



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 03:39 am BST

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

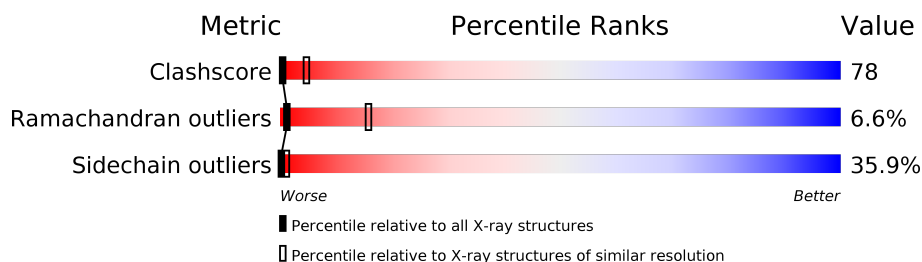
# 1 Overall quality at a glance

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	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ .

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	
2	H	150	

## 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			

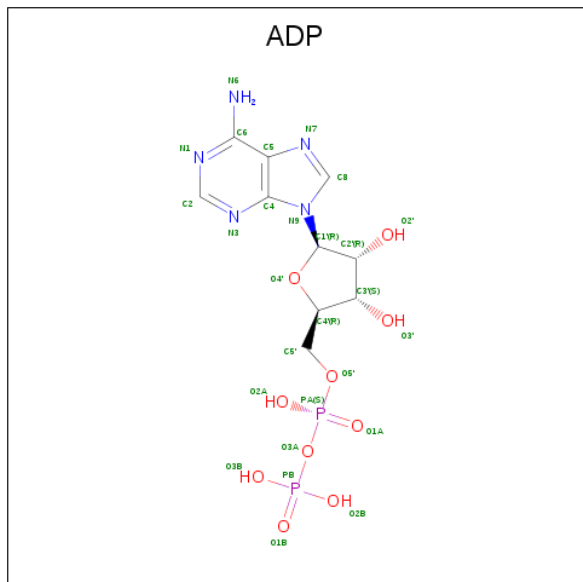
- Molecule 2 is a protein called MYOSIN.

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).

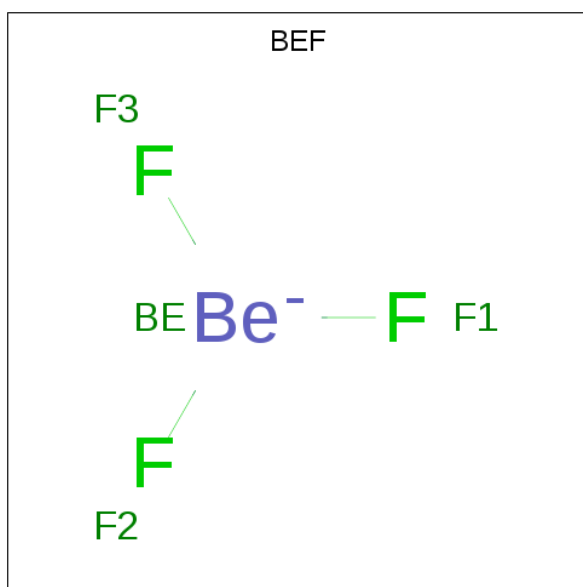
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- 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.

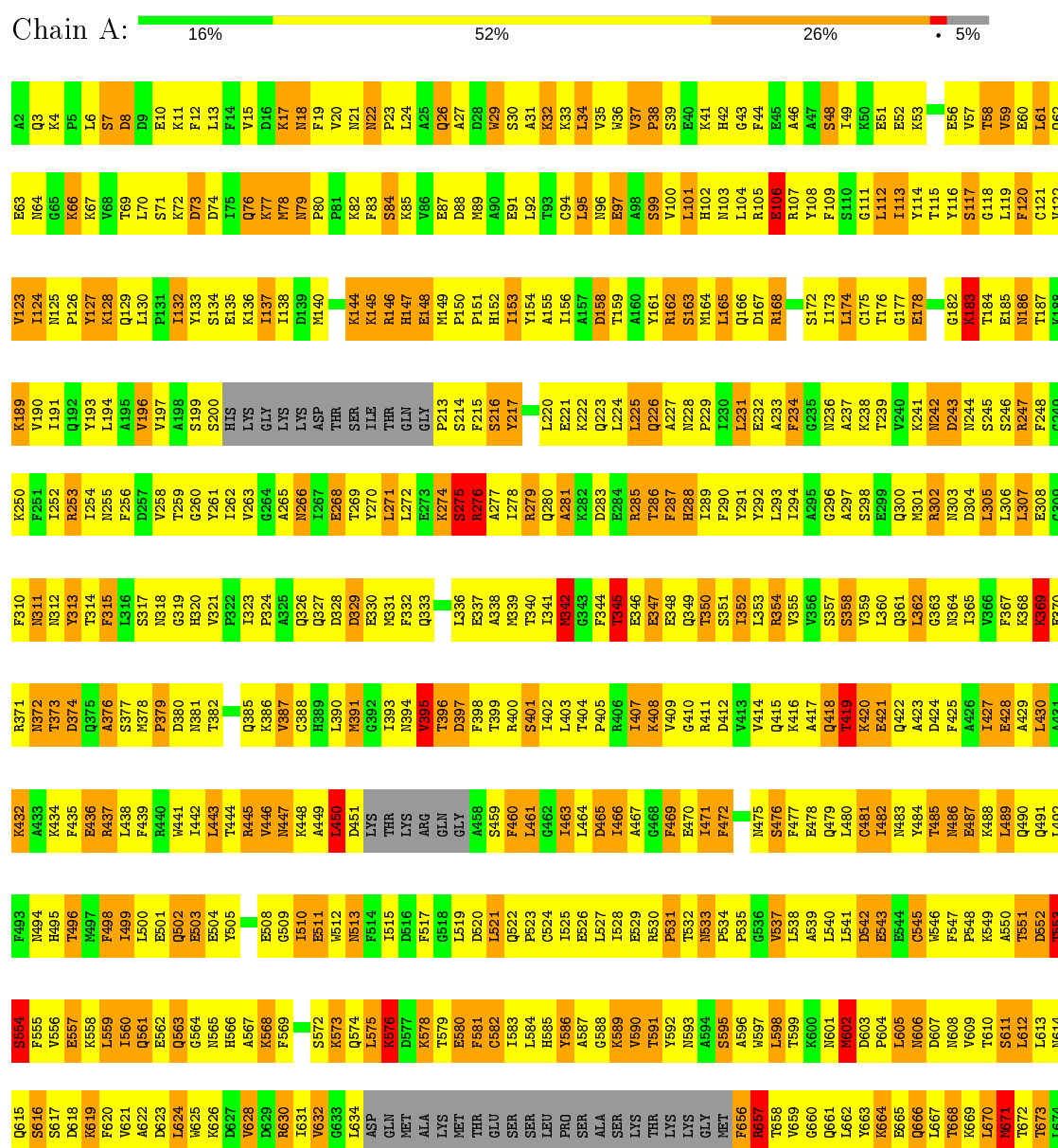
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	C	2	Total	O	0	0
			2	2		
6	E	2	Total	O	0	0
			2	2		
6	G	2	Total	O	0	0
			2	2		

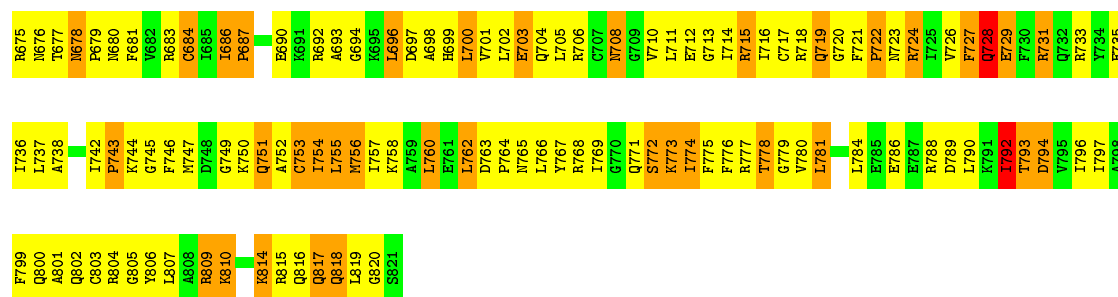
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

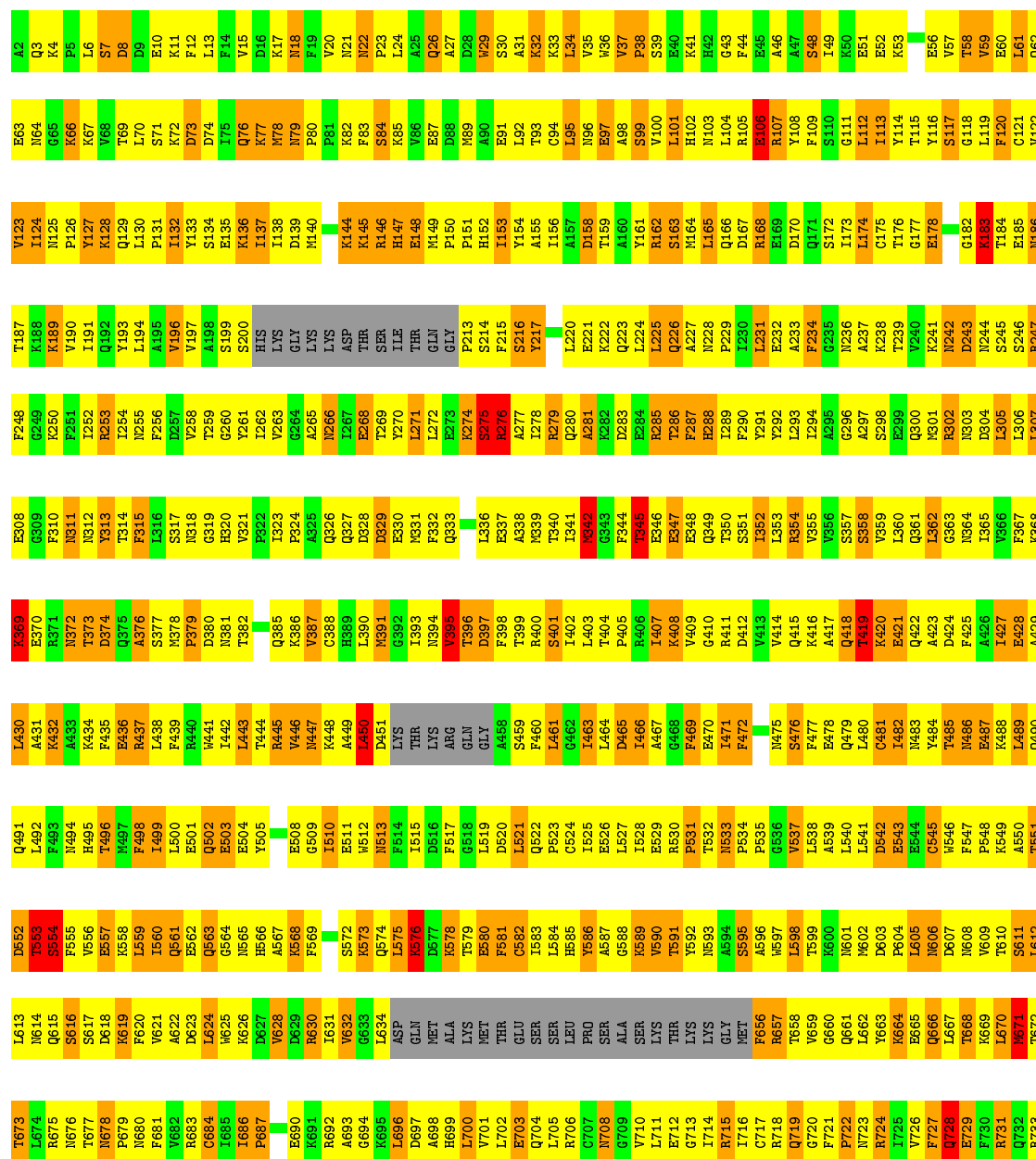
#### • Molecule 1: MYOSIN

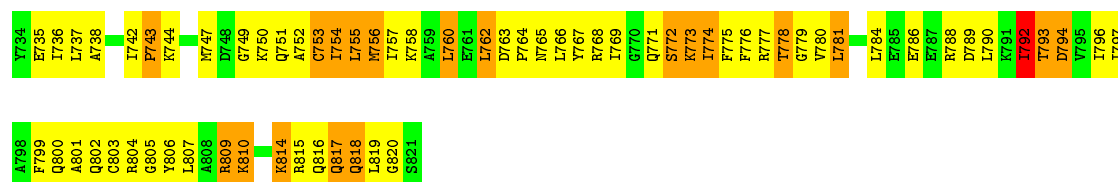




# • Molecule 1: MYOSIN

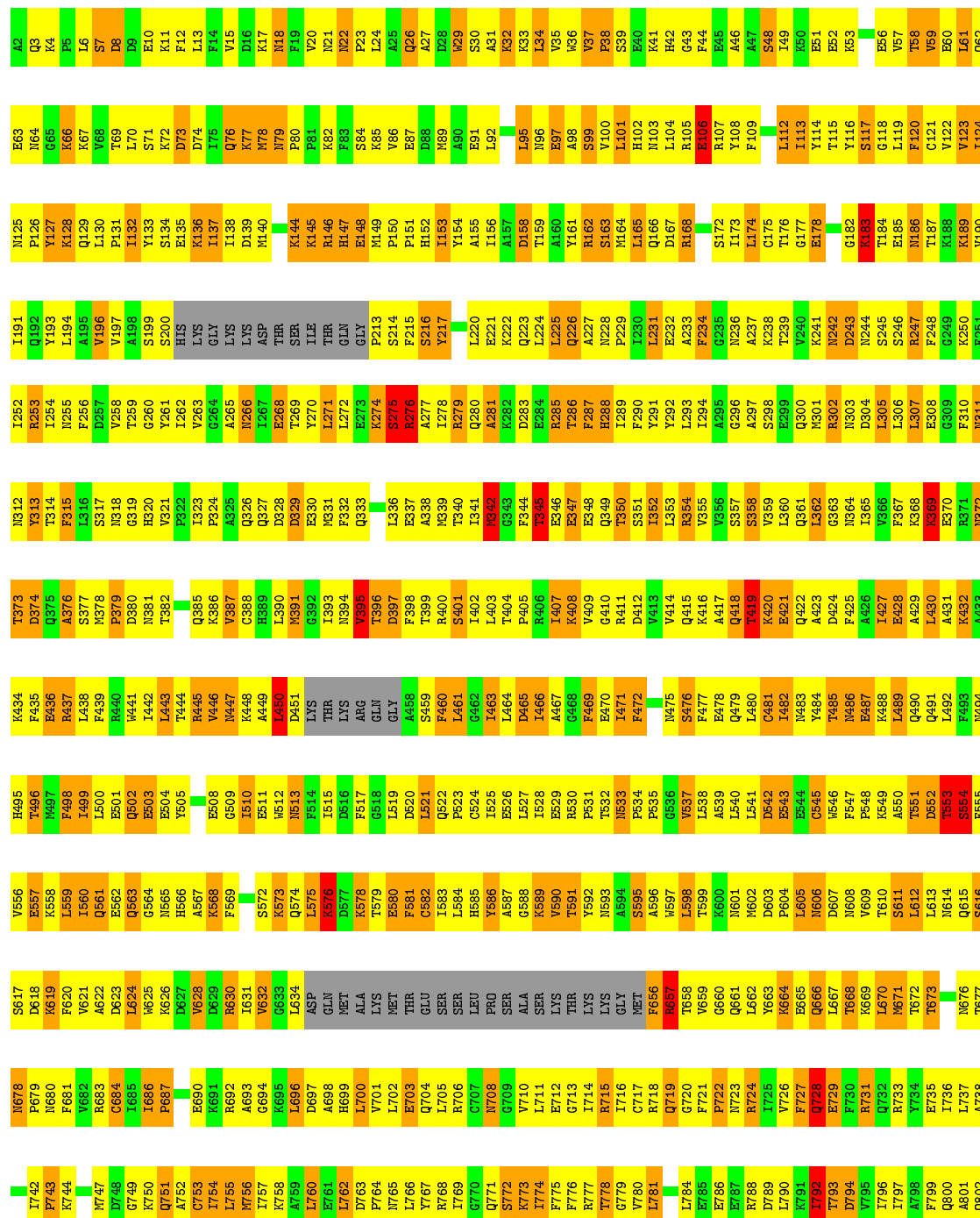
Chain C: 16% 52% 25% 5%





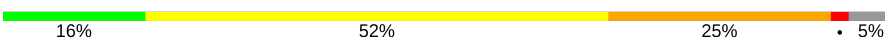
# Molecule 1: MYOSIN

Chain E: 16% 52% 26% 5%

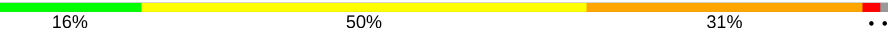


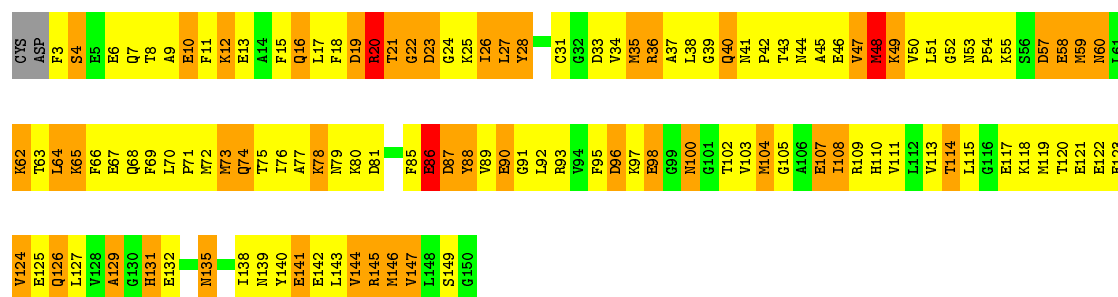
G803
R804
G805
Y806
L807
A808
R809
A810
A811
F812
A813
K814
R815
Q816
Q817
L818
G820
S821

• Molecule 1: MYOSIN


Chain G:  16% 52% 25% 5%

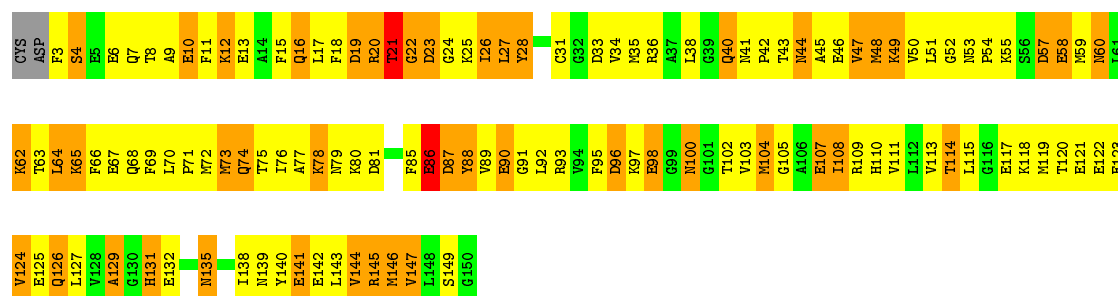
I736	Q800	R675	Q615	S554	F493	K432	R371	F310	K250	K189	N125	M64
A738	A801	T677	S616	F555	H495	A433	N372	N311	F251	V190	P126	G65
	Q802		S617	V556	N494	K434	T373	N312	T252	K128	Y127	K66
	C803	N678	D618	E557	T496	F435	D374	Y313	R253	Q192	K129	K67
	R804	P679	K619	K558	K497	E436	Q375	T314	T254	I193	Q129	V68
F743	G805	M680	F620	L559	F498	R437	A376	F315	N255	L194	L130	T69
K744	Y806	F681	V621	I560	L499	L438	S377	L316	F256	A196	P131	L70
	L807	V682	A622	Q561	L500	F439	M378	S317	D257	V195	I132	S71
M747	A808	R683	D623	E562	Q501	R440	P379	N318	T258	I197	K133	K72
D748	R809	G684	L624	Q563	E502	W441	D380	G319	T259	A198	S134	D73
K749	K810	L685	W625	G564	E503	I442	N381	H320	Q260	S199	E135	D74
K780		L686	K626	N565	E504	L443	T382	V321	Y261	S200	K136	F12
Q751	A811	P687	D627	H566	Y505	T444		P322	I262	H15	I137	Q76
A752	A813	A758	V628	A567		R445	Q385	I323	V263	L15	L138	K77
K814	K814	C753	D629	K568	E508	V446	K386	P324	G264	GLY	D139	M78
R815	R815	L754	R630	F569	G509	N447	V387	A325	A265	L15	M140	N18
L755	Q816	L755	I631		I510	K448	C388	Q326	N266	L15		P80
M756	Q817	M756	V632	S572	E511	A449	H589	Q27	I267	ASP		F61
	Q818		G633	K573	W512	L480	L390	D328	E268	THR		K82
	L819	L757	L634	Q574	N513	D451	M391	D329	T269	SER	K146	R83
G820	G820	A759	ASP	L575	F514	L15	G392	E330	Y270	I1E	H147	S84
	S821	L760	GLN	K576	I515	THR	I393	M331	L271	THR	E148	K85
		E761	MET	D577	D516	L15	N394	F332	L272	GLN	M149	V66
L762		L762	ALA	K578	F517	ARG	V395	Q333	E273	GLY	P150	Q26
D763	D763	L763	LYS	T579	G518	GLN	T396		K274	P88	P151	P87
P764	P764	V701	MET	E580	L519	GLY	D397	L336	S275	S214	H152	D28
N765	N765	L702	THR	F581	D520	A458	F398	E337	R276	A90	I153	W29
L766	L766	E703	GLU	C582	L521	S459	T399	A338	A277	S216	Y154	B31
Y767	Y767	Q704	SER	I583	Q522	F460	R400	M339	L278	Y217	A155	L92
R768	R768	L705	SER	L584	P523	L461	S401	T340	R279		I156	T93
I769	I769	R706	LEU	H585	C524	G462	I402	Q280	Q280	L220	A157	C94
	G770	G707	PRO	Y586	I525	I463	L403	M342	E221	E221	L158	L95
Q771	Q771	N708	SER	A587	E526	L464	T404	G343	K282	T159	V35	N96
S772	S772	G709	ALA	G588	L527	D465	P405	F344	Q223	Q223	A160	B37
K773	K773	V710	SER	K589	I528	I466	R406	T545	K284	L224	Y161	A98
I774	I774	L711	LYS	V590	E529	A467	I407	E346	R285	L225	R162	S99
F775	F775	E712	THR	T591	R530	G468	R408	E347	T286	Q226	S163	P38
F776	F776	G713	LYS	Y592	P531	F469	V409	E348	F287	L101	L101	S39
R777	R777	L714	LYS	N593	T532	E470	G410	Q349	H288	K164	E40	E40
T778	T778	R715	GLY	A594	N533	I471	R411	T350	I289	Q166	H102	K41
G779	G779	L716	MET	S595	P534	F472	D412	S351	F290	D167	N103	H42
V780	V780	C717	F656	A596	P535		V413	I352	Y291	L230	L104	G43
L781	L781	R657	R657	W597	G536	N475	V414	L353	Y292	L231	R168	F44
	L784	L784	T558	L598	V537	S476	Q415	R354	L293	A232	E106	E45
E785	E785	G720	V659	T599	A539	F477	K416	V355	I294	F234	E108	A46
E786	E786	F721	G660	K600	L639	E478	A417	V356	A295	Q171	F109	S48
E787	E787	P722	Q661	N601	E539	Q479	Q418	S357	G296	S172	K173	L49
	N723	N723	L662	M602	L541	L480	T419	S358	A297	I173	L174	K50
R788	R788	R724	V663	R603	L542	C481	R420	E297	A297	A237	L174	K50
D789	D789	L725	K664	L605	E543	I482	E421	V359	S298	K238	C175	E51
L790	L790	V726	E665	L605	E544	R483	Q422	Q361	E299	T239	T176	E52
K791	K791	F727	Q666	N606	C545	Y484	A423	Q361	Q300	G177	T115	E52
E792	E792	T727	L667	D607	F546	T485	D424	L362	N301	K241	E178	Y116
	Q728	Q728	L667	M608	L541	L480	F425	G363	R302	N242	A117	S117
T793	T793	E729	T668	R608	F547	N486	F425	N364	A297	K242	L174	K50
D794	D794	F730	K669	V609	P548	E487	A426	I365	S298	A237	L174	K50
V795	V795	R731	L670	T610	K549	K488	I427	V366	L305	N244	C175	E51
I796	I796	Q732	M671	S611	A550	E489	E428	Q361	E299	T239	T176	E52
T797	T797	R733	T672	L612	T551	Q490	A429	F367	Q300	G177	T115	E52
	A798	A798	L673	L613	D552	Q491	L430	K369	E298	F248	E178	Y116
F799	F799	R725	L674	N514	T552	I492	A434	E370	G298	C249	A117	S117

Chain B: 

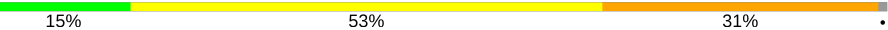


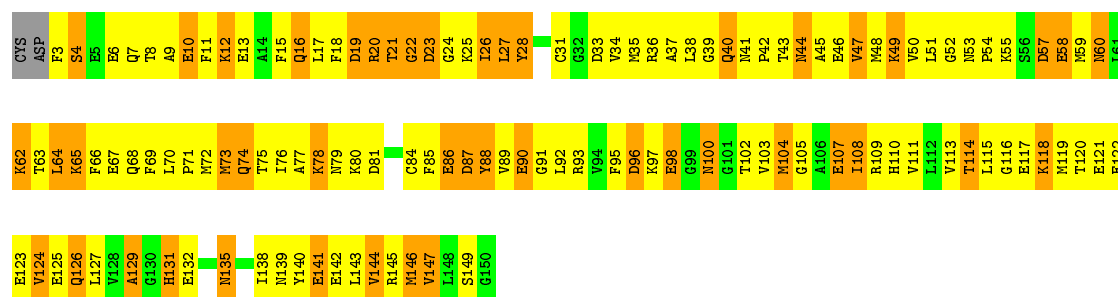
• Molecule 2: MYOSIN

Chain D: 

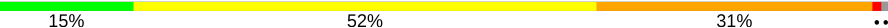


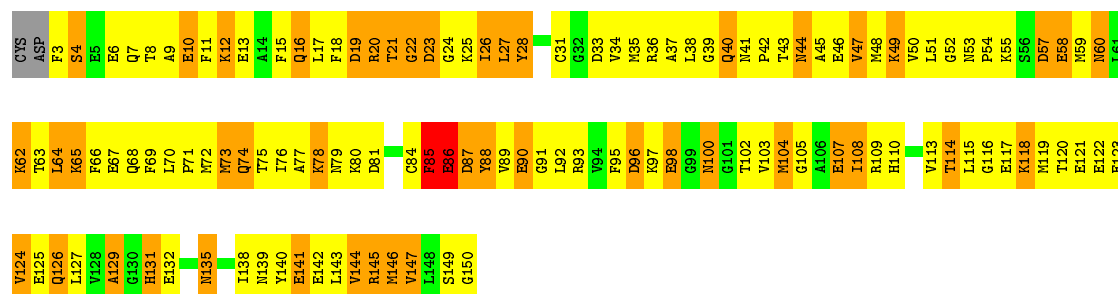
• Molecule 2: MYOSIN

Chain F: 



• Molecule 2: MYOSIN

Chain H: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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	14
1	C	773/820 (94%)	580 (75%)	138 (18%)	55 (7%)	1	14
1	E	773/820 (94%)	580 (75%)	138 (18%)	55 (7%)	1	14
1	G	773/820 (94%)	580 (75%)	138 (18%)	55 (7%)	1	14
2	B	146/150 (97%)	111 (76%)	29 (20%)	6 (4%)	3	25
2	D	146/150 (97%)	112 (77%)	28 (19%)	6 (4%)	3	25
2	F	146/150 (97%)	112 (77%)	29 (20%)	5 (3%)	3	30
2	H	146/150 (97%)	113 (77%)	26 (18%)	7 (5%)	2	22
All	All	3676/3880 (95%)	2767 (75%)	665 (18%)	244 (7%)	1	16

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	1
1	C	685/718 (95%)	446 (65%)	239 (35%)	0	1
1	E	685/718 (95%)	446 (65%)	239 (35%)	0	1
1	G	685/718 (95%)	446 (65%)	239 (35%)	0	1
2	B	127/129 (98%)	75 (59%)	52 (41%)	0	0
2	D	127/129 (98%)	74 (58%)	53 (42%)	0	0
2	F	127/129 (98%)	74 (58%)	53 (42%)	0	0
2	H	127/129 (98%)	73 (58%)	54 (42%)	0	0
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 [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	G	998	3,5	24,29,29	1.18	2 (8%)	29,45,45	1.33	3 (10%)
5	BEF	G	999	3,4	0,3,3	0.00	-	-		
4	ADP	A	998	3,5	24,29,29	1.18	2 (8%)	29,45,45	1.34	3 (10%)
5	BEF	E	999	3,4	0,3,3	0.00	-	-		
4	ADP	C	998	3,5	24,29,29	1.19	2 (8%)	29,45,45	1.33	3 (10%)
5	BEF	C	999	3,4	0,3,3	0.00	-	-		
5	BEF	A	999	3,4	0,3,3	0.00	-	-		
4	ADP	E	998	3,5	24,29,29	1.18	2 (8%)	29,45,45	1.33	3 (10%)

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	-	3/12/32/32	0/3/3/3
4	ADP	C	998	3,5	-	3/12/32/32	0/3/3/3
4	ADP	E	998	3,5	-	3/12/32/32	0/3/3/3
4	ADP	G	998	3,5	-	3/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	998	ADP	C2'-C1'	-3.44	1.48	1.53
4	G	998	ADP	C2'-C1'	-3.39	1.48	1.53
4	C	998	ADP	C2'-C1'	-3.39	1.48	1.53
4	E	998	ADP	C2'-C1'	-3.38	1.48	1.53
4	G	998	ADP	C2-N3	2.32	1.35	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	998	ADP	C5-C6-N6	5.05	128.02	120.35
4	E	998	ADP	C5-C6-N6	5.03	128.00	120.35
4	G	998	ADP	C5-C6-N6	5.03	128.00	120.35
4	C	998	ADP	C5-C6-N6	5.03	128.00	120.35
4	A	998	ADP	N6-C6-N1	-2.74	112.89	118.57

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	998	ADP	PA-O3A-PB-O2B
4	A	998	ADP	PA-O3A-PB-O2B
4	C	998	ADP	PA-O3A-PB-O2B
4	E	998	ADP	PA-O3A-PB-O2B
4	G	998	ADP	PA-O3A-PB-O1B

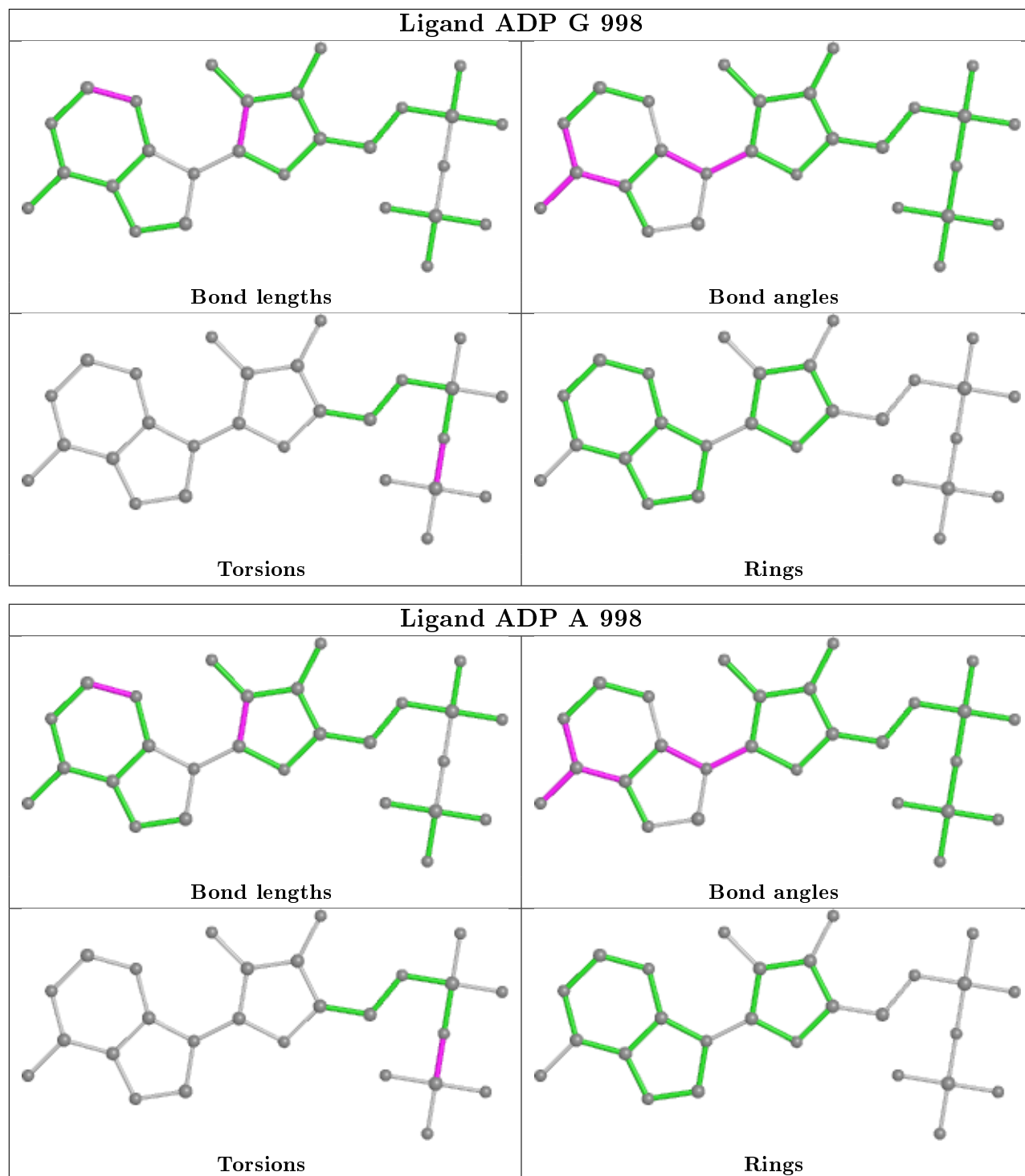
There are no ring outliers.

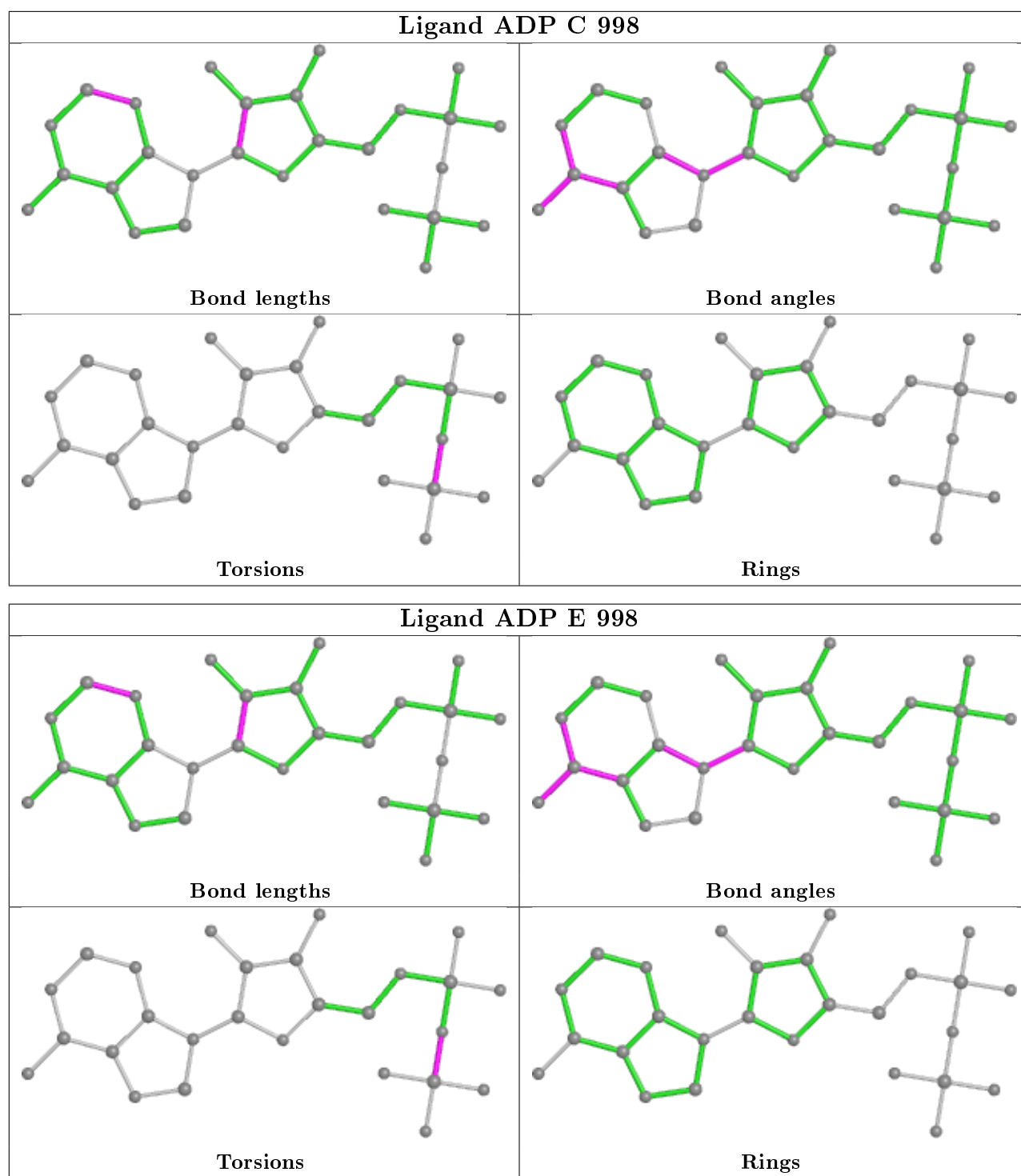
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	998	ADP	3	0
4	A	998	ADP	3	0
4	C	998	ADP	4	0
4	E	998	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.