



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:45 PM BST

PDB ID : 3J0J
EMDB ID: : EMD-5335
Title : Fitted atomic models of Thermus thermophilus V-ATPase subunits into cryo-EM map
Authors : Lau, W.C.Y.; Rubinstein, J.L.
Deposited on : 2011-08-24
Resolution : 9.70 Å(reported)
Based on PDB ID : 3A5C, 1R5Z, 3K5B

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

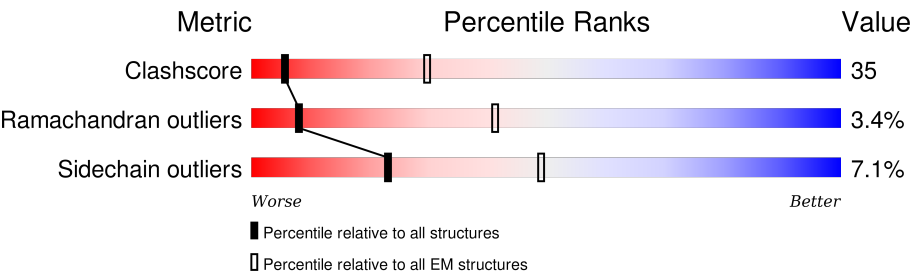
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 9.70 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.






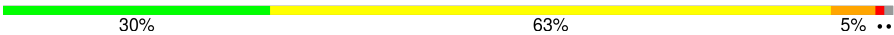
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	82% 13% . . .
1	B	578	85% 10% . .
1	C	578	83% 12% . .
2	D	478	83% 10% • 6%
2	E	478	82% 11% • 6%
2	F	478	82% 12% • 6%
3	G	223	• 23% 24% 8% 42%
4	H	104	79% 14% 7%
5	I	104	70% 24% . .

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Mol	Chain	Length	Quality of chain
5	K	104	 73% 22% • •
6	J	188	 64% 25% 7% • •
6	L	188	 64% 26% 6% • •
7	M	323	 30% 63% 5% • •

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22726 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	561	Total	C	N	O	0	0
			2752	1630	561	561		
1	B	561	Total	C	N	O	0	0
			2752	1630	561	561		
1	C	561	Total	C	N	O	0	0
			2752	1630	561	561		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	450	Total	C	N	O	0	0
			2212	1312	450	450		
2	E	450	Total	C	N	O	0	0
			2212	1312	450	450		
2	F	450	Total	C	N	O	0	0
			2212	1312	450	450		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	129	Total	C	N	O	0	0
			639	381	129	129		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	104	Total	C	N	O	0	0
			509	301	104	104		

- 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	S	0	0
			747	460	136	150	1		
5	K	100	Total	C	N	O	S	0	0
			747	460	136	150	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	17	GLY	-	EXPRESSION TAG	UNP Q5SIT5
K	17	GLY	-	EXPRESSION TAG	UNP Q5SIT5

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	184	Total	C	N	O	S	0	0
			1312	815	242	252	3		
6	L	184	Total	C	N	O	S	0	0
			1312	815	242	252	3		

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	S	0	0
			2514	1599	460	451	4		


- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

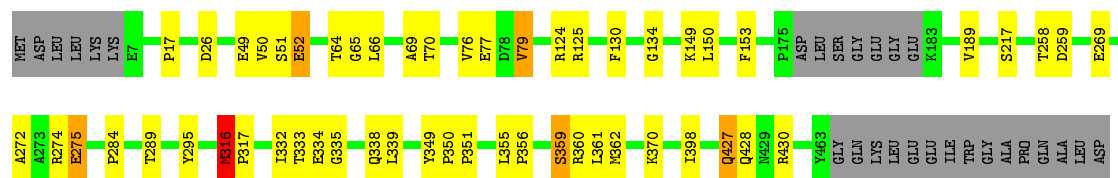


Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total 27	C 10	N 5	O 10	P 2	0
8	C	1	Total 27	C 10	N 5	O 10	P 2	0


- Molecule 1: V-type ATP synthase alpha chain

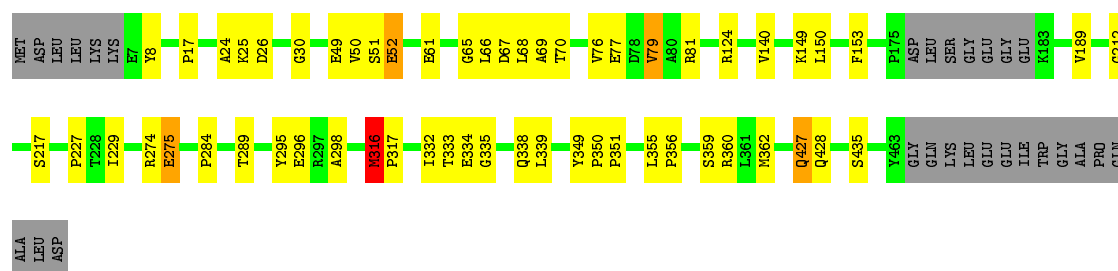


Chain D:  83% 10% • 6%




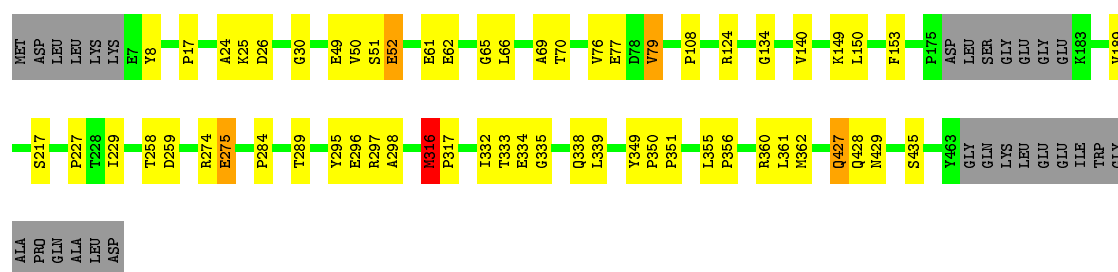
- Molecule 2: V-type ATP synthase beta chain

Chain E:  82% 11% • 6%




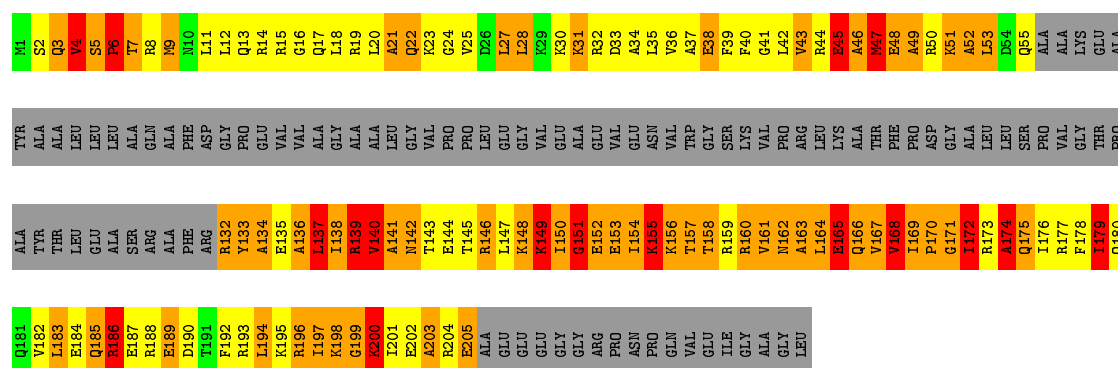
- Molecule 2: V-type ATP synthase beta chain

Chain F:  82% 12% • 6%




- Molecule 3: V-type ATP synthase subunit D

Chain G:  23% 24% 8% 42%



- Molecule 4: V-type ATP synthase subunit F

Chain H: 



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

Chain I: 



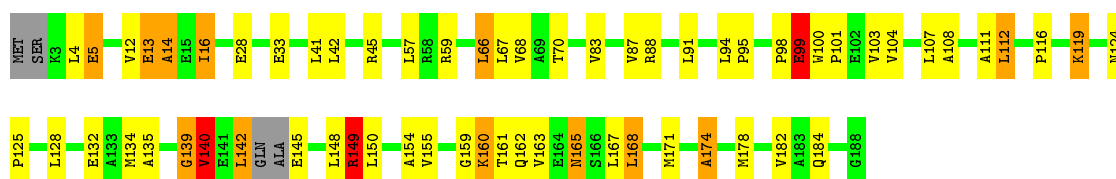
- Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

Chain K: 



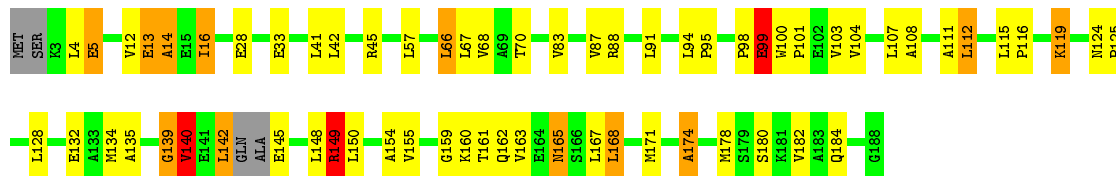
- Molecule 6: V-type ATP synthase subunit E

Chain J: 



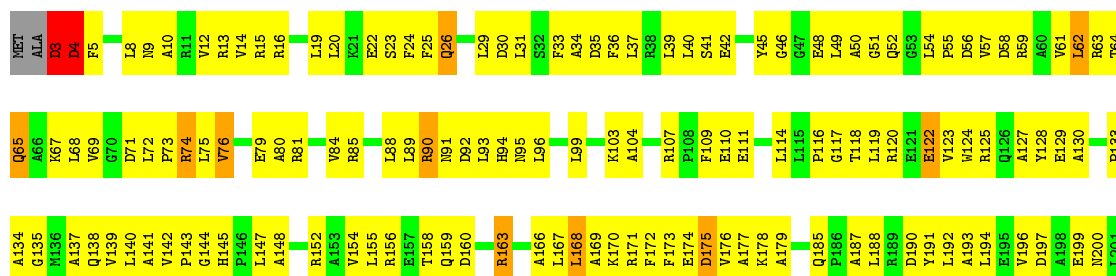
- Molecule 6: V-type ATP synthase subunit E

Chain L: 



- Molecule 7: V-type ATP synthase subunit C

Chain M: 






4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	46105	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Each particle	Depositor
Microscope	Tecnai F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.18	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	50000	Depositor
Image detector	Film	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	0.59	3/2750 (0.1%)	1.38	13/3815 (0.3%)
1	B	0.59	3/2750 (0.1%)	1.21	11/3815 (0.3%)
1	C	0.60	3/2750 (0.1%)	1.34	13/3815 (0.3%)
2	D	0.74	3/2210 (0.1%)	1.01	9/3068 (0.3%)
2	E	0.75	3/2210 (0.1%)	1.00	8/3068 (0.3%)
2	F	0.73	3/2210 (0.1%)	0.99	7/3068 (0.2%)
3	G	4.09	125/637 (19.6%)	2.63	50/885 (5.6%)
4	H	1.78	10/508 (2.0%)	2.16	15/703 (2.1%)
5	I	0.42	1/749 (0.1%)	0.48	0/1004
5	K	0.42	1/749 (0.1%)	0.48	0/1004
6	J	0.45	2/1325 (0.2%)	0.53	0/1798
6	L	0.45	2/1325 (0.2%)	0.53	0/1798
7	M	1.22	5/2553 (0.2%)	1.11	12/3447 (0.3%)
All	All	1.02	164/22726 (0.7%)	1.19	138/31288 (0.4%)

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	6
1	B	0	6
1	C	0	6
2	D	0	4
2	E	0	3
2	F	0	3
4	H	0	2
7	M	0	1
All	All	0	31

The worst 5 of 164 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	47	MET	CA-CB	-24.99	0.98	1.53
3	G	27	LEU	CA-CB	14.81	1.87	1.53
4	H	75	ALA	N-CA	13.46	1.73	1.46
3	G	7	THR	CA-CB	12.79	1.86	1.53
3	G	31	LYS	N-CA	12.37	1.71	1.46

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ASP	O-C-N	-39.91	58.85	122.70
1	B	325	ASP	O-C-N	-39.91	58.85	122.70
1	C	325	ASP	O-C-N	-39.84	58.95	122.70
1	C	70	PRO	C-N-CA	-27.46	53.06	121.70
4	H	76	GLY	N-CA-C	26.73	179.94	113.10

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Peptide
1	A	210	ARG	Mainchain
1	A	297	ALA	Mainchain
1	A	325	ASP	Mainchain
1	A	69	LEU	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	2752	0	1300	122	0
1	B	2752	0	1303	59	0
1	C	2752	0	1302	86	0
2	D	2212	0	1009	80	0
2	E	2212	0	1009	84	0
2	F	2212	0	1009	83	0
3	G	639	0	299	136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	509	0	255	23	0
5	I	747	0	726	21	0
5	K	747	0	726	18	0
6	J	1312	0	1240	74	0
6	L	1312	0	1240	56	0
7	M	2514	0	2583	624	0
8	A	27	0	12	0	0
8	C	27	0	12	4	0
All	All	22726	0	14025	1287	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 35.

The worst 5 of 1287 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)
7:M:33:PHE:CG	7:M:308:TYR:HD1	1.08	1.66
7:M:33:PHE:CD2	7:M:308:TYR:CD1	1.83	1.64
7:M:20:LEU:HD23	7:M:24:PHE:CD1	1.11	1.61
2:E:25:LYS:CA	6:J:161:THR:HG23	1.14	1.61
3:G:189:GLU:CB	3:G:189:GLU:CA	1.76	1.61

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	557/578 (96%)	493 (88%)	48 (9%)	16 (3%)	6	43
1	B	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	5	41
1	C	557/578 (96%)	492 (88%)	48 (9%)	17 (3%)	5	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	9	51
2	E	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	9	51
2	F	446/478 (93%)	420 (94%)	16 (4%)	10 (2%)	8	49
3	G	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	2
4	H	102/104 (98%)	90 (88%)	10 (10%)	2 (2%)	9	51
5	I	98/104 (94%)	90 (92%)	6 (6%)	2 (2%)	9	51
5	K	98/104 (94%)	90 (92%)	6 (6%)	2 (2%)	9	51
6	J	180/188 (96%)	156 (87%)	14 (8%)	10 (6%)	2	28
6	L	180/188 (96%)	156 (87%)	14 (8%)	10 (6%)	2	28
7	M	318/323 (98%)	281 (88%)	32 (10%)	5 (2%)	12	56
All	All	4110/4402 (93%)	3678 (90%)	293 (7%)	139 (3%)	8	40

5 of 139 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	A	19	MET
1	A	53	GLU
1	A	143	PHE
1	A	227	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	62/76 (82%)	59 (95%)	3 (5%)	31	67
5	K	62/76 (82%)	59 (95%)	3 (5%)	31	67
6	J	108/141 (77%)	94 (87%)	14 (13%)	5	28
6	L	108/141 (77%)	94 (87%)	14 (13%)	5	28
7	M	254/256 (99%)	246 (97%)	8 (3%)	47	77
All	All	594/690 (86%)	552 (93%)	42 (7%)	23	55

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	K	69	LEU
6	L	66	LEU
7	M	65	GLN
5	K	119	LEU
6	L	28	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
7	M	9	ASN
7	M	52	GLN
7	M	65	GLN
7	M	94	HIS
7	M	185	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](#)

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
8	ADP	A	600	-	24,29,29	1.11	3 (12%)	23,45,45	0.71	0
8	ADP	C	600	-	24,29,29	1.02	2 (8%)	23,45,45	1.08	3 (13%)

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
8	ADP	A	600	-	-	0/12/32/32	0/3/3/3
8	ADP	C	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)
8	C	600	ADP	PB-O2B	-2.70	1.45	1.54
8	A	600	ADP	PB-O2B	-2.59	1.45	1.54
8	C	600	ADP	PA-O1A	-2.36	1.42	1.51
8	A	600	ADP	PB-O3B	-2.15	1.47	1.54
8	A	600	ADP	O4'-C1'	2.42	1.44	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	600	ADP	C1'-N9-C4	-2.08	124.48	126.81
8	C	600	ADP	O4'-C4'-C3'	-2.02	101.06	105.16
8	C	600	ADP	O3B-PB-O2B	2.53	116.74	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	600	ADP	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.