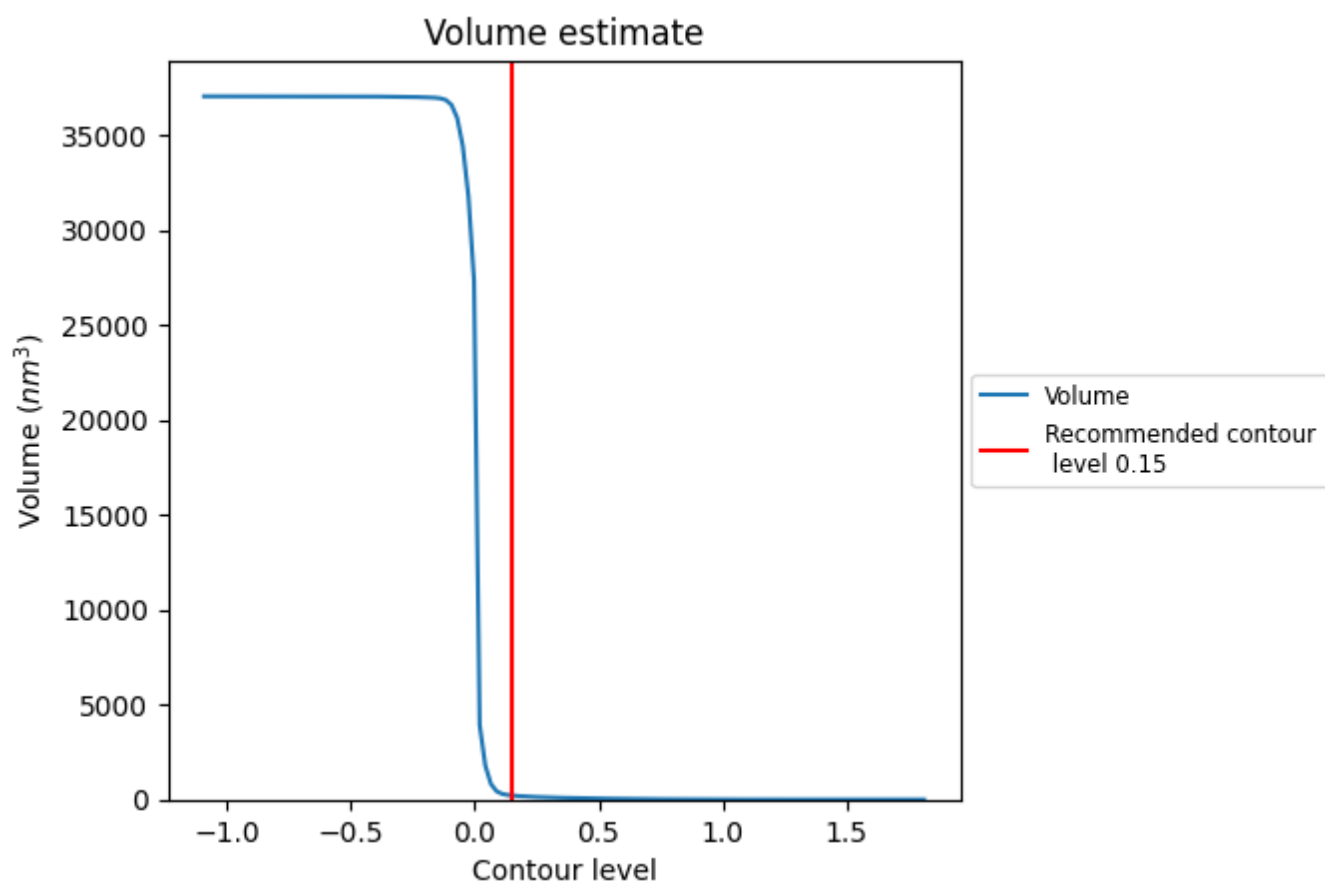
This section contains the results of statistical analysis of the map.

### 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.

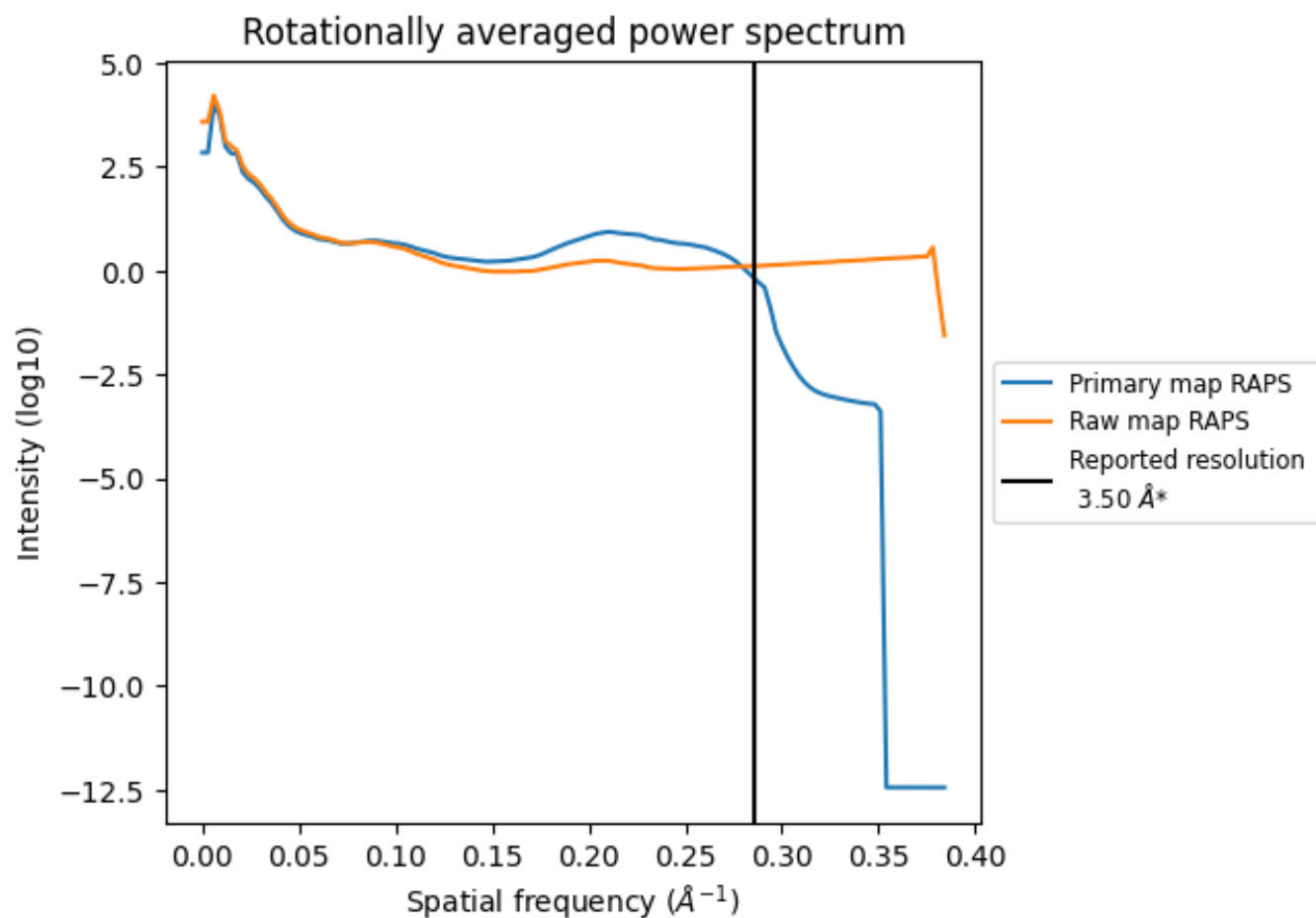
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 215 nm<sup>3</sup>; this corresponds to an approximate mass of 194 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 ⓘ



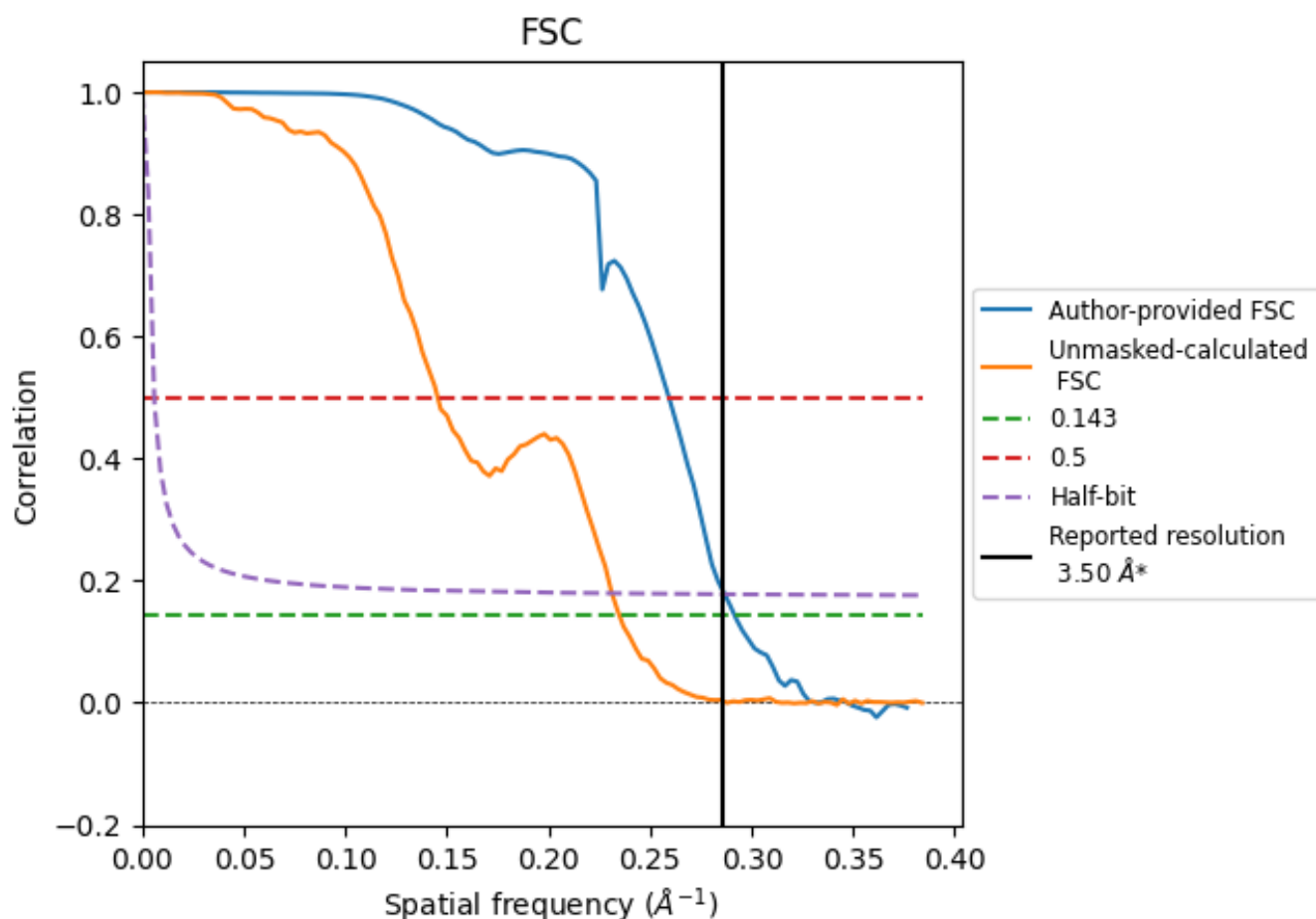
\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>



## 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  $0.286 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

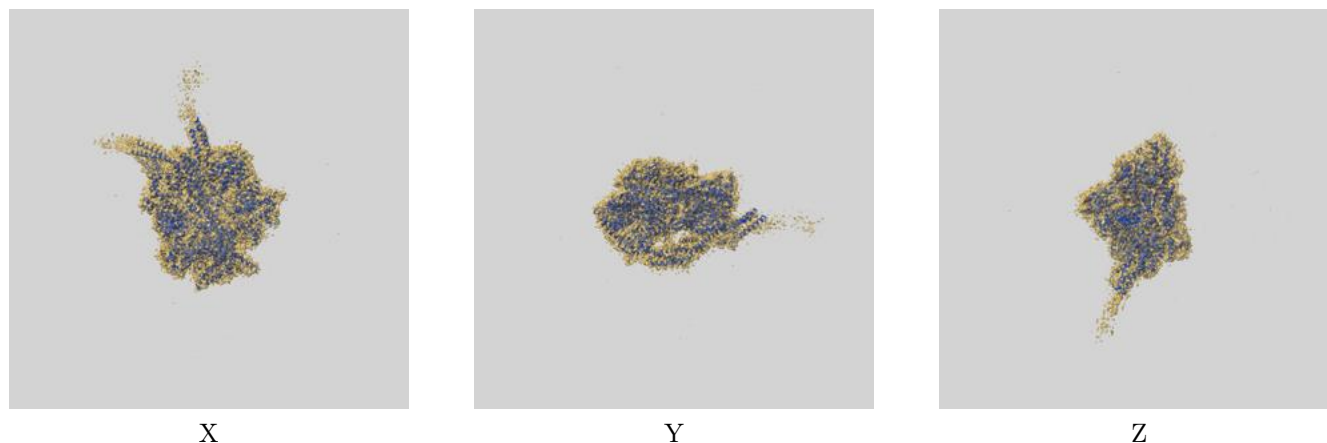
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.43	3.86	3.49
Unmasked-calculated*	4.26	6.87	4.32

\*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 4.26 differs from the reported value 3.5 by more than 10 %

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

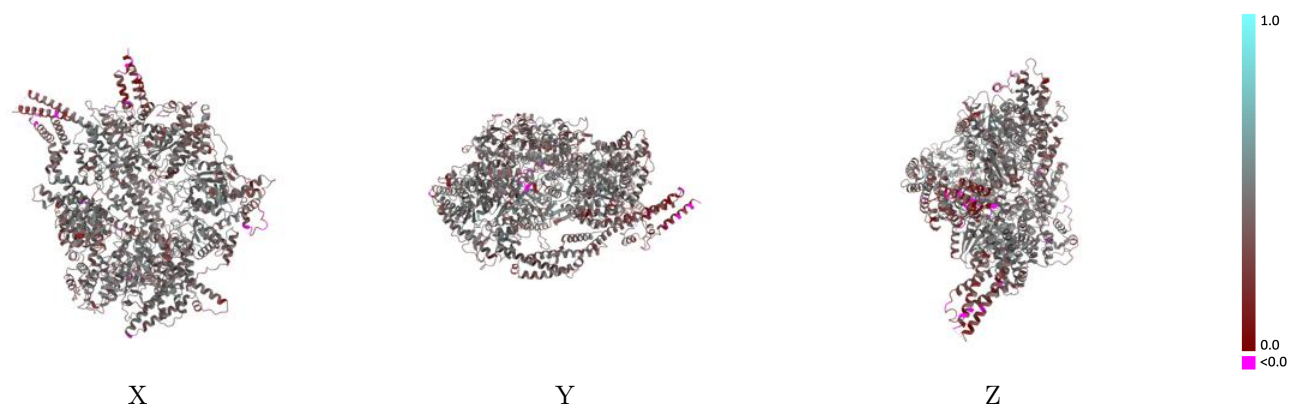
This section contains information regarding the fit between EMDB map EMD-46843 and PDB model 9DGP. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



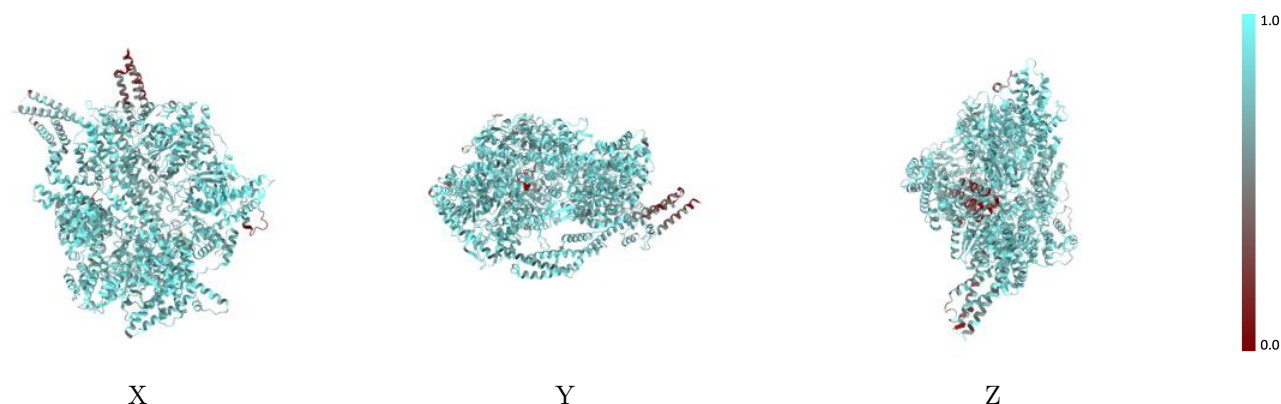
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



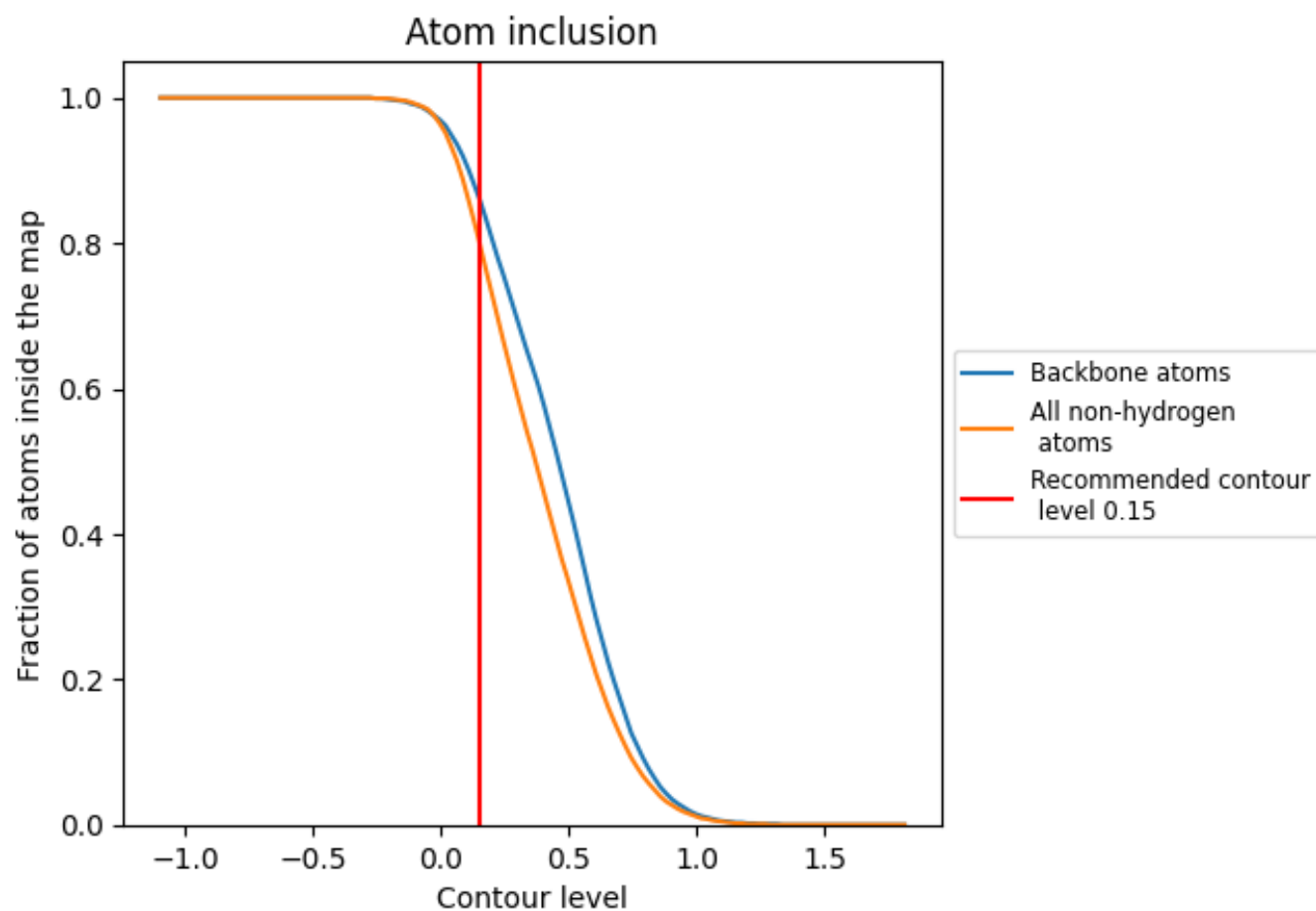
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8050	<div><div></div></div> 0.4120
A	<div><div></div></div> 0.8050	<div><div></div></div> 0.4120

