



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 16, 2018 – 05:14 PM EST

PDB ID : 5Y60
EMDB ID: : EMD-6813
Title : V/A-type ATPase/synthase from *Thermus thermophilus*, rotational state 3.
Authors : Nakanishi, A.; Kishikawa, J.; Tamakoshi, M.; Mitsuoka, K.; Yokoyama, K.
Deposited on : 2017-08-10
Resolution : 7.50 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.

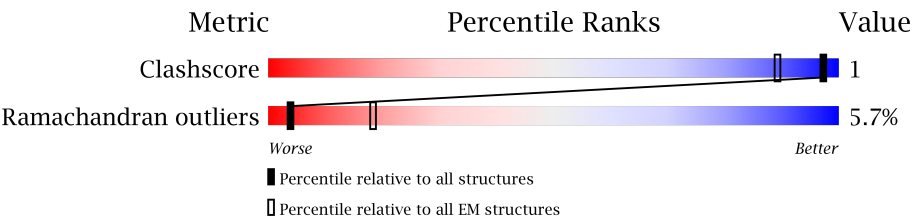
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

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 7.50 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	578	<div><div>91%</div><div>9%</div></div>
1	B	578	<div><div>90%</div><div>10%</div></div>
1	C	578	<div><div>88%</div><div>11%</div><div>.</div></div>
2	D	478	<div><div>90%</div><div>6%</div><div>.</div></div>
2	E	478	<div><div>85%</div><div>11%</div><div>.</div></div>
2	F	478	<div><div>84%</div><div>12%</div><div>.</div></div>
3	G	223	<div><div>84%</div><div>10%</div><div>6%</div></div>
4	H	104	<div><div>81%</div><div>14%</div><div>.</div><div>.</div></div>
5	I	120	<div><div>82%</div><div>.</div><div>17%</div></div>
5	K	120	<div><div>82%</div><div>.</div><div>17%</div></div>
6	J	188	<div><div>95%</div><div>.</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
6	L	188	 95% . .
7	M	323	 96% . .
8	N	652	 92% 5% .
9	O	99	 75% . 23%
9	P	99	 72% 5% 23%
9	Q	99	 76% . 23%
9	R	99	 77% 23%
9	S	99	 76% . 23%
9	T	99	 77% 23%
9	U	99	 76% . 23%
9	V	99	 76% . 23%
9	W	99	 76% . 23%
9	X	99	 75% . 23%
9	Y	99	 75% . . 23%
9	Z	99	 76% . 23%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 23433 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 ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	577	Total	C	N	O	0	0
			2307	1154	577	576		
1	B	577	Total	C	N	O	0	0
			2307	1154	577	576		
1	C	577	Total	C	N	O	0	0
			2307	1154	577	576		

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	459	Total	C	N	O	0	0
			1835	918	459	458		
2	E	459	Total	C	N	O	0	0
			1835	918	459	458		
2	F	459	Total	C	N	O	0	0
			1835	918	459	458		

- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	210	Total	C	N	O	0	0
			839	420	210	209		

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	100	Total	C	N	O	0	0
			399	200	100	99		

- Molecule 5 is a protein called V-type ATP synthase, subunit (VAPC-THERM).

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	100	Total	C	N	O	0	0
			399	200	100	99		
5	K	100	Total	C	N	O	0	0
			399	200	100	99		

- Molecule 6 is a protein called V-type ATP synthase subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	185	Total	C	N	O	0	0
			738	370	185	183		
6	L	185	Total	C	N	O	0	0
			738	370	185	183		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	134	MET	LEU	conflict	UNP P74901
J	171	MET	LEU	conflict	UNP P74901
J	178	MET	LEU	conflict	UNP P74901
L	134	MET	LEU	conflict	UNP P74901
L	171	MET	LEU	conflict	UNP P74901
L	178	MET	LEU	conflict	UNP P74901

- Molecule 7 is a protein called V-type ATP synthase subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	320	Total	C	N	O	0	0
			1279	640	320	319		

- Molecule 8 is a protein called V-type ATP synthase subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	N	632	Total	C	N	O	0	0
			2526	1264	632	630		

- Molecule 9 is a protein called V-type ATP synthase, subunit K.

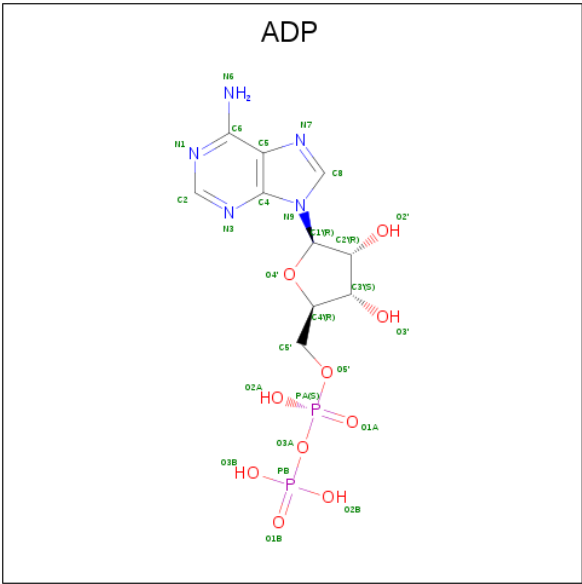
Mol	Chain	Residues	Atoms				AltConf	Trace
9	O	76	Total	C	N	O	0	0
			303	152	76	75		
9	P	76	Total	C	N	O	0	0
			303	152	76	75		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	76	Total	C	N	O	0	0
			303	152	76	75		
9	R	76	Total	C	N	O	0	0
			303	152	76	75		
9	S	76	Total	C	N	O	0	0
			303	152	76	75		
9	T	76	Total	C	N	O	0	0
			303	152	76	75		
9	U	76	Total	C	N	O	0	0
			303	152	76	75		
9	V	76	Total	C	N	O	0	0
			303	152	76	75		
9	W	76	Total	C	N	O	0	0
			303	152	76	75		
9	X	76	Total	C	N	O	0	0
			303	152	76	75		
9	Y	76	Total	C	N	O	0	0
			303	152	76	75		
9	Z	76	Total	C	N	O	0	0
			303	152	76	75		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

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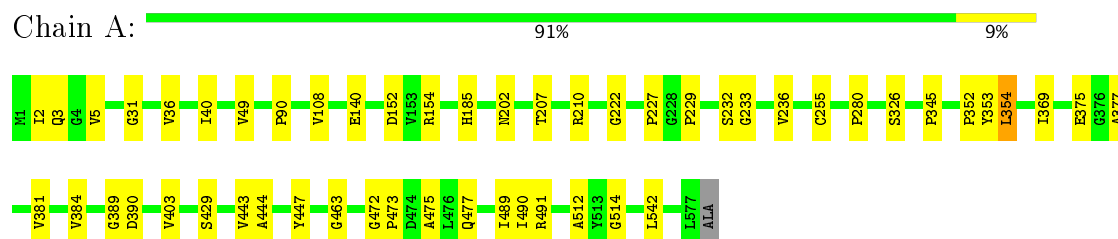
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	B	1	27	10	5	10	2	0

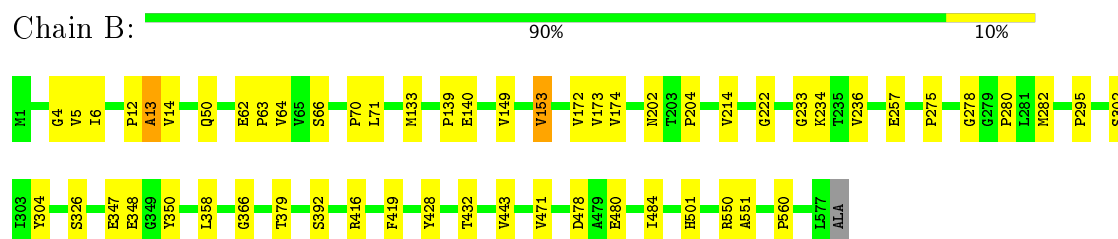
3 Residue-property plots

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.

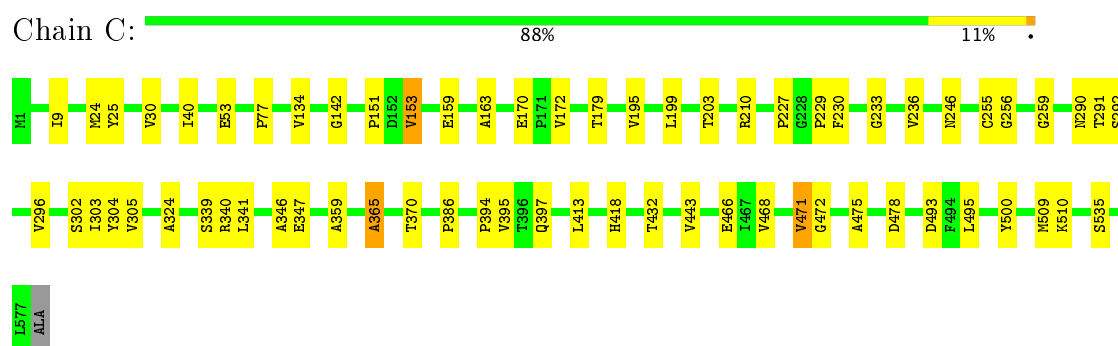
- Molecule 1: V-type ATP synthase alpha chain



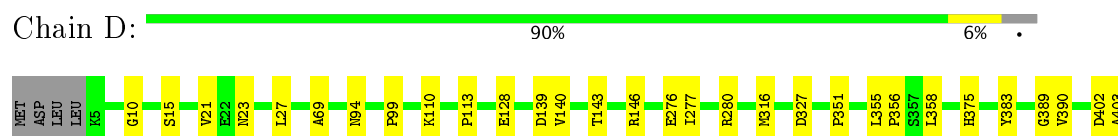
- Molecule 1: V-type ATP synthase alpha chain

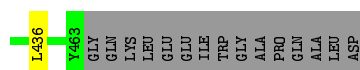


- Molecule 1: V-type ATP synthase alpha chain



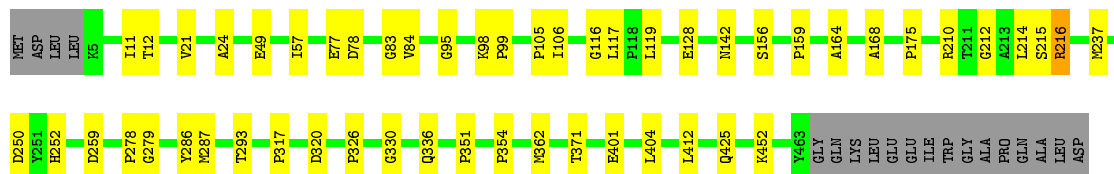
- Molecule 2: V-type ATP synthase beta chain





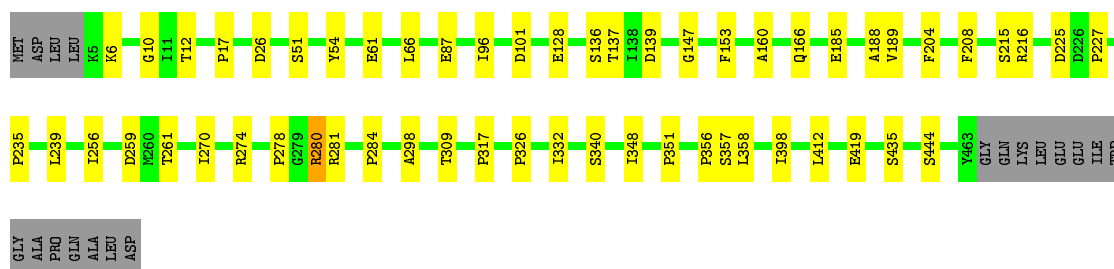
• Molecule 2: V-type ATP synthase beta chain

Chain E: 85% 11%



• Molecule 2: V-type ATP synthase beta chain

Chain F: 84% 12%



• Molecule 3: V-type ATP synthase subunit D

Chain G: 84% 10% 6%



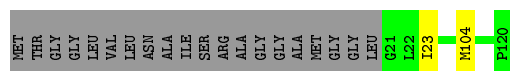
• Molecule 4: V-type ATP synthase subunit F

Chain H: 81% 14% 2%



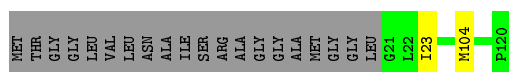
• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

Chain I: 82% 17%



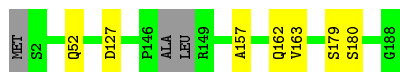
• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

Chain K: 82% 17%



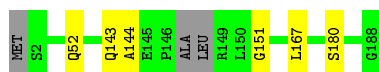
- Molecule 6: V-type ATP synthase subunit E

Chain J: 95%



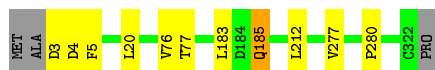
- Molecule 6: V-type ATP synthase subunit E

Chain L: 95%



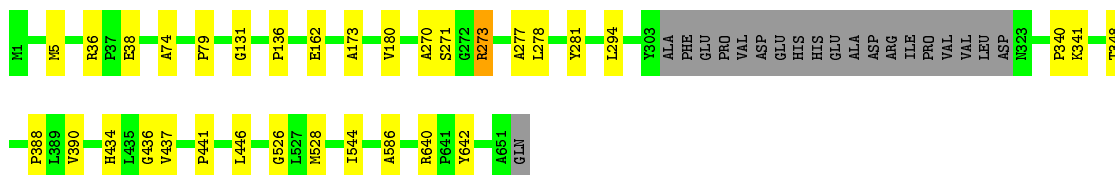
- Molecule 7: V-type ATP synthase subunit C

Chain M: 96%



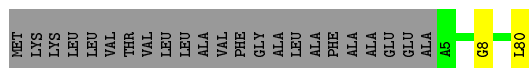
- Molecule 8: V-type ATP synthase subunit I

Chain N: 92% 5%



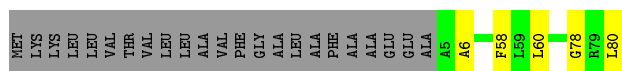
- Molecule 9: V-type ATP synthase, subunit K

Chain O: 75% 23%



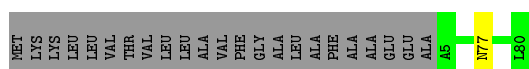
- Molecule 9: V-type ATP synthase, subunit K

Chain P: 72% 5% 23%

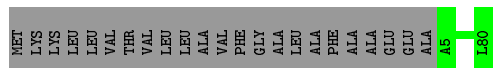
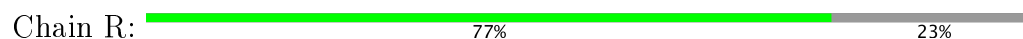


- Molecule 9: V-type ATP synthase, subunit K

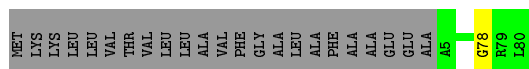
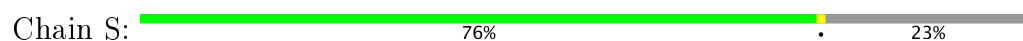
Chain Q: 76% 23%



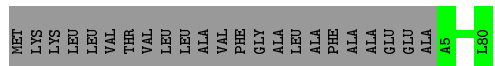
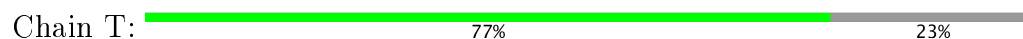
- Molecule 9: V-type ATP synthase, subunit K



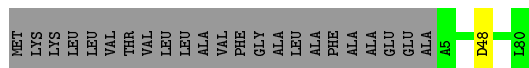
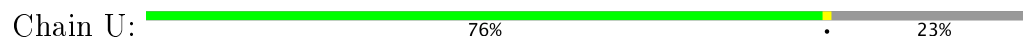
- Molecule 9: V-type ATP synthase, subunit K



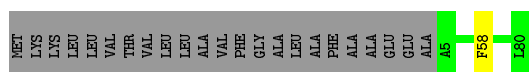
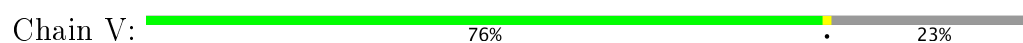
- Molecule 9: V-type ATP synthase, subunit K



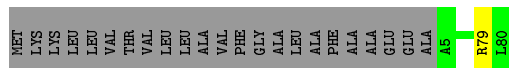
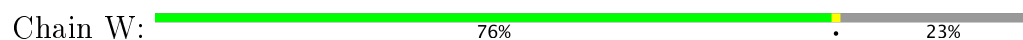
- Molecule 9: V-type ATP synthase, subunit K



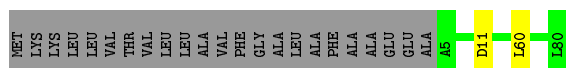
- Molecule 9: V-type ATP synthase, subunit K



- Molecule 9: V-type ATP synthase, subunit K



- Molecule 9: V-type ATP synthase, subunit K

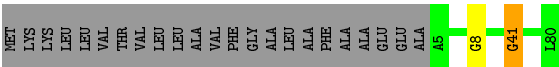


● Molecule 9: V-type ATP synthase, subunit K

Chain Y:

75%

23%



● Molecule 9: V-type ATP synthase, subunit K

Chain Z:

76%

23%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13851	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 ($e^-/\text{\AA}^2$)	26	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (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: 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	1.37	0/2306	1.29	9/2881 (0.3%)
1	B	1.37	1/2306 (0.0%)	1.32	10/2881 (0.3%)
1	C	1.34	0/2306	1.29	5/2881 (0.2%)
2	D	1.32	0/1834	1.31	4/2291 (0.2%)
2	E	1.41	0/1834	1.37	13/2291 (0.6%)
2	F	1.42	0/1834	1.36	8/2291 (0.3%)
3	G	1.32	0/838	1.29	1/1046 (0.1%)
4	H	1.24	0/398	1.36	3/496 (0.6%)
5	I	0.97	0/398	1.00	0/496
5	K	1.05	0/398	1.00	0/496
6	J	1.01	0/736	1.04	0/917
6	L	1.10	0/736	1.01	0/917
7	M	1.07	0/1278	1.04	2/1596 (0.1%)
8	N	1.03	0/2524	1.14	3/3152 (0.1%)
9	O	0.86	0/302	1.17	2/376 (0.5%)
9	P	0.89	0/302	1.19	1/376 (0.3%)
9	Q	0.89	0/302	1.03	0/376
9	R	0.86	0/302	1.13	0/376
9	S	0.89	0/302	1.06	1/376 (0.3%)
9	T	0.88	0/302	1.01	0/376
9	U	0.91	0/302	1.08	0/376
9	V	0.93	0/302	1.27	1/376 (0.3%)
9	W	0.85	0/302	1.12	0/376
9	X	0.88	0/302	1.11	1/376 (0.3%)
9	Y	0.85	0/302	1.03	1/376 (0.3%)
9	Z	0.94	0/302	1.12	0/376
All	All	1.22	1/23350 (0.0%)	1.23	65/29144 (0.2%)

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	1
2	F	0	2
7	M	0	3
9	P	0	1
9	U	0	1
9	Y	0	2
All	All	0	15

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4	GLY	CA-C	-5.40	1.43	1.51

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	HIS	C-N-CA	7.70	140.94	121.70
1	A	232	SER	C-N-CA	7.07	137.14	122.30
1	B	419	PHE	N-CA-C	-6.77	92.72	111.00
1	C	471	VAL	C-N-CA	6.75	136.47	122.30
2	E	12	THR	N-CA-C	-6.61	93.16	111.00

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	VAL	Mainchain
1	A	49	VAL	Mainchain
1	B	358	LEU	Mainchain,Peptide
1	B	379	THR	Mainchain
1	C	346	ALA	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	2307	0	654	2	0
1	B	2307	0	654	4	0
1	C	2307	0	654	4	0
2	D	1835	0	512	0	0
2	E	1835	0	512	1	0
2	F	1835	0	512	2	0
3	G	839	0	230	1	0
4	H	399	0	119	2	0
5	I	399	0	100	0	0
5	K	399	0	100	0	0
6	J	738	0	192	0	0
6	L	738	0	192	2	0
7	M	1279	0	357	0	0
8	N	2526	0	709	1	0
9	O	303	0	102	0	0
9	P	303	0	102	1	0
9	Q	303	0	102	0	0
9	R	303	0	102	0	0
9	S	303	0	102	0	0
9	T	303	0	102	0	0
9	U	303	0	102	0	0
9	V	303	0	102	0	0
9	W	303	0	102	0	0
9	X	303	0	102	1	0
9	Y	303	0	102	1	0
9	Z	303	0	102	0	0
10	A	27	0	12	0	0
10	B	27	0	12	1	0
All	All	23433	0	6745	20	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 20 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:B:6:ILE:H	1:B:62:GLU:H	1.51	0.58
6:L:151:GLY:HA2	6:L:167:LEU:H	1.69	0.57
1:A:352:PRO:C	1:A:354:LEU:H	2.08	0.56
1:C:24:MET:H	2:F:66:LEU:N	2.10	0.50
1:B:236:VAL:H	10:B:600:ADP:PA	2.35	0.49

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	575/578 (100%)	462 (80%)	75 (13%)	38 (7%)	1	21
1	B	575/578 (100%)	448 (78%)	86 (15%)	41 (7%)	1	19
1	C	575/578 (100%)	417 (72%)	102 (18%)	56 (10%)	1	13
2	D	457/478 (96%)	355 (78%)	75 (16%)	27 (6%)	2	23
2	E	457/478 (96%)	334 (73%)	84 (18%)	39 (8%)	1	15
2	F	457/478 (96%)	334 (73%)	79 (17%)	44 (10%)	1	13
3	G	208/223 (93%)	149 (72%)	39 (19%)	20 (10%)	1	13
4	H	98/104 (94%)	62 (63%)	24 (24%)	12 (12%)	0	7
5	I	98/120 (82%)	91 (93%)	5 (5%)	2 (2%)	9	46
5	K	98/120 (82%)	94 (96%)	2 (2%)	2 (2%)	9	46
6	J	181/188 (96%)	155 (86%)	19 (10%)	7 (4%)	3	31
6	L	181/188 (96%)	155 (86%)	22 (12%)	4 (2%)	8	44
7	M	318/323 (98%)	299 (94%)	12 (4%)	7 (2%)	8	44
8	N	628/652 (96%)	550 (88%)	49 (8%)	29 (5%)	3	28
9	O	74/99 (75%)	70 (95%)	4 (5%)	0	100	100
9	P	74/99 (75%)	71 (96%)	2 (3%)	1 (1%)	13	54
9	Q	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	13	54
9	R	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	S	74/99 (75%)	73 (99%)	1 (1%)	0	100	100
9	T	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	U	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	V	74/99 (75%)	74 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	W	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	13	54
9	X	74/99 (75%)	73 (99%)	1 (1%)	0	100	100
9	Y	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	Z	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	13	54
All	All	5794/6274 (92%)	4770 (82%)	692 (12%)	332 (6%)	4	24

5 of 332 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	THR
1	A	210	ARG
1	A	227	PRO
1	A	229	PRO
1	A	233	GLY

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](#)

2 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
10	ADP	A	600	-	25,29,29	1.10	3 (12%)	24,45,45	1.13	2 (8%)
10	ADP	B	600	-	25,29,29	1.50	2 (8%)	24,45,45	1.50	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
10	ADP	A	600	-	-	0/12/32/32	0/3/3/3
10	ADP	B	600	-	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	600	ADP	C8-N7	-2.40	1.30	1.34
10	A	600	ADP	C2'-C1'	-2.37	1.49	1.53
10	A	600	ADP	C8-N7	-2.05	1.30	1.34
10	A	600	ADP	PB-O3A	2.24	1.63	1.60
10	B	600	ADP	PB-O3A	5.79	1.69	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	600	ADP	C4'-O4'-C1'	-5.00	104.44	109.77
10	A	600	ADP	C1'-N9-C4	-2.15	122.92	126.64
10	A	600	ADP	N6-C6-N1	2.77	124.25	118.77
10	B	600	ADP	N6-C6-N1	3.40	125.51	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	600	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.