



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:50 PM GMT

PDB ID : 4AKH
Title : Dynein Motor Domain - AMPPNP complex
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on : 2012-02-22
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

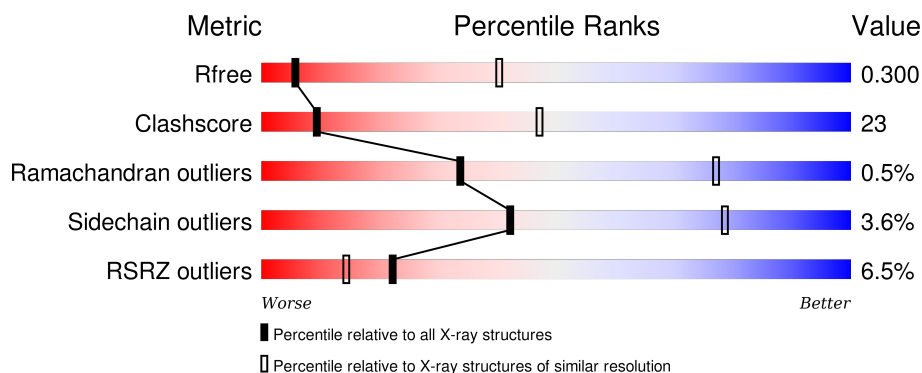
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2695	<div> <div>3%</div> <div>65%</div> <div>31%</div> <div>..</div> </div>
1	B	2695	<div> <div>10%</div> <div>67%</div> <div>30%</div> <div>..</div> </div>

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	ATP	B	5093	-	-	X	-
4	SO4	A	5095	-	-	X	-
4	SO4	B	5096	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 41642 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

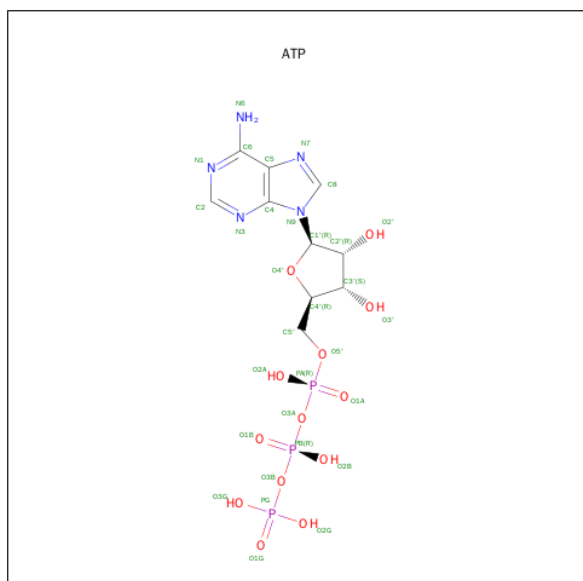
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			
1	B	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			

There are 4 discrepancies between the modelled and reference sequences:

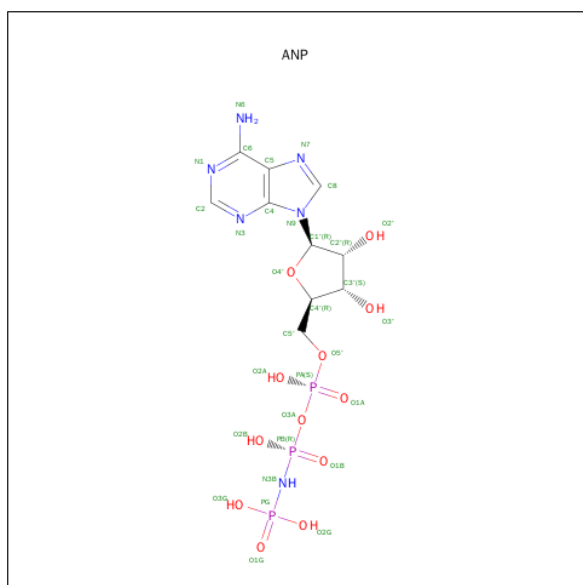
Chain	Residue	Modelled	Actual	Comment	Reference
A	1630	ILE	LEU	CONFLICT	UNP P36022
A	3782	ASP	GLU	CONFLICT	UNP P36022
B	1630	ILE	LEU	CONFLICT	UNP P36022
B	3782	ASP	GLU	CONFLICT	UNP P36022

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

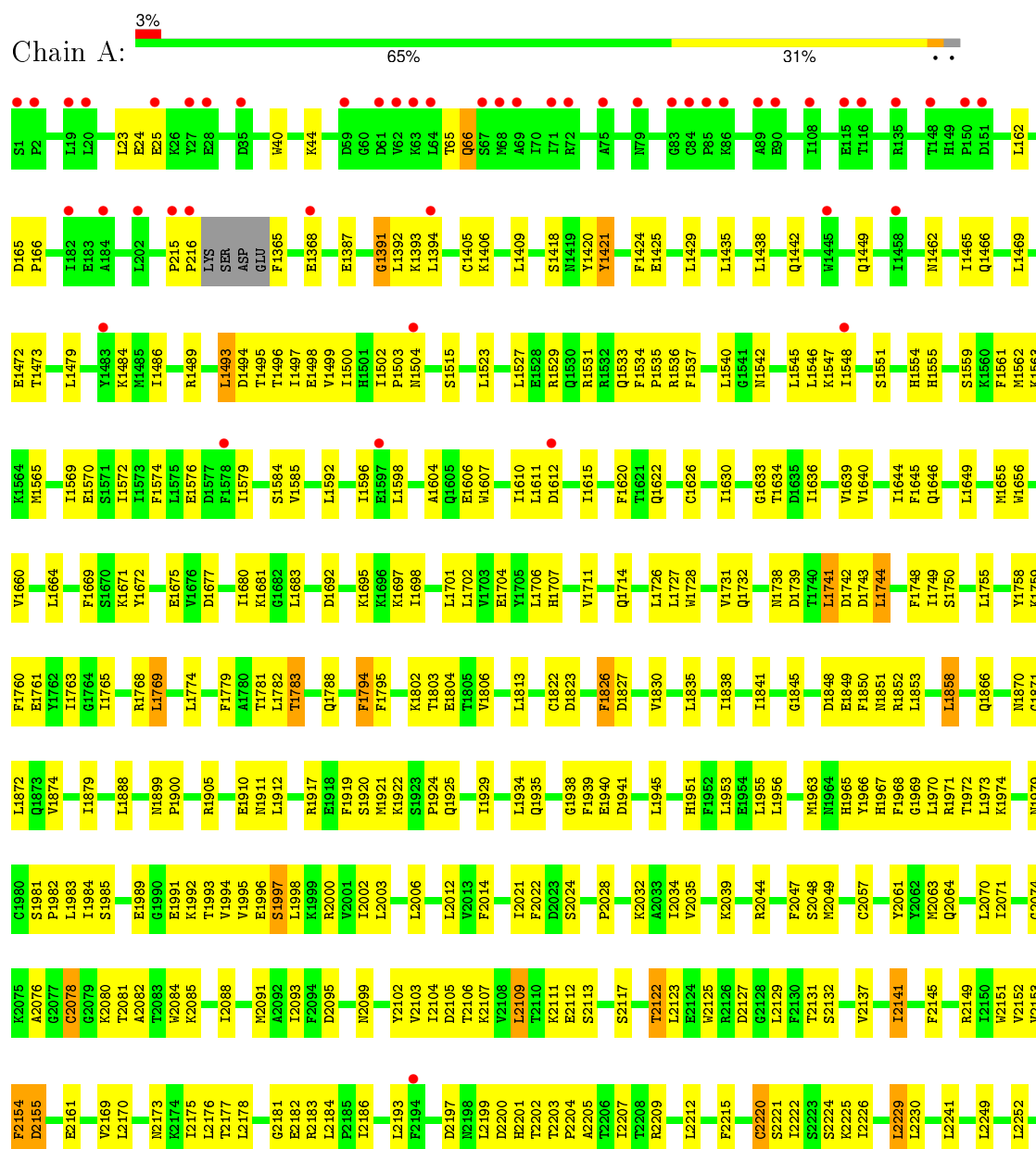
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

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

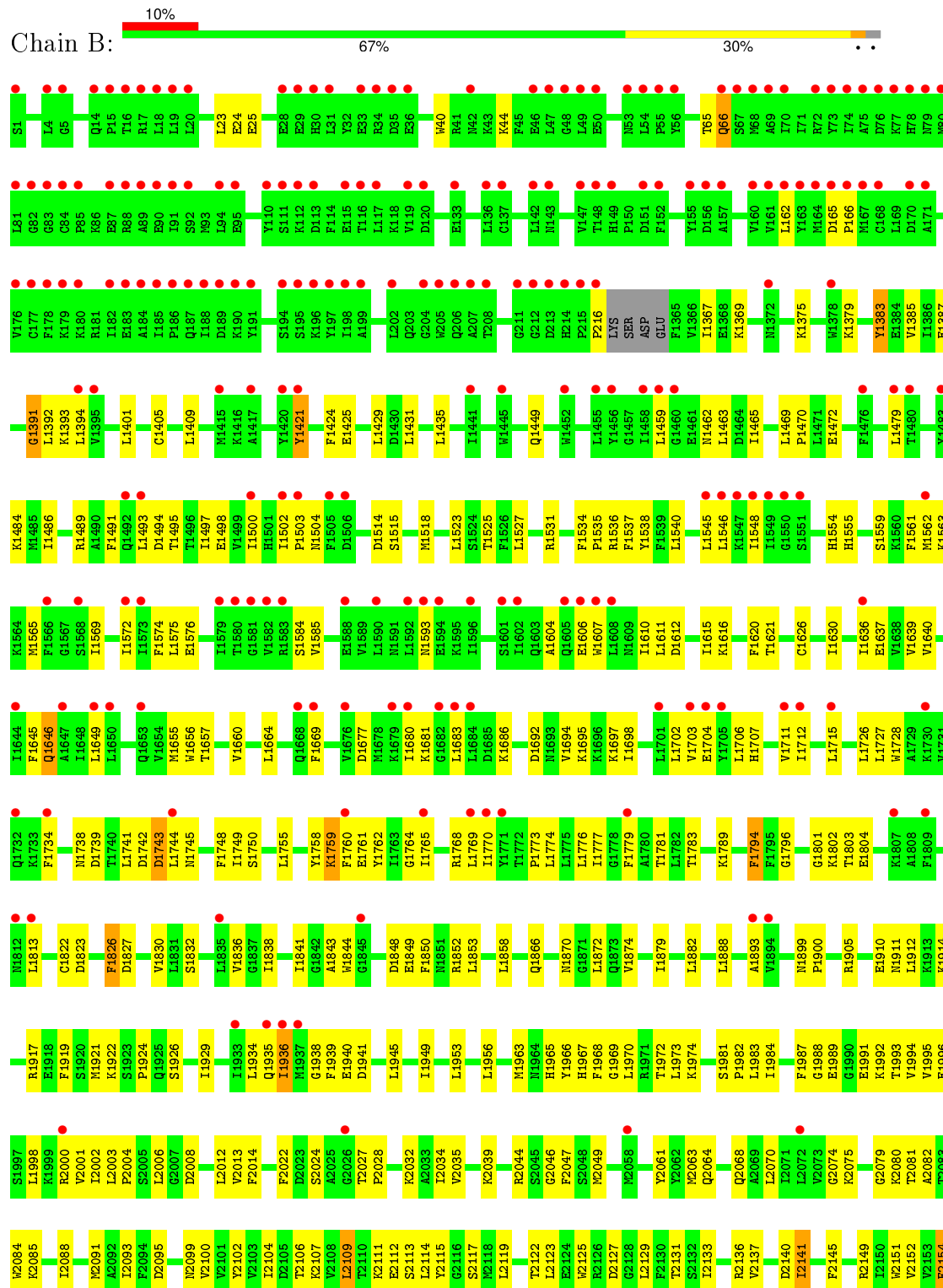
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



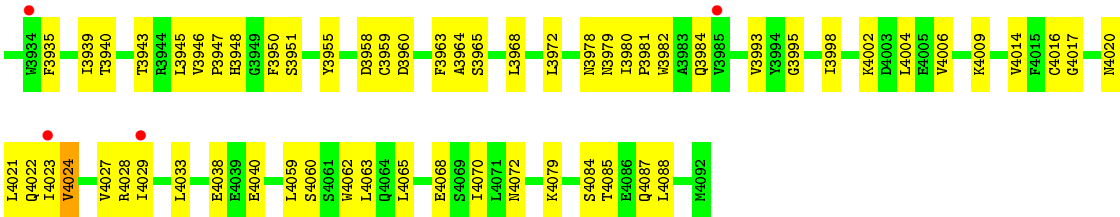
D3958	D3959	D3960	F3963	A3964	S3965	F3966	L3967	L3968	V3971	N3978	N3979	F3980	F3981	N3982	A3983	F3984	V3985	V3993	A3994	S3995	G3996	G3997	L3998	D3999	K4002	P4003	L4004	E4005	V4006	K4009	L4010	V4014	F4015	C4016	N4020	L4021	Q4022	L4023	V4024	R4028	L4029	L4033	L4034	Q4035	Q4036	F4037	E4038	F4039																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
R3792	R3797	F3798	K3799	L3800	L3801	E3802	A3804	K3805	A3806	S3807	K3808	L3809	S3810	L3811	K3812	F3813	K3814	L3815	K3816	G3817	F3818	M3819	F3820	N3821	L3822	N3823	S3832	K3833	G3836	S3730	G3837	K3838	L3839	L3840	I3844	Q3845	K3846	S3847	L3848	S3849	K3850	N3772	K3852	T3853	L3854	L3855	H3858	V3859	T3862	A3865	E3869	K3870	V3955																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
R3670	V3671	D3672	E3673	I3674	L3677	L3678	V3679	V3683	S3687	L3690	D3691	S3692	K3693	K3694	F3695	K3696	M3697	M3698	A3699	M3700	T3721	V3725	E3728	S3729	S3730	D3731	T3737	T3740	I3757	L3760	F3767	N3772	I3774	V3777	V3778	N3780	N3784	Y3785	F3786	M3788	V3777	V3778	N3780	N3784	Y3785	F3786	M3788	V3777	V3778	N3780	N3784	Y3785	F3786	M3788																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
L3578	E3579	N3580	L3583	L3587	K3588	E3589	K3592	E3593	N3596	K3600	L3601	E3602	E3603	F3607	D3612	N3613	L3614	V3615	E3618	G3622	L3628	F3629	S3630	M3631	L3632	E3633	K3634	F3641	Y3642	G3643	L3644	S3645	L3646	F3649	V3656	F3657	L3658	L3659	S3660	L3661	L3662	L3663	L3664	L3665	L3666	L3667	L3668	L3669	L3670	L3671	L3672	L3673	L3674	L3675	L3676	L3677	L3678	L3679	L3680	L3681	L3682	L3683	L3684	L3685	L3686	L3687	L3688	L3689	L3690	L3691	L3692	L3693	L3694	L3695	L3696	L3697	L3698	L3699	L3700	L3701	L3702	L3703	L3704	L3705	L3706	L3707	L3708	L3709	L3710	L3711	L3712	L3713	L3714	L3715	L3716	L3717	L3718	L3719	L3720	L3721	L3722	L3723	L3724	L3725	L3726	L3727	L3728	L3729	L3730	L3731	L3732	L3733	L3734	L3735	L3736	L3737	L3738	L3739	L3740	L3741	L3742	L3743	L3744	L3745	L3746	L3747	L3748	L3749	L3750	L3751	L3752	L3753	L3754	L3755	L3756	L3757	L3758	L3759	L3760	L3761	L3762	L3763	L3764	L3765	L3766	L3767	L3768	L3769	L3770	L3771	L3772	L3773	L3774	L3775	L3776	L3777	L3778	L3779	L3780	L3781	L3782	L3783	L3784	L3785	L3786	L3787	L3788	L3789	L3790	L3791	L3792	L3793	L3794	L3795	L3796	L3797	L3798	L3799	L3800	L3801	L3802	L3803	L3804	L3805	L3806	L3807	L3808	L3809	L3810	L3811	L3812	L3813	L3814	L3815	L3816	L3817	L3818	L3819	L3820	L3821	L3822	L3823	L3824	L3825	L3826	L3827	L3828	L3829	L3830	L3831	L3832	L3833	L3834	L3835	L3836	L3837	L3838	L3839	L3840	L3841	L3842	L3843	L3844	L3845	L3846	L3847	L3848	L3849	L3850	L3851	L3852	L3853	L3854	L3855	L3856	L3857	L3858	L3859	L3860	L3861	L3862	L3863	L3864	L3865	L3866	L3867	L3868	L3869	L3870	L3871	L3872	L3873	L3874	L3875	L3876	L3877	L3878	L3879	L3880	L3881	L3882	L3883	L3884	L3885	L3886	L3887	L3888	L3889	L3890	L3891	L3892	L3893	L3894	L3895	L3896	L3897	L3898	L3899	L3900	L3901	L3902	L3903	L3904	L3905	L3906	L3907	L3908	L3909	L3910	L3911	L3912	L3913	L3914	L3915	L3916	L3917	L3918	L3919	L3920	L3921	L3922	L3923	L3924	L3925	L3926	L3927	L3928	L3929	L3930	L3931	L3932	L3933	L3934	L3935	L3936	L3937	L3938	L3939	L3940	L3941	L3942	L3943	L3944	L3945	L3946	L3947	L3948	L3949	L3950	L3951	L3952	L3953	L3954	L3955	L3956	L3957	L3958	L3959	L3960	L3961	L3962	L3963	L3964	L3965	L3966	L3967	L3968	L3969	L3970	L3971	L3972	L3973	L3974	L3975	L3976	L3977	L3978	L3979	L3980	L3981	L3982	L3983	L3984	L3985	L3986	L3987	L3988	L3989	L3990	L3991	L3992	L3993	L3994	L3995	L3996	L3997	L3998	L3999	L4000	L4001	L4002	L4003	L4004	L4005	L4006	L4007	L4008	L4009	L4010	L4011	L4012	L4013	L4014	L4015	L4016	L4017	L4018	L4019	L4020	L4021	L4022	L4023	L4024	L4025	L4026	L4027	L4028	L4029	L4030	L4031	L4032	L4033	L4034	L4035	L4036	L4037	L4038	L4039	L4040	L4041	L4042	L4043	L4044	L4045	L4046	L4047	L4048	L4049	L4050	L4051	L4052	L4053	L4054	L4055	L4056	L4057	L4058	L4059	L4060	L4061	L4062	L4063	L4064	L4065	L4066	L4067	L4068	L4069	L4070	L4071	L4072	L4073	L4074	L4075	L4076	L4077	L4078	L4079	L4080	L4081	L4082	L4083	L4084	L4085	L4086	L4087	L4088	L4089	L4090	L4091	L4092	L4093	L4094	L4095	L4096	L4097	L4098	L4099	L4100	L4101	L4102	L4103	L4104	L4105	L4106	L4107	L4108	L4109	L4110	L4111	L4112	L4113	L4114	L4115	L4116	L4117	L4118	L4119	L4120	L4121	L4122	L4123	L4124	L4125	L4126	L4127	L4128	L4129	L4130	L4131	L4132	L4133	L4134	L4135	L4136	L4137	L4138	L4139	L4140	L4141	L4142	L4143	L4144	L4145	L4146	L4147	L4148	L4149	L4150	L4151	L4152	L4153	L4154	L4155	L4156	L4157	L4158	L4159	L4160	L4161	L4162	L4163	L4164	L4165	L4166	L4167	L4168	L4169	L4170	L4171	L4172	L4173	L4174	L4175	L4176	L4177	L4178	L4179	L4180	L4181	L4182	L4183	L4184	L4185	L4186	L4187	L4188	L4189	L4190	L4191	L4192	L4193	L4194	L4195	L4196	L4197	L4198	L4199	L4200	L4201	L4202	L4203	L4204	L4205	L4206	L4207	L4208	L4209	L4210	L4211	L4212	L4213	L4214	L4215	L4216	L4217	L4218	L4219	L4220	L4221	L4222	L4223	L4224	L4225	L4226	L4227	L4228	L4229	L4230	L4231	L4232	L4233	L4234	L4235	L4236	L4237	L4238	L4239	L4240	L4241	L4242	L4243	L4244	L4245	L4246	L4247	L4248	L4249	L4250	L4251	L4252	L4253	L4254	L4255	L4256	L4257	L4258	L4259	L4260	L4261	L4262	L4263	L4264	L4265	L4266	L4267	L4268	L4269	L4270	L4271	L4272	L4273	L4274	L4275	L4276	L4277	L4278	L4279	L4280	L4281	L4282	L4283	L4284	L4285	L4286	L4287	L4288	L4289	L4290	L4291	L4292	L4293	L4294	L4295	L4296	L4297	L4298	L4299	L4300	L4301	L4302	L4303	L4304	L4305	L4306	L4307	L4308	L4309	L4310	L4311	L4312	L4313	L4314	L4315	L4316	L4317	L4318	L4319	L4320	L4321	L4322	L4323	L4324	L4325	L4326	L4327	L4328	L4329	L4330	L4331	L4332	L4333	L4334	L4335	L4336	L4337	L4338	L4339	L4340	L4341	L4342	L4343	L4344	L4345	L4346	L4347	L4348	L4349	L4350	L4351	L4352	L4353	L4354	L4355	L4356	L4357	L4358	L4359	L4360	L4361	L4362	L4363	L4364	L4365	L4366	L4367	L4368	L4369	L4370	L4371	L4372	L4373	L4374	L4375	L4376	L4377	L4378	L4379	L4380	L4381	L4382	L4383	L4384	L4385	L4386	L4387	L4388	L4389	L4390	L4391	L4392	L4393	L4394	L4395	L4396	L4397	L4398	L4399	L4400	L4401	L4402	L4403	L4404	L4405	L4406	L4407	L4408	L4409	L4410	L4411	L4412	L4413	L4414	L4415	L4416	L4417	L4418	L4419	L4420	L4421	L4422	L4423	L4424	L4425	L4426	L4427	L4428	L4429	L4430	L4431	L4432	L4433	L4434	L4435	L4436	L4437	L4438	L4439	L4440	L4441	L4442	L4443	L4444	L4445	L4446	L4447	L4448	L4449	L4450	L4451	L4452	L4453	L4454	L4455	L4456	L4457	L4458	L4459	L4460	L4461	L4462	L4463	L4464	L4465	L4466	L4467	L4468	L4469	L4470	L4471	L4472	L4473	L4474	L4475	L4476	L4477	L4478	L4479	L4480	L4481	L4482	L4483	L4484	L4485	L4486	L4487	L4488	L4489	L4490	L4491	L4492	L4493	L4494	L4495	L4496	L4497	L4498	L4499	L4500	L4501	L4502	L4503	L4504	L4505	L4506	L4507	L4508	L4509	L4510	L4511	L4512	L4513	L4514	L4515	L4516	L4517	L4518	L4519	L4520	L4521	L4522	L4523	L4524	L4525	L4526	L4527	L4528	L4529	L4530	L4531	L4532	L4533	L4534	L4535	L4536	L4537	L4538	L4539	L4540	L4541	L4542	L4543	L4544	L4545	L4546	L4547	L4548	L4549	L4550	L4551	L4552	L4553	L4554	L4555	L4556	L4557	L4558	L4559	L4560	L4561	L4562	L4563	L4564	L4565	L4566	L4567	L4568	L4569	L4570	L4571	L4572	L4573	L4574	L4575	L4576	L4577	L4578	L4579	L4580	L4581	L4582	L4583	L4584	L4585	L4586	L4587	L4588	L4589	L4590	L4591	L4592	L4593	L4594	L4595	L4596	L4597	L4598	L4599	L4600	L4601	L4602	L4603	L4604	L4605	L4606	L4607	L4608	L4609	L4610	L4611	L4612	L4613	L4614	L4615	L4616	L4617	L4618	L4619	L4620	L4621	L4622	L4623	L4624	L4625	L4626	L4627	L4628	L4629	L4630	L4631	L4632	L4633	L4634	L4635	L4636	L4637	L4638	L4639	L4640	L4641	L4642	L4643	L4644	L4645	L4646	L4647	L4648	L4649	L4650	L4651	L4652	L4653	L4654	L4655	L4656	L4657	L4658	L4659	L4660	L4661	L4662	L4663	L4664	L4665	L4666	L4667	L4668	L4669	L4670	L4671	L4672	L4673	L4674	L4675	L4676	L4677	L4678	L4679	L4680	L4681	L4682	L4683	L4684	L4685	L4686	L4687	L4688	L4689	L4690	L4691	L4692	L4693	L4694	L4695	L4696	L4697	L4698	L4699	L4700	L4701	L4702	L4703	L4704	L4705	L4706	L4707	L4708	L4709	L4710	L4711	L4712	L4713	L4714	L4715	L4716	L4717	L4718	L4719	L4720	L4721	L4722	L4723	L4724	L4725	L4726	L4727	L4728	L4729	L4730	L4731	L4732	L4733	L4734	L4735	L4736	L4737	L4738	L4739	L4740	L4741	L4742	L4743	L4744	L4745	L4746	L4747	L4748	L4749	L4750	L4751	L4752	L4753	L4754	L4755	L4756	L4757	L4758	L4759	L4760	L4761	L4762	L4763	L4764	L4765	L4766	L4767	L4768	L4769	L4770	L4771	L4772	L4773	L4774	L4775	L4776	L4777	L4778	L4779	L4780	L4781	L4782	L4783	L4784	L4785	L4786	L4787	L4788	L4789	L4790	L4791	L4792	L4793	L4794	L4795	L4796	L4797	L4798	L4799	L4800	L4801	L4802	L4803	L4804	L4805	L4806	L4807	L4808	L4809	L4810	L4811	L4812	L4813	L4814	L4815	L4816	L4817	L4818	L4819	L4820	L4821	L48



• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	175.56Å 118.13Å 201.02Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 70.46 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-3.60) 99.2 (70.46-3.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.7.0019	Depositor
R, R_{free}	0.241 , 0.302 0.236 , 0.300	Depositor DCC
R_{free} test set	4766 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	127.5	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 117.1	EDS
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 94922 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	41642	wwPDB-VP
Average B, all atoms (Å ²)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, SO4, 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	0.53	0/21146	0.77	7/28618 (0.0%)
1	B	0.46	2/21146 (0.0%)	0.68	5/28618 (0.0%)
All	All	0.49	2/42292 (0.0%)	0.73	12/57236 (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	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3306	TRP	CE3-CZ3	-6.25	1.27	1.38
1	B	3306	TRP	CE2-CZ2	-5.22	1.30	1.39

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2012	LEU	CA-CB-CG	7.99	133.67	115.30
1	A	1741	LEU	CB-CG-CD1	6.69	122.38	111.00
1	A	3792	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	1782	LEU	CB-CG-CD2	-5.54	101.59	111.00
1	B	2460	ARG	NE-CZ-NH2	-5.52	117.54	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2119	LEU	Peptide
1	B	2620	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	20748	0	20206	952	0
1	B	20748	0	20206	909	0
2	A	31	0	12	8	0
2	B	31	0	12	17	0
3	A	31	0	13	7	0
3	B	31	0	13	7	0
4	A	10	0	0	3	0
4	B	10	0	0	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	41642	0	40462	1861	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 23.

The worst 5 of 1861 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:216:PRO:CB	1:A:1365:PHE:CE1	2.05	1.38
1:B:3303:LYS:HD2	1:B:3306:TRP:CD1	1.67	1.28
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.53	1.25
1:A:1368:GLU:HG2	1:A:1424:PHE:CZ	1.69	1.24
1:B:2467:THR:HB	1:B:2473:LEU:CD1	1.66	1.23

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 X-ray entries followed by that with respect to entries of similar resolution.

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	2640/2695 (98%)	2518 (95%)	110 (4%)	12 (0%)	34	77
1	B	2640/2695 (98%)	2515 (95%)	111 (4%)	14 (0%)	34	77
All	All	5280/5390 (98%)	5033 (95%)	221 (4%)	26 (0%)	34	77

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY
1	B	1391	GLY
1	B	3578	LEU
1	A	24	GLU
1	A	1633	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	2218/2453 (90%)	2138 (96%)	80 (4%)	42	78
1	B	2218/2453 (90%)	2137 (96%)	81 (4%)	41	77
All	All	4436/4906 (90%)	4275 (96%)	161 (4%)	42	78

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3940	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1826	PHE
1	B	3899	ASP
1	A	3958	ASP
1	B	1421	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	3962	GLN
1	B	1736	GLN
1	B	3783	ASN
1	A	3970	ASN
1	B	1501	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	ATP	A	5093	5	24,33,33	1.06	2 (8%)	31,52,52	2.00	5 (16%)
3	ANP	A	5094	-	27,33,33	3.06	6 (22%)	30,52,52	1.99	5 (16%)
4	SO4	A	5095	-	4,4,4	0.69	0	6,6,6	0.89	0
4	SO4	A	5096	-	4,4,4	0.54	0	6,6,6	0.21	0
2	ATP	B	5093	5	24,33,33	1.04	2 (8%)	31,52,52	1.98	5 (16%)
3	ANP	B	5094	-	27,33,33	3.12	6 (22%)	30,52,52	1.89	4 (13%)
4	SO4	B	5095	-	4,4,4	0.47	0	6,6,6	0.42	0
4	SO4	B	5096	-	4,4,4	0.44	0	6,6,6	0.19	0

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	ATP	A	5093	5	-	0/18/38/38	0/3/3/3
3	ANP	A	5094	-	-	0/12/38/38	0/3/3/3
4	SO4	A	5095	-	-	0/0/0/0	0/0/0/0
4	SO4	A	5096	-	-	0/0/0/0	0/0/0/0
2	ATP	B	5093	5	-	0/18/38/38	0/3/3/3
3	ANP	B	5094	-	-	1/12/38/38	0/3/3/3
4	SO4	B	5095	-	-	0/0/0/0	0/0/0/0
4	SO4	B	5096	-	-	0/0/0/0	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ANP	PG-O3G	-2.96	1.48	1.56
3	A	5094	ANP	PG-O3G	-2.91	1.48	1.56
3	A	5094	ANP	O4'-C1'	2.04	1.43	1.41
2	A	5093	ATP	O4'-C1'	2.07	1.43	1.41
3	B	5094	ANP	PB-O1B	2.13	1.48	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5094	ANP	N3-C2-N1	-7.14	123.42	128.89
3	B	5094	ANP	N3-C2-N1	-6.72	123.75	128.89
2	A	5093	ATP	N3-C2-N1	-6.69	123.77	128.89
2	B	5093	ATP	N3-C2-N1	-6.53	123.89	128.89
2	B	5093	ATP	PA-O3A-PB	-4.48	120.16	132.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5094	ANP	O1G-PG-N3B-PB

There are no ring outliers.

6 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5093	ATP	8	0
3	A	5094	ANP	7	0
4	A	5095	SO4	3	0
2	B	5093	ATP	17	0
3	B	5094	ANP	7	0
4	B	5096	SO4	3	0

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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2650/2695 (98%)	0.13	68 (2%) 59 44	69, 151, 281, 423	0
1	B	2650/2695 (98%)	0.66	278 (10%) 8 6	92, 193, 357, 500	0
All	All	5300/5390 (98%)	0.40	346 (6%) 22 14	69, 172, 321, 500	0

The worst 5 of 346 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	ASP	25.0
1	B	164	MET	22.5
1	B	213	ASP	20.8
1	B	29	GLU	20.0
1	B	163	TYR	19.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	A	5095	5/5	0.96	0.25	0.94	84,98,104,105	0
2	ATP	A	5093	31/31	0.95	0.29	0.19	88,123,185,204	0
3	ANP	B	5094	31/31	0.89	0.29	-0.05	112,145,237,257	0
3	ANP	A	5094	31/31	0.94	0.27	-0.31	111,140,238,248	0
2	ATP	B	5093	31/31	0.92	0.24	-0.35	99,141,184,200	0
4	SO4	B	5096	5/5	0.95	0.14	-0.78	155,168,174,176	0
5	MG	A	5097	1/1	0.99	0.22	-1.10	62,62,62,62	0
4	SO4	B	5095	5/5	0.84	0.18	-1.17	152,154,166,167	0
4	SO4	A	5096	5/5	0.96	0.20	-1.50	115,130,143,145	0
5	MG	B	5097	1/1	0.97	0.18	-	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.