



wwPDB EM Validation Summary Report ⓘ

Jan 22, 2025 – 07:04 PM JST

PDB ID : 8ZB7
EMDB ID : EMD-39896
Title : Human left ventricle ATM complex
Authors : Li, D.N.; Zhao, Q.Y.; Liu, C.
Deposited on : 2024-04-26
Resolution : 3.19 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

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

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:

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

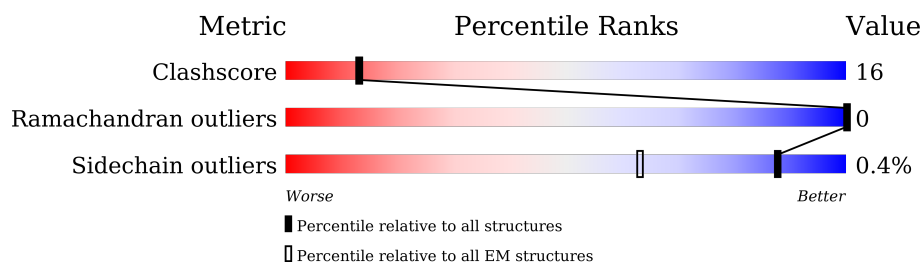
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.19 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.




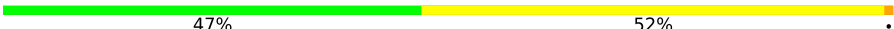
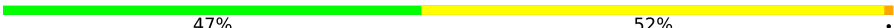
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	G	776	58% 37% .
1	H	776	59% 36% .
1	I	776	58% 38% .
1	J	776	57% 38% .
1	K	776	58% 37% .
1	M	776	59% 37% .
2	A	371	78% 22%
2	B	371	81% 19%
2	C	371	79% 21%

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Mol	Chain	Length	Quality of chain	
2	D	371		
2	E	371		
2	F	371		
3	L	166		.
3	N	166		.
3	O	166		.
3	P	166		.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 58698 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		
1	G	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		
1	H	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		
1	I	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		
1	J	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		
1	K	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		

- Molecule 2 is a protein called Actin, alpha cardiac muscle 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
2	C	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
2	D	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
2	E	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
2	F	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
2	A	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		

- Molecule 3 is a protein called Tropomyosin alpha-1 chain.

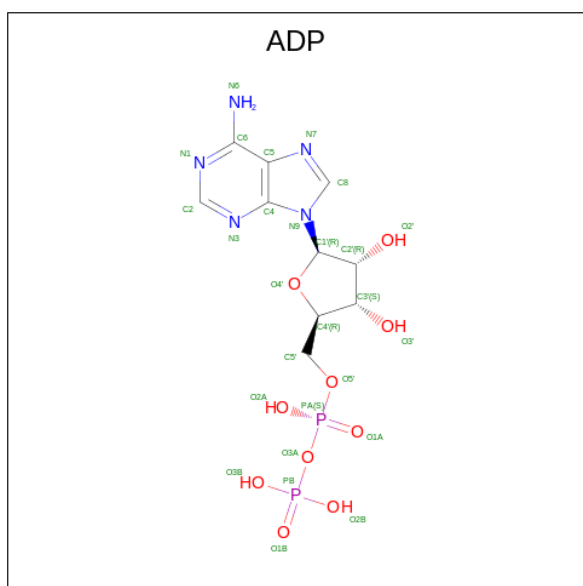
Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	166	Total	C	N	O	S	0	0
			1326	806	230	287	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	166	Total	C	N	O	S	0	0
			1326	806	230	287	3		
3	L	166	Total	C	N	O	S	0	0
			1326	806	230	287	3		
3	N	166	Total	C	N	O	S	0	0
			1326	806	230	287	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

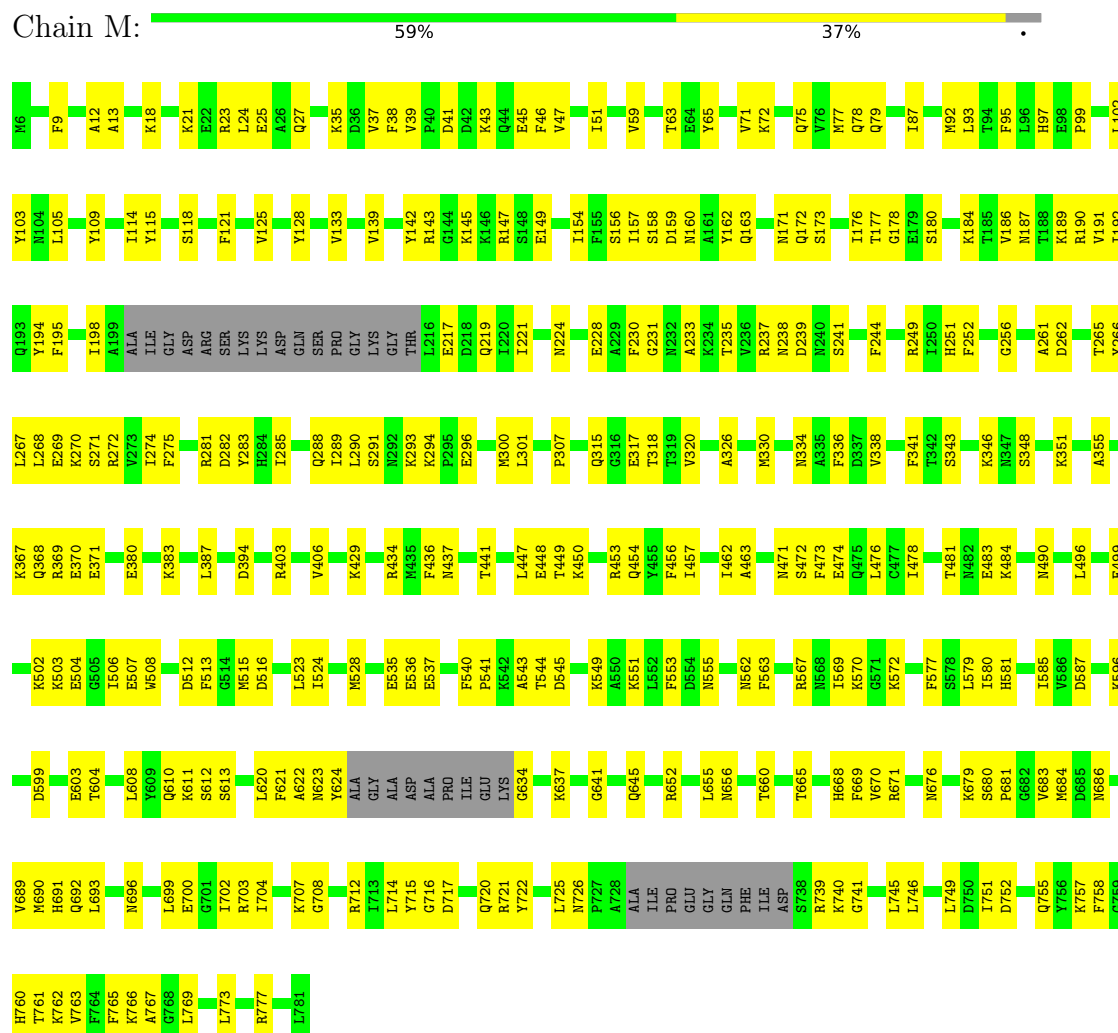


Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

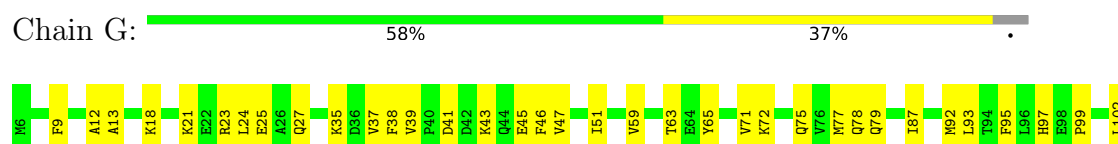
3 Residue-property plots

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.

• Molecule 1: Myosin-7



• Molecule 1: Myosin-7

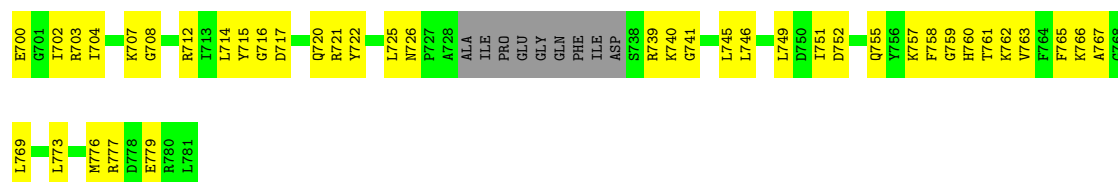


Y103	Q193	L267	Q368	E499	K596	V689	G759
N104	Y194	L268	R369	K502	K596	M690	H760
L105	F195	E269	E371	K503	D599	M691	T761
Y109	I198	K270	E371	K504	E603	M692	K762
I114	A199	S271	E380	G505	T604	L693	F763
Y115	ALA	R272	E380	I506	L608	M696	F765
Y118	ILE	W273	K383	E507	L609	L699	A767
S118	GLY	F275	L387	W508	Q610	E700	L769
F121	ASP	R281	L387	D512	Q611	G701	L773
F121	ARG	D282	D394	F513	S612	R702	R777
V125	SER	Y283	D394	G514	R703	R704	L781
V125	LYS	H284	R403	M515	S613	L704	
Y128	ASP	I285	R403	D516	L620	K707	
Y128	GLN	I289	V406	L517	A622	G708	
V133	SER	L290	T412	L523	M623	R712	
V139	GLY	K293	K429	I524	Y624	T713	
Y142	GLY	K294	R434	M528	ALA	L714	
R143	THR	E296	R434	E535	GLY	Y715	
G144	L216	E296	M435	E536	ALA	G716	
K145	D218	M300	F436	E537	ASP	D717	
K146	E217	L301	N437	F540	ALA	Q720	
R147	Q219	P307	T441	P541	PRO	R721	
S148	I220	L447	L447	K542	ILE	Y722	
E149	I221	E448	T449	T544	LYS	G634	
I154	N224	K315	K450	D545	K635	L725	
S156	E228	Q316	K450	K549	G636	N726	
I157	A229	E317	R453	K551	K637	A728	
S158	G231	T318	R453	K551	Q645	ALA	
D159	N232	V320	Y455	L552	R652	ILE	
M160	A233	A326	F456	F553	L655	PRO	
A161	K234	M330	I457	D554	M656	GLU	
Y162	T235	N334	I462	N555	T660	GLN	
Q163	V236	A335	A463	M562	ILE	ASP	
N171	R237	F336	N471	F563	T665	S738	
Q172	N238	D337	S472	R567	H668	R739	
S173	D239	V338	F473	I569	F669	K740	
I176	S241	F341	Q475	K570	V670	G741	
T177	F244	F341	Q475	G571	R671	L745	
G178	F244	T342	L476	K572	M676	L746	
E179	R249	S343	C477	K572	K679	L749	
S180	I250	K346	I478	F577	D750	T751	
K184	H251	R347	T481	S578	S680	D752	
T185	P252	S348	N482	L579	P681	Y755	
V186	G256	K351	E483	I580	G682	Q756	
N187	A261	L352	K484	H581	V683	K757	
T188	D262	A355	N490	I585	M684	F758	
K189	T265	L496	L496	D587	N686		
R190	Y266	K367					
V191							
K189							
R190							
V191							
I192							

● Molecule 1: Myosin-7

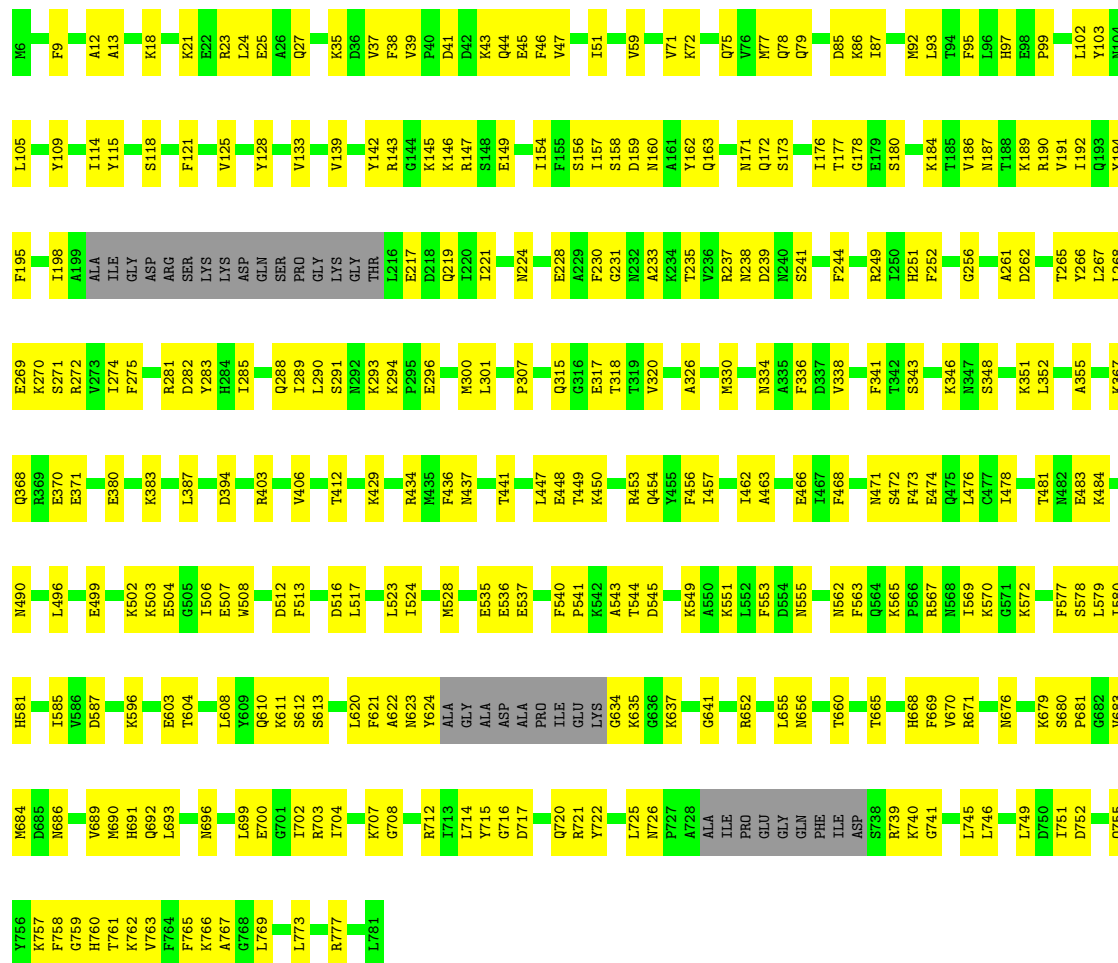
Chain H:  59% 36%

N6	Y103	F195	R272	K383	D512	S612
F9	N104	I198	V273	L387	F513	S613
A12	L105	A199	F275	L387	G514	L620
A13	Y109	ALA	R281	D394	M515	A622
K18	I114	ILE	D282	R403	D516	N623
K18	Y115	GLY	Y283	T412	L523	Y624
K21	S118	ARG	H284	T412	I524	ALA
E22	LYS	SER	I285	K429	M528	ALA
R23	LYS	ASP	L289	K429	E535	ASP
L24	LYS	LYS	L290	R434	E536	PRO
E25	ASP	GLN	K293	M435	E537	ILE
A26	GLN	SER	K294	N437	F540	GLY
Q27	SER	GLY	E296	T441	K549	LVS
K35	LYS	GLY	E296	L447	A543	G634
D36	THR	THR	M300	T441	K549	K635
V37	L216	L216	L301	L447	T544	G636
V39	Q219	Q219	P307	T449	D545	K637
P40	Q219	Q219	P307	T449	D545	K639
D41	N224	N224	Q315	R453	K549	Q645
D42	E228	E228	G316	Q454	K551	Q645
K43	E228	E228	E317	F455	L552	R652
Q44	F230	F230	T318	F456	T544	L655
F46	E149	E149	T319	I457	N555	N656
V47	I154	I154	V320	I462	N555	N656
T51	I154	I154	A326	A463	N562	T660
V59	S158	S158	M330	N471	F563	T665
T63	D159	D159	N334	F473	R567	H668
E64	A161	A161	A335	E474	I569	F669
V65	Y162	Y162	F336	Q475	K570	V670
V71	Q163	Q163	D337	L476	R671	R671
K72	N171	N171	V338	C477	F577	N676
Q75	Q172	Q172	F341	I478	L579	S680
N76	S173	S173	T342	T481	I580	P681
M77	I176	I176	S343	N482	H581	G682
Q78	T177	T177	K346	E483	T585	V683
Q79	G178	G178	N347	K484	D587	M684
S180	E179	E179	S348	N490	K596	N686
I87	S180	S180	K351	L496	D599	V689
M92	K184	K184	A355	E499	E603	M690
L93	T185	T185	K367	K502	T604	H691
T94	N187	N187	Q368	K503	G692	Q692
F95	T188	T188	R369	E504	L608	L693
L96	K189	K189	E370	G505	L609	N696
H97	R190	R190	E371	I506	Q610	L699
E98	V191	V191	E371	E507	K611	
P99	I192	I192	E380	W508		
Q193	Q193	Q193				
Y194	Y194	Y194				



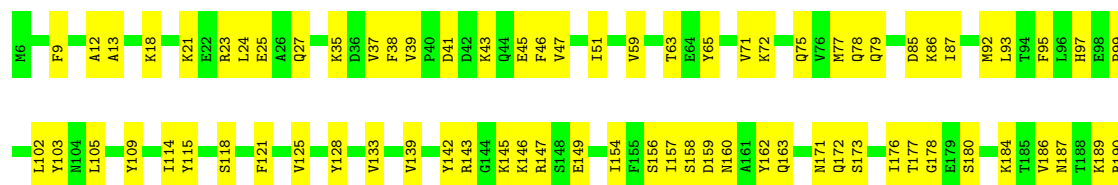
• Molecule 1: Myosin-7

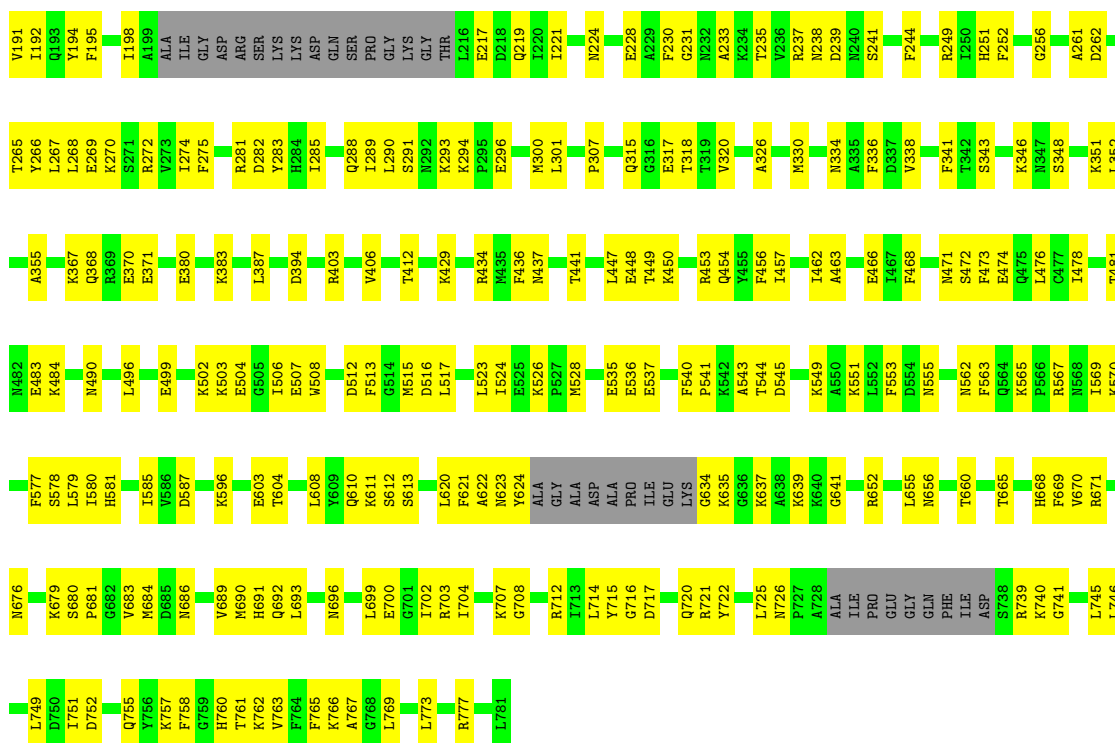
Chain I: 58% 38% •



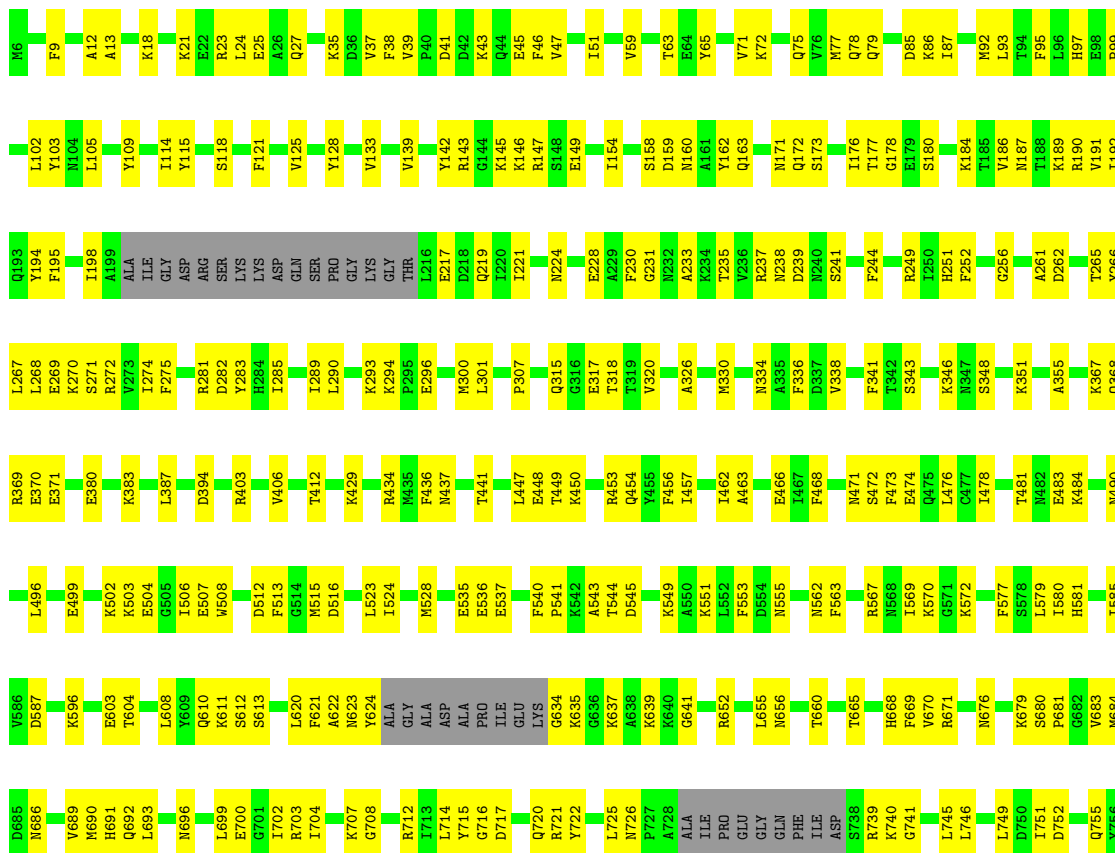
• Molecule 1: Myosin-7

Chain J: 57% 38% •





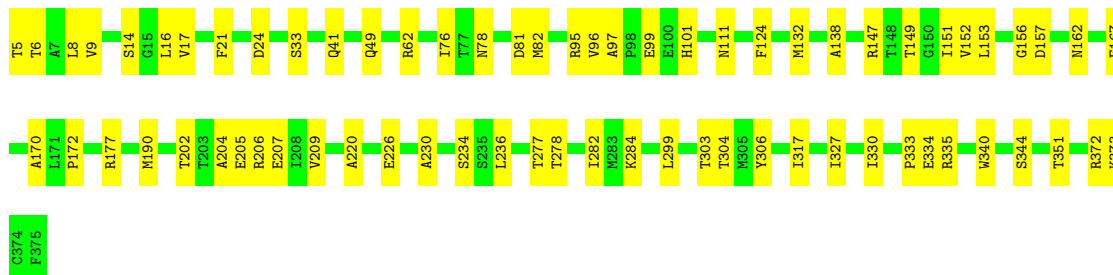
- Molecule 1: Myosin-7





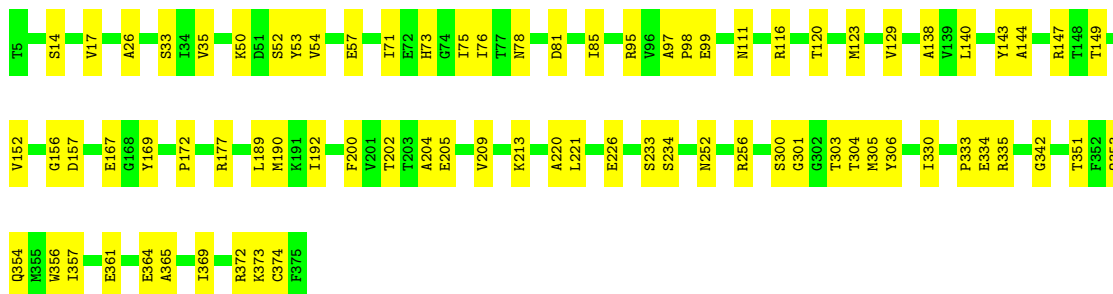
- Molecule 2: Actin, alpha cardiac muscle 1

Chain B: 81% 19%



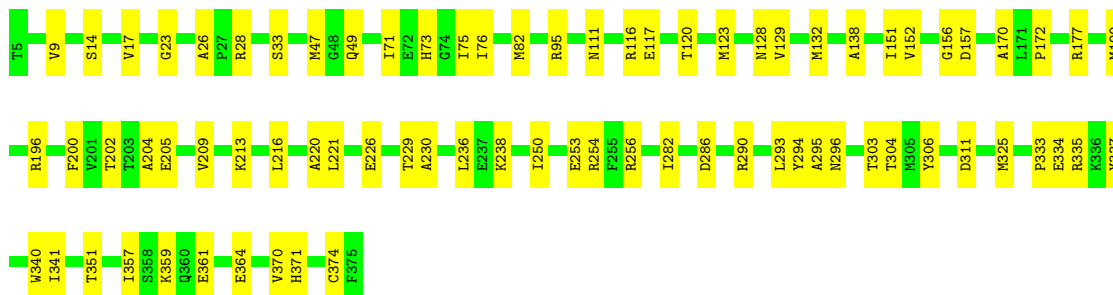
- Molecule 2: Actin, alpha cardiac muscle 1

Chain C: 79% 21%



- Molecule 2: Actin, alpha cardiac muscle 1

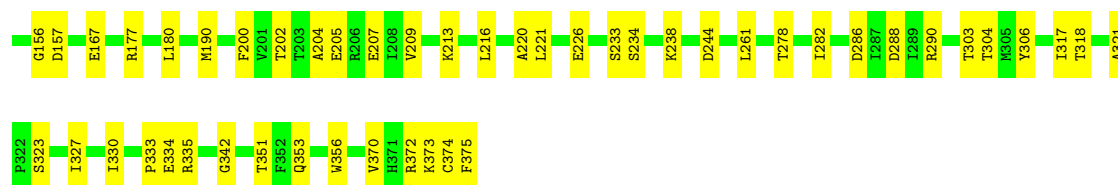
Chain D: 79% 21%



- Molecule 2: Actin, alpha cardiac muscle 1

Chain E: 78% 22%





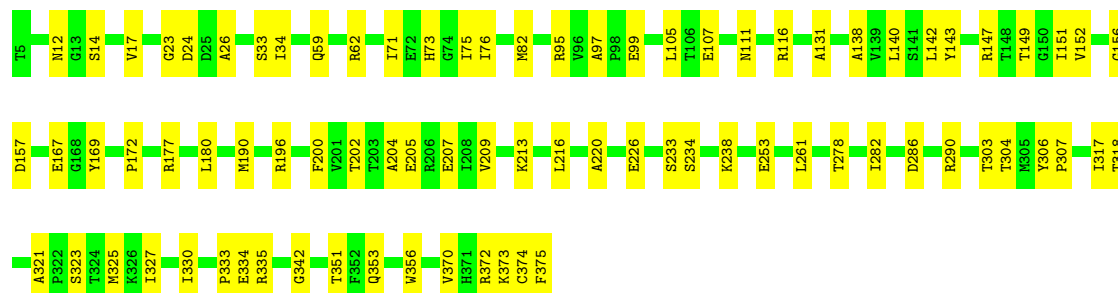
- Molecule 2: Actin, alpha cardiac muscle 1

Chain F: 80% 19%



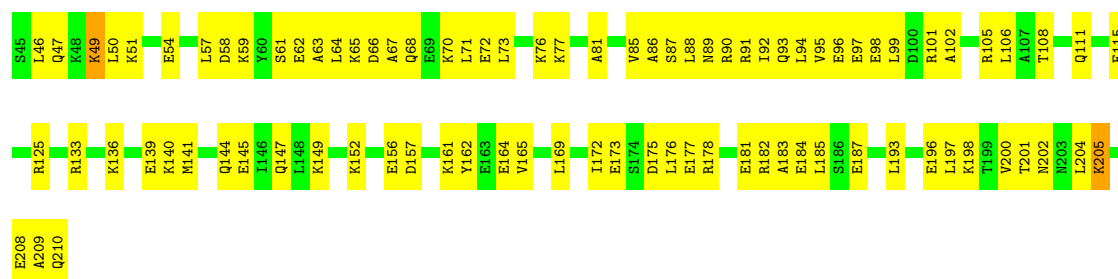
- Molecule 2: Actin, alpha cardiac muscle 1

Chain A: 78% 22%



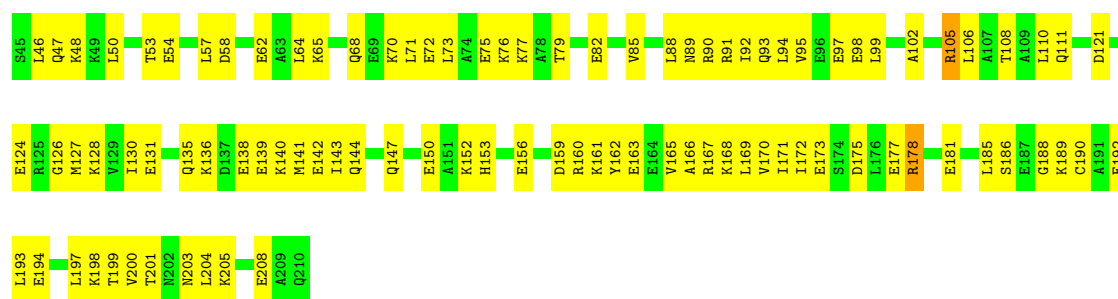
- Molecule 3: Tropomyosin alpha-1 chain

Chain O: 47% 52%



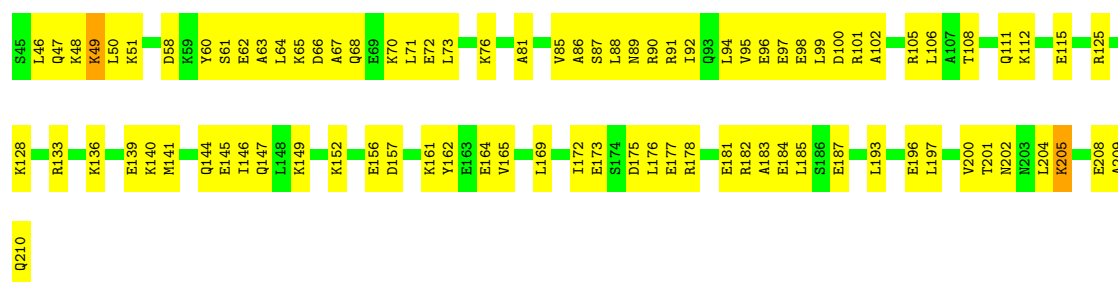
- Molecule 3: Tropomyosin alpha-1 chain

Chain P: 43% 56%



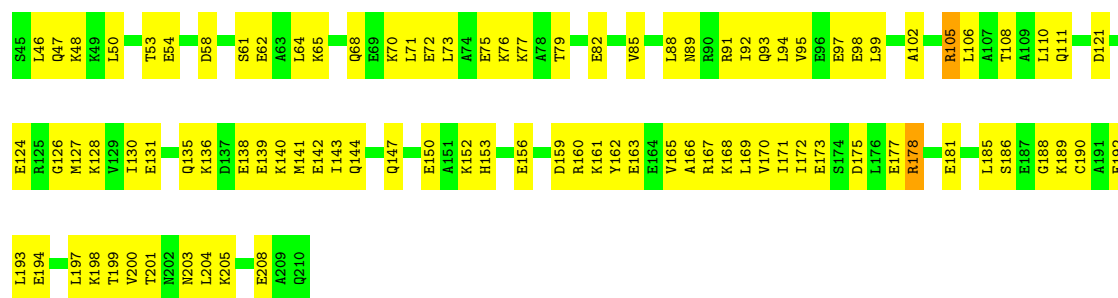
• Molecule 3: Tropomyosin alpha-1 chain

Chain L: 47% 52%



• Molecule 3: Tropomyosin alpha-1 chain

Chain N: 43% 55%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.66°, rise=27.3 Å, axial sym=C1	Depositor
Number of segments used	69013	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	G	0.32	0/6101	0.45	0/8217
1	H	0.32	0/6101	0.45	0/8217
1	I	0.32	0/6101	0.45	0/8217
1	J	0.32	0/6101	0.45	0/8217
1	K	0.32	0/6101	0.45	0/8217
1	M	0.32	0/6101	0.45	0/8217
2	A	0.58	0/2961	0.51	0/4011
2	B	0.53	0/2961	0.50	0/4011
2	C	0.55	0/2961	0.50	0/4011
2	D	0.57	0/2961	0.51	0/4011
2	E	0.58	0/2961	0.51	0/4011
2	F	0.57	0/2961	0.50	0/4011
3	L	0.28	0/1328	0.48	0/1770
3	N	0.28	0/1328	0.46	0/1770
3	O	0.28	0/1328	0.48	0/1770
3	P	0.28	0/1328	0.46	0/1770
All	All	0.40	0/59684	0.47	0/80448

There are no bond length outliers.

There are no bond angle outliers.

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	G	5974	0	5961	217	0
1	H	5974	0	5961	212	0
1	I	5974	0	5961	221	0
1	J	5974	0	5961	233	0
1	K	5974	0	5961	224	0
1	M	5974	0	5961	204	0
2	A	2898	0	2870	63	0
2	B	2898	0	2871	53	0
2	C	2898	0	2871	56	0
2	D	2898	0	2868	73	0
2	E	2898	0	2871	61	0
2	F	2898	0	2871	54	0
3	L	1326	0	1330	120	0
3	N	1326	0	1332	106	0
3	O	1326	0	1332	90	0
3	P	1326	0	1332	90	0
4	A	27	0	12	3	0
4	B	27	0	12	1	0
4	C	27	0	12	2	0
4	D	27	0	12	2	0
4	E	27	0	12	3	0
4	F	27	0	12	2	0
All	All	58698	0	58386	1879	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 1879 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:I:368:GLN:HE22	3:N:142:GLU:CB	1.15	1.57
1:J:368:GLN:HE22	3:L:100:ASP:CA	1.21	1.49
1:I:368:GLN:HE22	3:N:142:GLU:CA	1.21	1.48
1:I:368:GLN:NE2	3:N:142:GLU:HB3	1.30	1.45
1:J:368:GLN:NE2	3:L:100:ASP:CA	1.78	1.45

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	G	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
1	H	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
1	I	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
1	J	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
1	K	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
1	M	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
2	A	369/371 (100%)	347 (94%)	22 (6%)	0	100	100
2	B	369/371 (100%)	349 (95%)	20 (5%)	0	100	100
2	C	369/371 (100%)	352 (95%)	17 (5%)	0	100	100
2	D	369/371 (100%)	344 (93%)	25 (7%)	0	100	100
2	E	369/371 (100%)	347 (94%)	22 (6%)	0	100	100
2	F	369/371 (100%)	348 (94%)	21 (6%)	0	100	100
3	L	164/166 (99%)	164 (100%)	0	0	100	100
3	N	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
3	O	164/166 (99%)	164 (100%)	0	0	100	100
3	P	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
All	All	7274/7546 (96%)	6917 (95%)	357 (5%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	G	644/668 (96%)	642 (100%)	2 (0%)	91	96
1	H	644/668 (96%)	642 (100%)	2 (0%)	91	96
1	I	644/668 (96%)	642 (100%)	2 (0%)	91	96
1	J	644/668 (96%)	642 (100%)	2 (0%)	91	96
1	K	644/668 (96%)	642 (100%)	2 (0%)	91	96
1	M	644/668 (96%)	642 (100%)	2 (0%)	91	96
2	A	314/314 (100%)	313 (100%)	1 (0%)	91	96
2	B	314/314 (100%)	314 (100%)	0	100	100
2	C	314/314 (100%)	313 (100%)	1 (0%)	91	96
2	D	314/314 (100%)	314 (100%)	0	100	100
2	E	314/314 (100%)	313 (100%)	1 (0%)	91	96
2	F	314/314 (100%)	313 (100%)	1 (0%)	91	96
3	L	141/141 (100%)	139 (99%)	2 (1%)	62	82
3	N	141/141 (100%)	138 (98%)	3 (2%)	48	74
3	O	141/141 (100%)	139 (99%)	2 (1%)	62	82
3	P	141/141 (100%)	138 (98%)	3 (2%)	48	74
All	All	6312/6456 (98%)	6286 (100%)	26 (0%)	88	94

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	147	ARG
1	J	503	LYS
3	N	160	ARG
1	J	147	ARG
1	K	147	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	368	GLN
1	I	486	GLN
2	A	353	GLN
1	H	486	GLN
1	I	222	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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	B	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.45	4 (13%)
4	ADP	E	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.45	4 (13%)
4	ADP	A	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.45	4 (13%)
4	ADP	C	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.50	4 (13%)
4	ADP	F	401	-	24,29,29	0.92	1 (4%)	29,45,45	1.48	4 (13%)
4	ADP	D	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.44	4 (13%)

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	B	401	-	-	4/12/32/32	0/3/3/3
4	ADP	E	401	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	401	-	-	4/12/32/32	0/3/3/3
4	ADP	C	401	-	-	3/12/32/32	0/3/3/3
4	ADP	F	401	-	-	5/12/32/32	0/3/3/3
4	ADP	D	401	-	-	4/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	ADP	C5-C4	2.28	1.47	1.40
4	B	401	ADP	C5-C4	2.25	1.46	1.40
4	F	401	ADP	C5-C4	2.24	1.46	1.40
4	D	401	ADP	C5-C4	2.23	1.46	1.40
4	A	401	ADP	C5-C4	2.22	1.46	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	401	ADP	PA-O3A-PB	-3.87	119.54	132.83
4	C	401	ADP	PA-O3A-PB	-3.86	119.59	132.83
4	B	401	ADP	PA-O3A-PB	-3.66	120.26	132.83
4	D	401	ADP	PA-O3A-PB	-3.49	120.86	132.83
4	A	401	ADP	PA-O3A-PB	-3.37	121.26	132.83

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	ADP	C5'-O5'-PA-O2A
4	C	401	ADP	C5'-O5'-PA-O2A
4	D	401	ADP	C5'-O5'-PA-O2A
4	E	401	ADP	C5'-O5'-PA-O2A
4	F	401	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

6 monomers are involved in 13 short contacts:

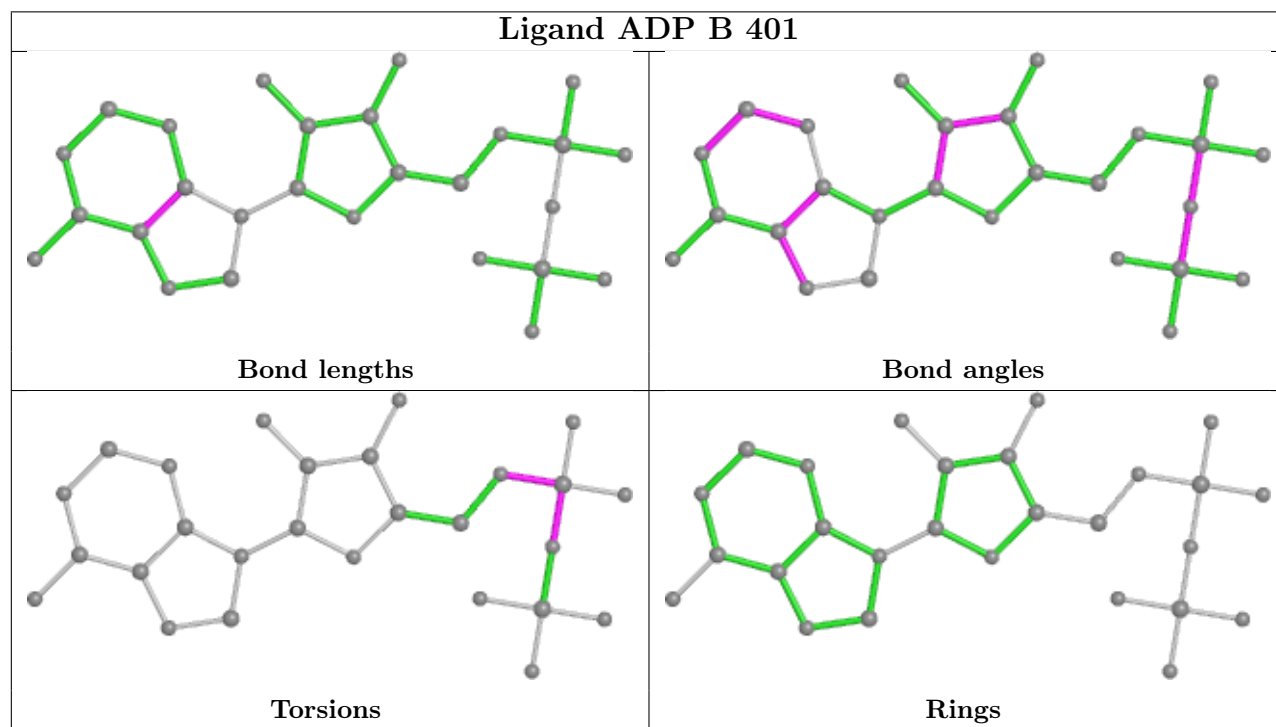
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	ADP	1	0
4	E	401	ADP	3	0
4	A	401	ADP	3	0

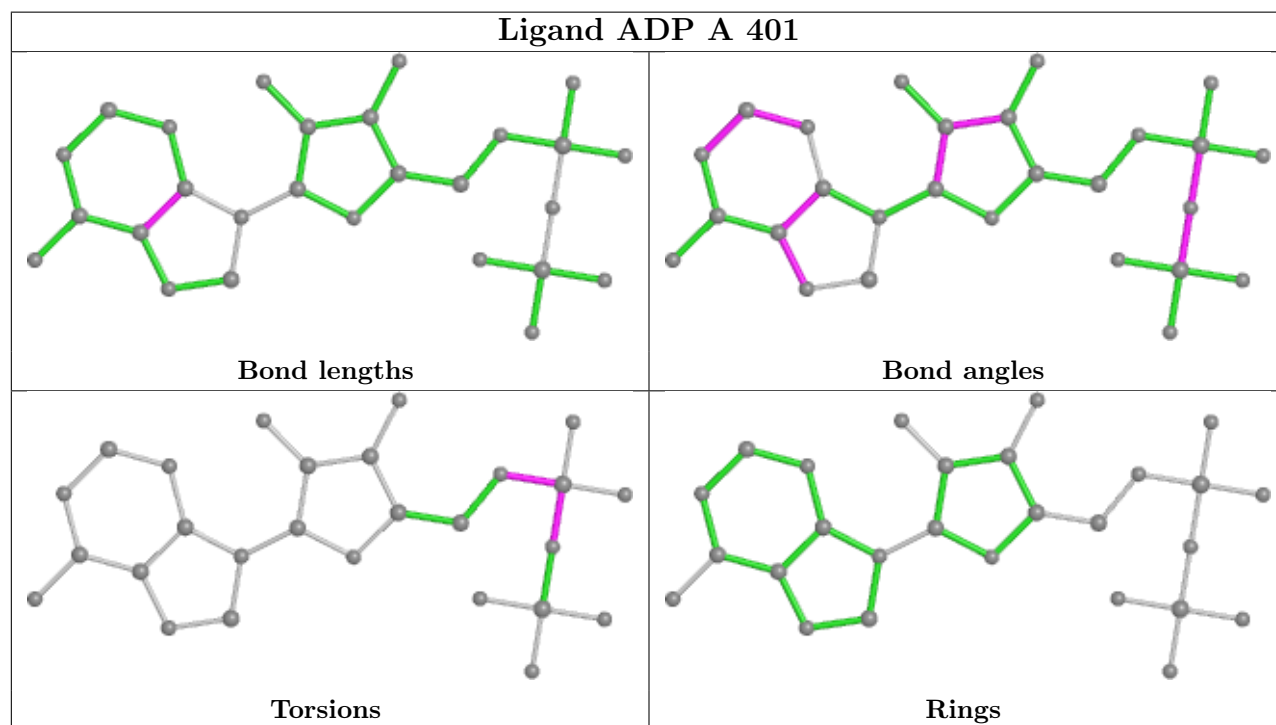
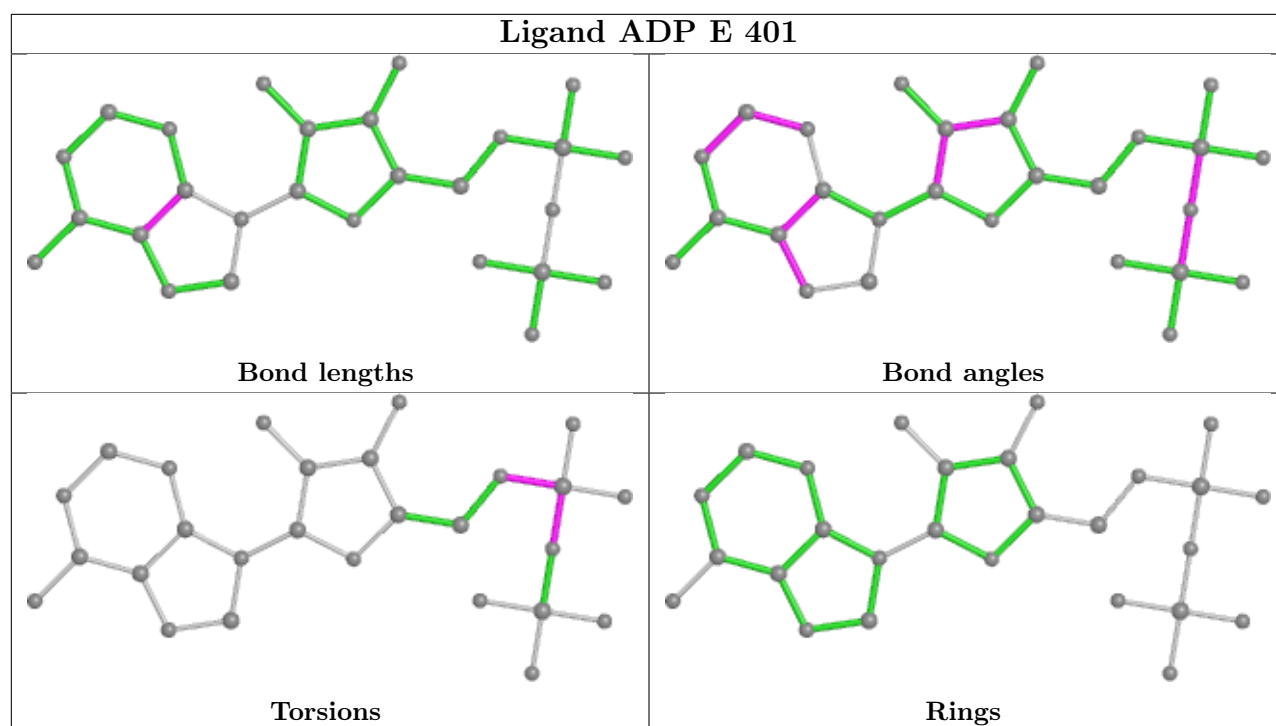
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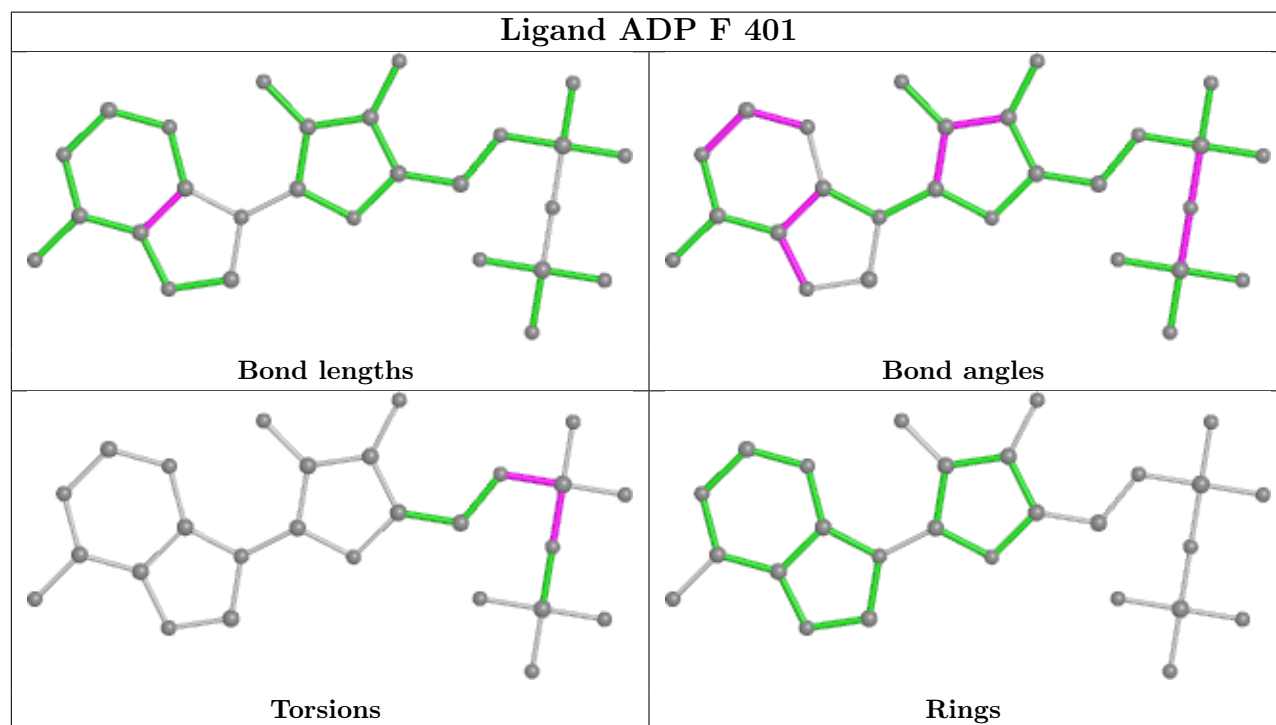
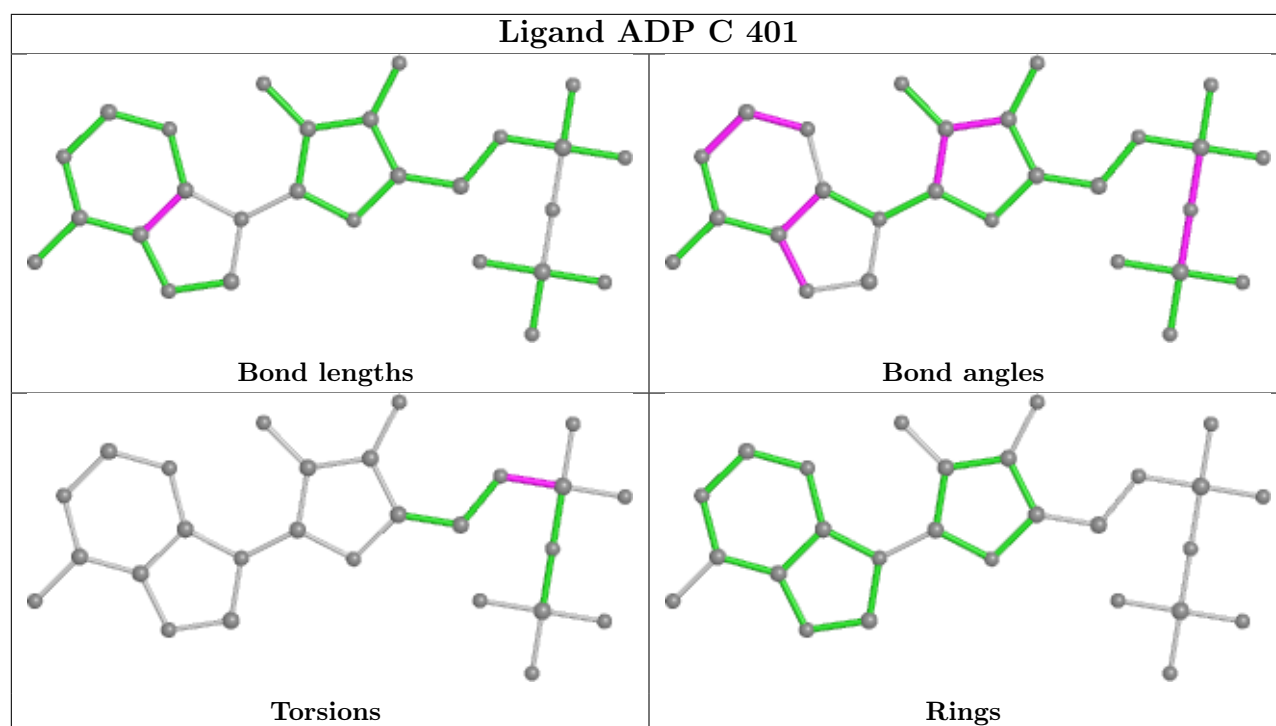
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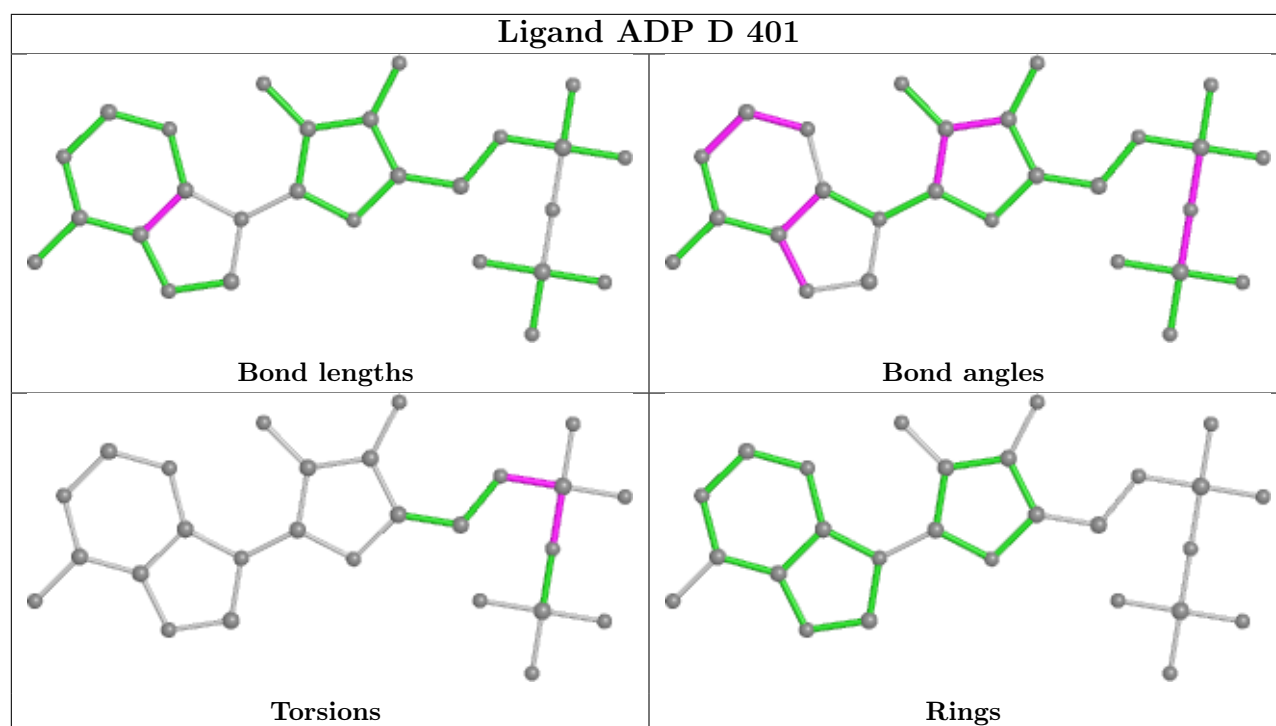
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	ADP	2	0
4	F	401	ADP	2	0
4	D	401	ADP	2	0

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 [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39896. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.