



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 23, 2017 – 10:59 AM EST

PDB ID : 5MVA
EMDB ID: : EMD-3576
Title : Structure of the thin filament at high calcium concentration
Authors : Paul, D.M.; Squire, J.M.; Morris, E.P.
Deposited on : unknown
Resolution : 27.70 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

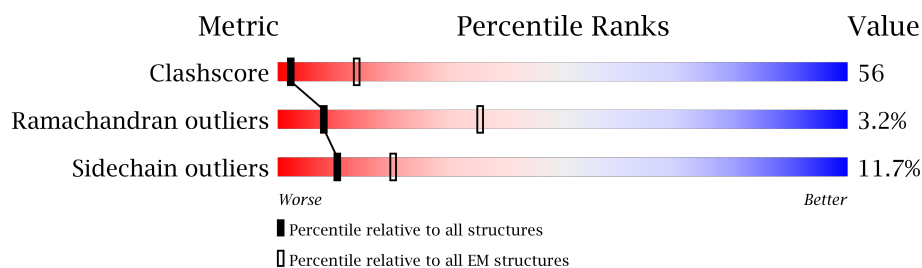
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 27.70 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	A	375	56% 35% 9% .
1	B	375	57% 33% 10% .
1	C	375	55% 35% 9% .
1	D	375	55% 35% 9% .
1	E	375	55% 35% 9% .
1	F	375	56% 35% 9% .
1	G	375	56% 35% 9% .
1	H	375	55% 35% 9% .
1	I	375	55% 34% 10% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	375	 55% 35% 9% .
1	K	375	 56% 34% 10% .
1	L	375	 55% 35% 9% .
1	M	375	 55% 34% 10% .
1	N	375	 55% 35% 9% .
1	O	375	 55% 34% 10% .
1	P	375	 55% 35% 9% .
1	Q	375	 56% 35% 9% .
1	R	375	 56% 35% 9% .
1	S	375	 56% 34% 9% .
1	T	375	 55% 35% 9% .
1	U	375	 56% 35% 9% .
1	V	375	 56% 34% 9% .
1	W	375	 56% 35% 9% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 68103 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 Actin, alpha skeletal muscle.

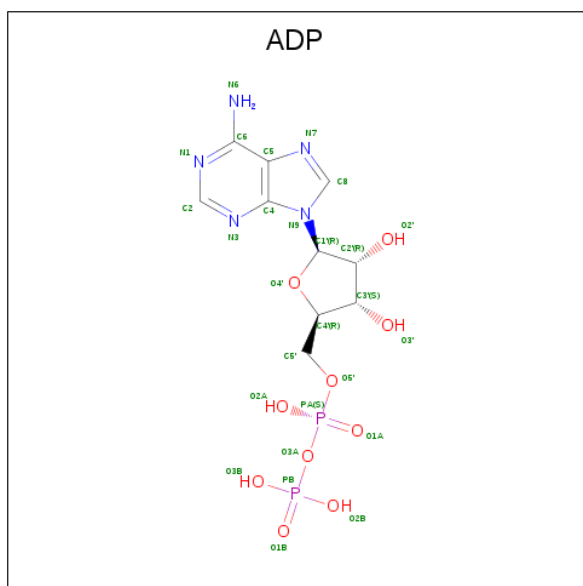
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	B	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	C	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	F	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	G	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	H	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	I	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	J	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	K	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	L	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	M	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	N	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	O	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	P	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	Q	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	S	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	T	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	U	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	V	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	W	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



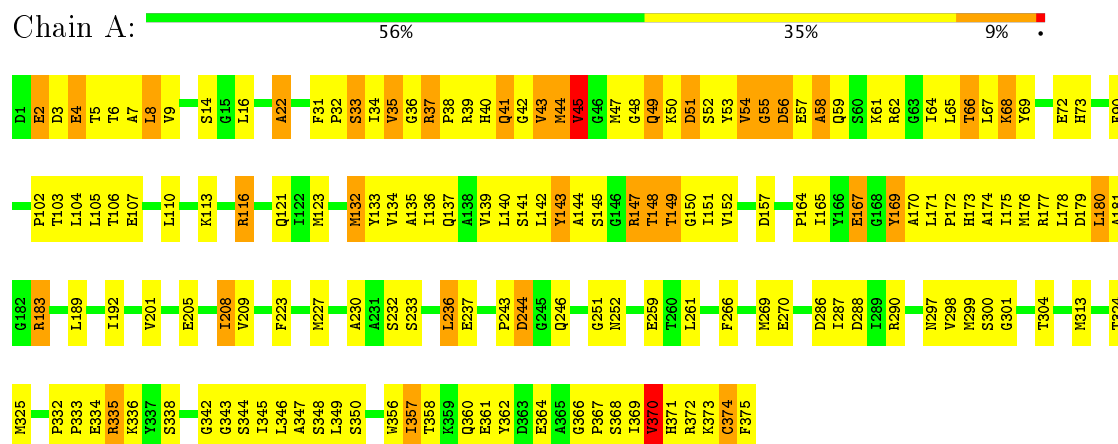
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	L	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	N	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	O	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	P	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	R	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	S	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	T	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	U	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	V	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	W	1	Total	C	N	O	P	0
			27	10	5	10	2	

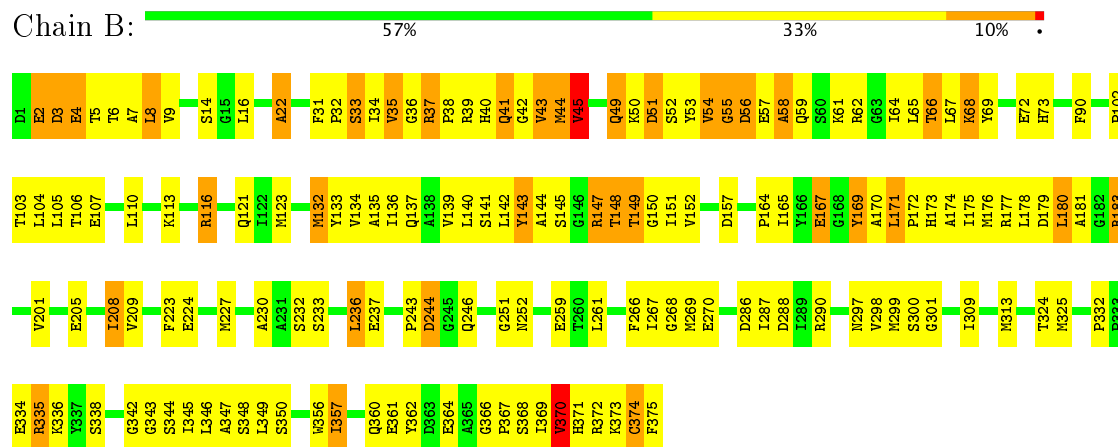
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

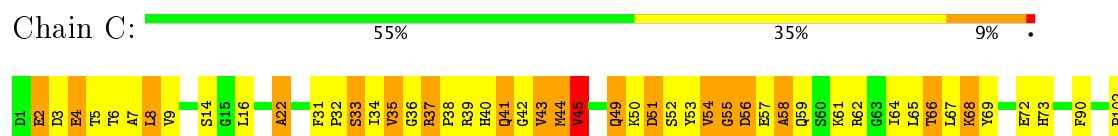
- Molecule 1: Actin, alpha skeletal muscle

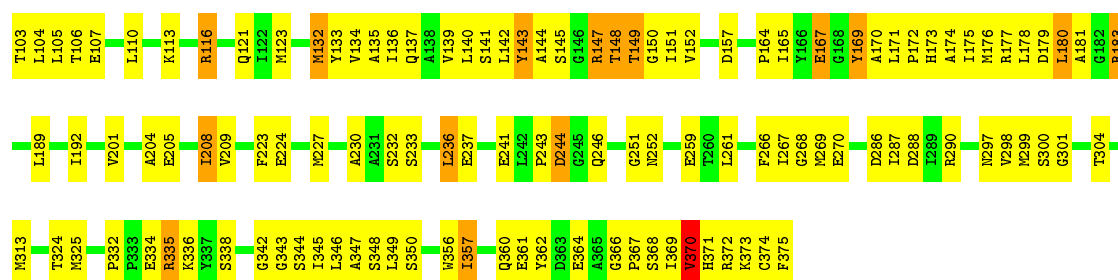


- Molecule 1: Actin, alpha skeletal muscle



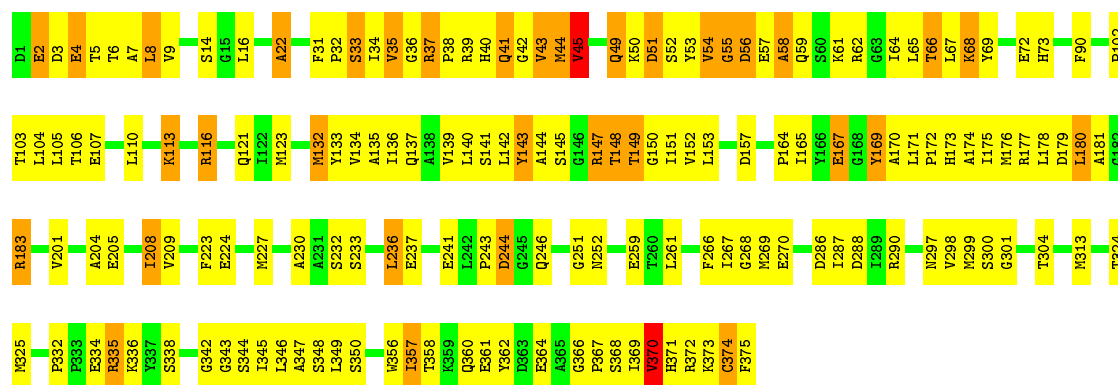
- Molecule 1: Actin, alpha skeletal muscle





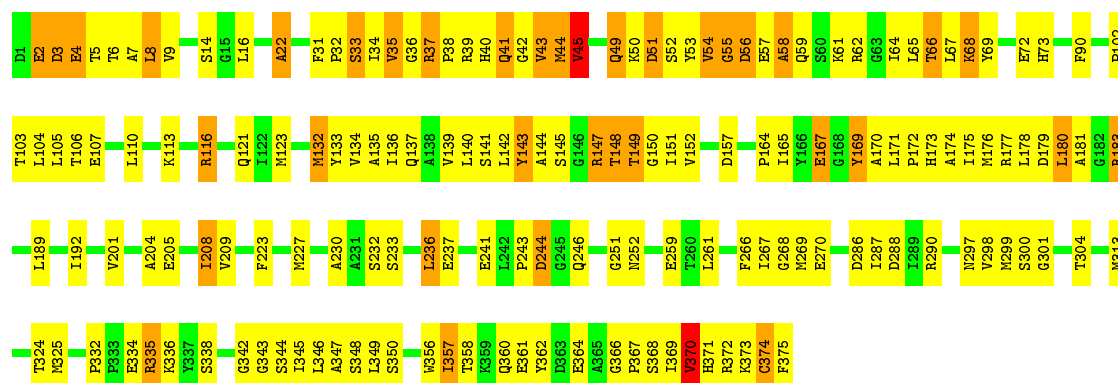
- Molecule 1: Actin, alpha skeletal muscle

Chain D: 55% 35% 9% .



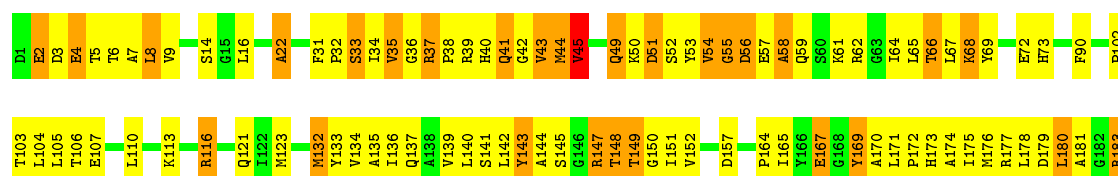
- Molecule 1: Actin, alpha skeletal muscle

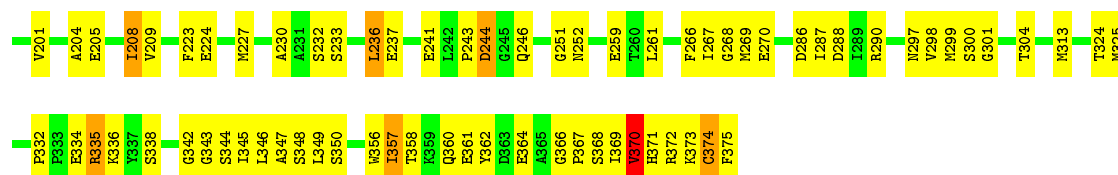
Chain E: 55% 35% 9% .



- Molecule 1: Actin, alpha skeletal muscle

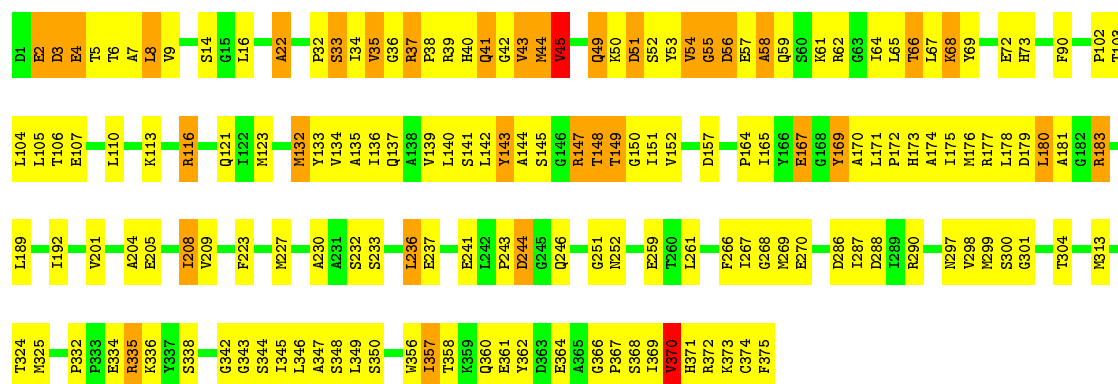
Chain F: 56% 35% 9% .





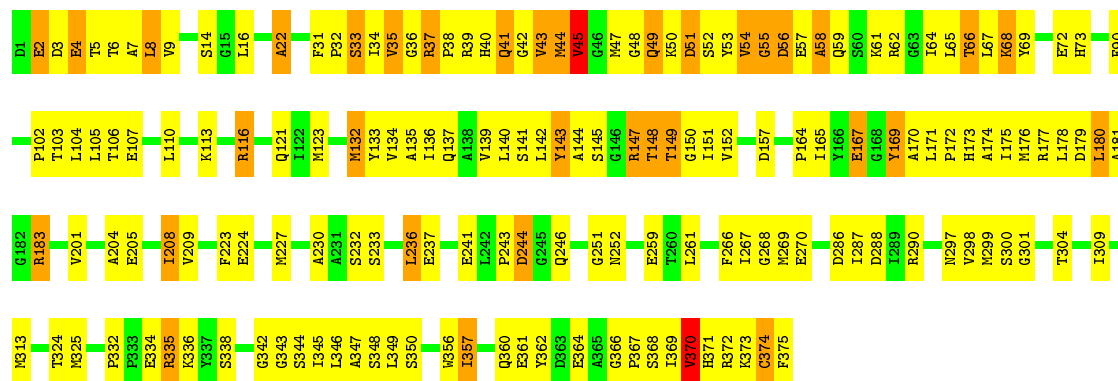
- Molecule 1: Actin, alpha skeletal muscle

Chain G: 56% 35% 9%



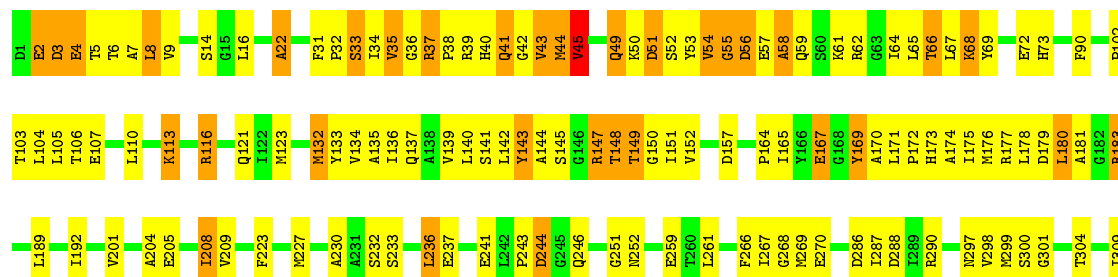
- Molecule 1: Actin, alpha skeletal muscle

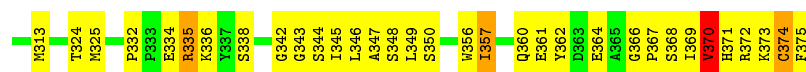
Chain H: 55% 35% 9%



- Molecule 1: Actin, alpha skeletal muscle

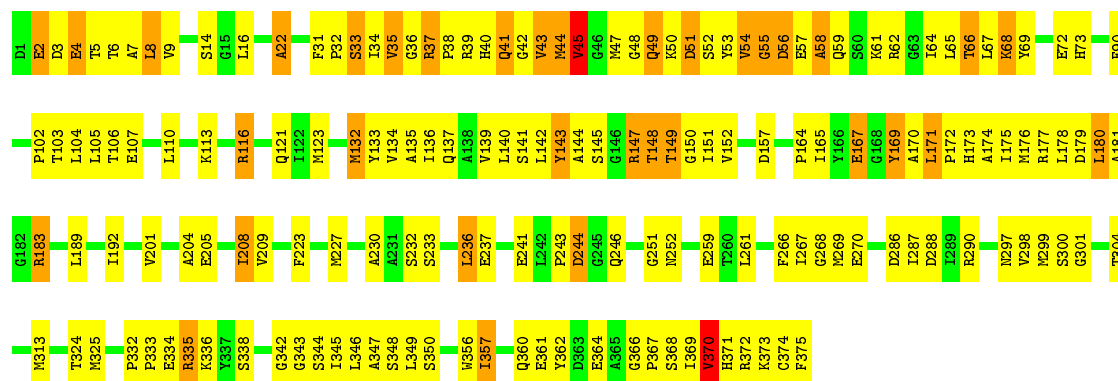
Chain I: 55% 34% 10%





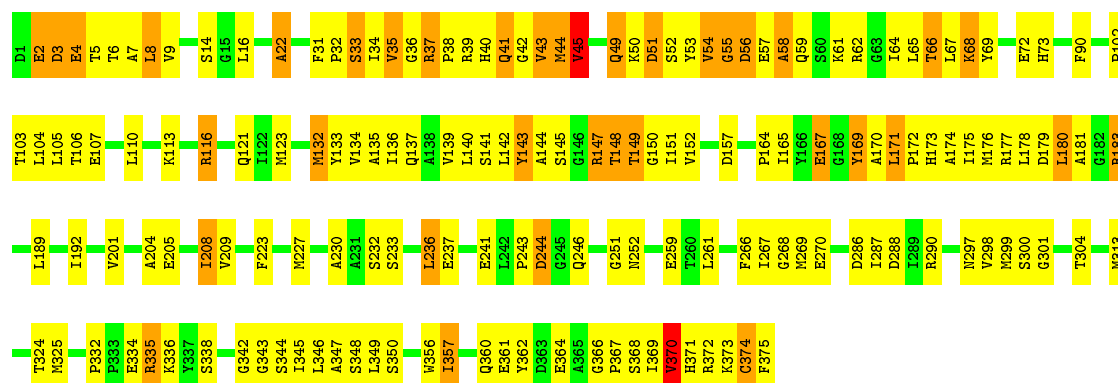
- Molecule 1: Actin, alpha skeletal muscle

Chain J: 55% 35% 9%



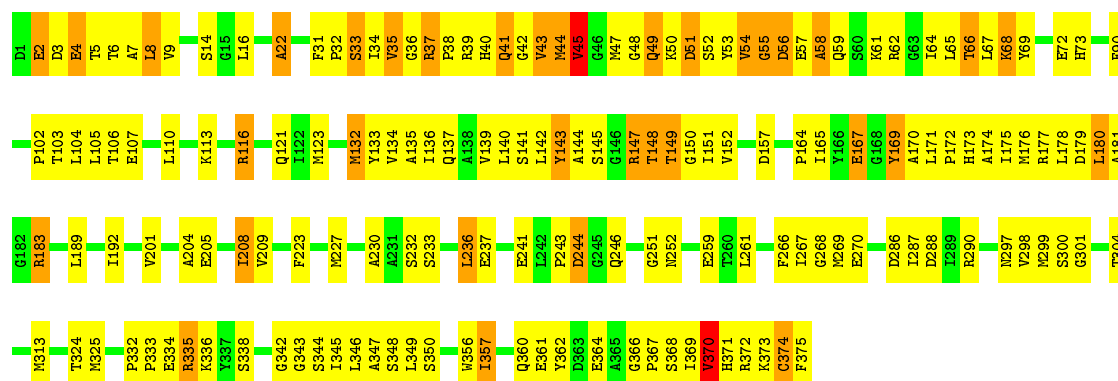
- Molecule 1: Actin, alpha skeletal muscle

Chain K: 56% 34% 10%

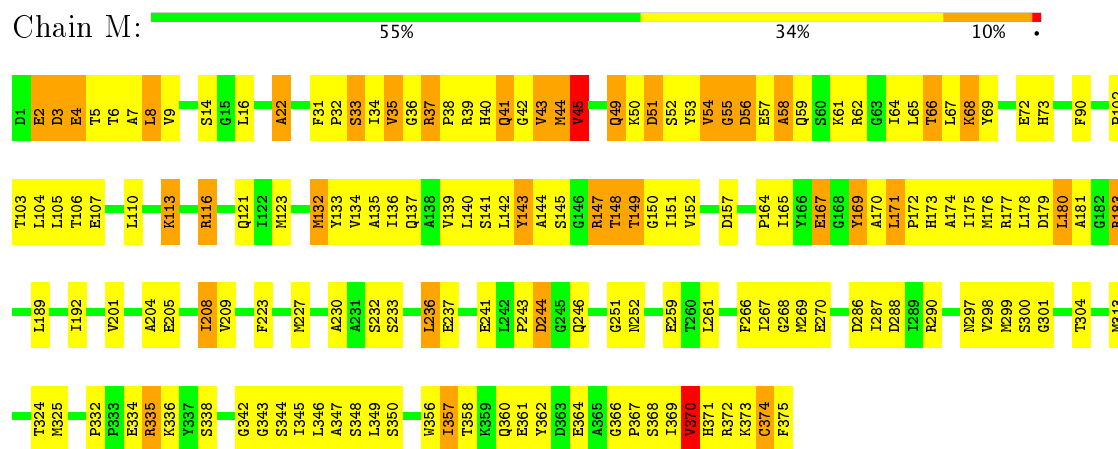


- Molecule 1: Actin, alpha skeletal muscle

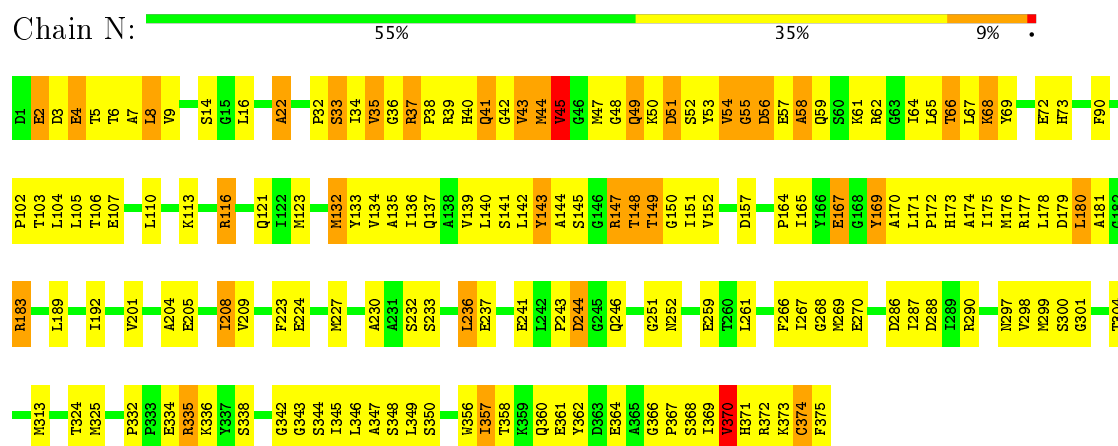
Chain L: 55% 35% 9%



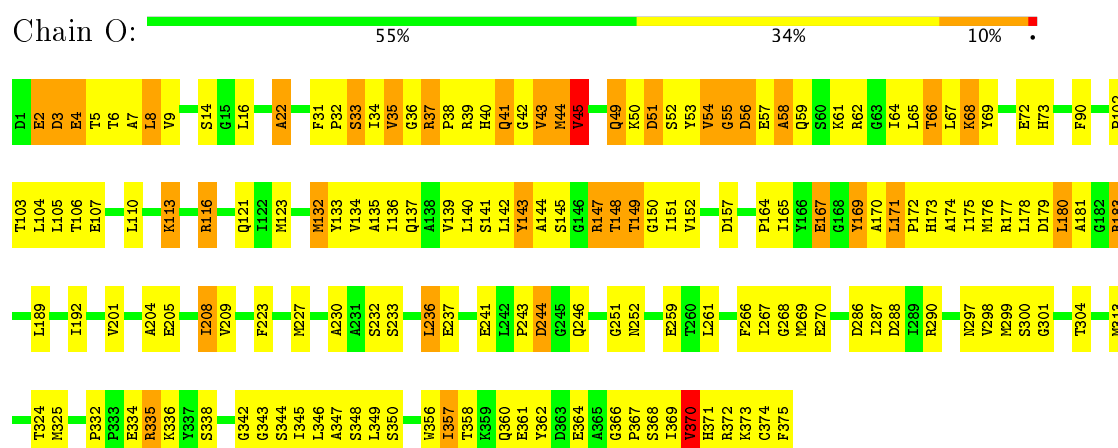
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle

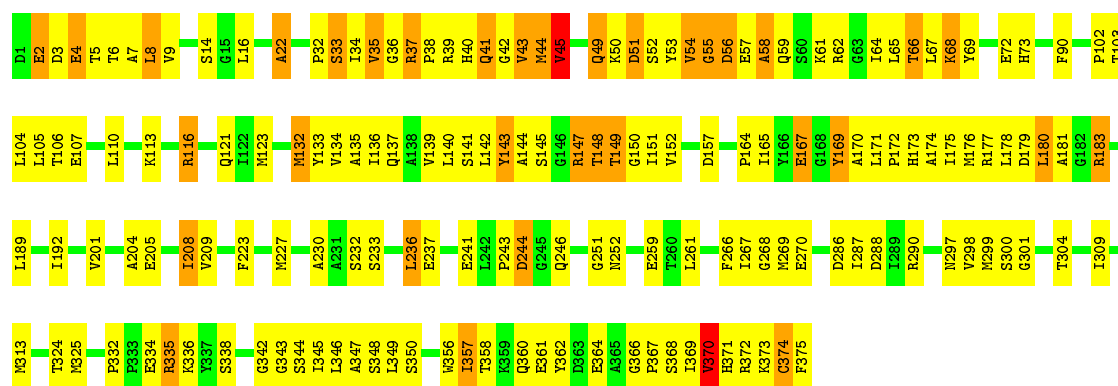


- Molecule 1: Actin, alpha skeletal muscle



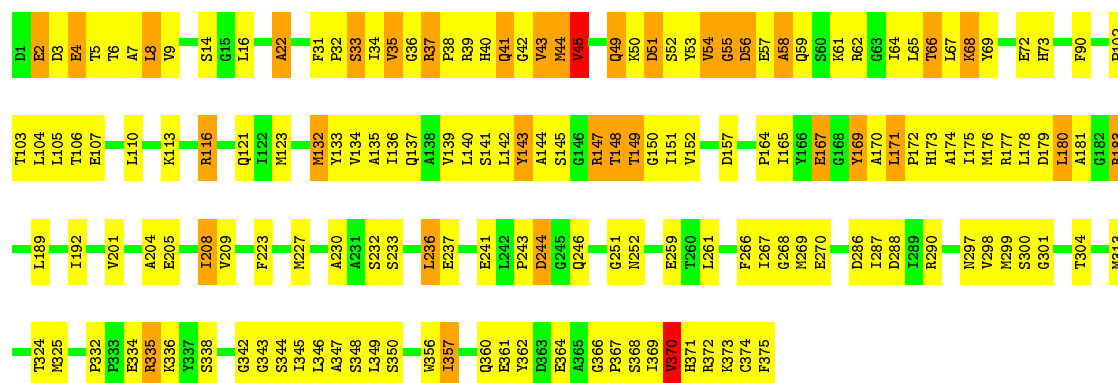
- Molecule 1: Actin, alpha skeletal muscle





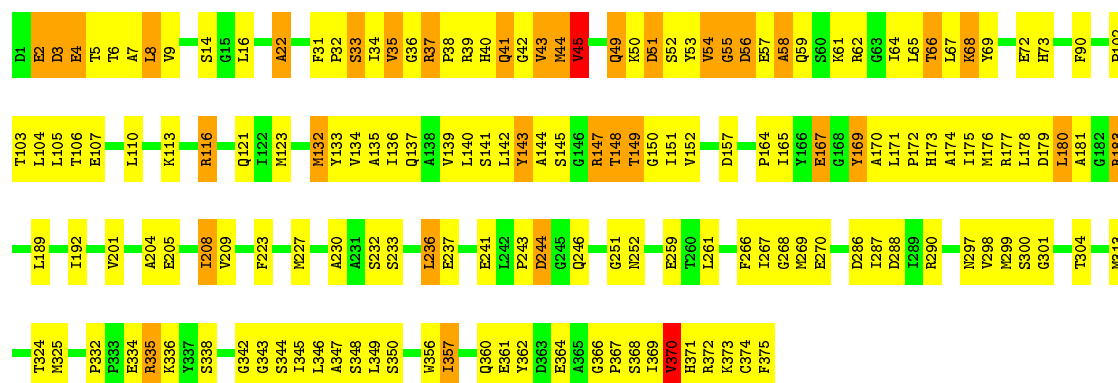
- Molecule 1: Actin, alpha skeletal muscle

Chain Q: 56% 35% 9%



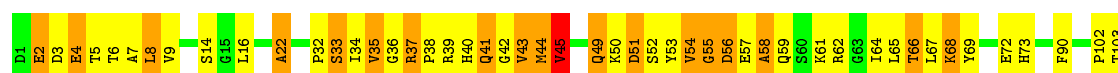
- Molecule 1: Actin, alpha skeletal muscle

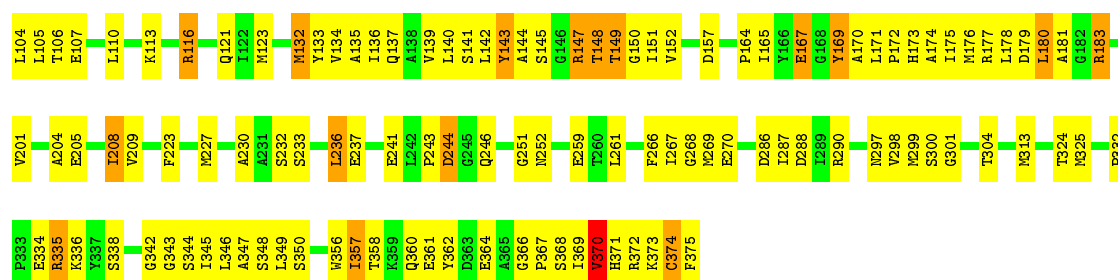
Chain R: 56% 35% 9%



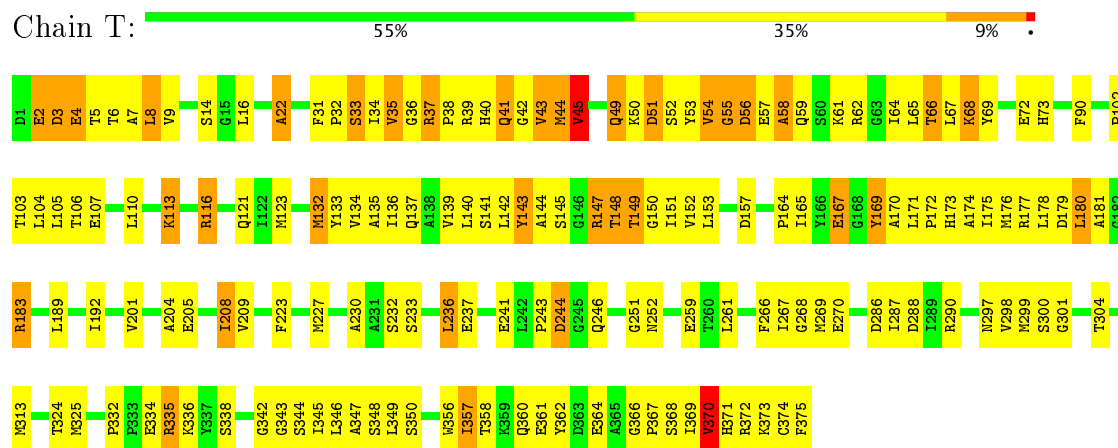
- Molecule 1: Actin, alpha skeletal muscle

Chain S: 56% 34% 9%

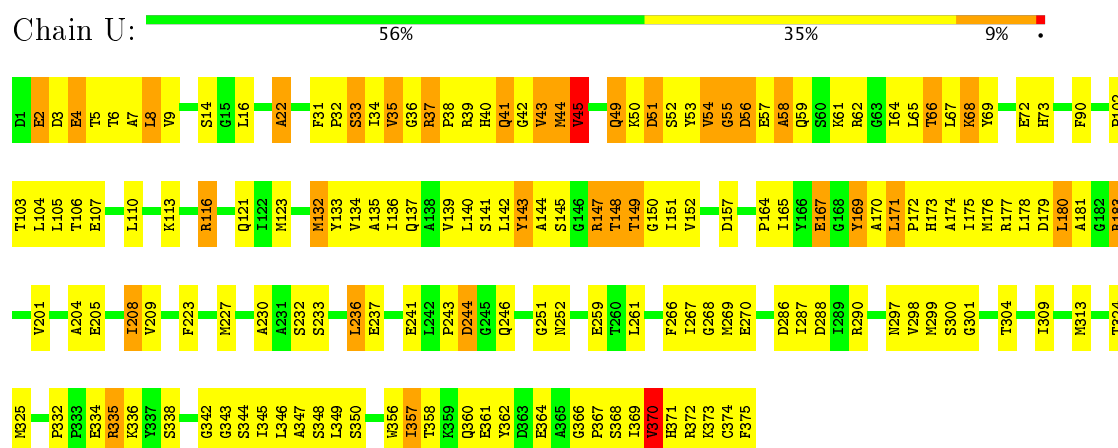




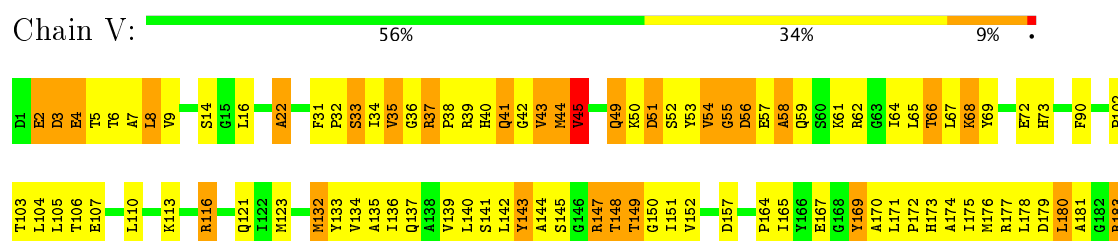
- Molecule 1: Actin, alpha skeletal muscle

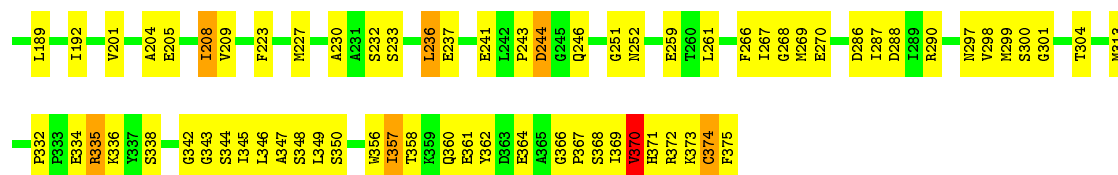


- Molecule 1: Actin, alpha skeletal muscle



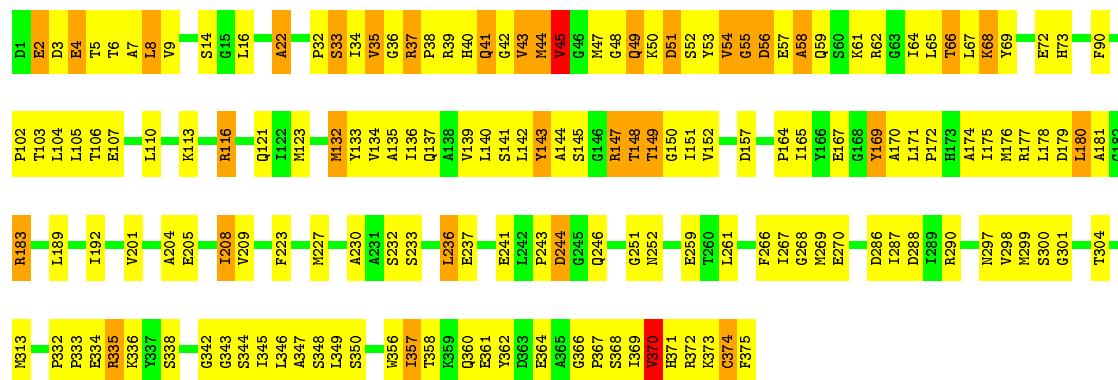
- Molecule 1: Actin, alpha skeletal muscle





• Molecule 1: Actin, alpha skeletal muscle

Chain W: 56% 35% 9%



4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	1680	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI/PHILIPS CM12	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	12	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	AGFA SCIENTA FILM	Depositor

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: HIC, 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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.66	0/2984	1.09	7/4040 (0.2%)
1	B	0.66	0/2984	1.09	7/4040 (0.2%)
1	C	0.66	0/2984	1.09	7/4040 (0.2%)
1	D	0.66	0/2984	1.09	7/4040 (0.2%)
1	E	0.66	0/2984	1.09	7/4040 (0.2%)
1	F	0.66	0/2984	1.09	7/4040 (0.2%)
1	G	0.66	0/2984	1.09	7/4040 (0.2%)
1	H	0.66	0/2984	1.09	7/4040 (0.2%)
1	I	0.66	0/2984	1.09	7/4040 (0.2%)
1	J	0.66	0/2984	1.09	7/4040 (0.2%)
1	K	0.66	0/2984	1.09	7/4040 (0.2%)
1	L	0.66	0/2984	1.09	7/4040 (0.2%)
1	M	0.66	0/2984	1.09	7/4040 (0.2%)
1	N	0.66	0/2984	1.09	7/4040 (0.2%)
1	O	0.66	0/2984	1.09	7/4040 (0.2%)
1	P	0.66	0/2984	1.09	7/4040 (0.2%)
1	Q	0.66	0/2984	1.09	7/4040 (0.2%)
1	R	0.66	0/2984	1.09	7/4040 (0.2%)
1	S	0.66	0/2984	1.09	7/4040 (0.2%)
1	T	0.66	0/2984	1.09	7/4040 (0.2%)
1	U	0.66	0/2984	1.09	7/4040 (0.2%)
1	V	0.66	0/2984	1.09	7/4040 (0.2%)
1	W	0.66	0/2984	1.09	7/4040 (0.2%)
All	All	0.66	0/68632	1.09	161/92920 (0.2%)

There are no bond length outliers.

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	201	VAL	O-C-N	-5.86	113.32	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	201	VAL	O-C-N	-5.86	113.33	122.70
1	J	201	VAL	O-C-N	-5.85	113.35	122.70
1	I	201	VAL	O-C-N	-5.84	113.35	122.70
1	K	201	VAL	O-C-N	-5.84	113.36	122.70

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	2934	0	2895	334	0
1	B	2934	0	2895	336	0
1	C	2934	0	2895	374	0
1	D	2934	0	2895	378	0
1	E	2934	0	2895	380	0
1	F	2934	0	2895	377	0
1	G	2934	0	2895	375	0
1	H	2934	0	2895	375	0
1	I	2934	0	2895	369	0
1	J	2934	0	2895	377	0
1	K	2934	0	2895	372	0
1	L	2934	0	2895	369	0
1	M	2934	0	2895	370	0
1	N	2934	0	2895	377	0
1	O	2934	0	2895	376	0
1	P	2934	0	2895	372	0
1	Q	2934	0	2895	375	0
1	R	2934	0	2895	370	0
1	S	2934	0	2895	371	0
1	T	2934	0	2895	374	0
1	U	2934	0	2895	375	0
1	V	2934	0	2895	337	0
1	W	2934	0	2895	333	0
2	A	27	0	12	4	0
2	B	27	0	12	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	27	0	12	4	0
2	D	27	0	12	5	0
2	E	27	0	12	4	0
2	F	27	0	12	4	0
2	G	27	0	12	4	0
2	H	27	0	12	4	0
2	I	27	0	12	4	0
2	J	27	0	12	4	0
2	K	27	0	12	5	0
2	L	27	0	12	4	0
2	M	27	0	12	4	0
2	N	27	0	12	4	0
2	O	27	0	12	4	0
2	P	27	0	12	4	0
2	Q	27	0	12	4	0
2	R	27	0	12	4	0
2	S	27	0	12	4	0
2	T	27	0	12	4	0
2	U	27	0	12	4	0
2	V	27	0	12	4	0
2	W	27	0	12	4	0
All	All	68103	0	66861	7549	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 56.

The worst 5 of 7549 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:R:59:GLN:O	1:R:62:ARG:HG3	1.43	1.19
1:T:59:GLN:O	1:T:62:ARG:HG3	1.43	1.19
1:W:59:GLN:O	1:W:62:ARG:HG3	1.43	1.19
1:A:59:GLN:O	1:A:62:ARG:HG3	1.43	1.19
1:H:59:GLN:O	1:H:62:ARG:HG3	1.43	1.18

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	A	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	B	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	C	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	D	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	E	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	F	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	G	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	H	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	I	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	J	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	K	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	L	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	M	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	N	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	O	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	P	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	Q	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	R	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	S	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	T	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	U	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	V	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
1	W	372/375 (99%)	329 (88%)	31 (8%)	12 (3%)	5	36
All	All	8556/8625 (99%)	7567 (88%)	713 (8%)	276 (3%)	8	36

5 of 276 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	41	GLN
1	A	44	MET
1	B	3	ASP
1	B	41	GLN

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	A	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	B	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	C	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	D	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	E	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	F	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	G	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	H	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	I	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	J	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	K	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	L	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	M	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	N	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	O	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	P	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	Q	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	R	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	S	317/317 (100%)	280 (88%)	37 (12%)	6	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	U	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	V	317/317 (100%)	280 (88%)	37 (12%)	6	27
1	W	317/317 (100%)	280 (88%)	37 (12%)	6	27
All	All	7291/7291 (100%)	6440 (88%)	851 (12%)	10	27

5 of 851 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	143	TYR
1	M	350	SER
1	V	66	THR
1	K	232	SER
1	L	208	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 136 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	92	ASN
1	M	353	GLN
1	V	49	GLN
1	K	173	HIS
1	L	173	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

23 non-standard protein/DNA/RNA residues 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
1	HIC	A	73	1	9,11,12	1.07	0	7,14,16	1.30	1 (14%)
1	HIC	B	73	1	9,11,12	1.07	0	7,14,16	1.31	1 (14%)
1	HIC	C	73	1	9,11,12	1.07	0	7,14,16	1.29	1 (14%)
1	HIC	D	73	1	9,11,12	1.07	0	7,14,16	1.31	1 (14%)
1	HIC	E	73	1	9,11,12	1.07	0	7,14,16	1.32	1 (14%)
1	HIC	F	73	1	9,11,12	1.07	0	7,14,16	1.31	1 (14%)
1	HIC	G	73	1	9,11,12	1.07	0	7,14,16	1.29	1 (14%)
1	HIC	H	73	1	9,11,12	1.08	0	7,14,16	1.31	1 (14%)
1	HIC	I	73	1	9,11,12	1.07	0	7,14,16	1.31	1 (14%)
1	HIC	J	73	1	9,11,12	1.07	0	7,14,16	1.32	1 (14%)
1	HIC	K	73	1	9,11,12	1.07	0	7,14,16	1.33	1 (14%)
1	HIC	L	73	1	9,11,12	1.07	0	7,14,16	1.30	1 (14%)
1	HIC	M	73	1	9,11,12	1.08	0	7,14,16	1.32	1 (14%)
1	HIC	N	73	1	9,11,12	1.08	0	7,14,16	1.31	1 (14%)
1	HIC	O	73	1	9,11,12	1.08	0	7,14,16	1.31	1 (14%)
1	HIC	P	73	1	9,11,12	1.07	0	7,14,16	1.30	1 (14%)
1	HIC	Q	73	1	9,11,12	1.08	0	7,14,16	1.32	1 (14%)
1	HIC	R	73	1	9,11,12	1.08	0	7,14,16	1.32	1 (14%)
1	HIC	S	73	1	9,11,12	1.08	0	7,14,16	1.32	1 (14%)
1	HIC	T	73	1	9,11,12	1.07	0	7,14,16	1.30	1 (14%)
1	HIC	U	73	1	9,11,12	1.08	0	7,14,16	1.32	1 (14%)
1	HIC	V	73	1	9,11,12	1.07	0	7,14,16	1.31	1 (14%)
1	HIC	W	73	1	9,11,12	1.09	0	7,14,16	1.33	1 (14%)

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
1	HIC	A	73	1	-	0/4/6/8	0/1/1/1
1	HIC	B	73	1	-	0/4/6/8	0/1/1/1
1	HIC	C	73	1	-	0/4/6/8	0/1/1/1
1	HIC	D	73	1	-	0/4/6/8	0/1/1/1
1	HIC	E	73	1	-	0/4/6/8	0/1/1/1
1	HIC	F	73	1	-	0/4/6/8	0/1/1/1
1	HIC	G	73	1	-	0/4/6/8	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HIC	H	73	1	-	0/4/6/8	0/1/1/1
1	HIC	I	73	1	-	0/4/6/8	0/1/1/1
1	HIC	J	73	1	-	0/4/6/8	0/1/1/1
1	HIC	K	73	1	-	0/4/6/8	0/1/1/1
1	HIC	L	73	1	-	0/4/6/8	0/1/1/1
1	HIC	M	73	1	-	0/4/6/8	0/1/1/1
1	HIC	N	73	1	-	0/4/6/8	0/1/1/1
1	HIC	O	73	1	-	0/4/6/8	0/1/1/1
1	HIC	P	73	1	-	0/4/6/8	0/1/1/1
1	HIC	Q	73	1	-	0/4/6/8	0/1/1/1
1	HIC	R	73	1	-	0/4/6/8	0/1/1/1
1	HIC	S	73	1	-	0/4/6/8	0/1/1/1
1	HIC	T	73	1	-	0/4/6/8	0/1/1/1
1	HIC	U	73	1	-	0/4/6/8	0/1/1/1
1	HIC	V	73	1	-	0/4/6/8	0/1/1/1
1	HIC	W	73	1	-	0/4/6/8	0/1/1/1

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	73	HIC	CG-CD2-NE2	2.23	110.13	107.78
1	C	73	HIC	CG-CD2-NE2	2.25	110.15	107.78
1	T	73	HIC	CG-CD2-NE2	2.25	110.16	107.78
1	A	73	HIC	CG-CD2-NE2	2.25	110.16	107.78
1	O	73	HIC	CG-CD2-NE2	2.25	110.16	107.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	73	HIC	2	0
1	B	73	HIC	2	0
1	C	73	HIC	2	0
1	D	73	HIC	2	0
1	E	73	HIC	2	0
1	F	73	HIC	2	0
1	G	73	HIC	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	73	HIC	2	0
1	I	73	HIC	2	0
1	J	73	HIC	2	0
1	K	73	HIC	2	0
1	L	73	HIC	2	0
1	M	73	HIC	2	0
1	N	73	HIC	2	0
1	O	73	HIC	2	0
1	P	73	HIC	2	0
1	Q	73	HIC	2	0
1	R	73	HIC	1	0
1	S	73	HIC	2	0
1	T	73	HIC	1	0
1	U	73	HIC	2	0
1	V	73	HIC	1	0
1	W	73	HIC	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

23 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$
2	ADP	A	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.62	3 (12%)
2	ADP	B	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.61	3 (12%)
2	ADP	C	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.62	3 (12%)
2	ADP	D	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.62	3 (12%)
2	ADP	E	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.61	3 (12%)
2	ADP	F	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.61	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	G	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.60	3 (12%)
2	ADP	H	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.61	3 (12%)
2	ADP	I	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.61	3 (12%)
2	ADP	J	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.60	3 (12%)
2	ADP	K	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.62	3 (12%)
2	ADP	L	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.61	3 (12%)
2	ADP	M	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.61	3 (12%)
2	ADP	N	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.61	3 (12%)
2	ADP	O	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.61	3 (12%)
2	ADP	P	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.61	3 (12%)
2	ADP	Q	401	-	25,29,29	1.13	1 (4%)	24,45,45	1.61	3 (12%)
2	ADP	R	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.61	3 (12%)
2	ADP	S	401	-	25,29,29	1.13	1 (4%)	24,45,45	1.61	3 (12%)
2	ADP	T	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.61	3 (12%)
2	ADP	U	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.61	3 (12%)
2	ADP	V	401	-	25,29,29	1.13	1 (4%)	24,45,45	1.61	3 (12%)
2	ADP	W	401	-	25,29,29	1.14	1 (4%)	24,45,45	1.62	3 (12%)

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
2	ADP	A	401	-	-	0/12/32/32	0/3/3/3
2	ADP	B	401	-	-	0/12/32/32	0/3/3/3
2	ADP	C	401	-	-	0/12/32/32	0/3/3/3
2	ADP	D	401	-	-	0/12/32/32	0/3/3/3
2	ADP	E	401	-	-	0/12/32/32	0/3/3/3
2	ADP	F	401	-	-	0/12/32/32	0/3/3/3
2	ADP	G	401	-	-	0/12/32/32	0/3/3/3
2	ADP	H	401	-	-	0/12/32/32	0/3/3/3
2	ADP	I	401	-	-	0/12/32/32	0/3/3/3
2	ADP	J	401	-	-	0/12/32/32	0/3/3/3
2	ADP	K	401	-	-	0/12/32/32	0/3/3/3
2	ADP	L	401	-	-	0/12/32/32	0/3/3/3
2	ADP	M	401	-	-	0/12/32/32	0/3/3/3
2	ADP	N	401	-	-	0/12/32/32	0/3/3/3
2	ADP	O	401	-	-	0/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	P	401	-	-	0/12/32/32	0/3/3/3
2	ADP	Q	401	-	-	0/12/32/32	0/3/3/3
2	ADP	R	401	-	-	0/12/32/32	0/3/3/3
2	ADP	S	401	-	-	0/12/32/32	0/3/3/3
2	ADP	T	401	-	-	0/12/32/32	0/3/3/3
2	ADP	U	401	-	-	0/12/32/32	0/3/3/3
2	ADP	V	401	-	-	0/12/32/32	0/3/3/3
2	ADP	W	401	-	-	0/12/32/32	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	401	ADP	C2-N1	2.89	1.39	1.33
2	Q	401	ADP	C2-N1	2.90	1.39	1.33
2	I	401	ADP	C2-N1	2.91	1.39	1.33
2	L	401	ADP	C2-N1	2.91	1.39	1.33
2	R	401	ADP	C2-N1	2.91	1.39	1.33

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	ADP	N3-C2-N1	-4.15	125.24	128.86
2	K	401	ADP	N3-C2-N1	-4.15	125.25	128.86
2	P	401	ADP	N3-C2-N1	-4.14	125.25	128.86
2	D	401	ADP	N3-C2-N1	-4.14	125.25	128.86
2	A	401	ADP	N3-C2-N1	-4.12	125.27	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 95 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ADP	4	0
2	B	401	ADP	5	0
2	C	401	ADP	4	0
2	D	401	ADP	5	0
2	E	401	ADP	4	0
2	F	401	ADP	4	0
2	G	401	ADP	4	0
2	H	401	ADP	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	401	ADP	4	0
2	J	401	ADP	4	0
2	K	401	ADP	5	0
2	L	401	ADP	4	0
2	M	401	ADP	4	0
2	N	401	ADP	4	0
2	O	401	ADP	4	0
2	P	401	ADP	4	0
2	Q	401	ADP	4	0
2	R	401	ADP	4	0
2	S	401	ADP	4	0
2	T	401	ADP	4	0
2	U	401	ADP	4	0
2	V	401	ADP	4	0
2	W	401	ADP	4	0

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.