



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 10, 2018 – 05:25 PM EST

PDB ID : 6BCX
EMDB ID: : EMD-7087
Title : mTORC1 structure refined to 3.0 angstroms
Authors : Pavletich, N.P.; Yang, H.
Deposited on : 2017-10-20
Resolution : 3.00 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-20030736

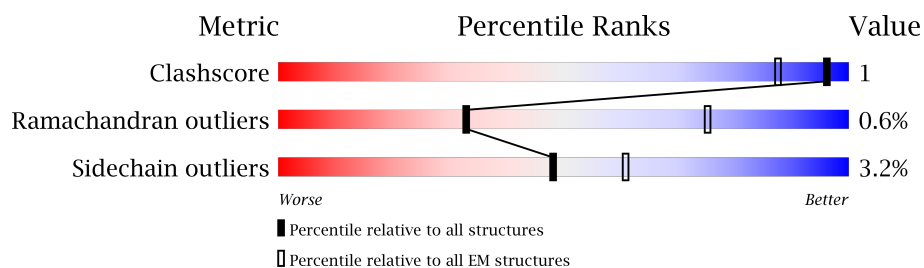
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	2549	
1	B	2549	
2	D	326	
2	E	326	
3	W	1343	
3	Y	1343	
4	X	122	
4	Z	122	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 113610 atoms, of which 57030 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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2178	Total	C	H	N	O	S	0	0
			35034	11082	17686	3038	3117	111		
1	B	2178	Total	C	H	N	O	S	0	0
			35034	11082	17686	3038	3117	111		

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	317	Total	C	H	N	O	S	0	0
			4809	1526	2353	436	476	18		
2	E	317	Total	C	H	N	O	S	0	0
			4809	1526	2353	436	476	18		

- Molecule 3 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	W	1052	Total	C	H	N	O	S	0	0
			16791	5361	8406	1450	1518	56		
3	Y	1052	Total	C	H	N	O	S	0	0
			16791	5361	8406	1450	1518	56		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-7	MET	-	initiating methionine	UNP Q8N122
W	-6	ASP	-	expression tag	UNP Q8N122
W	-5	TYR	-	expression tag	UNP Q8N122
W	-4	LYS	-	expression tag	UNP Q8N122
W	-3	ASP	-	expression tag	UNP Q8N122
W	-2	ASP	-	expression tag	UNP Q8N122
W	-1	ASP	-	expression tag	UNP Q8N122
W	0	ASP	-	expression tag	UNP Q8N122
W	1	LYS	-	expression tag	UNP Q8N122

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-7	MET	-	initiating methionine	UNP Q8N122
Y	-6	ASP	-	expression tag	UNP Q8N122
Y	-5	TYR	-	expression tag	UNP Q8N122
Y	-4	LYS	-	expression tag	UNP Q8N122
Y	-3	ASP	-	expression tag	UNP Q8N122
Y	-2	ASP	-	expression tag	UNP Q8N122
Y	-1	ASP	-	expression tag	UNP Q8N122
Y	0	ASP	-	expression tag	UNP Q8N122
Y	1	LYS	-	expression tag	UNP Q8N122

- Molecule 4 is a protein called Eukaryotic translation initiation factor 4E-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	X	8	Total	C	H	N	O	S	0	0
			126	42	58	9	16	1		
4	Z	8	Total	C	H	N	O	S	0	0
			126	42	58	9	16	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-3	GLY	-	expression tag	UNP Q13541
X	-2	SER	-	expression tag	UNP Q13541
X	-1	GLY	-	expression tag	UNP Q13541
X	0	ARG	-	expression tag	UNP Q13541
Z	-3	GLY	-	expression tag	UNP Q13541
Z	-2	SER	-	expression tag	UNP Q13541
Z	-1	GLY	-	expression tag	UNP Q13541
Z	0	ARG	-	expression tag	UNP Q13541

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

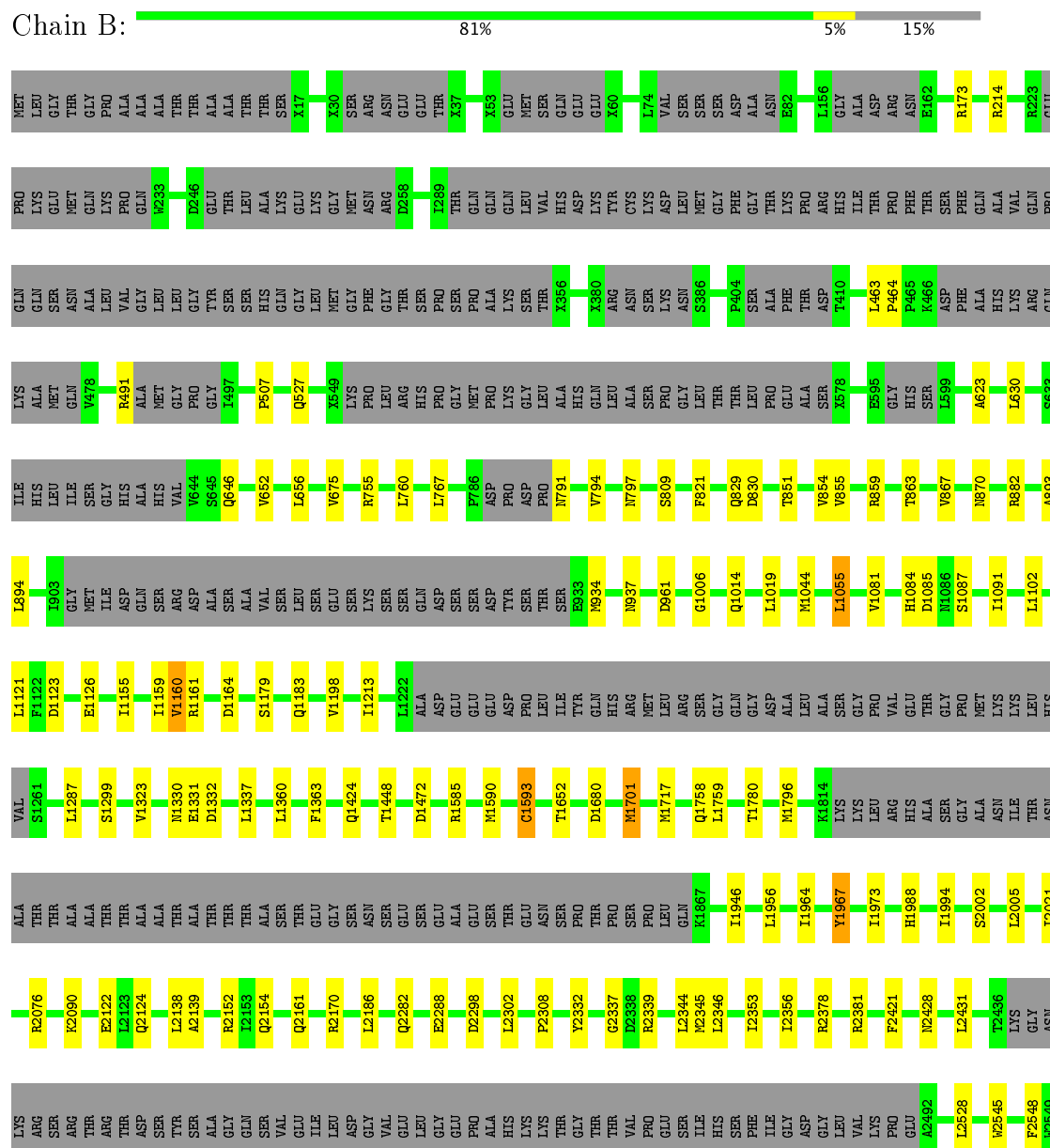
Mol	Chain	Residues	Atoms		AltConf
6	B	2	Total	Mg	0
			2	2	
6	A	2	Total	Mg	0
			2	2	

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.

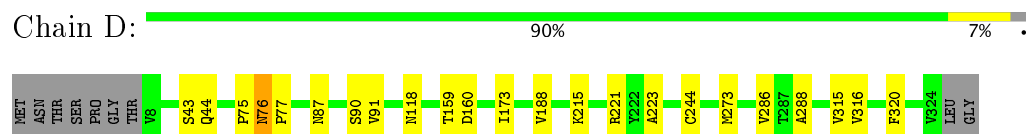
- Chain A: 81% 5% 15%

Position	Amino Acid	Conservation Level
1	F2548	High
2	W2549	High
3	I2021	Low
4	ASU	Low
5	R2076	Low
6	LYS	Low
7	K2090	Low
8	ARG	Low
9	SER	Low
10	E2122	Low
11	L2123	Low
12	THR	Low
13	Q2124	Low
14	THR	Low
15	L2138	Low
16	A2139	Low
17	SER	Low
18	R2152	Low
19	SER	Low
20	I2153	Low
21	GLY	Low
22	Q2154	Low
23	SER	Low
24	Q2161	Low
25	GLN	Low
26	VAL	Low
27	R2170	Low
28	ILE	Low
29	L2186	Low
30	ASP	Low
31	GLY	Low
32	VAL	Low
33	GLU	Low
34	E2288	Low
35	GLY	Low
36	D2298	Low
37	ALA	Low
38	L2302	Low
39	LYS	Low
40	P2308	Low
41	THR	Low
42	GLY	Low
43	Y2332	Low
44	THR	Low
45	G2337	Low
46	VAL	Low
47	R2339	Low
48	GLU	Low
49	L2344	Low
50	ILE	Low
51	L2346	Low
52	SER	Low
53	L2353	Low
54	ILE	Low
55	GLY	Low
56	ASP	Low
57	R2378	Low
58	LEU	Low
59	L2381	Low
60	VAL	Low
61	F2421	Low
62	N2428	Low
63	L2431	Low
64	A2492	Low
65	L2528	Low
66	P2545	Low
67	THR	Low
68	THR	Low
69	THR	Low
70	THR	Low
71	THR	Low
72	THR	Low
73	THR	Low
74	THR	Low
75	THR	Low
76	THR	Low
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93	THR	Low
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97	THR	Low
98	THR	Low
99	THR	Low
100	THR	Low

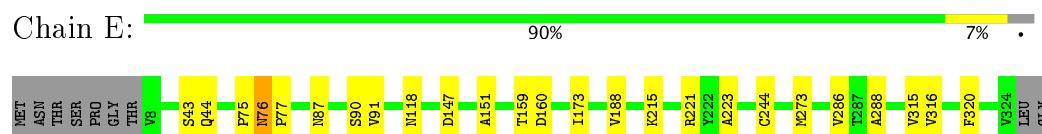
• Molecule 1: Serine/threonine-protein kinase mTOR



• Molecule 2: Target of rapamycin complex subunit LST8

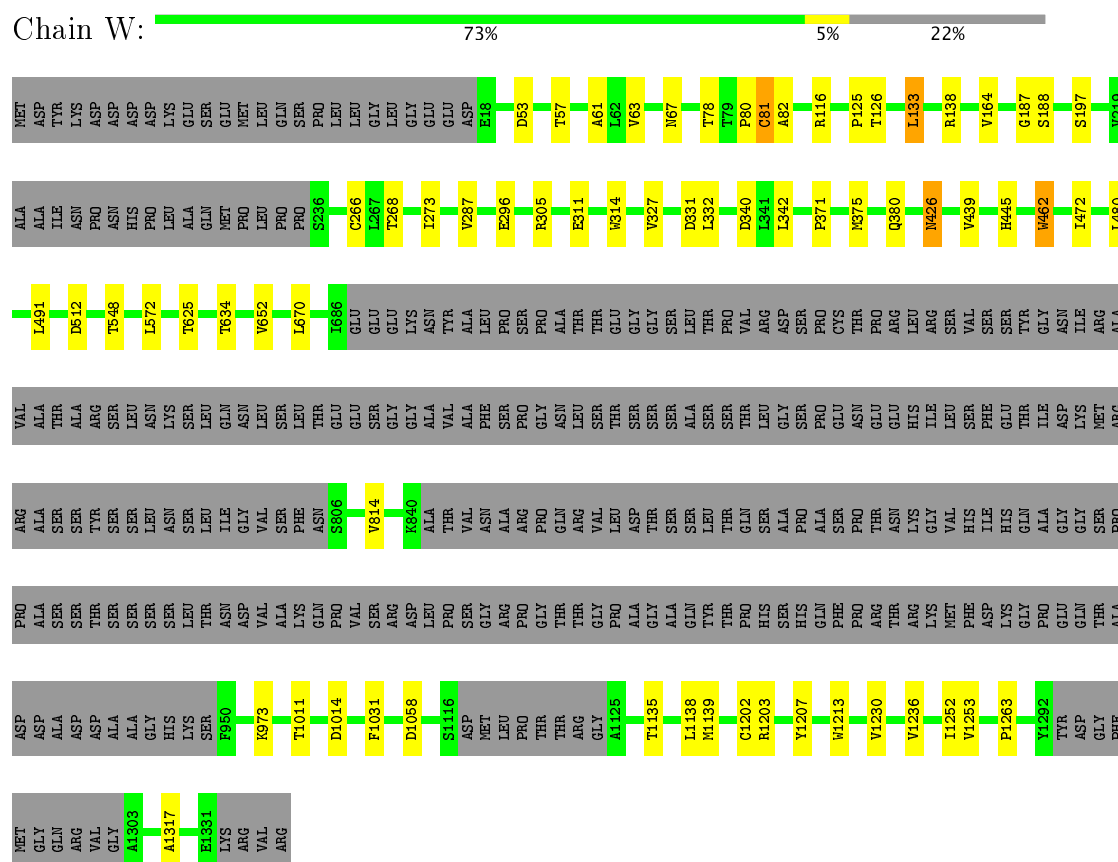


• Molecule 2: Target of rapamycin complex subunit LST8



- Molecule 3: Regulatory-associated protein of mTOR

Chain W:





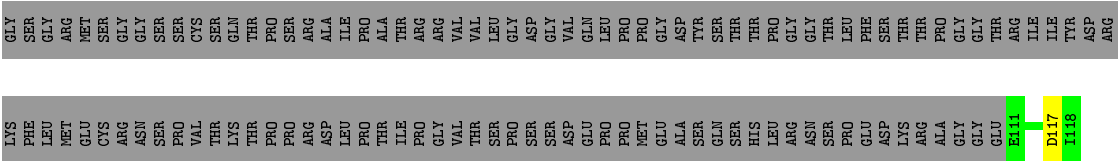
- Molecule 4: Eukaryotic translation initiation factor 4E-binding protein 1

Chain X: 6% 93%



- Molecule 4: Eukaryotic translation initiation factor 4E-binding protein 1

Chain Z: 6% 93%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	580768	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k 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: MG, ATP

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	0.42	0/17398	0.63	1/23547 (0.0%)
1	B	0.42	0/17398	0.62	1/23547 (0.0%)
2	D	0.39	0/2514	0.59	0/3426
2	E	0.39	0/2514	0.60	0/3426
3	W	0.41	0/8585	0.63	0/11680
3	Y	0.41	0/8585	0.63	0/11680
4	X	0.50	0/68	0.58	0/89
4	Z	0.51	0/68	0.58	0/89
All	All	0.41	0/57130	0.62	2/77484 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1055	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	1055	LEU	CA-CB-CG	5.43	127.79	115.30

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	17348	17686	17376	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	17348	17686	17376	34	0
2	D	2456	2353	2341	9	0
2	E	2456	2353	2341	9	0
3	W	8385	8406	8375	18	0
3	Y	8385	8406	8375	15	0
4	X	68	58	57	0	0
4	Z	68	58	57	0	0
5	A	31	12	12	0	0
5	B	31	12	12	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
All	All	56580	57030	56322	113	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 1.

The worst 5 of 113 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:2378:ARG:NH2	1:A:2545:TRP:O	2.18	0.77
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.18	0.77
3:Y:426:ASN:N	3:Y:426:ASN:HD22	1.96	0.63
3:W:426:ASN:HD22	3:W:426:ASN:N	1.96	0.60
1:B:755:ARG:HB2	1:B:797:ASN:HD22	1.68	0.58

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	2088/2549 (82%)	1972 (94%)	107 (5%)	9 (0%)	38 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	2088/2549 (82%)	1973 (94%)	106 (5%)	9 (0%)	38	78
2	D	315/326 (97%)	279 (89%)	32 (10%)	4 (1%)	14	51
2	E	315/326 (97%)	279 (89%)	32 (10%)	4 (1%)	14	51
3	W	1040/1343 (77%)	948 (91%)	85 (8%)	7 (1%)	25	67
3	Y	1040/1343 (77%)	948 (91%)	85 (8%)	7 (1%)	25	67
4	X	6/122 (5%)	6 (100%)	0	0	100	100
4	Z	6/122 (5%)	5 (83%)	1 (17%)	0	100	100
All	All	6898/8680 (80%)	6410 (93%)	448 (6%)	40 (1%)	33	70

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	893	ALA
3	W	53	ASP
1	B	893	ALA
3	Y	53	ASP
1	A	1006	GLY

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	1861/2166 (86%)	1803 (97%)	58 (3%)	45	80
1	B	1861/2166 (86%)	1804 (97%)	57 (3%)	45	80
2	D	269/276 (98%)	263 (98%)	6 (2%)	57	86
2	E	269/276 (98%)	263 (98%)	6 (2%)	57	86
3	W	928/1171 (79%)	895 (96%)	33 (4%)	40	77
3	Y	928/1171 (79%)	895 (96%)	33 (4%)	40	77
4	X	8/104 (8%)	7 (88%)	1 (12%)	5	23
4	Z	8/104 (8%)	7 (88%)	1 (12%)	5	23
All	All	6132/7434 (82%)	5937 (97%)	195 (3%)	48	79

5 of 195 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	W	634	THR
1	B	894	LEU
3	Y	472	ILE
3	W	1011	THR
1	B	214	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
3	W	426	ASN
1	B	646	GLN
3	Y	412	GLN
1	B	193	ASN
1	B	791	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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
5	ATP	A	3000	6	27,33,33	1.03	1 (3%)	25,52,52	1.79	2 (8%)
5	ATP	B	3000	6	27,33,33	1.06	1 (3%)	25,52,52	1.85	4 (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
5	ATP	A	3000	6	-	0/18/38/38	0/3/3/3
5	ATP	B	3000	6	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3000	ATP	C5-C4	3.09	1.47	1.40
5	B	3000	ATP	C5-C4	3.34	1.48	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3000	ATP	N3-C2-N1	-7.08	122.70	128.86
5	A	3000	ATP	N3-C2-N1	-7.03	122.73	128.86
5	B	3000	ATP	C4-C5-N7	-3.23	106.29	109.41
5	A	3000	ATP	C4-C5-N7	-3.04	106.47	109.41
5	B	3000	ATP	C1'-N9-C4	-2.33	122.62	126.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.