



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 12, 2018 – 09:25 PM EDT

PDB ID : 5VC7
EMDB ID: : EMD-8658
Title : VCP like ATPase from T. acidophilum (VAT) - conformation 1
Authors : Ripstein, Z.A.; Huang, R.; Augustyniak, R.; Kay, L.E.; Rubinstein, J.L.
Deposited on : 2017-03-31
Resolution : 3.90 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

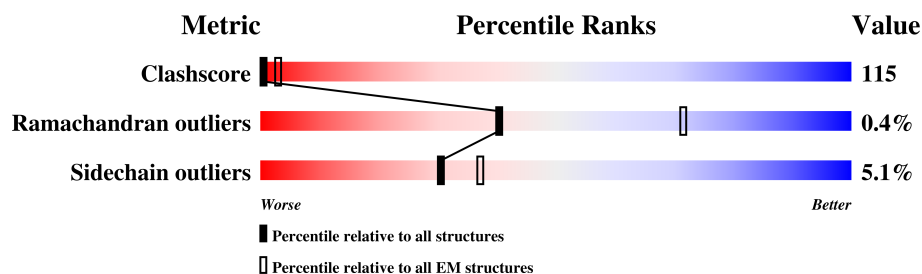
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

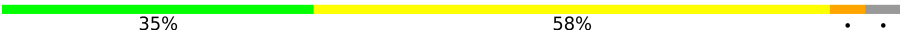
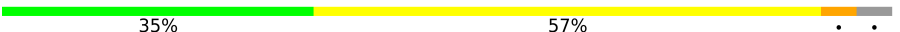



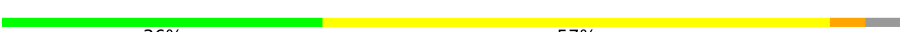
The reported resolution of this entry is 3.90 Å.

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	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	564		35% 58% . .
1	C	564		35% 57% . .
1	D	564		36% 57% . .
1	E	564		36% 57% . .
1	F	564		36% 57% . .
1	G	564		36% 57% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23442 atoms, of which 144 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.

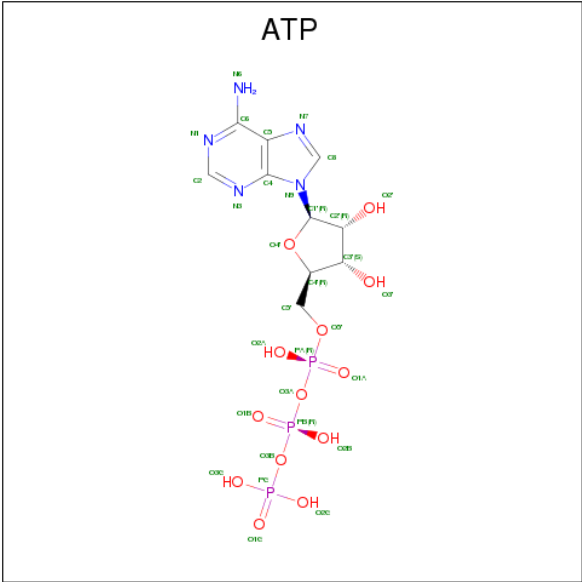
- Molecule 1 is a protein called VCP-like ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	544	Total	C	N	O	S	0	0
			3821	2440	665	706	10		
1	C	544	Total	C	N	O	S	0	0
			3821	2440	665	706	10		
1	D	544	Total	C	N	O	S	0	0
			3821	2440	665	706	10		
1	E	544	Total	C	N	O	S	0	0
			3821	2440	665	706	10		
1	F	544	Total	C	N	O	S	0	0
			3821	2440	665	706	10		
1	G	544	Total	C	N	O	S	0	0
			3821	2440	665	706	10		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	MET	-	expression tag	UNP O05209
C	182	MET	-	expression tag	UNP O05209
D	182	MET	-	expression tag	UNP O05209
E	182	MET	-	expression tag	UNP O05209
F	182	MET	-	expression tag	UNP O05209
G	182	MET	-	expression tag	UNP O05209

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

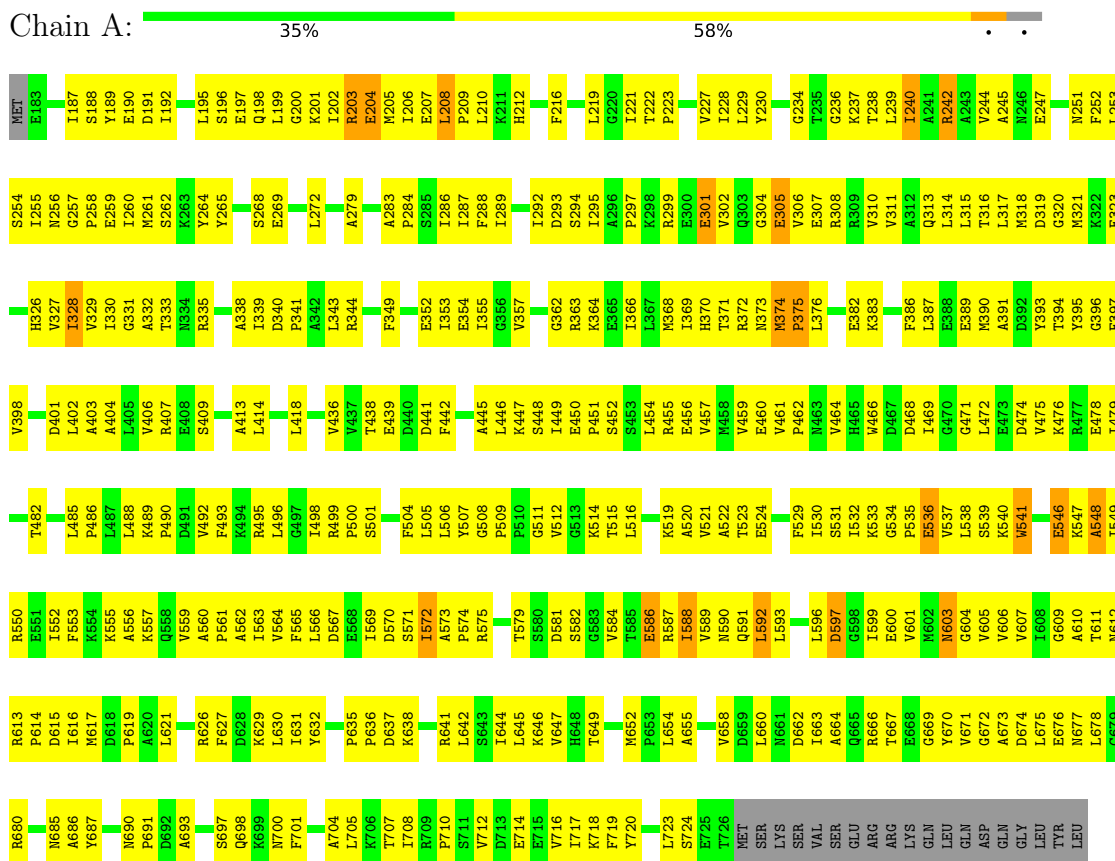


Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	A	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	C	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	C	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	D	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	D	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	E	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	E	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	F	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	F	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	G	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	G	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	

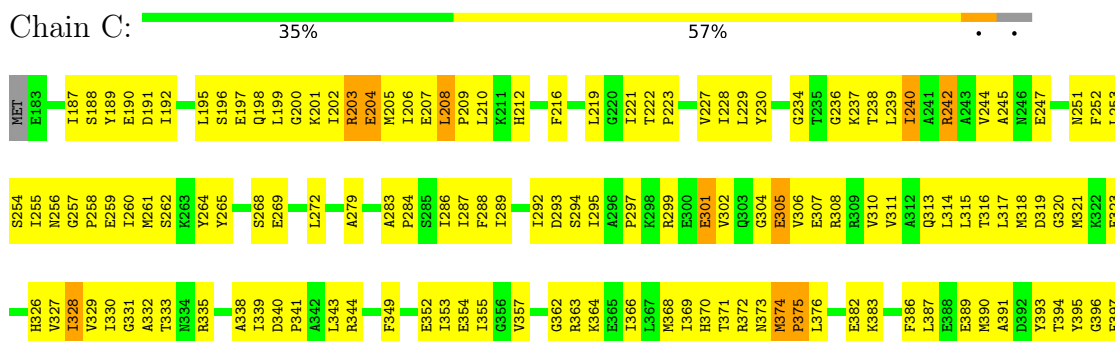
3 Residue-property plots

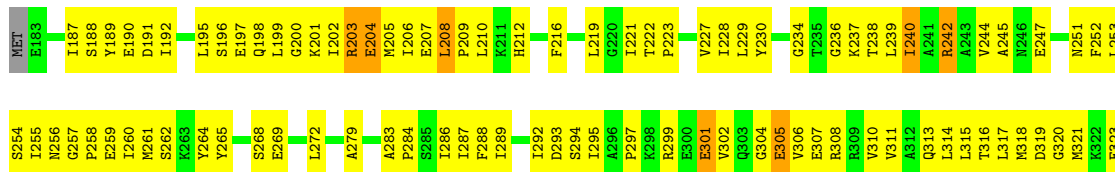
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

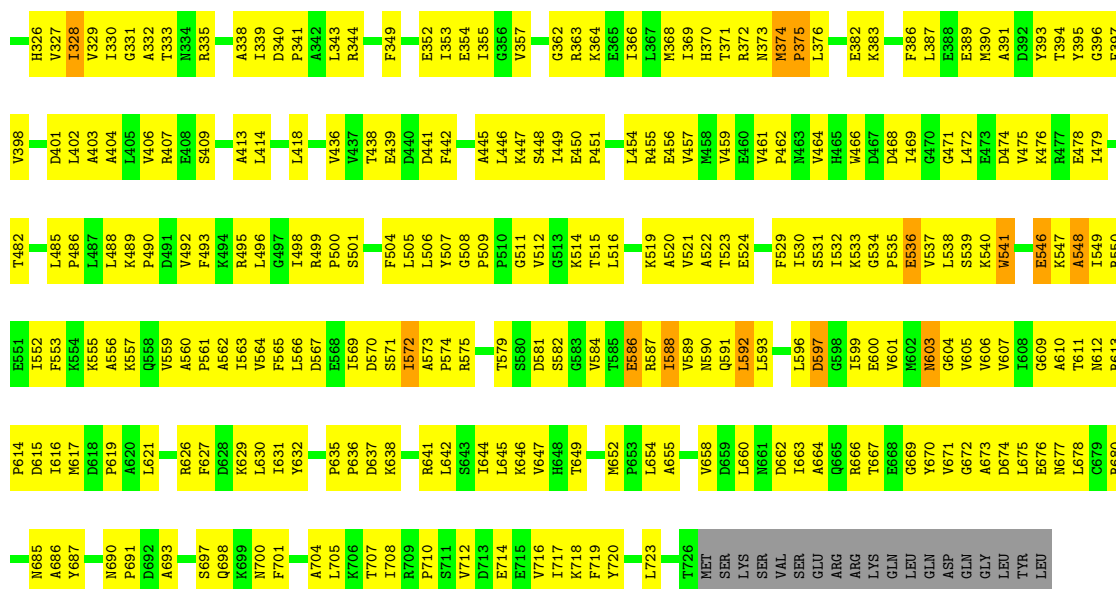
• Molecule 1: VCP-like ATPase



• Molecule 1: VCP-like ATPase

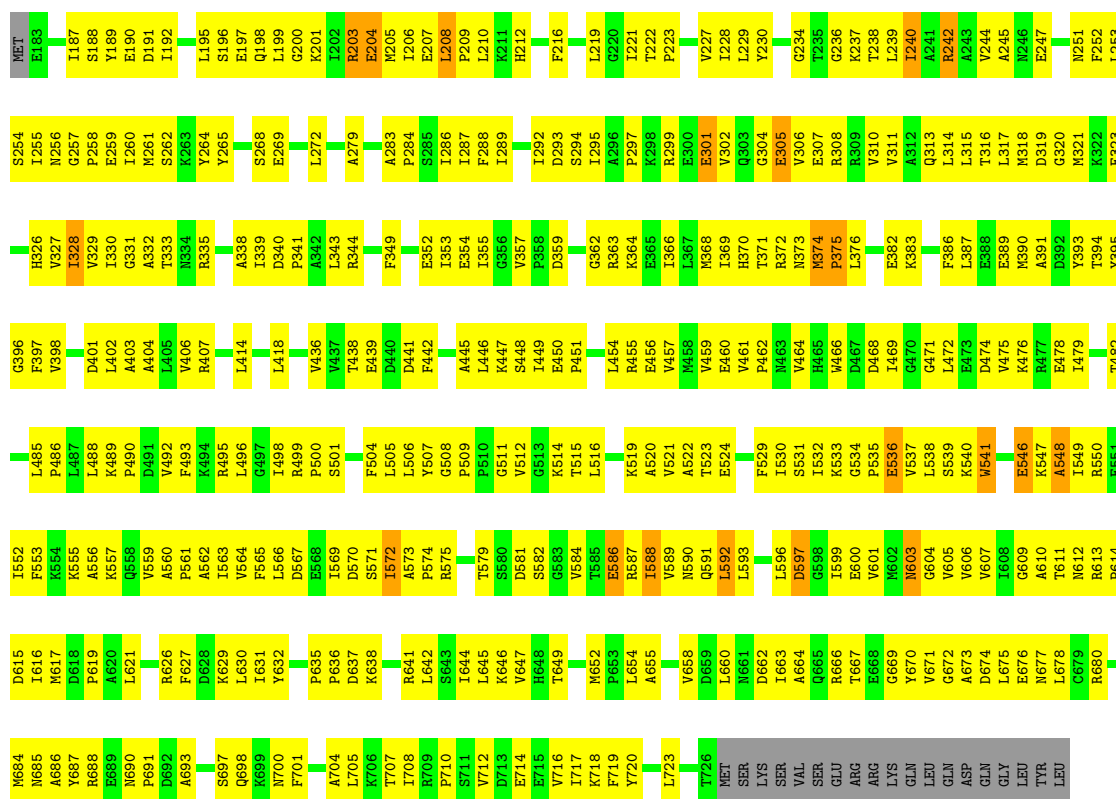






• Molecule 1: VCP-like ATPase

Chain F: 36% 57%



• Molecule 1: VCP-like ATPase

Chain G: 36% 57%



N685	A686	V687	N690	P691	D692	A693	S697	Q698	K699	N700	F701	A704	L705	K706	T707	I708	R709	P710	S711	V712	D713	E714	E715	V716	I717	K718	F719	Y720	L723	I726	SER	LYS	SER	VAL	GLN	ARG	ARG	LYS	GLN	LEU	GLN	ASP	GLN	GLY	LEU	TYR	LEU										
D615	I616	M617	D618	P619	A620	L621	R626	F627	D628	K629	L630	I631	Y632	P635	P636	D637	K638	R641	L642	S643	I644	L645	K646	V647	H648	T649	M652	P653	L654	A655	V658	D659	L660	N661	D662	I663	A664	Q665	R666	T667	E668	G669	Y670	V671	Q672	A673	D674	L675	E676	N677	L678	G679	R680				
I552	F553	K554	K555	A556	K557	Q558	V559	A560	P561	A562	I563	V564	F565	L566	D567	E568	I569	D570	S571	I572	A573	P574	R575	T579	S580	D581	S582	G583	V584	T585	E586	R587	I588	V589	N590	Q591	L592	L593	L596	D597	G598	I599	E600	V601	N602	N603	G604	V605	V606	V607	I608	G609	A610	T611	N612	R613	P614
D401	L402	A403	A404	L405	V406	R407	V492	K493	R494	R495	L496	G497	I498	R499	P500	V436	V437	T438	E439	D440	F441	F442	A445	L446	K447	S448	I449	E450	P451	L454	R455	A456	V457	A458	V459	E460	V461	P462	N463	V464	L465	L466	L467	D468	E469	G470	L471	L472	E473	D474	V475	K476	E477	A478	I479	T482	
H326	V327	I328	V329	I330	G331	A332	T333	N334	R335	A338	I339	D340	P341	A342	L343	R344	F349	A283	E352	I353	E354	I355	G356	V357	G362	R363	K364	E365	I366	L367	M368	I369	H370	T371	R372	N373	M374	P375	L376	E382	K383	F386	L387	E388	E389	A391	D392	Y393	T394	Y395	G396	F397	V398				
S254	I255	N256	G257	P258	E259	T260	K261	S262	K263	Y264	Y265	S268	E269	L272	A279	A283	P284	S285	I286	I287	F288	I289	I292	D293	K294	I295	A296	P297	K298	R299	E300	E301	V302	Q303	G304	P305	V306	F307	R308	V309	V310	V311	A312	Q313	L314	L315	T316	T317	K318	D319	G320	E323					

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	75205	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	25000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.39	0/3888	0.61	2/5320 (0.0%)
1	C	0.39	0/3888	0.61	2/5320 (0.0%)
1	D	0.39	0/3888	0.61	2/5320 (0.0%)
1	E	0.39	0/3888	0.61	2/5320 (0.0%)
1	F	0.39	0/3888	0.61	2/5320 (0.0%)
1	G	0.39	0/3888	0.61	2/5320 (0.0%)
All	All	0.39	0/23328	0.61	12/31920 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	MET	C-N-CD	5.43	139.81	128.40
1	D	374	MET	C-N-CD	5.42	139.78	128.40
1	E	374	MET	C-N-CD	5.41	139.77	128.40
1	G	374	MET	C-N-CD	5.41	139.76	128.40
1	C	374	MET	C-N-CD	5.41	139.75	128.40

There are no chirality outliers.

There are no planarity outliers.

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	3821	0	3595	915	0
1	C	3821	0	3595	907	0
1	D	3821	0	3595	922	0
1	E	3821	0	3595	921	0
1	F	3821	0	3595	918	0
1	G	3821	0	3595	914	0
2	A	62	24	24	5	0
2	C	62	24	24	5	0
2	D	62	24	24	5	0
2	E	62	24	24	5	0
2	F	62	24	24	4	0
2	G	62	24	24	4	0
All	All	23298	144	21714	5185	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 115.

The worst 5 of 5185 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:F:541:TRP:CZ2	1:F:548:ALA:HB1	1.12	1.65
1:G:541:TRP:CZ2	1:G:548:ALA:HB1	1.12	1.64
1:G:237:LYS:CA	1:G:240:ILE:HD11	1.23	1.64
1:F:237:LYS:CA	1:F:240:ILE:HD11	1.23	1.64
1:E:541:TRP:CZ2	1:E:548:ALA:CB	1.78	1.63

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	542/564 (96%)	532 (98%)	8 (2%)	2 (0%)	36 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	542/564 (96%)	532 (98%)	8 (2%)	2 (0%)	36	74
1	D	542/564 (96%)	532 (98%)	8 (2%)	2 (0%)	36	74
1	E	542/564 (96%)	532 (98%)	8 (2%)	2 (0%)	36	74
1	F	542/564 (96%)	532 (98%)	8 (2%)	2 (0%)	36	74
1	G	542/564 (96%)	532 (98%)	8 (2%)	2 (0%)	36	74
All	All	3252/3384 (96%)	3192 (98%)	48 (2%)	12 (0%)	40	74

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	PRO
1	A	548	ALA
1	C	375	PRO
1	C	548	ALA
1	D	375	PRO

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	350/486 (72%)	332 (95%)	18 (5%)	26	60
1	C	350/486 (72%)	332 (95%)	18 (5%)	26	60
1	D	350/486 (72%)	332 (95%)	18 (5%)	26	60
1	E	350/486 (72%)	332 (95%)	18 (5%)	26	60
1	F	350/486 (72%)	332 (95%)	18 (5%)	26	60
1	G	350/486 (72%)	332 (95%)	18 (5%)	26	60
All	All	2100/2916 (72%)	1992 (95%)	108 (5%)	30	60

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	546	GLU

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Mol	Chain	Res	Type
1	E	301	GLU
1	G	352	GLU
1	D	586	GLU
1	E	203	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	326	HIS
1	E	651	ASN
1	G	326	HIS
1	D	700	ASN
1	G	590	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](#)

12 ligands are modelled in this entry.

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
2	ATP	A	801	1	27,33,33	0.96	1 (3%)	27,52,52	2.22	4 (14%)
2	ATP	A	802	-	27,33,33	0.98	1 (3%)	27,52,52	2.05	4 (14%)
2	ATP	C	801	1	27,33,33	0.97	1 (3%)	27,52,52	2.22	4 (14%)
2	ATP	C	802	-	27,33,33	0.97	1 (3%)	27,52,52	2.06	4 (14%)
2	ATP	D	801	1	27,33,33	0.97	1 (3%)	27,52,52	2.22	4 (14%)
2	ATP	D	802	-	27,33,33	0.98	1 (3%)	27,52,52	2.06	4 (14%)
2	ATP	E	801	1	27,33,33	0.97	1 (3%)	27,52,52	2.22	4 (14%)
2	ATP	E	802	-	27,33,33	0.97	1 (3%)	27,52,52	2.06	4 (14%)
2	ATP	F	801	1	27,33,33	0.96	1 (3%)	27,52,52	2.22	4 (14%)
2	ATP	F	802	-	27,33,33	0.97	1 (3%)	27,52,52	2.06	4 (14%)
2	ATP	G	801	1	27,33,33	0.97	1 (3%)	27,52,52	2.22	4 (14%)
2	ATP	G	802	-	27,33,33	0.98	1 (3%)	27,52,52	2.05	4 (14%)

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
2	ATP	A	801	1	-	0/18/38/38	0/3/3/3
2	ATP	A	802	-	-	0/18/38/38	0/3/3/3
2	ATP	C	801	1	-	0/18/38/38	0/3/3/3
2	ATP	C	802	-	-	0/18/38/38	0/3/3/3
2	ATP	D	801	1	-	0/18/38/38	0/3/3/3
2	ATP	D	802	-	-	0/18/38/38	0/3/3/3
2	ATP	E	801	1	-	0/18/38/38	0/3/3/3
2	ATP	E	802	-	-	0/18/38/38	0/3/3/3
2	ATP	F	801	1	-	0/18/38/38	0/3/3/3
2	ATP	F	802	-	-	0/18/38/38	0/3/3/3
2	ATP	G	801	1	-	0/18/38/38	0/3/3/3
2	ATP	G	802	-	-	0/18/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	802	ATP	C5-C4	2.84	1.46	1.40
2	A	802	ATP	C5-C4	2.85	1.46	1.40
2	E	802	ATP	C5-C4	2.85	1.46	1.40
2	F	802	ATP	C5-C4	2.86	1.46	1.40
2	G	802	ATP	C5-C4	2.87	1.47	1.40

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	ATP	N3-C2-N1	-6.99	122.88	128.86
2	A	801	ATP	N3-C2-N1	-6.96	122.90	128.86
2	C	801	ATP	N3-C2-N1	-6.96	122.91	128.86
2	G	801	ATP	N3-C2-N1	-6.95	122.91	128.86
2	F	801	ATP	N3-C2-N1	-6.94	122.93	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ATP	1	0
2	A	802	ATP	4	0
2	C	801	ATP	1	0
2	C	802	ATP	4	0
2	D	801	ATP	1	0
2	D	802	ATP	4	0
2	E	801	ATP	1	0
2	E	802	ATP	4	0
2	F	801	ATP	1	0
2	F	802	ATP	3	0
2	G	801	ATP	1	0
2	G	802	ATP	3	0

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.