



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:42 PM GMT

PDB ID : 1LKX
Title : MOTOR DOMAIN OF MYOE, A CLASS-I MYOSIN
Authors : Kollmar, M.; Durrwang, U.; Kliche, W.; Manstein, D.J.; Kull, F.J.
Deposited on : 2002-04-26
Resolution : 3.00 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

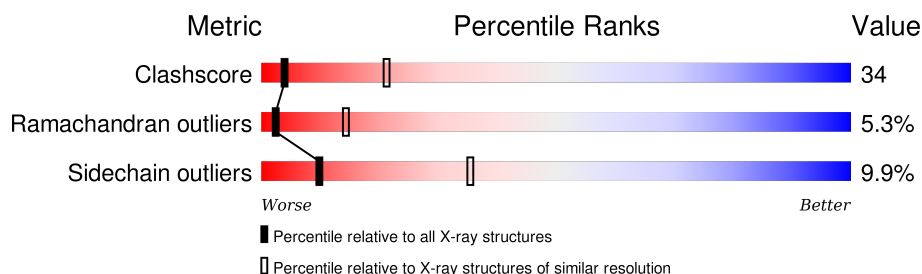
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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	697	
1	B	697	
1	C	697	
1	D	697	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21265 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 IE HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	0	0	0
			5192	3285	890	988	29			
1	B	650	Total	C	N	O	S	0	0	0
			5188	3282	889	988	29			
1	C	679	Total	C	N	O	S	0	0	0
			5422	3427	932	1033	30			
1	D	660	Total	C	N	O	S	0	0	0
			5267	3329	903	1005	30			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLU	ASP	SEE REMARK 999	UNP Q03479
A	48	THR	ARG	SEE REMARK 999	UNP Q03479
A	77	MET	ILE	SEE REMARK 999	UNP Q03479
A	?	-	ILE	SEE REMARK 999	UNP Q03479
A	?	-	ARG	SEE REMARK 999	UNP Q03479
A	137	LEU	PHE	SEE REMARK 999	UNP Q03479
A	138	ASP	GLN	SEE REMARK 999	UNP Q03479
A	215	ASP	ASN	SEE REMARK 999	UNP Q03479
A	371	ILE	LEU	SEE REMARK 999	UNP Q03479
A	372	ILE	SER	SEE REMARK 999	UNP Q03479
A	373	ASN	ILE	SEE REMARK 999	UNP Q03479
A	374	CYS	VAL	SEE REMARK 999	UNP Q03479
A	375	THR	HIS	SEE REMARK 999	UNP Q03479
A	376	THR	ARG	SEE REMARK 999	UNP Q03479
A	378	LYS	-	SEE REMARK 999	UNP Q03479
A	380	PRO	THR	SEE REMARK 999	UNP Q03479
A	427	VAL	-	SEE REMARK 999	UNP Q03479
A	428	ARG	-	SEE REMARK 999	UNP Q03479
A	429	GLU	LYS	SEE REMARK 999	UNP Q03479
A	440	ASN	-	SEE REMARK 999	UNP Q03479
A	498	ILE	ASN	SEE REMARK 999	UNP Q03479

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Chain	Residue	Modelled	Actual	Comment	Reference
A	604	VAL	ASP	SEE REMARK 999	UNP Q03479
A	681	ASN	ILE	SEE REMARK 999	UNP Q03479
A	683	THR	ARG	SEE REMARK 999	UNP Q03479
B	26	GLU	ASP	SEE REMARK 999	UNP Q03479
B	48	THR	ARG	SEE REMARK 999	UNP Q03479
B	77	MET	ILE	SEE REMARK 999	UNP Q03479
B	?	-	ILE	SEE REMARK 999	UNP Q03479
B	?	-	ARG	SEE REMARK 999	UNP Q03479
B	137	LEU	PHE	SEE REMARK 999	UNP Q03479
B	138	ASP	GLN	SEE REMARK 999	UNP Q03479
B	215	ASP	ASN	SEE REMARK 999	UNP Q03479
B	371	ILE	LEU	SEE REMARK 999	UNP Q03479
B	372	ILE	SER	SEE REMARK 999	UNP Q03479
B	373	ASN	ILE	SEE REMARK 999	UNP Q03479
B	374	CYS	VAL	SEE REMARK 999	UNP Q03479
B	375	THR	HIS	SEE REMARK 999	UNP Q03479
B	376	THR	ARG	SEE REMARK 999	UNP Q03479
B	378	LYS	-	SEE REMARK 999	UNP Q03479
B	380	PRO	THR	SEE REMARK 999	UNP Q03479
B	427	VAL	-	SEE REMARK 999	UNP Q03479
B	428	ARG	-	SEE REMARK 999	UNP Q03479
B	429	GLU	LYS	SEE REMARK 999	UNP Q03479
B	440	ASN	-	SEE REMARK 999	UNP Q03479
B	498	ILE	ASN	SEE REMARK 999	UNP Q03479
B	604	VAL	ASP	SEE REMARK 999	UNP Q03479
B	681	ASN	ILE	SEE REMARK 999	UNP Q03479
B	683	THR	ARG	SEE REMARK 999	UNP Q03479
C	26	GLU	ASP	SEE REMARK 999	UNP Q03479
C	48	THR	ARG	SEE REMARK 999	UNP Q03479
C	77	MET	ILE	SEE REMARK 999	UNP Q03479
C	?	-	ILE	SEE REMARK 999	UNP Q03479
C	?	-	ARG	SEE REMARK 999	UNP Q03479
C	137	LEU	PHE	SEE REMARK 999	UNP Q03479
C	138	ASP	GLN	SEE REMARK 999	UNP Q03479
C	215	ASP	ASN	SEE REMARK 999	UNP Q03479
C	371	ILE	LEU	SEE REMARK 999	UNP Q03479
C	372	ILE	SER	SEE REMARK 999	UNP Q03479
C	373	ASN	ILE	SEE REMARK 999	UNP Q03479
C	374	CYS	VAL	SEE REMARK 999	UNP Q03479
C	375	THR	HIS	SEE REMARK 999	UNP Q03479
C	376	THR	ARG	SEE REMARK 999	UNP Q03479
C	378	LYS	-	SEE REMARK 999	UNP Q03479

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Chain	Residue	Modelled	Actual	Comment	Reference
C	380	PRO	THR	SEE REMARK 999	UNP Q03479
C	427	VAL	-	SEE REMARK 999	UNP Q03479
C	428	ARG	-	SEE REMARK 999	UNP Q03479
C	429	GLU	LYS	SEE REMARK 999	UNP Q03479
C	440	ASN	-	SEE REMARK 999	UNP Q03479
C	498	ILE	ASN	SEE REMARK 999	UNP Q03479
C	604	VAL	ASP	SEE REMARK 999	UNP Q03479
C	681	ASN	ILE	SEE REMARK 999	UNP Q03479
C	683	THR	ARG	SEE REMARK 999	UNP Q03479
D	26	GLU	ASP	SEE REMARK 999	UNP Q03479
D	48	THR	ARG	SEE REMARK 999	UNP Q03479
D	77	MET	ILE	SEE REMARK 999	UNP Q03479
D	?	-	ILE	SEE REMARK 999	UNP Q03479
D	?	-	ARG	SEE REMARK 999	UNP Q03479
D	137	LEU	PHE	SEE REMARK 999	UNP Q03479
D	138	ASP	GLN	SEE REMARK 999	UNP Q03479
D	215	ASP	ASN	SEE REMARK 999	UNP Q03479
D	371	ILE	LEU	SEE REMARK 999	UNP Q03479
D	372	ILE	SER	SEE REMARK 999	UNP Q03479
D	373	ASN	ILE	SEE REMARK 999	UNP Q03479
D	374	CYS	VAL	SEE REMARK 999	UNP Q03479
D	375	THR	HIS	SEE REMARK 999	UNP Q03479
D	376	THR	ARG	SEE REMARK 999	UNP Q03479
D	378	LYS	-	SEE REMARK 999	UNP Q03479
D	380	PRO	THR	SEE REMARK 999	UNP Q03479
D	427	VAL	-	SEE REMARK 999	UNP Q03479
D	428	ARG	-	SEE REMARK 999	UNP Q03479
D	429	GLU	LYS	SEE REMARK 999	UNP Q03479
D	440	ASN	-	SEE REMARK 999	UNP Q03479
D	498	ILE	ASN	SEE REMARK 999	UNP Q03479
D	604	VAL	ASP	SEE REMARK 999	UNP Q03479
D	681	ASN	ILE	SEE REMARK 999	UNP Q03479
D	683	THR	ARG	SEE REMARK 999	UNP Q03479

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

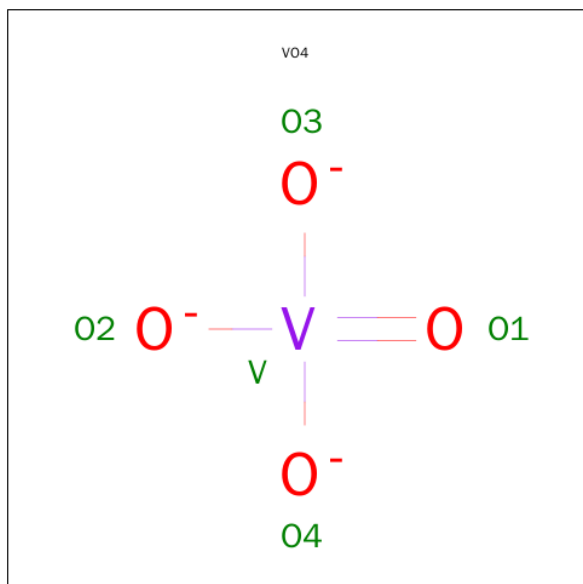
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

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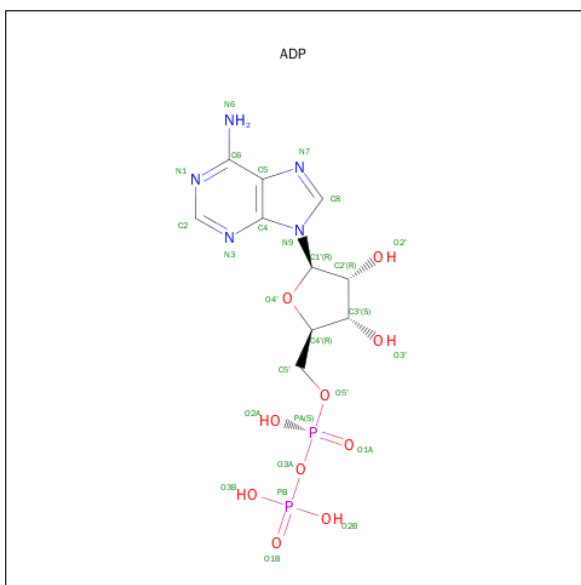
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is VANADATE ION (three-letter code: VO4) (formula: O₄V).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	V	0	0
			5	4	1		
3	B	1	Total	O	V	0	0
			5	4	1		
3	C	1	Total	O	V	0	0
			5	4	1		
3	D	1	Total	O	V	0	0
			5	4	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 5 is water.

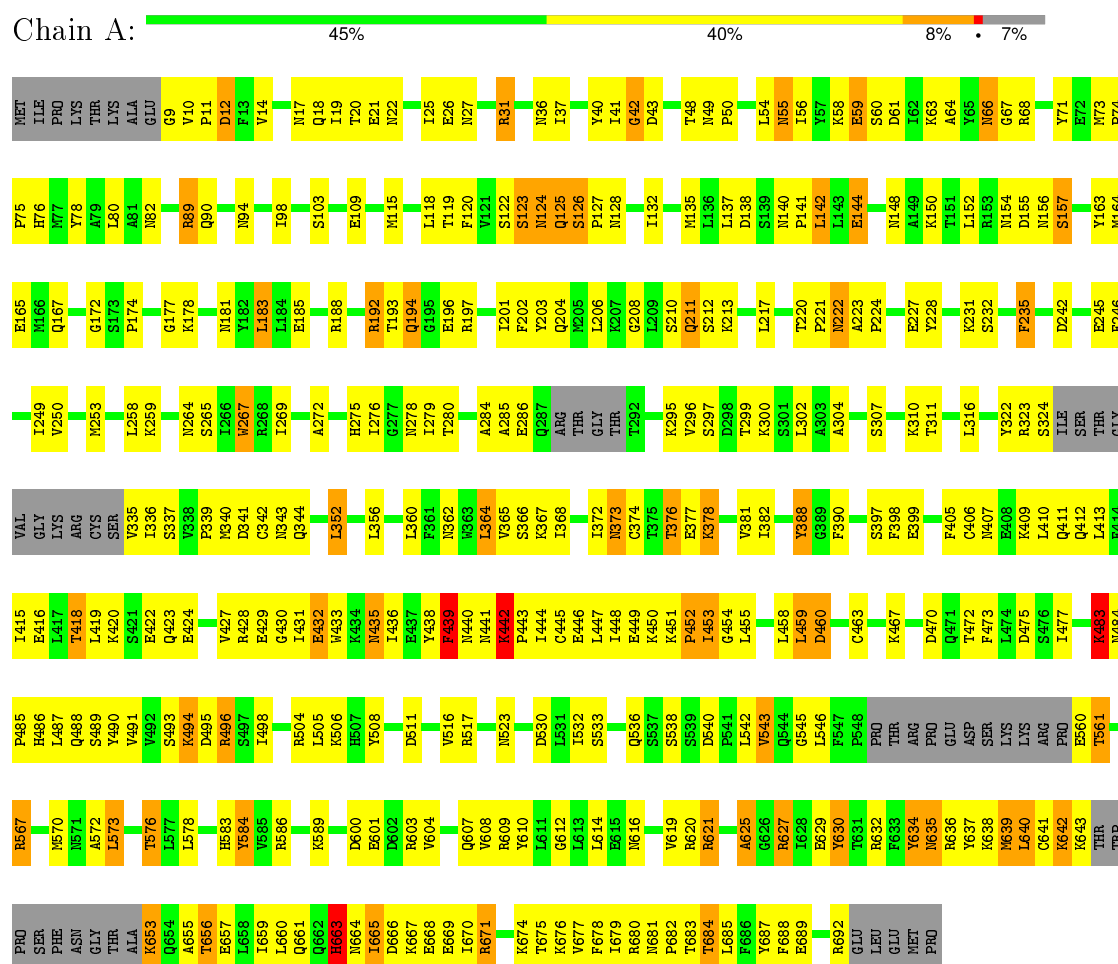
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	18	Total O 18 18	0	0
5	B	16	Total O 16 16	0	0
5	C	19	Total O 19 19	0	0
5	D	11	Total O 11 11	0	0

3 Residue-property plots

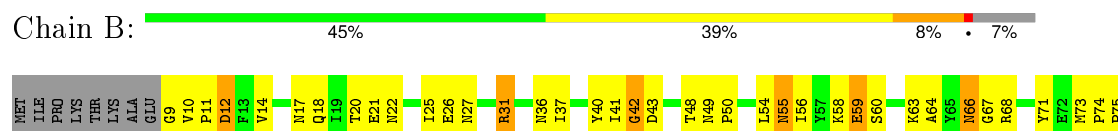
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 IE HEAVY CHAIN



• Molecule 1: MYOSIN IE HEAVY CHAIN

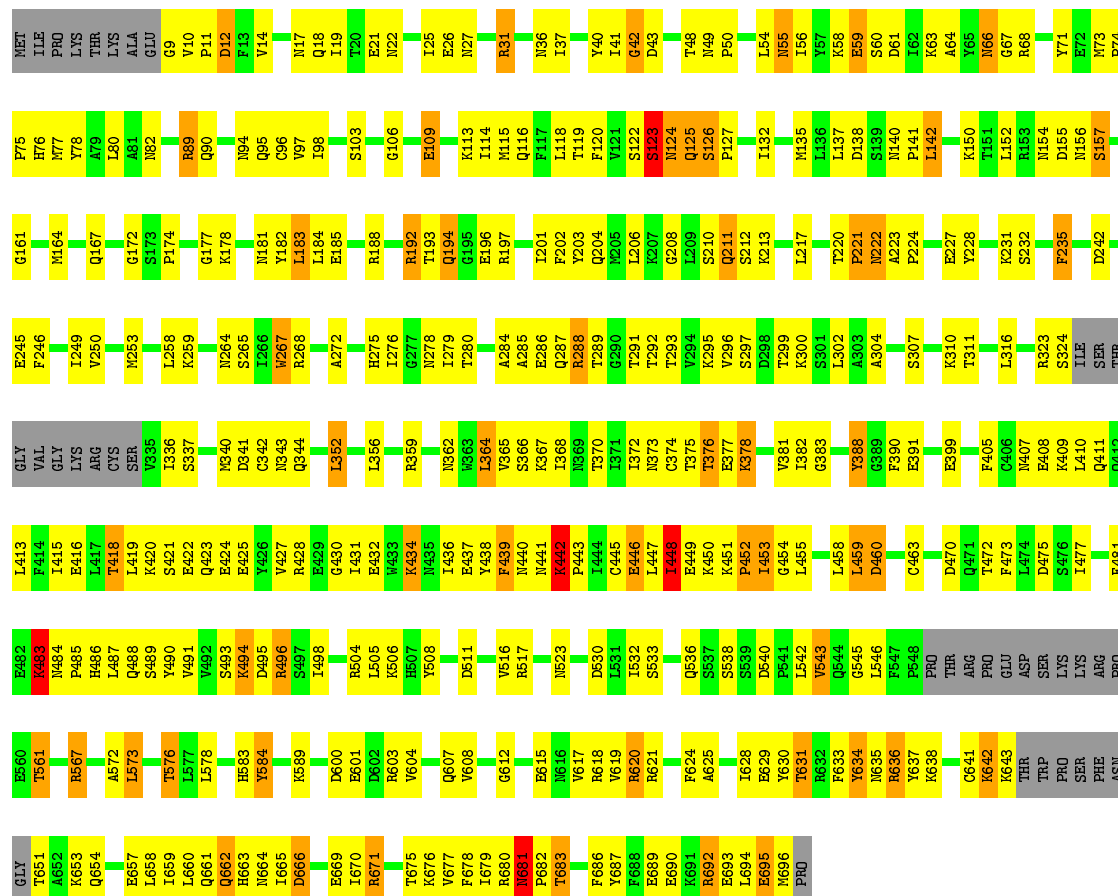


E165	E166	Q167	E169	H76	H77	H78	A79	L80	A81	H82	R89	Q90	S91	Q92	R93	H94	I98	E109	M115	L118	T119	F120	G121	S122	S123	I124	Q125	S126	P127	H128	I132	S133	G134	M135	L136	L137	D138	S139	K213	L214	P141	L142	L143	E144	N148	A223	P224	E227	Y228	N154	D155	N156	S157	F235	T239																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
T240	D241	D242	E245	F246	A170	A171	G172	S173	P174	R89	Q90	S91	Q92	R93	H94	I98	E109	M115	L118	T119	F120	G121	S122	S123	I124	Q125	S126	P127	H128	I132	S133	G134	M135	L136	L137	D138	S139	K213	L214	P141	L142	L143	E144	N148	A223	P224	E227	Y228	N154	D155	N156	S157	F235	T239																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
GLY	LYS	ARG	CYS	SER	V335	L336	S337	V338	P339	M340	D341	C342	N343	Q344	L352	L356	N362	W363	L364	V365	S366	K367	I368	A282	E283	A284	G374	T375	T376	E377	K378	V381	I382	Y388	F390	S397	F398	E399	F405	C406	N407	E408	K409	L410	Q411	Q412	L413	E416	L417	Q488	T418																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
L419	K420	Q423	Y426	V427	R428	E429	R504	L505	K506	H507	Y508	D511	V516	R517	N523	D530	I532	S533	Q536	S537	S538	S539	P541	L542	L543	L544	L545	L548	L549	D460	C463	D470	Q473	T472	F473	L474	D475	S476	L477	F481	E482	K483	T561	N484	P485	H486	L487	Q488	S489																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
Y490	V491	V492	S493	K494	D495	R496	S497	L498	R504	L505	K506	H507	Y508	D511	V516	R517	N523	D530	I532	S533	Q536	S537	S538	S539	P541	L542	L543	L544	L545	L548	L549	D460	C463	D470	Q473	T472	F473	L474	D475	S476	L477	F481	E482	K483	T561	N484	P485	H486	L487	Q488	S489																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
T576	L577	L578	H583	Y584	H589	D600	R601	D602	R603	V604	Q607	V608	V610	V611	V616	R617	L614	E615	V619	R620	R621	A622	G623	F624	K450	K451	K452	K453	L454	L455	L458	L459	D460	C463	D470	Q473	T472	F473	L474	D475	S476	L477	F481	E482	K483	T561	N484	P485	H486	L487	Q488	S489																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
E657	L658	L659	L660	Q661	H663	L664	L665	D666	K667	E668	E669	L670	R671	T675	K676	V677	F678	L679	N681	P682	T683	T684	L685	G623	F624	K450	K451	K452	K453	L454	L455	L458	L459	D460	C463	D470	Q473	T472	F473	L474	D475	S476	L477	F481	E482	K483	T561	N484	P485	H486	L487	Q488	S489																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	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	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	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	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	L1704	L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719	L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734	L1735	L1736	L1737	L1738	L1739	L1740	L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748



• Molecule 1: MYOSIN IE HEAVY CHAIN

Chain D: 45% 41% 8% 5%



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 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.82Å 143.67Å 236.05Å 90.00° 94.86° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21265	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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: VO4, MG, 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	0.41	0/5280	0.61	1/7108 (0.0%)
1	B	0.41	0/5276	0.61	1/7104 (0.0%)
1	C	0.42	0/5521	0.63	1/7442 (0.0%)
1	D	0.42	0/5356	0.63	2/7212 (0.0%)
All	All	0.42	0/21433	0.62	5/28866 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	483	LYS	N-CA-C	-6.56	93.30	111.00
1	D	483	LYS	N-CA-C	-6.49	93.49	111.00
1	B	483	LYS	N-CA-C	-6.40	93.72	111.00
1	C	483	LYS	N-CA-C	-6.38	93.77	111.00
1	D	442	LYS	N-CA-C	5.20	125.04	111.00

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	5192	0	5189	366	0
1	B	5188	0	5182	351	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5422	0	5415	417	0
1	D	5267	0	5265	357	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	1	0
4	A	27	0	12	2	0
4	B	27	0	12	2	0
4	C	27	0	12	2	0
4	D	27	0	12	3	0
5	A	18	0	0	4	0
5	B	16	0	0	2	0
5	C	19	0	0	2	0
5	D	11	0	0	2	0
All	All	21265	0	21099	1458	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 34.

The worst 5 of 1458 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:C:131:ARG:HD3	1:D:259:LYS:HE2	1.24	1.17
1:C:635:ASN:HA	1:C:638:LYS:HD2	1.28	1.16
1:D:642:LYS:HD2	1:D:642:LYS:H	1.00	1.09
1:B:656:THR:HG21	1:B:677:VAL:HG21	1.37	1.06
1:C:288:ARG:H	1:C:288:ARG:HD3	1.22	1.03

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	640/697 (92%)	529 (83%)	80 (12%)	31 (5%)	3	17
1	B	640/697 (92%)	541 (84%)	64 (10%)	35 (6%)	2	13
1	C	675/697 (97%)	553 (82%)	80 (12%)	42 (6%)	2	10
1	D	652/697 (94%)	557 (85%)	66 (10%)	29 (4%)	3	18
All	All	2607/2788 (94%)	2180 (84%)	290 (11%)	137 (5%)	2	14

5 of 137 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	157	SER
1	A	376	THR
1	A	439	PHE
1	A	442	LYS

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	575/616 (93%)	520 (90%)	55 (10%)	10	38
1	B	574/616 (93%)	519 (90%)	55 (10%)	10	38
1	C	601/616 (98%)	538 (90%)	63 (10%)	8	32
1	D	583/616 (95%)	525 (90%)	58 (10%)	10	35
All	All	2333/2464 (95%)	2102 (90%)	231 (10%)	10	35

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	653	LYS
1	C	265	SER
1	D	496	ARG

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Mol	Chain	Res	Type
1	B	677	VAL
1	C	125	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	373	ASN
1	C	76	HIS
1	D	362	ASN
1	B	423	GLN
1	B	654	GLN

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 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	791	3,2	22,29,29	1.63	5 (22%)	27,45,45	1.53	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	VO4	A	792	2,4	1,4,4	1.64	0	0,6,6	0.00	-
4	ADP	B	794	3,2	22,29,29	1.68	5 (22%)	27,45,45	1.43	6 (22%)
3	VO4	B	795	2,4	1,4,4	1.52	0	0,6,6	0.00	-
4	ADP	C	891	3,2	22,29,29	1.63	5 (22%)	27,45,45	1.37	4 (14%)
3	VO4	C	892	2,4	1,4,4	1.22	0	0,6,6	0.00	-
4	ADP	D	894	3,2	22,29,29	1.63	6 (27%)	27,45,45	1.34	7 (25%)
3	VO4	D	895	2,4	1,4,4	1.60	0	0,6,6	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	791	3,2	-	0/12/32/32	0/3/3/3
3	VO4	A	792	2,4	-	0/0/0/0	0/0/0/0
4	ADP	B	794	3,2	-	0/12/32/32	0/3/3/3
3	VO4	B	795	2,4	-	0/0/0/0	0/0/0/0
4	ADP	C	891	3,2	-	0/12/32/32	0/3/3/3
3	VO4	C	892	2,4	-	0/0/0/0	0/0/0/0
4	ADP	D	894	3,2	-	0/12/32/32	0/3/3/3
3	VO4	D	895	2,4	-	0/0/0/0	0/0/0/0

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	794	ADP	C8-N7	-2.86	1.29	1.34
4	C	891	ADP	PB-O2B	-2.58	1.45	1.54
4	C	891	ADP	C8-N7	-2.57	1.29	1.34
4	A	791	ADP	C8-N7	-2.55	1.29	1.34
4	D	894	ADP	PB-O2B	-2.44	1.45	1.54

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	791	ADP	N3-C2-N1	-3.54	126.18	128.89
4	B	794	ADP	N3-C2-N1	-3.16	126.47	128.89
4	C	891	ADP	N3-C2-N1	-3.03	126.58	128.89
4	D	894	ADP	N3-C2-N1	-2.78	126.77	128.89
4	B	794	ADP	O3B-PB-O1B	-2.29	103.19	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	791	ADP	2	0
3	A	792	VO4	1	0
4	B	794	ADP	2	0
4	C	891	ADP	2	0
3	C	892	VO4	1	0
4	D	894	ADP	3	0
3	D	895	VO4	1	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.