



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 18, 2017 – 08:31 AM EDT

PDB ID : 5VOZ
EMDB ID: : EMD-8726
Title : Yeast V-ATPase in complex with Legionella pneumophila effector SidK (rotational state 3)
Authors : Zhao, J.
Deposited on : unknown
Resolution : 7.60 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation 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) : rb-20029824

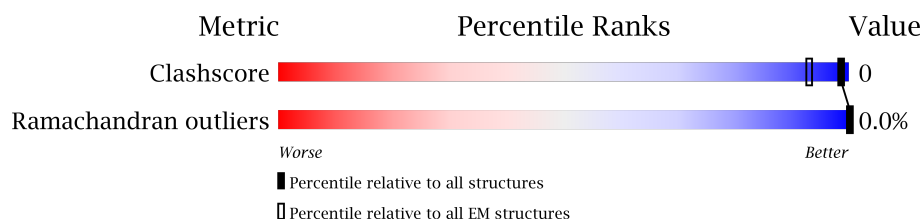
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.60 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.





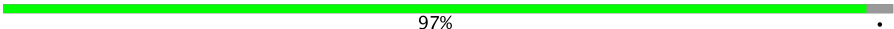
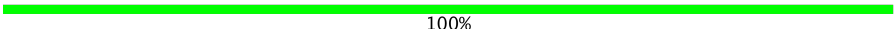
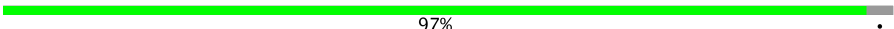

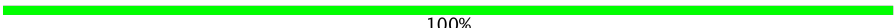











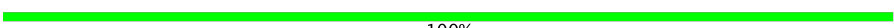



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120

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	617	 96% .
1	C	617	 96% .
1	E	617	 96% .
2	B	517	 88% 12%
2	D	517	 88% 12%
2	F	517	 88% 12%
3	G	233	 94% 6%
3	I	233	 93% 7%
3	K	233	 93% 7%
4	H	114	 92% 8%
4	J	114	 92% 8%

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Mol	Chain	Length	Quality of chain
4	L	114	 92% 8%
5	M	256	 81% 18%
6	N	118	 97%
7	O	392	 100%
8	P	478	 97%
9	Q	345	 99%
10	R	213	 100%
11	S	164	 90% 10%
12	T	160	 94% 6%
12	U	160	 94% 6%
12	V	160	 93% 7%
12	W	160	 94% 6%
12	X	160	 93% 6%
12	Y	160	 94% 6%
12	Z	160	 93% 8%
12	a	160	 93% 8%
13	b	840	 75% 25%
14	c	73	 77% 22%
15	d	54	 100%
16	e	573	 44% 56%
16	f	573	 44% 56%
16	g	573	 44% 56%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 34724 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 V-type proton ATPase catalytic subunit A,V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	593	Total	C	N	O	0	0
			2371	1186	593	592		
1	C	593	Total	C	N	O	0	0
			2371	1186	593	592		
1	E	593	Total	C	N	O	0	0
			2371	1186	593	592		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	457	Total	C	N	O	0	0
			1827	914	457	456		
2	D	457	Total	C	N	O	0	0
			1827	914	457	456		
2	F	457	Total	C	N	O	0	0
			1827	914	457	456		

- Molecule 3 is a protein called V-type proton ATPase subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	218	Total	C	N	O	0	0
			871	436	218	217		
3	I	217	Total	C	N	O	0	0
			867	434	217	216		
3	K	217	Total	C	N	O	0	0
			867	434	217	216		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	105	Total	C	N	O	0	0
			419	210	105	104		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	105	Total	C	N	O	0	0
			419	210	105	104		
4	L	105	Total	C	N	O	0	0
			419	210	105	104		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	210	Total	C	N	O	0	0
			839	420	210	209		

- Molecule 6 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	115	Total	C	N	O	0	0
			459	230	115	114		

- Molecule 7 is a protein called V-type proton ATPase subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	392	Total	C	N	O	0	0
			1567	784	392	391		

- Molecule 8 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	462	Total	C	N	O	0	0
			1847	924	462	461		

- Molecule 9 is a protein called V-type proton ATPase subunit d.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	345	Total	C	N	O	0	0
			1379	690	345	344		

- Molecule 10 is a protein called V-type proton ATPase subunit c”.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	R	213	Total	C	N	O	0	0
			851	426	213	212		

- Molecule 11 is a protein called V-type proton ATPase subunit c'.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	S	147	Total	C	N	O	0	0
			587	294	147	146		

- Molecule 12 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	T	150	Total	C	N	O	0	0
			599	300	150	149		
12	U	150	Total	C	N	O	0	0
			599	300	150	149		
12	V	149	Total	C	N	O	0	0
			595	298	149	148		
12	W	150	Total	C	N	O	0	0
			599	300	150	149		
12	X	150	Total	C	N	O	0	0
			599	300	150	149		
12	Y	150	Total	C	N	O	0	0
			599	300	150	149		
12	Z	148	Total	C	N	O	0	0
			591	296	148	147		
12	a	148	Total	C	N	O	0	0
			591	296	148	147		

- Molecule 13 is a protein called V-type proton ATPase subunit a, vacuolar isoform.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	b	634	Total	C	N	O	0	0
			2529	1268	634	627		

- Molecule 14 is a protein called V-type proton ATPase subunit e.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	c	57	Total	C	N	O	0	0
			227	114	57	56		

- Molecule 15 is a protein called V-type proton ATPase subunit f.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	d	54	Total	C	N	O	0	0
			214	108	54	52		

- Molecule 16 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	e	250	Total 999	C 500	N 250	O 249	0	0
16	f	250	Total 999	C 500	N 250	O 249	0	0
16	g	250	Total 999	C 500	N 250	O 249	0	0

There are 3 discrepancies between the modelled and reference sequences:

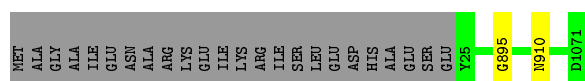
Chain	Residue	Modelled	Actual	Comment	Reference
e	89	LEU	GLN	conflict	UNP G8UUS6
f	89	LEU	GLN	conflict	UNP G8UUS6
g	89	LEU	GLN	conflict	UNP G8UUS6

3 Residue-property plots [i](#)

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.

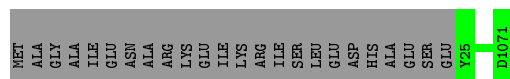
- Molecule 1: V-type proton ATPase catalytic subunit A,V-type proton ATPase catalytic subunit A

Chain A:  96%



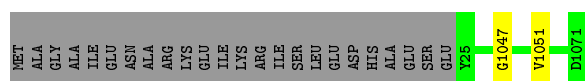
- Molecule 1: V-type proton ATPase catalytic subunit A,V-type proton ATPase catalytic subunit A

Chain C:  96%




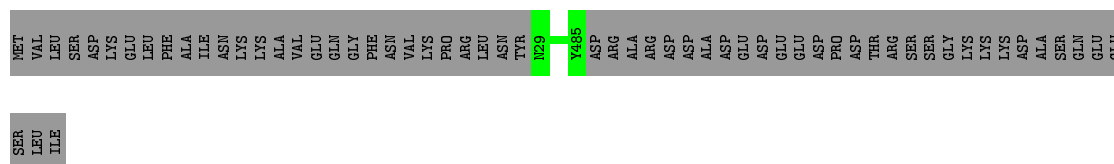
- Molecule 1: V-type proton ATPase catalytic subunit A,V-type proton ATPase catalytic subunit A

Chain E:  96%



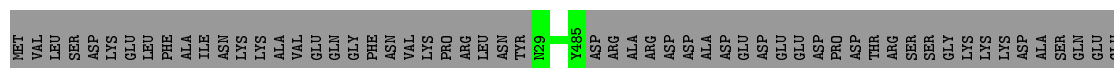
- Molecule 2: V-type proton ATPase subunit B

Chain B:  88% 12%



- Molecule 2: V-type proton ATPase subunit B

Chain D:  88% 12%



SER
LEU
ILE

- Molecule 2: V-type proton ATPase subunit B

Chain F:  88% 12%

MET VAL SER ASP LYS GLU LEU PHE ALA ILE ASN LYS VAL GLN GLY PHE VAL LYS PRO ARG LEU ASN TYR N29 Y465 ASP ARG ALA ARG ASP ASP ALA ASP GLU ASP GLU ASP PRO THR ARG SER GLY LYS LYS LYS ASP ALA SER GLN GLU

SER
LEU
ILE

- Molecule 3: V-type proton ATPase subunit E

Chain G:  94% 6%

MET SER SER ALA ILE THR A7 G224 PRO SER LYS THR ARG LYS LYS PHE ASP

- Molecule 3: V-type proton ATPase subunit E

Chain I:  93% 7%

MET SER SER ALA ILE THR ALA L4 G224 PRO SER LYS THR ARG LYS LYS PHE ASP

- Molecule 3: V-type proton ATPase subunit E

Chain K:  93% 7%

MET SER SER ALA ILE THR ALA L4 G224 PRO SER LYS THR ARG LYS LYS PHE ASP

- Molecule 4: V-type proton ATPase subunit G

Chain H:  92% 8%

MET S2 S106 ALA GLU VAL HIS ILE ASN ALA LEU

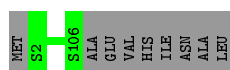
- Molecule 4: V-type proton ATPase subunit G

Chain J:  92% 8%

MET S2 S106 ALA GLU VAL HIS ILE ASN ALA LEU

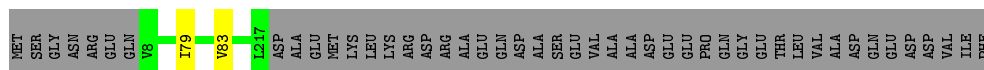
- Molecule 4: V-type proton ATPase subunit G

Chain L:  92% 8%



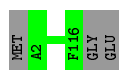
- Molecule 5: V-type proton ATPase subunit D

Chain M: 81% 18%



- Molecule 6: V-type proton ATPase subunit F

Chain N: 97%



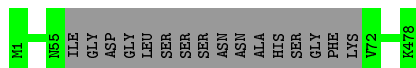
- Molecule 7: V-type proton ATPase subunit C

Chain O: 100%

There are no outlier residues recorded for this chain.

- Molecule 8: V-type proton ATPase subunit H

Chain P: 97%



- Molecule 9: V-type proton ATPase subunit d

Chain Q: 99%



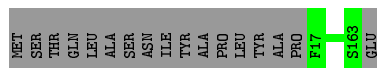
- Molecule 10: V-type proton ATPase subunit c''

Chain R: 100%

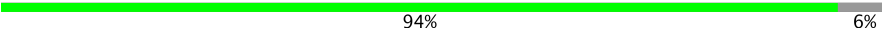
There are no outlier residues recorded for this chain.

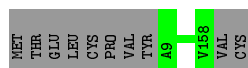
- Molecule 11: V-type proton ATPase subunit c'

Chain S: 90% 10%



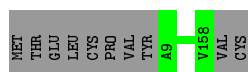
- Molecule 12: V-type proton ATPase subunit c

Chain T:  94% 6%



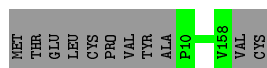
- Molecule 12: V-type proton ATPase subunit c

Chain U:  94% 6%



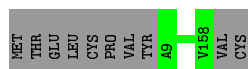
- Molecule 12: V-type proton ATPase subunit c

Chain V:  93% 7%



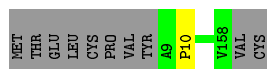
- Molecule 12: V-type proton ATPase subunit c

Chain W:  94% 6%



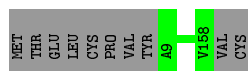
- Molecule 12: V-type proton ATPase subunit c

Chain X:  93% 6%



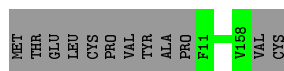
- Molecule 12: V-type proton ATPase subunit c

Chain Y:  94% 6%



- Molecule 12: V-type proton ATPase subunit c

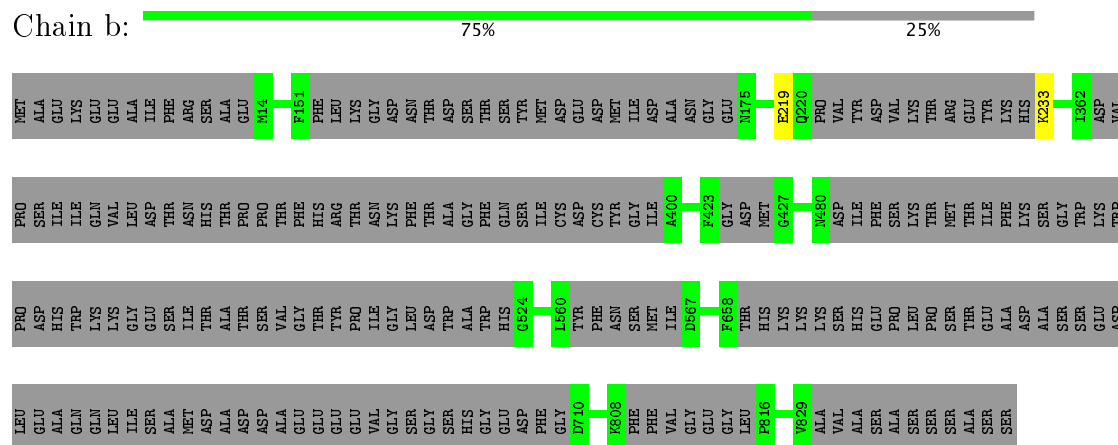
Chain Z:  93% 8%



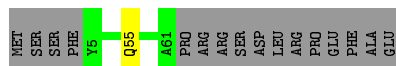
- Molecule 12: V-type proton ATPase subunit c

Chain a:  93% 8%

- Molecule 13: V-type proton ATPase subunit a, vacuolar isoform



- Molecule 14: V-type proton ATPase subunit e

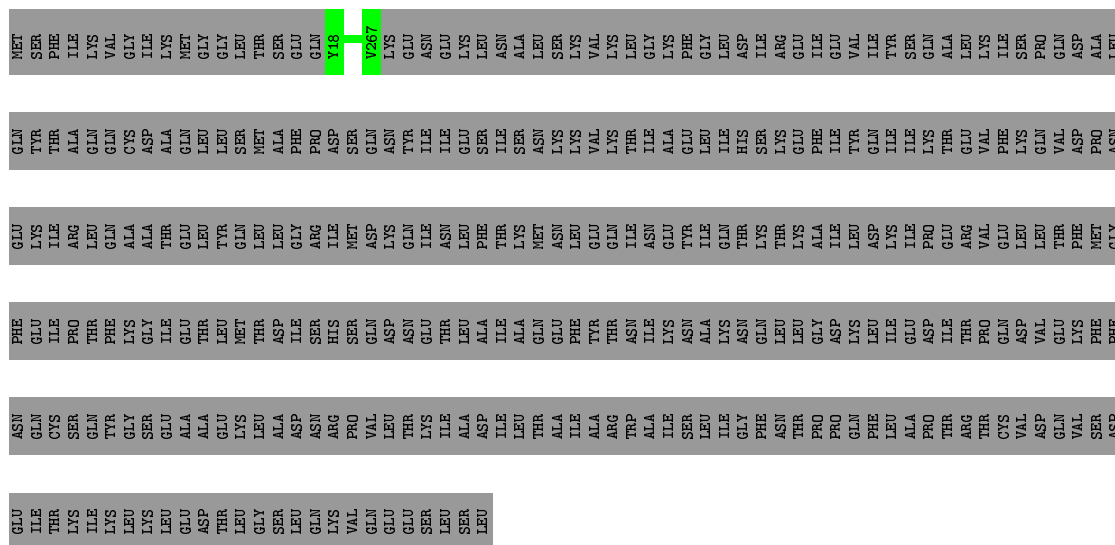


- Molecule 15: V-type proton ATPase subunit f



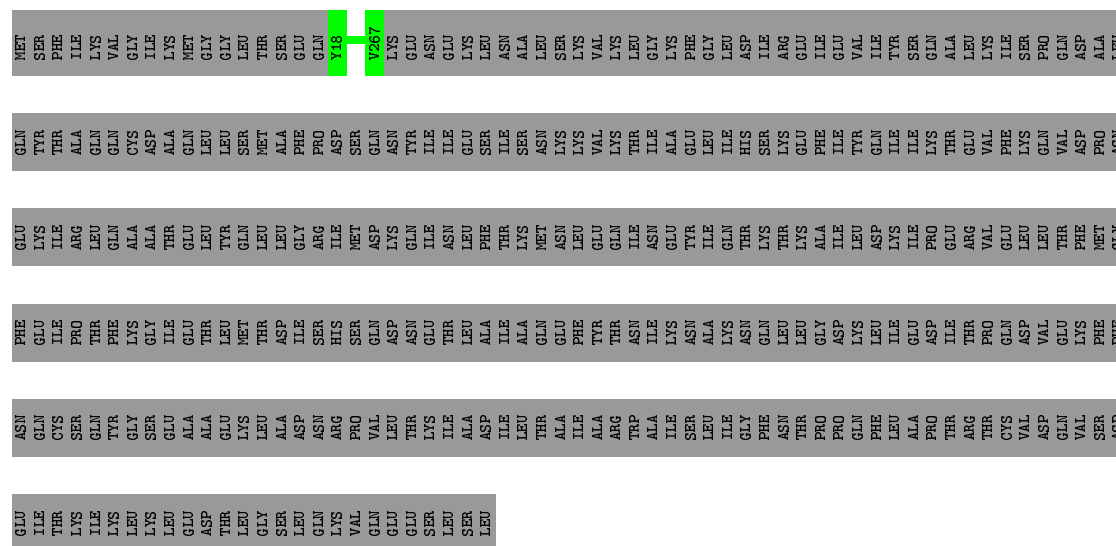
There are no outlier residues recorded for this chain.

- Molecule 16: Uncharacterized protein



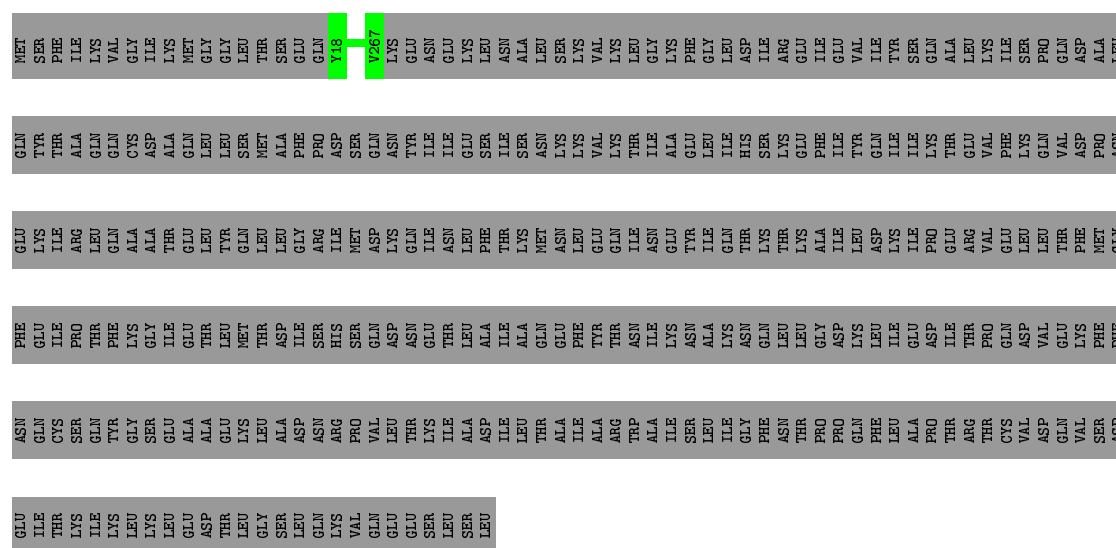
- Molecule 16: Uncharacterized protein

Chain f:  44% 56%



- Molecule 16: Uncharacterized protein

Chain g:  44% 56%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	13061	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 ($e^-/\text{\AA}^2$)	1.2	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 ⓘ

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	0.23	0/2370	0.44	0/2961
1	C	0.23	0/2370	0.44	0/2961
1	E	0.23	0/2370	0.44	0/2961
10	R	0.23	0/850	0.41	0/1061
11	S	0.22	0/586	0.41	0/731
12	T	0.23	0/598	0.39	0/746
12	U	0.23	0/598	0.39	0/746
12	V	0.23	0/594	0.39	0/741
12	W	0.22	0/598	0.39	0/746
12	X	0.23	0/598	0.39	0/746
12	Y	0.23	0/598	0.40	0/746
12	Z	0.23	0/590	0.41	0/736
12	a	0.23	0/590	0.39	0/736
13	b	0.26	1/2520 (0.0%)	0.46	1/3136 (0.0%)
14	c	0.21	0/226	0.44	0/281
16	e	0.22	0/998	0.38	0/1246
16	f	0.22	0/998	0.37	0/1246
16	g	0.22	0/998	0.39	0/1246
2	B	0.23	0/1826	0.43	0/2281
2	D	0.23	0/1826	0.45	0/2281
2	F	0.23	0/1826	0.45	0/2281
3	G	0.25	0/870	0.39	0/1086
3	I	0.24	0/866	0.39	0/1081
3	K	0.24	0/866	0.40	0/1081
4	H	0.22	0/418	0.36	0/521
4	J	0.23	0/418	0.36	0/521
4	L	0.23	0/418	0.35	0/521
5	M	0.24	0/838	0.38	0/1046
6	N	0.22	0/458	0.44	0/571
7	O	0.23	0/1566	0.43	0/1956
8	P	0.22	0/1845	0.36	0/2303
9	Q	0.22	0/1378	0.40	0/1721
All	All	0.23	1/34469 (0.0%)	0.42	1/43024 (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
13	b	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	233	LYS	C-N	6.48	1.49	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	233	LYS	C-N-CA	-7.89	101.96	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	b	219	GLU	Mainchain

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	2371	0	662	1	0
1	C	2371	0	662	0	0
1	E	2371	0	662	1	0
2	B	1827	0	501	0	0
2	D	1827	0	501	0	0
2	F	1827	0	501	0	0
3	G	871	0	226	0	0
3	I	867	0	225	0	0
3	K	867	0	225	0	0
4	H	419	0	115	0	0
4	J	419	0	115	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	419	0	115	0	0
5	M	839	0	228	1	0
6	N	459	0	117	0	0
7	O	1567	0	404	0	0
8	P	1847	0	480	0	0
9	Q	1379	0	370	1	0
10	R	851	0	261	0	0
11	S	587	0	186	0	0
12	T	599	0	189	0	0
12	U	599	0	189	0	0
12	V	595	0	189	0	0
12	W	599	0	189	0	0
12	X	599	0	189	0	0
12	Y	599	0	189	0	0
12	Z	591	0	188	0	0
12	a	591	0	188	0	0
13	b	2529	0	681	0	0
14	c	227	0	56	0	0
15	d	214	0	4	0	0
16	e	999	0	256	0	0
16	f	999	0	256	0	0
16	g	999	0	256	0	0
All	All	34724	0	9575	4	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 0.

All (4) 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:A:895:GLY:HA3	1:A:910:ASN:H	1.73	0.52
1:E:1047:GLY:N	1:E:1051:VAL:O	2.43	0.47
5:M:79:ILE:O	5:M:83:VAL:N	2.46	0.43
9:Q:196:VAL:O	9:Q:200:ILE:CA	2.68	0.42

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	591/617 (96%)	570 (96%)	21 (4%)	0	100	100
1	C	591/617 (96%)	557 (94%)	34 (6%)	0	100	100
1	E	591/617 (96%)	565 (96%)	26 (4%)	0	100	100
2	B	455/517 (88%)	442 (97%)	13 (3%)	0	100	100
2	D	455/517 (88%)	444 (98%)	11 (2%)	0	100	100
2	F	455/517 (88%)	445 (98%)	10 (2%)	0	100	100
3	G	216/233 (93%)	214 (99%)	2 (1%)	0	100	100
3	I	215/233 (92%)	213 (99%)	2 (1%)	0	100	100
3	K	215/233 (92%)	212 (99%)	3 (1%)	0	100	100
4	H	103/114 (90%)	103 (100%)	0	0	100	100
4	J	103/114 (90%)	102 (99%)	1 (1%)	0	100	100
4	L	103/114 (90%)	103 (100%)	0	0	100	100
5	M	208/256 (81%)	202 (97%)	6 (3%)	0	100	100
6	N	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
7	O	390/392 (100%)	374 (96%)	16 (4%)	0	100	100
8	P	458/478 (96%)	439 (96%)	19 (4%)	0	100	100
9	Q	343/345 (99%)	330 (96%)	13 (4%)	0	100	100
10	R	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
11	S	145/164 (88%)	143 (99%)	2 (1%)	0	100	100
12	T	148/160 (92%)	144 (97%)	4 (3%)	0	100	100
12	U	148/160 (92%)	145 (98%)	3 (2%)	0	100	100
12	V	147/160 (92%)	142 (97%)	5 (3%)	0	100	100
12	W	148/160 (92%)	144 (97%)	4 (3%)	0	100	100
12	X	148/160 (92%)	144 (97%)	3 (2%)	1 (1%)	25	68
12	Y	148/160 (92%)	145 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Z	146/160 (91%)	145 (99%)	1 (1%)	0	100	100
12	a	146/160 (91%)	144 (99%)	2 (1%)	0	100	100
13	b	616/840 (73%)	594 (96%)	22 (4%)	0	100	100
14	c	55/73 (75%)	43 (78%)	11 (20%)	1 (2%)	10	49
16	e	248/573 (43%)	245 (99%)	3 (1%)	0	100	100
16	f	248/573 (43%)	244 (98%)	4 (2%)	0	100	100
16	g	248/573 (43%)	244 (98%)	4 (2%)	0	100	100
All	All	8555/10321 (83%)	8287 (97%)	266 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	X	10	PRO
14	c	55	GLN

5.3.2 Protein sidechains [i](#)

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

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	d	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	d	31:UNK	C	78:UNK	N	10.76