wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 02:34 PM EST

PDB ID	:	1BR1
Title	:	SMOOTH MUSCLE MYOSIN MOTOR DOMAIN-ESSENTIAL LIGHT CHAIN COMPLEX WITH MGADP.ALF4 BOUND AT THE ACTIVE SITE
Authors	:	Dominguez, R.; Trybus, K.M.; Cohen, C.
Deposited on	:	1998-08-26
Resolution	:	3.50 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:

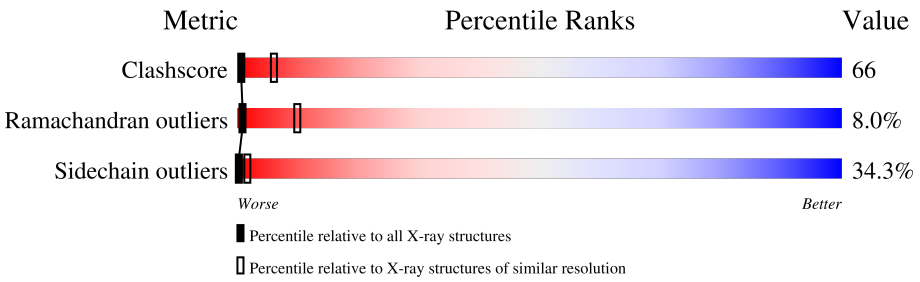
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.50 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	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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	19% 51% 24% • •
1	C	820	19% 51% 24% • •
1	E	820	19% 51% 24% • •
1	G	820	19% 50% 24% • •
2	B	150	18% 53% 27% ••
2	D	150	17% 51% 30% •
2	F	150	19% 53% 25% ••
2	H	150	17% 52% 29% ••

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 30132 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
			Total	C	N	O	S			
1	A	787	6337	4036	1089	1183	29	0	0	0
1	C	787	6337	4036	1089	1183	29	0	0	0
1	E	787	6337	4036	1089	1183	29	0	0	0
1	G	787	6337	4036	1089	1183	29	0	0	0

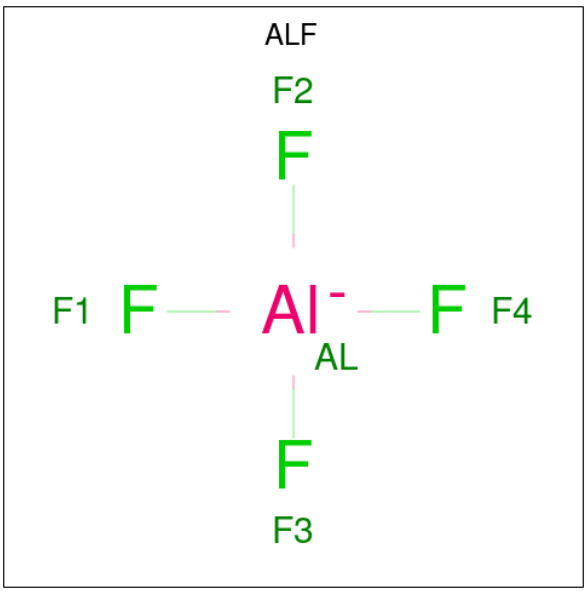
- Molecule 2 is a protein called MYOSIN.

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

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

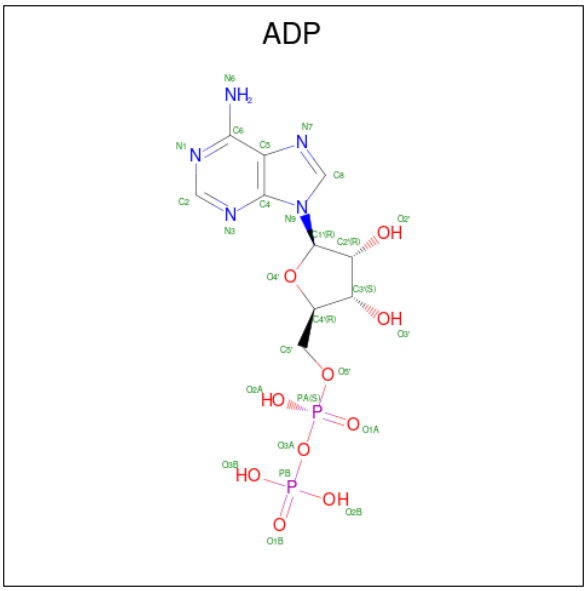
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	C	1	1	1	0	0
3	E	1	1	1	0	0
3	G	1	1	1	0	0

- Molecule 4 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



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

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



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

- 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		

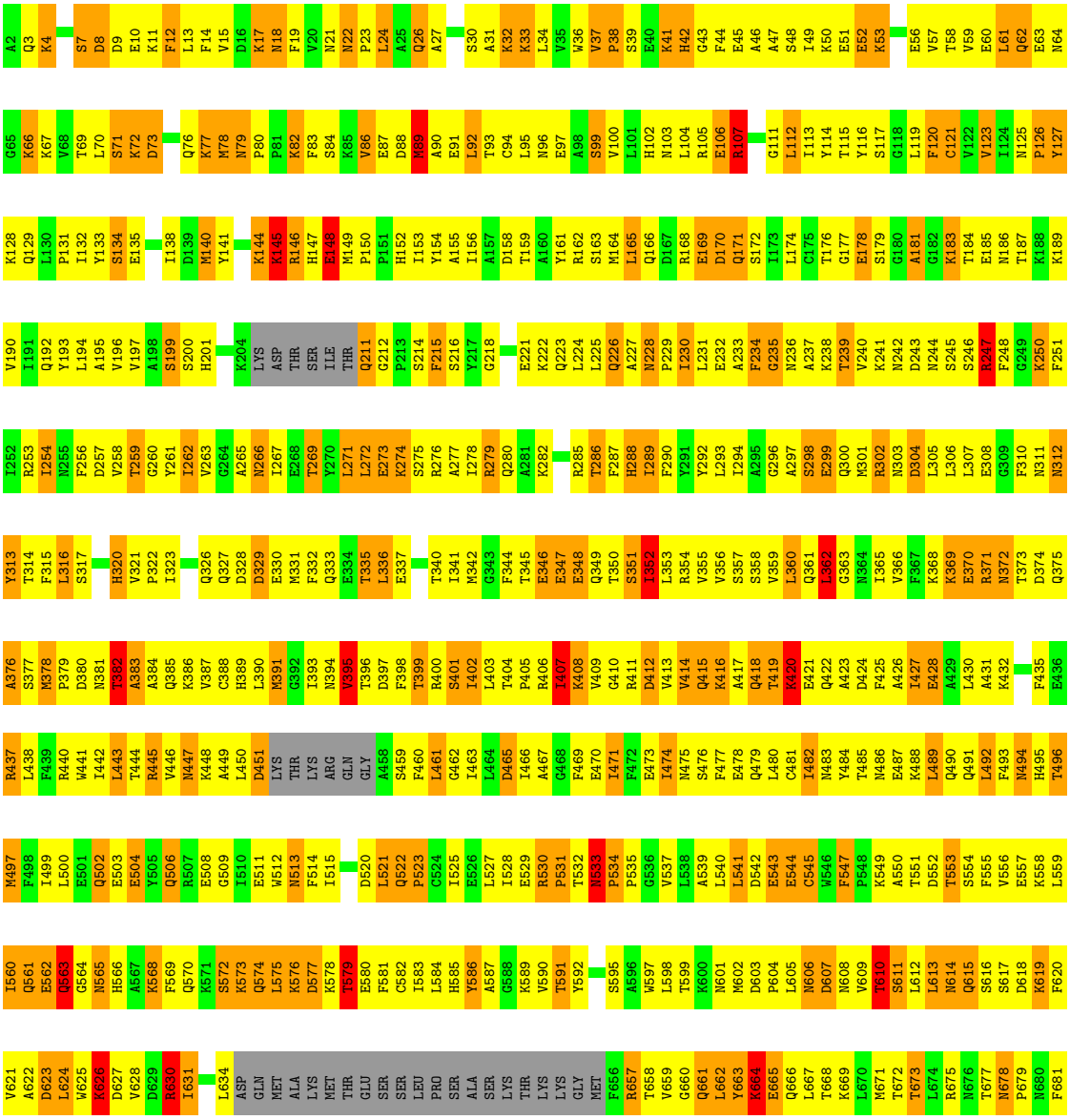
3 Residue-property plots (i)

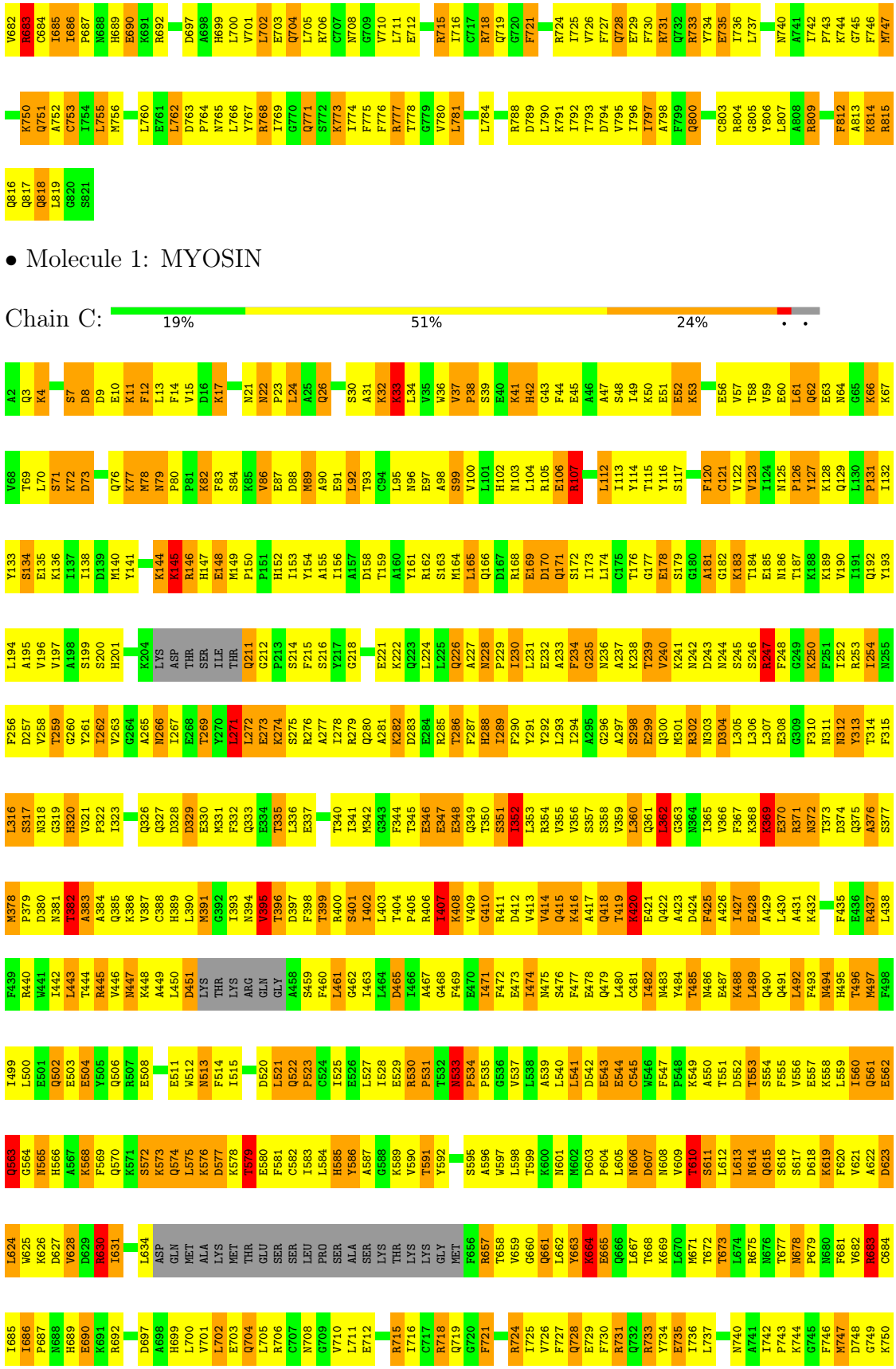
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

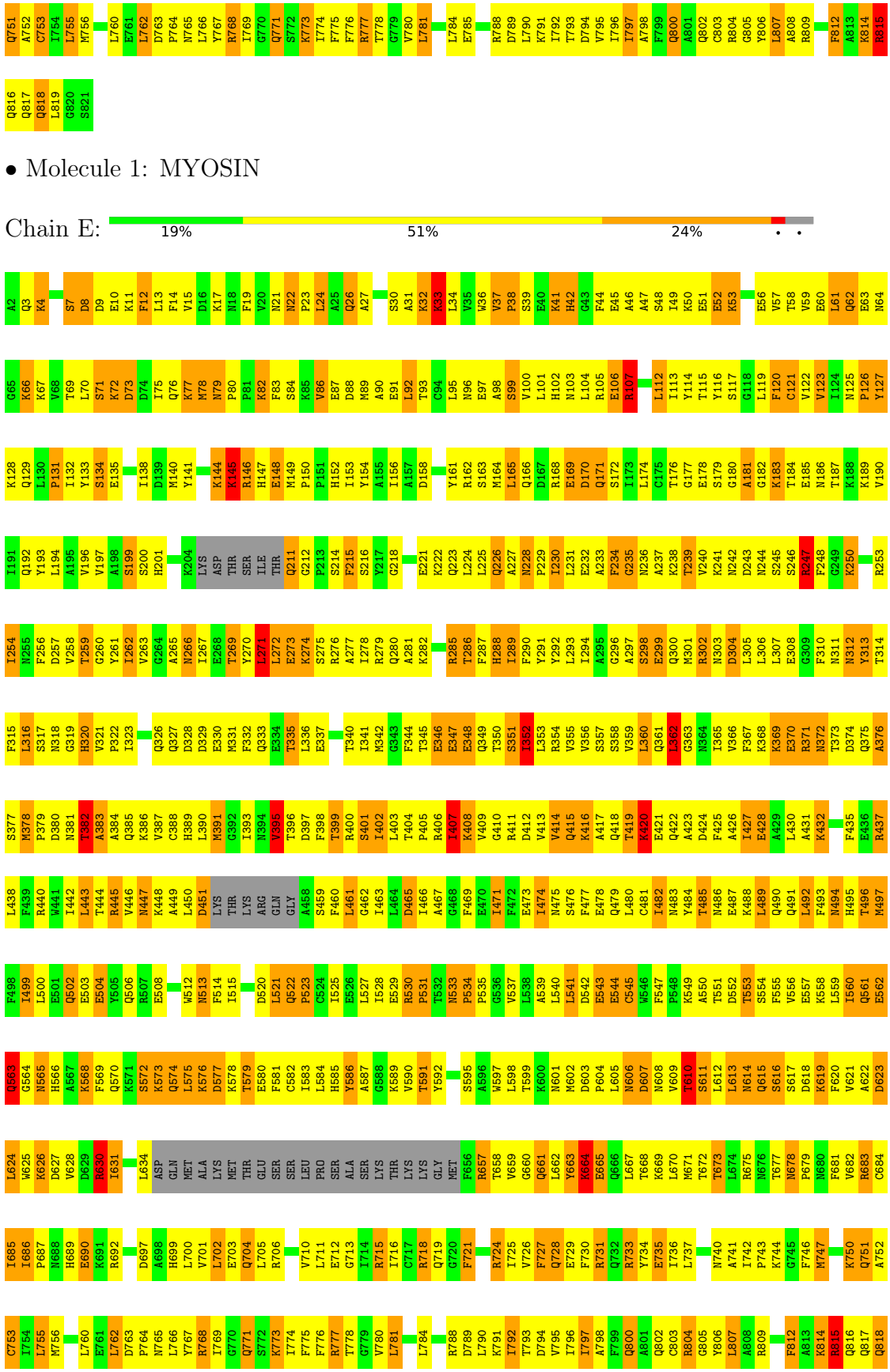
Chain A: 19% 51% 24%





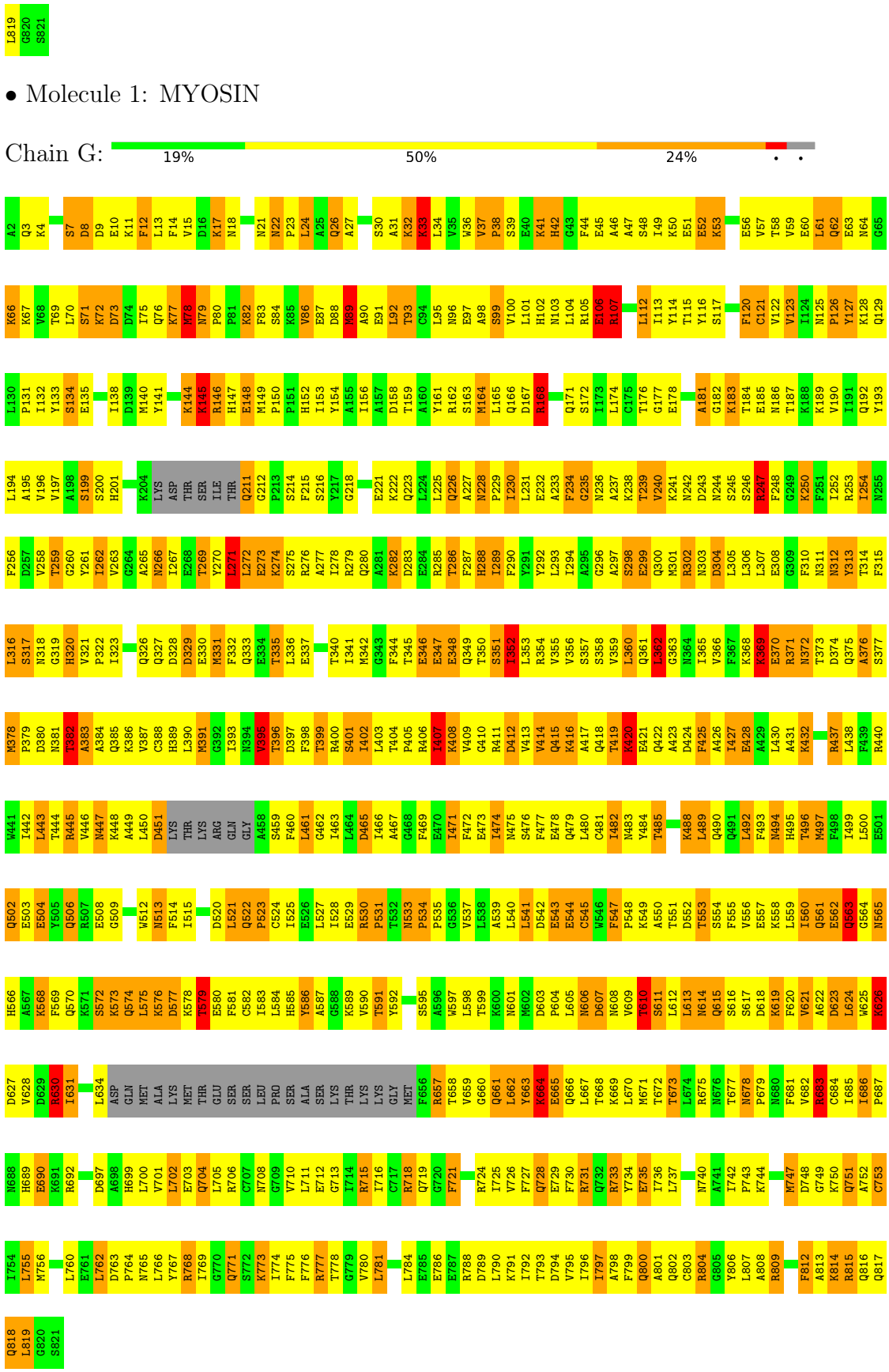
• Molecule 1: MYOSIN

Chain C: 19% 51% 24%



• Molecule 1: MYOSIN

Chain E: 19% 51% 24%


L819 G820 S821
• Molecule 1: MYOSIN
Chain G:
19%
50%
24%
• •
• Molecule 2: MYOSIN

Chain B: 18% 53% 27%

CYS ASP F3 S4 Q7 T8 A9 E10 F11 K12 E13 A14 F15 Q16 L17 F18 D19 R20 T21 G22 D23 G24 K25 I26 L27 Y28 S29 Q30 C31 V34 M35 R36 A37 L38 G39 Q40 N41 P42 T43 E46 V47 M48 K49 V50 L51 G52 N53 P54 K55 S56 D57 E58 M59 N60 L61 K62 T63

L64 K65 F66 E67 Q68 F69 L70 P71 M72 M73 Q74 T75 I76 A77 K78 N79 K80 D81 Q82 G83 C84 F85 E86 D87 Y88 V89 E90 G91 L92 R93 V94 F95 D96 K97 E98 G99 N100 V103 M104 G105 A106 E107 I108 R109 H110 V111 L112 V113 T114 L115 G116 E117 K118 M119 T120 E123 V124 E125

V128 A129 E132 D133 S134 N135 G136 C137 I138 N139 Y140 E141 E142 L143 V144 R145 M146 V147 L148 S149 G150

- Molecule 2: MYOSIN

Chain D: 17% 51% 30%

CYS ASP F3 S4 Q7 T8 A9 E10 F11 K12 E13 A14 F15 Q16 L17 F18 D19 R20 T21 G22 D23 G24 K25 I26 L27 Y28 S29 Q30 C31 V34 M35 R36 A37 L38 G39 Q40 N41 P42 T43 E46 V47 M48 K49 V50 L51 G52 N53 P54 K55 S56 D57 E58 M59 N60 L61 K62 T63

L64 K65 F66 E67 Q68 F69 L70 P71 M72 M73 Q74 T75 I76 A77 K78 N79 K80 D81 Q82 G83 C84 F85 E86 D87 Y88 V89 E90 G91 L92 R93 V94 F95 D96 K97 E98 G99 N100 V103 M104 G105 A106 E107 I108 R109 H110 V111 L112 V113 T114 L115 G116 E117 K118 M119 T120 E123 V124 E125

Q126 L127 V128 A129 E132 D133 S134 N135 G136 C137 I138 N139 Y140 E141 E142 L143 V144 R145 M146 V147 L148 S149 G150

- Molecule 2: MYOSIN

Chain F: 19% 53% 25%

CYS ASP F3 S4 Q7 T8 A9 E10 F11 K12 E13 A14 F15 F18 D19 R20 T21 G22 D23 G24 K25 I26 L27 Y28 S29 Q30 C31 V34 M35 R36 A37 L38 G39 Q40 N41 P42 T43 N44 A45 E46 V47 M48 K49 V50 L51 G52 N53 P54 K55 S56 D57 E58 M59 N60 L61 K62 T63

L64 K65 F66 E67 Q68 F69 L70 P71 M72 M73 Q74 T75 I76 A77 K78 N79 K80 D81 Q82 G83 C84 F85 E86 D87 Y88 V89 E90 G91 L92 R93 V94 F95 D96 K97 E98 G99 N100 V103 M104 G105 A106 E107 I108 R109 H110 V111 L112 V113 T114 L115 G116 E117 K118 M119 T120 E123 V124 E125

Q126 L127 V128 A129 E132 D133 S134 N135 G136 C137 I138 N139 Y140 E141 E142 L143 V144 R145 M146 V147 L148 S149 G150

- Molecule 2: MYOSIN

Chain H: 17% 52% 29%

CYS ASP F3 S4 Q7 T8 A9 E10 F11 K12 E13 A14 F15 F18 D19 R20 T21 G22 D23 G24 K25 I26 L27 Y28 S29 Q30 C31 V34 M35 R36 A37 L38 G39 Q40 N41 P42 T43 N44 A45 E46 V47 M48 K49 V50 L51 G52 N53 P54 K55 S56 D57 E58 M59 N60 L61 K62 T63

L64 K65 F66 E67 Q68 F69 L70 P71 M72 M73 Q74 T75 I76 A77 K78 N79 K80 D81 Q82 G83 C84 F85 E86 D87 Y88 V89 E90 G91 L92 R93 V94 F95 D96 K97 E98 G99 N100 V103 M104 G105 A106 E107 I108 R109 H110 V111 L112 V113 T114 L115 G116 E117 K118 M119 T120 E121 E122 E123 V124

E125 V128 A129 E132 D133 S134 N135 G136 C137 I138 N139 Y140 E141 E142 L143 V144 R145 M146 V147 L148 S149 G150

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 – 3.50	Depositor
% Data completeness (in resolution range)	91.5 (10.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.227 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	30132	wwPDB-VP
Average B, all atoms (Å^2)	50.0	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: ALF, ADP, MG

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	0.57	0/6456	0.74	9/8700 (0.1%)
1	C	0.57	0/6456	0.74	8/8700 (0.1%)
1	E	0.57	0/6456	0.74	8/8700 (0.1%)
1	G	0.57	0/6456	0.74	9/8700 (0.1%)
2	B	0.46	0/1176	0.60	0/1575
2	D	0.46	0/1176	0.62	1/1575 (0.1%)
2	F	0.49	0/1176	0.66	2/1575 (0.1%)
2	H	0.57	0/1176	0.65	0/1575
All	All	0.56	0/30528	0.73	37/41100 (0.1%)

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	630	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	G	630	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	A	285	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	A	247	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	E	285	ARG	NE-CZ-NH2	7.51	124.05	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	6337	0	6346	865	5
1	C	6337	0	6346	858	0
1	E	6337	0	6346	841	4
1	G	6337	0	6346	860	12
2	B	1161	0	1126	146	0
2	D	1161	0	1126	151	8
2	F	1161	0	1126	152	5
2	H	1161	0	1126	163	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	5	0	0	1	0
4	C	5	0	0	1	0
4	E	5	0	0	1	0
4	G	5	0	0	1	0
5	A	27	0	12	1	0
5	C	27	0	12	4	0
5	E	27	0	12	4	0
5	G	27	0	12	3	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	30132	0	29936	3959	17

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 66.

The worst 5 of 3959 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)
2:F:89:VAL:HG12	2:F:144:VAL:HG21	1.29	1.14
1:C:8:ASP:HA	1:C:11:LYS:HD2	1.31	1.11
2:D:89:VAL:HG12	2:D:144:VAL:HG21	1.29	1.10
1:A:8:ASP:HA	1:A:11:LYS:HD2	1.32	1.09
1:G:8:ASP:HA	1:G:11:LYS:HD2	1.28	1.08

The worst 5 of 17 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)
1:E:19:PHE:CE1	1:G:786:GLU:OE2[1_556]	1.59	0.61
1:E:19:PHE:CD1	1:G:786:GLU:OE2[1_556]	1.66	0.54
2:D:23:ASP:N	1:G:371:ARG:NH2[1_545]	1.81	0.39
2:D:22:GLY:N	1:G:371:ARG:CZ[1_545]	1.88	0.32
1:A:371:ARG:NH1	2:F:22:GLY:N[1_544]	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	779/820 (95%)	549 (70%)	172 (22%)	58 (7%)	1 11
1	C	779/820 (95%)	553 (71%)	163 (21%)	63 (8%)	1 9
1	E	779/820 (95%)	547 (70%)	173 (22%)	59 (8%)	1 10
1	G	779/820 (95%)	552 (71%)	165 (21%)	62 (8%)	1 10
2	B	146/150 (97%)	102 (70%)	30 (20%)	14 (10%)	0 8
2	D	146/150 (97%)	104 (71%)	28 (19%)	14 (10%)	0 8
2	F	146/150 (97%)	101 (69%)	33 (23%)	12 (8%)	1 9
2	H	146/150 (97%)	104 (71%)	28 (19%)	14 (10%)	0 8
All	All	3700/3880 (95%)	2612 (71%)	792 (21%)	296 (8%)	1 10

5 of 296 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	LYS
1	A	170	ASP
1	A	383	ALA
1	A	395	VAL
1	A	414	VAL

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	689/718 (96%)	449 (65%)	240 (35%)	0 1
1	C	689/718 (96%)	449 (65%)	240 (35%)	0 1
1	E	689/718 (96%)	452 (66%)	237 (34%)	0 1
1	G	689/718 (96%)	450 (65%)	239 (35%)	0 1
2	B	127/129 (98%)	86 (68%)	41 (32%)	0 2
2	D	127/129 (98%)	86 (68%)	41 (32%)	0 2
2	F	127/129 (98%)	87 (68%)	40 (32%)	0 2
2	H	127/129 (98%)	85 (67%)	42 (33%)	0 2
All	All	3264/3388 (96%)	2144 (66%)	1120 (34%)	0 1

5 of 1120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	336	LEU
1	G	412	ASP
1	G	335	THR
1	G	702	LEU
1	C	399	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	601	ASN
1	G	751	GLN
1	C	533	ASN
1	C	495	HIS
1	G	783	HIS

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	$\#\|Z\| > 2$
4	ALF	C	999	5,6,1,3	0,4,4	-	-	-		
5	ADP	G	998	4,3	24,29,29	0.79	0	29,45,45	1.25	3 (10%)
4	ALF	A	999	5,6,1,3	0,4,4	-	-	-		
5	ADP	A	998	4,3	24,29,29	0.80	0	29,45,45	1.25	3 (10%)
4	ALF	E	999	5,6,1,3	0,4,4	-	-	-		
5	ADP	E	998	4,3	24,29,29	0.78	0	29,45,45	1.25	3 (10%)
4	ALF	G	999	5,6,1,3	0,4,4	-	-	-		
5	ADP	C	998	4,3	24,29,29	0.79	0	29,45,45	1.26	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
5	ADP	G	998	4,3	-	5/12/32/32	0/3/3/3
5	ADP	E	998	4,3	-	5/12/32/32	0/3/3/3
5	ADP	A	998	4,3	-	5/12/32/32	0/3/3/3
5	ADP	C	998	4,3	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	998	ADP	C5-C6-N6	2.86	124.70	120.35
5	G	998	ADP	C5-C6-N6	2.84	124.67	120.35
5	E	998	ADP	C5-C6-N6	2.83	124.65	120.35
5	A	998	ADP	C5-C6-N6	2.81	124.63	120.35
5	E	998	ADP	O3'-C3'-C2'	2.48	119.84	111.82

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	998	ADP	C5'-O5'-PA-O1A
5	A	998	ADP	C5'-O5'-PA-O2A
5	C	998	ADP	C5'-O5'-PA-O1A
5	C	998	ADP	C5'-O5'-PA-O2A
5	E	998	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

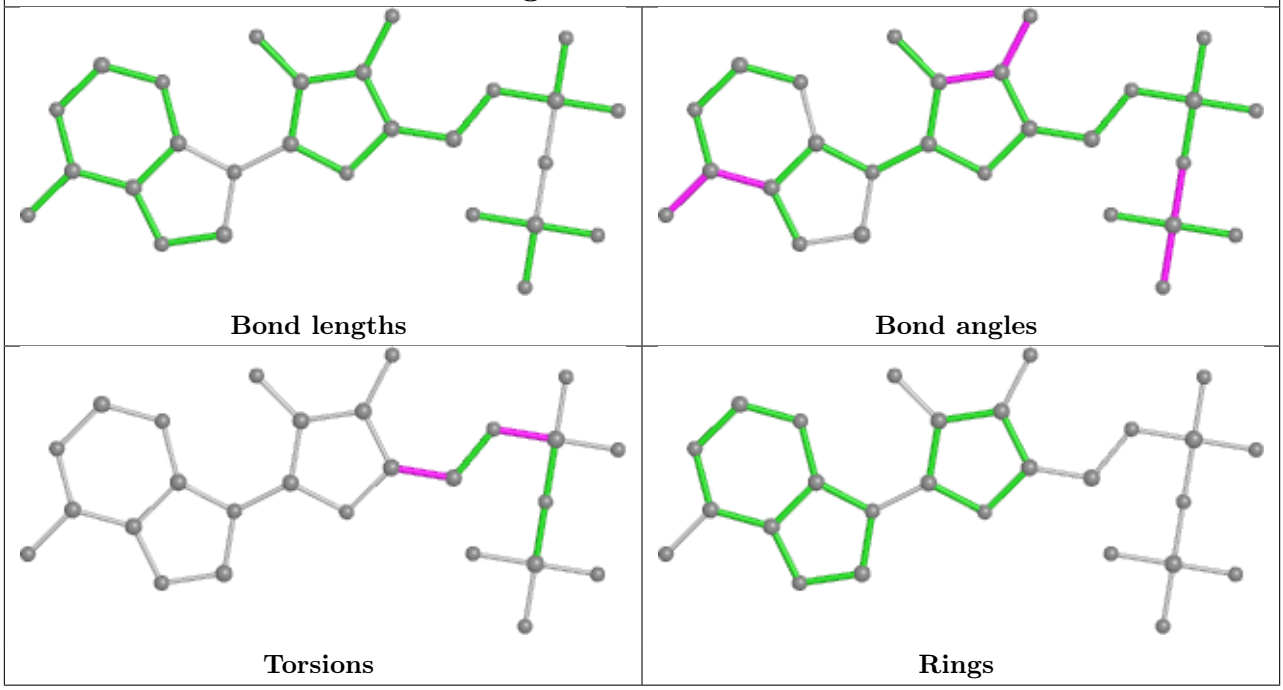
8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	999	ALF	1	0
5	G	998	ADP	3	0
4	A	999	ALF	1	0
5	A	998	ADP	1	0
4	E	999	ALF	1	0
5	E	998	ADP	4	0
4	G	999	ALF	1	0
5	C	998	ADP	4	0

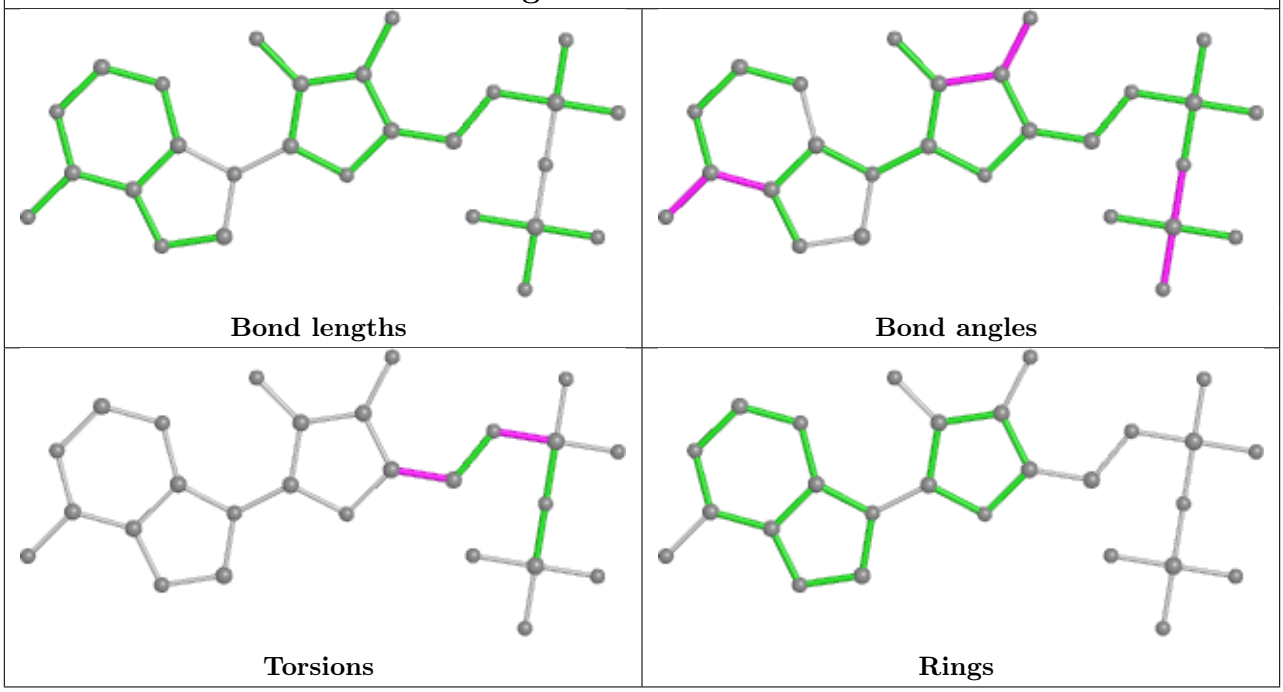
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

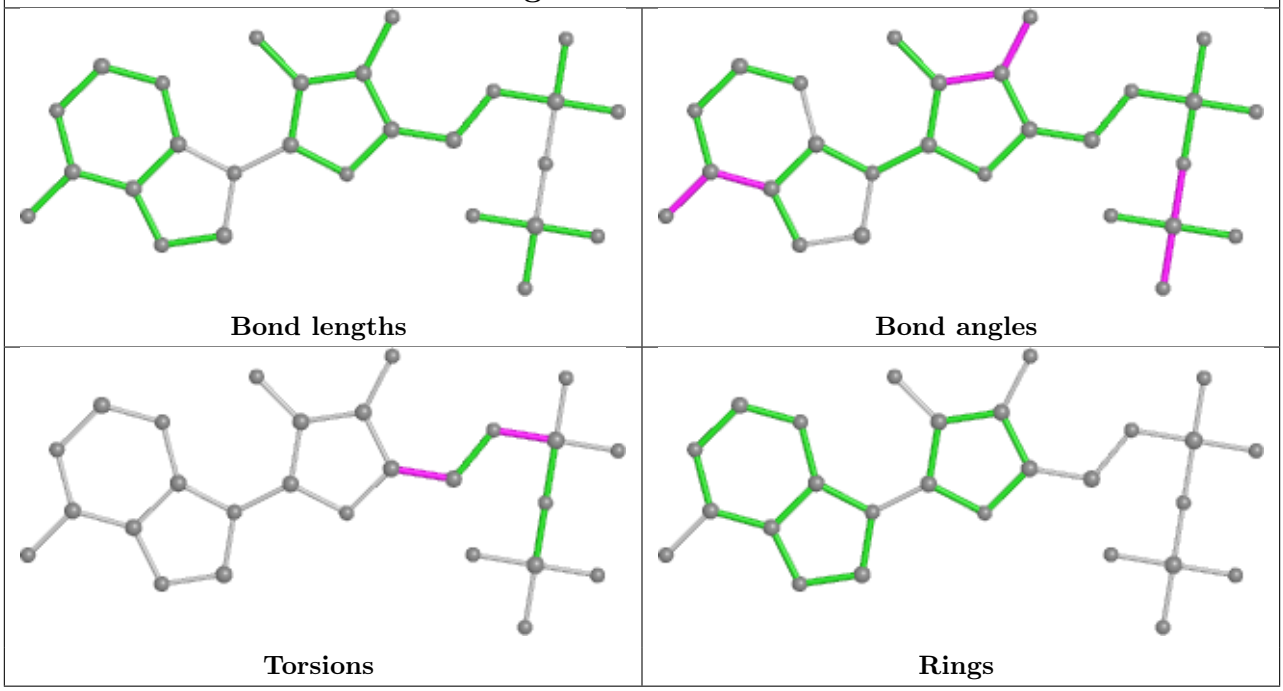
Ligand ADP G 998



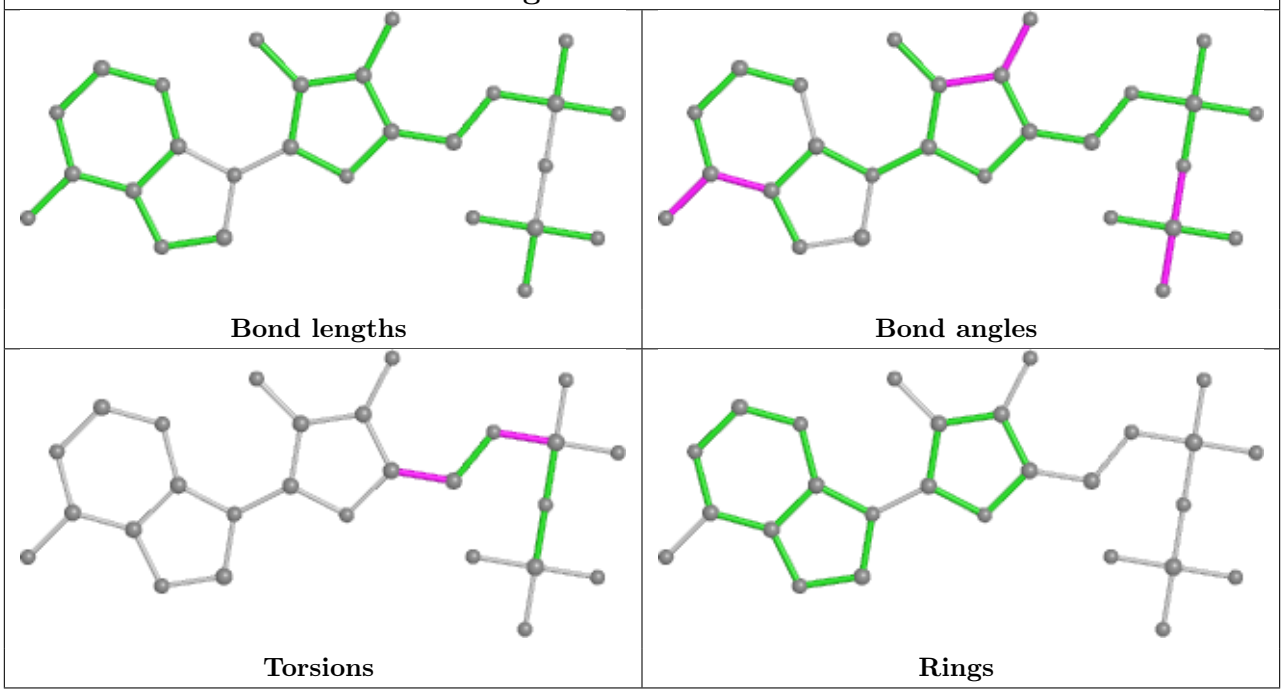
Ligand ADP A 998



Ligand ADP E 998



Ligand ADP C 998



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 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.