



## wwPDB EM Map/Model Validation Report ⓘ

Oct 24, 2016 – 01:56 PM EDT

PDB ID : 3JAZ  
EMDB ID: : EMD-6371  
Title : Atomic model of cytoplasmic polyhedrosis virus with ATP  
Authors : Yu, X.K.; Jiang, J.S.; Sun, J.C.; Zhou, Z.H.  
Deposited on : 2015-07-06  
Resolution : 3.10 Å(reported)

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 : unknown  
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-20027939

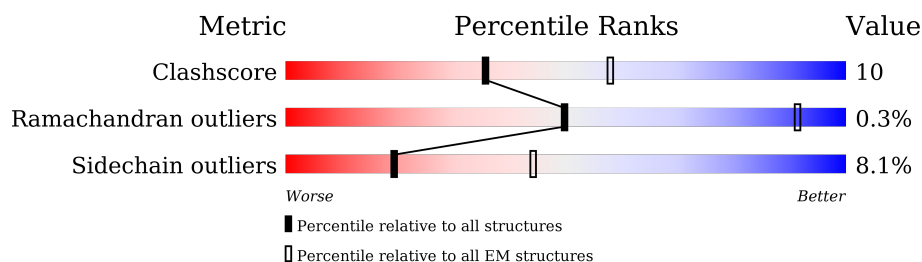
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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	1058	68% 28% .
2	B	1333	63% 24% . 11%
2	C	1333	69% 23% . 6%
3	D	448	45% 17% . 35%
3	E	448	46% 17% . 35%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32244 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 Structural protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1057	Total	C	N	O	S	0	0
			8434	5345	1457	1587	45		

- Molecule 2 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1191	Total	C	N	O	S	0	0
			9397	5937	1634	1789	37		
2	C	1250	Total	C	N	O	S	0	0
			9851	6219	1712	1882	38		

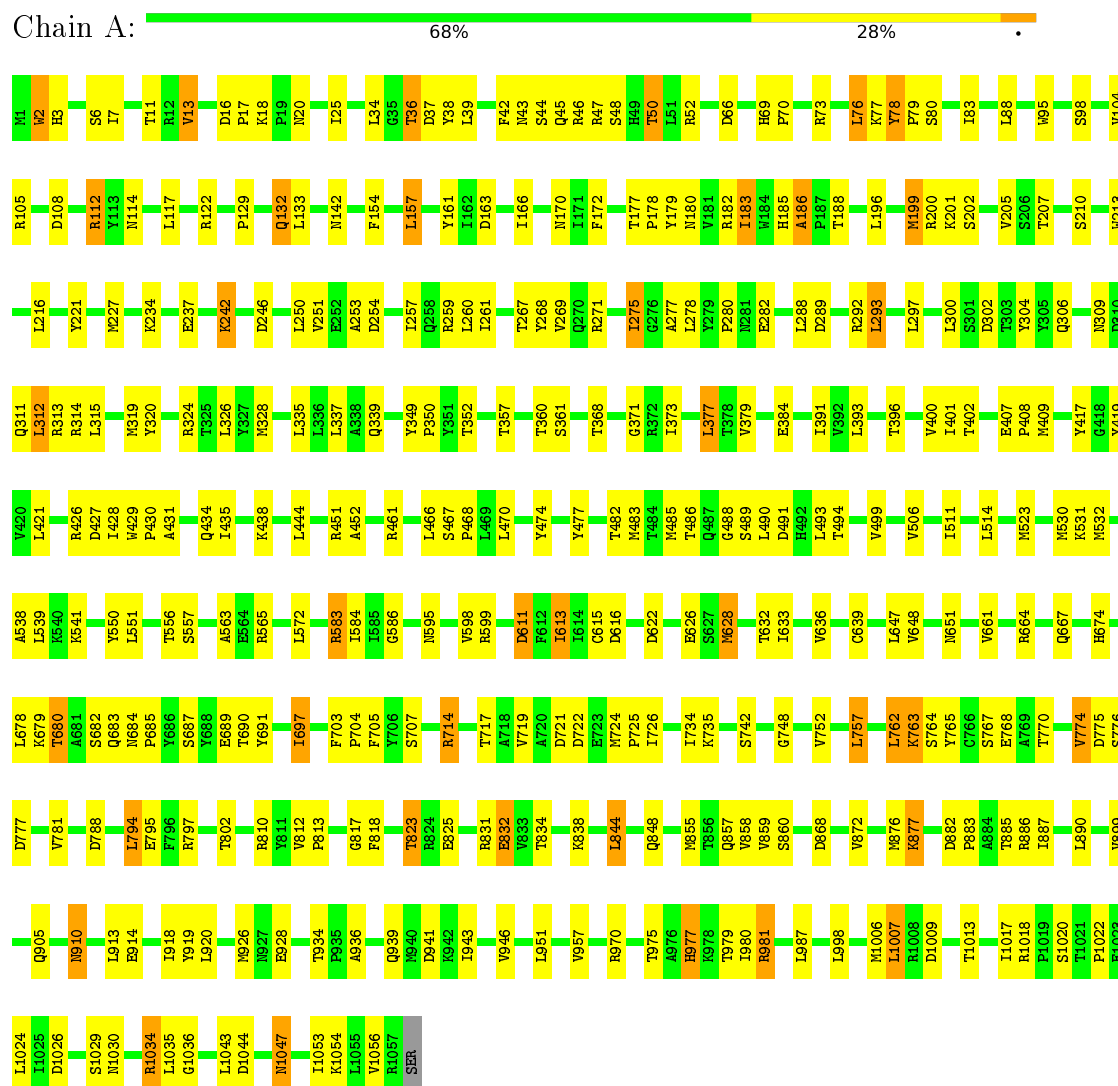
- Molecule 3 is a protein called Viral structural protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		
3	E	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		

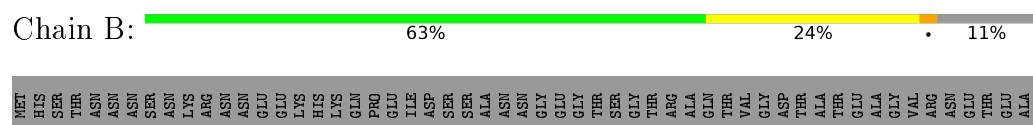
### 3 Residue-property plots

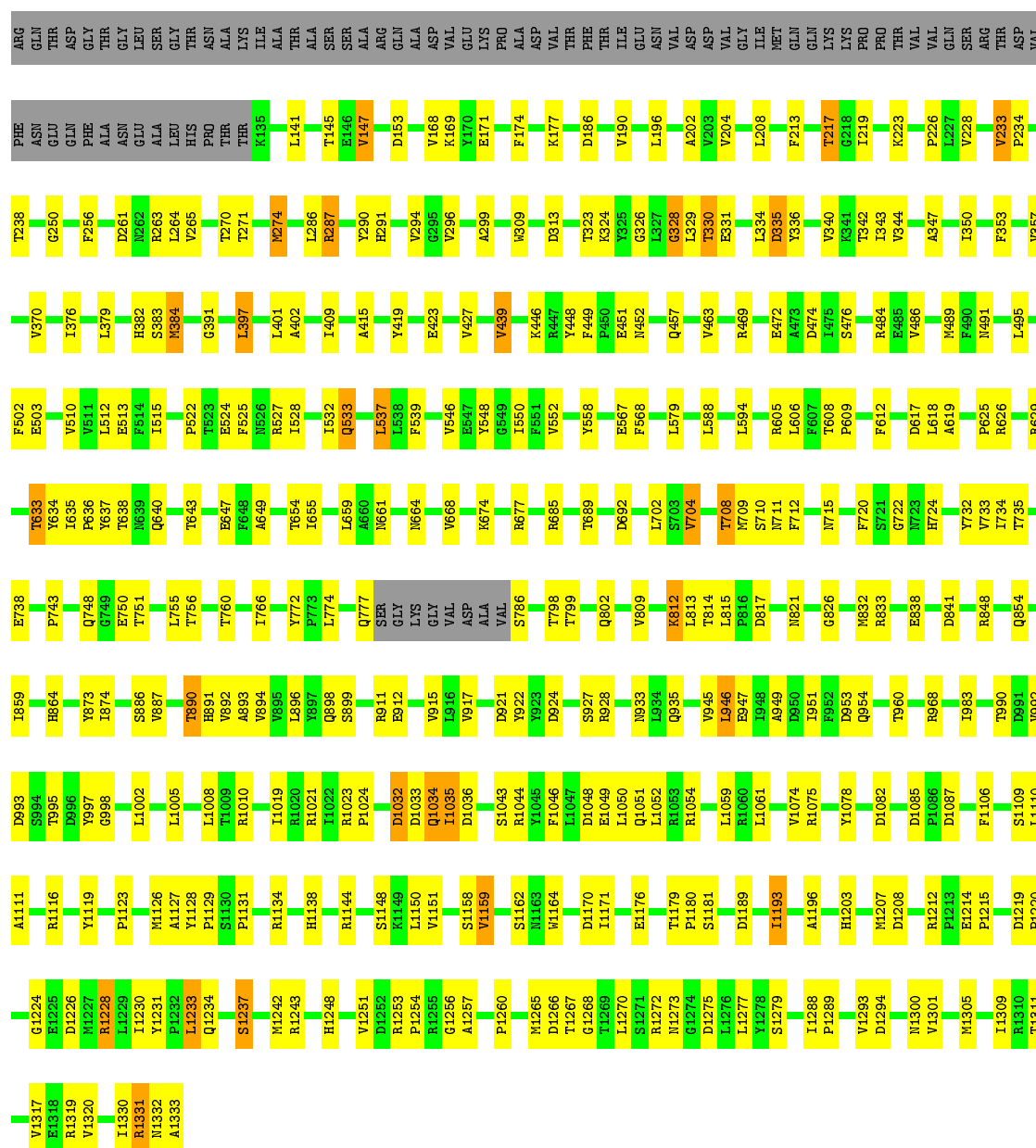
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: Structural protein VP3



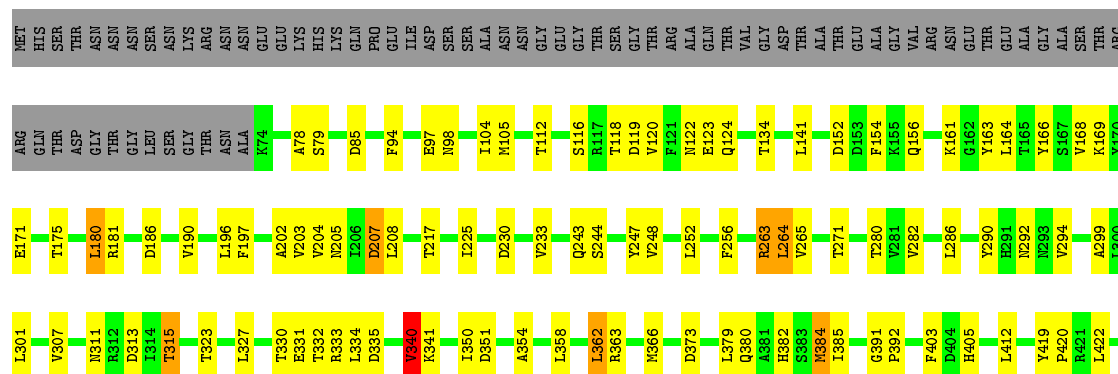
#### • Molecule 2: Capsid protein VP1

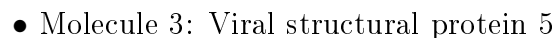




### • Molecule 2: Capsid protein VP1

Chain C:  69% 23% 6%





ILE	THR	ARG	V239	T116	M1
	ASP	HIS	V240		L2
THR	ALA	ASN	V241	I119	Y9
GLN	TRP	ARG	R242	P120	
SER	THR	TYR	V243	F121	
ASP	GLU	MET	V244		F17
SER	GLU	THR		F130	T18
VAL	PHE	GLU	R247		I19
LEU	ALA	ASN		T133	R20
	GLU	PHE	R250	T133	N21
	VAL	LYS	V251	Y134	
	GLU	GLY	L252	A135	A26
PRO	PRO	LEU	L253		
THR	THR	SER	E253	N139	T29
THR	THR	PRO	Y254	D148	Q30
VAL	VAL	ILE	R261		F31
THR	THR	ALA	T262	D151	
GLU	GLU	LEU	A263		L35
ARG	ARG	ALA		L160	
HIS	HIS	GLN	T268	A161	L44
GLN	GLN	LYS	I269		V45
ILE	ILE	LYS		D164	K46
GLY	GLY	HIS	R275		K47
THR	THR	GLU		R167	
ASP	ASP	MET	K281	V171	E53
PRO	PRO	MET	F282		T54
GLU	GLU	LEU	L283		H55
GLN	GLN	HIS	I284	V174	L56
THR	THR	THR	L285	K175	P67
GLN	GLN	HIS	T286	R176	
LEU	LEU	GLU	F287	A177	R60
ILE	ILE	ILE		K178	N61
ILE	ILE	HIS	A292		V62
SER	SER	SER	ALA	L186	P63
GLN	GLN	MET	SER	I187	G64
ASP	ASP	ASP	ALA	S188	
ALA	ALA	ASP	ALA	L189	I68
VAL	VAL	ILE	MET	S190	E69
ILE	ILE	ASP	ILE	R191	
VAL	VAL	GLY	ARG	D192	D70
VAL	VAL	SER	SER	V193	
HIS	HIS	ILE	MET	V194	F77
GLN	GLN	LYS	PRO	N195	G78
ALA	ALA	ASN	ASP	W196	I79
SER	SER	MET	MET		
SER	SER	VAL	HIS	L199	H87
ASP	ASP	GLU	THR		G88
VAL	VAL	ARG	PRO		Y89
ASP	ASP	GLU	ARG	D204	F90
GLU	GLU	GLU	THR		S91
ASN	ASN	VAL	THR	R214	R92
GLU	GLU	ASN	ILE		L93
TYR	TYR	LYS	THR	D222	
GLY	GLY	MET	PRO		N100
ASN	ASN	ASN	ALA	M226	
SER	SER	GLU	ALA		L105
VAL	VAL	ILE	GLY	F229	G106
SER	SER	ILE	GLU	I230	L107
GLU	GLU	ASP	ASN		
GLU	GLU	ALA	ALA		
LEU	LEU	MET	LEU	T233	Y112
THR	THR	ASN	VAL		

- Molecule 3: Viral structural protein 5

M1	L2	Y9	I19	D22	G23	T24	T29	Q30	F31	L35	V45	T48	E53	L56	V62	V66	I68	F77	S80	F90	S91	R92	L93	S94	L98	R104	L105	G109	E115	N118	F121	P124	V127	T133	L134
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GLN SER ASP	TRP	ARG	R250	A135
	THR	TYR	V251	K336
	GLU	MET	L252	L137
	GLU	THR	E253	G138
	PHE	GLU		N139
	ALA	ASN		
SER VAL LEU	GLU	PHE	N258	T142
	VAL	LYS	S259	
	GLU	GLY	D260	R146
	PRO	LEU	R261	L147
	THR	SER	T262	D148
	THR	PRO	A263	
	VAL	ILE	T266	D151
	TYR	ALA		
	GLU	LEU	D272	L158
	ARG	ALA	L273	E159
	HIS	GLN	S274	L160
	GLN	LYS		
	ILE	LYS	E277	D164
	GLY	HIS		
	THR	GLU	K281	R167
	ASP	MET	F282	
	PRO	MET	L283	V171
	GLU	LEU	G284	
	GLN	HIS	L285	R176
	THR	THR	T286	A177
	GLN	HIS	F287	
	LEU	GLU	T288	D180
	ILE	ILE		S181
	SER	HIS	A292	W182
	GLN	SER	ALA	E183
	ASP	MET	SER	G184
	ALA	ASP	ALA	S185
	ALA	ILE	MET	
	VAL	ASP	ILE	L189
	ILE	GLY	ARG	
	VAL	ILE	SER	V194
	HIS	ILE	MET	
	GLN	LYS	PRO	L199
	ALA	ASN	ASP	
	SER	MET	MET	D204
	SER	VAL	HIS	
	ASP	GLU	THR	R221
	VAL	ARG	PRO	
	ASP	GLU	ARG	F224
	GLU	THR	THR	R225
	ASN	VAL	SER	M226
	GLU	ASN	ILE	M227
	TYR	LYS	THR	L228
	GLY	MET	PRO	F229
	ASN	ASN	ALA	
	SER	GLU	GLY	T233
	VAL	ILE	GLU	
	SER	ASP	ASN	V239
	GLU	ALA	LEU	V240
	LEU	MET	LEU	
	THR	ASN	VAL	V244
	ILE	THR	ARG	
	ASP	ALA	HIS	R247
	THR	PRO	ASN	

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	19447	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.29	0/8619	0.52	3/11737 (0.0%)
2	B	0.34	0/9590	0.55	1/13056 (0.0%)
2	C	0.33	0/10052	0.56	0/13687
3	D	0.33	0/2327	0.55	0/3163
3	E	0.31	0/2327	0.53	0/3163
All	All	0.32	0/32915	0.55	4/44806 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ALA	C-N-CD	-8.47	101.96	120.60
1	A	186	ALA	C-N-CA	5.95	146.99	122.00
1	A	78	TYR	C-N-CD	-5.78	107.88	120.60
2	B	274	MET	CG-SD-CE	5.07	108.32	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	328	GLY	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	8434	0	8399	184	0
2	B	9397	0	9315	209	0
2	C	9851	0	9762	195	0
3	D	2281	0	2282	53	0
3	E	2281	0	2282	48	0
All	All	32244	0	32040	660	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 10.

The worst 5 of 660 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:812:LYS:NZ	2:B:812:LYS:HB3	1.55	1.12
2:B:812:LYS:NZ	2:B:812:LYS:CB	2.12	1.11
2:B:812:LYS:HZ3	2:B:812:LYS:HB3	0.95	1.10
1:A:277:ALA:HB3	1:A:319:MET:HE1	1.54	0.89
2:B:812:LYS:CB	2:B:812:LYS:HZ2	1.86	0.88

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	1055/1058 (100%)	1011 (96%)	41 (4%)	3 (0%)	46 80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1187/1333 (89%)	1133 (96%)	49 (4%)	5 (0%)	39	75
2	C	1246/1333 (94%)	1180 (95%)	63 (5%)	3 (0%)	52	84
3	D	290/448 (65%)	283 (98%)	5 (2%)	2 (1%)	26	65
3	E	290/448 (65%)	282 (97%)	7 (2%)	1 (0%)	46	80
All	All	4068/4620 (88%)	3889 (96%)	165 (4%)	14 (0%)	50	80

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
2	B	1035	ILE
2	B	1123	PRO
2	C	1267	THR
3	D	61	ASN

### 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	942/943 (100%)	852 (90%)	90 (10%)	10	37
2	B	1038/1153 (90%)	967 (93%)	71 (7%)	20	55
2	C	1089/1153 (94%)	1011 (93%)	78 (7%)	18	53
3	D	240/379 (63%)	218 (91%)	22 (9%)	11	40
3	E	240/379 (63%)	214 (89%)	26 (11%)	8	30
All	All	3549/4007 (89%)	3262 (92%)	287 (8%)	19	47

5 of 287 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	755	LEU
2	B	1331	ARG
3	E	48	THR
2	B	812	LYS

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Mol	Chain	Res	Type
2	B	1138	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1030	ASN
2	B	491	ASN
2	C	981	HIS
1	A	667	GLN
2	C	430	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.