



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 12:03 PM UTC

PDB ID : 1BR4 / pdb_00001br4
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

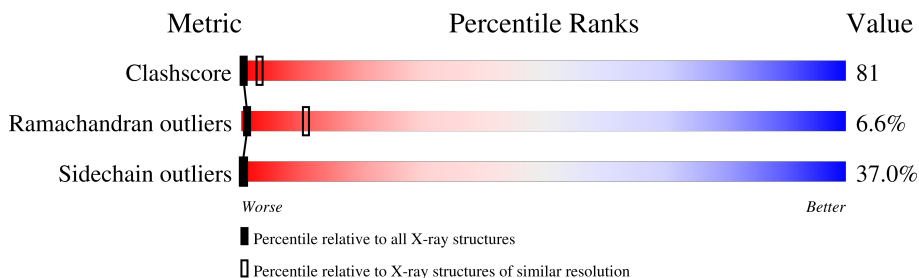
1 Overall quality at a glance

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	190562	1092 (3.72-3.52)
Ramachandran outliers	187476	1057 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	15% 50% 27% • 5%
1	C	820	15% 50% 26% • 5%
1	E	820	15% 50% 26% • 5%
1	G	820	15% 50% 26% • 5%
2	B	150	15% 50% 32% ..
2	D	150	15% 52% 29% ..
2	F	150	15% 53% 31% ..
2	H	150	14% 52% 31% ..

2 Entry composition

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			

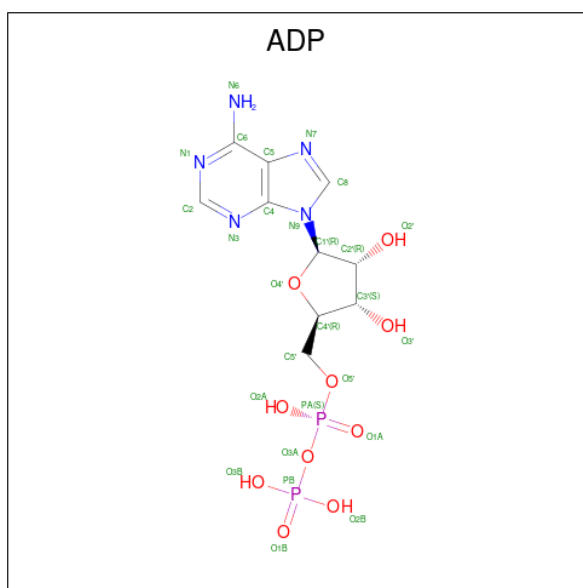
- Molecule 2 is a protein called MYOSIN.

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 (CCD ID: MG) (formula: Mg).

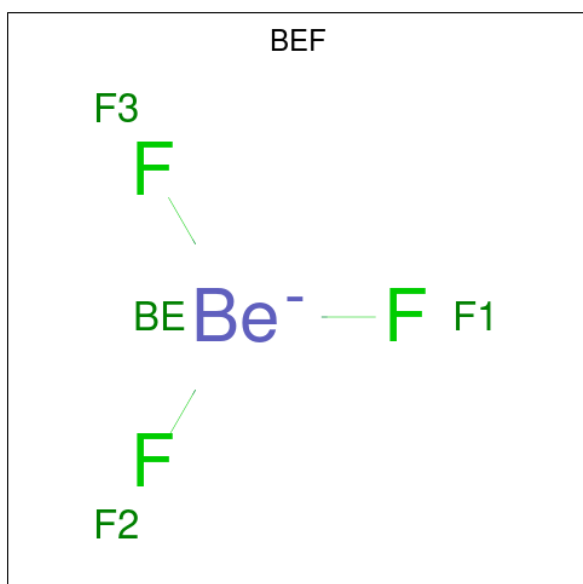
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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 (CCD ID: BEF) (formula: BeF_3).



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

- Molecule 6 is water.

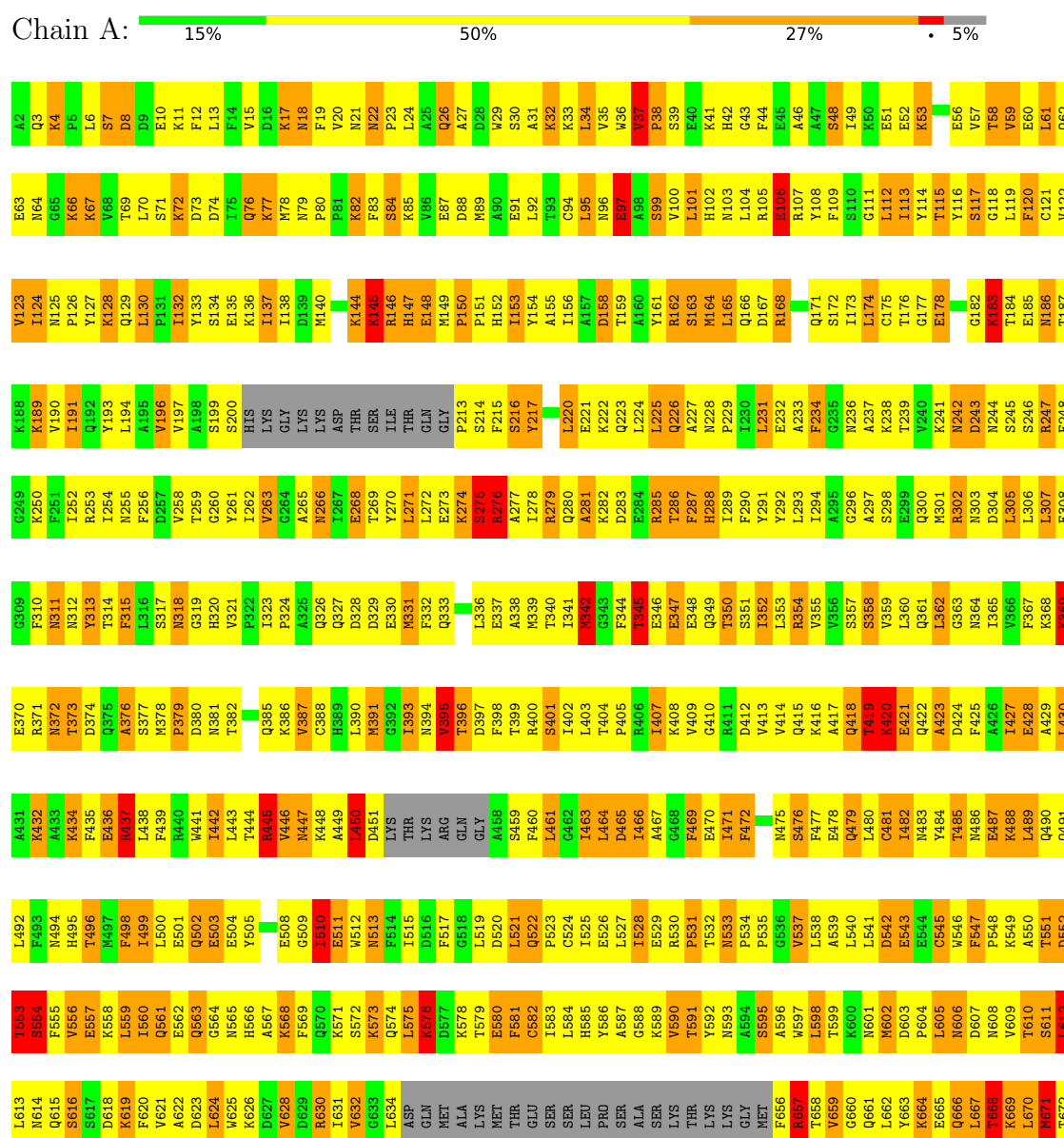
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	O 2	0	0
6	C	2	Total 2	O 2	0	0
6	E	2	Total 2	O 2	0	0
6	G	2	Total 2	O 2	0	0

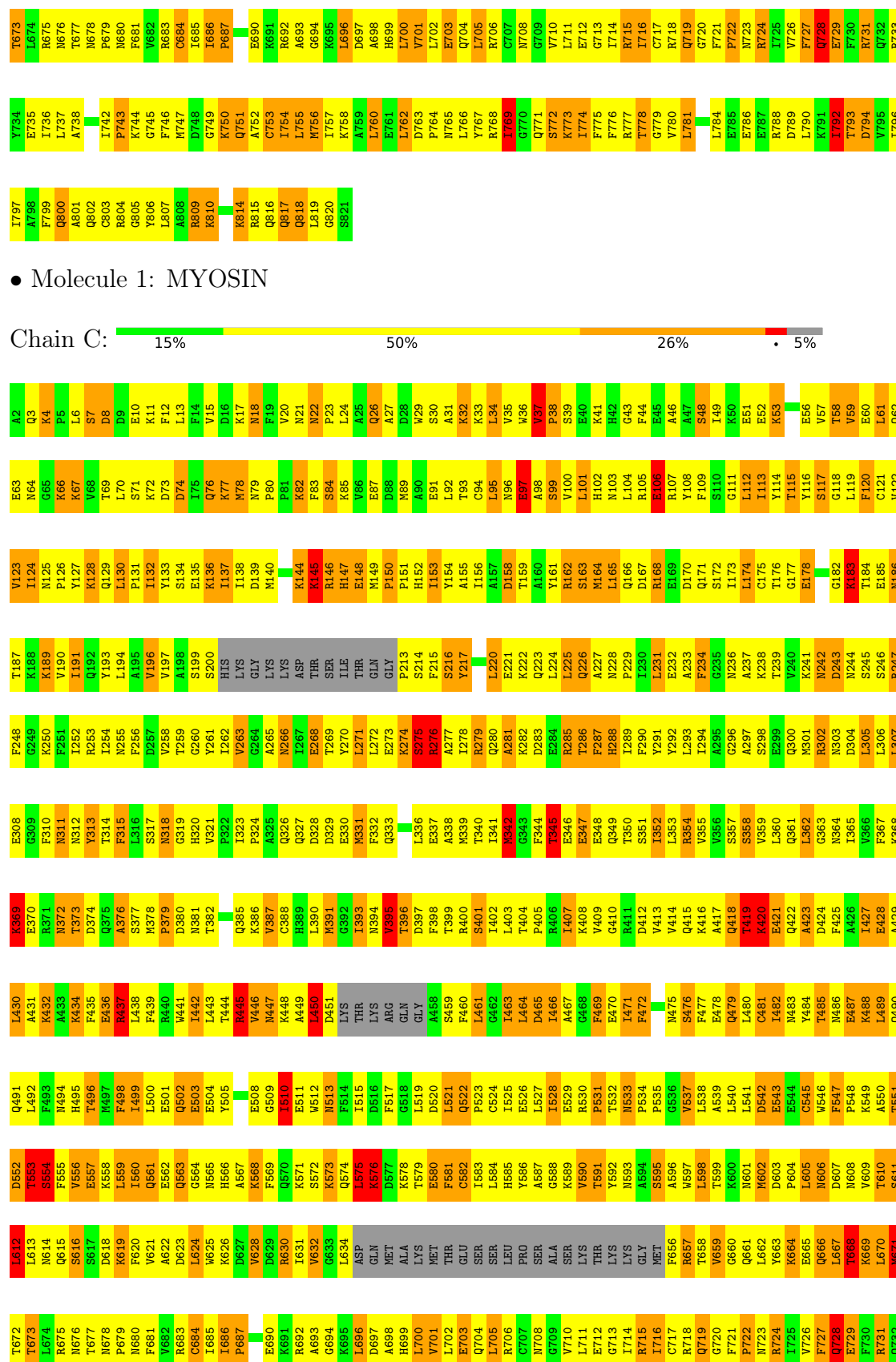
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

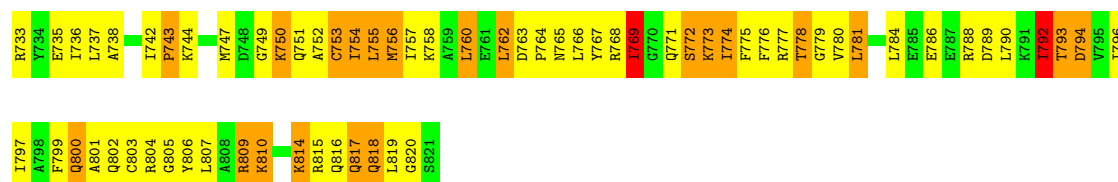
Note EDS was not executed.

• Molecule 1: MYOSIN



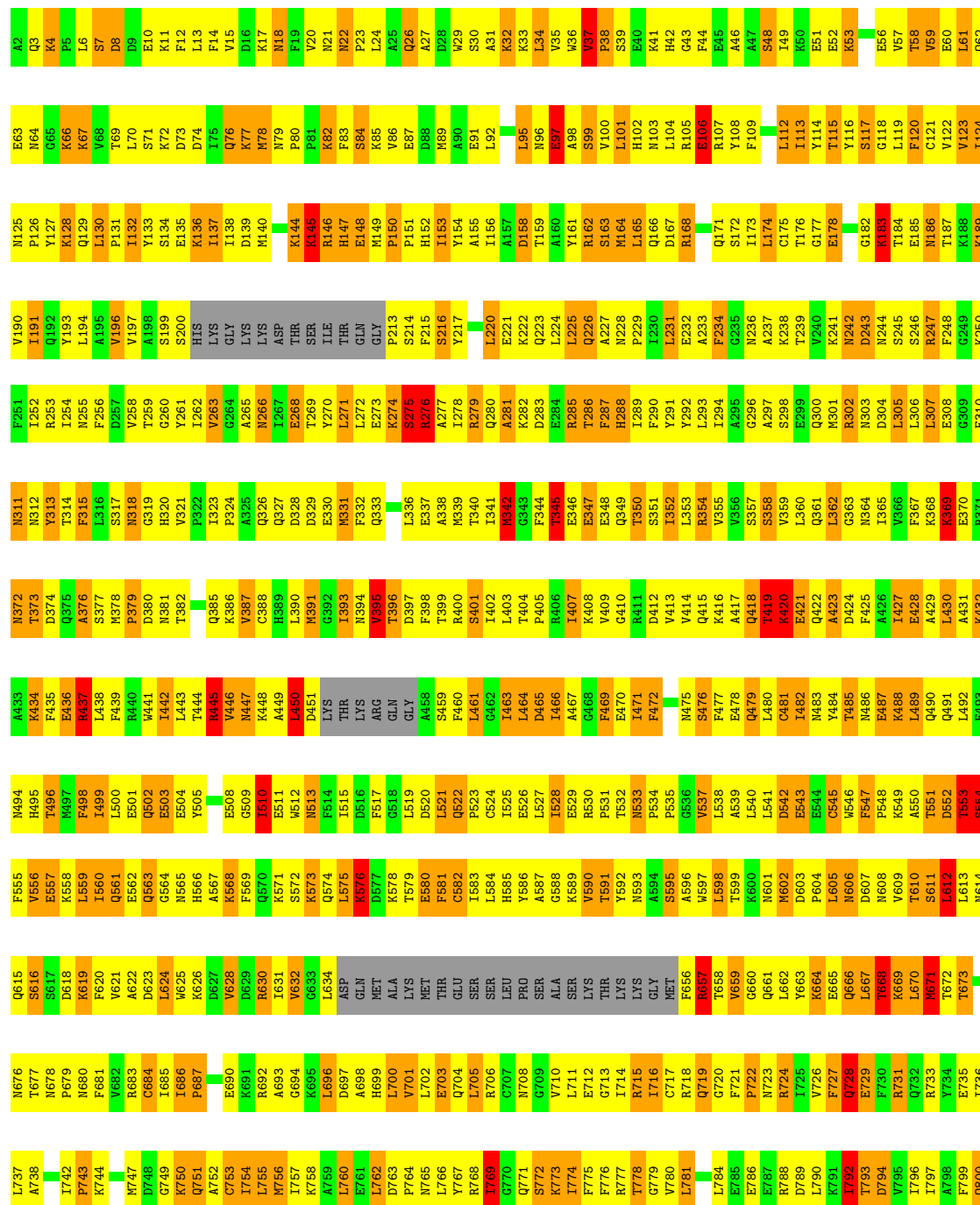


● Molecule 1: MYOSIN



• Molecule 1: MYOSIN

Chain E: 15% 50% 26% 5%



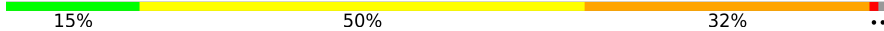
A801
Q802
C803
R804
G805
Y806
L807
A808
R809
K810
A811
F812
A813
K814
R815
Q816
Q817
L819
G820
S821

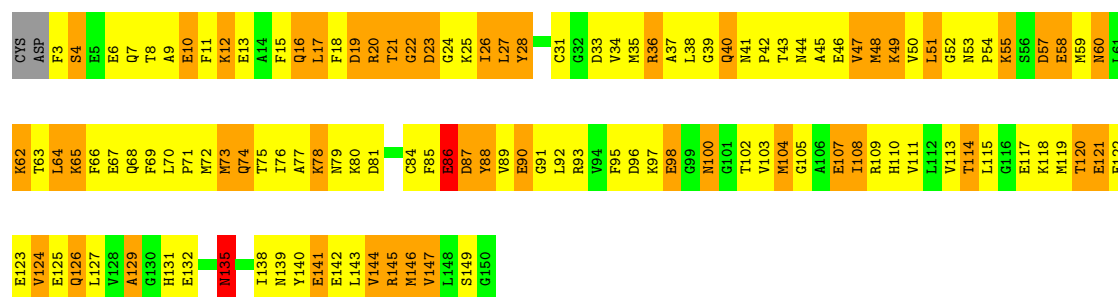
• Molecule 1: MYOSIN

Chain G: 15% 50% 26% 5%

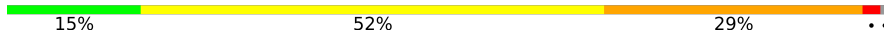
A2 Q3 K4 P5 L6 S7 D8 D9 E10 K11 F12
V15 D16 K17 N18 F19 V20 N21 N22 P23 P24 L24 A25 Q26 E27 D28 W29 S30 A31 L32 K33 L34 V35 V36 V37
N64 G65 K66 K67 V68 T69 L70 S71 K72 K73 K74 K75 K76 K77 K78 K79 K80 K81 K82 K83 K84 K85 K86 K87 K88 K89 K90 K91 K92 K93 K94 K95 K96 K97 K98 K99 K100 K101 K102 K103 K104 K105 K106 K107 K108 K109 K110 K111 K112 K113 K114 K115 K116 K117 K118 K119 K120 K121 K122 K123 K124 K125 K126 K127 K128 K129 K130 K131 K132 K133 K134 K135 K136 K137 K138 K139 K140 K141 K142 K143 K144 K145 K146 K147 K148 K149 K150 K151 K152 K153 K154 K155 K156 K157 K158 K159 K160 K161 K162 K163 K164 K165 K166 K167 K168 K169 K170 K171 K172 K173 K174 K175 K176 K177 K178 K179 K180 K181 K182 K183 K184 K185 K186 K187 K188 K189 K190 K191 K192 K193 K194 K195 K196 K197 K198 K199 K200 K201 K202 K203 K204 K205 K206 K207 K208 K209 K210 K211 K212 K213 K214 K215 K216 K217 K218 K219 K220 K221 K222 K223 K224 K225 K226 K227 K228 K229 K230 K231 K232 K233 K234 K235 K236 K237 K238 K239 K240 K241 K242 K243 K244 K245 K246 K247 K248 K249 K250 K251 K252 K253 K254 K255 K256 K257 K258 K259 K260 K261 K262 K263 K264 K265 K266 K267 K268 K269 K270 K271 K272 K273 K274 K275 K276 K277 K278 K279 K280 K281 K282 K283 K284 K285 K286 K287 K288 K289 K290 K291 K292 K293 K294 K295 K296 K297 K298 K299 K300 K301 K302 K303 K304 K305 K306 K307 K308 K309 K310 K311 K312 K313 K314 K315 K316 K317 K318 K319 K320 K321 K322 K323 K324 K325 K326 K327 K328 K329 K330 K331 K332 K333 K334 K335 K336 K337 K338 K339 K340 K341 K342 K343 K344 K345 K346 K347 K348 K349 K350 K351 K352 K353 K354 K355 K356 K357 K358 K359 K360 K361 K362 K363 K364 K365 K366 K367 K368 K369 K370 K371 K372 K373 K374 K375 K376 K377 K378 K379 K380 K381 K382 K383 K384 K385 K386 K387 K388 K389 K390 K391 K392 K393 K394 K395 K396 K397 K398 K399 K400 K401 K402 K403 K404 K405 K406 K407 K408 K409 K410 K411 K412 K413 K414 K415 K416 K417 K418 K419 K420 K421 K422 K423 K424 K425 K426 K427 K428 K429 K430 K431 K432 K433 K434 K435 K436 K437 K438 K439 K440 K441 K442 K443 K444 K445 K446 K447 K448 K449 K450 K451 K452 K453 K454 K455 K456 K457 K458 K459 K460 K461 K462 K463 K464 K465 K466 K467 K468 K469 K470 K471 K472 K473 K474 K475 K476 K477 K478 K479 K480 K481 K482 K483 K484 K485 K486 K487 K488 K489 K490 K491 K492 K493 K494 K495 K496 K497 K498 K499 K500 K501 K502 K503 K504 K505 K506 K507 K508 K509 K510 K511 K512 K513 K514 K515 K516 K517 K518 K519 K520 K521 K522 K523 K524 K525 K526 K527 K528 K529 K530 K531 K532 K533 K534 K535 K536 K537 K538 K539 K540 K541 K542 K543 K544 K545 K546 K547 K548 K549 K550 K551 K552 K553 K554 K555 K556 K557 K558 K559 K560 K561 K562 K563 K564 K565 K566 K567 K568 K569 K570 K571 K572 K573 K574 K575 K576 K577 K578 K579 K580 K581 K582 K583 K584 K585 K586 K587 K588 K589 K590 K591 K592 K593 K594 K595 K596 K597 K598 K599 K600 K601 K602 K603 K604 K605 K606 K607 K608 K609 K610 K611 K612 K613 K614 K615 K616 K617 K618 K619 K620 K621 K622 K623 K624 K625 K626 K627 K628 K629 K630 K631 K632 K633 K634 K635 K636 K637 K638 K639 K640 K641 K642 K643 K644 K645 K646 K647 K648 K649 K650 K651 K652 K653 K654 K655 K656 K657 K658 K659 K660 K661 K662 K663 K664 K665 K666 K667 K668 K669 K670 K671 K672 K673 K674 K675 K676 K677 K678 K679 K680 K681 K682 K683 K684 K685 K686 K687 K688 K689 K690 K691 K692 K693 K694 K695 K696 K697 K698 K699 K700 K701 K702 K703 K704 K705 K706 K707 K708 K709 K710 K711 K712 K713 K714 K715 K716 K717 K718 K719 K720 K721 K722 K723 K724 K725 K726 K727 K728 K729 K730 K731 K732 K733 K734 K735 K736 K737 K738 K739 K740 K741 K742 K743 K744 K745 K746 K747 K748 K749 K750 K751 K752 K753 K754 K755 K756 K757 K758 K759 K760 K761 K762 K763 K764 K765 K766 K767 K768 K769 K770 K771 K772 K773 K774 K775 K776 K777 K778 K779 K780 K781 K782 K783 K784 K785 K786 K787 K788 K789 K790 K791 K792 K793 K794 K795 K796 K797 K798 K799 K800 K801 K802 K803 K804 K805 K806 K807 K808 K809 K810 K811 K812 K813 K814 K815 K816 K817 K818 K819 K820 K821

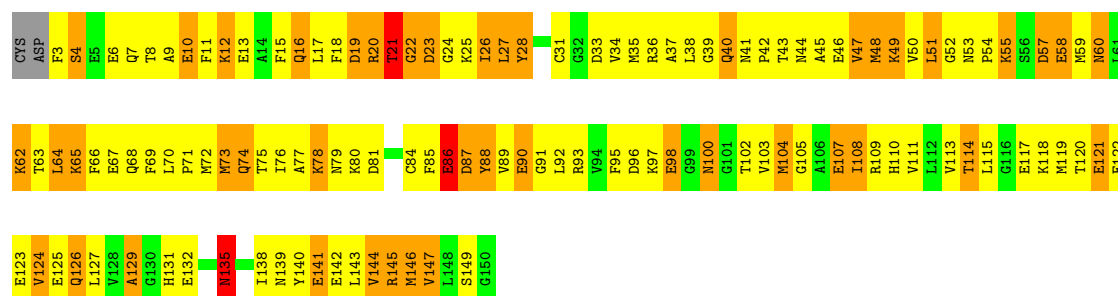
• Molecule 2: MYOSIN

Chain B: 

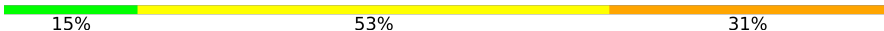


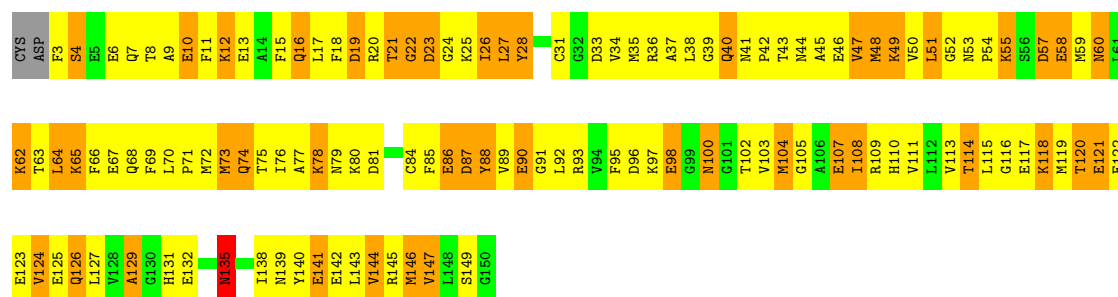
• Molecule 2: MYOSIN

Chain D: 

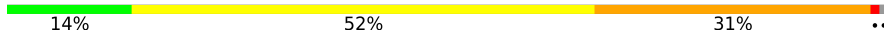


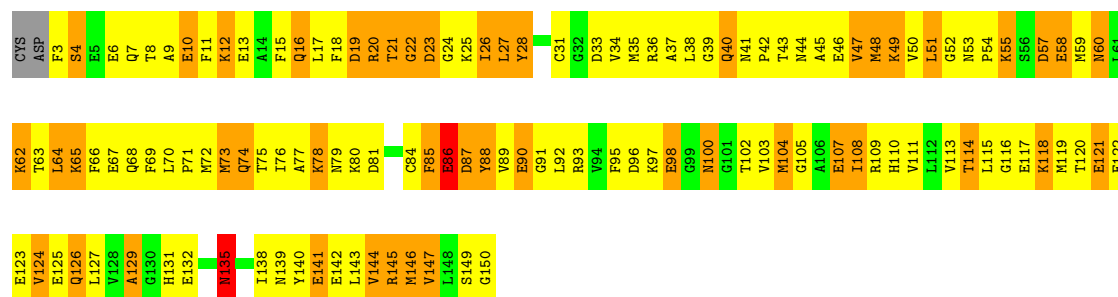
• Molecule 2: MYOSIN

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, 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, BEF

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	0.51	0/6410	1.08	22/8640 (0.3%)
1	C	0.52	0/6410	1.08	22/8640 (0.3%)
1	E	0.53	0/6410	1.08	21/8640 (0.2%)
1	G	0.52	0/6410	1.08	22/8640 (0.3%)
2	B	0.64	0/1176	1.15	3/1575 (0.2%)
2	D	0.55	0/1176	1.12	2/1575 (0.1%)
2	F	0.54	0/1176	1.11	1/1575 (0.1%)
2	H	0.56	0/1176	1.11	1/1575 (0.1%)
All	All	0.53	0/30344	1.09	94/40860 (0.2%)

There are no bond length outliers.

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	668	THR	N-CA-C	-8.51	103.42	113.88
1	E	668	THR	N-CA-C	-8.49	103.43	113.88
1	G	668	THR	N-CA-C	-8.48	103.45	113.88
1	C	668	THR	N-CA-C	-8.48	103.45	113.88
1	C	74	ASP	N-CA-C	-8.31	102.34	114.39

There are no chirality outliers.

There are no planarity outliers.

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	6292	0	6301	1020	3
1	C	6292	0	6301	993	0
1	E	6292	0	6301	1016	0
1	G	6292	0	6301	1016	11
2	B	1161	0	1126	228	0
2	D	1161	0	1126	221	11
2	F	1161	0	1126	228	3
2	H	1161	0	1126	229	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	4834	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 81.

The worst 5 of 4834 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	9
1	C	773/820 (94%)	580 (75%)	138 (18%)	55 (7%)	1	9
1	E	773/820 (94%)	580 (75%)	138 (18%)	55 (7%)	1	9
1	G	773/820 (94%)	580 (75%)	138 (18%)	55 (7%)	1	9
2	B	146/150 (97%)	111 (76%)	29 (20%)	6 (4%)	2	18
2	D	146/150 (97%)	112 (77%)	28 (19%)	6 (4%)	2	18
2	F	146/150 (97%)	112 (77%)	29 (20%)	5 (3%)	3	21
2	H	146/150 (97%)	113 (77%)	26 (18%)	7 (5%)	2	15
All	All	3676/3880 (95%)	2767 (75%)	665 (18%)	244 (7%)	1	11

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%)	439 (64%)	246 (36%)	0	0
1	C	685/718 (95%)	437 (64%)	248 (36%)	0	0
1	E	685/718 (95%)	438 (64%)	247 (36%)	0	0
1	G	685/718 (95%)	437 (64%)	248 (36%)	0	0
2	B	127/129 (98%)	74 (58%)	53 (42%)	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%)	74 (58%)	53 (42%)	0	0
All	All	3248/3388 (96%)	2047 (63%)	1201 (37%)	0	0

5 of 1201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	95	LEU
1	G	817	GLN
1	G	178	GLU
1	G	91	GLU
1	G	481	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	303	ASN
1	G	320	HIS
1	G	680	ASN
1	C	372	ASN
1	C	320	HIS

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 oligosaccharides 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	998	3,5	28,29,29	1.05	1 (3%)	43,45,45	1.09	3 (6%)
5	BEF	C	999	3,4	0,3,3	-	-	-		
4	ADP	G	998	3,5	28,29,29	1.06	1 (3%)	43,45,45	1.09	3 (6%)
5	BEF	G	999	3,4	0,3,3	-	-	-		
4	ADP	E	998	3,5	28,29,29	1.06	1 (3%)	43,45,45	1.08	3 (6%)
4	ADP	C	998	3,5	28,29,29	1.06	1 (3%)	43,45,45	1.09	3 (6%)
5	BEF	E	999	3,4	0,3,3	-	-	-		
5	BEF	A	999	3,4	0,3,3	-	-	-		

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	-	3/16/32/32	0/3/3/3
4	ADP	G	998	3,5	-	3/16/32/32	0/3/3/3
4	ADP	C	998	3,5	-	3/16/32/32	0/3/3/3
4	ADP	E	998	3,5	-	3/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	998	ADP	PA-O3A	-2.42	1.56	1.59
4	C	998	ADP	PA-O3A	-2.39	1.56	1.59
4	A	998	ADP	PA-O3A	-2.37	1.56	1.59
4	E	998	ADP	PA-O3A	-2.32	1.57	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	998	ADP	O4'-C1'-N9	3.73	115.25	108.09
4	G	998	ADP	O4'-C1'-N9	3.72	115.23	108.09
4	A	998	ADP	O4'-C1'-N9	3.71	115.22	108.09
4	C	998	ADP	O4'-C1'-N9	3.70	115.20	108.09
4	A	998	ADP	N6-C6-N1	-2.46	112.89	118.38

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

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

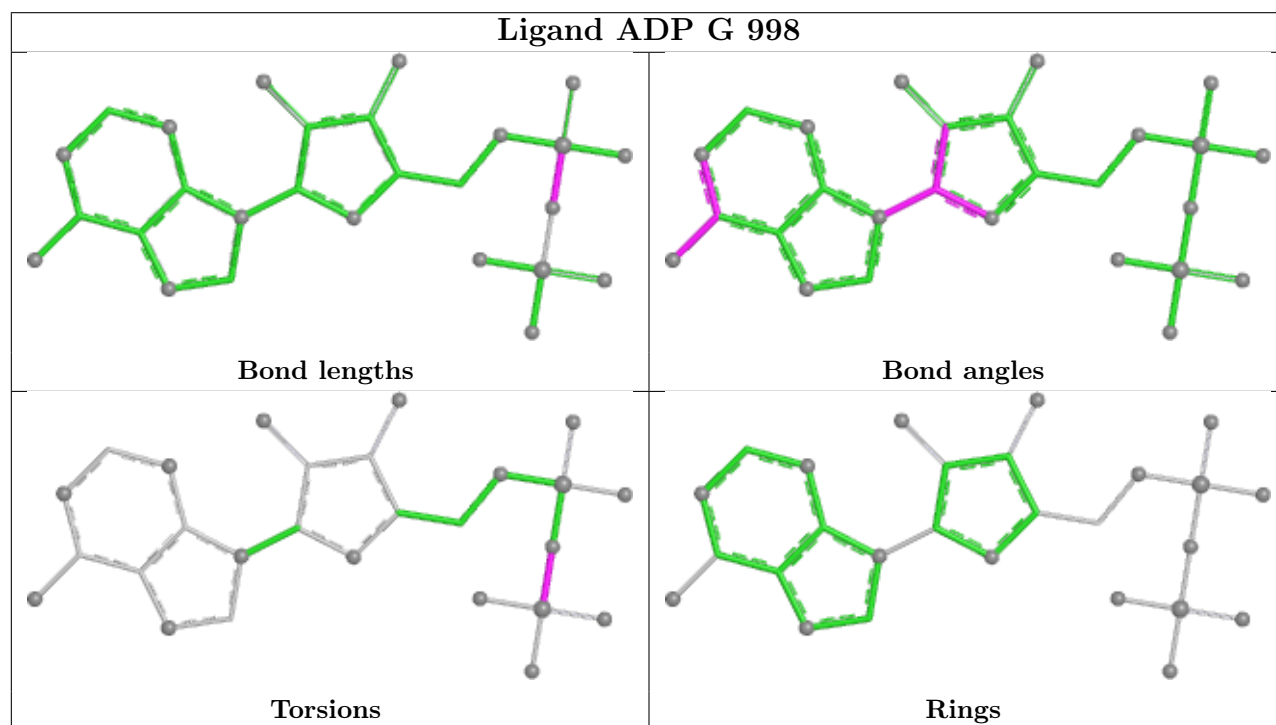
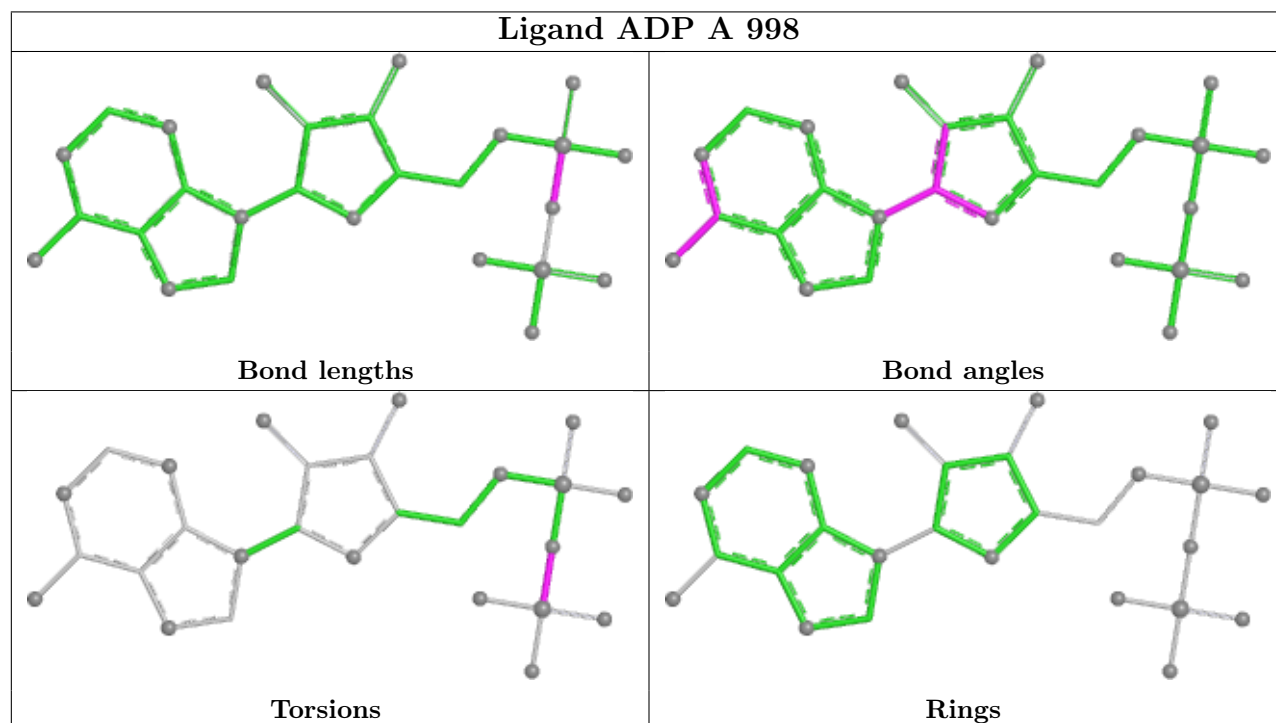
There are no ring outliers.

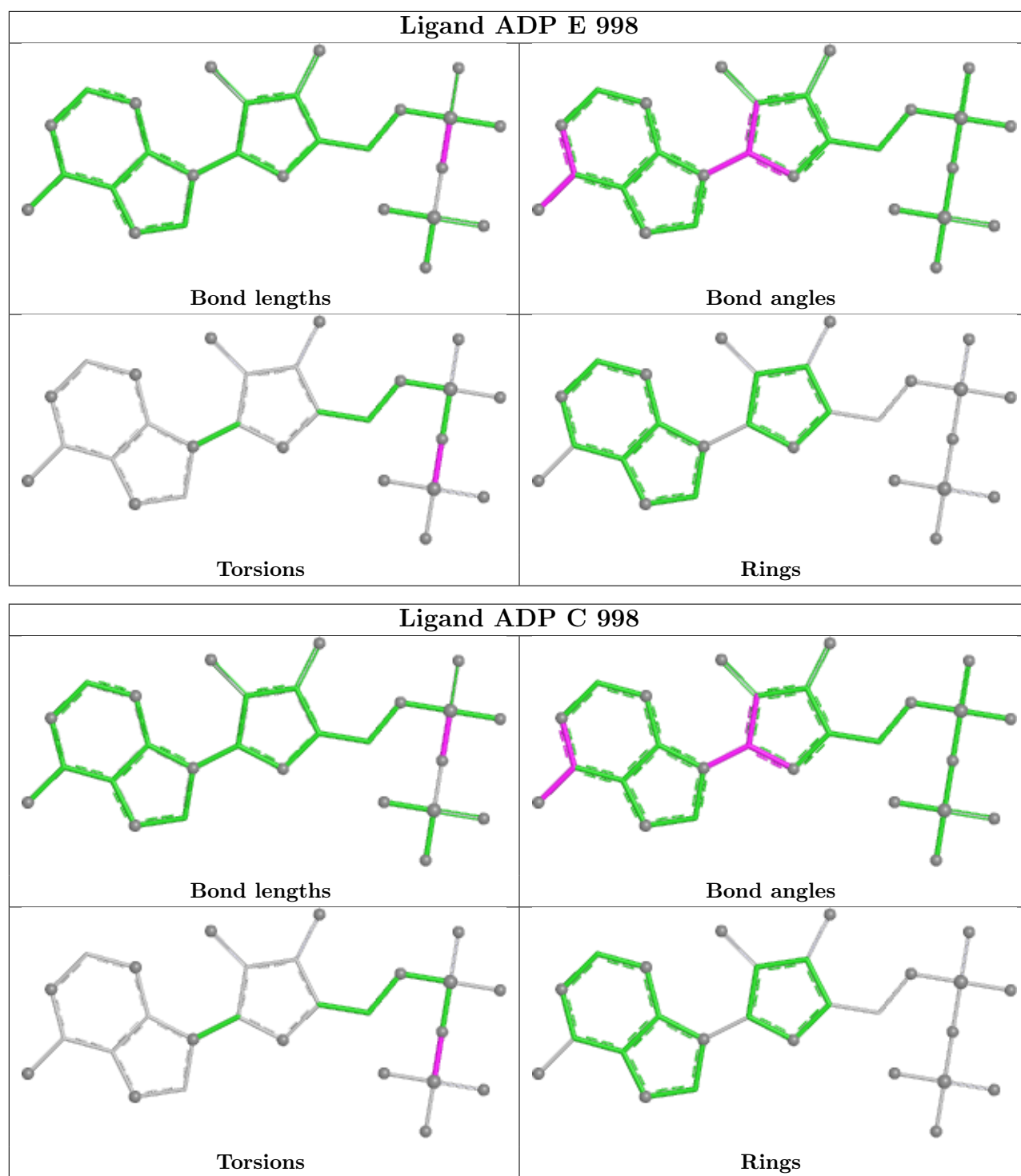
4 monomers are involved in 12 short contacts:

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

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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.