



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:50 PM BST

PDB ID : 3J7V
EMDB ID: : EMD-6034
Title : Capsid Expansion Mechanism Of Bacteriophage T7 Revealed By Multi-State Atomic Models Derived From Cryo-EM Reconstructions
Authors : Guo, F.; Liu, Z.; Fang, P.A.; Zhang, Q.; Wright, E.T.; Wu, W.; Zhang, C.; Vago, F.; Ren, Y.; Jakata, J.; Chiu, W.; Serwer, P.; Jiang, W.
Deposited on : 2014-08-12
Resolution : 4.50 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

A user guide is available at

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

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) : trunk27241

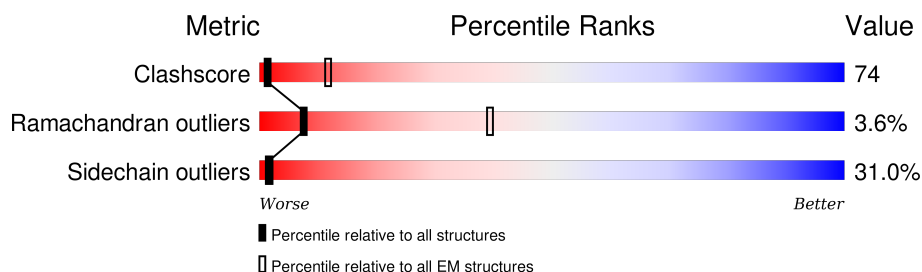
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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	345	 30% 42% 13% • 13%
1	B	345	 29% 40% 19% • 10%
1	C	345	 23% 40% 21% • 14%
1	D	345	 31% 37% 17% • 14%
1	E	345	 28% 39% 16% • 15%
1	F	345	 32% 39% 14% • 13%
1	G	345	 31% 43% 17% • 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15873 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.

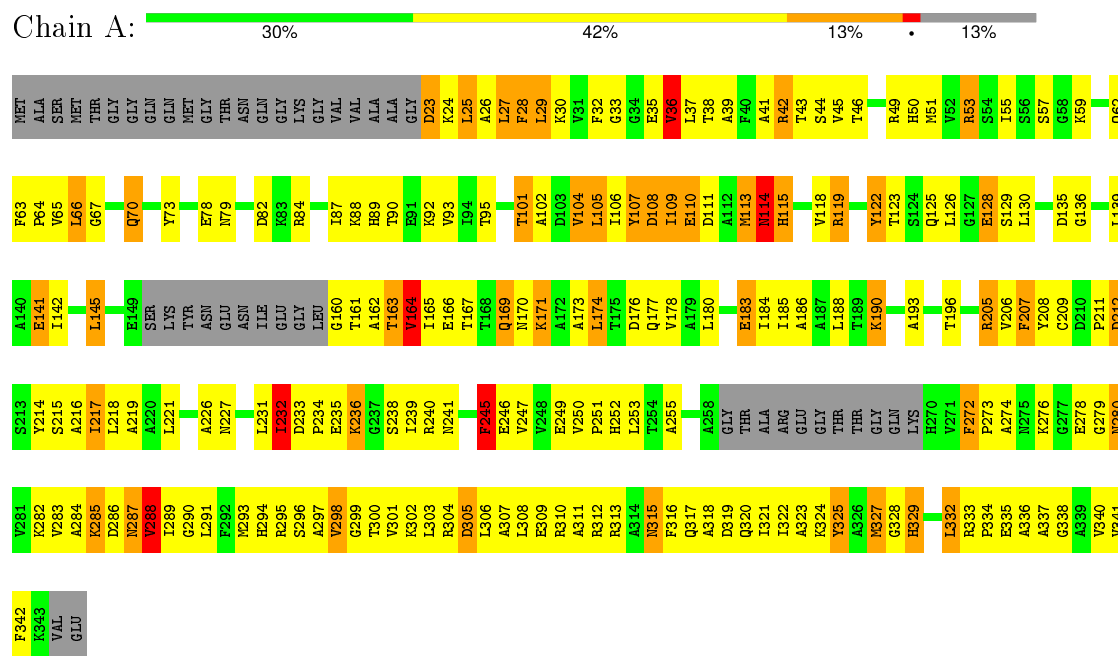
- Molecule 1 is a protein called Major capsid protein 10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	300	Total	C	N	O	S	0	0
			2250	1418	396	427	9		
1	B	309	Total	C	N	O	S	0	0
			2321	1462	406	444	9		
1	C	296	Total	C	N	O	S	0	0
			2234	1411	393	421	9		
1	D	298	Total	C	N	O	S	0	0
			2241	1413	394	425	9		
1	E	293	Total	C	N	O	S	0	0
			2208	1393	387	419	9		
1	F	299	Total	C	N	O	S	0	0
			2245	1415	395	426	9		
1	G	317	Total	C	N	O	S	0	0
			2374	1492	419	454	9		

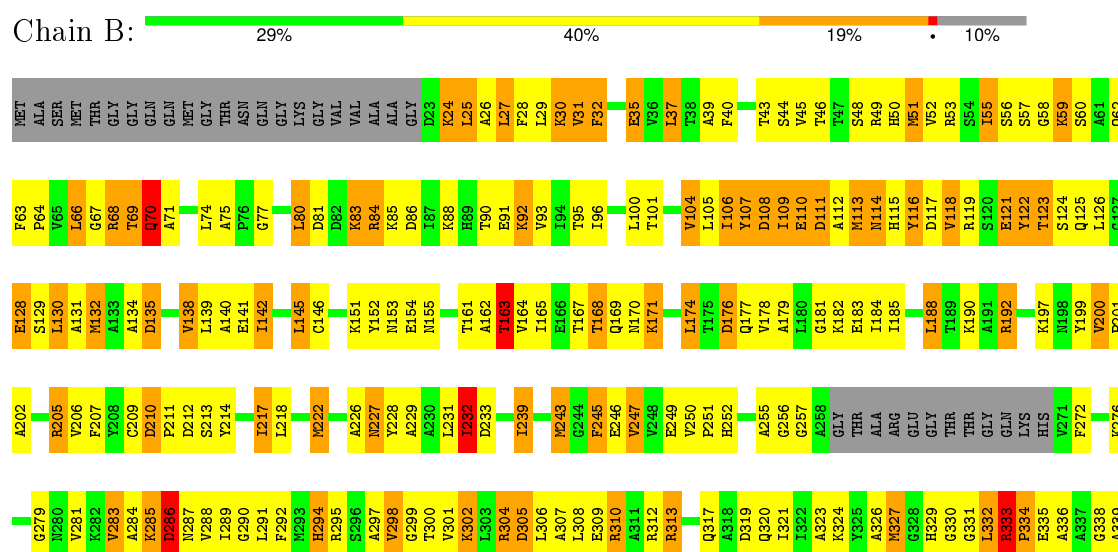
3 Residue-property plots

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: Major capsid protein 10A

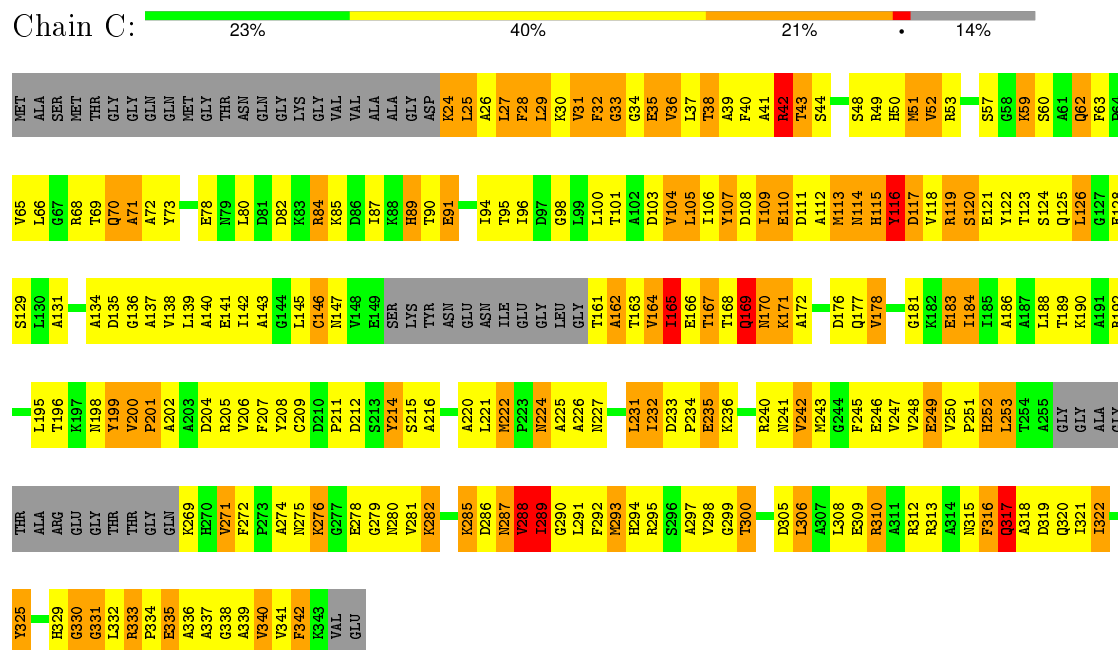


- Molecule 1: Major capsid protein 10A

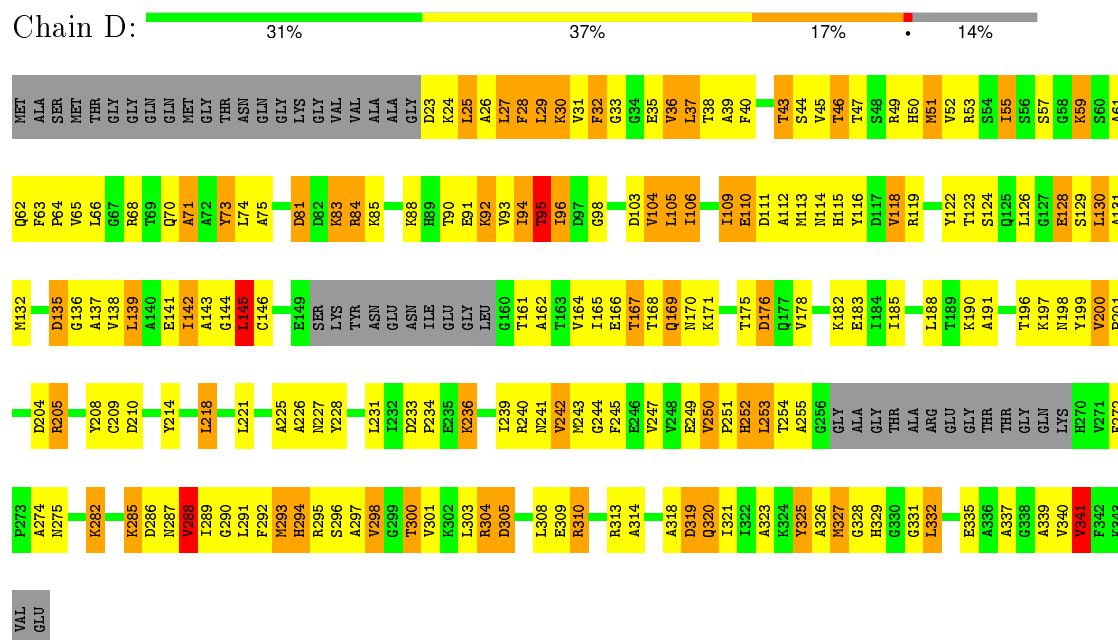


V340
V341
F342
K343
VAL
GLU

• Molecule 1: Major capsid protein 10A

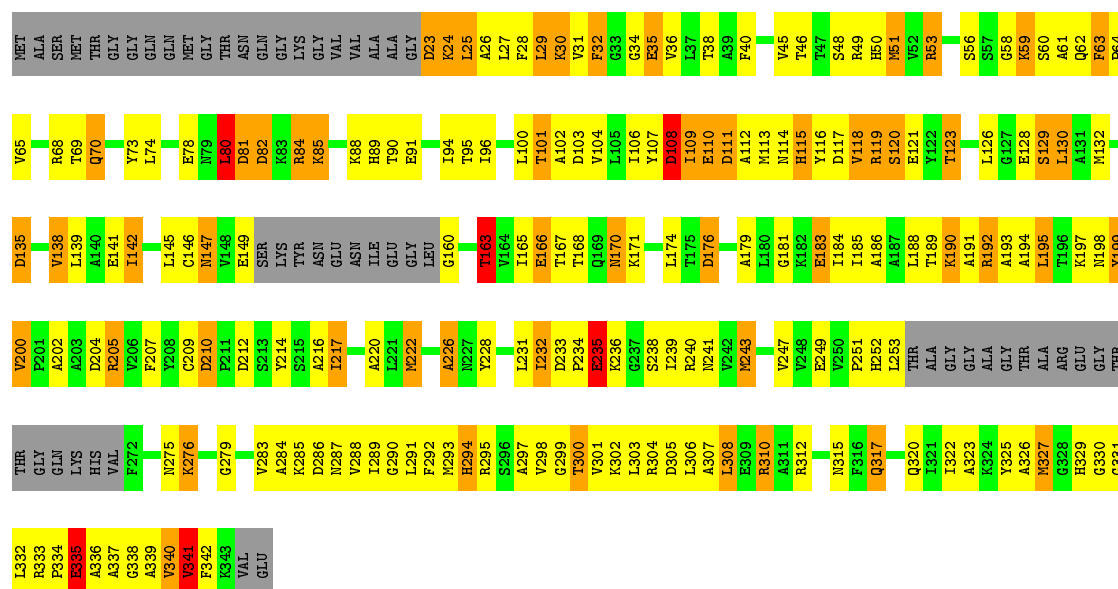


• Molecule 1: Major capsid protein 10A



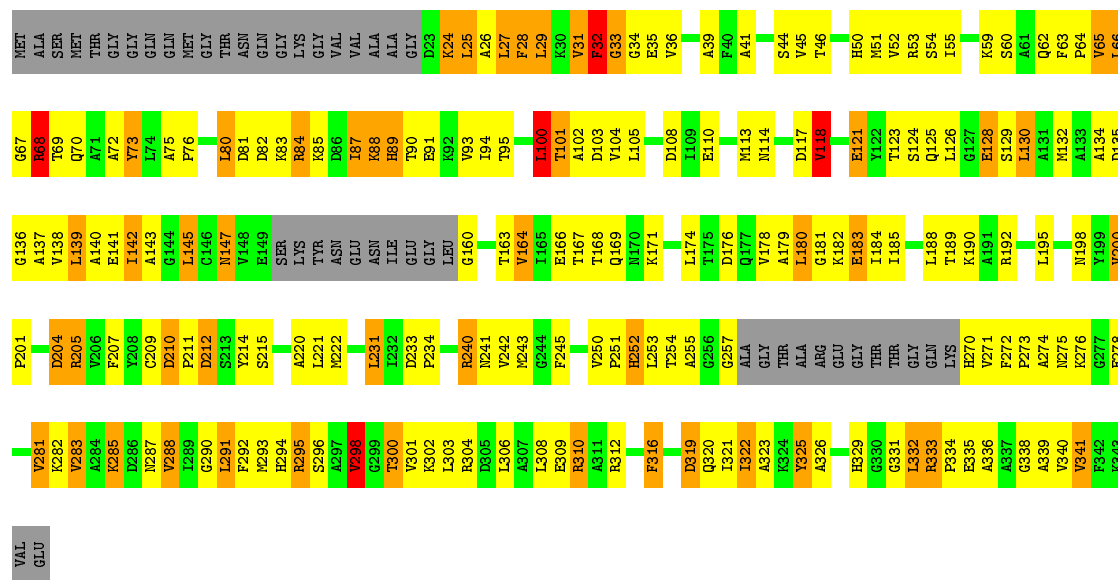
• Molecule 1: Major capsid protein 10A





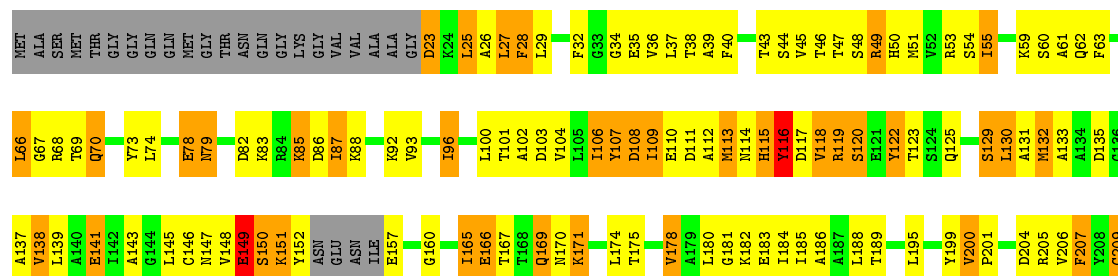
• Molecule 1: Major capsid protein 10A

Chain F: 32% 39% 14% 13%



• Molecule 1: Major capsid protein 10A

Chain G: 31% 43% 17% 8%



D210	E278
P211	
	V281
Y214	
S215	A284
A216	K285
I217	D286
L218	
A219	L291
A220	F292
L221	M293
M222	H294
P223	R295
N224	S296
	A297
L231	V298
I232	G299
D233	T300
P234	V301
E235	K302
K236	L303
G237	R304
S238	D305
I239	L306
K240	A307
N241	L308
V242	E309
M243	R310
G244	A311
F245	R312
E246	R313
V247	A314
Y248	
E249	A318
V250	D319
P251	Q320
H252	I321
L253	I322
T254	A323
A255	K324
G256	Y325
G257	A326
A258	M327
G259	G328
T260	H329
A261	
R262	L332
E263	R333
G264	P334
T265	E335
T266	A336
G267	
Q268	V340
K269	V341
H270	F342
V271	K343
F272	VAL
P273	GLU
A274	
N275	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	27520	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4500	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	0.35	0/2282	0.69	1/3087 (0.0%)
1	B	0.40	0/2354	0.82	3/3185 (0.1%)
1	C	0.45	0/2266	0.82	2/3065 (0.1%)
1	D	0.38	0/2273	0.74	2/3075 (0.1%)
1	E	0.38	0/2239	0.70	2/3028 (0.1%)
1	F	0.37	0/2277	0.70	2/3080 (0.1%)
1	G	0.30	0/2408	0.65	1/3256 (0.0%)
All	All	0.38	0/16099	0.73	13/21776 (0.1%)

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	5
1	B	0	3
1	C	0	6
1	D	0	5
1	E	0	7
1	F	0	3
1	G	0	1
All	All	0	30

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	ARG	C-N-CD	-20.55	75.40	120.60
1	B	70	GLN	CB-CA-C	-7.36	95.67	110.40
1	C	200	VAL	C-N-CD	6.03	141.06	128.40
1	E	80	LEU	CA-CB-CG	5.80	128.65	115.30
1	C	331	GLY	N-CA-C	5.50	126.84	113.10

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ASP	Peptide
1	A	114	ASN	Peptide
1	A	316	PHE	Peptide
1	A	329	HIS	Peptide
1	A	332	LEU	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	2250	0	2279	343	0
1	B	2321	0	2348	415	0
1	C	2234	0	2271	465	0
1	D	2241	0	2272	281	0
1	E	2208	0	2240	372	0
1	F	2245	0	2275	229	0
1	G	2374	0	2403	333	0
All	All	15873	0	16088	2351	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 74.

The worst 5 of 2351 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:B:28:PHE:CE1	1:B:112:ALA:HA	1.24	1.71
1:B:251:PRO:HB2	1:C:199:TYR:CZ	1.09	1.60
1:E:298:VAL:C	1:E:333:ARG:HH12	1.06	1.57
1:E:189:THR:HG22	1:E:243:MET:SD	1.45	1.55
1:E:25:LEU:HD21	1:E:310:ARG:CZ	1.08	1.55

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	294/345 (85%)	224 (76%)	61 (21%)	9 (3%)	5	44
1	B	305/345 (88%)	229 (75%)	67 (22%)	9 (3%)	5	44
1	C	290/345 (84%)	206 (71%)	65 (22%)	19 (7%)	1	25
1	D	292/345 (85%)	213 (73%)	70 (24%)	9 (3%)	5	44
1	E	287/345 (83%)	214 (75%)	65 (23%)	8 (3%)	6	46
1	F	293/345 (85%)	225 (77%)	61 (21%)	7 (2%)	7	49
1	G	313/345 (91%)	240 (77%)	60 (19%)	13 (4%)	3	35
All	All	2074/2415 (86%)	1551 (75%)	449 (22%)	74 (4%)	7	40

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	VAL
1	A	288	VAL
1	B	70	GLN
1	B	114	ASN
1	B	232	ILE

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	230/261 (88%)	168 (73%)	62 (27%)	0	5
1	B	238/261 (91%)	157 (66%)	81 (34%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	230/261 (88%)	151 (66%)	79 (34%)	0	2
1	D	230/261 (88%)	160 (70%)	70 (30%)	0	3
1	E	227/261 (87%)	157 (69%)	70 (31%)	0	3
1	F	230/261 (88%)	167 (73%)	63 (27%)	0	5
1	G	242/261 (93%)	163 (67%)	79 (33%)	0	3
All	All	1627/1827 (89%)	1123 (69%)	504 (31%)	2	3

5 of 504 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	32	PHE
1	D	308	LEU
1	G	171	LYS
1	D	51	MET
1	D	128	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	294	HIS
1	E	177	GLN
1	G	115	HIS
1	E	70	GLN
1	B	287	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 [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.