



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:40 PM UTC

PDB ID : 8PQZ / pdb_00008pqz
EMDB ID : EMD-17829
Title : Cytoplasmic dynein-1 A1/A2 motor domains bound to LIS1
Authors : Singh, K.; Lau, C.K.; Manigrasso, G.; Gassmann, R.; Carter, A.P.
Deposited on : 2023-07-12
Resolution : 5.50 Å(reported)
Based on initial model : 7Z8G

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

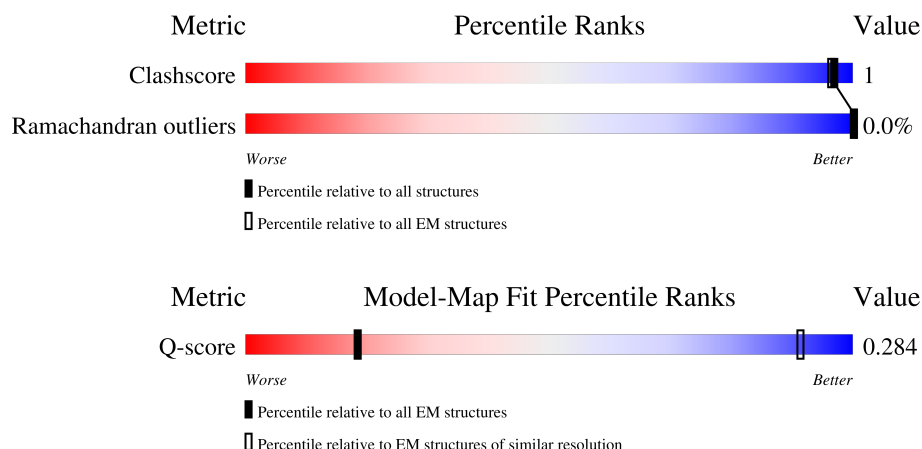
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 5.50 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.



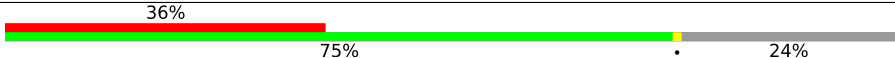
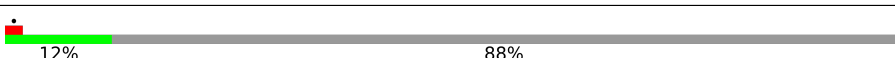
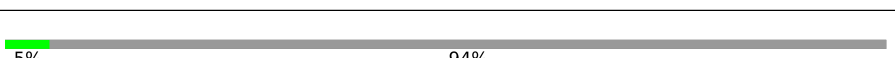
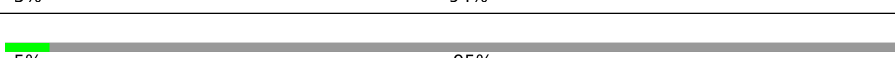
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	520 (5.00 - 6.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	J	4646	
2	B	410	
2	C	410	
2	D	410	

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Mol	Chain	Length	Quality of chain
2	E	410	 18% 82%
2	K	410	 52% 75% 24%
2	L	410	 36% 75% 24%
3	F	1281	 12% 88%
3	G	1281	 12% 88%
4	H	612	 5% 94%
4	I	612	 5% 95%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 37643 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
1	A	2892	Total	C	N	O	0	0
			14326	8542	2892	2892		
1	J	2892	Total	C	N	O	0	0
			14326	8542	2892	2892		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1567	GLU	ARG	engineered mutation	UNP Q14204
A	1610	GLU	LYS	engineered mutation	UNP Q14204
J	1567	GLU	ARG	engineered mutation	UNP Q14204
J	1610	GLU	LYS	engineered mutation	UNP Q14204

- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	313	Total	C	N	O	0	0
			1547	921	313	313		
2	C	313	Total	C	N	O	0	0
			1547	921	313	313		
2	D	75	Total	C	N	O	0	0
			373	223	75	75		
2	E	75	Total	C	N	O	0	0
			373	223	75	75		
2	K	313	Total	C	N	O	0	0
			1547	921	313	313		
2	L	313	Total	C	N	O	0	0
			1547	921	313	313		

- Molecule 3 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	150	Total	C	N	O	0	0
			747	447	150	150		
3	G	150	Total	C	N	O	0	0
			747	447	150	150		

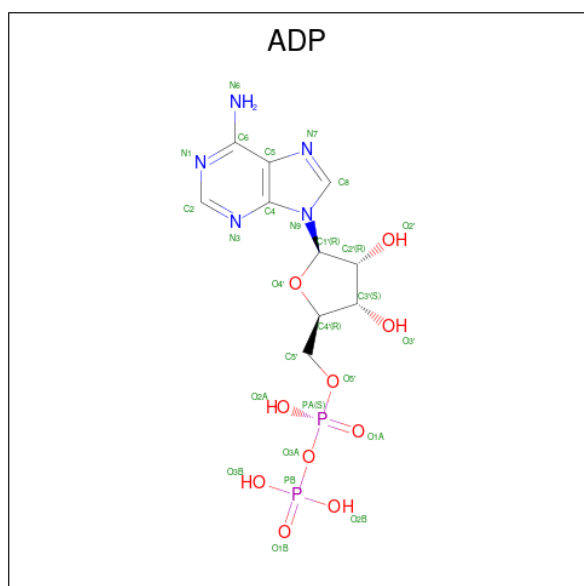
- Molecule 4 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	34	Total	C	N	O	0	0
			170	102	34	34		
4	I	33	Total	C	N	O	0	0
			165	99	33	33		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	484	SER	THR	conflict	UNP Q13409
H	499	GLY	ASP	conflict	UNP Q13409
I	484	SER	THR	conflict	UNP Q13409
I	499	GLY	ASP	conflict	UNP Q13409

- Molecule 5 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
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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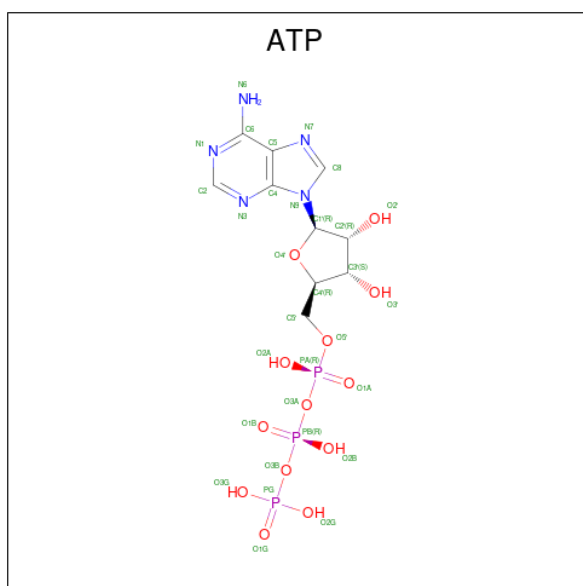
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Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	Mg	0
			2	2	
6	J	2	Total	Mg	0
			2	2	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

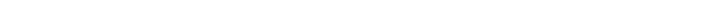


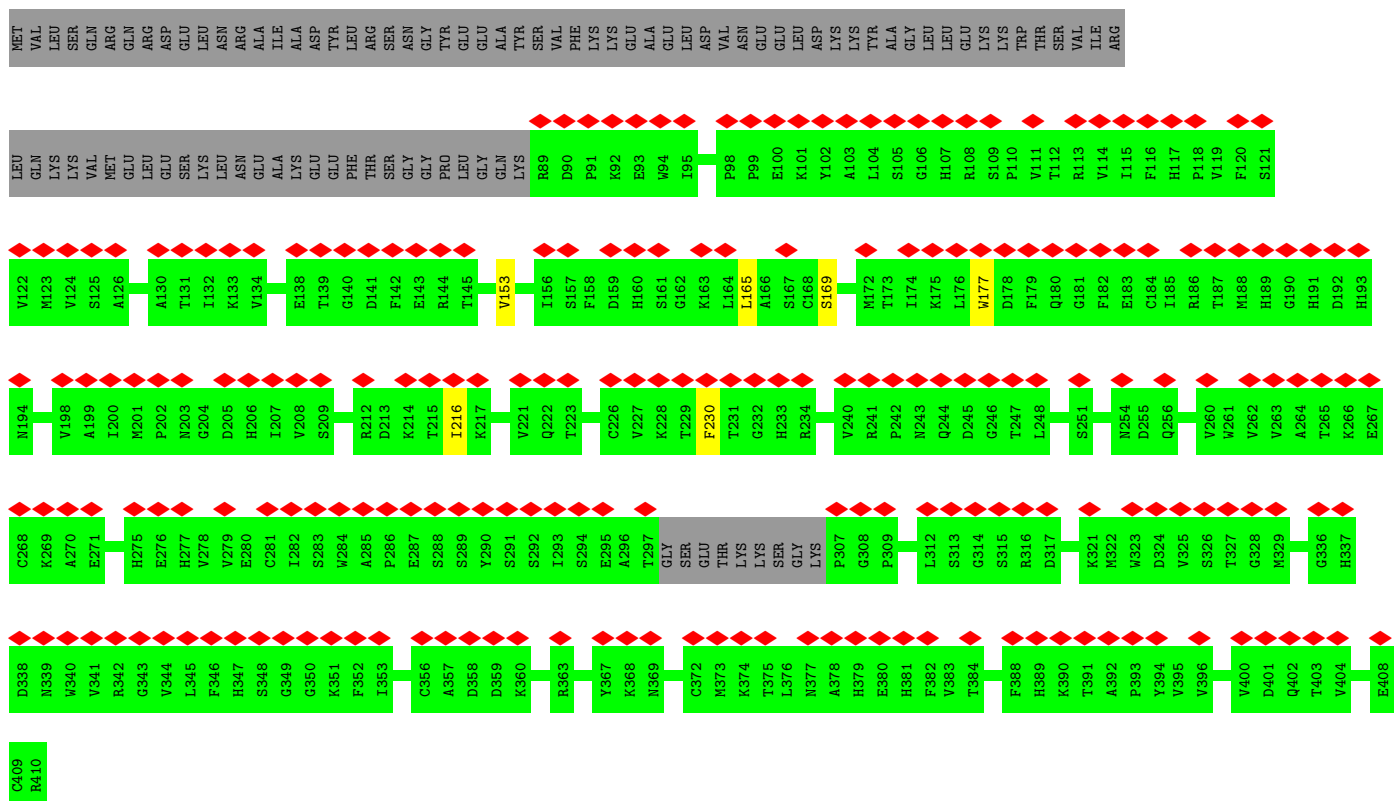


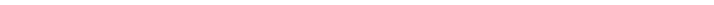


N4463	V4456	K4457	G4458	R4462	H4466	P4470	A4471	G4472	V4475	K4487	Q4488	L4489	Q4490	M4491	L4494	A4495	A4496	A4497	S4498	GLY	GLY	ALA	K4502	E4503	L4504	K4505	M4506	L4511	G4512	G4513	L4514	F4515	Y4527	V4528	A4529	Q4530	A4531	M4532	S4533	N4534	S4535	L4536	E4537	V4545	THR	THR	SER	GLN	GLY					
D4279	S4280	E4281	F4282	K4283	L4284	A4285	C4286	K4287	V4288	D4289	G4290	H4291	K4292	D4298	R4302	E4303	E4304	F4305	D4314	N4326	A4327	E4328	K4329	V4330	T4333	G4336	V4337	D4338	S4341	L4344	K4345	M4346	Q4347	M4348	L4349	E4350	ASP	GLU	ASP	ASP	LEU	ALA	TYR	ALA	THR	GLU	GLU	LYS	LYS	THR	ARG			
THR	ASP	SER	THR	SER	ASP	GLY	ARG	PRO	ALA	TRP	MET	ARG	T4379	N4386	L4390	T4394	L4395	S4396	H4397	L4398	K4399	R4400	T4401	VAL	E4403	M4404	V4417	K4418	M4419	G4420	A4421	K4422	L4423	L4424	Q4425	D4426	V4427	R4428	Q4429	D4430	L4431	A4432	D4433	V4434	V4435	Q4436	V4437	G4440	K4441	K4442	K4443	M4446		
V4146	F4147	E4148	S4162	S4163	Q4191	L4199	S4210	D4217	D4224	T4225	A4227	K4228	G4229	N4232	P4235	D4236	K4237	L4238	P4239	N4240	K4244	T4245	L4246	M4247	A4248	Q4249	S4250	T4251	Y4252	G4253	G4254	R4255	V4256	D4257	N4258	A4259	F4260	D4261	Q4262	L4265	N4266	L4269	E4270	R4276	S4277	F4278								
Q3994	R3997	P3998	A4003	T4011	N4012	E4015	S4016	F4017	M4018	S4019	E4034	V4046	P4047	V4055	E4056	D4057	L4058	E4061	Q4062	N4063	I4066	A4080	D4081	H4100	L4101	A4102	P4103	G4104	K4111	A4120	F4125	M4128	E4129	I4130	M4131	P4132	K4133	R4140	A4141	G4142	R4143													
N3912	E3913	I3914	V3915	L3916	S3917	A3918	G3919	S3920	T3921	P3922	R3923	I3924	Q3925	G3926	L3927	T3928	V3929	E3930	Q3931	A3932	C3940	L3941	K3945	L3946	L3947	I3948	A3949	K3950	V3951	Q3952	A3953	D3954	E3955	Q3956	F3957	G3958	I3959	D3962	S3963	S3964	S3965	P3966	E3967	Q3968	V3970	P3971	W3974	SER	GLU	GLU	T3978	P3979	A3980	T3981
S3817	Q3820	I3821	H3822	F3823	L3824	Y3825	L3829	Q3830	L3833	H3843	P3844	H3845	L3846	LYS	GLY	V3849	T3850	D3851	H3852	T3853	Q3854	A3867	A3872	R3873	G3874	M3875	L3876	H3877	Q3878	D3879	H3880	A3884	M3885	K3891	L3892	K3893	S3894	T3895	VAL	G3897	T3900	Y3901	D3902	A3903	H3907	F3908	L3909	R3910	G3911					
T3810	R3611	L3615	D3616	D3617	Q3636	D3637	V3638	E3639	S3640	Y3641	D3642	P3643	G3658	T3663	L3664	G3665	D3666	Q3667	D3668	I3669	D3670	L3671	S3672	P3673	L3679	R3682	D3683	P3684	T3685	V3686	E3687	F3688	P3689	P3690	C3693	S3694	N3700	F3701	T3702	V3703	T3704	Q3711	C3712	L3713	N3714	D3723	V3724	D3725	E3726					
K3497	N3498	S3501	A3504	S3510	A3511	A3512	F3513	I3514	A3515	Y3516	A3517	G3518	Y3519	F3520	D3521	R3525	Q3537	R3544	T3545	D3546	I3547	A3548	R3549	T3550	E3551	Y3552	L3553	S3554	N3555	A3556	D3557	E3558	A3564	S3565	S3566	C3573	A3577	F3583	N3584	R3585	L3588	V3489	E3487	E3490	K3491	S3492	S3493	E3494	T3495	F3496				
ILE	ARG	ASP	GLU	ALA	ILE	ILE	TYR	LYS	GLY	E3450	Y3451	A3452	V3453	L3454	I3455	S3456	E3457	A3458	Q3459	A3460	I3461	K3462	A3463	D3464	L3465	A3466	A3467	R3549	LEU	ASN	PHE	SER	ASP	ASP	ALA	ILE	ARG	GLU	LYS	MET	GLN	LYS	ALA	ASN	TYR	GLN	VAL	GLU	ASN	PRO	MET			
TYR	ASN	TYR	GLU	ALA	LEU	VAL	ASN	ARG	ALA	ALA	ALA	TYR	LYS	TRP	ALA	ILE	GLN	ARG	SER	ASN	ILE	ILE	MET	ARG	GLU	ASN	PHE	GLU	LEU	GLN	GLU	LYS	LEU	ASP	ASP	ALA	ILE	ARG	GLU	LYS	MET	GLN	LYS	ALA	ASN	TYR	GLN	VAL	GLU	ASN	PRO	MET		

[illegible]

Chain K:  52% 75% 24%



Chain L:  36% 75% 24%



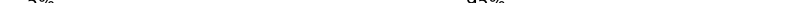
• Molecule 3: Dynactin subunit 1





[illegible]

- Molecule 4: Cytoplasmic dynein 1 intermediate chain 2

Chain I:  5% 95%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31898	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0086	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.20	0/14312	0.50	3/19934 (0.0%)
1	J	0.17	0/14312	0.46	1/19934 (0.0%)
2	B	0.17	0/1545	0.48	0/2149
2	C	0.17	0/1545	0.48	0/2149
2	D	0.21	0/372	0.55	0/518
2	E	0.17	0/372	0.47	0/518
2	K	0.18	0/1545	0.48	0/2149
2	L	0.16	0/1545	0.46	0/2149
3	F	0.21	0/746	0.45	0/1041
3	G	0.27	0/746	0.53	1/1041 (0.1%)
4	H	0.35	0/169	1.07	3/235 (1.3%)
4	I	0.27	0/164	0.75	0/228
All	All	0.19	0/37373	0.48	8/52045 (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	J	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	16	GLN	N-CA-CB	6.41	120.85	110.40
3	G	498	GLU	N-CA-CB	5.79	119.25	110.28
1	A	3823	PHE	N-CA-C	5.58	119.39	112.47
1	J	2344	GLU	N-CA-CB	5.47	118.06	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2685	GLN	CA-C-N	-5.18	113.00	122.38
1	A	2685	GLN	C-N-CA	-5.18	113.00	122.38
4	H	15	LYS	CA-C-N	-5.05	112.31	121.14
4	H	15	LYS	C-N-CA	-5.05	112.31	121.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	2343	PHE	Peptide

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	14326	0	6331	7	0
1	J	14326	0	6331	12	0
2	B	1547	0	676	5	0
2	C	1547	0	676	8	0
2	D	373	0	172	0	0
2	E	373	0	172	0	0
2	K	1547	0	676	3	0
2	L	1547	0	676	3	0
3	F	747	0	344	0	0
3	G	747	0	344	0	0
4	H	170	0	73	0	0
4	I	165	0	71	0	0
5	A	81	0	36	1	0
5	J	81	0	36	0	0
6	A	2	0	0	0	0
6	J	2	0	0	0	0
7	A	31	0	12	1	0
7	J	31	0	12	0	0
All	All	37643	0	16638	38	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 1.

All (38) 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)
2:C:219:TRP:HA	2:C:226:CYS:HA	1.85	0.58
1:A:1880:VAL:H	5:A:4801:ADP:HN62	1.52	0.56
2:L:208:VAL:HA	2:L:218:MET:HA	1.88	0.55
1:J:1479:ASN:HA	1:J:1485:ARG:HA	1.91	0.52
1:J:2639:CYS:HA	1:J:2652:PRO:HA	1.90	0.51
2:B:216:ILE:O	2:B:230:PHE:N	2.43	0.51
1:J:4557:SER:N	1:J:4590:LEU:O	2.45	0.50
1:A:2538:GLU:O	1:A:2546:SER:N	2.43	0.49
2:B:92:LYS:HA	2:B:349:GLY:HA3	1.95	0.49
2:L:196:SER:H	2:L:211:SER:HA	1.78	0.48
2:C:249:ILE:O	2:C:261:TRP:N	2.45	0.48
1:J:3475:SER:O	1:J:3479:LEU:N	2.43	0.48
2:C:242:PRO:HA	2:C:249:ILE:HA	1.95	0.48
2:K:165:LEU:N	2:K:177:TRP:O	2.45	0.47
2:K:216:ILE:O	2:K:230:PHE:N	2.48	0.47
1:A:4557:SER:N	1:A:4590:LEU:O	2.48	0.47
2:K:153:VAL:HA	2:K:169:SER:HA	1.99	0.45
1:A:3083:PRO:O	1:A:3087:ASN:N	2.50	0.44
2:C:96:PRO:HA	2:C:409:CYS:HA	1.99	0.44
2:C:260:VAL:O	2:C:269:LYS:N	2.50	0.44
2:C:218:MET:O	2:C:227:VAL:N	2.51	0.44
2:C:238:ARG:H	2:C:253:SER:HA	1.83	0.44
1:A:2230:LYS:N	7:A:4803:ATP:O2B	2.50	0.44
1:A:4286:CYS:HA	1:A:4293:ASP:HA	1.98	0.43
1:J:1885:THR:O	1:J:1889:TYR:N	2.48	0.43
1:J:4417:VAL:O	1:J:4421:ALA:N	2.51	0.43
2:C:220:GLU:N	2:C:225:TYR:O	2.49	0.43
1:J:1708:GLU:O	1:J:1712:THR:N	2.48	0.42
1:J:2324:LEU:HA	1:J:2334:SER:HA	2.01	0.42
2:B:322:MET:O	2:B:331:LEU:N	2.52	0.42
1:J:4567:GLY:N	1:J:4581:ILE:O	2.50	0.42
1:J:2593:LEU:O	1:J:2712:CYS:N	2.53	0.41
2:B:101:LYS:N	2:B:406:VAL:O	2.51	0.41
2:B:282:ILE:HA	2:B:313:SER:HA	2.02	0.41
1:J:3154:LEU:HA	1:J:3157:ALA:HB3	2.03	0.41
2:L:279:VAL:HA	2:L:315:SER:HA	2.03	0.41
1:A:1905:PHE:O	1:A:2041:MET:N	2.52	0.41
1:J:2493:TYR:O	1:J:2497:ALA:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2864/4646 (62%)	2762 (96%)	101 (4%)	1 (0%)	100	100
1	J	2864/4646 (62%)	2773 (97%)	91 (3%)	0	100	100
2	B	309/410 (75%)	293 (95%)	16 (5%)	0	100	100
2	C	309/410 (75%)	291 (94%)	18 (6%)	0	100	100
2	D	73/410 (18%)	72 (99%)	1 (1%)	0	100	100
2	E	73/410 (18%)	73 (100%)	0	0	100	100
2	K	309/410 (75%)	294 (95%)	15 (5%)	0	100	100
2	L	309/410 (75%)	293 (95%)	16 (5%)	0	100	100
3	F	148/1281 (12%)	148 (100%)	0	0	100	100
3	G	148/1281 (12%)	148 (100%)	0	0	100	100
4	H	32/612 (5%)	32 (100%)	0	0	100	100
4	I	31/612 (5%)	31 (100%)	0	0	100	100
All	All	7469/15538 (48%)	7210 (96%)	258 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1965	GLU

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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$
5	ADP	J	4801	6	28,29,29	1.41	4 (14%)	43,45,45	1.86	9 (20%)
7	ATP	J	4803	6	32,33,33	0.40	0	48,52,52	0.44	0
5	ADP	A	4806	-	28,29,29	1.41	4 (14%)	43,45,45	1.86	10 (23%)
5	ADP	J	4806	-	28,29,29	1.41	4 (14%)	43,45,45	1.86	9 (20%)
5	ADP	A	4805	-	28,29,29	1.43	5 (17%)	43,45,45	2.02	9 (20%)
5	ADP	J	4805	-	28,29,29	1.41	5 (17%)	43,45,45	1.86	10 (23%)
7	ATP	A	4803	6	32,33,33	0.30	0	48,52,52	0.40	0
5	ADP	A	4801	6	28,29,29	1.42	4 (14%)	43,45,45	1.83	7 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	J	4801	6	-	2/16/32/32	0/3/3/3
7	ATP	J	4803	6	-	4/22/38/38	0/3/3/3
5	ADP	A	4806	-	-	3/16/32/32	0/3/3/3
5	ADP	J	4806	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	A	4805	-	-	2/16/32/32	0/3/3/3
5	ADP	J	4805	-	-	0/16/32/32	0/3/3/3
7	ATP	A	4803	6	-	3/22/38/38	0/3/3/3
5	ADP	A	4801	6	-	4/16/32/32	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4805	ADP	C5-C4	4.86	1.47	1.39
5	A	4806	ADP	C5-C4	4.74	1.47	1.39
5	J	4806	ADP	C5-C4	4.74	1.47	1.39
5	J	4801	ADP	C5-C4	4.71	1.47	1.39
5	J	4805	ADP	C5-C4	4.71	1.47	1.39
5	A	4801	ADP	C5-C4	4.68	1.47	1.39
5	A	4805	ADP	C5-C6	2.74	1.48	1.41
5	J	4806	ADP	C5-C6	2.70	1.48	1.41
5	A	4801	ADP	C5-C6	2.70	1.48	1.41
5	J	4801	ADP	C5-C6	2.69	1.48	1.41
5	A	4806	ADP	C5-C6	2.67	1.48	1.41
5	J	4805	ADP	C5-C6	2.64	1.48	1.41
5	A	4801	ADP	C5-N7	-2.41	1.34	1.39
5	A	4805	ADP	C5-N7	-2.36	1.34	1.39
5	J	4806	ADP	C8-N7	2.35	1.36	1.31
5	A	4806	ADP	C5-N7	-2.33	1.34	1.39
5	A	4806	ADP	C8-N7	2.31	1.36	1.31
5	J	4801	ADP	C8-N7	2.29	1.36	1.31
5	J	4805	ADP	C5-N7	-2.29	1.34	1.39
5	J	4801	ADP	C5-N7	-2.28	1.34	1.39
5	J	4806	ADP	C5-N7	-2.27	1.34	1.39
5	J	4805	ADP	C8-N7	2.25	1.36	1.31
5	A	4801	ADP	C8-N7	2.24	1.36	1.31
5	A	4805	ADP	C8-N7	2.20	1.35	1.31
5	A	4805	ADP	PA-O3A	2.19	1.61	1.59
5	J	4805	ADP	PA-O3A	2.02	1.61	1.59

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	4805	ADP	C5-C4-N3	-6.94	117.17	126.72
5	A	4801	ADP	C5-C4-N3	-6.22	118.15	126.72
5	J	4806	ADP	C5-C4-N3	-5.98	118.49	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	4801	ADP	C5-C4-N3	-5.90	118.59	126.72
5	A	4806	ADP	C5-C4-N3	-5.85	118.66	126.72
5	A	4805	ADP	N3-C4-N9	5.82	137.06	127.17
5	J	4805	ADP	C5-C4-N3	-5.72	118.84	126.72
5	J	4805	ADP	N3-C4-N9	4.80	135.33	127.17
5	J	4801	ADP	N3-C4-N9	4.75	135.24	127.17
5	A	4801	ADP	N3-C4-N9	4.73	135.22	127.17
5	A	4806	ADP	N3-C4-N9	4.71	135.18	127.17
5	J	4806	ADP	N3-C4-N9	4.70	135.17	127.17
5	A	4805	ADP	C2-N3-C4	4.28	122.29	111.83
5	A	4801	ADP	C2-N3-C4	3.96	121.51	111.83
5	J	4806	ADP	C2-N3-C4	3.85	121.23	111.83
5	J	4805	ADP	C2-N3-C4	3.83	121.18	111.83
5	J	4805	ADP	N3-C2-N1	-3.82	122.81	128.58
5	A	4806	ADP	C2-N3-C4	3.78	121.06	111.83
5	J	4801	ADP	C2-N3-C4	3.69	120.85	111.83
5	A	4805	ADP	N3-C2-N1	-3.55	123.20	128.58
5	J	4806	ADP	C4-C5-N7	-3.46	106.62	110.58
5	A	4801	ADP	C4-C5-N7	-3.44	106.65	110.58
5	A	4806	ADP	N3-C2-N1	-3.42	123.40	128.58
5	J	4806	ADP	N3-C2-N1	-3.42	123.41	128.58
5	A	4801	ADP	N3-C2-N1	-3.38	123.46	128.58
5	A	4806	ADP	C4-C5-N7	-3.37	106.73	110.58
5	J	4801	ADP	C4-C5-N7	-3.32	106.79	110.58
5	J	4801	ADP	N3-C2-N1	-3.20	123.73	128.58
5	A	4805	ADP	C3'-C2'-C1'	3.08	107.28	101.46
5	J	4805	ADP	C4-C5-N7	-3.05	107.10	110.58
5	A	4805	ADP	C4-C5-N7	-2.98	107.17	110.58
5	J	4805	ADP	C4-N9-C8	2.81	108.69	105.74
5	A	4806	ADP	C4-N9-C8	2.63	108.50	105.74
5	A	4806	ADP	C3'-C2'-C1'	2.62	106.42	101.46
5	J	4806	ADP	C3'-C2'-C1'	2.56	106.30	101.46
5	J	4805	ADP	C3'-C2'-C1'	2.54	106.27	101.46
5	J	4801	ADP	C4-N9-C8	2.53	108.39	105.74
5	J	4806	ADP	C5-N7-C8	2.53	107.42	103.45
5	J	4806	ADP	C4-N9-C8	2.52	108.38	105.74
5	J	4801	ADP	C3'-C2'-C1'	2.51	106.20	101.46
5	A	4806	ADP	C5-N7-C8	2.41	107.24	103.45
5	J	4805	ADP	C2-N1-C6	2.41	122.69	118.73
5	A	4801	ADP	C3'-C2'-C1'	2.41	106.01	101.46
5	J	4801	ADP	C5-N7-C8	2.40	107.22	103.45
5	A	4805	ADP	C5-N7-C8	2.37	107.17	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	4805	ADP	C5-N7-C8	2.34	107.13	103.45
5	A	4801	ADP	C5-N7-C8	2.31	107.08	103.45
5	A	4805	ADP	C4-N9-C8	2.25	108.10	105.74
5	A	4805	ADP	C1'-N9-C8	-2.21	122.20	127.09
5	J	4801	ADP	C2'-C1'-N9	-2.10	108.09	113.30
5	J	4806	ADP	C6-C5-N7	2.10	136.13	132.09
5	A	4806	ADP	C2-N1-C6	2.07	122.12	118.73
5	A	4806	ADP	C6-C5-N7	2.06	136.06	132.09
5	J	4805	ADP	C6-C5-N7	2.03	136.00	132.09

There are no chirality outliers.

All (20) torsion outliers are listed below:

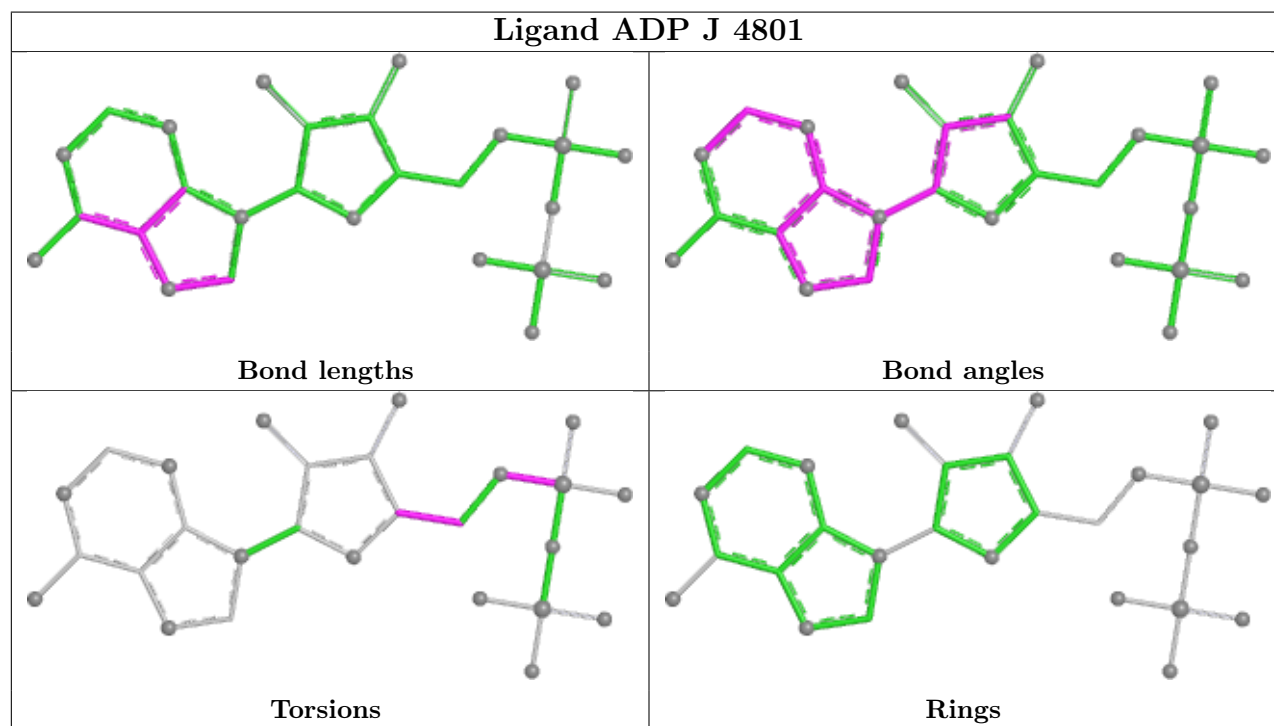
Mol	Chain	Res	Type	Atoms
5	A	4801	ADP	C5'-O5'-PA-O1A
5	A	4801	ADP	C5'-O5'-PA-O3A
5	A	4801	ADP	O4'-C4'-C5'-O5'
5	A	4806	ADP	O4'-C4'-C5'-O5'
5	J	4806	ADP	O4'-C4'-C5'-O5'
7	J	4803	ATP	C5'-O5'-PA-O3A
5	A	4806	ADP	C3'-C4'-C5'-O5'
5	J	4806	ADP	C3'-C4'-C5'-O5'
5	A	4801	ADP	C3'-C4'-C5'-O5'
7	J	4803	ATP	O4'-C4'-C5'-O5'
7	J	4803	ATP	C3'-C4'-C5'-O5'
5	A	4806	ADP	C5'-O5'-PA-O1A
5	J	4801	ADP	C5'-O5'-PA-O1A
7	J	4803	ATP	C5'-O5'-PA-O1A
7	A	4803	ATP	O4'-C4'-C5'-O5'
7	A	4803	ATP	PA-O3A-PB-O2B
5	A	4805	ADP	O4'-C4'-C5'-O5'
5	J	4801	ADP	O4'-C4'-C5'-O5'
5	A	4805	ADP	C2'-C1'-N9-C8
7	A	4803	ATP	C3'-C4'-C5'-O5'

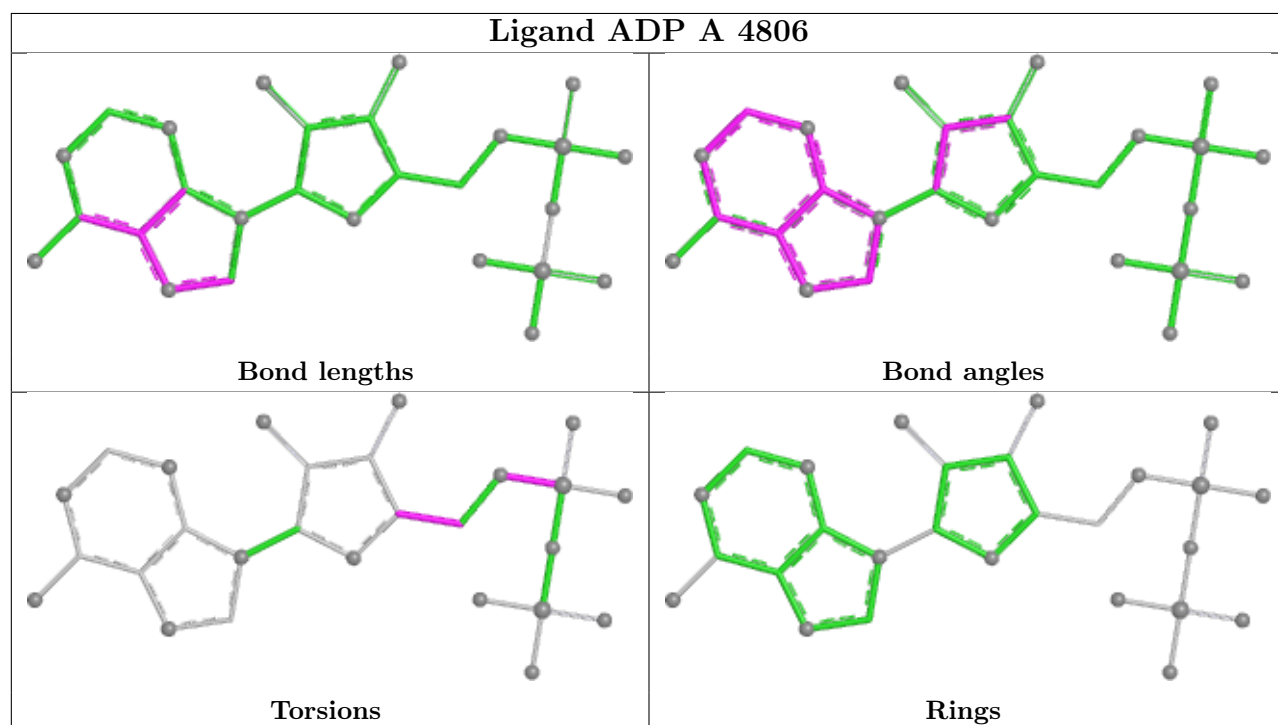
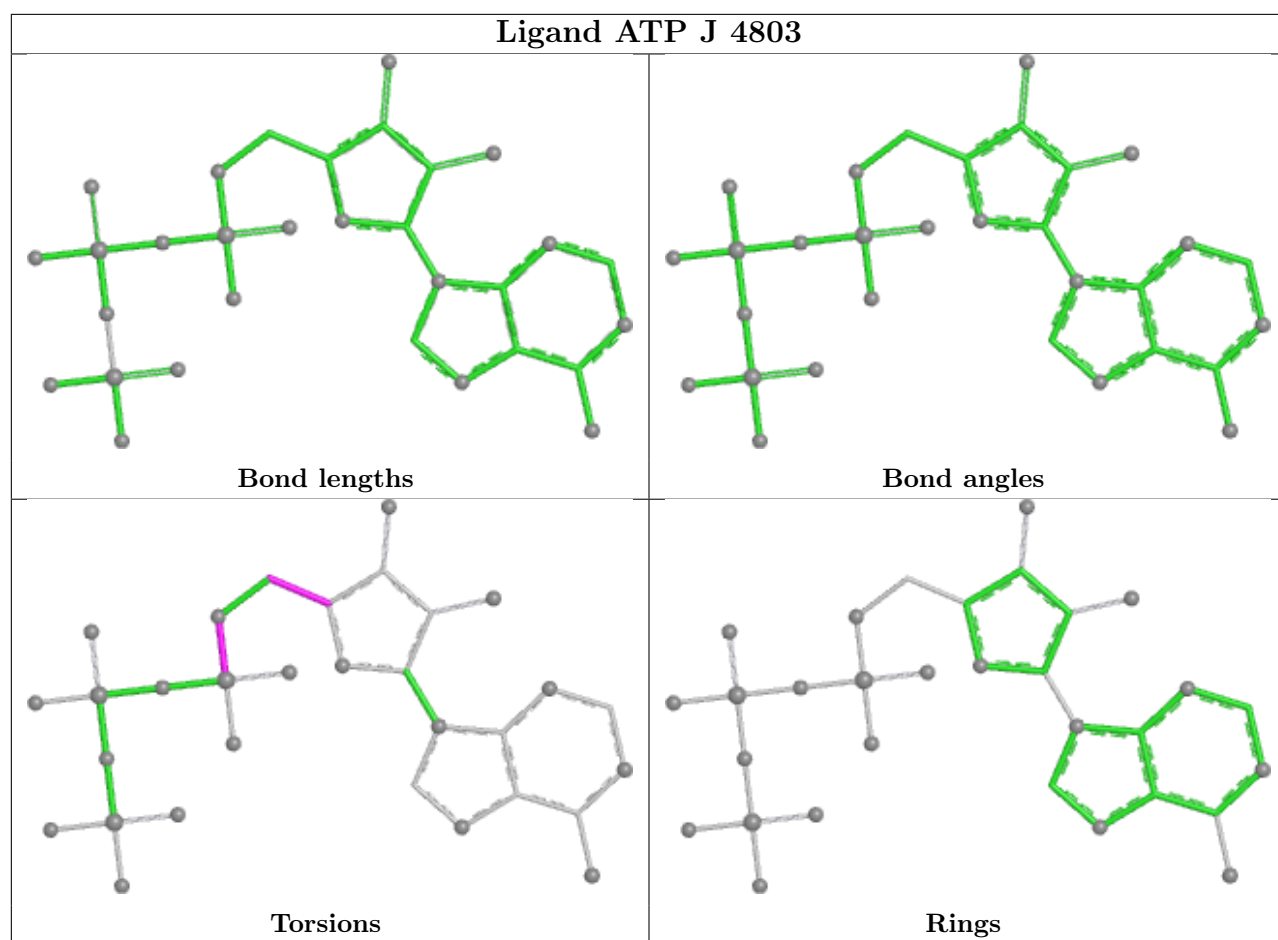
There are no ring outliers.

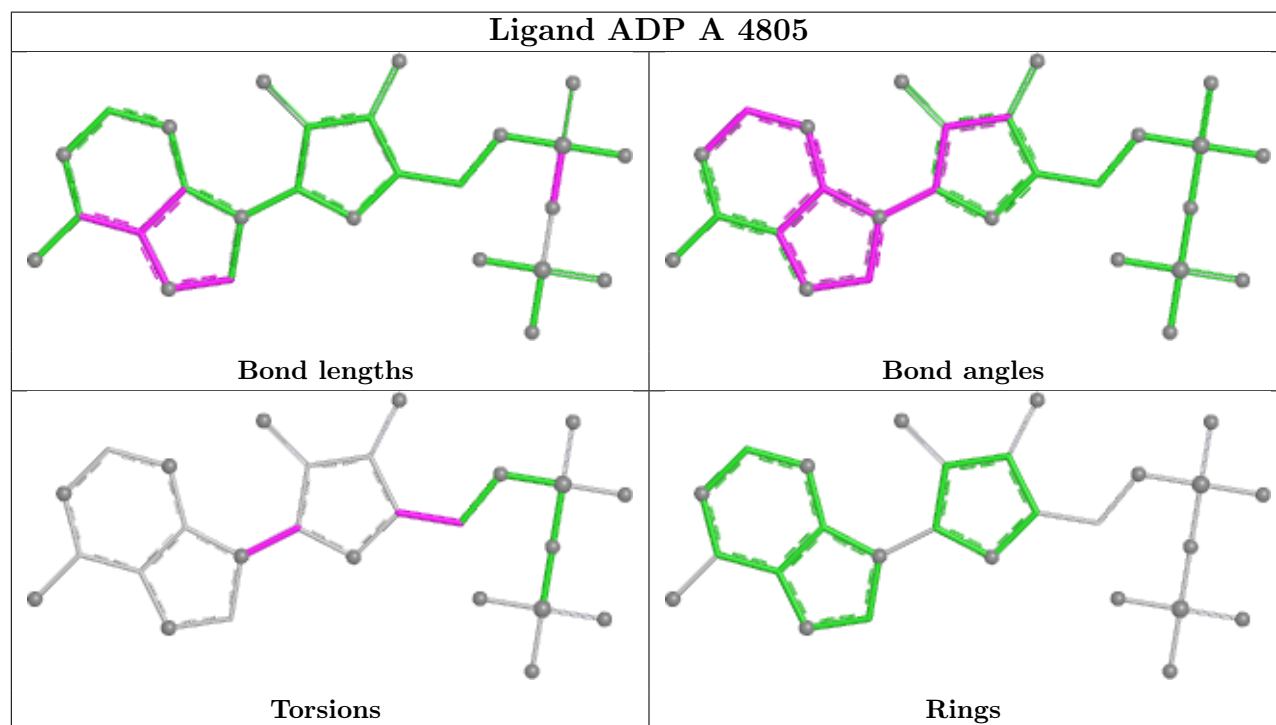
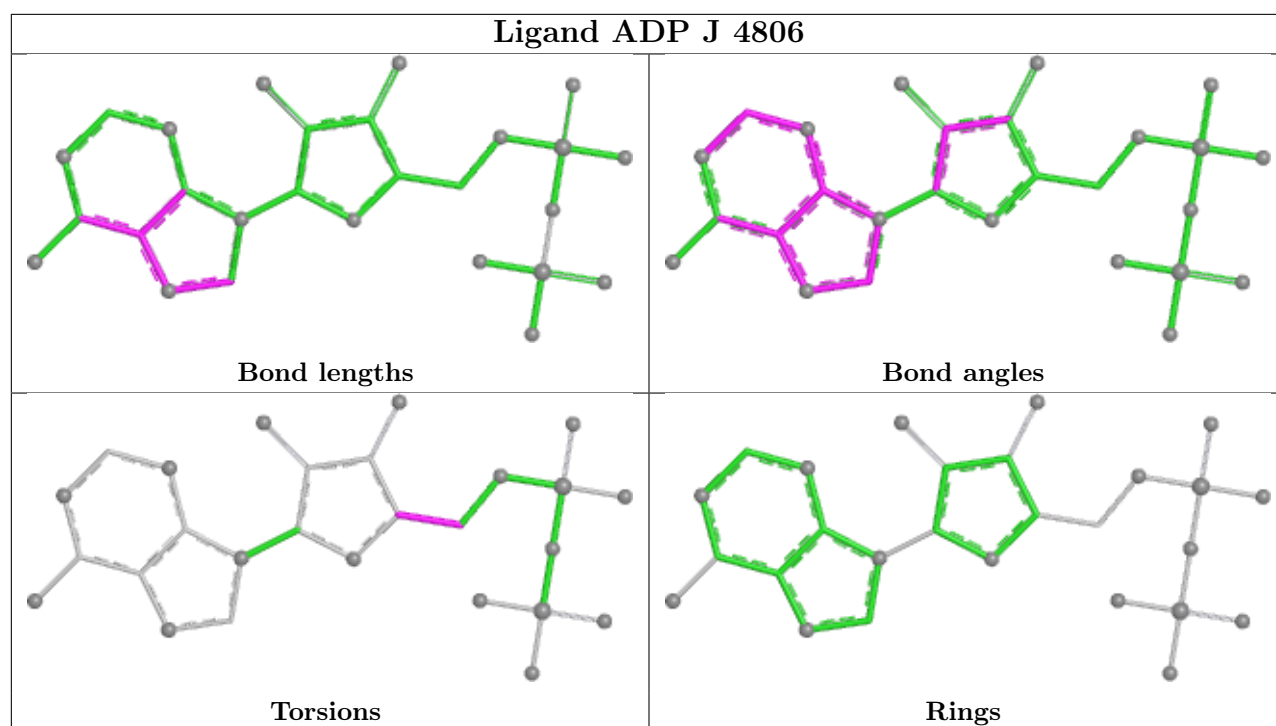
2 monomers are involved in 2 short contacts:

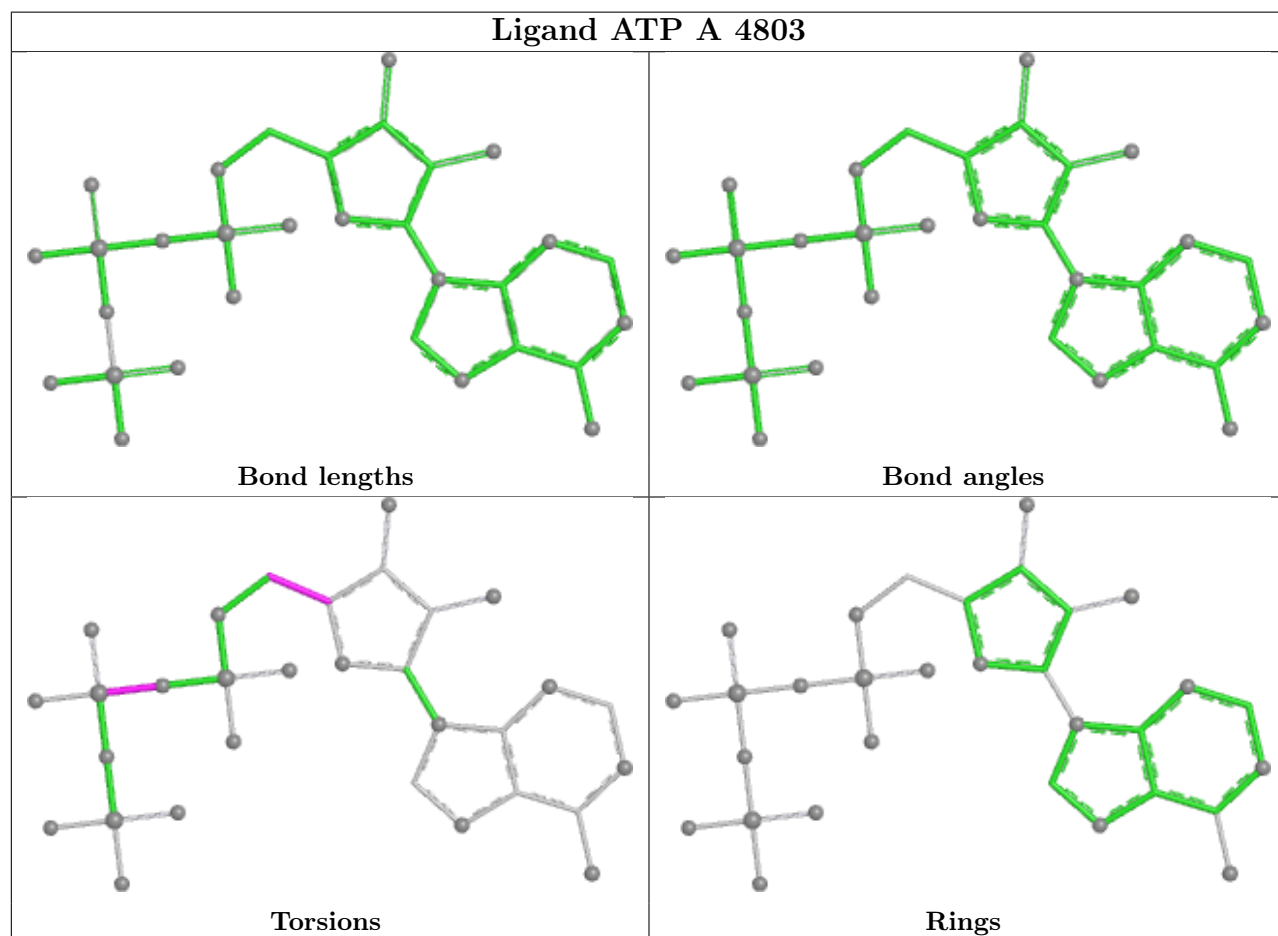
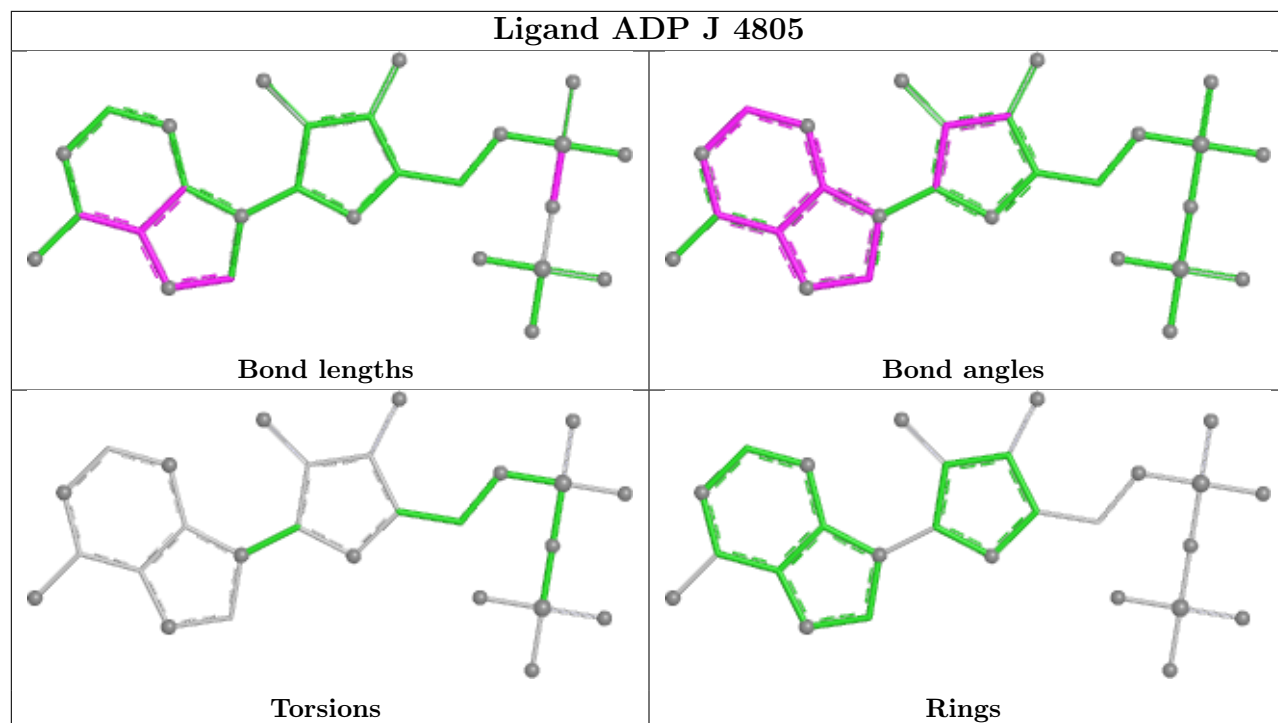
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	4803	ATP	1	0
5	A	4801	ADP	1	0

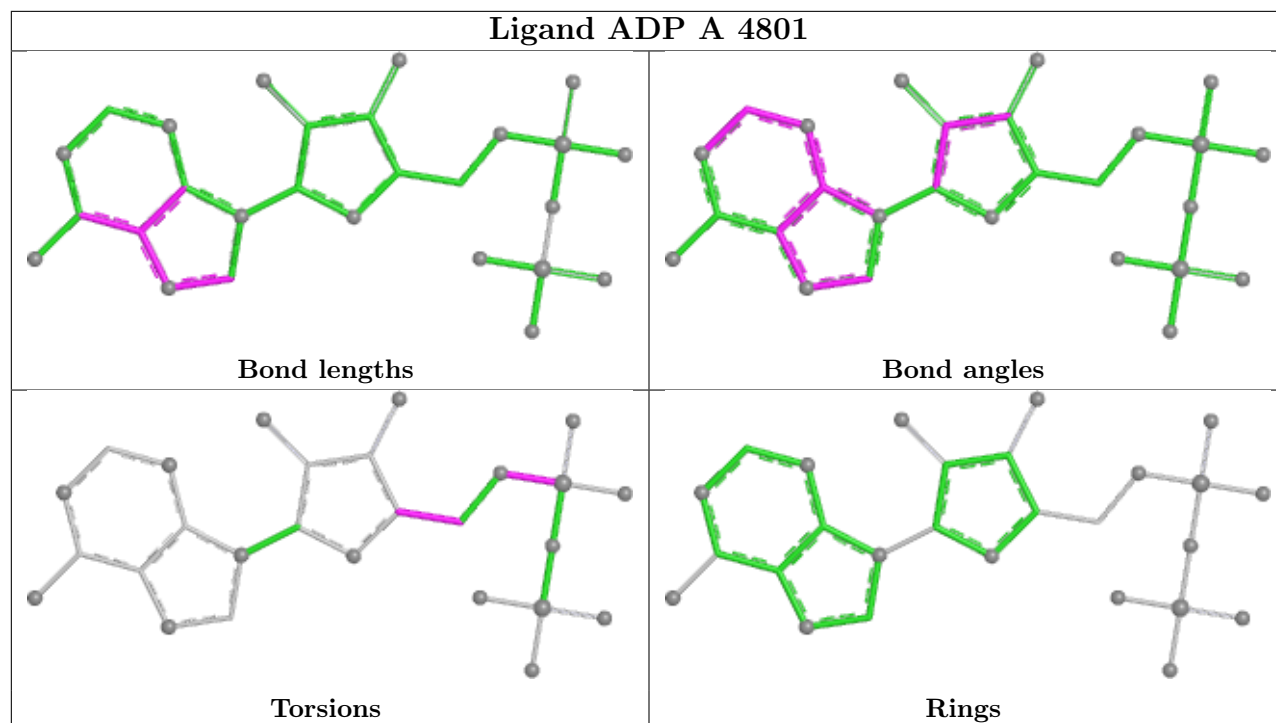
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

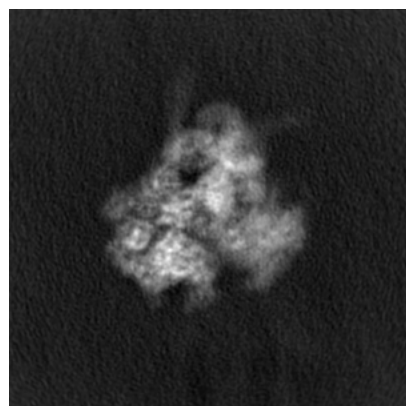
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17829. These allow visual inspection of the internal detail of the map and identification of artifacts.

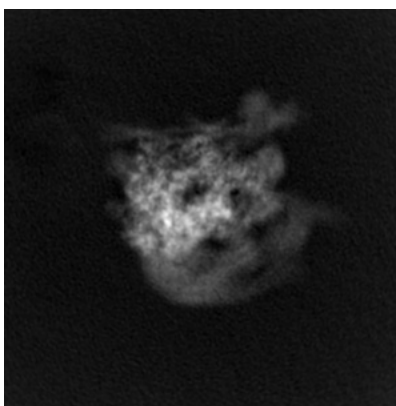
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

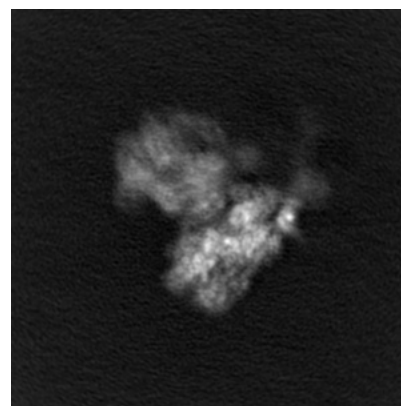
6.1.1 Primary map



X

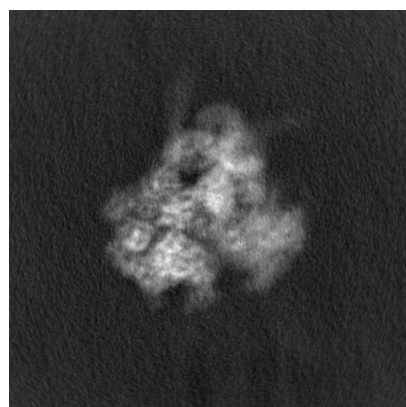


Y

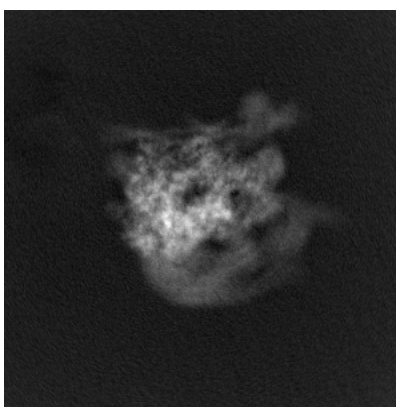


Z

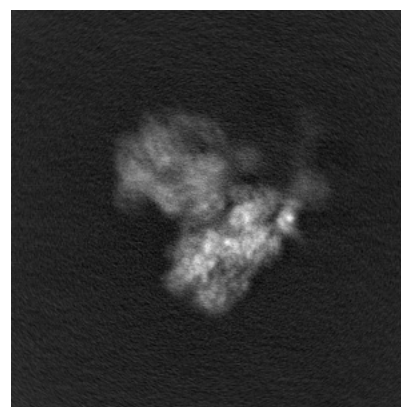
6.1.2 Raw map



X



Y

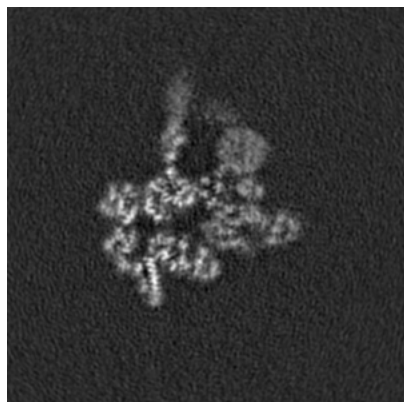


Z

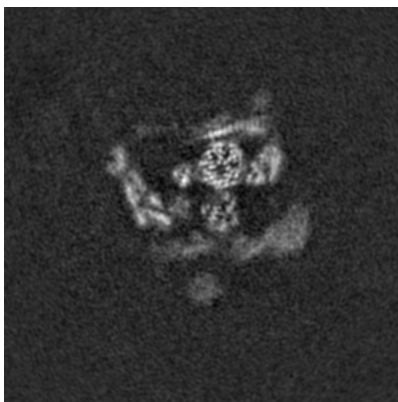
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

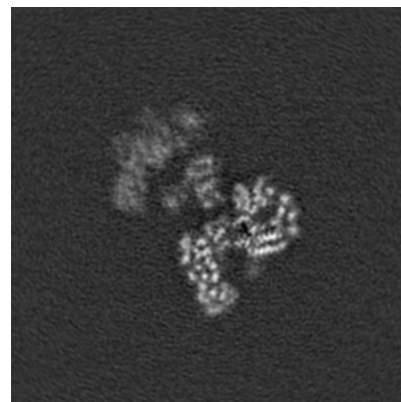
6.2.1 Primary map



X Index: 180

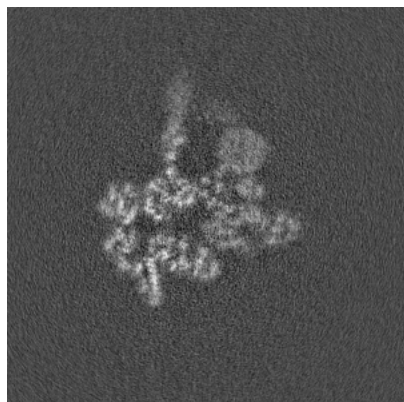


Y Index: 180

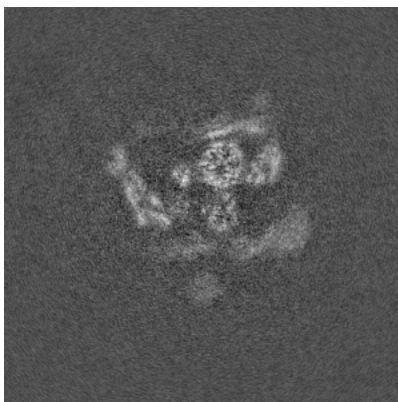


Z Index: 180

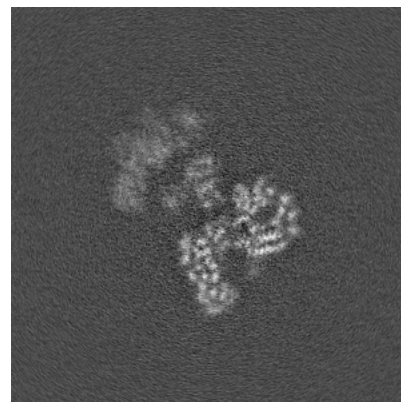
6.2.2 Raw map



X Index: 180



Y Index: 180

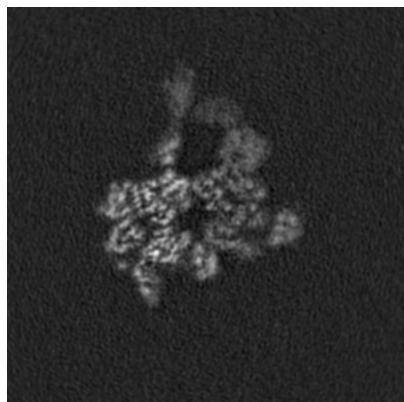


Z Index: 180

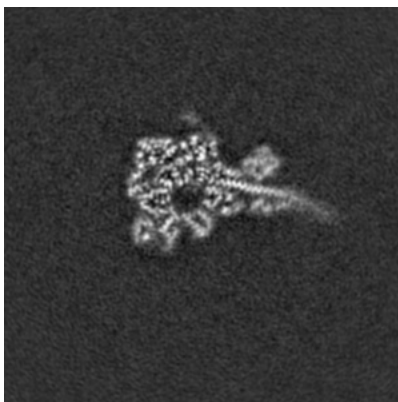
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

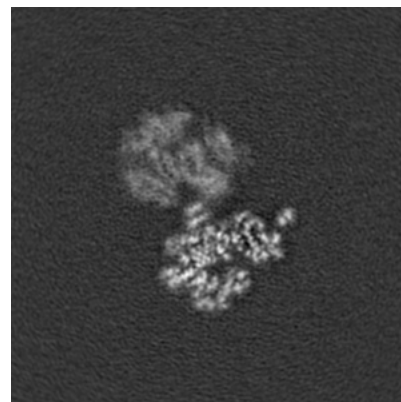
6.3.1 Primary map



X Index: 176

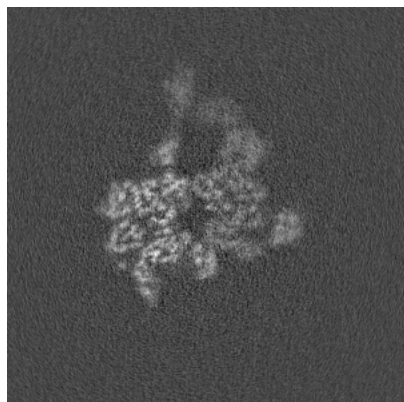


Y Index: 150

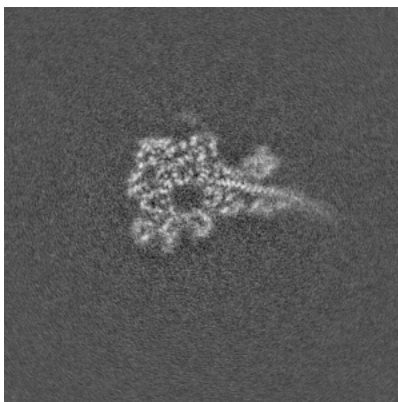


Z Index: 146

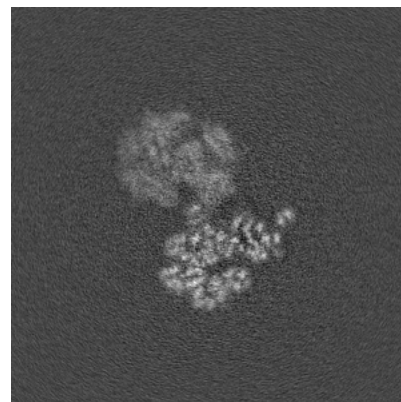
6.3.2 Raw map



X Index: 175



Y Index: 149

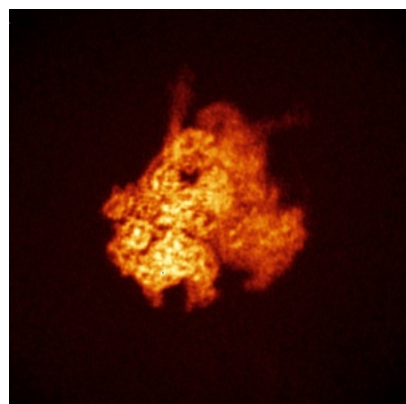


Z Index: 148

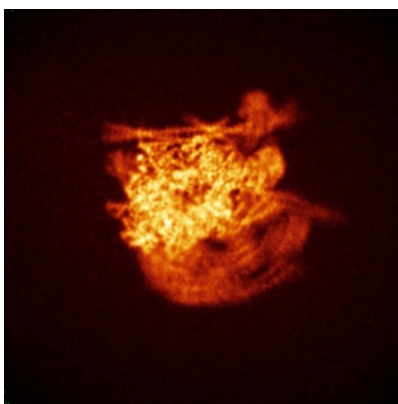
The images above show the largest variance slices of the map in three orthogonal directions.

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

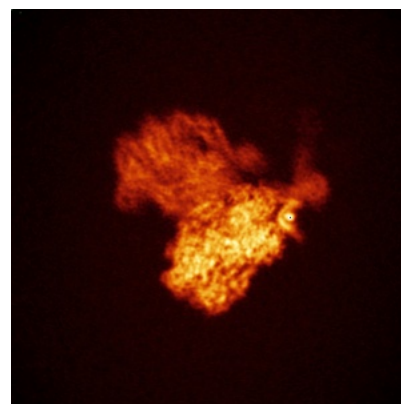
6.4.1 Primary map



X

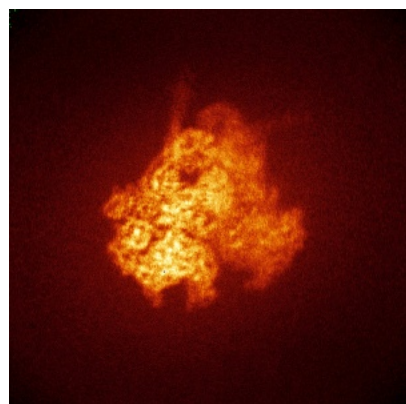


Y

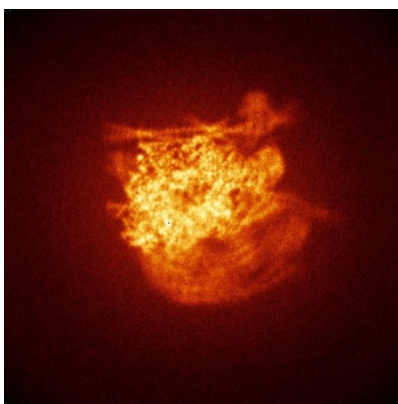


Z

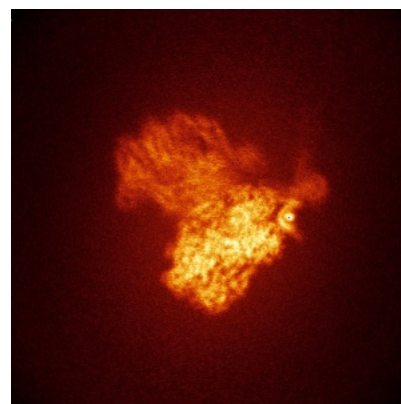
6.4.2 Raw map



X



Y



Z

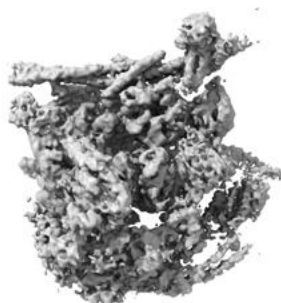
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

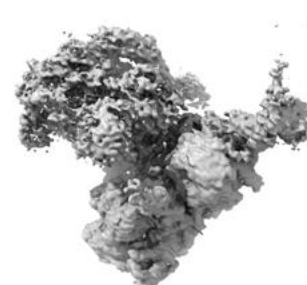
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0086. 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.

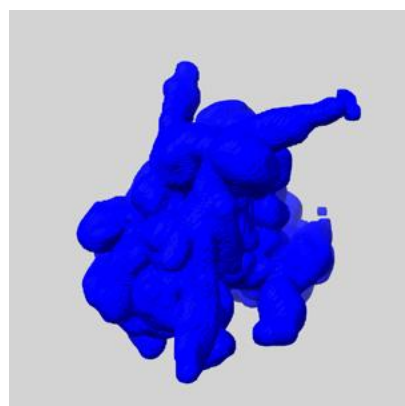
6.6 Mask visualisation [i](#)

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

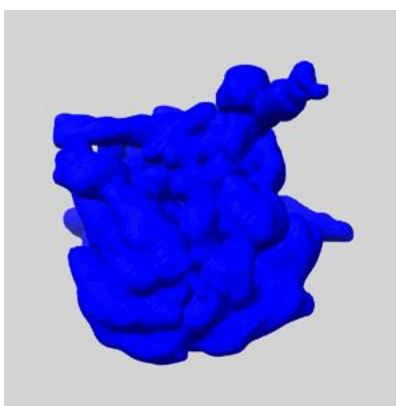
A mask typically either:

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

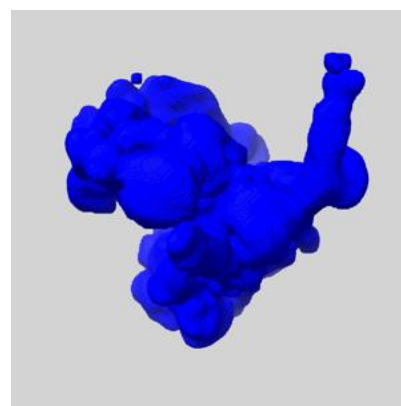
6.6.1 emd_17829_msk_1.map [i](#)



X



Y

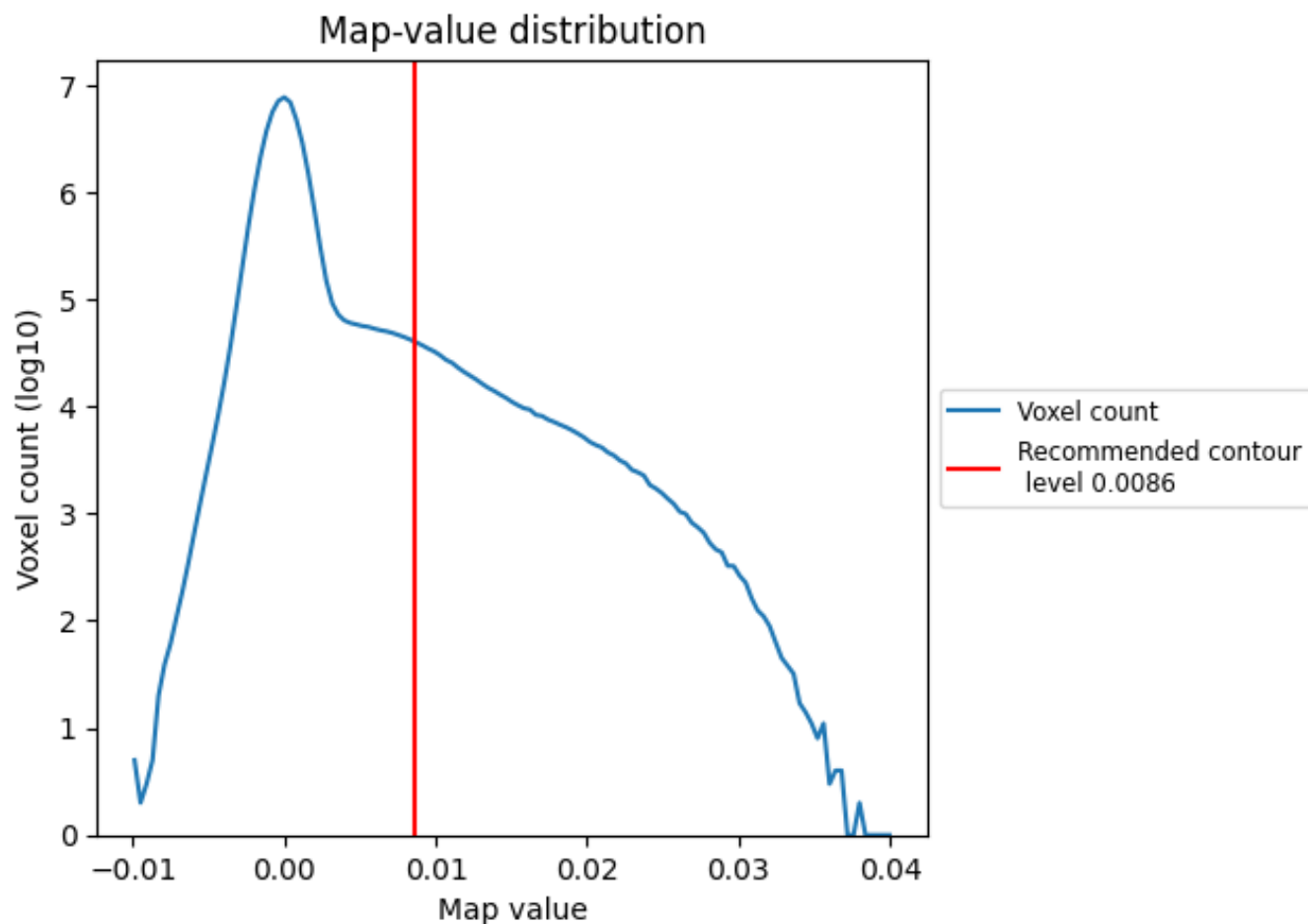


Z

7 Map analysis [i](#)

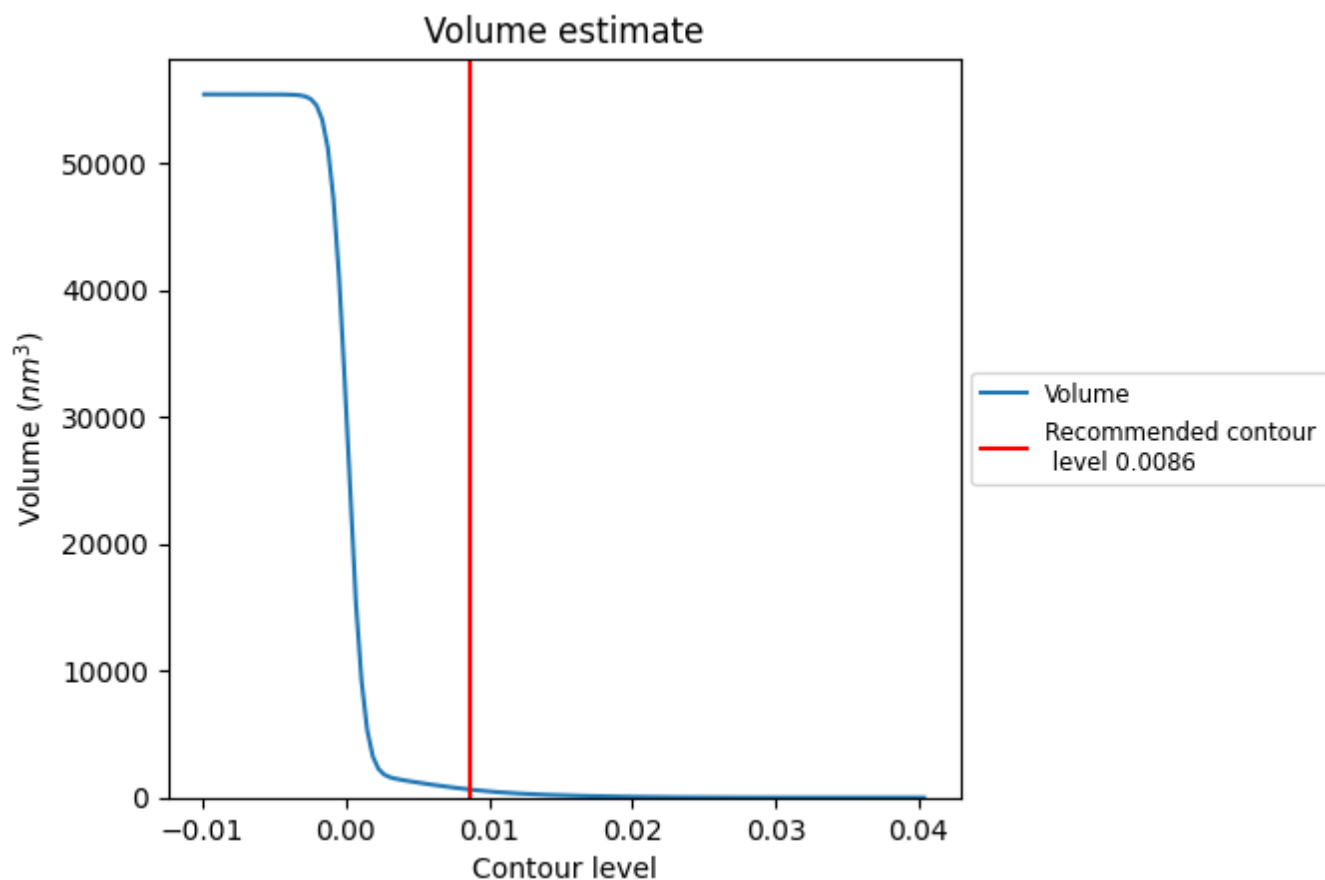
This section contains the results of statistical analysis of the map.

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.

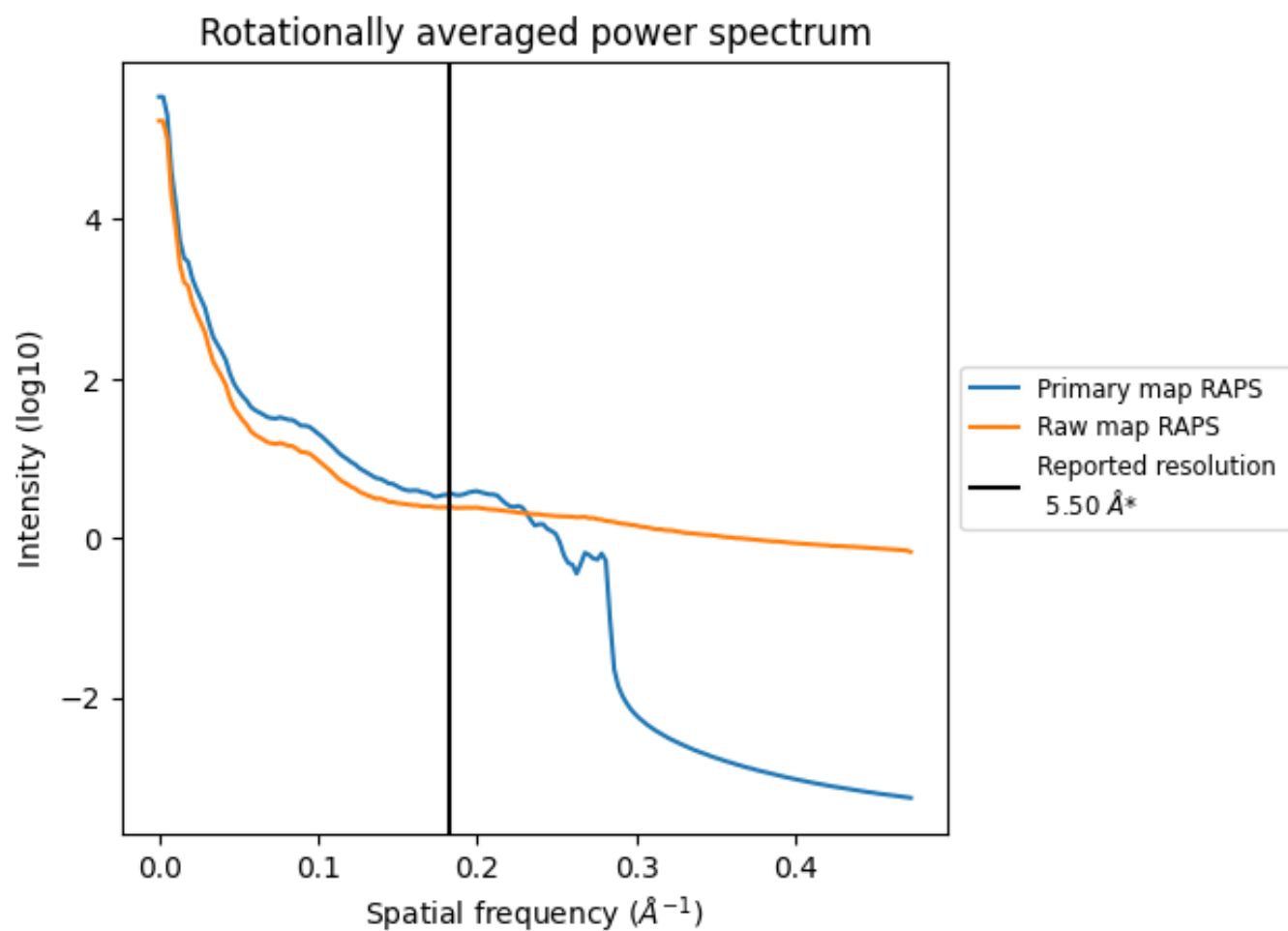
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 642 nm^3 ; this corresponds to an approximate mass of 580 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 ⓘ

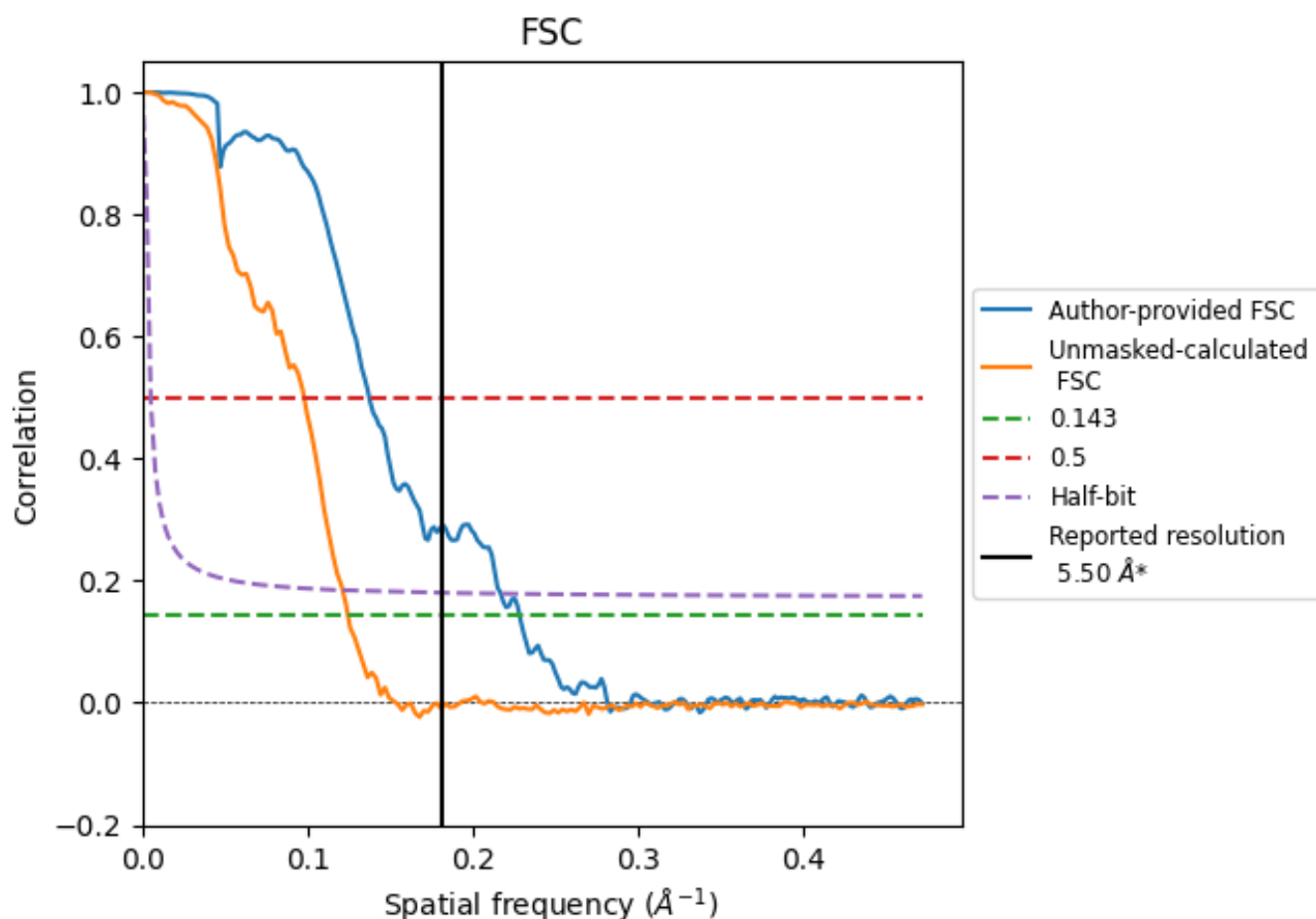


*Reported resolution corresponds to spatial frequency of 0.182 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.182 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.50	-	-
Author-provided FSC curve	4.38	7.27	4.60
Unmasked-calculated*	8.03	10.21	8.24

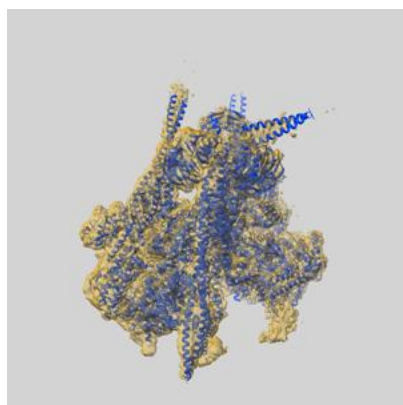
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.38 differs from the reported value 5.5 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.03 differs from the reported value 5.5 by more than 10 %

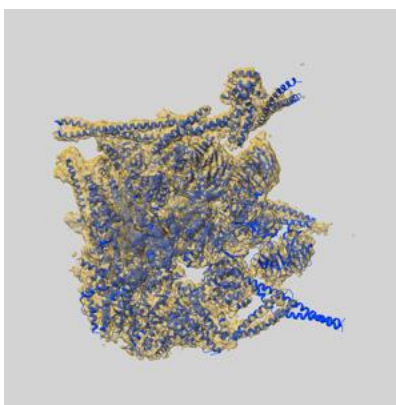
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17829 and PDB model 8PQZ. Per-residue inclusion information can be found in section 3 on page 7.

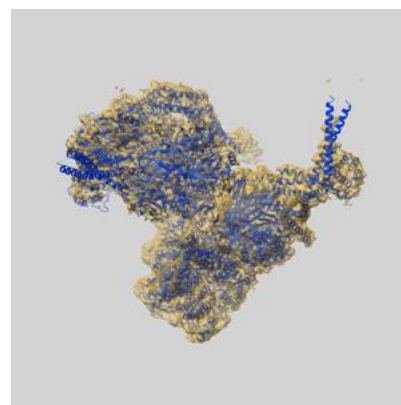
9.1 Map-model overlay [i](#)



X



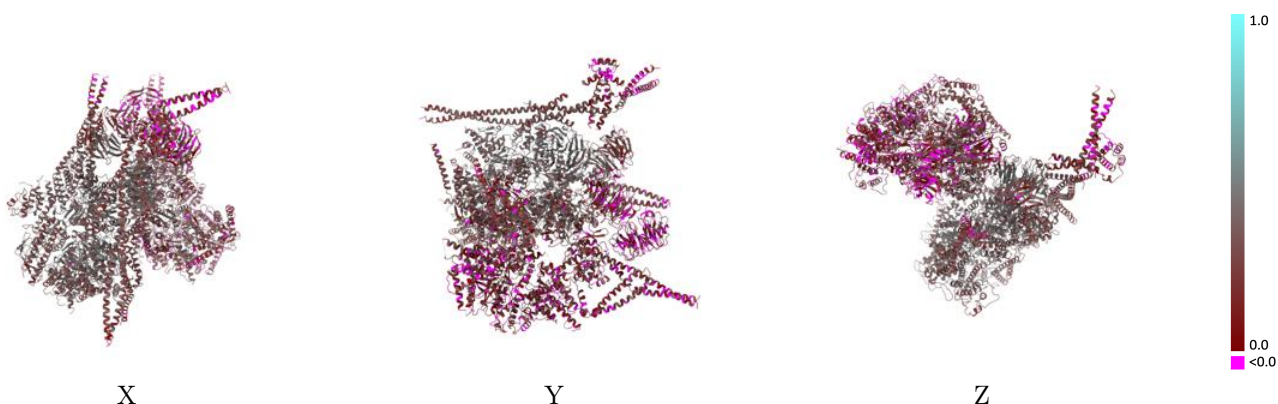
Y



Z

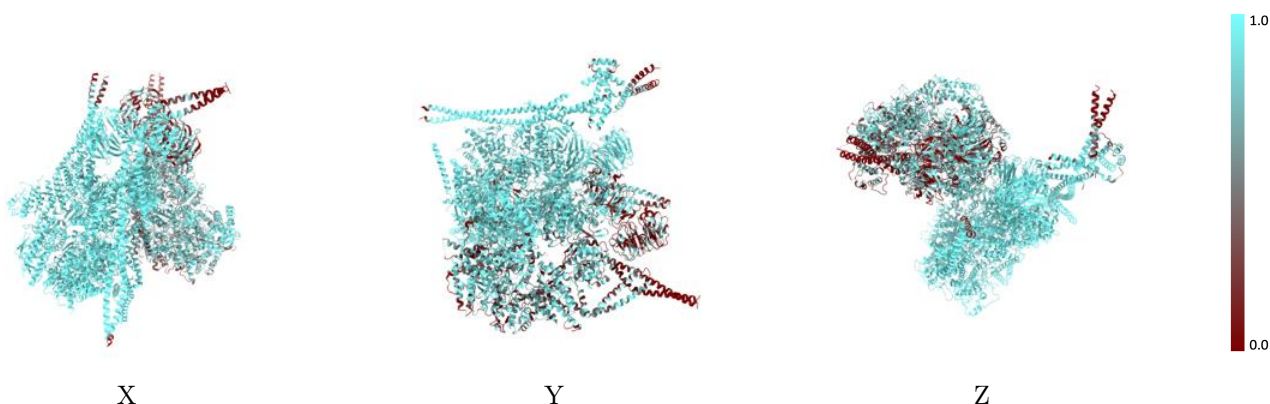
The images above show the 3D surface view of the map at the recommended contour level 0.0086 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



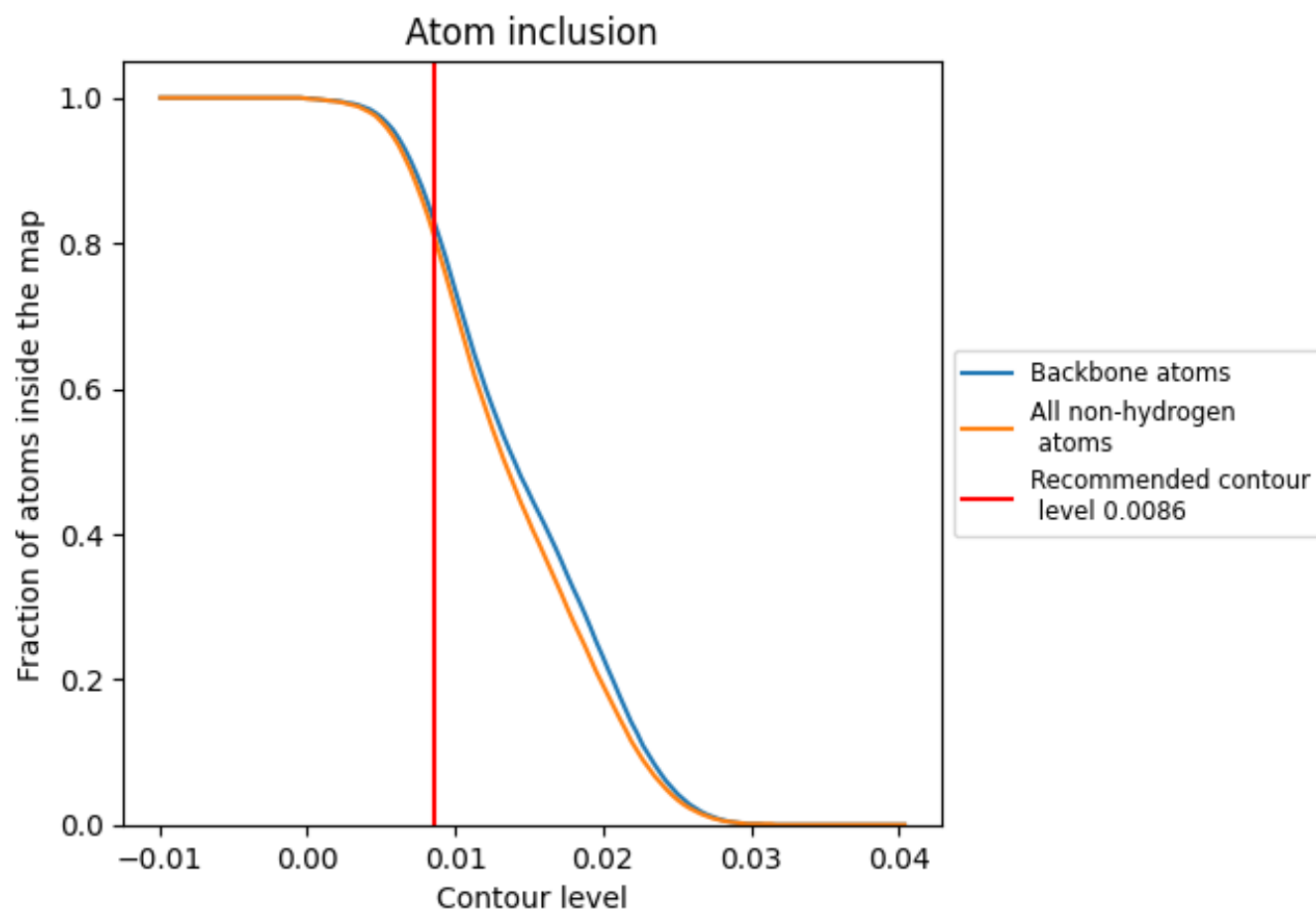
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0086).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 81% 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 (0.0086) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.2840
A	0.9860	0.3770
B	0.9880	0.3160
C	0.9900	0.4270
D	0.8500	0.1830
E	0.7990	0.1390
F	0.8220	0.2430
G	0.7910	0.2580
H	0.9590	0.2960
I	0.9640	0.3020
J	0.6720	0.2150
K	0.3150	0.0820
L	0.5190	0.1710

