



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:29 pm GMT

PDB ID : 5G4G
EMDB ID: : EMD-3435
Title : Structure of the ATPgS-bound VAT complex
Authors : Huang, R.; Ripstein, Z.A.; Augustyniak, R.; Lazniewski, M.; Ginalski, K.;
Kay, L.E.; Rubinstein, J.L.
Deposited on : 2016-05-12
Resolution : 7.80 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
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) : recalc29047

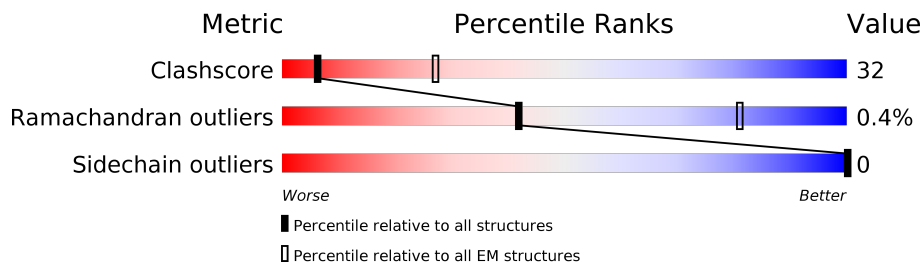
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.80 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	721	63% 37% .
1	B	721	63% 36% .
1	C	721	63% 36% .
1	D	721	63% 37% .
1	E	721	63% 36% .
1	F	721	63% 37% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33462 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.

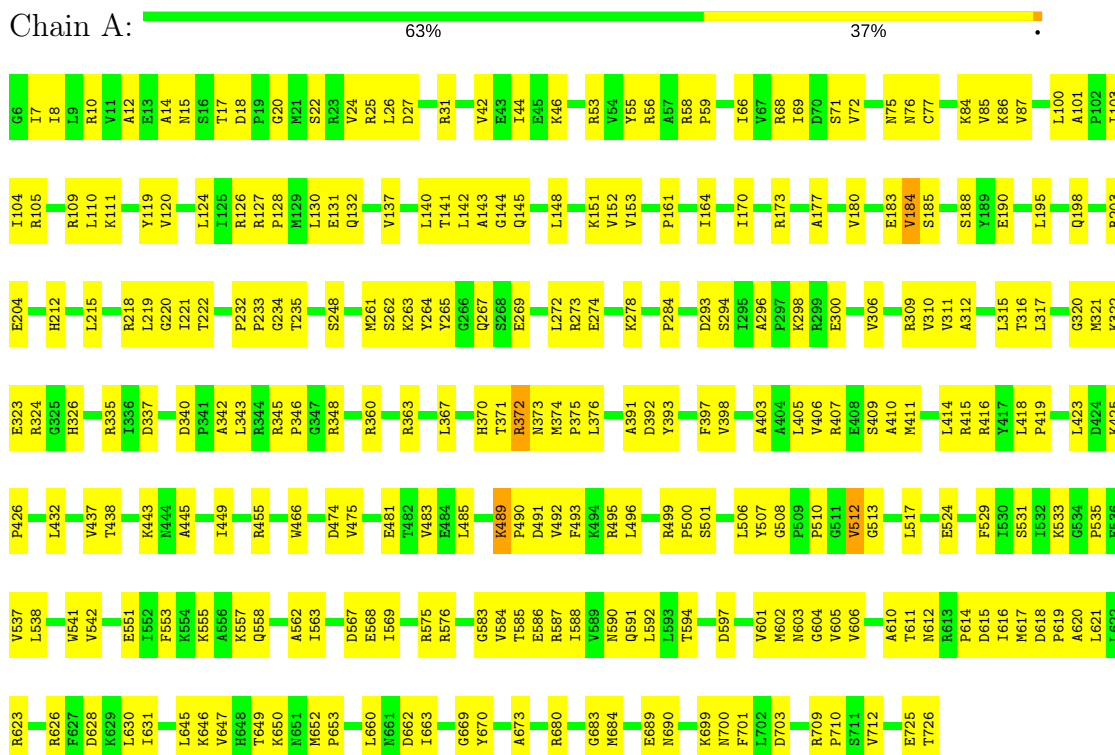
- Molecule 1 is a protein called VCP-LIKE ATPASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	721	Total	C	N	O	S	0	0
			5577	3489	990	1078	20		
1	B	721	Total	C	N	O	S	0	0
			5577	3489	990	1078	20		
1	C	721	Total	C	N	O	S	0	0
			5577	3489	990	1078	20		
1	D	721	Total	C	N	O	S	0	0
			5577	3489	990	1078	20		
1	E	721	Total	C	N	O	S	0	0
			5577	3489	990	1078	20		
1	F	721	Total	C	N	O	S	0	0
			5577	3489	990	1078	20		

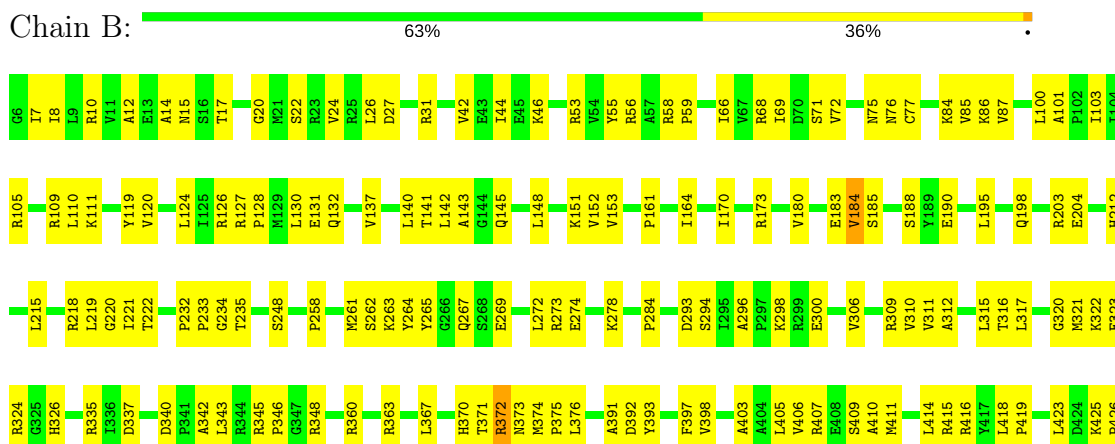
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

• Molecule 1: VCP-LIKE ATPASE



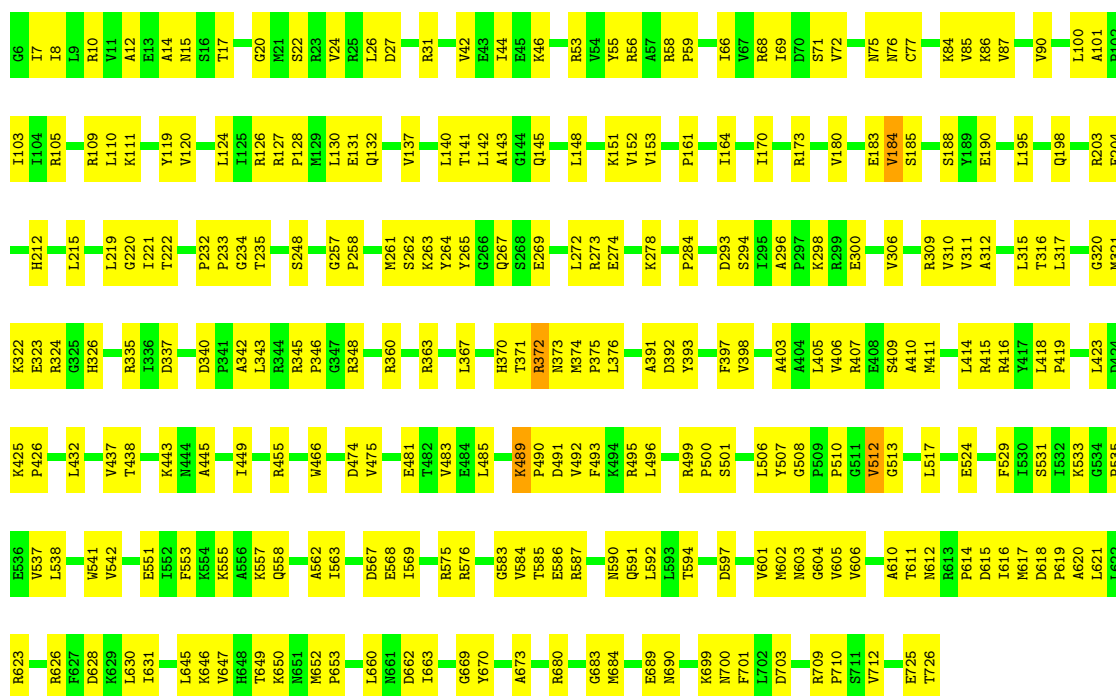
• Molecule 1: VCP-LIKE ATPASE





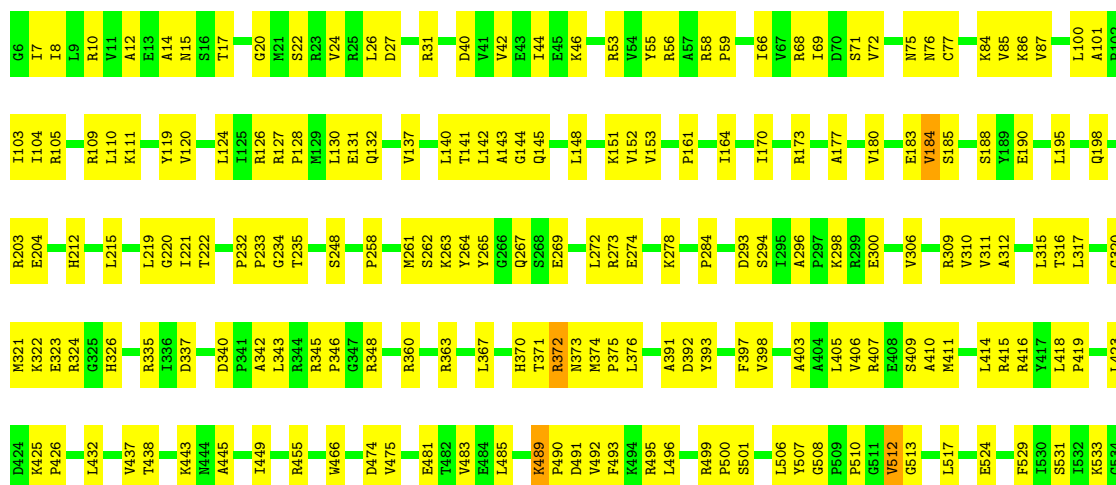
• Molecule 1: VCP-LIKE ATPASE

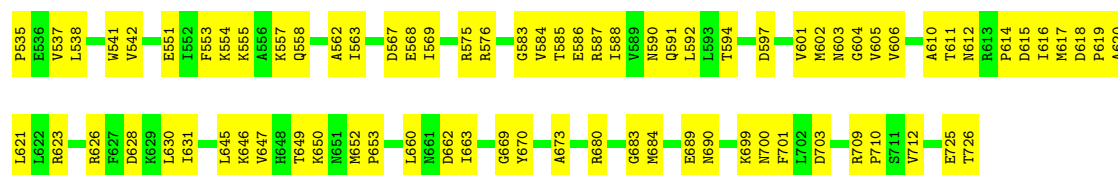
Chain C:  63% 36%



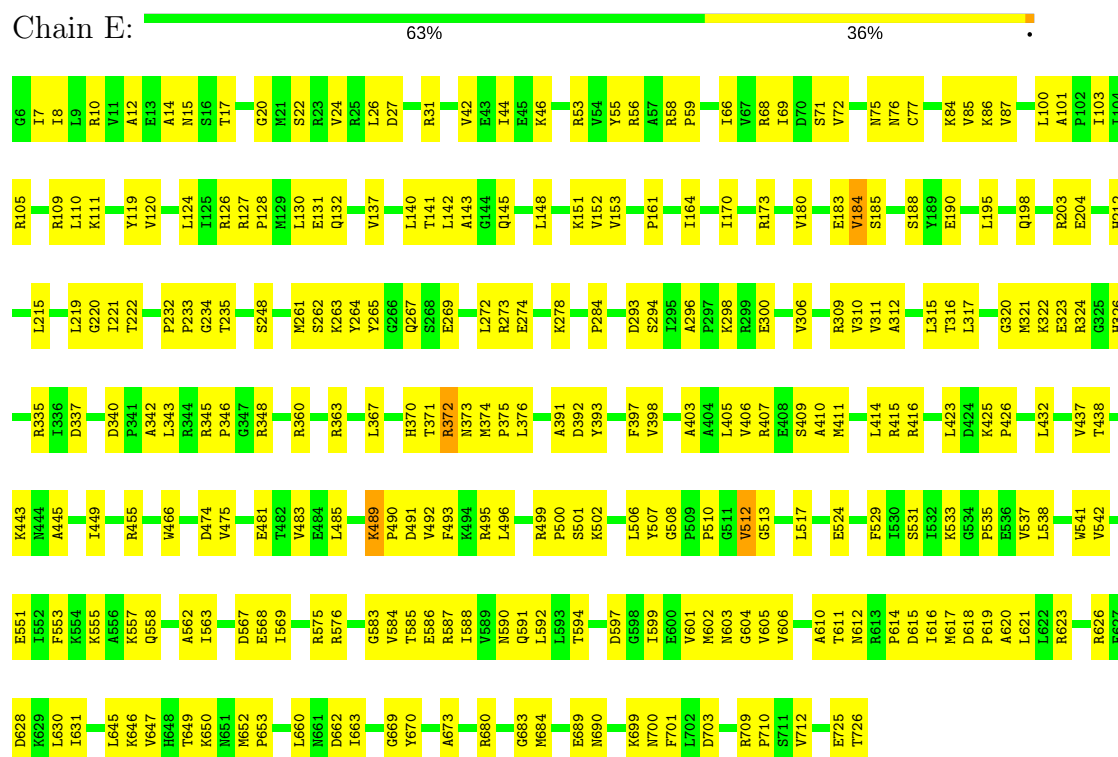
• Molecule 1: VCP-LIKE ATPASE

Chain D:  63% 37%

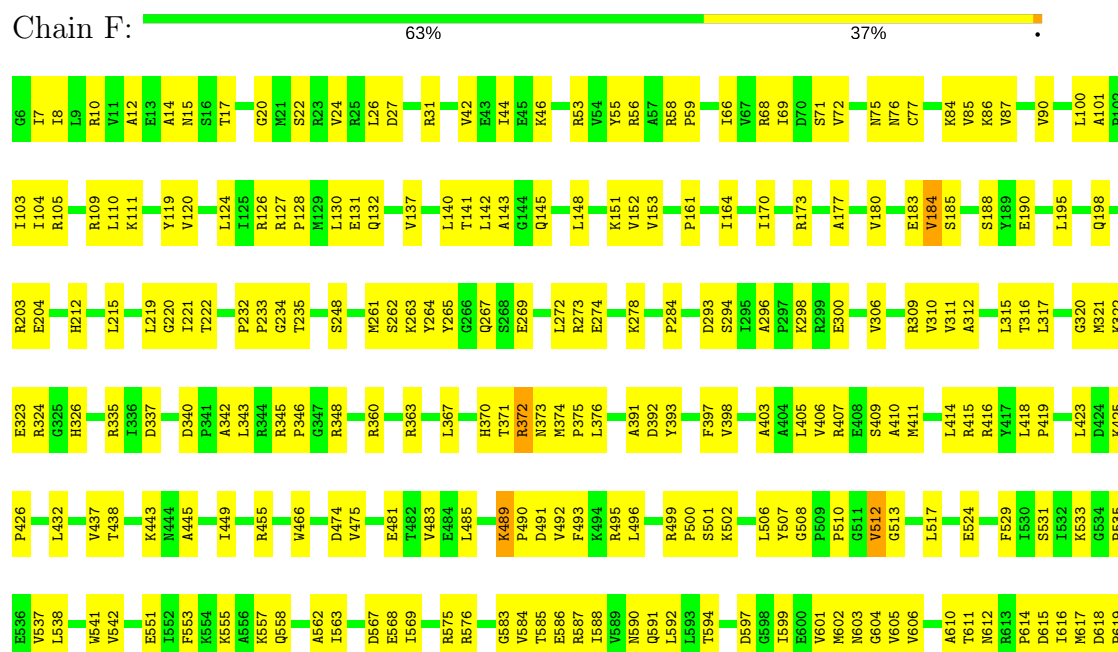




• Molecule 1: VCP-LIKE ATPASE



• Molecule 1: VCP-LIKE ATPASE



A620	L621	L622	R623	R626	R627	D628	R629	L630	I631	L645	R646	V647	H648	T649	R650	H651	H652	P653	L660	H661	D662	I663	G669	Y670	A673	R680	G683	H684	E689	H690	R699	N700	F701	L702	D703	R709	P710	S711	V712	E725	T726
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH MICROGRAPH	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	34483	Depositor
Image detector	GATAN K2 SUMMIT (4K X 4K)	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	0.25	0/5660	0.48	0/7663
1	B	0.25	0/5660	0.48	0/7663
1	C	0.25	0/5660	0.48	0/7663
1	D	0.25	0/5660	0.48	0/7663
1	E	0.25	0/5660	0.48	0/7663
1	F	0.25	0/5660	0.48	0/7663
All	All	0.25	0/33960	0.48	0/45978

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	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
All	All	0	18

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	324	ARG	Peptide
1	A	372	ARG	Peptide
1	A	489	LYS	Peptide
1	B	324	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	B	372	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	5577	0	5500	540	0
1	B	5577	0	5500	535	0
1	C	5577	0	5500	544	0
1	D	5577	0	5500	542	0
1	E	5577	0	5500	531	0
1	F	5577	0	5500	533	0
All	All	33462	0	33000	2129	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 32.

The worst 5 of 2129 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:261:MET:SD	1:E:312:ALA:HA	1.26	1.75
1:A:312:ALA:HA	1:D:261:MET:SD	1.26	1.75
1:E:261:MET:SD	1:F:312:ALA:HA	1.26	1.71
1:B:261:MET:SD	1:C:312:ALA:HA	1.26	1.70
1:D:312:ALA:HA	1:F:261:MET:SD	1.26	1.69

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	719/721 (100%)	646 (90%)	70 (10%)	3 (0%)	38	77
1	B	719/721 (100%)	646 (90%)	70 (10%)	3 (0%)	38	77
1	C	719/721 (100%)	646 (90%)	70 (10%)	3 (0%)	38	77
1	D	719/721 (100%)	646 (90%)	70 (10%)	3 (0%)	38	77
1	E	719/721 (100%)	647 (90%)	69 (10%)	3 (0%)	38	77
1	F	719/721 (100%)	646 (90%)	70 (10%)	3 (0%)	38	77
All	All	4314/4326 (100%)	3877 (90%)	419 (10%)	18 (0%)	42	77

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	615	ASP
1	B	615	ASP
1	C	615	ASP
1	D	615	ASP
1	E	615	ASP

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	558/621 (90%)	558 (100%)	0	100	100
1	B	558/621 (90%)	558 (100%)	0	100	100
1	C	558/621 (90%)	558 (100%)	0	100	100
1	D	558/621 (90%)	558 (100%)	0	100	100
1	E	558/621 (90%)	558 (100%)	0	100	100
1	F	558/621 (90%)	558 (100%)	0	100	100
All	All	3348/3726 (90%)	3348 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	690	ASN
1	D	267	GLN
1	E	690	ASN
1	C	267	GLN
1	C	591	GLN

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.