



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 17, 2017 – 02:20 PM EST

PDB ID : 5H53
EMDB ID: : EMD-6664
Title : The structure of rabbit skeletal muscle actomyosin rigor complex at 5.2 angstrom.
Authors : Fujii, T.; Namba, K.
Deposited on : 2016-11-04
Resolution : 5.20 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 : 1.7.1 (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) : rb-20028442

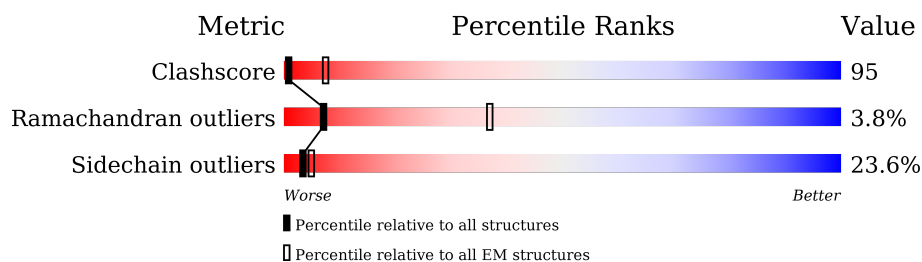
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.20 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 ≥ 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	845	<div> <div>19%</div> <div>58%</div> <div>20%</div> <div>.</div> </div>
2	B	146	<div> <div>18%</div> <div>49%</div> <div>25%</div> <div>8%</div> </div>
3	C	153	<div> <div>7%</div> <div>49%</div> <div>32%</div> <div>12%</div> </div>
4	D	375	<div> <div>30%</div> <div>55%</div> <div>15%</div> <div>.</div> </div>
4	E	375	<div> <div>35%</div> <div>51%</div> <div>13%</div> <div>.</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15077 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 Skeletal muscle myosin heavy chain MyHC-EO/IIL.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	845	Total	C	N	O	S	0	0
			6795	4340	1155	1256	44		

- Molecule 2 is a protein called Myosin regulatory light chain 2, skeletal muscle isoform type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	146	Total	C	N	O	S	0	0
			1157	729	189	232	7		

- Molecule 3 is a protein called Myosin light chain 1/3, skeletal muscle isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	153	Total	C	N	O	S	0	0
			1203	751	199	246	7		

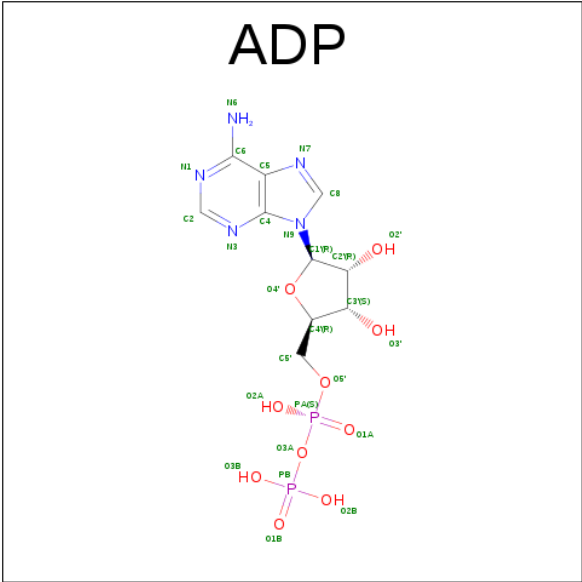
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	193	ASP	-	expression tag	UNP P02602

- Molecule 4 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
4	E	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

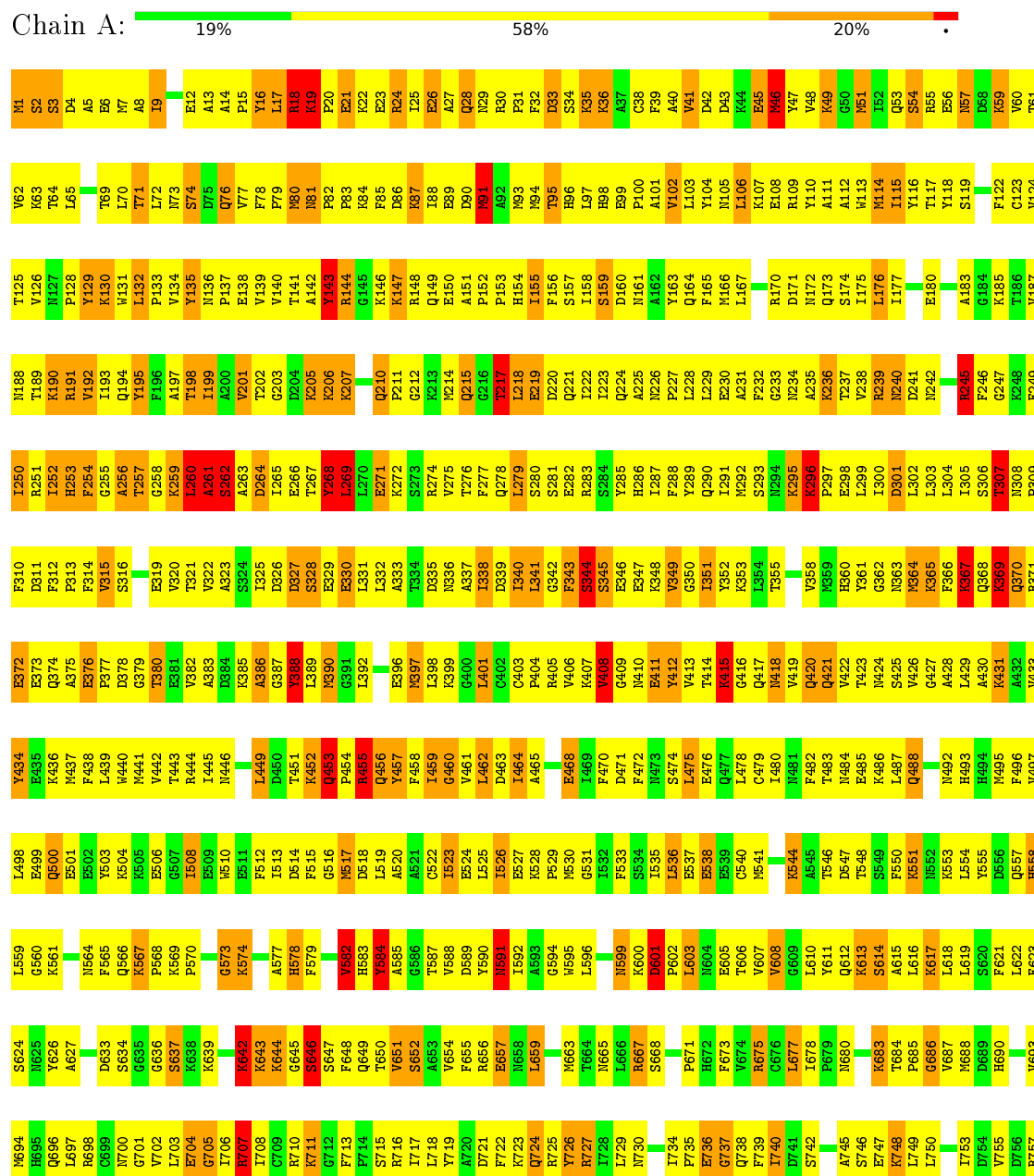


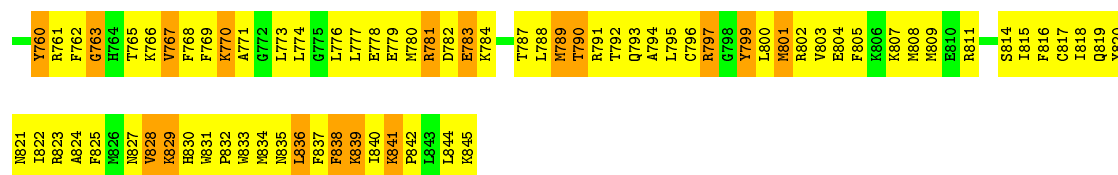
Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

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 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.

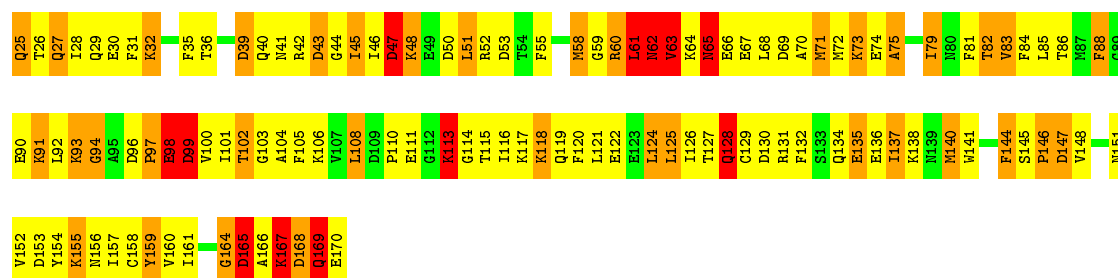
- Molecule 1: Skeletal muscle myosin heavy chain MyHC-EO/IIL





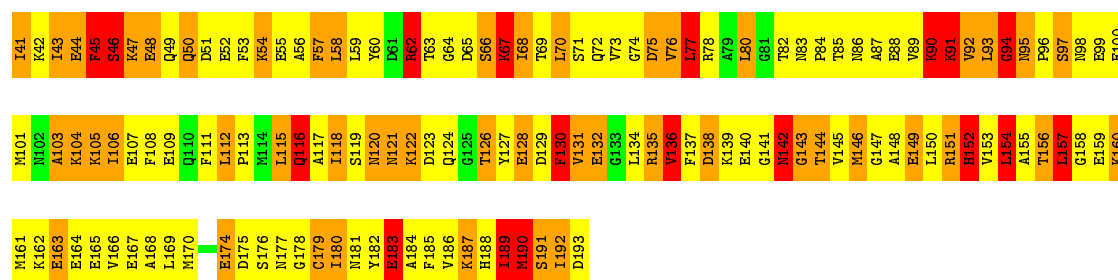
• Molecule 2: Myosin regulatory light chain 2, skeletal muscle isoform type 1

Chain B: 18% 49% 25% 8%



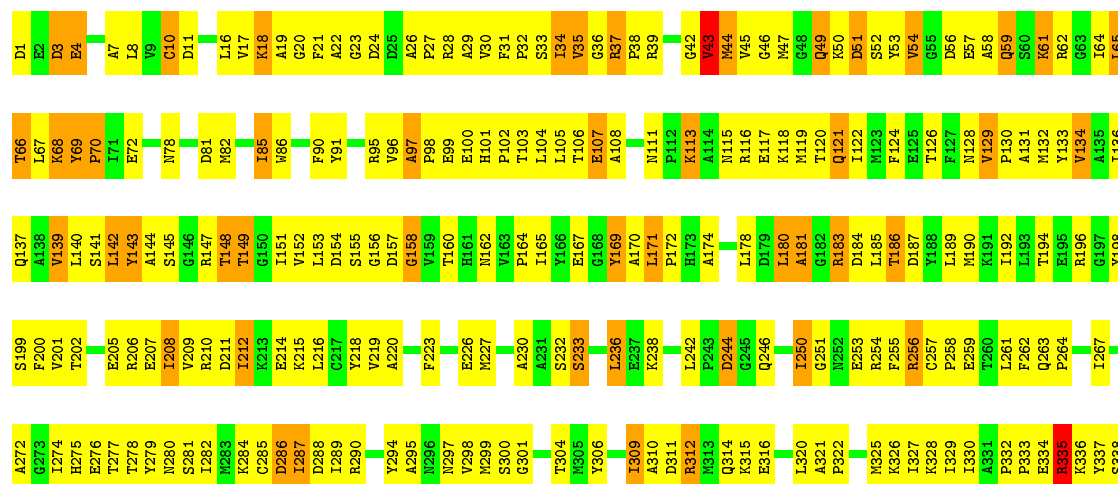
• Molecule 3: Myosin light chain 1/3, skeletal muscle isoform

Chain C: 7% 49% 32% 12%



• Molecule 4: Actin, alpha skeletal muscle

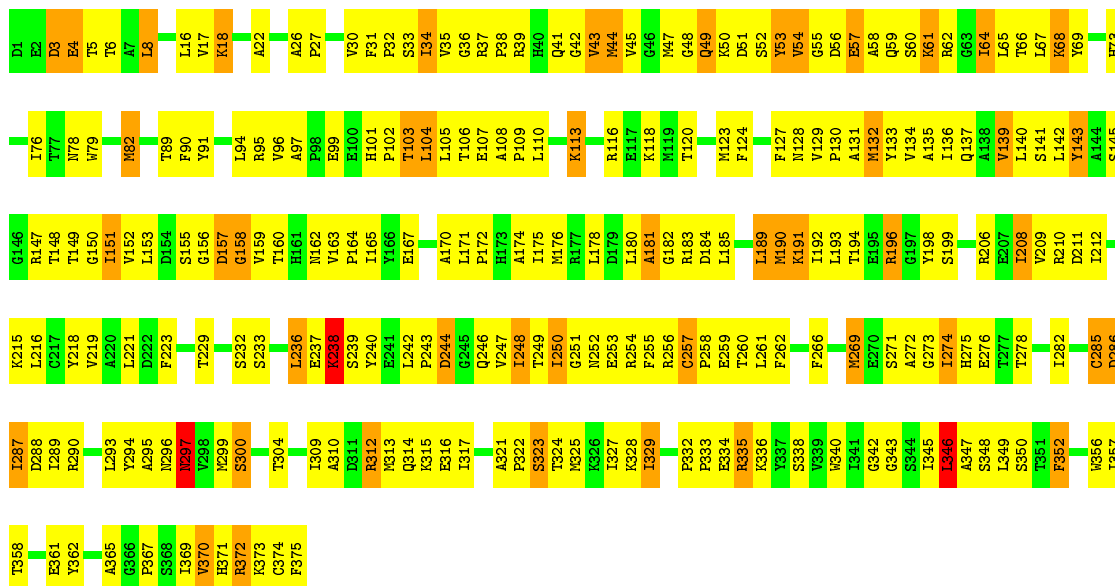
Chain D: 30% 55% 15%





• Molecule 4: Actin, alpha skeletal muscle

Chain E: 35% 51% 13%



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	31535	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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	1.03	3/6941 (0.0%)	1.45	52/9343 (0.6%)
2	B	0.96	1/1175 (0.1%)	1.78	8/1578 (0.5%)
3	C	1.02	1/1218 (0.1%)	1.33	4/1632 (0.2%)
4	D	1.02	5/2984 (0.2%)	1.15	4/4040 (0.1%)
4	E	0.97	0/2984	1.14	6/4040 (0.1%)
All	All	1.01	10/15302 (0.1%)	1.36	74/20633 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	31
2	B	0	18
3	C	0	22
4	D	0	2
4	E	0	2
All	All	0	75

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	538	GLU	CD-OE2	11.79	1.38	1.25
1	A	538	GLU	CG-CD	-10.73	1.35	1.51
4	D	212	ILE	C-N	8.81	1.54	1.34
1	A	538	GLU	CB-CG	7.55	1.66	1.52
3	C	183	GLU	CB-CG	6.51	1.64	1.52

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	99	ASP	CB-CG-OD1	-40.40	81.94	118.30
2	B	99	ASP	CB-CG-OD2	-25.09	95.72	118.30
1	A	180	GLU	CG-CD-OE1	-23.88	70.54	118.30
1	A	747	GLU	CG-CD-OE1	-23.65	71.00	118.30
1	A	747	GLU	CG-CD-OE2	-23.28	71.74	118.30

There are no chirality outliers.

5 of 75 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	TYR	Peptide
1	A	18	ARG	Peptide
1	A	203	GLY	Peptide
1	A	217	THR	Peptide
1	A	239	ARG	Peptide

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	6795	0	6785	1589	0
2	B	1157	0	1127	222	0
3	C	1203	0	1176	410	0
4	D	2934	0	2894	381	0
4	E	2934	0	2895	382	0
5	D	27	0	12	7	0
5	E	27	0	12	4	0
All	All	15077	0	14901	2860	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 95.

The worst 5 of 2860 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:B:79:ILE:HG13	2:B:83:VAL:HG13	1.20	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:361:GLU:HB3	4:E:369:ILE:HD13	1.25	1.19
1:A:390:MET:HB3	1:A:392:LEU:HD23	1.19	1.18
1:A:800:LEU:HG	3:C:162:LYS:HE2	1.19	1.17
4:D:142:LEU:HD21	4:D:165:ILE:HD13	1.17	1.17

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	843/845 (100%)	776 (92%)	42 (5%)	25 (3%)	5	42
2	B	144/146 (99%)	116 (81%)	17 (12%)	11 (8%)	1	20
3	C	151/153 (99%)	121 (80%)	15 (10%)	15 (10%)	1	14
4	D	372/375 (99%)	338 (91%)	24 (6%)	10 (3%)	6	44
4	E	372/375 (99%)	343 (92%)	18 (5%)	11 (3%)	5	42
All	All	1882/1894 (99%)	1694 (90%)	116 (6%)	72 (4%)	7	37

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	SER
1	A	46	MET
1	A	215	GLN
1	A	269	LEU

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	738/738 (100%)	566 (77%)	172 (23%)	1	8
2	B	125/125 (100%)	86 (69%)	39 (31%)	0	3
3	C	131/131 (100%)	76 (58%)	55 (42%)	0	0
4	D	317/317 (100%)	255 (80%)	62 (20%)	1	13
4	E	317/317 (100%)	261 (82%)	56 (18%)	2	17
All	All	1628/1628 (100%)	1244 (76%)	384 (24%)	3	7

5 of 384 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	31	PHE
3	C	47	LYS
4	E	191	LYS
2	B	47	ASP
2	B	108	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	672	HIS
1	A	835	ASN
4	E	59	GLN
1	A	690	HIS
1	A	819	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
4	HIC	D	73	4	6,11,12	1.14	0	6,14,16	1.37	2 (33%)
4	HIC	E	73	4	6,11,12	1.14	0	6,14,16	1.42	2 (33%)

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	HIC	D	73	4	-	0/4/6/8	0/1/1/1
4	HIC	E	73	4	-	0/4/6/8	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	E	73	HIC	O-C-CA	-2.21	119.80	125.72
4	D	73	HIC	O-C-CA	-2.17	119.91	125.72
4	D	73	HIC	CG-CD2-NE2	2.08	110.02	107.63
4	E	73	HIC	CG-CD2-NE2	2.19	110.14	107.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	73	HIC	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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
5	ADP	D	401	-	24,29,29	1.21	2 (8%)	23,45,45	1.55	3 (13%)
5	ADP	E	401	-	24,29,29	1.22	2 (8%)	23,45,45	1.54	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
5	ADP	D	401	-	-	0/12/32/32	0/3/3/3
5	ADP	E	401	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	401	ADP	PB-O2B	-2.06	1.47	1.54
5	D	401	ADP	PB-O2B	-2.01	1.47	1.54
5	D	401	ADP	C2-N1	2.83	1.39	1.33
5	E	401	ADP	C2-N1	2.92	1.39	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	401	ADP	N3-C2-N1	-4.69	125.19	128.87
5	E	401	ADP	N3-C2-N1	-4.62	125.24	128.87
5	E	401	ADP	C2-N1-C6	2.15	122.61	118.77
5	D	401	ADP	C2-N1-C6	2.17	122.65	118.77
5	E	401	ADP	O3B-PB-O2B	2.33	115.98	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	401	ADP	7	0
5	E	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.