



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 09:01 AM EDT

PDB ID : 5NUG  
EMDB ID: : EMD-3698  
Title : Motor domains from human cytoplasmic dynein-1 in the phi-particle conformation  
Authors : Zhang, K.; Foster, H.E.; Carter, A.P.  
Deposited on : unknown  
Resolution : 3.80 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

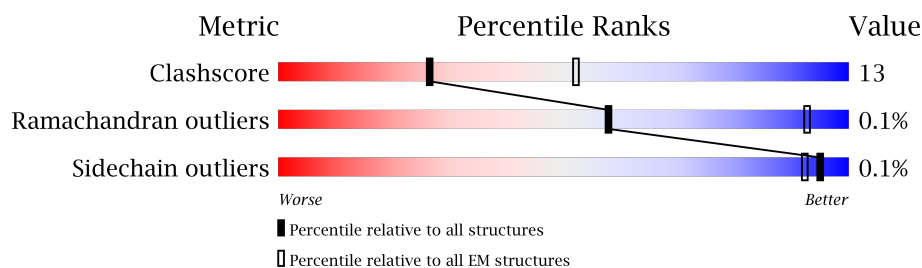
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	4646	
1	B	4646	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	A	4801	-	-	X	-
2	ADP	B	4801	-	-	X	-

## 2 Entry composition [i](#)

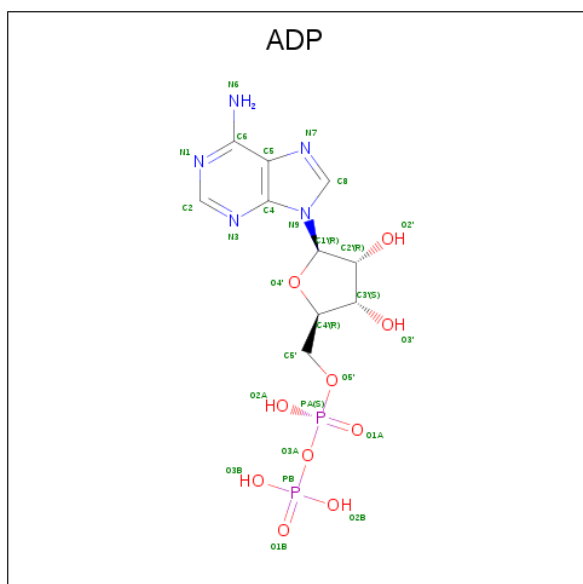
There are 4 unique types of molecules in this entry. The entry contains 46232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	2920	Total	C	N	O	S	0	0
			23003	14686	3978	4227	112		
1	B	2920	Total	C	N	O	S	0	0
			23003	14686	3978	4227	112		

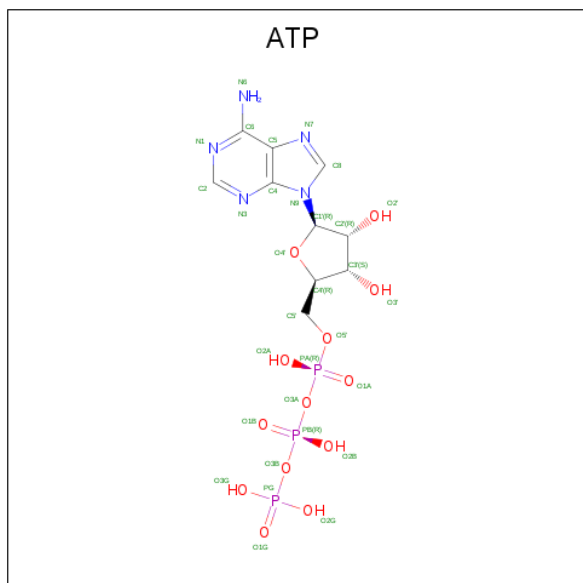
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			81	30	15	30	6	
2	B	1	Total	C	N	O	P	0
			81	30	15	30	6	

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



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

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

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



- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

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PROTEIN DATA BANK

 **EMDataBank**  
Unified Data Resource for 3DEM

L2348	L2238	A2100	N1931	L1752	LYS	ALA	ALA	VAL	TRP	ARG	GLU	ALA	ASN	GLU	PHE	LEU	ASN	PHE	LEU
T2355	I2253	V2103	C1932	I1756	ASN	TYR	TYR	ALA	GLU	PHE	HIS	LEU	LEU	LEU	GLN	LEU	ASN	LEU	ASN
R2358	I2254	K2104	E1934	E1444	ALA	GLU	GLU	GLU	LYS	PHE	SER	VAL	GLN	THR	THR	THR	ASP	GLN	GLU
C2359	P2256	E2114	T1935	N1761	V1452	VAL	PHE	LEU	PRO	PRO	ILE	ILE	MET	ASN	THR	GLU	LYS	GLU	VAL
		LYS	W1954	V1762		GLN	GLN	GLN	VAL	SER	SER	ARG	PRO	GLN	VAL	ILE	VAL	VAL	THR
L2369	L2264	GLU	D1958	A1765	W1490	LEU	LEU	LYS	ASN	TYR	ARG	ARG	PRO	TYR	TYR	LEU	LEU	GLU	GLU
S2370	Y2265	ARG	E1959	L1766	V1504	LEU	LEU	GLY	LEU	ILE	GLN	GLY	VAL	VAL	VAL	LEU	LEU	LEU	THR
M2373	W2275	GLY	F1960	S1767		GLY	GLY	VAL	ARG	ASP	GLU	THR	ALA	ASN	GLY	GLY	GLY	CYS	CYS
N2377	Z2276	GLU	N1961	S1768	P1511	GLY	TYR	TRP	ARG	ASN	GLU	PHE	LEU	ASN	ILE	ILE	ILE	ILE	GLU
R2381	D2277	ALA	R1962	GLY	Y1512	GLY	GLY	TRP	PRO	ILE	GLU	ASN	GLU	GLU	ARG	GLU	GLU	GLU	VAL
	L2278	ASP	L1963	GLY	E1524	LYS	LYS	GLU	GLU	GLY	HIS	ALA	SER	GLU	ILE	GLU	LYS	LYS	VAL
L2385	L2279	GLY	E1964	GLY	D1525	ILE	ILE	LEU	ALA	GLY	SER	GLU	TYR	TYR	GLU	ALA	GLY	GLU	GLU
	V2283	GLY	A1970	ASP	K1526	ASN	ASN	SER	LEU	TRP	VAL	GLU	SER	SER	ASP	GLY	ASP	ARG	ARG
L2284	L2284	GLU	I1978	A1775	R1529	MET	MET	LYS	GLN	TRP	GLY	THR	LYS	ALA	LEU	LEU	LEU	ASN	ASN
R2285	E2128	ILE	I1978	L1778		LEU	VAL	VAL	ALA	GLY	ASP	LYS	LYS	VAL	ARG	TYR	GLU	GLU	GLU
E2294	I2136	GLU	A1981	L1778	W1537	ILE	ILE	TRP	LEU	ALA	THR	ALA	LYS	VAL	VAL	VAL	VAL	VAL	ILE
L2295	L2137	ASP	H1985	V1781	I1538	GLU	GLN	GLN	ILE	PHE	SER	PHE	ASN	GLY	THR	LEU	THR	ARG	ILE
Q2299	L1792	LYS	H1985	L1792	Q1541	LEU	LYS	ASP	TYR	ASP	THR	GLY	PRO	VAL	THR	GLN	GLN	LEU	LEU
W2300	L1808	GLN	S1986	L1808	V1546	SER	SER	GLN	GLY	MET	ASP	VAL	SER	VAL	VAL	GLU	VAL	VAL	VAL
I2301	P2147	GLU	PRO	L1808		GLU	GLU	MET	PHE	ARG	ALA	VAL	GLU	GLU	GLU	MET	LEU	THR	THR
V2302	K2148	ARG	ASN	L1811	I1550	ALA	ALA	LYS	GLY	ARG	VAL	ILE	VAL	VAL	VAL	PHE	LEU	CYS	GLY
F2303	L1812	TYR	TYR	L1812		LEU	LEU	GLU	GLY	LYS	THR	ASP	GLN	GLU	ALA	ALA	GLY	GLY	GLY
D2304	L1812	ASP	ASP	L1812	I1571	LYS	ASP	GLN	ARG	ASP	PHE	TYR	GLN	GLU	SER	GLU	LYS	LYS	LYS
	Q1848	LYS	THR	Q1848		ASP	ASP	PRO	LEU	SER	ILE	GLY	TYR	LYS	TYR	LEU	ALA	ASP	LYS
V2307	L2154	GLY	GLY	L2154	L1578	ARG	ARG	TRP	LYS	ALA	THR	VAL	VAL	VAL	VAL	MET	GLU	HIS	GLU
D2308	P2155	GLU	SER	L2155	L1578	HIS	HIS	VAL	LYS	ILE	TYR	VAL	LYS	LYS	VAL	VAL	VAL	LYS	VAL
P2309	L2156	ASP	ALA	T1822		TRP	TRP	SER	ASP	GLN	ILE	GLN	GLN	VAL	VAL	THR	GLN	LYS	VAL
E2310	L2157	GLY	P1996	L1825	L1607	LYS	LYS	VAL	GLU	GLN	GLN	SER	TRP	GLN	TRP	LEU	ALA	PHE	ALA
W2311	L2182	GLY	I1997	L1825	R1628	LEU	LEU	GLN	GLY	GLN	SER	LYS	LEU	SER	LEU	SER	GLU	LEU	LEU
V2312	E2312	GLY	T1998	L1825		GLY	GLY	PRO	LYS	VAL	LEU	VAL	VAL	GLN	GLN	VAL	VAL	ILE	ILE
C2313	L2182	GLU	T1998	L1825		LEU	LEU	GLN	GLY	VAL	LEU	VAL	VAL	GLN	GLN	VAL	VAL	GLU	GLU
GLU	P2185	ALA	C1999	I1830	V1632	MET	MET	ARG	CYS	ALA	LYS	ASN	ASN	TYR	TYR	ASP	ILE	ALA	ALA
A2409	V2185	ALA	M2012	D1831		LYS	LYS	LYS	ALA	ASN	ARG	LEU	LEU	GLN	GLN	MET	ASP	LEU	LEU
	Y2190	GLY	N2019	A1833	D1636	ARG	ARG	ARG	ALA	GLN	ILE	TYR	LYS	GLN	THR	THR	ASP	GLY	GLY
I2446	L2191	GLY	N2019	E1871	L1637	HIS	HIS	GLN	LYS	MET	LYS	ASP	LYS	GLN	SER	SER	VAL	VAL	VAL
R2451	L2319	GLY	R2025	L1879	I1641	ASN	ASN	ASN	GLU	LYS	GLN	SER	ASP	ASP	THR	ASP	GLN	GLN	GLN
L2452	D2320	GLY	R2046	L1879		VAL	VAL	ASP	LEU	VAL	PHE	HIS	VAL	GLN	THR	MET	PRO	VAL	VAL
R2453	L2325	GLY	R2046	Y1889	S1644	VAL	VAL	LEU	LEU	GLU	GLN	GLU	GLU	VAL	VAL	GLY	VAL	VAL	VAL
C2454	P2328	GLY	I2049	L1882	V1647	SER	SER	LEU	THR	ASP	GLU	VAL	VAL	VAL	VAL	GLY	HIS	ASP	SER
		GLY				GLU	GLU	ASN	ASP	ARG	GLU	VAL	LEU	VAL	VAL	VAL	LYS	ASP	THR
S2457	L2333	GLY	G2058	M1882	V1647	LEU	LEU	GLN	THR	ALA	LEU	SER	LEU	GLU	GLU	HIS	LEU	LEU	LYS
L2458	S2334	GLY	L2208	T1893	L1650	THR	THR	LEU	THR	GLY	TYR	LYS	ASN	TYR	ASN	PRO	ASN	ASN	ASN
M2461	L2335	GLY	I2069	L1896	K1656	LYS	LYS	LEU	LEU	VAL	GLU	PHE	GLY	ARG	GLY	GLY	GLY	GLY	PRO
		GLY				GLY	GLY	SER	LEU	SER	ASN	GLY	LEU	LEU	LEU	GLU	GLU	GLU	GLU
Q2464	N2338	GLY	I2213	E4914	T1698	ILE	ILE	PHE	GLY	ARG	GLN	GLN	GLY	GLY	GLY	THR	LYS	LYS	VAL
		GLY				THR	THR	ALA	GLY	THR	GLN	MET	GLU	GLU	GLU	THR	LYS	LYS	GLN
Y2472	I2341	GLY	E2078	A1948	L1713	ASP	ASP	ARG	SER	ASP	LEU	LEU	GLU	ASP	ASP	ILE	ILE	ASN	ARG
Y2493	M2342	GLY	Q2079	L1923	L1749	VAL	VAL	LEU	GLU	GLU	LEU	LEU	LYS	ASN	ASN	LEU	LEU	ASN	PRO
E2344	E2344	GLY	Q2079	L1923	L1749	ASP	ASP	ARG	ARG	LEU	LEU	LEU	LYS	ASN	ASN	LEU	LEU	ASN	ALA
Y2496	V2345	GLY	R2091	V1927	W1754	GLN	GLN	TRP	VAL	THR	LYS	MET	VAL	ASN	THR	THR	VAL	VAL	GLU
		GLY				LEU	LEU	GLN	GLN	ASP	GLN	THR	GLN	GLN	ASP	GLN	GLN	GLN	THR

V4642	V4545	PRO	L4138	T3895	W3562	LEU	ALA	VAL	D3178	Y2967	M2752	L2805	T2498
L4643	ALA	ALA	L4139	G3897	L3567	GLN	GLU	LYS	F3179	LYS	M2752	L2805	L2499
C4644	TRP	TRP	R4143	L3567	L3567	LEU	LEU	ILE	I3180	L2509	L2509	L2805	W2500
T4645	SER	ARG	R4176	F3905	L3572	GLU	SER	LYS	H3200	L2612	L2612	L2805	S2501
E4646	GLN	TRP	R4177	I3924	C3573	ASP	ASP	LYS	H3200	L2612	L2612	L2805	L2502
	GLY		A4177	I3924	T3574	ASP	ALA	GLN	V3203	M2615	M2615	L2805	L2514
	ALA		R4178	T3574	T3574	ALA	ILE	HIS	G3204	E2616	E2616	L2805	G2515
	THR	L4388	F4186	W3974	I3578	LVS	ARG	LEU	L2770	V2617	V2617	L2805	R2519
	LEU		SER	W3974	L3578	ASP	GLU	VAL	R3206	M3008	D2787	L2805	R2538
	ASP	I4391	GLU	W3974	L3580	ASN	GLU	GLU	K3207	M3009	P2796	L2805	L2534
	ALA	P4392	I4190	GLU	L3580	GLN	MET	VAL	T3208	T3010	P2796	L2805	L2538
	CYS	L4395	L4223	T3978	N3584	GLN	LVS	ARG	I3222	E3016	E2819	L2805	L2534
S4557				I3978	R3585	ALA	ASN	MET	L3222	F3021	I2824	L2805	L2538
				V4009	L3588	LVS	ASN	VAL	A3236	F3021	I2824	L2805	L2538
V4560	W4240	T4401	W4240	ASN	L3588	ASN	TRP	ALA	A3236	F3021	I2824	L2805	L2538
T4561	VAL	VAL	S3809	GLU	I3589	GLU	MET	ASN	L2830	C2639	L2830	L2805	L2538
G4562	L4013	E4403	L4013	VAL	F3599	VAL	SER	PRO	L3029	L3029	L2830	L2805	L2538
L4563	A4248		A4248	GLU	F3599	GLU	ASN	PRO	L3029	L3029	L2830	L2805	L2538
K4564	Q4249	L4424	Q4249	GLU	F3599	GLU	ASN	PRO	L3029	L3029	L2830	L2805	L2538
S4250	S4250	L4424	S4250	GLN	F3599	GLN	MET	VAL	L3029	L3029	L2830	L2805	L2538
I4251	I4251	V4427	I4251	GLN	F3599	GLN	MET	VAL	L3029	L3029	L2830	L2805	L2538
Y4252	Y4252	V4427	Y4252	GLN	F3599	GLN	MET	VAL	L3029	L3029	L2830	L2805	L2538
		D4430	L4265	V4041	P3632	LVS	TRP	LEU	S3082	S3082	T2852	L2805	L2538
L4577		L4431	L4265	V4041	L3633	LVS	TRP	LEU	S3082	S3082	T2852	L2805	L2538
L4587		V4434	N4266	L4042	V3638	ALA	ILE	GLU	D2862	D2862	I2862	L2805	L2538
T4588		V4434	L4058	L4042	V3638	ALA	ILE	GLU	D2862	D2862	I2862	L2805	L2538
Q4589		V4434	F4273	F3823	E3639	VAL	VAL	GLU	D2862	D2862	I2862	L2805	L2538
L4590		V4437	T4067	F3823	E3639	VAL	VAL	GLU	D2862	D2862	I2862	L2805	L2538
R4591		V4447	S4073	L3824	Y3825	ASN	ASN	LEU	W3093	W3093	L2871	L2805	L2538
W4592		Y4447	S4073	L3824	Y3825	ASN	ASN	LEU	W3093	W3093	L2871	L2805	L2538
		L4451	A4083	F3832	F3832	ALA	ALA	CYS	W3097	W3097	L2871	L2805	L2538
Q4595		T4468	K4342	F3832	F3832	ALA	ALA	CYS	W3097	W3097	L2871	L2805	L2538
THR	ASN	T4468	T4086	I3835	I3661	CYS	GLY	GLY	S3098	S3098	S2874	L2805	L2538
THR	THR	T4468	L4349	I3836	I3662	PRO	PRO	ILE	E3100	E3100	V2893	L2805	L2538
GLU	GLU	S4483	E4350	I3836	I3662	L3508	MET	THR	Q3104	Q3104	Q2686	L2805	L2538
LVS	LVS	I4486	GLU	F3675	L3509	L3509	VAL	THR	ASP	ASP	Y2901	L2805	L2538
ALA	ALA	I4486	ASP	LVS	F3676	LVS	TRP	ASP	LYS	LYS	V2907	L2805	L2538
		S4498	ASP	GLY	I3677	A3516	TRP	TRP	F3109	F3109	V2907	L2805	L2538
S4603		S4498	ASP	GLY	I3677	A3517	ALA	LYS	MET	MET	L2910	L2805	L2538
V4604	LEU	GLY	LEU	S3680	S3680	A3517	ALA	LYS	MET	MET	L2910	L2805	L2538
V4605	ALA	GLY	ALA	S3681	S3681	F3520	ALA	ILE	VAL	VAL	L2911	L2805	L2538
T4606	TRP	T4606	T4098	L3682	L3682	D3521	GLN	ARG	LYS	F2708	F2708	L2805	L2538
L4607	ALA	K4502	V4099	D3683	D3683	Q3522	LEU	SER	GLU	W2709	W2709	L2805	L2538
P4608	GLU		GLU	F3688	F3688	Q3522	ASN	ILE	ASP	ASP	L2922	L2805	L2538
V4609	THR	L4106	THR	S3694	S3694	R3525	TRP	ILE	LEU	LEU	L2922	L2805	L2538
V4610	GLU	H4507	GLU	S3694	S3694	R3525	TRP	ILE	LEU	LEU	L2922	L2805	L2538
L4611	LYS	H4509	LYS	P4148	M3875	F3529	ASP	MET	ASP	ASP	L2922	L2805	L2538
	THR	C4510	LVS	T3703	L3876	F3529	ASP	ARG	LYS	F3149	M2713	L2805	L2538
I4619	THR	L4511	THR	F4122	T3704	W3532	MET	GLU	VAL	W3150	L2936	L2805	L2538
	ARG		ARG	F4122	T3704	W3532	ASN	ASN	PRO	H3151	L2937	L2805	L2538
V4622	THR	T4522	THR	F4125	T3882	L3536	LYS	PHE	ALA	W3148	L2938	L2805	L2538
P4623	ASP	F4125	ASP	L4126	F3883	L3536	ARG	ILE	ALA	W3148	L2938	L2805	L2538
F4624	SER	Q4526	SER	L4127	A3884	N3540	VAL	PRO	VAL	T3153	L2941	L2805	L2538
	THR	Y4527	THR	T4127	L3887	N3540	GLU	THR	ILE	T3153	L2941	L2805	L2538
F4635	SER	W4528	SER	M4128	L3887	T3550	LEU	VAL	ALA	T3172	V2958	L2805	L2538
	ASP	A4529	ASP	E4129	R3888	T3550	ARG	ASN	GLN	F3173	L2961	L2805	L2538
V4640	GLY	L4130	GLY	I4130	R3889	S3554	ASN	PRE	ASN	R3174	L2962	L2805	L2538
E4641	ASP	S4523	ASP	N4137	I3890	S3554	GLU	SER	ALA	H3175	T3082	L2805	L2538

- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

Chain B:



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WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

**EMDataBank**  
Unified Data Resource for 3DEM

C4644	T4645	E4646	THR	THR	ALA	TRP	PRO	L4138	T3895	L3770	L3572	GLU	SER
			ALA	THR	TRP	ALA	ALA	L4139	VAL	L3773	L3573	ASP	ASP
			TRP	GLN	MET	MET		G3897			T3574	ALA	ALA
			GLY	GLY	ARG	ARG		R4143	F3905	E3776		LYS	ARG
			ALA	ALA	T4379	T4379		R4176	I3924	V3797	I3578	ASP	GLU
			THR	THR				A4177			M3578	ASN	LYS
			LEU	LEU	W4387	W4387		R4178	I3924		L3580	GLN	MET
			ASP	ASP	L4388	L4388						LYS	LYS
			ALA	ALA				F4186	S3974	Y3801		LYS	ASN
			CYS	CYS	I4391	I4391		SER	GLU	P3803	N3584	ALA	ASN
			S4557	S4557	P4392	P4392		GLU	GLU	L3804	R3585	ASN	TYR
								T3978			L3588	GLU	MET
											I3589	VAL	SER
			V4560	V4560	L4395	L4395		V4009		C3808	F3599	GLU	ASN
			G4561	G4561	T4401	T4401		S3809		S3810		Q3435	PRO
			L4563	L4563	VAL	VAL		S3811		I3811	Y3451	SER	SER
			K4564	K4564	E4403	E4403		N4012			I3609	TYR	ASN
			L4565	L4565				L4013		T3814		I3455	THR
			Q4566	Q4566	L4424	L4424		L4027		M3815	P3632	S3456	GLU
										E3816	L3633	I3456	ILE
			L4577	L4577	V4427	V4427		W4035		S3817		Q3459	VAL
								Y4251		I3818	V3638	ASN	VAL
			L4587	L4587	D4430	D4430		Y4252			E3639	ARG	ASN
			T4588	T4588	L4431	L4431		W4041		I3821		L3465	ALA
			Q4589	Q4589				L4042		H3822	L3645	L3478	ALA
			L4590	L4590	V4434	V4434		L4058		F3823		I3478	SER
			R4591	R4591						L3824	V3648	I3482	LEU
			W4592	W4592	V4437	V4437		T4067		Y3825		I3482	ALA
											R3654	CYS	ALA
			Q4595	Q4595	Y4447	Y4447		S4073		F3832		R3486	GLY
			THR	THR							L3661	PRO	GLY
			ASN	ASN	L4451	L4451		A4083		I3835		L3508	MET
			GLU	GLU	S4483	S4483		T4086		Y3836	F3675	L3509	VAL
			LYS	LYS							V3676		LYS
			ALA	ALA	I4486	I4486		L4349		L3846	I3677	Y3516	TRP
			S4603	S4603				W4088		LYS		A3517	ALA
			V4604	V4604	G4498	G4498		A4087		GLY	S3680	ILE	ALA
			T4606	T4606	GLY	GLY		W4088		S3649	T3681	ALA	ALA
			L4607	L4607	ALA	ALA		S4090		L3856	R3682	GLN	GLN
			P4608	P4608				W4094			D3683	LEU	LEU
			V4609	V4609	K4502	K4502		V4094		F3668		ASN	ASN
			Y4610	Y4610	I4507	I4507		K4097			R3525	TYR	TYR
			L4611	L4611	H4508	H4508		W4098		V3871	F3529	ALA	ALA
					C4510	C4510		V4099		T3702		ASP	ASP
			I4619	I4619	V4509	V4509		L4106		V3703	W3532	LEU	MET
										T3704		LYS	LYS
					L4511	L4511		P4118		L3876	L3536	ARG	ARG
												VAL	VAL
			V4622	V4622	T4522	T4522		F4122			N3540	GLU	GLU
			D4623	D4623						T3882		PRO	PRO
			F4624	F4624	Q4526	Q4526		F4125		F3883	V3716	LEU	LEU
					Y4527	Y4527		L4126		A3884	L3717	ARG	ARG
			F4635	F4635	V4528	V4528		T4127			L3553	ASN	ASN
					A4529	A4529		M4128			S3554	GLU	GLU
			V4640	V4640				E4129		L3887		LEU	LEU
			A4641	A4641	S4533	S4533		I4130		A3888	L3749	GLN	GLN
			V4642	V4642						R3889		LYS	LYS
			L4643	L4643	V4545	V4545		N4137		I3890	T3769	LEU	LEU

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	233227	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 ( $e^-/\text{\AA}^2$ )	1.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	106061	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.43	0/23474	0.71	4/31851 (0.0%)
1	B	0.43	0/23474	0.71	4/31851 (0.0%)
All	All	0.43	0/46948	0.71	8/63702 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3821	ILE	N-CA-C	5.74	126.51	111.00
1	B	3821	ILE	N-CA-C	5.74	126.51	111.00
1	A	4250	SER	N-CA-C	5.52	125.91	111.00
1	B	4250	SER	N-CA-C	5.52	125.91	111.00
1	B	3578	ILE	CB-CA-C	-5.10	101.40	111.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23003	0	22805	587	0
1	B	23003	0	22805	582	0
2	A	81	0	36	13	0
2	B	81	0	36	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	4	0
3	B	31	0	12	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	46232	0	45706	1155	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 13.

The worst 5 of 1155 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:3638:VAL:HG12	1:A:3681:THR:CG2	1.29	1.60
1:B:3638:VAL:HG12	1:B:3681:THR:CG2	1.29	1.54
1:B:3749:LEU:HD13	1:B:3773:LEU:CD1	1.44	1.46
1:B:2584:TRP:CZ3	1:B:2732:PRO:HG2	1.50	1.45
1:A:3749:LEU:HD13	1:A:3773:LEU:CD1	1.44	1.43

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	2888/4646 (62%)	2714 (94%)	171 (6%)	3 (0%)	55	88
1	B	2888/4646 (62%)	2714 (94%)	171 (6%)	3 (0%)	55	88
All	All	5776/9292 (62%)	5428 (94%)	342 (6%)	6 (0%)	58	88

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1647	VAL
1	B	1647	VAL
1	A	1964	GLU
1	B	1964	GLU
1	A	1511	PRO

### 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	2472/4125 (60%)	2469 (100%)	3 (0%)	94	98
1	B	2472/4125 (60%)	2469 (100%)	3 (0%)	94	98
All	All	4944/8250 (60%)	4938 (100%)	6 (0%)	95	98

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3905	PHE
1	B	3905	PHE
1	B	2796	PRO
1	A	3825	TYR
1	B	3825	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4488	GLN
1	B	1856	GLN
1	B	4131	ASN
1	A	4490	GLN
1	B	1612	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 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$
2	ADP	A	4801	-	25,29,29	1.14	2 (8%)	24,45,45	1.79	3 (12%)
3	ATP	A	4802	4	27,33,33	1.04	1 (3%)	25,52,52	1.91	4 (16%)
2	ADP	A	4804	-	25,29,29	0.94	1 (4%)	24,45,45	1.85	3 (12%)
2	ADP	A	4805	-	25,29,29	0.87	1 (4%)	24,45,45	1.82	4 (16%)
2	ADP	B	4801	-	25,29,29	1.14	2 (8%)	24,45,45	1.79	3 (12%)
3	ATP	B	4802	4	27,33,33	1.03	1 (3%)	25,52,52	1.91	4 (16%)
2	ADP	B	4804	-	25,29,29	0.93	1 (4%)	24,45,45	1.84	3 (12%)
2	ADP	B	4805	-	25,29,29	0.87	2 (8%)	24,45,45	1.82	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4801	-	-	0/12/32/32	0/3/3/3
3	ATP	A	4802	4	-	0/18/38/38	0/3/3/3
2	ADP	A	4804	-	-	0/12/32/32	0/3/3/3
2	ADP	A	4805	-	-	0/12/32/32	0/3/3/3
2	ADP	B	4801	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	4802	4	-	0/18/38/38	0/3/3/3
2	ADP	B	4804	-	-	0/12/32/32	0/3/3/3
2	ADP	B	4805	-	-	0/12/32/32	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4805	ADP	C5-N7	-2.01	1.32	1.39
2	B	4801	ADP	C2-N3	2.31	1.36	1.32
2	A	4801	ADP	C2-N3	2.37	1.36	1.32
2	A	4805	ADP	C5-C4	2.53	1.46	1.40
2	B	4805	ADP	C5-C4	2.53	1.46	1.40

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4802	ATP	N3-C2-N1	-7.51	122.31	128.86
3	A	4802	ATP	N3-C2-N1	-7.51	122.31	128.86
2	A	4805	ADP	N3-C2-N1	-6.86	122.88	128.86
2	B	4805	ADP	N3-C2-N1	-6.86	122.88	128.86
2	B	4801	ADP	N3-C2-N1	-6.47	123.22	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4801	ADP	11	0
3	A	4802	ATP	4	0
2	A	4804	ADP	2	0
2	B	4801	ADP	11	0
3	B	4802	ATP	4	0
2	B	4804	ADP	2	0

## 5.7 Other polymers

There are no such residues in this entry.



## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3803:PRO	C	3804:LEU	N	2.62
1	B	3803:PRO	C	3804:LEU	N	2.62
1	A	3203:VAL	C	3204:GLY	N	2.58
1	B	3203:VAL	C	3204:GLY	N	2.58