



# wwPDB EM Model Validation Summary Report ⓘ

Mar 9, 2020 – 10:27 AM EDT

PDB ID : 6VQ9  
EMDB ID : EMD-21345  
Title : Mammalian V-ATPase from rat brain soluble V1 region rotational state 1 with SidK and ADP (from focused refinement)  
Authors : Abbas, Y.M.; Rubinstein, J.L.  
Deposited on : 2020-02-04  
Resolution : 3.60 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

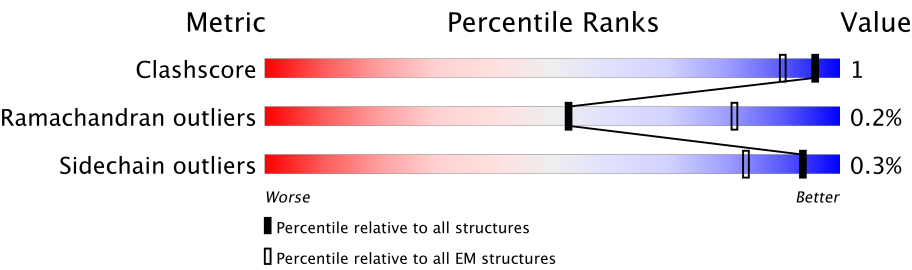
MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.8

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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 and their fit to the map. 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 respectively. 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	617	96% ..
1	B	617	96% ..
1	C	617	94% ..
2	D	511	86% . 10%
2	E	511	88% . 10%
2	F	511	85% . 10%
3	H	247	43% . 56%
4	I	226	67% . 29%
4	J	226	69% . 29%

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Mol	Chain	Length	Quality of chain
4	K	226	 71%29%
5	M	118	 40%60%
5	N	118	 40%60%
5	O	118	 40%60%
6	Q	301	 71%•26%
6	R	301	 68%•30%
6	S	301	 76%•23%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 36114 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 ATPase H<sup>+</sup>-transporting V1 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	600	Total	C	N	O	S	0	0
			4651	2949	786	889	27		
1	B	600	Total	C	N	O	S	0	0
			4651	2949	786	889	27		
1	C	600	Total	C	N	O	S	0	0
			4651	2949	786	889	27		

- Molecule 2 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	459	Total	C	N	O	S	0	0
			3595	2282	613	680	20		
2	E	459	Total	C	N	O	S	0	0
			3595	2282	613	680	20		
2	F	459	Total	C	N	O	S	0	0
			3595	2282	613	680	20		

- Molecule 3 is a protein called ATPase H<sup>+</sup>-transporting V1 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	109	Total	C	N	O	S	0	0
			914	580	171	161	2		

- Molecule 4 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	161	Total	C	N	O	S	0	0
			1288	814	232	235	7		
4	J	161	Total	C	N	O	S	0	0
			1288	814	232	235	7		
4	K	161	Total	C	N	O	S	0	0
			1288	814	232	235	7		

- Molecule 5 is a protein called V-type proton ATPase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	47	Total	C	N	O	S	0	0
			382	228	80	71	3		
5	N	47	Total	C	N	O	S	0	0
			382	228	80	71	3		
5	O	47	Total	C	N	O	S	0	0
			382	228	80	71	3		

- Molecule 6 is a protein called Effector protein SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	224	Total	C	N	O	S	0	0
			1824	1162	306	346	10		
6	R	212	Total	C	N	O	S	0	0
			1722	1096	292	325	9		
6	S	232	Total	C	N	O	S	0	0
			1878	1197	316	354	11		

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	0	GLY	-	expression tag	UNP Q5ZWW6
Q	279	ASP	-	expression tag	UNP Q5ZWW6
Q	280	TYR	-	expression tag	UNP Q5ZWW6
Q	281	LYS	-	expression tag	UNP Q5ZWW6
Q	282	ASP	-	expression tag	UNP Q5ZWW6
Q	283	HIS	-	expression tag	UNP Q5ZWW6
Q	284	ASP	-	expression tag	UNP Q5ZWW6
Q	285	GLY	-	expression tag	UNP Q5ZWW6
Q	286	ASP	-	expression tag	UNP Q5ZWW6
Q	287	TYR	-	expression tag	UNP Q5ZWW6
Q	288	LYS	-	expression tag	UNP Q5ZWW6
Q	289	ASP	-	expression tag	UNP Q5ZWW6
Q	290	HIS	-	expression tag	UNP Q5ZWW6
Q	291	ASP	-	expression tag	UNP Q5ZWW6
Q	292	ILE	-	expression tag	UNP Q5ZWW6
Q	293	ASP	-	expression tag	UNP Q5ZWW6
Q	294	TYR	-	expression tag	UNP Q5ZWW6
Q	295	LYS	-	expression tag	UNP Q5ZWW6
Q	296	ASP	-	expression tag	UNP Q5ZWW6
Q	297	ASP	-	expression tag	UNP Q5ZWW6
Q	298	ASP	-	expression tag	UNP Q5ZWW6

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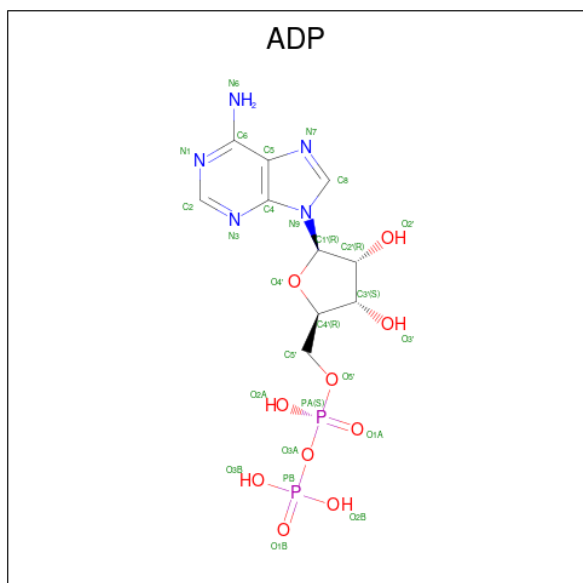
Chain	Residue	Modelled	Actual	Comment	Reference
Q	299	ASP	-	expression tag	UNP Q5ZWW6
Q	300	LYS	-	expression tag	UNP Q5ZWW6
R	0	GLY	-	expression tag	UNP Q5ZWW6
R	279	ASP	-	expression tag	UNP Q5ZWW6
R	280	TYR	-	expression tag	UNP Q5ZWW6
R	281	LYS	-	expression tag	UNP Q5ZWW6
R	282	ASP	-	expression tag	UNP Q5ZWW6
R	283	HIS	-	expression tag	UNP Q5ZWW6
R	284	ASP	-	expression tag	UNP Q5ZWW6
R	285	GLY	-	expression tag	UNP Q5ZWW6
R	286	ASP	-	expression tag	UNP Q5ZWW6
R	287	TYR	-	expression tag	UNP Q5ZWW6
R	288	LYS	-	expression tag	UNP Q5ZWW6
R	289	ASP	-	expression tag	UNP Q5ZWW6
R	290	HIS	-	expression tag	UNP Q5ZWW6
R	291	ASP	-	expression tag	UNP Q5ZWW6
R	292	ILE	-	expression tag	UNP Q5ZWW6
R	293	ASP	-	expression tag	UNP Q5ZWW6
R	294	TYR	-	expression tag	UNP Q5ZWW6
R	295	LYS	-	expression tag	UNP Q5ZWW6
R	296	ASP	-	expression tag	UNP Q5ZWW6
R	297	ASP	-	expression tag	UNP Q5ZWW6
R	298	ASP	-	expression tag	UNP Q5ZWW6
R	299	ASP	-	expression tag	UNP Q5ZWW6
R	300	LYS	-	expression tag	UNP Q5ZWW6
S	0	GLY	-	expression tag	UNP Q5ZWW6
S	279	ASP	-	expression tag	UNP Q5ZWW6
S	280	TYR	-	expression tag	UNP Q5ZWW6
S	281	LYS	-	expression tag	UNP Q5ZWW6
S	282	ASP	-	expression tag	UNP Q5ZWW6
S	283	HIS	-	expression tag	UNP Q5ZWW6
S	284	ASP	-	expression tag	UNP Q5ZWW6
S	285	GLY	-	expression tag	UNP Q5ZWW6
S	286	ASP	-	expression tag	UNP Q5ZWW6
S	287	TYR	-	expression tag	UNP Q5ZWW6
S	288	LYS	-	expression tag	UNP Q5ZWW6
S	289	ASP	-	expression tag	UNP Q5ZWW6
S	290	HIS	-	expression tag	UNP Q5ZWW6
S	291	ASP	-	expression tag	UNP Q5ZWW6
S	292	ILE	-	expression tag	UNP Q5ZWW6
S	293	ASP	-	expression tag	UNP Q5ZWW6
S	294	TYR	-	expression tag	UNP Q5ZWW6

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Chain	Residue	Modelled	Actual	Comment	Reference
S	295	LYS	-	expression tag	UNP Q5ZWW6
S	296	ASP	-	expression tag	UNP Q5ZWW6
S	297	ASP	-	expression tag	UNP Q5ZWW6
S	298	ASP	-	expression tag	UNP Q5ZWW6
S	299	ASP	-	expression tag	UNP Q5ZWW6
S	300	LYS	-	expression tag	UNP Q5ZWW6

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
7	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

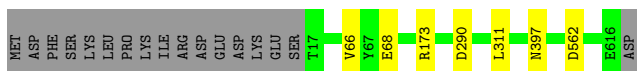
Mol	Chain	Residues	Atoms		AltConf
8	C	1	Total	Mg	0
			1	1	

### 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: ATPase H<sup>+</sup>-transporting V1 subunit A

Chain A:  96%



- Molecule 1: ATPase H<sup>+</sup>-transporting V1 subunit A

Chain B:  96%




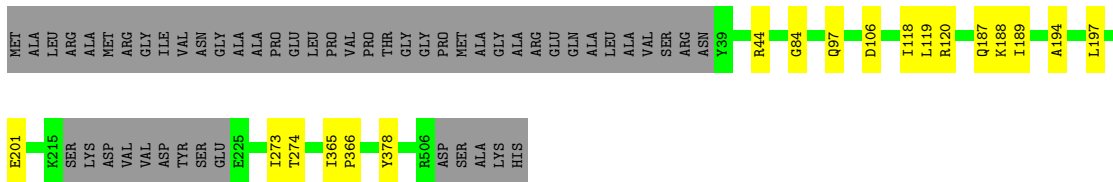
- Molecule 1: ATPase H<sup>+</sup>-transporting V1 subunit A

Chain C:  94%




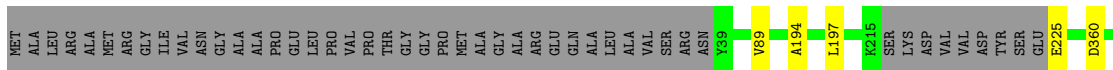
- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain D:  86% 10%

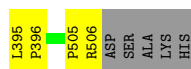


- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain E:  88% 10%

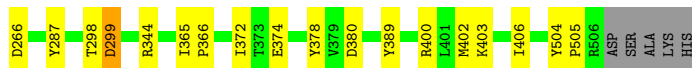
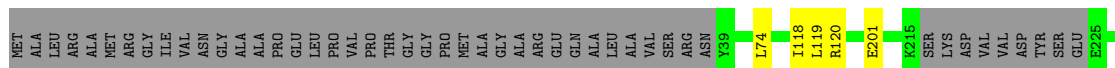






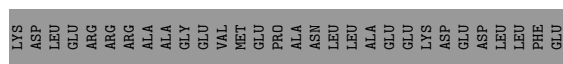
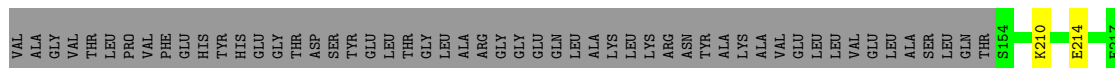
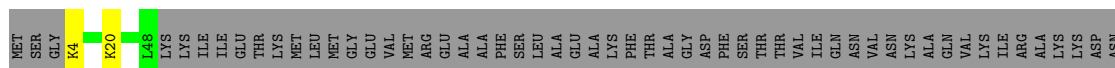
- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain F: 85% 10%



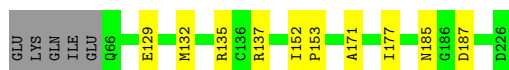
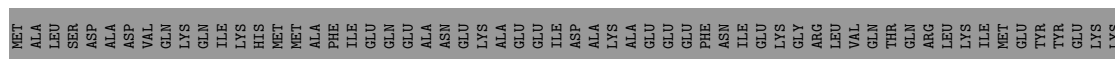
- Molecule 3: ATPase H<sup>+</sup>-transporting V1 subunit D

Chain H: 43% 56%



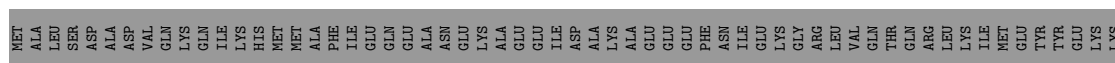
- Molecule 4: V-type proton ATPase subunit E 1

Chain I: 67% 29%



- Molecule 4: V-type proton ATPase subunit E 1

Chain J: 69% 29%



- Molecule 4: V-type proton ATPase subunit E 1

Chain K: 71% 29%

MET	ALA	LEU	SER	ASP	ALA	ASP	VAL	GLN	GLN	LYS	ILE	LYS	HIS	MET	MET	ALA	PHE	ILE	GLU	GLN	GLU	ALA	ASN	GLU	LYS	ALA	GLU	ILE	ASP	ALA	ALA	GLU	GLU	GLU	PHE	ASN	GLU	LYS	GLY	ARG	LEU	VAL	GLN	THR	ARG	LEU	LYS	ILE	MET	GLU	TYR	LYS	GLN	LYS
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GLU	LYS	GLN	ILE	GLU	D66	D228
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● Molecule 5: V-type proton ATPase subunit G



MET	ALA	SER	GLN	SER	GLN	GLY	ILE	GLN	GLN	LEU	LEU	GLN	ALA	GLU	LYS	ARG	ALA	ALA	GLU	LYS	VAL	ALA	ASP	ALA	ARG	LYS	ARG	ALA	ARG	LEU	LYS	GLN	ALA	LYS	GLU	GLU	GLU	ALA	MET	MET	GLU	VAL	GLU	GLN	TYR	ARG	ARG	GLU	ARG	GLN	GLN	PHE	SER	LYS	GLN	GLN
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ALA	ALA	MET	GLY	SER	GLN	GLY	ASN	LEU	S70	I116	THR	VAL
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● Molecule 5: V-type proton ATPase subunit G



MET	ALA	SER	GLN	SER	GLN	GLY	ILE	GLN	GLN	LEU	LEU	GLN	ALA	GLU	LYS	ARG	ALA	ALA	GLU	LYS	VAL	ALA	ASP	ALA	ARG	LYS	ARG	ALA	ARG	LEU	LYS	GLN	ALA	LYS	GLU	GLU	ALA	MET	MET	GLU	VAL	GLU	GLN	TYR	ARG	ARG	GLU	ARG	GLN	GLN	PHE	SER	LYS	GLN	GLN
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ALA	ALA	MET	GLY	SER	GLN	GLY	ASN	LEU	S70	I116	THR	VAL
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● Molecule 5: V-type proton ATPase subunit G



MET	ALA	SER	GLN	SER	GLN	GLY	ILE	GLN	GLN	LEU	LEU	GLN	ALA	GLU	LYS	ARG	ALA	ALA	GLU	LYS	VAL	ALA	ASP	ALA	ARG	LYS	ARG	ALA	ARG	LEU	LYS	GLN	ALA	LYS	GLU	GLU	ALA	GLN	MET	MET	GLU	VAL	GLU	GLN	TYR	ARG	ARG	GLU	ARG	GLN	GLN	PHE	SER	LYS	GLN	GLN
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ALA	ALA	MET	GLY	SER	GLN	GLY	ASN	LEU	S70	I116	THR	VAL
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● Molecule 6: Effector protein SidK



GLY	MET	PHE	ILE	LYS	VAL	GLY	ILE	LYS	MET	GLY	G12	Y28	Y60	R61	S99	P100	K114	K123	E170	D171	P235	LYS	LEU	SER	SER	LYS	VAL	LEU	GLN	ASP	LYS	LEU	SER	SER	GLN	ASP	VAL	LEU	THR	LYS	THR	LEU	LEU	ASP	SER	ILE	ASP	ARG
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ILE	VAL	LYS	GLU	ASN	LYS	LEU	ALA	LYS	SER	GLY	ASP	TYR	LYS	ASP	HIS	GLY	ASP	TYR	LYS	ASP	ILE	ASP	LYS	ASP	LEU	ASP	ASP	ASP	LYS
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● Molecule 6: Effector protein SidK



GLY	MET	PHE	LYS	VAL	G7	I8	K9	Y28	Y126	K148	E195	E210	P218	ALA	GLU	GLN	ILE	ILE	LEU	VAL	LYS	THR	MET	ILE	ASP	TYR	ALA	MET	PRO	LYS	LEU	SER	SER	LYS	VAL	GLN	ASP	LYS	LEU	THR	ALA	SER	SER	SER	ASP	VAL	LEU	THR
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LYS THR LEU ASP SER ILE ASP ARG ILE VAL LYS GLU ASN  
THR LEU ASP SER ILE ASP ARG ILE VAL LYS GLU ASN

● Molecule 6: Effector protein SidK



GLY MET SER PHE I4 G12 Y28 D138 P235  
GLY MET SER PHE I4 G12 Y28 D138 P235

HIS ASP GLY ASP TYR LYS ASP HIS ASP ILE ASP TYR LYS ASP  
HIS ASP GLY ASP TYR LYS ASP HIS ASP ILE ASP TYR LYS ASP

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	90648	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	43	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

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	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.73	1/4746 (0.0%)	0.55	0/6425
1	B	0.72	0/4746	0.53	0/6425
1	C	0.71	0/4746	0.53	0/6425
2	D	0.68	0/3666	0.52	0/4967
2	E	0.70	0/3666	0.52	0/4967
2	F	0.70	0/3666	0.52	0/4967
3	H	0.78	0/921	0.45	0/1224
4	I	0.61	0/1300	0.49	0/1746
4	J	0.60	0/1300	0.48	0/1746
4	K	0.60	0/1300	0.48	0/1746
5	M	0.68	0/385	0.48	0/517
5	N	0.67	0/385	0.45	0/517
5	O	0.66	0/385	0.47	0/517
6	Q	0.69	0/1858	0.50	0/2505
6	R	0.70	0/1754	0.49	0/2362
6	S	0.70	0/1912	0.51	0/2575
All	All	0.70	1/36736 (0.0%)	0.52	0/49631

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	290	ASP	C-N	-5.25	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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	4651	0	4643	3	0
1	B	4651	0	4644	6	0
1	C	4651	0	4643	20	0
2	D	3595	0	3602	10	0
2	E	3595	0	3602	7	0
2	F	3595	0	3602	21	0
3	H	914	0	992	3	0
4	I	1288	0	1366	5	0
4	J	1288	0	1366	4	0
4	K	1288	0	1366	0	0
5	M	382	0	384	0	0
5	N	382	0	384	0	0
5	O	382	0	384	0	0
6	Q	1824	0	1835	5	0
6	R	1722	0	1733	7	0
6	S	1878	0	1898	2	0
7	C	27	0	12	1	0
8	C	1	0	0	0	0
All	All	36114	0	36456	74	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 1.

The worst 5 of 74 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:525:TYR:CE2	2:F:403:LYS:HD2	2.00	0.95
2:F:374:GLU:HA	2:F:400:ARG:HD2	1.57	0.86
1:C:525:TYR:CE2	2:F:403:LYS:CD	2.62	0.83
1:C:525:TYR:CD2	2:F:403:LYS:HD2	2.16	0.79
1:C:525:TYR:CE2	2:F:403:LYS:HE3	2.22	0.75

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	598/617 (97%)	578 (97%)	20 (3%)	0	100	100
1	B	598/617 (97%)	575 (96%)	22 (4%)	1 (0%)	49	83
1	C	598/617 (97%)	572 (96%)	25 (4%)	1 (0%)	49	83
2	D	455/511 (89%)	442 (97%)	11 (2%)	2 (0%)	36	75
2	E	455/511 (89%)	443 (97%)	12 (3%)	0	100	100
2	F	455/511 (89%)	443 (97%)	9 (2%)	3 (1%)	24	66
3	H	105/247 (42%)	104 (99%)	1 (1%)	0	100	100
4	I	159/226 (70%)	159 (100%)	0	0	100	100
4	J	159/226 (70%)	157 (99%)	2 (1%)	0	100	100
4	K	159/226 (70%)	159 (100%)	0	0	100	100
5	M	45/118 (38%)	44 (98%)	1 (2%)	0	100	100
5	N	45/118 (38%)	44 (98%)	1 (2%)	0	100	100
5	O	45/118 (38%)	44 (98%)	1 (2%)	0	100	100
6	Q	222/301 (74%)	215 (97%)	7 (3%)	0	100	100
6	R	210/301 (70%)	204 (97%)	6 (3%)	0	100	100
6	S	230/301 (76%)	223 (97%)	6 (3%)	1 (0%)	36	75
All	All	4538/5566 (82%)	4406 (97%)	124 (3%)	8 (0%)	53	83

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	119	LEU
2	F	299	ASP
1	C	350	SER
2	F	119	LEU
6	S	12	GLY

### 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	507/524 (97%)	505 (100%)	2 (0%)	92	97
1	B	507/524 (97%)	505 (100%)	2 (0%)	92	97
1	C	507/524 (97%)	504 (99%)	3 (1%)	87	95
2	D	393/431 (91%)	392 (100%)	1 (0%)	93	98
2	E	393/431 (91%)	393 (100%)	0	100	100
2	F	393/431 (91%)	390 (99%)	3 (1%)	83	93
3	H	100/212 (47%)	100 (100%)	0	100	100
4	I	141/198 (71%)	141 (100%)	0	100	100
4	J	141/198 (71%)	141 (100%)	0	100	100
4	K	141/198 (71%)	141 (100%)	0	100	100
5	M	43/100 (43%)	43 (100%)	0	100	100
5	N	43/100 (43%)	43 (100%)	0	100	100
5	O	43/100 (43%)	43 (100%)	0	100	100
6	Q	203/274 (74%)	203 (100%)	0	100	100
6	R	191/274 (70%)	191 (100%)	0	100	100
6	S	208/274 (76%)	208 (100%)	0	100	100
All	All	3954/4793 (82%)	3943 (100%)	11 (0%)	93	98

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	173	ARG
1	C	400	ARG
2	F	74	LEU
1	B	296	MET
2	D	44	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:



Mol	Chain	Res	Type
2	E	181	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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
7	ADP	C	701	8	24,29,29	0.68	0	25,45,45	0.72	1 (4%)

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
7	ADP	C	701	8	-	4/12/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
7	C	701	ADP	C5-C6-N6	2.12	123.71	120.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

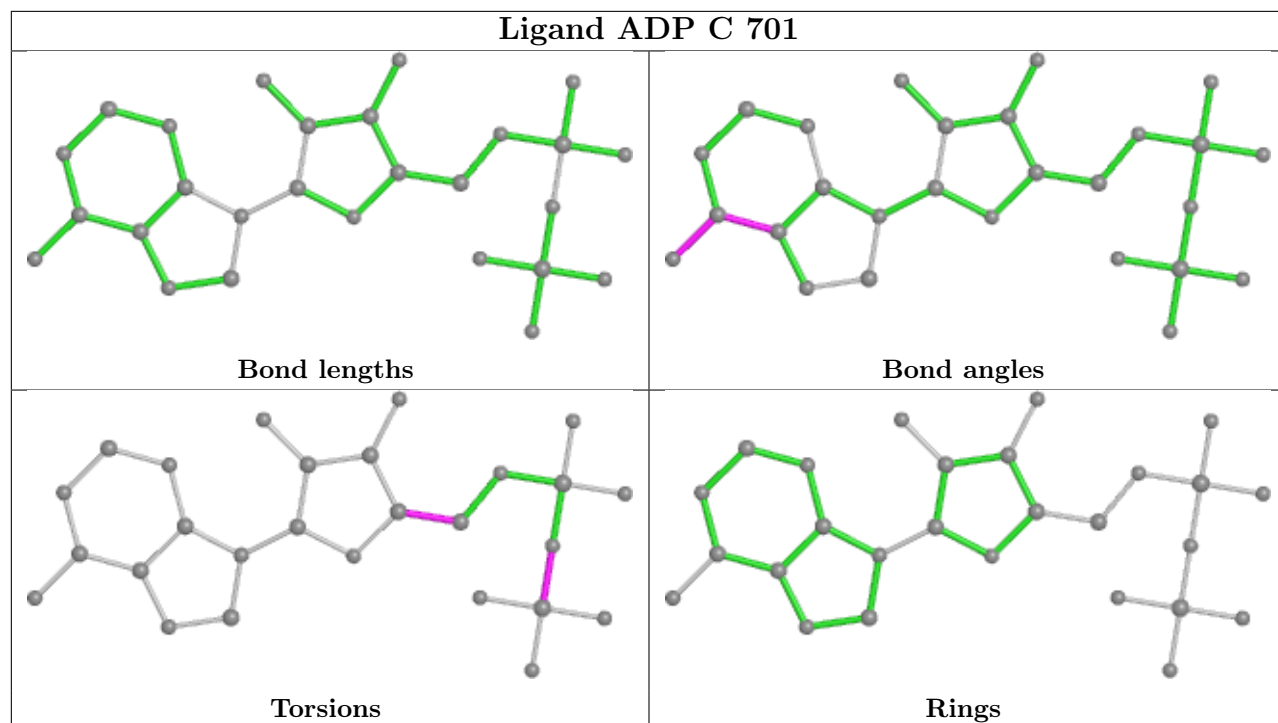
Mol	Chain	Res	Type	Atoms
7	C	701	ADP	O4'-C4'-C5'-O5'
7	C	701	ADP	C3'-C4'-C5'-O5'
7	C	701	ADP	PA-O3A-PB-O1B
7	C	701	ADP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	701	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.