



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:02 PM BST

PDB ID : 4A7F  
EMDB ID: : EMD-1987  
Title : Structure of the Actin-Tropomyosin-Myosin Complex (rigor ATM 3)  
Authors : Behrmann, E.; Mueller, M.; Penczek, P.A.; Mannherz, H.G.; Manstein, D.J.;  
Raunser, S.  
Deposited on : 2011-11-14  
Resolution : 7.70 Å(reported)  
Based on PDB ID : 3MFP;1LKX

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could  
stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

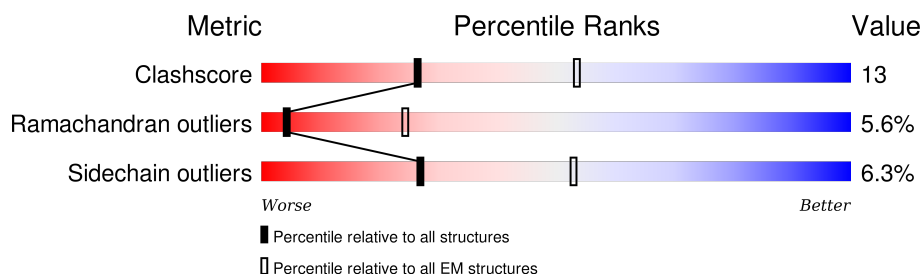
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.70 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 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	68% 22% 7% .
1	D	375	66% 25% 6% .
1	E	375	67% 24% 6% .
1	F	375	67% 24% 7% .
1	I	375	66% 25% 7% .
2	B	136	98% .
2	H	136	99% .
3	C	697	75% 21% ..
3	G	697	73% 22% ..

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Mol	Chain	Length	Quality of chain
3	J	697	<div><div></div><div>74%</div><div>22%</div><div>..</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33500 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	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	I	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		

- Molecule 2 is a protein called TROPOMYOSIN 1 ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	136	Total	C	N	O	S	0	0
			1104	673	189	239	3		
2	H	136	Total	C	N	O	S	0	0
			1104	673	189	239	3		

- Molecule 3 is a protein called MYOSIN IE HEAVY CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	689	Total	C	N	O	S	0	0
			5494	3469	946	1048	31		
3	G	689	Total	C	N	O	S	0	0
			5494	3469	946	1048	31		
3	J	689	Total	C	N	O	S	0	0
			5494	3469	946	1048	31		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	77	MET	ILE	CONFLICT	UNP Q03479

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Chain	Residue	Modelled	Actual	Comment	Reference
C	215	ASP	ASN	CONFLICT	UNP Q03479
C	334	GLU	SER	ENGINEERED MUTATION	UNP Q03479
G	77	MET	ILE	CONFLICT	UNP Q03479
G	215	ASP	ASN	CONFLICT	UNP Q03479
G	334	GLU	SER	ENGINEERED MUTATION	UNP Q03479
J	77	MET	ILE	CONFLICT	UNP Q03479
J	215	ASP	ASN	CONFLICT	UNP Q03479
J	334	GLU	SER	ENGINEERED MUTATION	UNP Q03479

- # ADP
- 

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

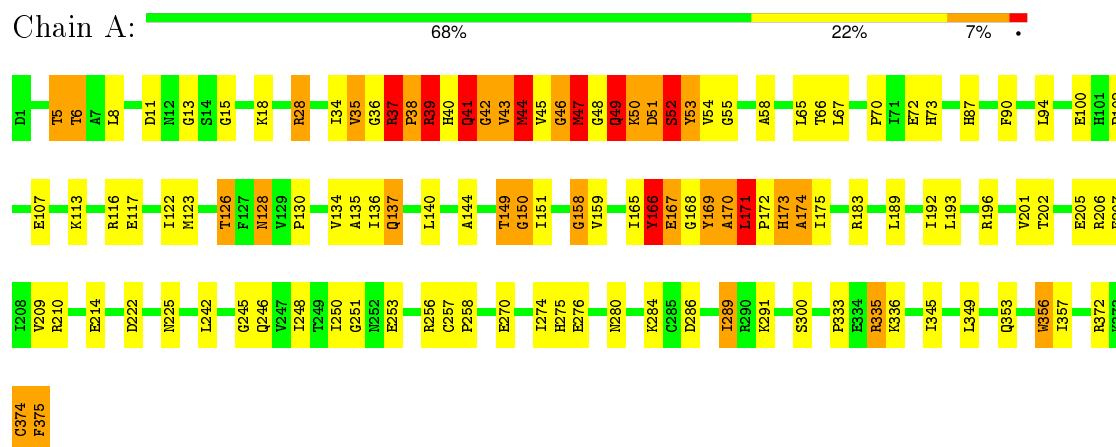
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Mol	Chain	Residues	Atoms		AltConf
5	I	1	Total 1	Ca 1	0
5	A	1	Total 1	Ca 1	0
5	D	1	Total 1	Ca 1	0
5	F	1	Total 1	Ca 1	0
5	E	1	Total 1	Ca 1	0

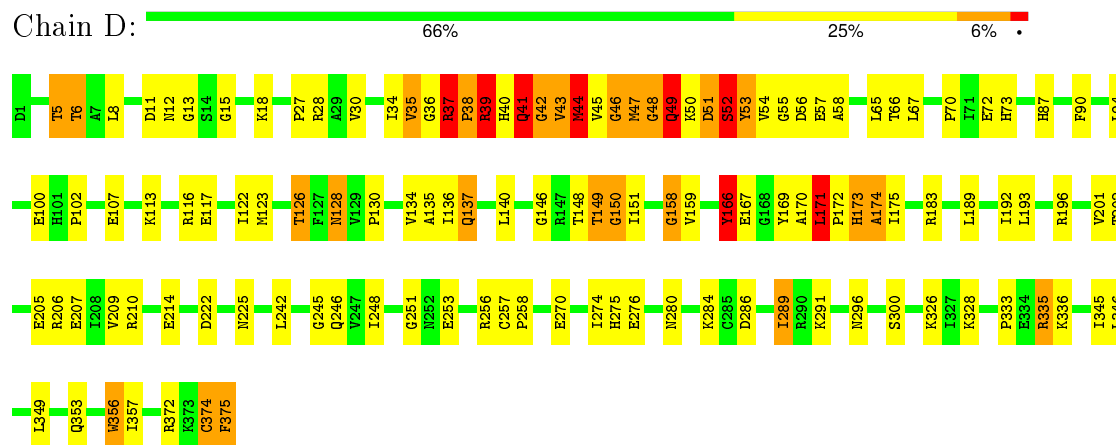
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

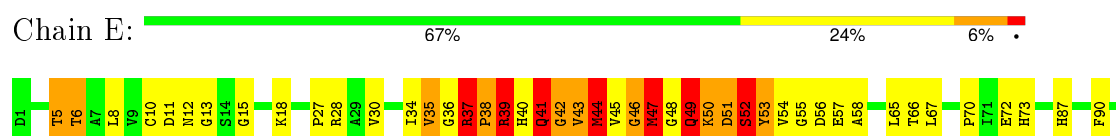
- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

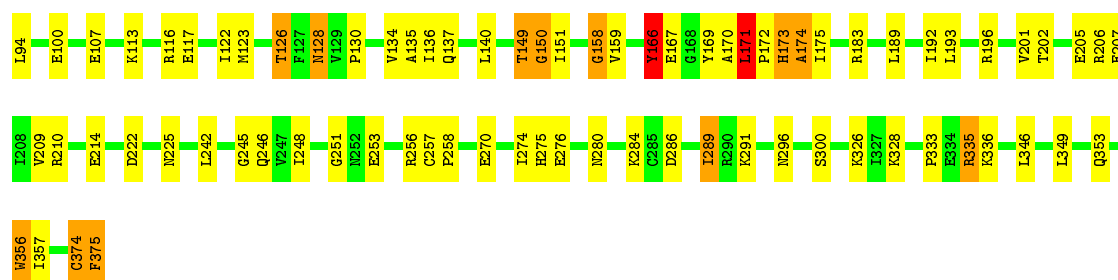


- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

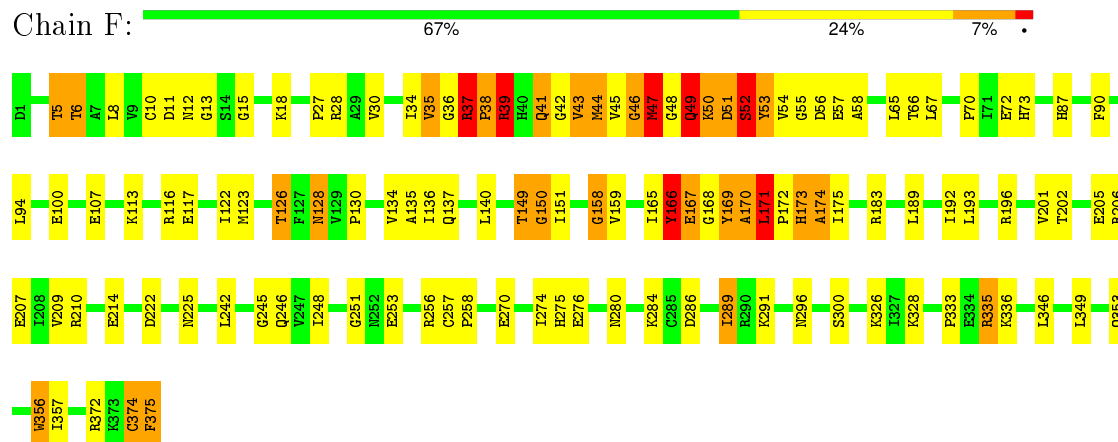


- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

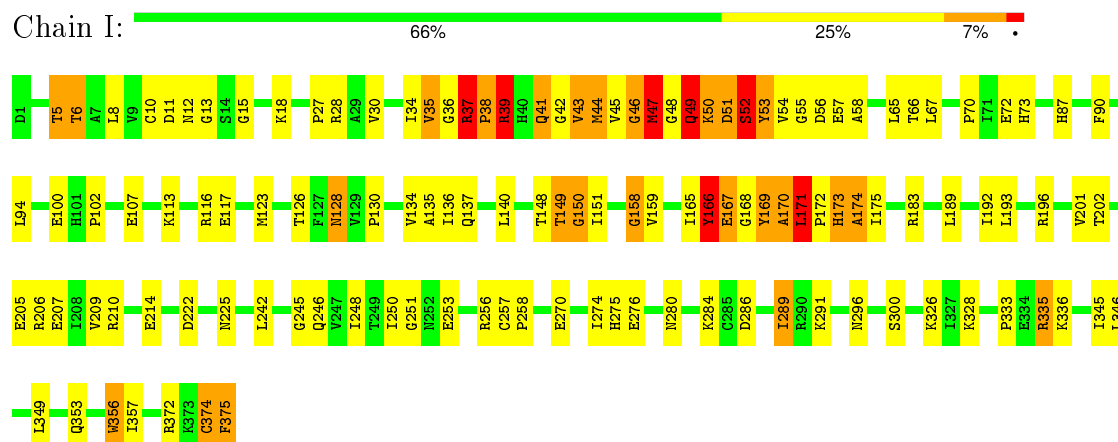




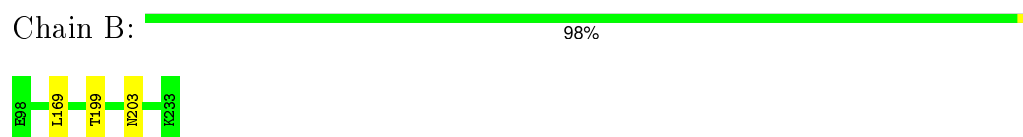
- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



- Molecule 2: TROPOMYOSIN 1 ALPHA



- Molecule 2: TROPOMYOSIN 1 ALPHA

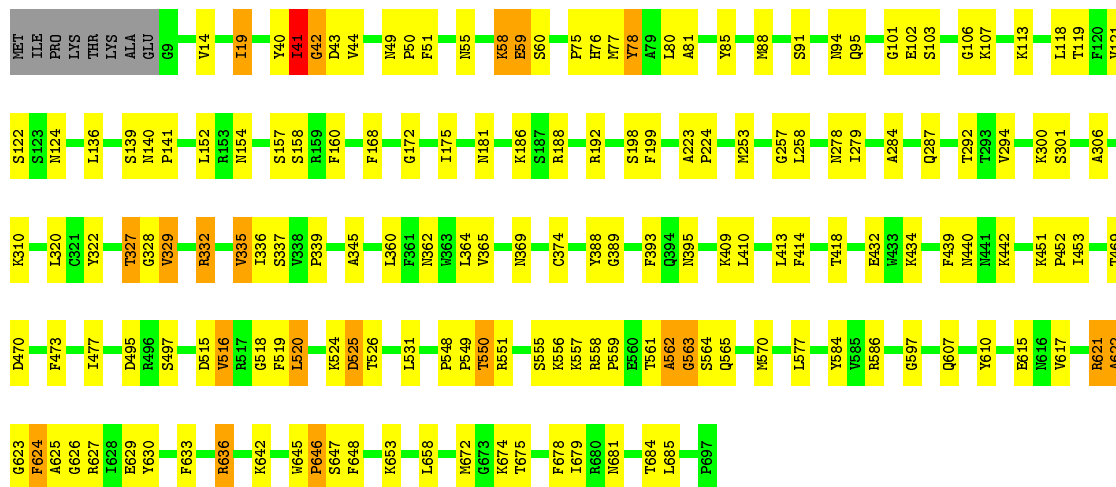






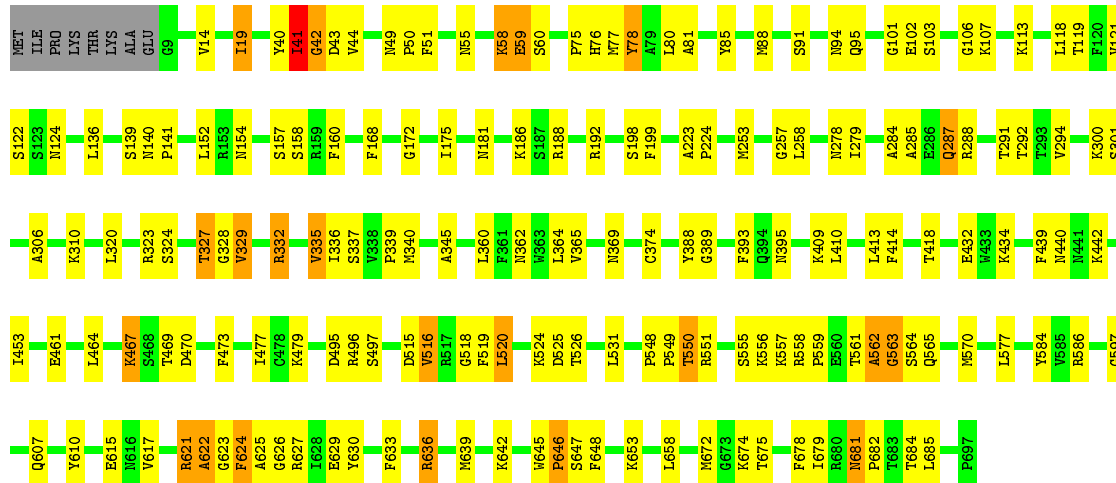
• Molecule 3: MYOSIN IE HEAVY CHAIN

Chain C: 75% 21% ..



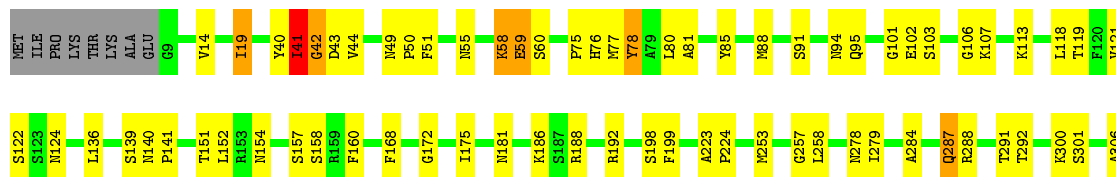
• Molecule 3: MYOSIN IE HEAVY CHAIN

Chain G: 73% 22% ..



• Molecule 3: MYOSIN IE HEAVY CHAIN

Chain J: 74% 22% ..



K310	K320	R323	S324	T327	G328	V329	R332	V335	I336	S337	V338	P339	M340	L360	F361	N362	N363	L364	V365	N369	C374	Y388	G389	F393	N394	N395	K409	L410	L413	F414	T418	E432	N433	K434	F439	N440	N441	K442	I453	E461				
L464	I465	A466	K467	S468	T469	D470	F473	I477	D495	R496	S497	D515	V516	R517	G518	F519	L520	K524	D525	T526	L531	P548	P549	T550	R551	S555	K556	K557	R558	P559	E560	T561	A562	G563	S564	Q565	M570	L577	Y584	V585	R586	G597	Q607	Y610
E615	R621	A622	G623	F624	A625	G626	R627	L628	E629	Y630	F633	R636	K642	K645	P646	S647	F648	K653	L658	N672	G673	K674	T675	F678	I679	R680	N681	P682	T683	T684	L685	P697												

## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	INDIVIDUAL PARTICLES	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.7	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	80000	Depositor
Image detector	TVIPS TEMCAM-F816 (CMOS)	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: CA, 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	0.91	10/2984 (0.3%)	0.65	8/4040 (0.2%)
1	D	0.89	9/2984 (0.3%)	0.63	8/4040 (0.2%)
1	E	0.88	10/2984 (0.3%)	0.64	8/4040 (0.2%)
1	F	0.88	10/2984 (0.3%)	0.64	8/4040 (0.2%)
1	I	0.88	10/2984 (0.3%)	0.64	8/4040 (0.2%)
2	B	0.31	0/1107	0.31	0/1471
2	H	0.22	0/1107	0.35	0/1471
3	C	0.26	0/5592	0.39	0/7533
3	G	0.22	0/5592	0.37	0/7533
3	J	0.22	0/5592	0.37	0/7533
All	All	0.62	49/33910 (0.1%)	0.51	40/45741 (0.1%)

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	166	TYR	CD2-CE2	19.81	1.69	1.39
1	D	166	TYR	CD2-CE2	19.81	1.69	1.39
1	A	166	TYR	CD2-CE2	19.79	1.69	1.39
1	I	166	TYR	CD2-CE2	19.77	1.69	1.39
1	F	166	TYR	CD2-CE2	19.73	1.69	1.39

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	39	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	A	39	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	F	39	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	E	39	ARG	NE-CZ-NH2	-10.01	115.30	120.30
1	D	39	ARG	NE-CZ-NH2	-9.96	115.32	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	2934	0	2895	160	0
1	D	2934	0	2895	139	0
1	E	2934	0	2895	125	0
1	F	2934	0	2895	127	0
1	I	2934	0	2895	138	0
2	B	1104	0	1104	2	0
2	H	1104	0	1104	4	0
3	C	5494	0	5490	88	0
3	G	5494	0	5490	98	0
3	J	5494	0	5490	93	0
4	A	27	0	12	7	0
4	D	27	0	12	7	0
4	E	27	0	12	7	0
4	F	27	0	12	7	0
4	I	27	0	12	7	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
All	All	33500	0	33213	877	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 13.

The worst 5 of 877 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:44:MET:SD	1:I:169:TYR:HE1	1.32	1.51
1:A:169:TYR:HE1	1:D:44:MET:SD	1.39	1.46
1:E:44:MET:SD	1:F:169:TYR:HE1	1.44	1.38
1:A:44:MET:SD	1:I:169:TYR:CE1	2.14	1.38
1:I:53:TYR:O	1:I:58:ALA:CB	1.75	1.35

There are no symmetry-related clashes.

## 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 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%)	292 (78%)	53 (14%)	27 (7%)	1	21
1	D	372/375 (99%)	292 (78%)	53 (14%)	27 (7%)	1	21
1	E	372/375 (99%)	292 (78%)	53 (14%)	27 (7%)	1	21
1	F	372/375 (99%)	292 (78%)	53 (14%)	27 (7%)	1	21
1	I	372/375 (99%)	293 (79%)	52 (14%)	27 (7%)	1	21
2	B	134/136 (98%)	134 (100%)	0	0	100	100
2	H	134/136 (98%)	134 (100%)	0	0	100	100
3	C	683/697 (98%)	551 (81%)	99 (14%)	33 (5%)	3	32
3	G	683/697 (98%)	551 (81%)	99 (14%)	33 (5%)	3	32
3	J	683/697 (98%)	551 (81%)	99 (14%)	33 (5%)	3	32
All	All	4177/4238 (99%)	3382 (81%)	561 (13%)	234 (6%)	4	28

5 of 234 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	37	ARG
1	A	38	PRO
1	A	44	MET
1	A	47	MET

### 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 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%)	286 (90%)	31 (10%)	10	39
1	D	317/317 (100%)	288 (91%)	29 (9%)	12	43
1	E	317/317 (100%)	286 (90%)	31 (10%)	10	39
1	F	317/317 (100%)	286 (90%)	31 (10%)	10	39
1	I	317/317 (100%)	286 (90%)	31 (10%)	10	39
2	B	118/118 (100%)	118 (100%)	0	100	100
2	H	118/118 (100%)	118 (100%)	0	100	100
3	C	609/616 (99%)	585 (96%)	24 (4%)	39	72
3	G	609/616 (99%)	582 (96%)	27 (4%)	35	69
3	J	609/616 (99%)	582 (96%)	27 (4%)	35	69
All	All	3648/3669 (99%)	3417 (94%)	231 (6%)	27	59

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	183	ARG
1	F	151	ILE
3	J	388	TYR
1	E	206	ARG
1	F	39	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	354	GLN
1	F	354	GLN
3	J	313	GLN
1	F	137	GLN
1	F	161	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	6,11,12	1.22	0	6,14,16	1.48	1 (16%)
1	HIC	D	73	1	6,11,12	1.21	0	6,14,16	1.48	1 (16%)
1	HIC	E	73	1	6,11,12	1.23	0	6,14,16	1.48	1 (16%)
1	HIC	F	73	1	6,11,12	1.22	1 (16%)	6,14,16	1.49	1 (16%)
1	HIC	I	73	1	6,11,12	1.22	0	6,14,16	1.48	1 (16%)

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	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	I	73	1	-	0/4/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	73	HIC	CB-CA	2.02	1.58	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	73	HIC	O-C-CA	-2.98	117.72	125.72
1	I	73	HIC	O-C-CA	-2.98	117.73	125.72
1	E	73	HIC	O-C-CA	-2.97	117.75	125.72
1	A	73	HIC	O-C-CA	-2.97	117.76	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	73	HIC	O-C-CA	-2.96	117.79	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	73	HIC	1	0
1	D	73	HIC	1	0
1	E	73	HIC	1	0
1	F	73	HIC	1	0
1	I	73	HIC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	ADP	A	376	-	24,29,29	1.16	1 (4%)	23,45,45	1.51	3 (13%)
4	ADP	D	376	-	24,29,29	1.16	1 (4%)	23,45,45	1.51	3 (13%)
4	ADP	E	376	-	24,29,29	1.16	1 (4%)	23,45,45	1.51	3 (13%)
4	ADP	F	376	-	24,29,29	1.16	1 (4%)	23,45,45	1.49	3 (13%)
4	ADP	I	376	-	24,29,29	1.17	1 (4%)	23,45,45	1.51	3 (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	A	376	-	-	0/12/32/32	0/3/3/3
4	ADP	D	376	-	-	0/12/32/32	0/3/3/3
4	ADP	E	376	-	-	0/12/32/32	0/3/3/3
4	ADP	F	376	-	-	0/12/32/32	0/3/3/3
4	ADP	I	376	-	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	376	ADP	C2-N1	2.88	1.39	1.33
4	A	376	ADP	C2-N1	2.88	1.39	1.33
4	F	376	ADP	C2-N1	2.88	1.39	1.33
4	I	376	ADP	C2-N1	2.89	1.39	1.33
4	D	376	ADP	C2-N1	2.92	1.39	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	376	ADP	N3-C2-N1	-4.67	125.20	128.87
4	D	376	ADP	N3-C2-N1	-4.64	125.22	128.87
4	I	376	ADP	N3-C2-N1	-4.64	125.22	128.87
4	A	376	ADP	N3-C2-N1	-4.63	125.23	128.87
4	F	376	ADP	N3-C2-N1	-4.55	125.30	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	376	ADP	7	0
4	D	376	ADP	7	0
4	E	376	ADP	7	0
4	F	376	ADP	7	0
4	I	376	ADP	7	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.