wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 01:40 PM EST

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

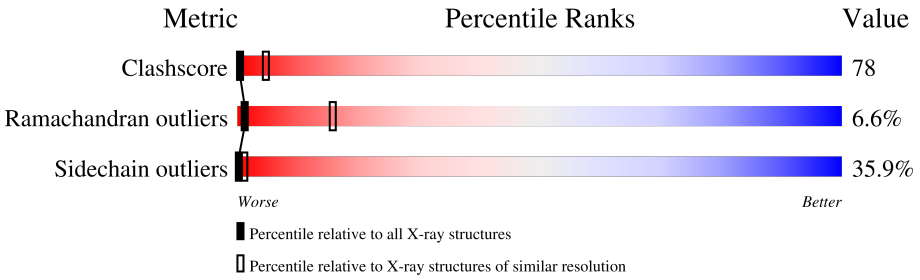
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	820	16% 52% 26% • 5%
1	C	820	16% 52% 25% • 5%
1	E	820	16% 52% 26% • 5%
1	G	820	16% 52% 25% • 5%
2	B	150	16% 50% 31% ••
2	D	150	17% 50% 30% ••
2	F	150	15% 53% 31% •
2	H	150	15% 52% 31% ••

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			

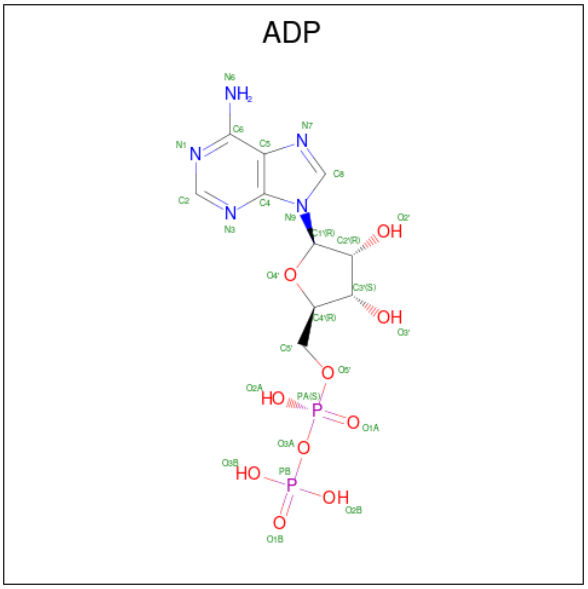
- Molecule 2 is a protein called MYOSIN.

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).

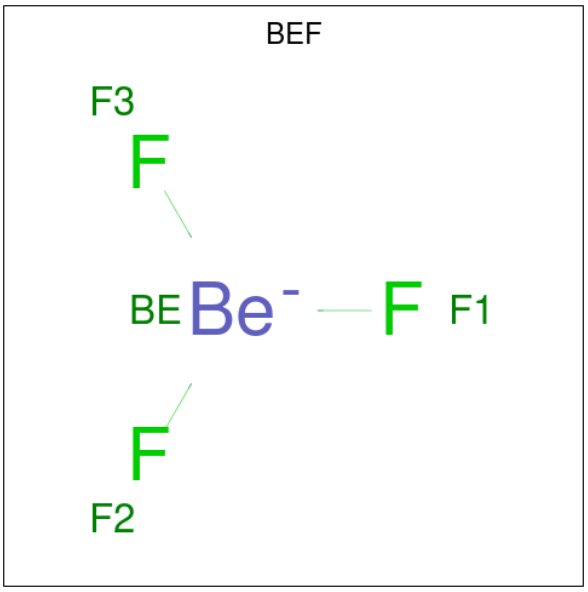
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (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 4 1 3	0	0
5	C	1	Total Be F 4 1 3	0	0
5	E	1	Total Be F 4 1 3	0	0
5	G	1	Total Be F 4 1 3	0	0

- Molecule 6 is water.

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

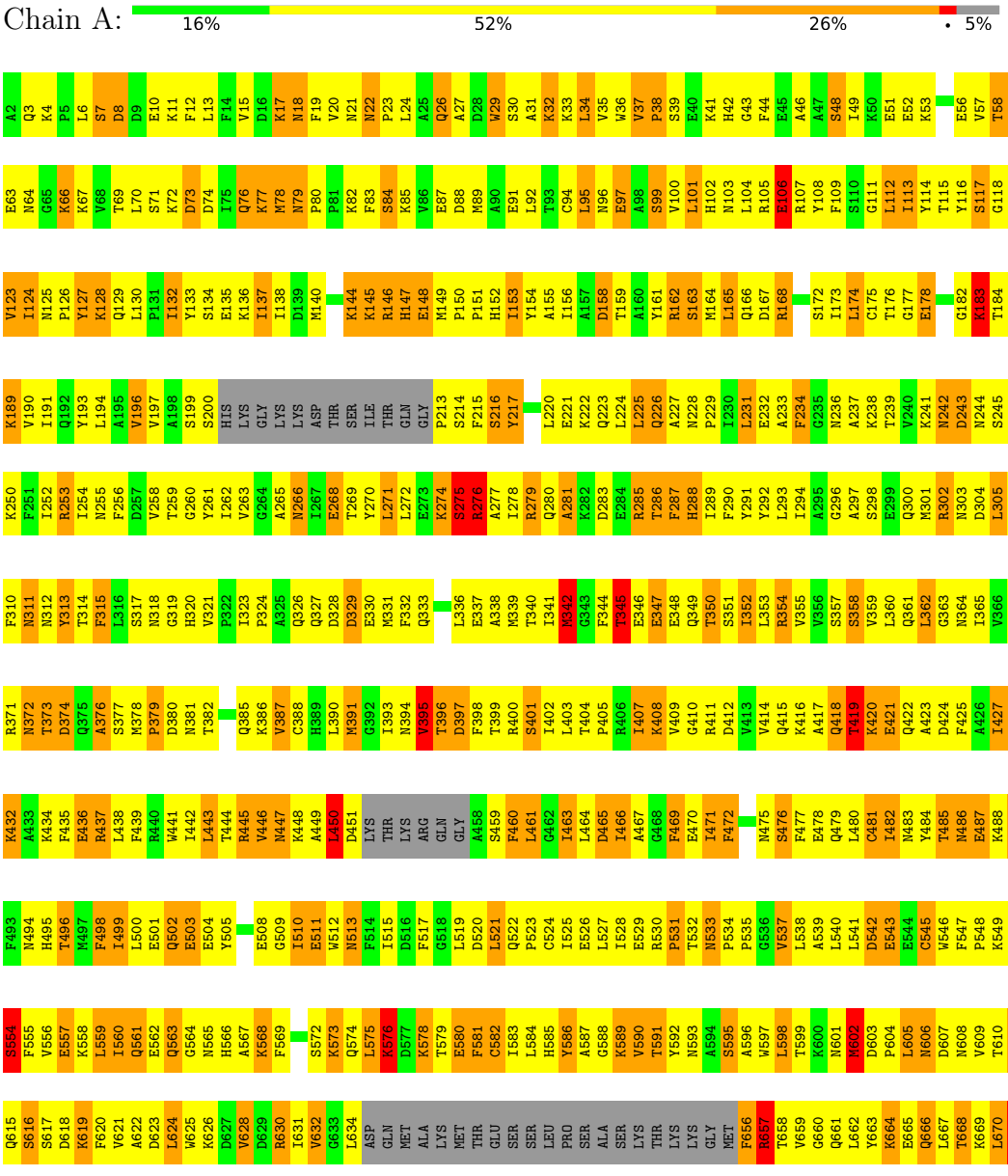
3 Residue-property plots (i)

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

Chain A:



R675 N676 T677 N678 P679 N680 F681 V682 R683 C684 I685 I686 P687 – E690 K691 R692 A693 G694 K695 L696 D697 A698 H699 L700 V701 L702 E703 Q704 L705 R706 C707 N708 G709 V710 L711 E712 G713 I714 R715 I716 C717 R718 Q719 G720 F721 P722 N723 R724 I725 V726 F727 Q728 E729 F730 R731 Q732 R733 Y734 E735

I736 L737 A738 – I742 P743 K744 G745 F746 M747 D748 G749 K750 Q751 A752 C753 I754 L755 M756 I757 K758 A759 L760 E761 L762 D763 P764 N765 L766 Y767 R768 I769 G770 Q771 S772 K773 I774 F775 F776 R777 T778 G779 V780 L781 – L784 E785 E786 E787 R788 D789 L790 K791 I792 T793 D794 V795 I796 I797 A798

F799 Q800 A801 Q802 C803 R804 G805 Y806 L807 A808 R809 K810 – K814 R815 Q816 Q817 Q818 L819 G820 S821

- Molecule 1: MYOSIN

Chain C: 16% 52% 25% • 5%

A2 Q3 K4 P5 L6 S7 D8 D9 E10 K11 F12 L13 F14 V15 D16 K17 N18 F19 V20 N21 N22 P23 L24 A25 Q26 A27 D28 W29 S30 A31 K32 K33 L34 V35 W36 V37 P38 S39 E40 K41 H42 G43 F44 E45 A46 A47 S48 I49 K50 E51 E52 K53 – E56 V57 T58 V59 E60 L61 Q62

E63 N64 G65 K66 K67 V68 T69 L70 S71 K72 D73 D74 I75 Q76 K77 M78 N79 P80 P81 K82 F83 S84 K85 V86 E87 D88 M89 A90 E91 L92 T93 C94 L95 N96 E97 A98 S99 V100 L101 H102 N103 L104 R105 E106 R107 Y108 F109 S110 G111 L112 I113 Y114 T115 Y116 S117 G118 L119 F120 C121 V122

V123 I124 N125 P126 Y127 K128 Q129 L130 P131 I132 Y133 S134 E135 K136 I137 I138 D139 M140 – K144 K145 R146 H147 E148 M149 P150 P151 H152 I153 Y154 A155 I156 A157 D158 T159 A160 Y161 R162 S163 M164 L165 Q166 D167 R168 E169 D170 Q171 S172 I173 L174 C175 T176 G177 E178 – G182 K183 T184 E185 N186

T187 K188 K189 V190 I191 Q192 Y193 L194 A195 V196 V197 A198 S199 S200 HIS LYS GLY LYS LYS ASP THR SER ILE THR GLN GLY P213 S214 F215 S216 Y217 – L220 E221 K222 Q223 L224 L225 Q226 A227 N228 P229 I230 L231 E232 A233 F234 G235 N236 A237 K238 T239 V240 K241 N242 D243 N244 S245 S246 R247

F248 G249 K250 F251 I252 R253 I254 N255 F256 D257 V258 T259 G260 Y261 I262 V263 G264 A265 N266 I267 E268 T269 Y270 L271 L272 E273 K274 S275 R276 A277 I278 R279 Q280 A281 K282 D283 E284 R285 T286 F287 H288 I289 F290 Y291 Y292 L293 I294 A295 G296 A297 S298 E299 Q300 M301 R302 N303 D304 L305 L306 L307

E308 G309 F310 N311 N312 Y313 T314 F315 L316 S317 N318 G319 H320 V321 P322 I323 P324 A325 Q326 Q327 D328 D329 E330 M331 F332 Q333 – L336 E337 A338 M339 T340 I341 M342 G343 F344 T345 E346 E347 E348 Q349 T350 S351 I352 L353 R354 V355 V356 S357 S358 V359 L360 Q361 L362 G363 N364 I365 V366 F367 K368

K369 E370 R371 N372 T373 D374 Q375 A376 S377 M378 P379 D380 N381 T382 – Q385 K386 V387 C388 H389 L390 M391 G392 I393 N394 V395 T396 D397 F398 T399 R400 S401 I402 L403 T404 P405 R406 I407 K408 V409 G410 R411 D412 V413 V414 Q415 K416 A417 Q418 T419 K420 E421 Q422 A423 D424 F425 A426 I427 E428 A429

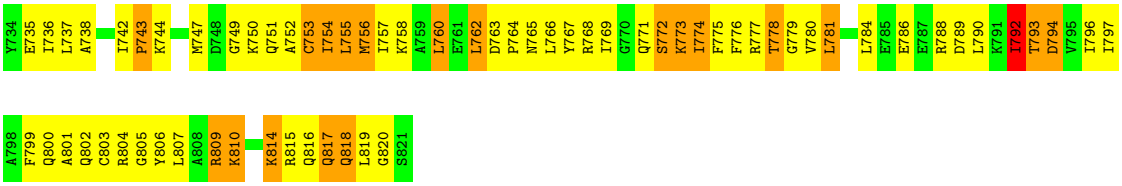
L430 A431 K432 A433 K434 F435 E436 R437 L438 F439 R440 W441 I442 L443 T444 R445 V446 N447 K448 A449 L450 D451 LYS THR LYS ARG GLN GLY A458 S459 F460 L461 G462 I463 L464 D465 I466 A467 G468 F469 E470 I471 F472 – N475 S476 F477 E478 Q479 L480 C481 I482 N483 Y484 T485 N486 E487 K488 L489 Q490

Q491 L492 F493 N494 H495 T496 M497 F498 I499 L500 E501 Q502 E503 E504 Y505 – E508 G509 I510 E511 W512 N513 F514 I515 D516 F517 G518 L519 D520 L521 Q522 P523 C524 I525 E526 L527 I528 E529 R530 P531 T532 N533 P534 P535 G536 V537 L538 A539 L540 L541 D542 E543 E544 C545 W546 F547 P548 K549 A550 T551

D552 T553 S554 F555 V556 E557 K558 L559 I560 Q561 E562 Q563 G564 N565 H566 A567 K568 F569 – S572 K573 Q574 L575 K576 D577 K578 T579 E580 F581 C582 I583 L584 H585 Y586 A587 G588 K589 V590 T591 Y592 N593 A594 S595 A596 W597 L598 T599 K600 N601 M602 D603 P604 L605 N606 D607 N608 V609 T610 S611 L612

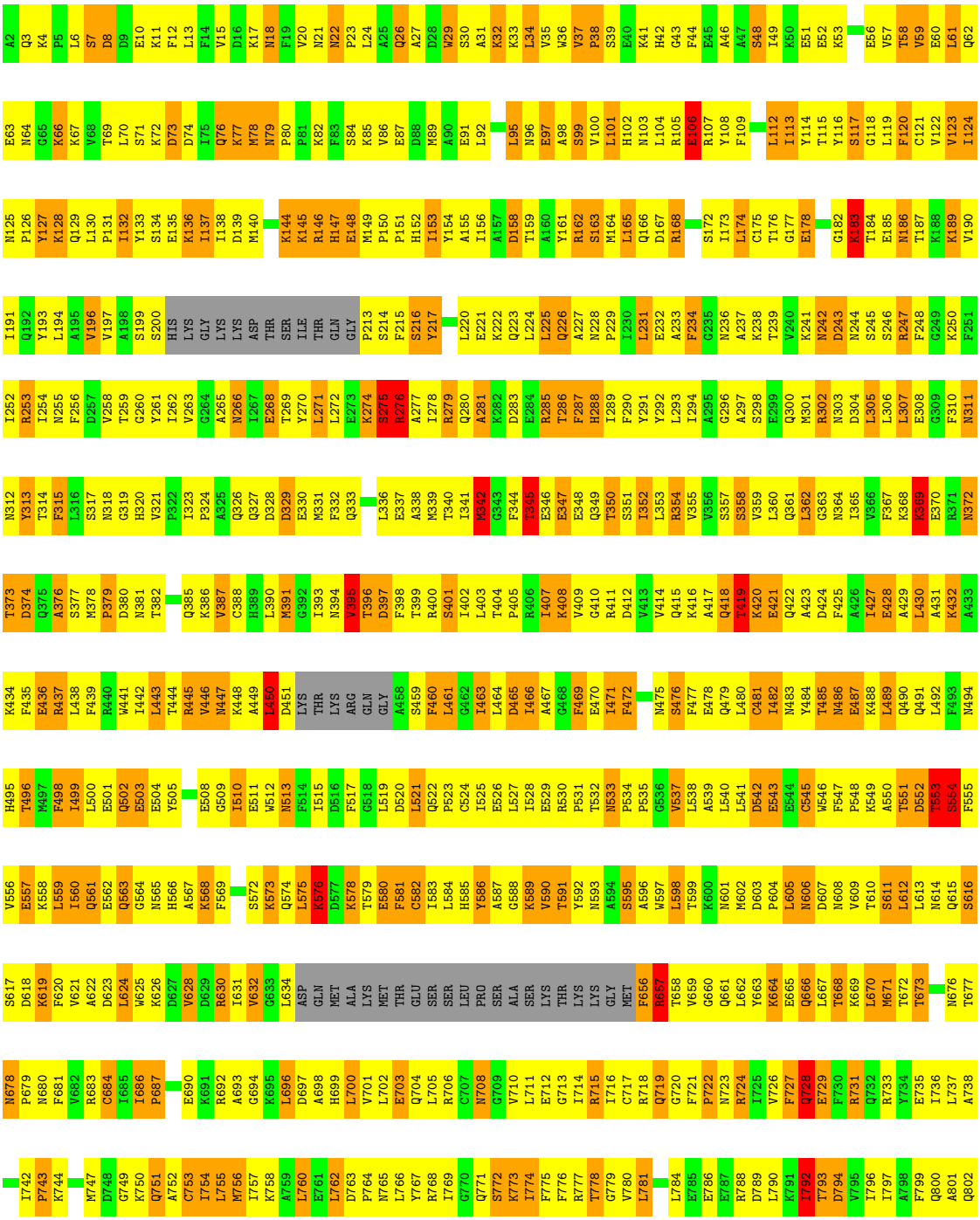
L613 N614 Q615 S616 S617 D618 K619 F620 V621 A622 D623 L624 W625 K626 D627 V628 D629 R630 I631 V632 G633 L634 ASP GLN MET ALA LYS MET THR GLU SER SER LEU PRO SER ALA SER LYS THR LYS LYS GLY MET F656 R657 T658 V659 G660 Q661 L662 Y663 K664 E665 Q666 L667 T668 K669 L670 M671 T672

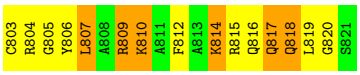
T673 L674 R675 N676 T677 N678 P679 N680 F681 V682 R683 C684 I685 I686 P687 – E690 K691 R692 A693 G694 K695 L696 D697 A698 H699 L700 V701 L702 E703 Q704 L705 R706 C707 N708 G709 V710 L711 E712 G713 I714 R715 I716 C717 R718 Q719 G720 F721 P722 N723 R724 I725 V726 F727 Q728 E729 F730 R731 Q732 R733



• Molecule 1: MYOSIN

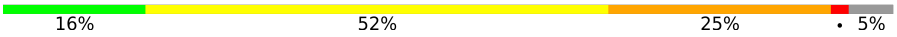
Chain E:

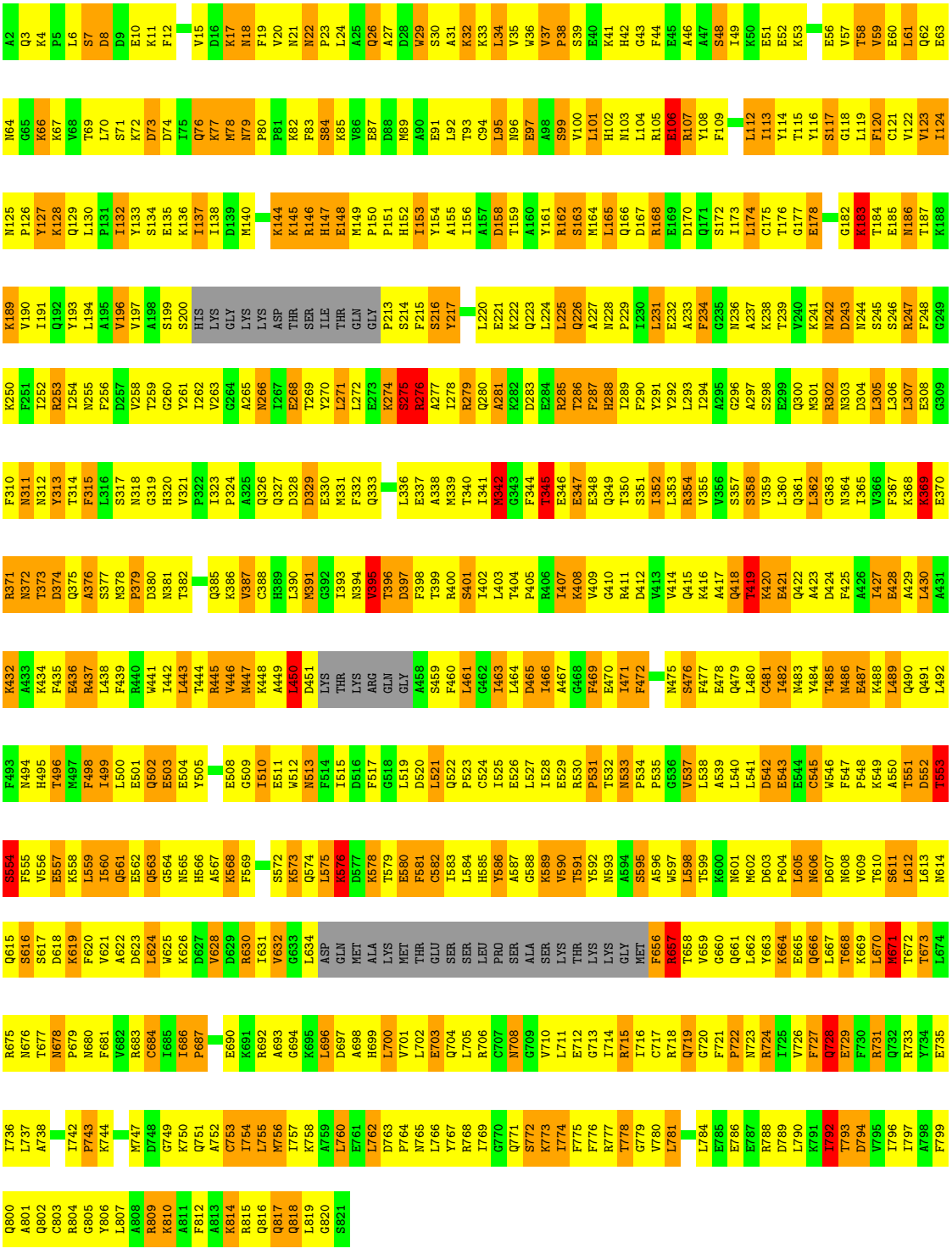




• Molecule 1: MYOSIN

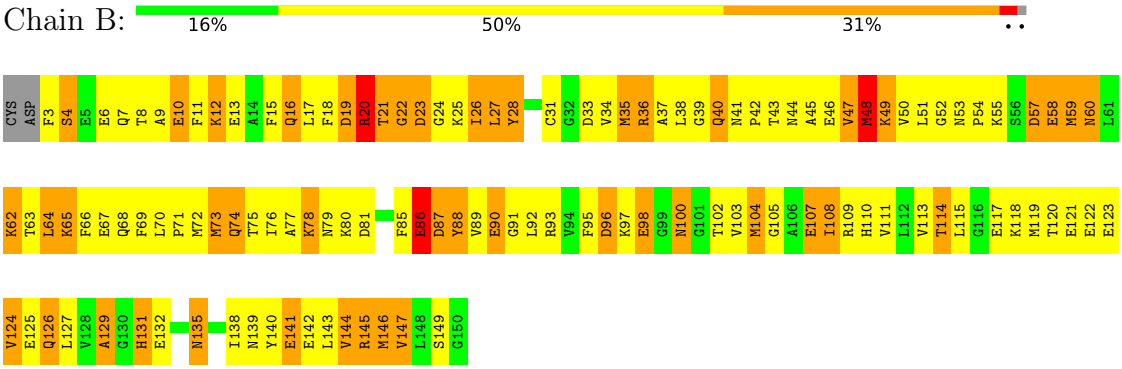
Chain G:





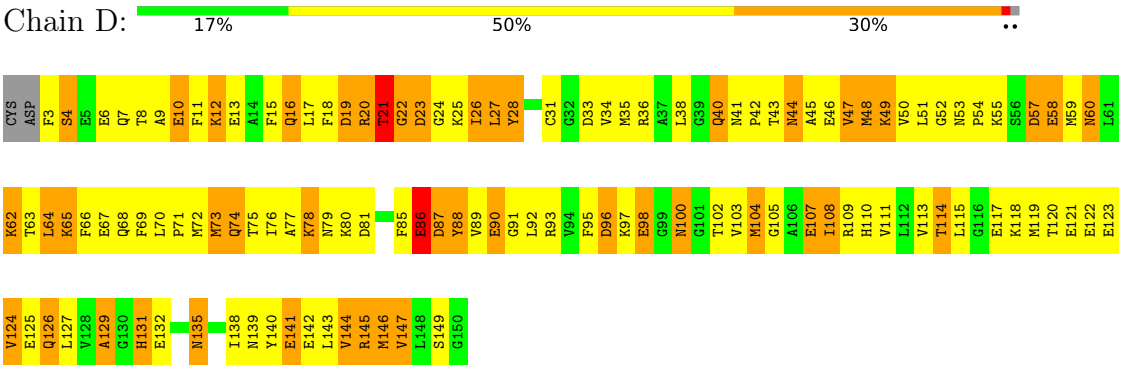
• Molecule 2: MYOSIN

Chain B:



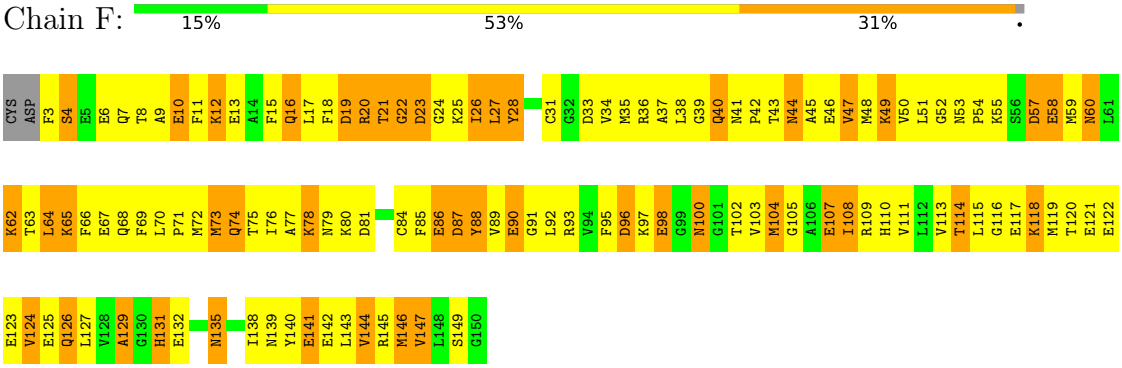
• Molecule 2: MYOSIN

Chain D:



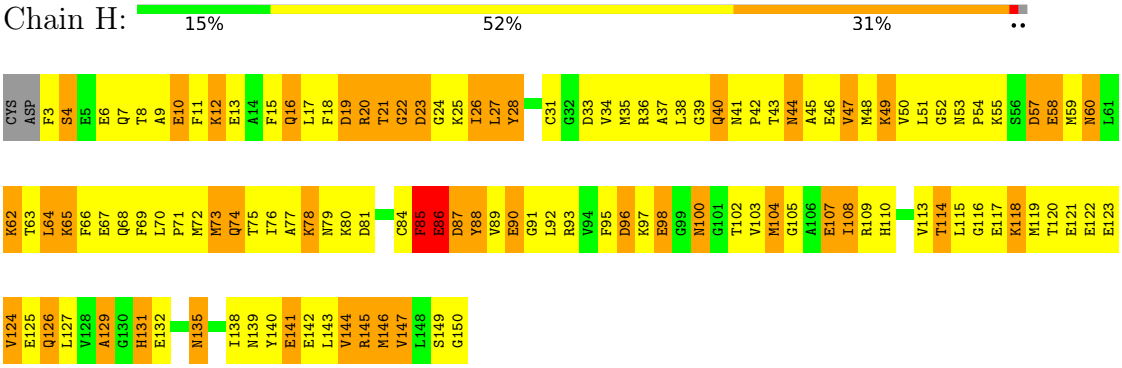
• Molecule 2: MYOSIN

Chain F:



• Molecule 2: MYOSIN

Chain H:



4 Data and refinement statistics (i)

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: ADP, MG, 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	0.47	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(^{o})	Ideal(^{o})
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

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 (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	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	G	183	LYS
2	H	88	TYR
1	G	276	ARG
1	G	178	GLU
1	G	574	GLN

Sometimes 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	816	GLN
1	G	513	ASN
1	E	303	ASN
1	G	490	GLN
1	G	728	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 monosaccharides 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	$\#\|Z\| > 2$
5	BEF	A	999	4,3	0,3,3	-	-	-		
5	BEF	E	999	4,3	0,3,3	-	-	-		
4	ADP	E	998	5,3	24,29,29	1.18	2 (8%)	29,45,45	1.33	3 (10%)
5	BEF	G	999	4,3	0,3,3	-	-	-		
5	BEF	C	999	4,3	0,3,3	-	-	-		
4	ADP	C	998	5,3	24,29,29	1.19	2 (8%)	29,45,45	1.33	3 (10%)
4	ADP	G	998	5,3	24,29,29	1.18	2 (8%)	29,45,45	1.33	3 (10%)
4	ADP	A	998	5,3	24,29,29	1.18	2 (8%)	29,45,45	1.34	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	C	998	5,3	-	3/12/32/32	0/3/3/3
4	ADP	G	998	5,3	-	3/12/32/32	0/3/3/3
4	ADP	A	998	5,3	-	3/12/32/32	0/3/3/3
4	ADP	E	998	5,3	-	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(^{o})	Ideal(^{o})
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	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.

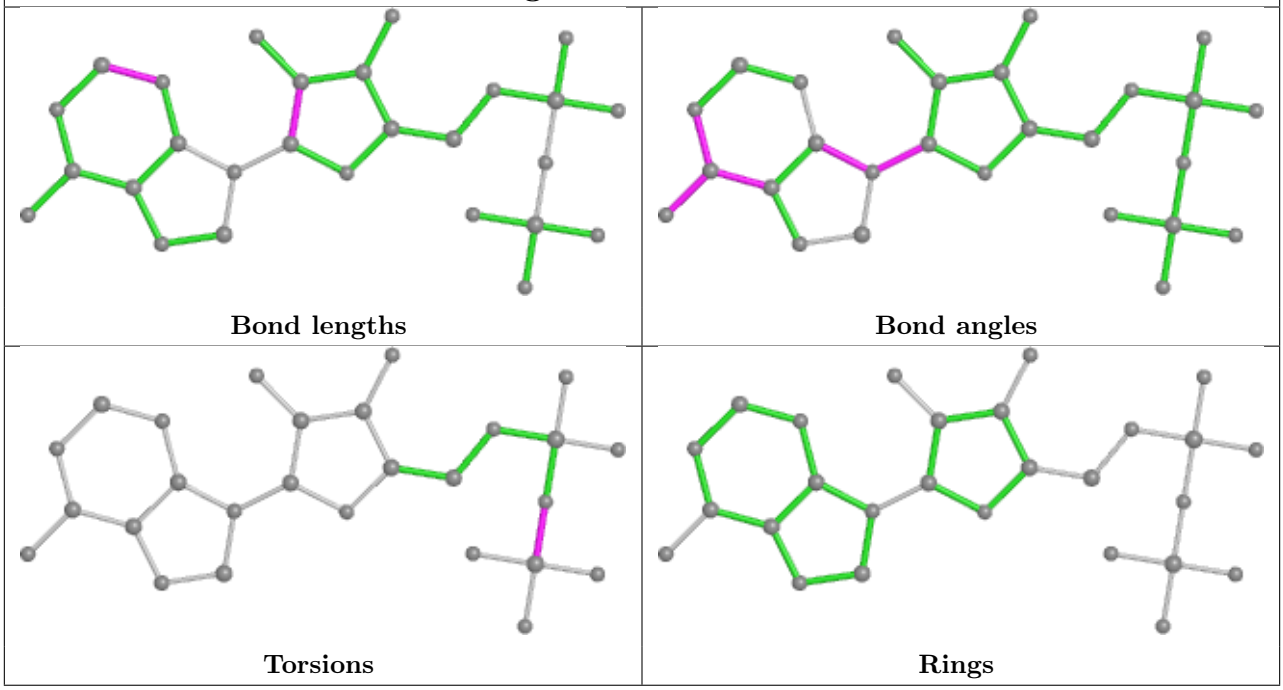
4 monomers are involved in 12 short contacts:

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

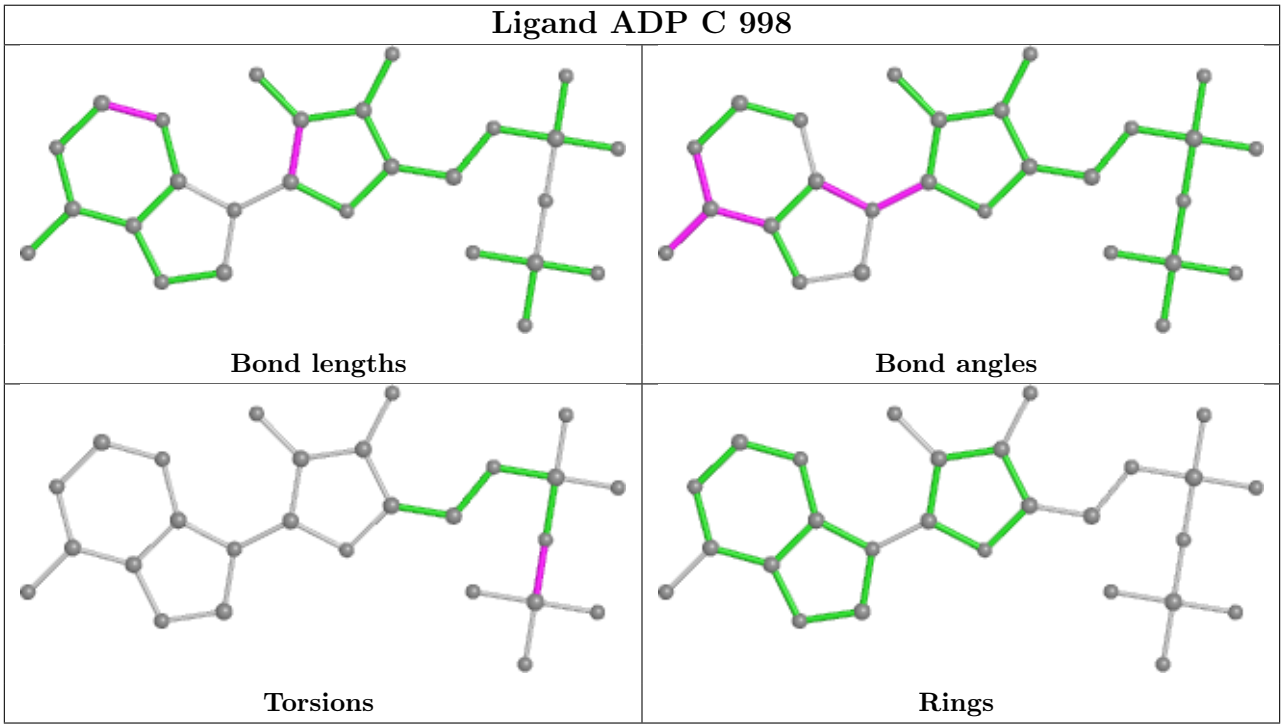
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

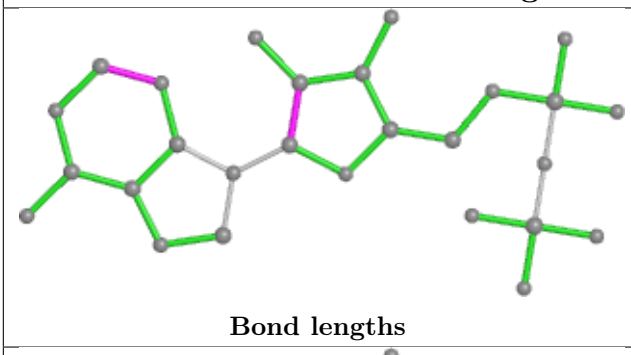
Ligand ADP E 998



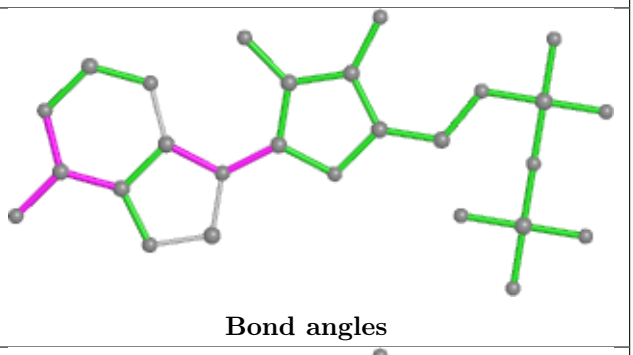
Ligand ADP C 998



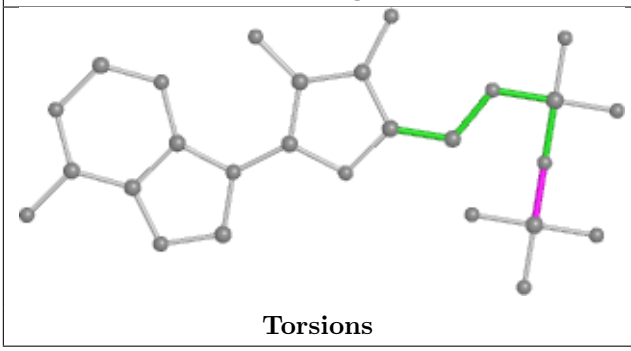
Ligand ADP G 998



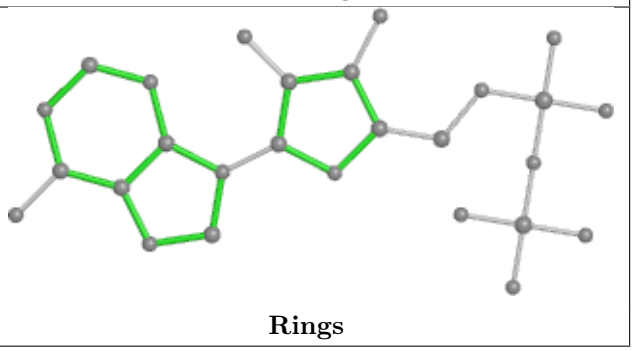
Bond lengths



Bond angles

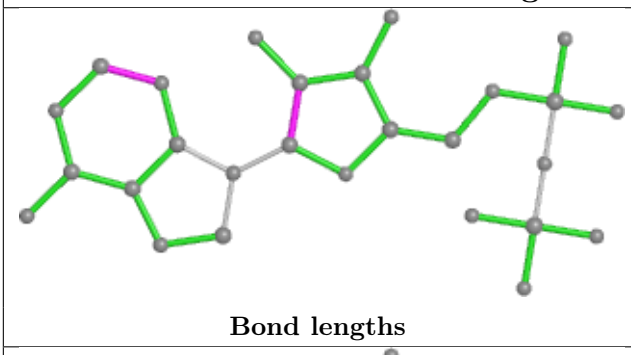


Torsions

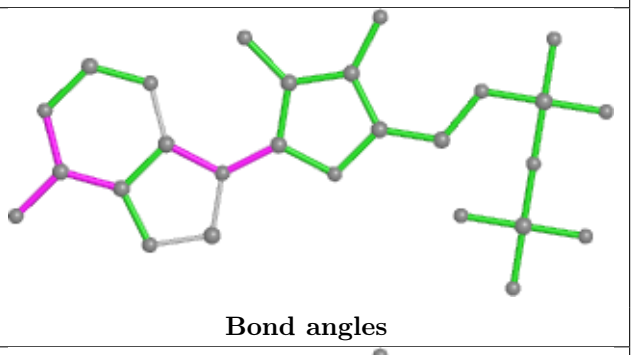


Rings

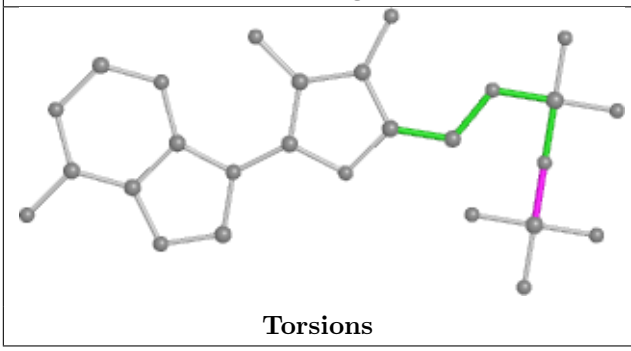
Ligand ADP A 998



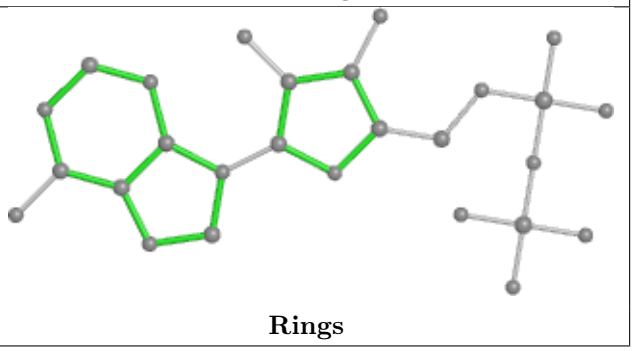
Bond lengths



Bond angles



Torsions



Rings

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

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.