wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:41 PM BST

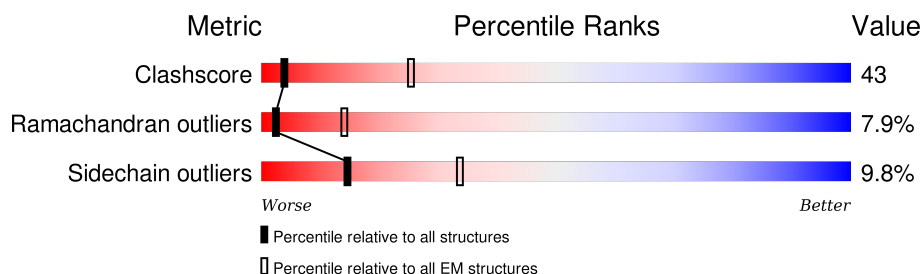|		
PDB ID	:	3IZG
EMDB ID:	:	EMD-1321
Title	:	Bacteriophage T7 prohead shell EM-derived atomic model
Authors	:	Ionel, A.; Velazquez-Muriel, J.A.; Agirrezabala, X.; Luque, D.; Cuervo, A.; Caston, J.R.; Valpuesta, J.M.; Martin-Benito, J.; Carrascosa, J.L.
Deposited on	:	2010-10-27
Resolution	:	10.90 Å(reported)

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 10.90 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	Percentile Ranks	Value
Clashscore		43
Ramachandran outliers		7.9%
Sidechain outliers		9.8%

Worse *Better*

▮ Percentile relative to all structures
◨ Percentile relative to all EM structures

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	345	31% 31% 8% • 29%
1	B	345	30% 34% 6% • 29%
1	C	345	29% 34% 7% • 29%
1	D	345	31% 31% 8% • 29%
1	E	345	33% 32% 5% • 29%
1	F	345	27% 37% 5% • 29%
1	G	345	34% 30% 6% • 29%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12831 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	G	246	Total	C	N	O	S	0	0
			1833	1147	321	357	8		
1	A	246	Total	C	N	O	S	0	0
			1833	1147	321	357	8		
1	B	246	Total	C	N	O	S	0	0
			1833	1147	321	357	8		
1	C	246	Total	C	N	O	S	0	0
			1833	1147	321	357	8		
1	D	246	Total	C	N	O	S	0	0
			1833	1147	321	357	8		
1	E	246	Total	C	N	O	S	0	0
			1833	1147	321	357	8		
1	F	246	Total	C	N	O	S	0	0
			1833	1147	321	357	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: Major capsid protein 10A
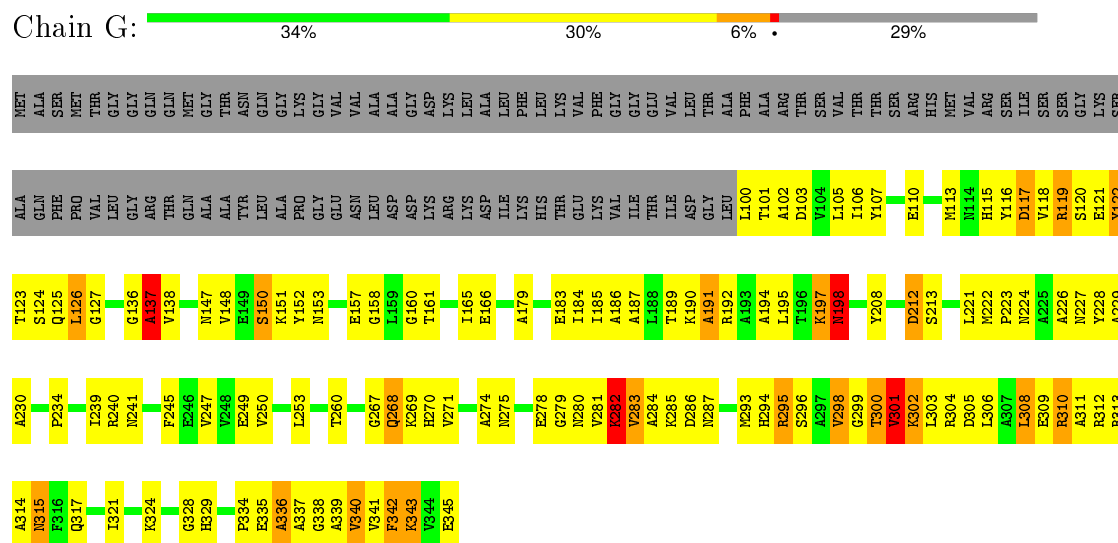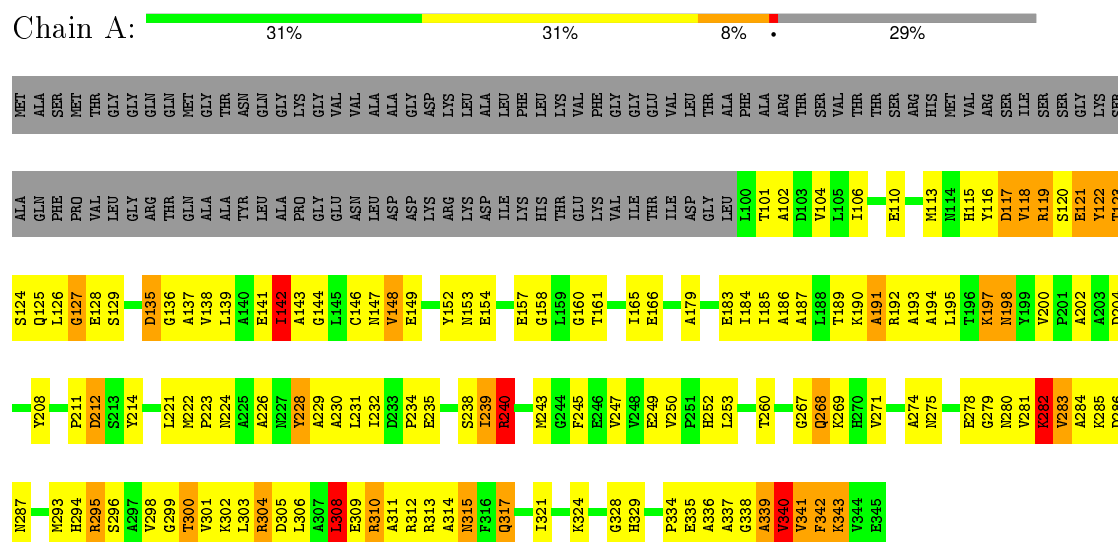
Chain G:

- Molecule 1: Major capsid protein 10A

Chain A:

- Molecule 1: Major capsid protein 10A

Chain B:

• Molecule 1: Major capsid protein 10A

Chain C:　　29%　　34%　　7%　•　29%

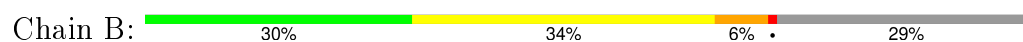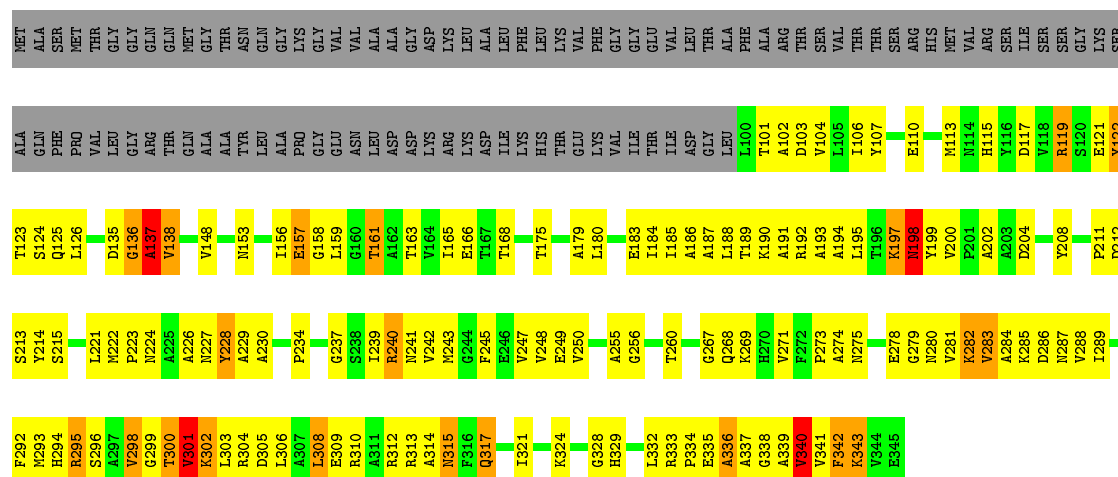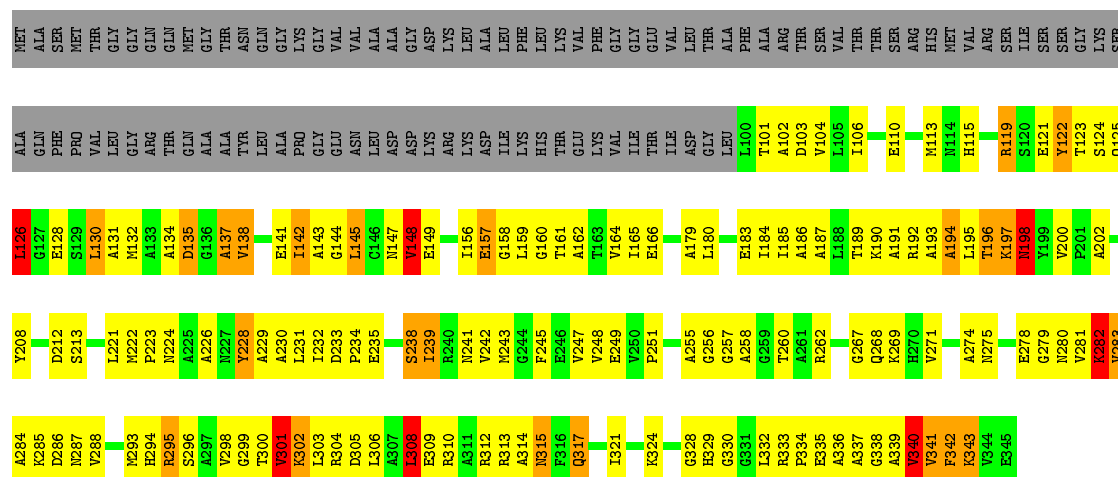• Molecule 1: Major capsid protein 10A

Chain D:　　31%　　31%　　8%　•　29%
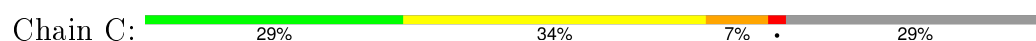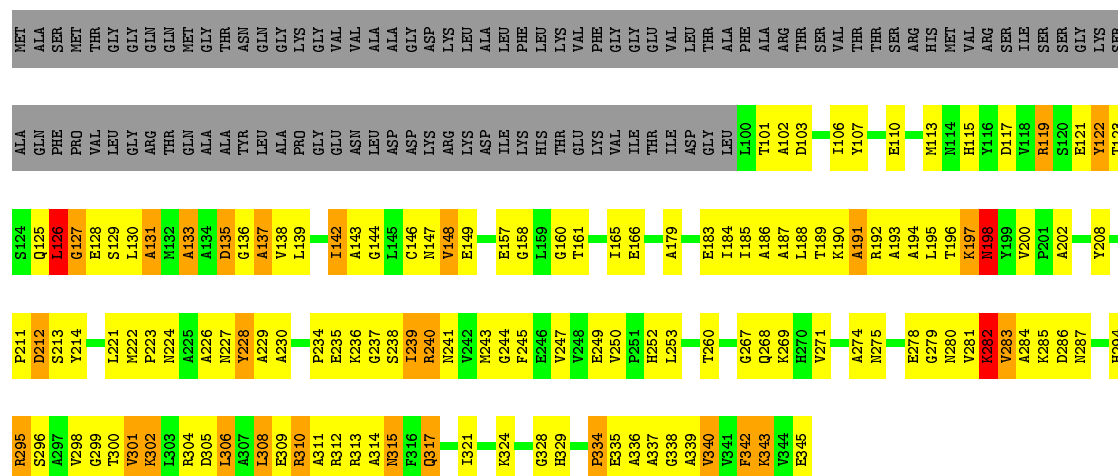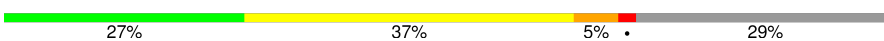
• Molecule 1: Major capsid protein 10A
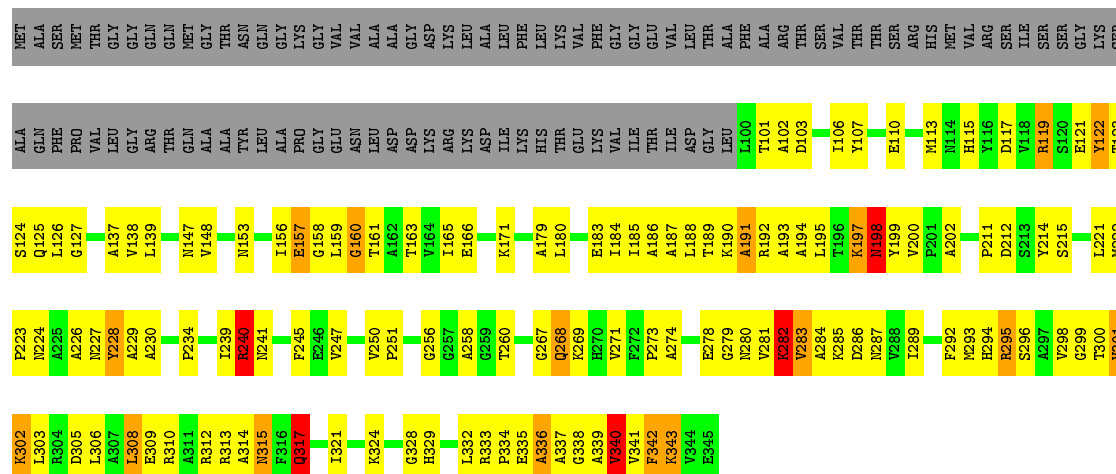
Chain E:

• Molecule 1: Major capsid protein 10A

Chain F:
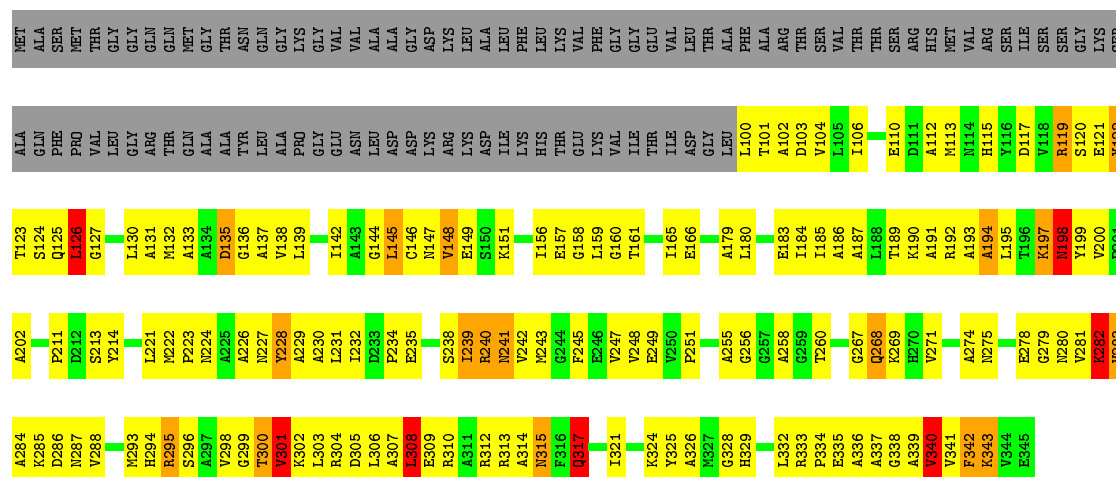
4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Wiener filter, defocus groups	Depositor
Microscope	Tecnai G2	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	10	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.36	0/1859	0.78	4/2518 (0.2%)
1	B	0.36	0/1859	0.97	4/2518 (0.2%)
1	C	0.43	1/1859 (0.1%)	0.99	7/2518 (0.3%)
1	D	0.35	0/1859	1.18	9/2518 (0.4%)
1	E	0.37	0/1859	1.14	6/2518 (0.2%)
1	F	0.36	0/1859	1.05	8/2518 (0.3%)
1	G	0.38	1/1859 (0.1%)	0.98	5/2518 (0.2%)
All	All	0.37	2/13013 (0.0%)	1.02	43/17626 (0.2%)

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	2
1	B	0	3
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	3
1	G	0	4
All	All	0	17

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	301	VAL	C-O	10.12	1.42	1.23
1	G	301	VAL	C-O	5.44	1.33	1.23

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	317	GLN	CG-CD-OE1	-32.03	57.54	121.60
1	C	317	GLN	CG-CD-OE1	-31.99	57.62	121.60
1	G	317	GLN	CG-CD-OE1	-31.93	57.73	121.60
1	F	317	GLN	CG-CD-OE1	-30.51	60.58	121.60
1	D	317	GLN	CG-CD-OE1	-30.32	60.96	121.60

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	THR	Peptide
1	G	136	GLY	Peptide
1	G	137	ALA	Peptide
1	G	300	THR	Peptide
1	G	301	VAL	Mainchain

5.2 Too-close contacts (i)

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	1833	0	1832	185	0
1	B	1833	0	1832	165	0
1	C	1833	0	1832	177	0
1	D	1833	0	1831	145	0
1	E	1833	0	1830	157	0
1	F	1833	0	1832	164	0
1	G	1833	0	1832	184	0
All	All	12831	0	12821	1107	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 43.

The worst 5 of 1107 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:C:137:ALA:HB3	1:C:138:VAL:HB	1.20	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ALA:HB1	1:B:138:VAL:HB	1.13	1.08
1:E:313:ARG:HD2	1:E:334:PRO:HB3	1.30	1.05
1:E:156:ILE:HB	1:F:135:ASP:HB3	1.36	1.04
1:B:313:ARG:HD2	1:B:334:PRO:HB3	1.39	1.04

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	244/345 (71%)	180 (74%)	42 (17%)	22 (9%)	1	17
1	B	244/345 (71%)	183 (75%)	46 (19%)	15 (6%)	2	26
1	C	244/345 (71%)	183 (75%)	38 (16%)	23 (9%)	1	16
1	D	244/345 (71%)	179 (73%)	38 (16%)	27 (11%)	0	11
1	E	244/345 (71%)	186 (76%)	44 (18%)	14 (6%)	2	28
1	F	244/345 (71%)	179 (73%)	47 (19%)	18 (7%)	1	21
1	G	244/345 (71%)	186 (76%)	42 (17%)	16 (7%)	1	24
All	All	1708/2415 (71%)	1276 (75%)	297 (17%)	135 (8%)	2	19

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	240	ARG
1	G	302	LYS
1	A	127	GLY
1	A	239	ILE
1	A	283	VAL

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	184/261 (70%)	160 (87%)	24 (13%)	5	28
1	B	184/261 (70%)	165 (90%)	19 (10%)	9	37
1	C	184/261 (70%)	163 (89%)	21 (11%)	7	33
1	D	184/261 (70%)	169 (92%)	15 (8%)	14	49
1	E	184/261 (70%)	170 (92%)	14 (8%)	16	53
1	F	184/261 (70%)	167 (91%)	17 (9%)	11	43
1	G	184/261 (70%)	168 (91%)	16 (9%)	13	45
All	All	1288/1827 (70%)	1162 (90%)	126 (10%)	14	39

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	340	VAL
1	C	293	MET
1	F	282	LYS
1	B	343	LYS
1	C	148	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	287	ASN
1	D	155	ASN
1	F	315	ASN
1	C	315	ASN
1	C	320	GLN

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 ⓘ

There are no ligands in this entry.

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.