



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:49 PM GMT

PDB ID : 4AKG
Title : Dynein Motor Domain - ATP complex
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on : 2012-02-22
Resolution : 3.30 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

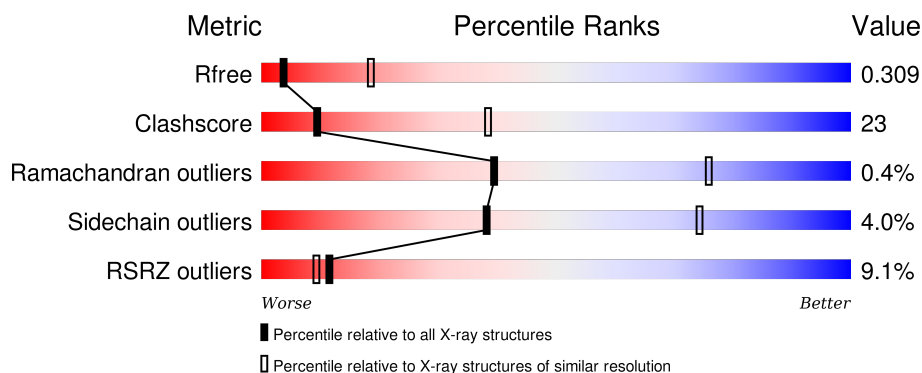
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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>5%</div> <div>64%</div> <div>32%</div> <div>..</div> </div>
1	B	2695	<div> <div>12%</div> <div>68%</div> <div>29%</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	A	5093	-	-	X	-
2	ATP	B	5093	-	-	X	-
4	MG	A	5095	-	-	-	X
4	MG	B	5095	-	-	-	X
5	SO4	A	5096	-	-	-	X
5	SO4	A	5097	-	-	X	-
5	SO4	B	5096	-	-	X	X
5	SO4	B	5097	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 41634 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.

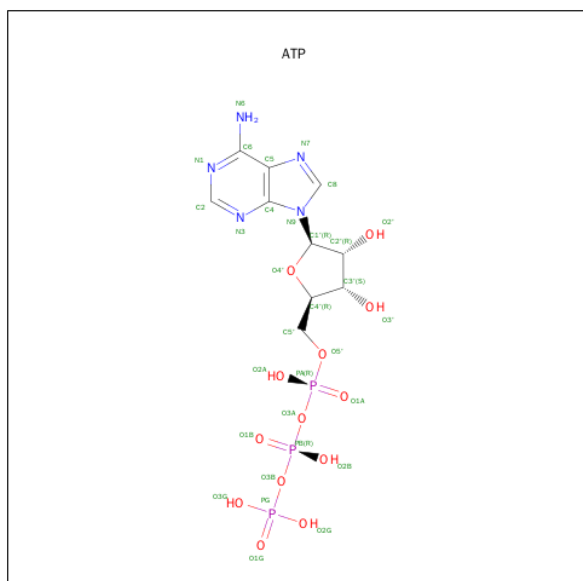
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

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:

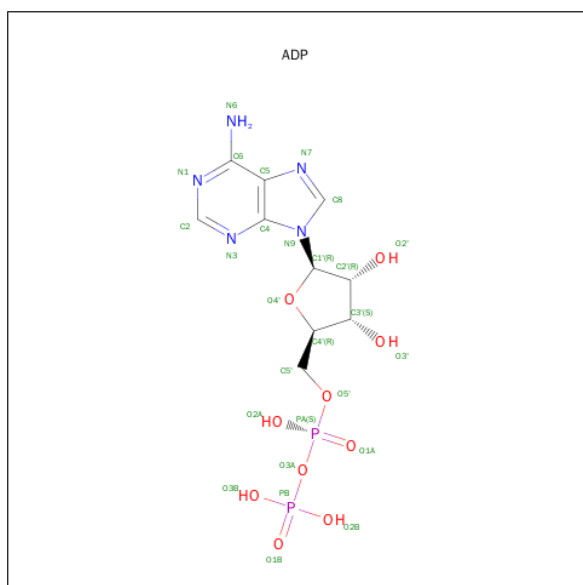
Chain	Residue	Modelled	Actual	Comment	Reference
A	1630	ILE	LEU	CONFLICT	UNP P36022
A	3782	ASP	GLU	CONFLICT	UNP P36022
B	1630	ILE	LEU	CONFLICT	UNP P36022
B	3782	ASP	GLU	CONFLICT	UNP P36022

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



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

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

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

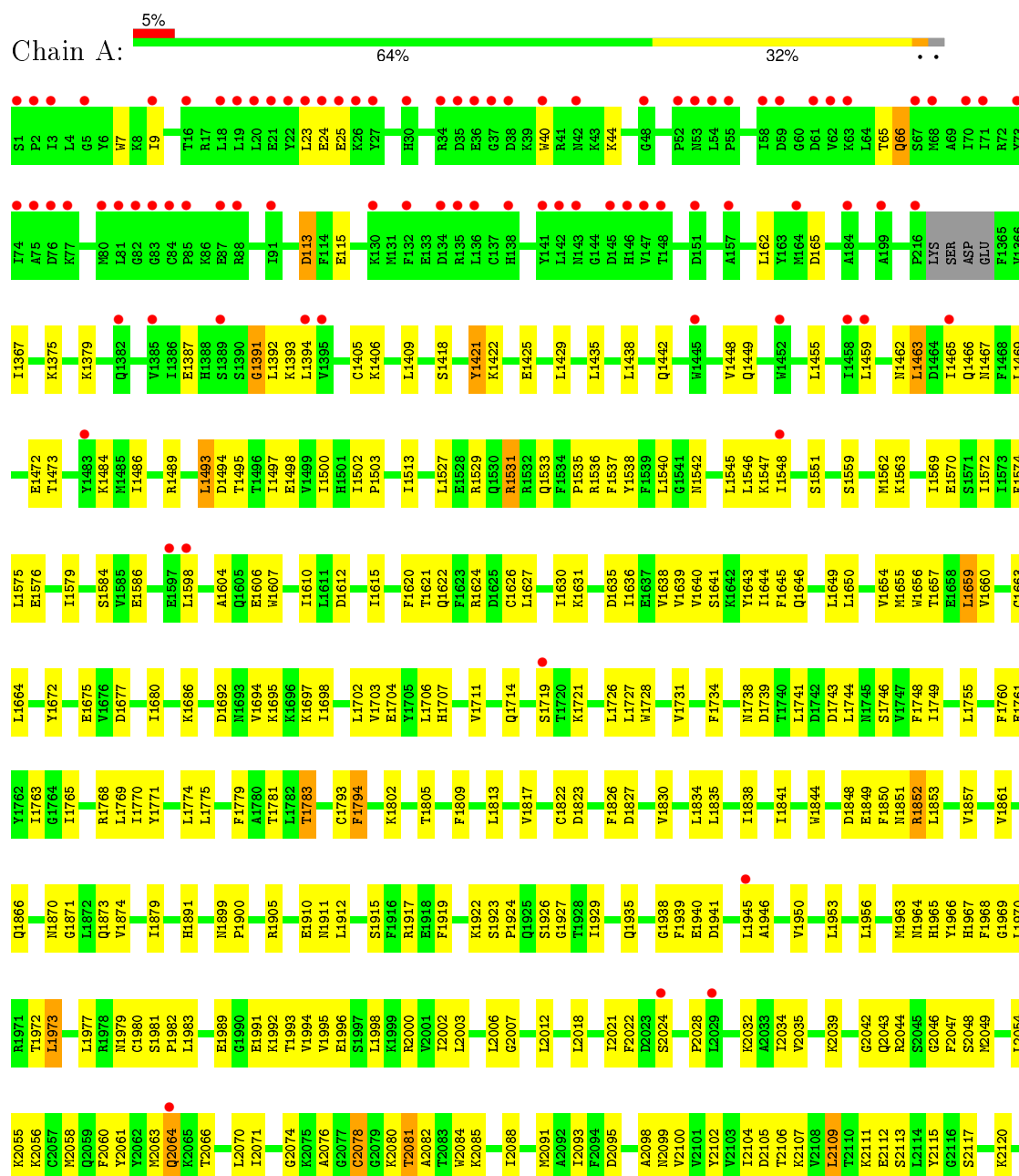


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

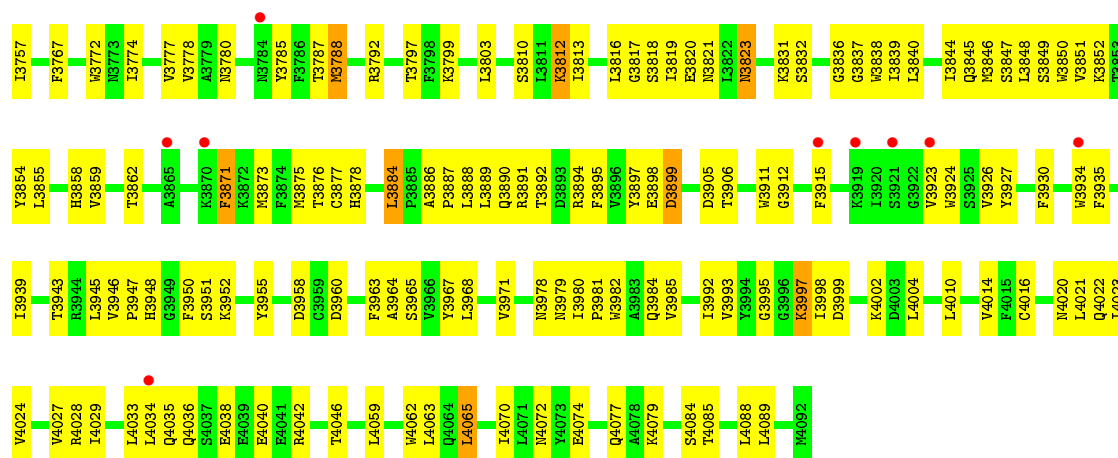
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

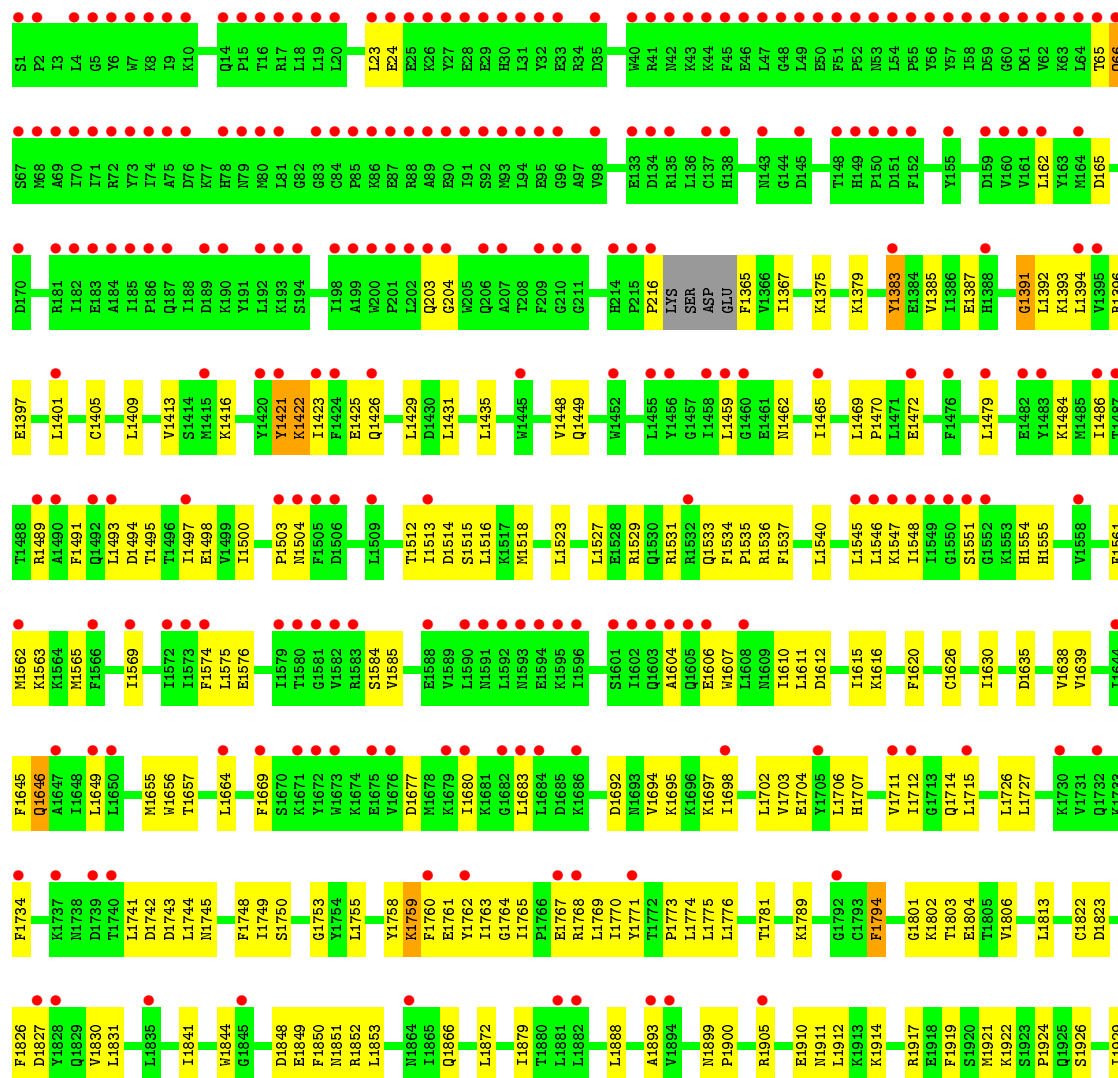
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC

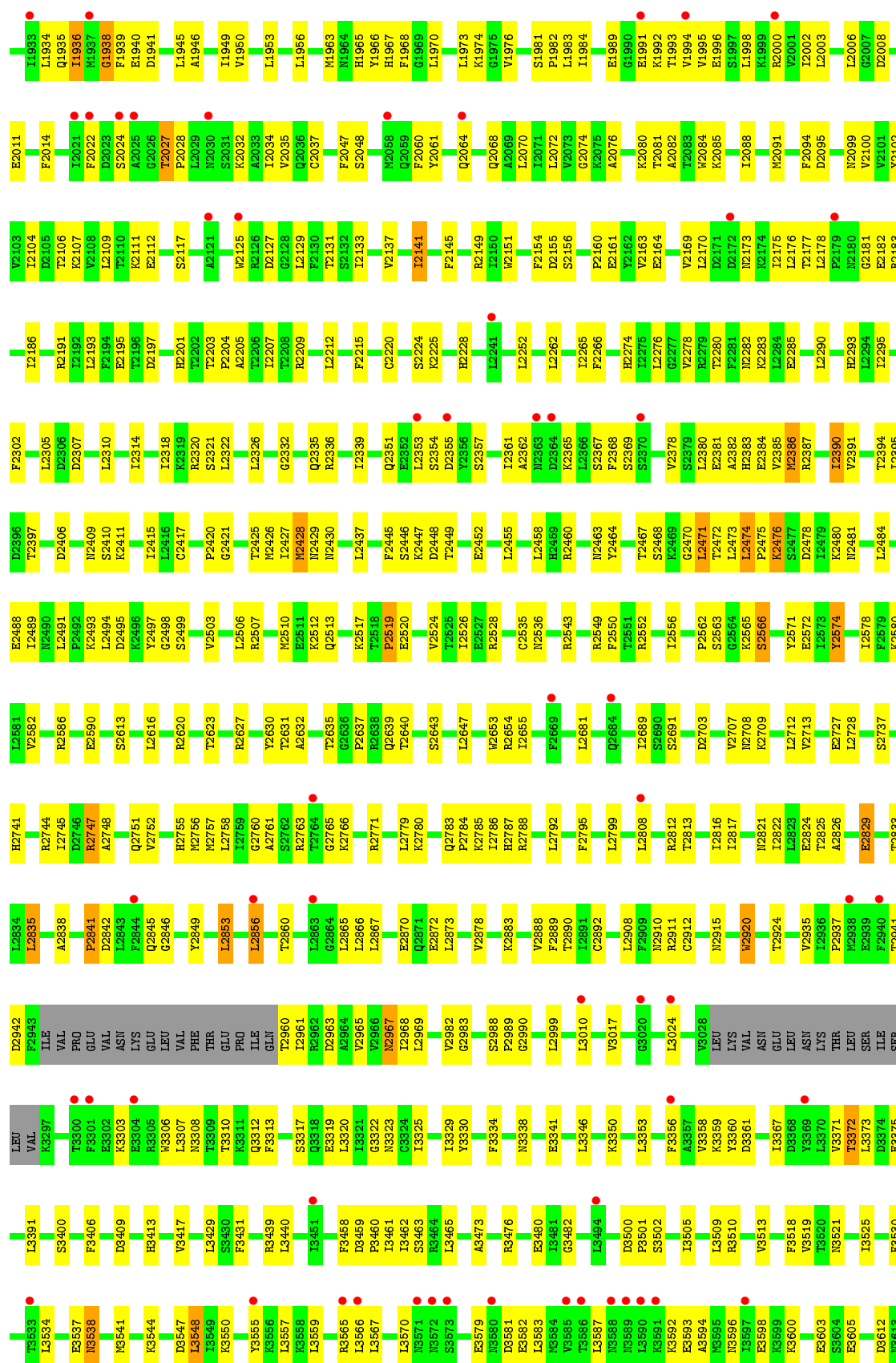






● Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC





K4002	F3915	L3841	S3727	L3614
D4003	F3916		E3728	V3615
L4004	T3917	T3844	S3729	
E4005	G3918	Q3845		Y3618
V4006	K3919	K3846	F3734	
	L3920	S3847	K3735	G3622
K4009		L3848	L3736	
	V3923	S3849	T3737	I3628
V4014	K3924	K3850	T3740	M3631
F4015	S3925	V3851		
C4016	V3926		R3745	F3641
G4017	V3927	Y3854		
		L3855	F3767	S3645
N4020	F3930	H3856	F3768	I3646
L4021		K3857	V3769	
Q4022	K3934	H3858		K3654
I4023	F3935	V3859	W3772	R3655
V4024		E3860	K3773	V3656
	I3939		I3774	F3657
V4027		K3865		I3658
R4028	T3943	E3866	V3777	LYS
I4029	K3944		V3778	SER
	L3945	E3869		ARG
E4038	V3946	K3870	A3779	GLU
	P3947	F3871	M3780	THR
L4049		K3872		ALA
E4054	F3950	K3873	Y3785	ALA
P4055	S3951	F3874	F3786	ARG
		K3875	T3787	
	Y3955	T3876		ALA
L4059		C3877	R3792	ARG
S4060	K3958	H3878		T3669
S4061	C3959		K3799	R3670
W4062	D3960	D3882		V3671
L4063		K3883	L3803	
Q4064	F3963	L3884		I3674
L4065	A3964	P3885	S3807	
	S3965	A3886	K3808	L3677
I4070		F3887	E3809	L3678
E4074	L3968	L3888	S3810	Y3679
	E3969	L3889	L3811	
Q4077	N3970	K3890	K3812	
A4078	V3971		I3813	Y3683
K4079	L3972	F3895	L3814	
		V3896	P3815	S3687
T4085	N3978	Y3897	L3816	
E4086	K3979	E3898	G3817	L3690
Q4087	I3980	D3899	G3818	D3691
L4088	P3981	I3900	I3819	K3692
	K3982	P3901	E3820	K3693
	A3983		M3821	F3694
	Q3984	D3905	L3822	
	V3985	T3906	N3823	M3698
		V3907		A3699
	V3993	K3908	I3834	M3700
	V3994			T3701
	G3995			M3702
		M3911	G3837	
	I3998	G3912	W3838	T3705
		S3913	I3839	
		Q3914	L3840	L3726

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	175.33Å 117.92Å 202.76Å 90.00° 90.21° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 48.81 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-3.30) 96.1 (48.81-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.33Å)	Xtriage
Refinement program	REFMAC NULL	Depositor
R, R_{free}	0.239 , 0.305 0.239 , 0.309	Depositor DCC
R_{free} test set	5981 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	113.9	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 102.4	EDS
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 119750 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	41634	wwPDB-VP
Average B, all atoms (Å ²)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: ATP, MG, SO4, 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 >5	RMSZ	# Z >5
1	A	0.62	7/21146 (0.0%)	0.85	21/28618 (0.1%)
1	B	0.51	2/21146 (0.0%)	0.72	4/28618 (0.0%)
All	All	0.57	9/42292 (0.0%)	0.79	25/57236 (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	A	0	3
1	B	0	1
All	All	0	4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2064	GLN	CA-C	-8.38	1.31	1.52
1	B	2841	PRO	N-CD	-7.95	1.36	1.47
1	A	2495	ASP	C-N	-7.35	1.17	1.34
1	B	1759	LYS	C-O	6.47	1.35	1.23
1	A	2488	GLU	CD-OE1	5.63	1.31	1.25

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2412	ARG	NE-CZ-NH2	9.64	125.12	120.30
1	B	2471	LEU	CA-CB-CG	8.90	135.76	115.30
1	A	3459	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	A	2012	LEU	CA-CB-CG	7.53	132.62	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2212	LEU	CB-CG-CD1	-7.18	98.80	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ASP	Peptide
1	A	2007	GLY	Peptide
1	A	2521	ASN	Peptide
1	B	2727	GLU	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	20748	0	20205	957	0
1	B	20748	0	20206	896	0
2	A	31	0	12	10	0
2	B	31	0	12	24	0
3	A	27	0	12	2	0
3	B	27	0	12	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	0	2	0
5	B	10	0	0	4	0
All	All	41634	0	40459	1855	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 1855 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:2380:LEU:CD2	1:A:2390:ILE:HD11	1.55	1.33
1:B:1826:PHE:CE2	1:B:1831:LEU:HB2	1.66	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.55	1.24
1:B:216:PRO:O	1:B:1365:PHE:HD1	1.21	1.22
1:B:216:PRO:O	1:B:1365:PHE:CD1	1.94	1.20

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%)	2511 (95%)	118 (4%)	11 (0%)	39	76
1	B	2640/2695 (98%)	2525 (96%)	107 (4%)	8 (0%)	46	81
All	All	5280/5390 (98%)	5036 (95%)	225 (4%)	19 (0%)	39	76

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY
1	A	2495	ASP
1	B	1391	GLY
1	A	2476	LYS
1	A	2728	LEU

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%)	2115 (95%)	103 (5%)	33	71
1	B	2218/2453 (90%)	2145 (97%)	73 (3%)	45	78
All	All	4436/4906 (90%)	4260 (96%)	176 (4%)	38	74

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3729	SER
1	A	3997	LYS
1	B	3737	THR
1	A	3788	MET
1	A	3899	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4020	ASN
1	B	1851	ASN
1	B	3890	GLN
1	A	4077	GLN
1	B	1707	HIS

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	ATP	A	5093	4	24,33,33	0.98	1 (4%)	31,52,52	1.99	5 (16%)
3	ADP	A	5094	-	22,29,29	1.26	1 (4%)	27,45,45	2.36	5 (18%)
5	SO4	A	5096	-	4,4,4	1.48	1 (25%)	6,6,6	1.34	1 (16%)
5	SO4	A	5097	-	4,4,4	0.61	0	6,6,6	0.58	0
2	ATP	B	5093	4	24,33,33	1.08	1 (4%)	31,52,52	1.91	6 (19%)
3	ADP	B	5094	-	22,29,29	1.31	3 (13%)	27,45,45	2.46	8 (29%)
5	SO4	B	5096	-	4,4,4	1.25	1 (25%)	6,6,6	1.94	1 (16%)
5	SO4	B	5097	-	4,4,4	0.46	0	6,6,6	0.44	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	4	-	0/18/38/38	0/3/3/3
3	ADP	A	5094	-	-	0/12/32/32	0/3/3/3
5	SO4	A	5096	-	-	0/0/0/0	0/0/0/0
5	SO4	A	5097	-	-	0/0/0/0	0/0/0/0
2	ATP	B	5093	4	-	0/18/38/38	0/3/3/3
3	ADP	B	5094	-	-	0/12/32/32	0/3/3/3
5	SO4	B	5096	-	-	0/0/0/0	0/0/0/0
5	SO4	B	5097	-	-	0/0/0/0	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ADP	PB-O3B	-2.10	1.47	1.54
5	B	5096	SO4	O2-S	2.05	1.54	1.47
3	B	5094	ADP	C4-N3	2.55	1.39	1.35
5	A	5096	SO4	O1-S	2.89	1.57	1.47
2	A	5093	ATP	C5-C4	3.13	1.47	1.40

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5094	ADP	N3-C2-N1	-10.12	121.14	128.89
3	B	5094	ADP	N3-C2-N1	-9.35	121.73	128.89
2	A	5093	ATP	N3-C2-N1	-6.70	123.77	128.89
2	B	5093	ATP	N3-C2-N1	-5.61	124.60	128.89
2	B	5093	ATP	PA-O3A-PB	-4.38	120.43	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5093	ATP	10	0
3	A	5094	ADP	2	0
5	A	5097	SO4	2	0
2	B	5093	ATP	24	0
3	B	5094	ADP	6	0
5	B	5096	SO4	2	0
5	B	5097	SO4	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.21	147 (5%)	29 23	62, 134, 265, 480	1 (0%)
1	B	2650/2695 (98%)	0.70	336 (12%)	5 4	83, 185, 334, 500	1 (0%)
All	All	5300/5390 (98%)	0.46	483 (9%)	11 9	62, 158, 303, 500	2 (0%)

The worst 5 of 483 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	SER	19.7
1	B	59	ASP	17.7
1	B	69	ALA	17.3
1	B	31	LEU	16.5
1	B	60	GLY	15.3

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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
5	SO4	A	5096	5/5	0.91	0.45	6.98	77,106,130,132	0
4	MG	A	5095	1/1	0.89	0.40	5.42	76,76,76,76	0
5	SO4	B	5096	5/5	0.87	0.53	3.27	86,103,146,179	0
4	MG	B	5095	1/1	0.97	0.34	2.52	86,86,86,86	0
5	SO4	A	5097	5/5	0.97	0.21	1.25	82,93,104,115	0
2	ATP	A	5093	31/31	0.93	0.28	1.24	78,92,129,144	0
2	ATP	B	5093	31/31	0.92	0.26	0.57	93,138,174,217	0
5	SO4	B	5097	5/5	0.97	0.17	0.44	157,162,176,183	0
3	ADP	B	5094	27/27	0.90	0.27	0.26	81,114,155,168	0
3	ADP	A	5094	27/27	0.94	0.25	-0.12	91,101,113,131	0

6.5 Other polymers [i](#)

There are no such residues in this entry.