



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:39 PM GMT

PDB ID : 1BR4
Title : SMOOTH MUSCLE MYOSIN MOTOR DOMAIN-ESSENTIAL LIGHT CHAIN COMPLEX WITH MGADP.BEF3 BOUND AT THE ACTIVE SITE
Authors : Dominguez, R.; Trybus, K.M.; Cohen, C.
Deposited on : 1998-08-27
Resolution : 3.62 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

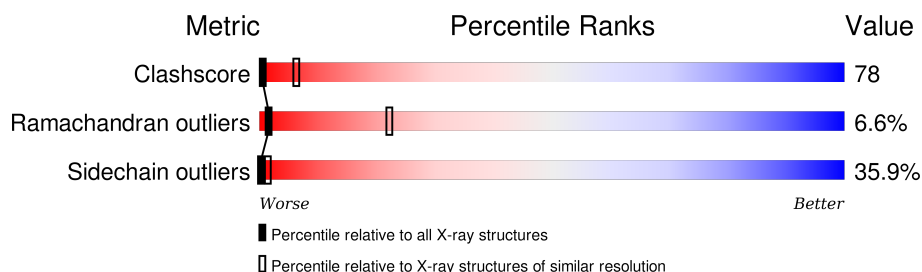
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.62 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))
Clashscore	102246	1043 (3.78-3.46)
Ramachandran outliers	100387	1003 (3.78-3.46)
Sidechain outliers	100360	1003 (3.78-3.46)


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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	820	
1	C	820	
1	E	820	
1	G	820	
2	B	150	
2	D	150	
2	F	150	

Continued on next page...

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Mol	Chain	Length	Quality of chain
2	H	150	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: green (15%), yellow (52%), and orange (31%). The segments are labeled with their respective percentages. The bar ends with a small red segment and two black dots.

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 29948 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 MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			6292	4009	1078	1176	29			
1	C	781	Total	C	N	O	S	0	0	0
			6292	4009	1078	1176	29			
1	E	781	Total	C	N	O	S	0	0	0
			6292	4009	1078	1176	29			
1	G	781	Total	C	N	O	S	0	0	0
			6292	4009	1078	1176	29			

- Molecule 2 is a protein called MYOSIN.

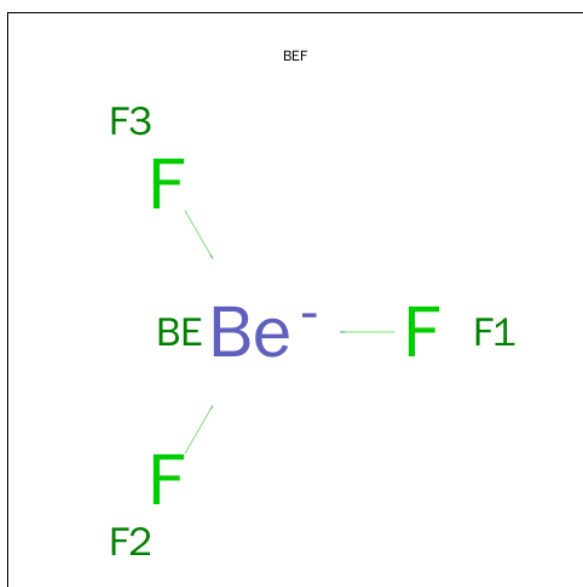
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	148	Total	C	N	O	S	0	0	0
			1161	722	193	235	11			
2	D	148	Total	C	N	O	S	0	0	0
			1161	722	193	235	11			
2	F	148	Total	C	N	O	S	0	0	0
			1161	722	193	235	11			
2	H	148	Total	C	N	O	S	0	0	0
			1161	722	193	235	11			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

-

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Be	F	0	0
			4	1	3		
5	C	1	Total	Be	F	0	0
			4	1	3		
5	E	1	Total	Be	F	0	0
			4	1	3		
5	G	1	Total	Be	F	0	0
			4	1	3		

- Molecule 6 is water.

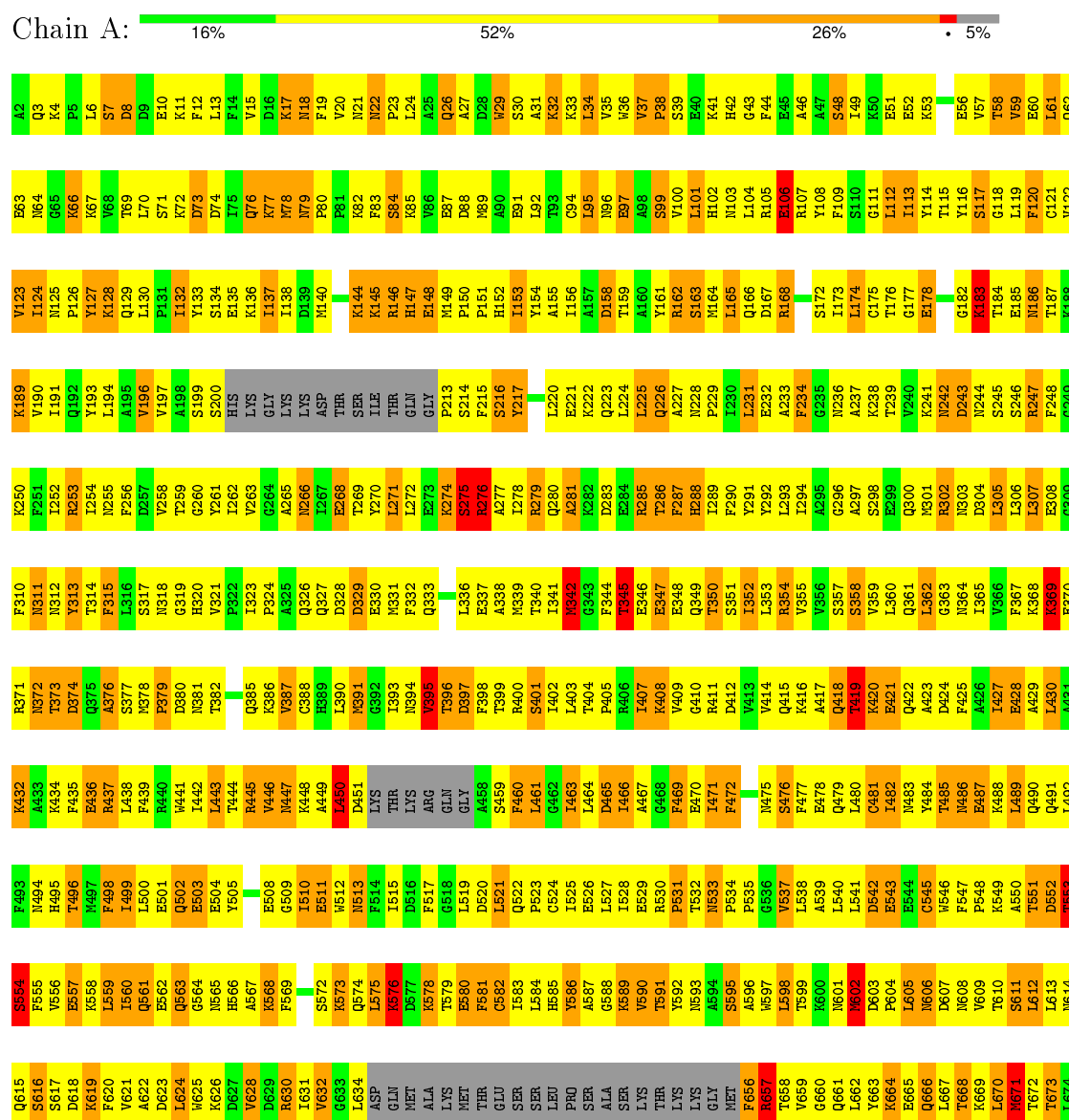
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	C	2	Total	O	0	0
			2	2		
6	E	2	Total	O	0	0
			2	2		
6	G	2	Total	O	0	0
			2	2		

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.

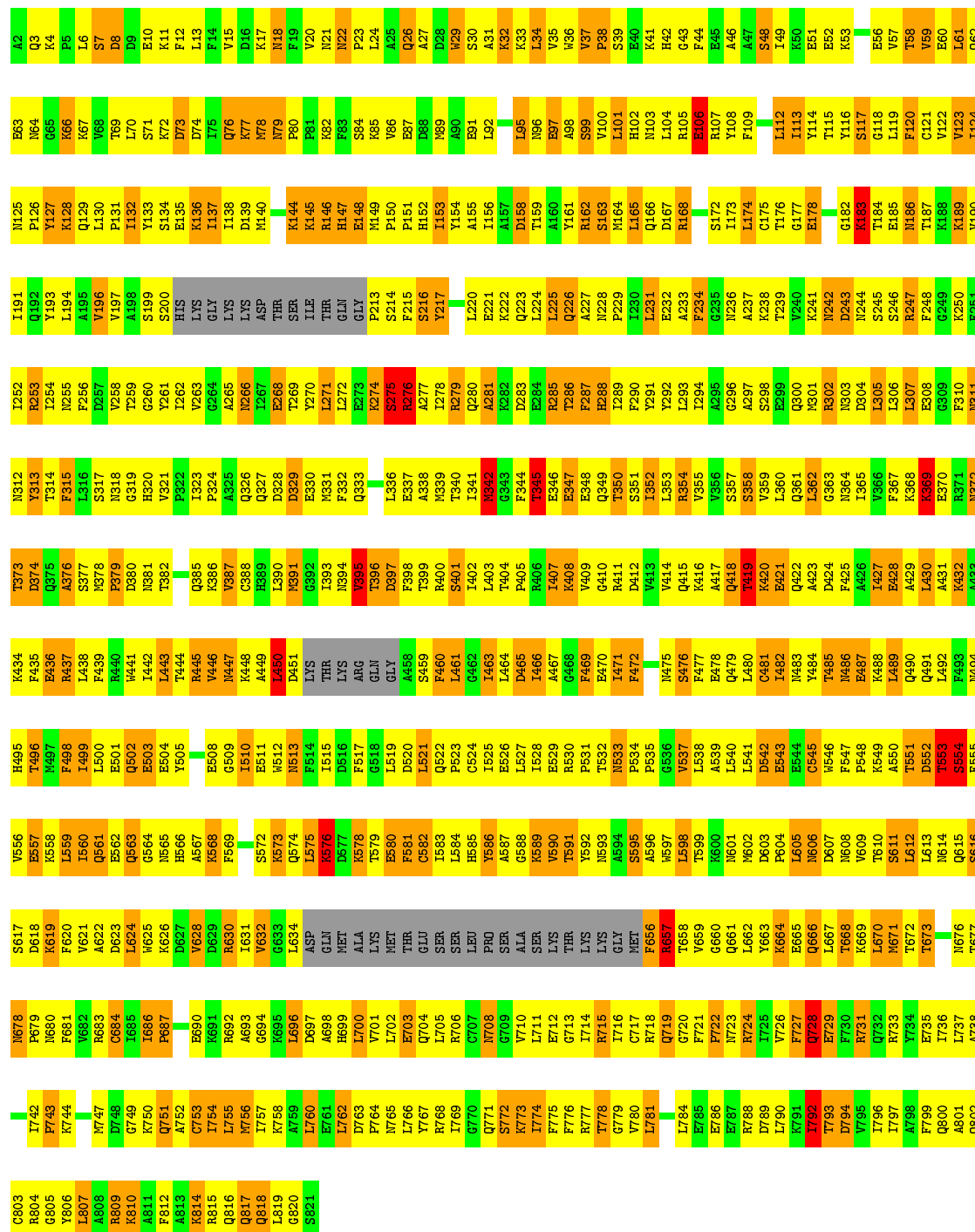
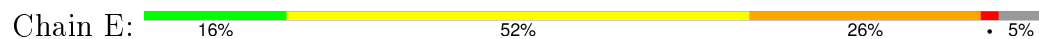
Note EDS was not executed.

• Molecule 1: MYOSIN

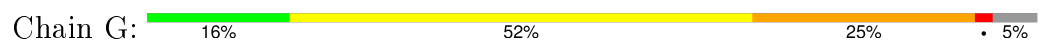




• Molecule 1: MYOSIN



• Molecule 1: MYOSIN



Q800	A801	Q802	C803	R804	G805	Y806	L807	A808	R809	K810	A811	F812	F813	A814	R815	L816	L817	L818	L819	L820	S821		F822	E823	D824	V825	E826	G827	N828	L829	R830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000																																															
K189	V190	I191	Q192	Y193	L194	A195	V196	I197	A198	N199	E200	K201	L202	L203	L204	L205	L206	L207	L208	L209	L210	L211	L212	L213	L214	L215	L216	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240	K241	N242	D243	D244	S245	S246	R247	F248	G249	K250	F251	L252	R253	L254	N255	F256	V257	V258	T259	G260	K261	L262	V263	G264	A265	K266	L267	E268	T269	L270	L271	L272	L273	E274	K275	R276	L277	E278	L279	L280	L281	K282	L283	L284	L285	T286	F287	H288	L289	F290	Y291	Y292	L293	L294	A295	G296	A297	S298	E299	Q300	K301	R302	N303	D304	L305	L306	L307	K308	E309	F310	N311	N312	Y313	T314	F315	L316	S317	N318	G319	K320	V321	P322	L323	P324	A325	Q326	Q327	D328	D329	E330	N331	F332	Q333		L336	E337	A338	N339	T340	L341	K342	G343	P344	E345	E346	K347	V348	V349	G400	R401	T350	S351	L352	L353	R354	V355	V356	S357	S358	V359	L360	Q361	L362	G363	N364	L365	V366	F367	K368	E369	E370		K371	N372	T373	D374	Q375	R376	S377	K378	P379	D380	N381	T382		Q385	K386	V387	K388	L389	M390	G391	N393	N394	V395	T396	D397	F398	T399	R400	S401	L402	L403	L404	L405	R406	I407	K408	V409	G410	R411	T412		V413	V414	L415	L416	L417		N475	S476	F477	L478	L479	L480	L481	L482	L483	C484	T485	N486	F487	P488	K489	A490	T491	L492
S554	F555	V556	E557	K558	L559	L560	Q561	E562	Q563	E564	N565	H566	A567	K568	F569		S572	K573	Q574	L575	D576	K577	K578	T579	E580	F581	C582	L583	L584	L585	L586	A587	K588	L589	T590	L591	L592	N593	S594	A595	V596	L597	L598	T599	K600	N601	L602	L603	L604	L605	L606	D607	N608	V609	T610	S611	L612	L613	N614		Q615	S616	S617	D618	K619	F620	R621	A622	D623	W624	W625	K626	D627	V628	D629	R630	L631	V632	G633	L634	A635	G636	M637	ALA	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	Q660	Q661	L662	V663	K664	E665	Q666	L667	T668	K669	F670	L671	L672	L673	L674																																																																																																																															
R675	L676	T677	N678	N679	N680	F681	V682	F683	G684	L685	L686	P687		E690	F691	R692	A693	G694	K695	L696	D697	A698	H699	L700	V701	L702	E703	Q704	L705	L706	G707	N708	S709	L710	L711	L712	L713	L714	L715	L716	C717	R718	Q719	G720	F721	P722	N723	R724	L725	V726	F727	Q728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	N765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	G779	V780	L781		L784	E785	L786	L787	L788	L789	L790	L791	N792	L793	L794	L795	L796	L797	L798	F799																																																																																																																														
Q800	A801	Q802	C803	R804	G805	Y806	L807	A808	R809	K810	A811	F812	A813	R814	R815	L816	L817	L818	L819	L820	S821		F822	E823	D824	V825	E826	G827	N828	L829	R830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000																																															

• Molecule 2: MYOSIN

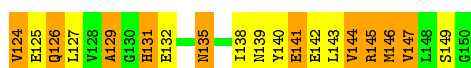
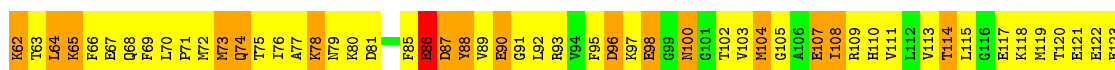
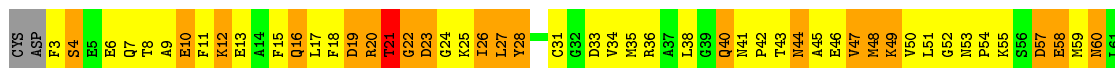
Chain B: 16% 50% 31% . .

CYS	ASP	K62	T63	K65	L64	K66	F66	E67	Q68	F69	L70	F71	M72	M73	Q74	T75	L76	A77	K78	M79	K80	D81	F85	E86	D87	Y88	V89	E90	G91	L92	R93	Y94	G95	D96	R97	E98	G99	N100	G101	T102	V103	M104	G105	A106	E107	L108	R109	H110	V111	L112	V113	T114	L115	N116	P117	K118	S119	M120	E121	E122	L123
ASP	F3	S4	E5	E6	Q7	T8	A9	E10	F11	K12	K13	E14	F15	Q16	L17	F18	D19	R20	T21	D22	G24	I26	L27	Y28	G31	G32	D33	V34	R35	R36	A37	L38	G39	Q40	M41	P42	T43	G44	A45	E46	V47	K48	V49	L51	G52	N53	P54	K55	D56	S57	E58	M59	N60	L61							



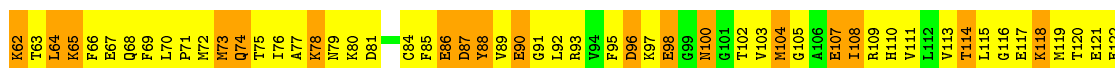
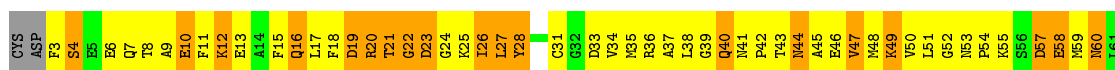
• Molecule 2: MYOSIN

Chain D: 17% 50% 30% ..



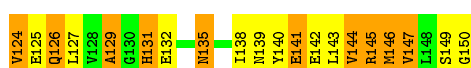
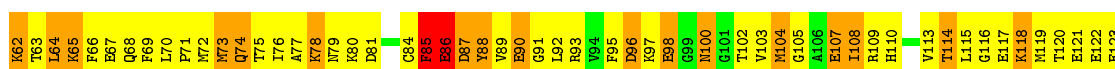
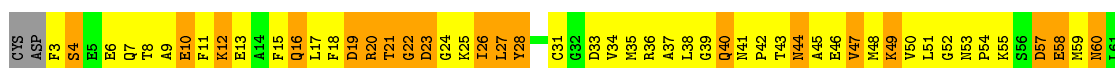
• Molecule 2: MYOSIN

Chain F: 15% 53% 31% .



• Molecule 2: MYOSIN

Chain H: 15% 52% 31% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	95.32Å 144.66Å 147.29Å 111.21° 106.10° 92.58°	Depositor
Resolution (Å)	10.00 – 3.62	Depositor
% Data completeness (in resolution range)	95.7 (10.00-3.62)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.277 , 0.352	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29948	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BEF, 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	0.47	0/6410	0.73	4/8640 (0.0%)
1	C	0.48	0/6410	0.74	2/8640 (0.0%)
1	E	0.49	0/6410	0.75	3/8640 (0.0%)
1	G	0.48	0/6410	0.75	4/8640 (0.0%)
2	B	0.64	0/1176	0.91	5/1575 (0.3%)
2	D	0.59	0/1176	0.86	1/1575 (0.1%)
2	F	0.59	0/1176	0.86	1/1575 (0.1%)
2	H	0.58	0/1176	0.84	0/1575
All	All	0.50	0/30344	0.77	20/40860 (0.0%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	ARG	NE-CZ-NH2	7.51	124.05	120.30
1	E	276	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	A	279	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	C	276	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	G	276	ARG	NE-CZ-NH2	7.38	123.99	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6292	0	6301	979	3
1	C	6292	0	6301	952	0
1	E	6292	0	6301	973	0
1	G	6292	0	6301	975	11
2	B	1161	0	1126	223	0
2	D	1161	0	1126	211	11
2	F	1161	0	1126	221	3
2	H	1161	0	1126	220	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	27	0	12	3	0
4	C	27	0	12	4	0
4	E	27	0	12	2	0
4	G	27	0	12	3	0
5	A	4	0	0	0	0
5	C	4	0	0	0	0
5	E	4	0	0	0	0
5	G	4	0	0	0	0
6	A	2	0	0	0	0
6	C	2	0	0	0	0
6	E	2	0	0	0	0
6	G	2	0	0	0	0
All	All	29948	0	29756	4645	14

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 78.

The worst 5 of 4645 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:814:LYS:O	1:A:817:GLN:HG3	1.28	1.32
1:C:814:LYS:O	1:C:817:GLN:HG3	1.27	1.32
1:A:747:MET:SD	1:G:812:PHE:HZ	1.53	1.31
1:G:814:LYS:O	1:G:817:GLN:HG3	1.28	1.29
1:E:814:LYS:O	1:E:817:GLN:HG3	1.28	1.24

The worst 5 of 14 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:GLY:N	1:G:371:ARG:CZ[1_545]	1.62	0.58
2:D:22:GLY:CA	1:G:371:ARG:NE[1_545]	1.63	0.57
2:D:22:GLY:N	1:G:371:ARG:NE[1_545]	1.74	0.46
2:D:23:ASP:N	1:G:371:ARG:NH2[1_545]	1.83	0.37
2:D:22:GLY:N	1:G:371:ARG:NH1[1_545]	1.91	0.29

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	773/820 (94%)	579 (75%)	139 (18%)	55 (7%)	1	19
1	C	773/820 (94%)	580 (75%)	138 (18%)	55 (7%)	1	19
1	E	773/820 (94%)	580 (75%)	138 (18%)	55 (7%)	1	19
1	G	773/820 (94%)	580 (75%)	138 (18%)	55 (7%)	1	19
2	B	146/150 (97%)	111 (76%)	29 (20%)	6 (4%)	3	34
2	D	146/150 (97%)	112 (77%)	28 (19%)	6 (4%)	3	34
2	F	146/150 (97%)	112 (77%)	29 (20%)	5 (3%)	5	41
2	H	146/150 (97%)	113 (77%)	26 (18%)	7 (5%)	3	30
All	All	3676/3880 (95%)	2767 (75%)	665 (18%)	244 (7%)	1	22

5 of 244 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	PRO
1	A	145	LYS
1	A	183	LYS
1	A	233	ALA
1	A	288	HIS

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 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	685/718 (95%)	447 (65%)	238 (35%)	0	2
1	C	685/718 (95%)	446 (65%)	239 (35%)	0	2
1	E	685/718 (95%)	446 (65%)	239 (35%)	0	2
1	G	685/718 (95%)	446 (65%)	239 (35%)	0	2
2	B	127/129 (98%)	75 (59%)	52 (41%)	0	1
2	D	127/129 (98%)	74 (58%)	53 (42%)	0	1
2	F	127/129 (98%)	74 (58%)	53 (42%)	0	1
2	H	127/129 (98%)	73 (58%)	54 (42%)	0	1
All	All	3248/3388 (96%)	2081 (64%)	1167 (36%)	0	1

5 of 1167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	817	GLN
1	E	258	VAL
1	G	686	ILE
2	D	47	VAL
1	E	37	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	751	GLN
1	E	288	HIS
1	G	689	HIS
2	D	7	GLN
2	D	139	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
4	ADP	A	998	3,5	22,29,29	1.01	2 (9%)	27,45,45	1.32	4 (14%)
5	BEF	A	999	3,4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	C	998	3,5	22,29,29	1.02	2 (9%)	27,45,45	1.32	4 (14%)
5	BEF	C	999	3,4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	E	998	3,5	22,29,29	1.01	2 (9%)	27,45,45	1.31	4 (14%)
5	BEF	E	999	3,4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	G	998	3,5	22,29,29	1.01	2 (9%)	27,45,45	1.32	4 (14%)
5	BEF	G	999	3,4	0,3,3	0.00	-	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	998	3,5	-	0/12/32/32	0/3/3/3
5	BEF	A	999	3,4	-	0/0/0/0	0/0/0/0
4	ADP	C	998	3,5	-	0/12/32/32	0/3/3/3
5	BEF	C	999	3,4	-	0/0/0/0	0/0/0/0
4	ADP	E	998	3,5	-	0/12/32/32	0/3/3/3
5	BEF	E	999	3,4	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	G	998	3,5	-	0/12/32/32	0/3/3/3
5	BEF	G	999	3,4	-	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)
4	C	998	ADP	O4'-C1'	-2.30	1.38	1.41
4	E	998	ADP	O4'-C1'	-2.28	1.38	1.41
4	G	998	ADP	O4'-C1'	-2.23	1.38	1.41
4	A	998	ADP	O4'-C1'	-2.23	1.38	1.41
4	A	998	ADP	C2-N3	2.01	1.35	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	998	ADP	C1'-N9-C4	-2.99	122.43	126.94
4	G	998	ADP	C1'-N9-C4	-2.97	122.46	126.94
4	C	998	ADP	C1'-N9-C4	-2.96	122.48	126.94
4	E	998	ADP	C1'-N9-C4	-2.96	122.48	126.94
4	A	998	ADP	N6-C6-N1	-2.94	112.89	119.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	998	ADP	3	0
4	C	998	ADP	4	0
4	E	998	ADP	2	0
4	G	998	ADP	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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.