



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 3, 2017 – 04:12 PM EDT

PDB ID : 5UIE
EMDB ID: : EMD-8549
Title : Vps4-Vta1 complex
Authors : Monroe, N.; Shen, P.; Han, H.; Sundquist, W.I.; Hill, C.P.
Deposited on : unknown
Resolution : 5.70 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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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) : rb-20029824

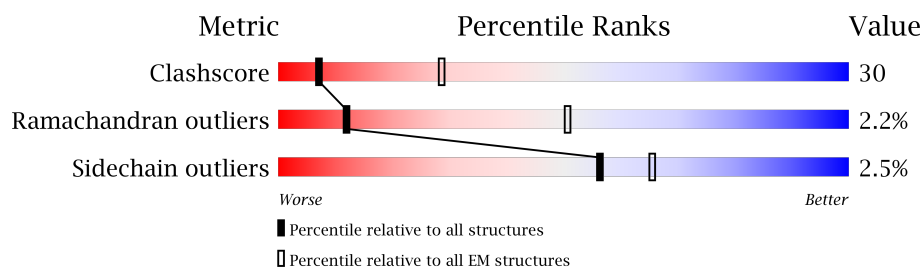
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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	437	
1	B	437	
1	C	437	
1	D	437	
1	E	437	
1	F	437	
2	G	9	
3	H	330	
3	I	330	

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Mol	Chain	Length	Quality of chain
3	J	330	<div><div></div><div></div><div></div></div> 8% 87%
3	K	330	<div><div></div><div></div><div></div></div> 9% 5% 86%
3	L	330	<div><div></div><div></div><div></div></div> 5% 8% 87%
3	M	330	<div><div></div><div></div><div></div></div> 9% 5% 86%
3	N	330	<div><div></div><div></div><div></div></div> 5% 8% 87%
3	O	330	<div><div></div><div></div><div></div></div> 5% 8% 87%
3	P	330	<div><div></div><div></div><div></div></div> 5% 8% 87%
3	Q	330	<div><div></div><div></div><div></div></div> 5% 7% 87%
3	R	330	<div><div></div><div></div><div></div></div> 5% 7% 87%
3	S	330	<div><div></div><div></div><div></div></div> 5% 8% 87%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18682 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 Vacuolar protein sorting-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	312	Total	C	N	O	S	0	0
			2412	1522	409	472	9		
1	B	311	Total	C	N	O	S	0	0
			2407	1519	408	471	9		
1	C	311	Total	C	N	O	S	0	0
			2407	1519	408	471	9		
1	D	311	Total	C	N	O	S	0	0
			2407	1519	408	471	9		
1	E	308	Total	C	N	O	S	0	0
			2387	1507	405	466	9		
1	F	302	Total	C	N	O	S	0	0
			2344	1484	396	455	9		

- Molecule 2 is a protein called DOA4-independent degradation protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	9	Total	C	N	O	0	0
			43	26	8	9		

- Molecule 3 is a protein called Vacuolar protein sorting-associated protein VTA1.

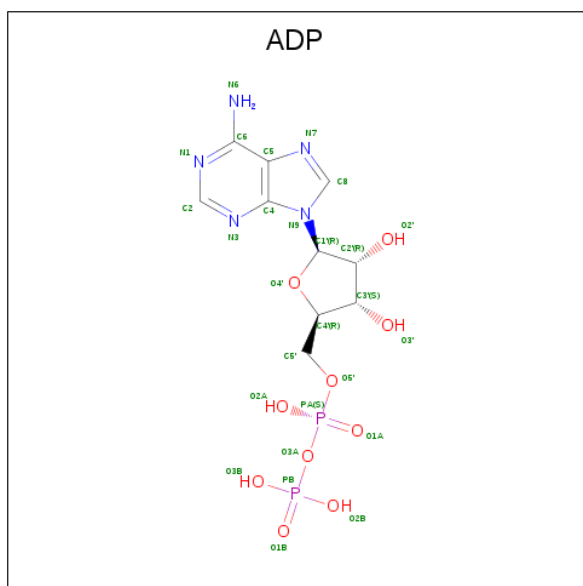
Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	42	Total	C	N	O		0	0
			331	209	54	68			
3	I	51	Total	C	N	O	S	0	0
			404	255	65	83	1		
3	J	42	Total	C	N	O		0	0
			331	209	54	68			
3	K	47	Total	C	N	O	S	0	0
			371	236	60	74	1		
3	L	42	Total	C	N	O		0	0
			331	209	54	68			
3	M	47	Total	C	N	O	S	0	0
			371	236	60	74	1		

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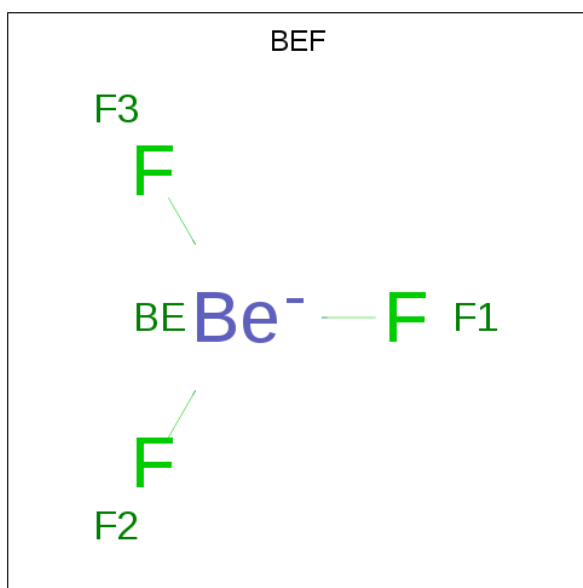
Mol	Chain	Residues	Atoms				AltConf	Trace
3	N	42	Total	C	N	O	0	0
			331	209	54	68		
3	O	42	Total	C	N	O	0	0
			331	209	54	68		
3	P	42	Total	C	N	O	0	0
			331	209	54	68		
3	Q	42	Total	C	N	O	0	0
			331	209	54	68		
3	R	42	Total	C	N	O	0	0
			331	209	54	68		
3	S	42	Total	C	N	O	0	0
			331	209	54	68		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).

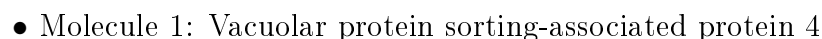


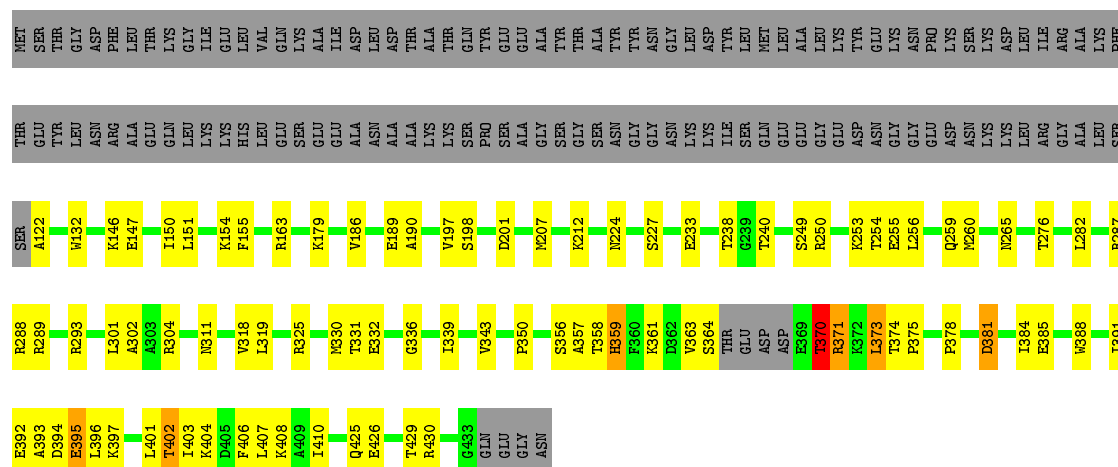
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Be	F	0
			4	1	3	
5	C	1	Total	Be	F	0
			8	2	6	
5	C	1	Total	Be	F	0
			8	2	6	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

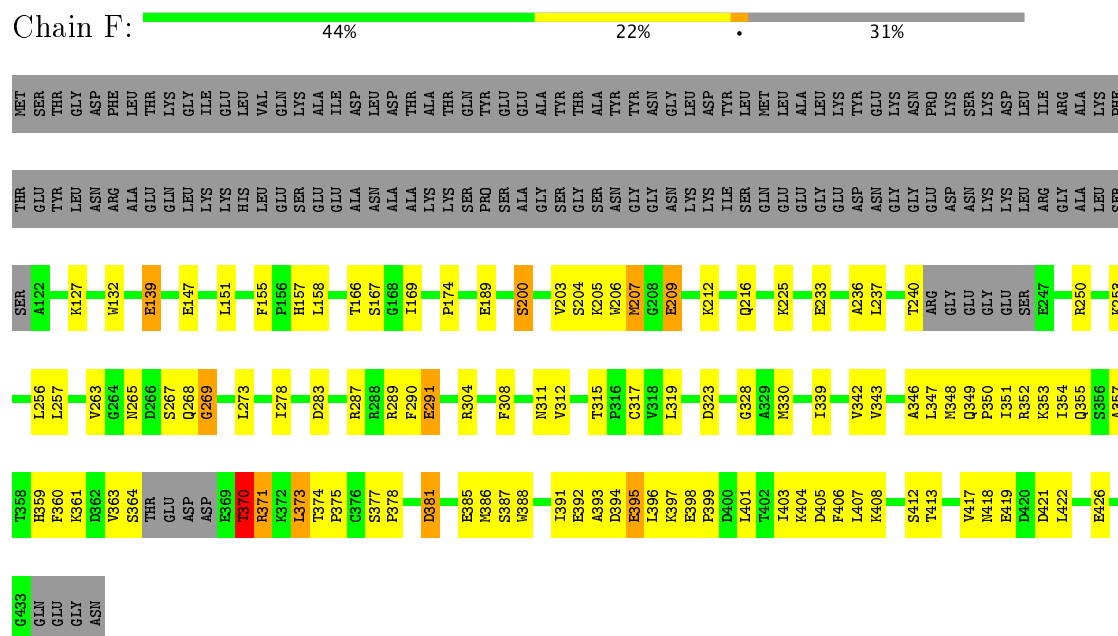
Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Mg	0
			1	1	
6	A	1	Total	Mg	0
			1	1	
6	C	1	Total	Mg	0
			1	1	

- Molecule 1: Vacuolar protein sorting-associated protein 4





- Molecule 1: Vacuolar protein sorting-associated protein 4

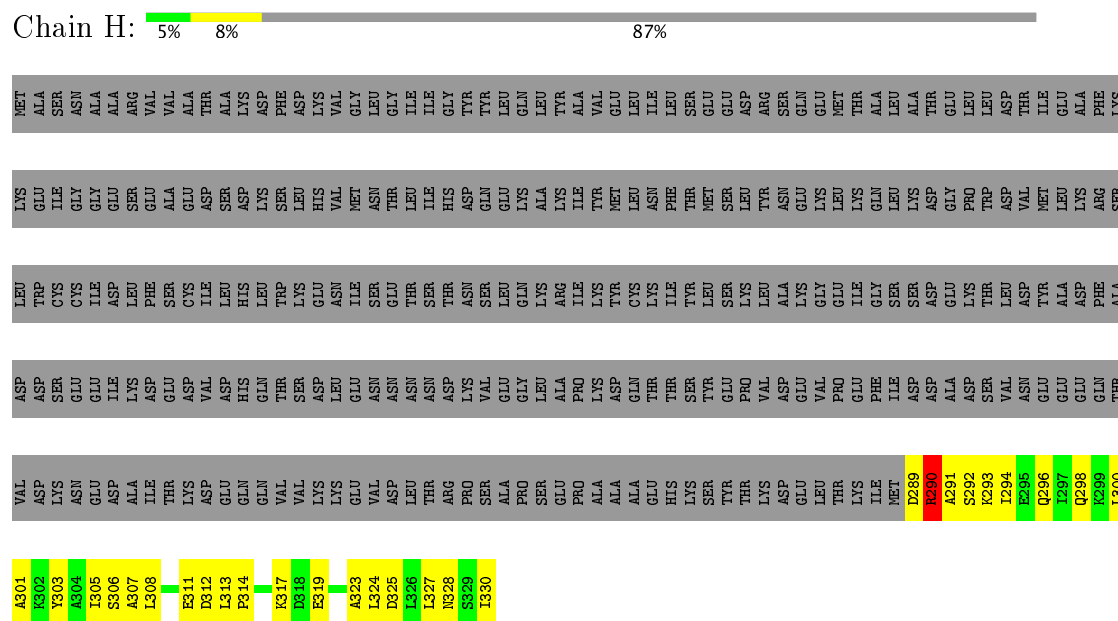


- Molecule 2: DOA4-independent degradation protein 4



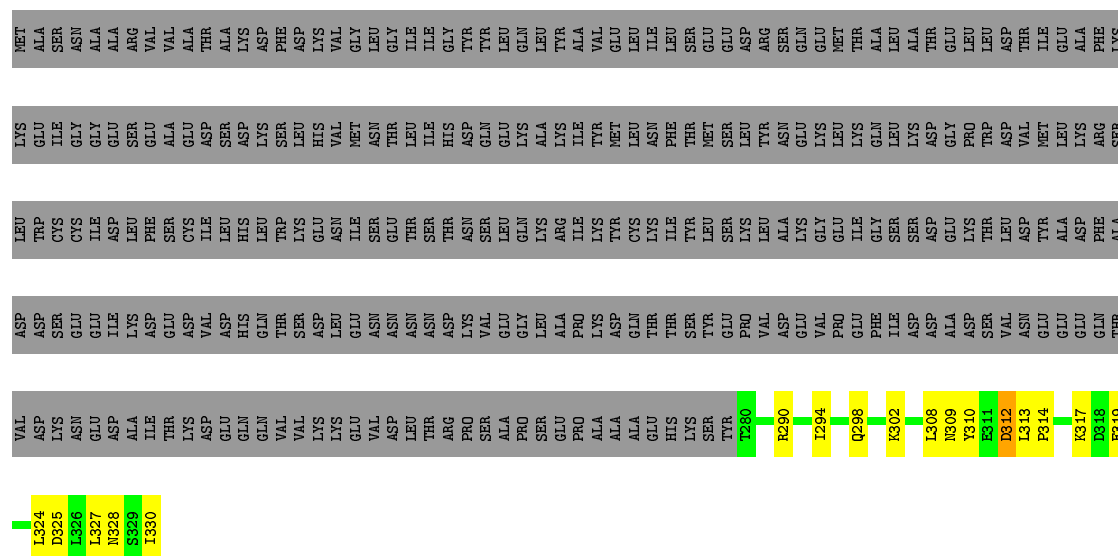
There are no outlier residues recorded for this chain.

- Molecule 3: Vacuolar protein sorting-associated protein VTA1



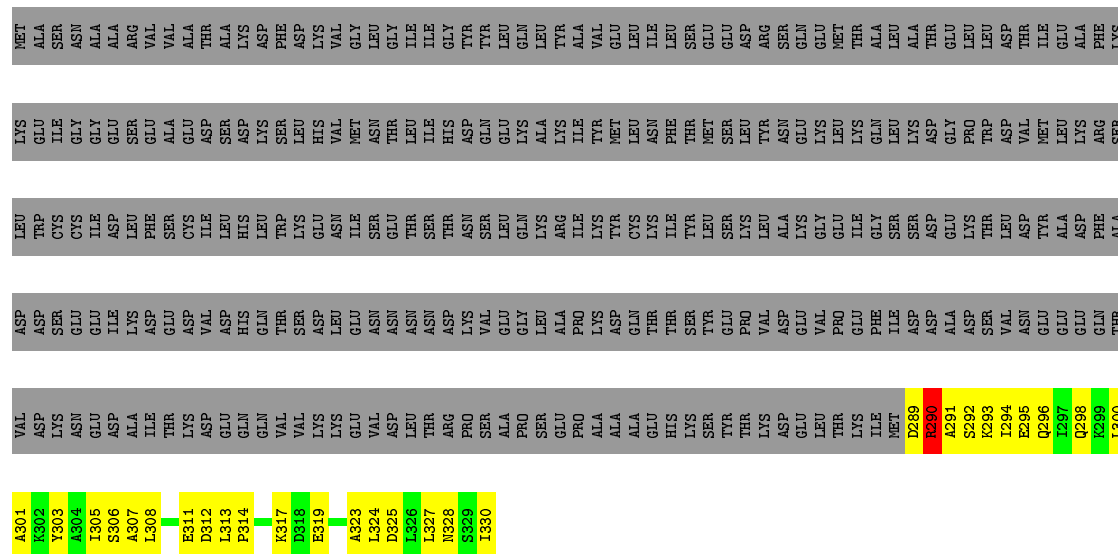
- Molecule 3: Vacuolar protein sorting-associated protein VTA1





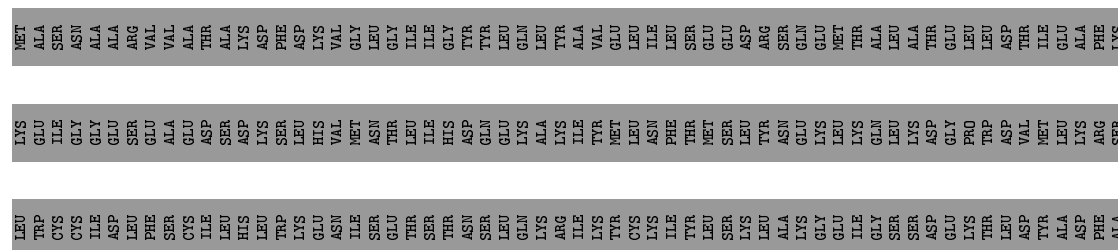
- Molecule 3: Vacuolar protein sorting-associated protein VTA1

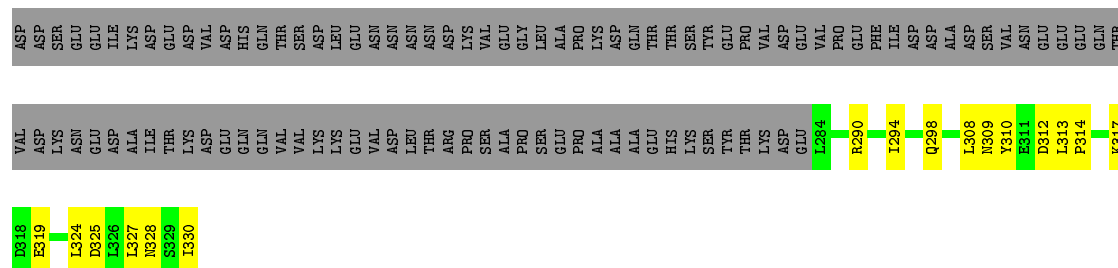
Chain J: 8% 87%



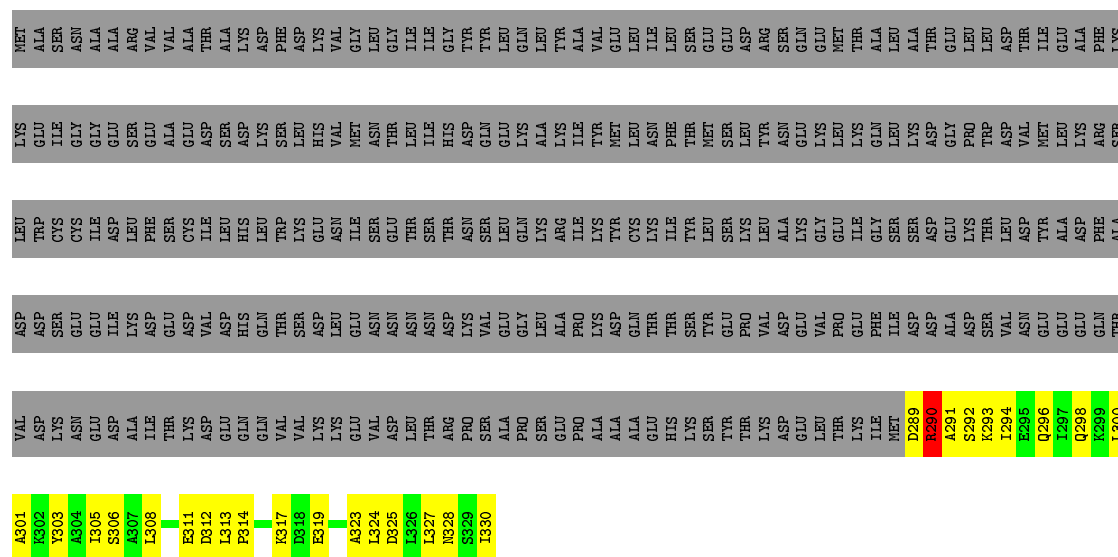
- Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain K:  9% 5% 86%

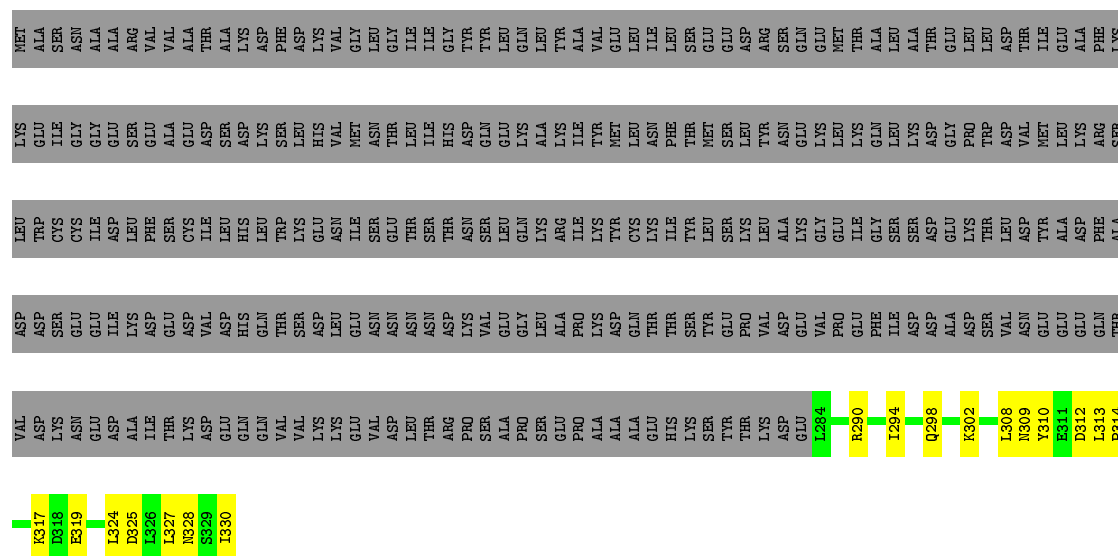




- Molecule 3: Vacuolar protein sorting-associated protein VTA1



- Molecule 3: Vacuolar protein sorting-associated protein VTA1



- Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain N: 5% 8% 87%

[illegible]

- Molecule 3: Vacuolar protein sorting-associated protein VTA1

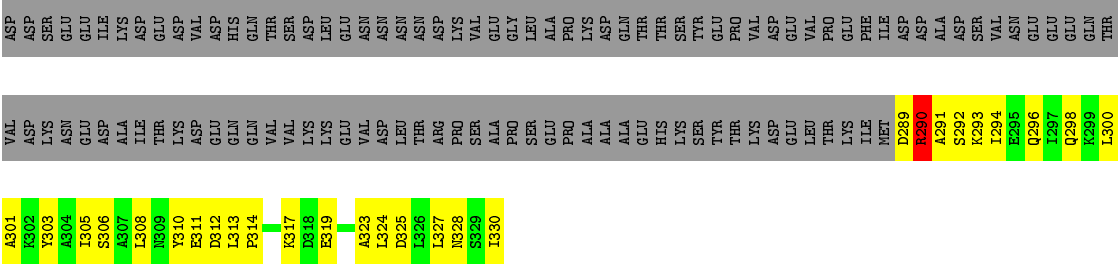
Chain O: 5% 8% 87%

A301	VAL	ASP	TRP	LEU	LYS	MET
I305	ASP	ASP	CYS	CYS	CYS	ALA
L308	ASN	GLU	ILE	ASP	GLY	ASN
	GLU	ILE	ASP	GLY	ALA	ALA
N309	ALA	LYS	LEU	ASP	ARG	ARG
E311	ILE	ASP	PHE	GLU	VAL	VAL
D312	THR	GLU	SER	SER	ALA	ALA
L313	LYS	ASP	CYS	CYS	GLU	VAL
P314	ASP	VAL	ILE	ILE	ASP	THR
K317	GLU	ASP	LEU	LEU	SER	ALA
	GLN	HIS	HIS	HIS	ASP	LYS
D318	GLN	GLN	GLN	LEU	LYS	ASP
E319	VAL	THR	TRP	TRP	SER	PHE
A323	VAL	SER	SER	LYS	LEU	ASP
	LYS	ASP	GLU	HIS	SER	LYS
L324	LYS	LEU	ASN	VAL	VAL	VAL
D325	GLU	GLU	ILE	ILE	GLY	GLY
L326	VAL	ASN	SER	SER	ASN	LEU
L327	ASP	ASN	GLU	THR	THR	GLY
N328	LEU	ASN	THR	SER	ILE	ILE
S329	THR	ASN	THR	THR	ILE	ILE
I330	ANG	ASP	HIS	THR	GLY	GLY
	PRO	LYS	ASN	ASN	ASP	TYR
D331	SER	VAL	SER	SER	GLN	TYR
	ALA	GLU	LEU	GLU	LEU	LEU
Q332	PRO	GLY	GLN	LYS	LYS	GLN
	SER	LEU	LYS	ALA	ALA	LEU
Q333	GLU	ALA	ARG	ARG	LYS	TYR
	PRO	PHE	ILE	ILE	ILE	ALA
Q334	ALA	LYS	LYS	LYS	TYR	VAL
	ALA	ASP	THR	THR	THR	GLU
Q335	GLU	THR	THR	THR	THR	VAL
	HIS	THR	THR	THR	THR	GLU
Q336	LYS	SER	THR	THR	THR	GLU
	THR	GLU	SER	LYS	LEU	GLU
Q337	LYS	VAL	LEU	LEU	TYR	ASP
	ASP	ASP	ALA	ALA	ASN	ARG
Q338	GLU	GLU	LYS	LYS	GLU	SER
	LEU	VAL	GLY	GLY	GLY	GLN
Q339	THR	PHE	ILE	GLY	GLN	ALA
	ILE	ASP	SER	SER	LEU	LEU
Q340	MET	ILE	SER	SER	LYS	LEU
	D289	ASP	ASP	GLY	LYS	ALA
Q341	E290	ALA	GLU	GLU	GLY	THR
	A291	ASP	GLU	GLU	GLY	GLU
Q342	S292	SER	THR	THR	PRO	LEU
	K293	VAL	LEU	THR	LYS	LEU
Q343	I294	ASN	ASP	THR	TRP	LEU
	E295	GLU	THR	THR	ASP	ASP
Q344	Q296	GLU	ALA	ALA	VAL	THR
	I297	GLU	ASP	LYS	THR	ILE
Q345	Q298	GLU	PHE	ALA	LEU	GLU
	K299	GLN	ILE	THR	ARG	ALA

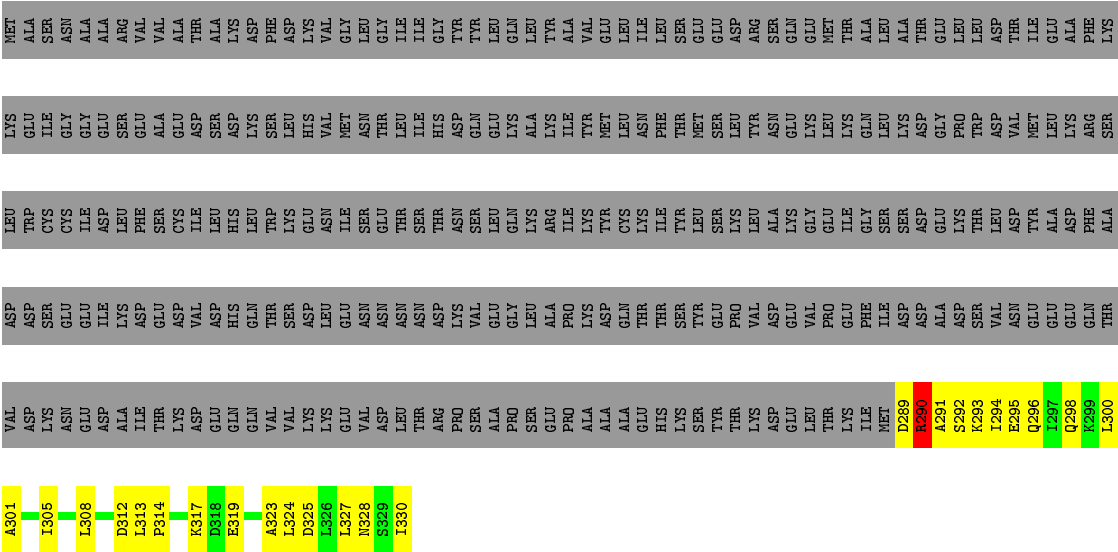
- Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain P: 5% 8% 87%

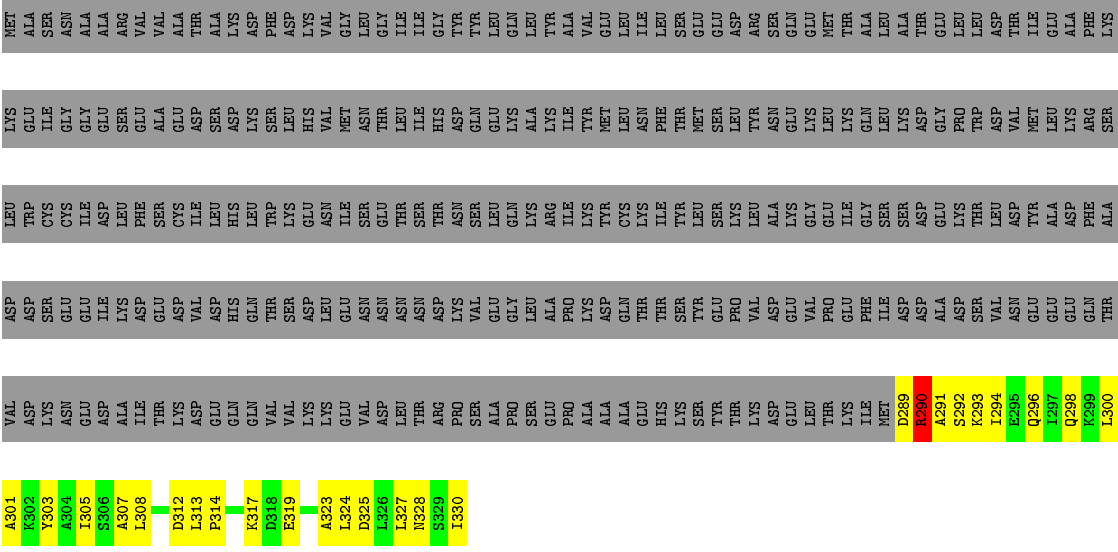
[illegible]



● Molecule 3: Vacuolar protein sorting-associated protein VTA1



● Molecule 3: Vacuolar protein sorting-associated protein VTA1



● Molecule 3: Vacuolar protein sorting-associated protein VTA1

Chain S:  5% 8% 87%

[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.3	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (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, BEF, ACE, 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 >2	RMSZ	# Z >2
1	A	0.35	0/2453	0.55	0/3315
1	B	0.36	0/2448	0.55	0/3308
1	C	0.36	0/2448	0.55	0/3308
1	D	0.36	0/2448	0.56	0/3308
1	E	0.35	0/2428	0.57	0/3281
1	F	0.60	0/2384	0.69	2/3222 (0.1%)
3	H	0.52	0/333	0.75	0/447
3	I	0.54	0/406	0.66	0/544
3	J	0.52	0/333	0.75	0/447
3	K	0.52	0/373	0.68	0/500
3	L	0.52	0/333	0.75	0/447
3	M	0.52	0/373	0.68	0/500
3	N	0.52	0/333	0.75	0/447
3	O	0.52	0/333	0.75	0/447
3	P	0.52	0/333	0.75	0/447
3	Q	0.52	0/333	0.75	0/447
3	R	0.53	0/333	0.75	0/447
3	S	0.53	0/333	0.75	0/447
All	All	0.43	0/18758	0.61	2/25309 (0.0%)

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	1
1	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	9

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	269	GLY	N-CA-C	5.16	126.00	113.10
1	F	287	ARG	NE-CZ-NH1	5.15	122.88	120.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	LYS	Peptide
1	A	250	ARG	Sidechain
1	B	205	LYS	Peptide
1	B	270	VAL	Mainchain
1	B	414	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	2412	0	2435	178	0
1	B	2407	0	2430	179	0
1	C	2407	0	2430	124	0
1	D	2407	0	2430	147	0
1	E	2387	0	2407	154	0
1	F	2344	0	2371	208	0
2	G	43	0	12	0	0
3	H	331	0	344	36	0
3	I	404	0	425	36	0
3	J	331	0	344	37	0
3	K	371	0	395	24	0
3	L	331	0	344	39	0
3	M	371	0	395	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	331	0	344	36	0
3	O	331	0	344	38	0
3	P	331	0	344	39	0
3	Q	331	0	344	29	0
3	R	331	0	344	27	0
3	S	331	0	344	59	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	2	0
4	E	27	0	12	1	0
5	A	4	0	0	0	0
5	C	8	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
All	All	18682	0	18886	1118	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 30.

The worst 5 of 1118 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:354:ILE:HD13	1:C:375:PRO:CG	1.31	1.61
1:F:354:ILE:CG2	1:F:396:LEU:HD21	1.20	1.59
1:B:354:ILE:HA	1:B:375:PRO:CG	1.14	1.59
1:C:354:ILE:HD13	1:C:375:PRO:CD	1.31	1.55
1:D:389:THR:CG2	1:E:154:LYS:HZ1	1.16	1.54

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	308/437 (70%)	280 (91%)	23 (8%)	5 (2%)	11	51
1	B	307/437 (70%)	271 (88%)	31 (10%)	5 (2%)	11	51
1	C	307/437 (70%)	275 (90%)	27 (9%)	5 (2%)	11	51
1	D	307/437 (70%)	272 (89%)	30 (10%)	5 (2%)	11	51
1	E	304/437 (70%)	268 (88%)	31 (10%)	5 (2%)	11	51
1	F	296/437 (68%)	275 (93%)	15 (5%)	6 (2%)	9	47
3	H	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	I	49/330 (15%)	43 (88%)	5 (10%)	1 (2%)	9	47
3	J	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	K	45/330 (14%)	39 (87%)	5 (11%)	1 (2%)	8	44
3	L	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	M	45/330 (14%)	39 (87%)	5 (11%)	1 (2%)	8	44
3	N	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	O	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	P	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	Q	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	R	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
3	S	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	27
All	All	2328/6582 (35%)	2041 (88%)	235 (10%)	52 (2%)	12	44

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	HIS
1	A	371	ARG
1	A	395	GLU
1	B	359	HIS
1	B	371	ARG

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	265/367 (72%)	262 (99%)	3 (1%)	78	89
1	B	265/367 (72%)	259 (98%)	6 (2%)	56	78
1	C	265/367 (72%)	262 (99%)	3 (1%)	78	89
1	D	265/367 (72%)	261 (98%)	4 (2%)	70	85
1	E	262/367 (71%)	259 (99%)	3 (1%)	78	89
1	F	258/367 (70%)	247 (96%)	11 (4%)	33	64
3	H	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	I	45/294 (15%)	44 (98%)	1 (2%)	57	79
3	J	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	K	41/294 (14%)	40 (98%)	1 (2%)	54	77
3	L	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	M	41/294 (14%)	40 (98%)	1 (2%)	54	77
3	N	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	O	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	P	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	Q	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	R	36/294 (12%)	34 (94%)	2 (6%)	25	57
3	S	36/294 (12%)	34 (94%)	2 (6%)	25	57
All	All	2031/5730 (35%)	1980 (98%)	51 (2%)	56	77

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	240	THR
1	F	412	SER
3	R	290	ARG
1	F	291	GLU
1	F	417	VAL

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

Mol	Chain	Res	Type
3	H	296	GLN

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Mol	Chain	Res	Type
3	J	296	GLN
3	P	296	GLN
1	F	265	ASN
3	Q	296	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](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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$
4	ADP	A	501	5	25,29,29	0.93	1 (4%)	24,45,45	0.97	1 (4%)
5	BEF	A	502	4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	B	501	5	25,29,29	0.95	1 (4%)	24,45,45	0.90	1 (4%)
5	BEF	C	501	4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	C	502	5	25,29,29	0.82	0	24,45,45	0.98	1 (4%)
5	BEF	C	503	4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	D	501	-	25,29,29	0.95	1 (4%)	24,45,45	1.61	2 (8%)
4	ADP	E	501	-	25,29,29	0.99	1 (4%)	24,45,45	1.58	2 (8%)

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
4	ADP	A	501	5	-	0/12/32/32	0/3/3/3
5	BEF	A	502	4	-	0/0/0/0	0/0/0/0
4	ADP	B	501	5	-	0/12/32/32	0/3/3/3
5	BEF	C	501	4	-	0/0/0/0	0/0/0/0
4	ADP	C	502	5	-	0/12/32/32	0/3/3/3
5	BEF	C	503	4	-	0/0/0/0	0/0/0/0
4	ADP	D	501	-	-	0/12/32/32	0/3/3/3
4	ADP	E	501	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	ADP	PB-O3A	-2.06	1.56	1.60
4	A	501	ADP	PB-O1B	2.10	1.57	1.50
4	D	501	ADP	C5-C4	3.05	1.47	1.40
4	E	501	ADP	C5-C4	3.15	1.47	1.40

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	501	ADP	N3-C2-N1	-5.68	123.91	128.86
4	D	501	ADP	N3-C2-N1	-5.45	124.11	128.86
4	D	501	ADP	C4-C5-N7	-2.94	106.57	109.41
4	E	501	ADP	C4-C5-N7	-2.81	106.70	109.41
4	B	501	ADP	O2A-PA-O5'	2.33	119.14	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	ADP	1	0
4	B	501	ADP	1	0
5	C	501	BEF	1	0
4	C	502	ADP	1	0
4	D	501	ADP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	501	ADP	1	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.