wwPDB EM Validation Summary Report (i)

May 13, 2024 – 09:40 pm BST

PDB ID	:	6T8O
EMDB ID	:	EMD-10402
Title	:	Stalled FtsK motor domain bound to dsDNA end
Authors	:	Jean, N.L.; Lowe, J.
Deposited on	:	2019-10-24
Resolution	:	3.99 Å(reported)
Based on initial model	:	2IUU

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

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

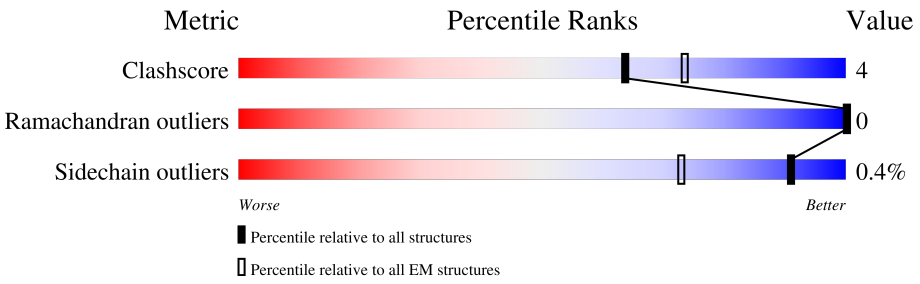
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.99 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 of the bar indicate the fraction of residues that contain outliers for >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	491	68% 12% 20%
1	B	491	69% 11% 20%
1	C	491	71% 10% 19%
1	D	491	68% 12% 19%
1	E	491	73% 8% 19%
1	F	491	72% 9% 19%
2	G	14	93% 7%
2	H	14	93% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18806 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 DNA translocase FtsK.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	395	3014	1917	521	561	15	0	0
1	B	392	2991	1903	517	556	15	0	0
1	C	398	3038	1935	524	564	15	0	0
1	D	396	3018	1921	521	561	15	0	0
1	E	396	3021	1922	522	562	15	0	0
1	F	397	3029	1928	523	563	15	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	MET	-	initiating methionine	UNP Q9I0M3
A	729	LYS	-	expression tag	UNP Q9I0M3
A	730	LEU	-	expression tag	UNP Q9I0M3
A	731	HIS	-	expression tag	UNP Q9I0M3
A	732	HIS	-	expression tag	UNP Q9I0M3
A	733	HIS	-	expression tag	UNP Q9I0M3
A	734	HIS	-	expression tag	UNP Q9I0M3
A	735	HIS	-	expression tag	UNP Q9I0M3
A	736	HIS	-	expression tag	UNP Q9I0M3
B	246	MET	-	initiating methionine	UNP Q9I0M3
B	729	LYS	-	expression tag	UNP Q9I0M3
B	730	LEU	-	expression tag	UNP Q9I0M3
B	731	HIS	-	expression tag	UNP Q9I0M3
B	732	HIS	-	expression tag	UNP Q9I0M3
B	733	HIS	-	expression tag	UNP Q9I0M3
B	734	HIS	-	expression tag	UNP Q9I0M3
B	735	HIS	-	expression tag	UNP Q9I0M3
B	736	HIS	-	expression tag	UNP Q9I0M3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	246	MET	-	initiating methionine	UNP Q9I0M3
C	729	LYS	-	expression tag	UNP Q9I0M3
C	730	LEU	-	expression tag	UNP Q9I0M3
C	731	HIS	-	expression tag	UNP Q9I0M3
C	732	HIS	-	expression tag	UNP Q9I0M3
C	733	HIS	-	expression tag	UNP Q9I0M3
C	734	HIS	-	expression tag	UNP Q9I0M3
C	735	HIS	-	expression tag	UNP Q9I0M3
C	736	HIS	-	expression tag	UNP Q9I0M3
D	246	MET	-	initiating methionine	UNP Q9I0M3
D	729	LYS	-	expression tag	UNP Q9I0M3
D	730	LEU	-	expression tag	UNP Q9I0M3
D	731	HIS	-	expression tag	UNP Q9I0M3
D	732	HIS	-	expression tag	UNP Q9I0M3
D	733	HIS	-	expression tag	UNP Q9I0M3
D	734	HIS	-	expression tag	UNP Q9I0M3
D	735	HIS	-	expression tag	UNP Q9I0M3
D	736	HIS	-	expression tag	UNP Q9I0M3
E	246	MET	-	initiating methionine	UNP Q9I0M3
E	729	LYS	-	expression tag	UNP Q9I0M3
E	730	LEU	-	expression tag	UNP Q9I0M3
E	731	HIS	-	expression tag	UNP Q9I0M3
E	732	HIS	-	expression tag	UNP Q9I0M3
E	733	HIS	-	expression tag	UNP Q9I0M3
E	734	HIS	-	expression tag	UNP Q9I0M3
E	735	HIS	-	expression tag	UNP Q9I0M3
E	736	HIS	-	expression tag	UNP Q9I0M3
F	246	MET	-	initiating methionine	UNP Q9I0M3
F	729	LYS	-	expression tag	UNP Q9I0M3
F	730	LEU	-	expression tag	UNP Q9I0M3
F	731	HIS	-	expression tag	UNP Q9I0M3
F	732	HIS	-	expression tag	UNP Q9I0M3
F	733	HIS	-	expression tag	UNP Q9I0M3
F	734	HIS	-	expression tag	UNP Q9I0M3
F	735	HIS	-	expression tag	UNP Q9I0M3
F	736	HIS	-	expression tag	UNP Q9I0M3

- Molecule 2 is a DNA chain called dsDNA substrate.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	G	13	267	130	47	77	13	0	0

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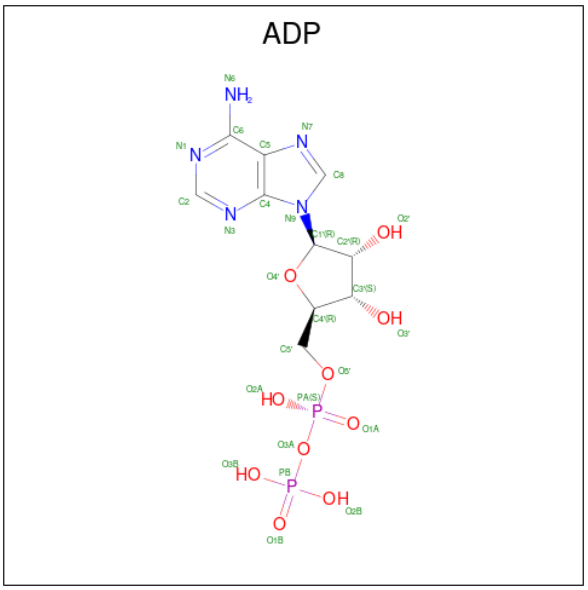
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	H	13	266	130	44	79	13	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



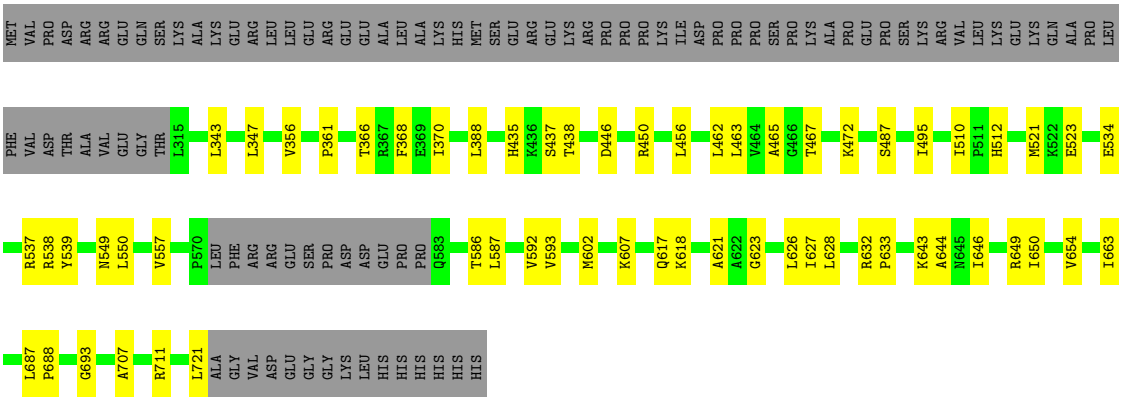
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	27	10	5	10	2	0
3	B	1	27	10	5	10	2	0
3	C	1	27	10	5	10	2	0
3	D	1	27	10	5	10	2	0
3	E	1	27	10	5	10	2	0
3	F	1	27	10	5	10	2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

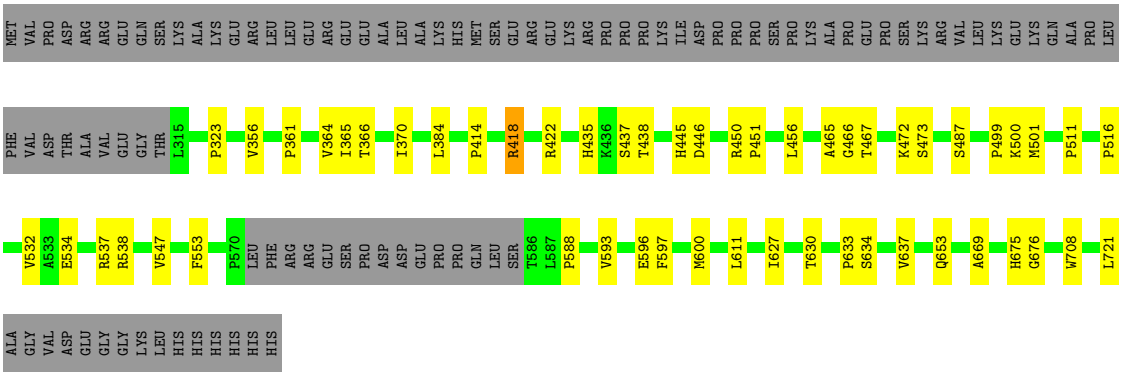
- Molecule 1: DNA translocase FtsK

Chain A:



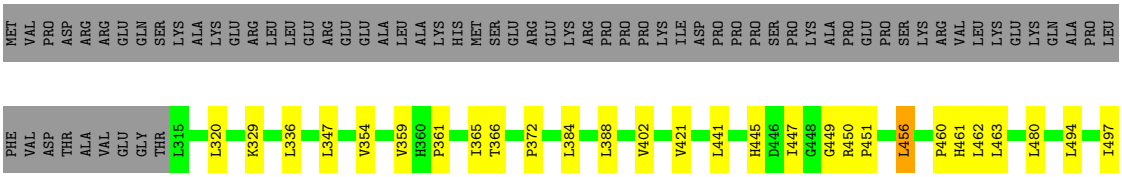
- Molecule 1: DNA translocase FtsK

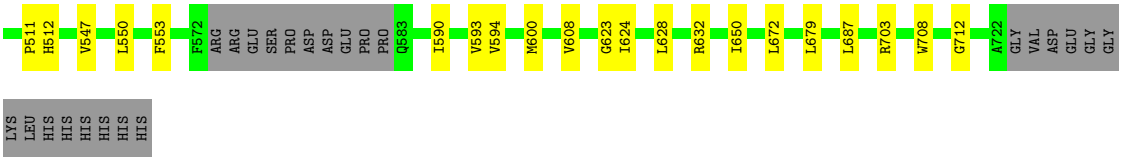
Chain B:



- Molecule 1: DNA translocase FtsK

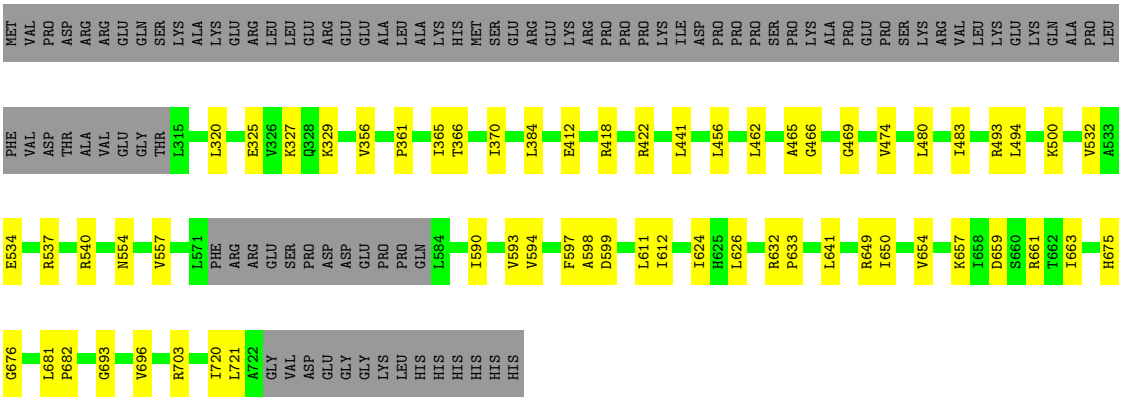
Chain C:





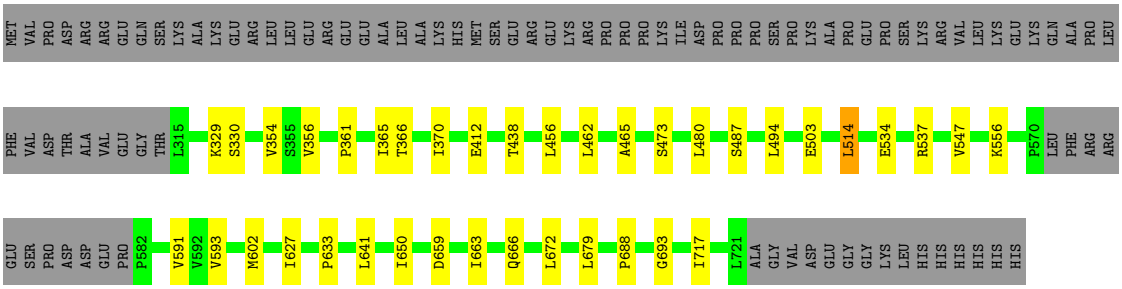
• Molecule 1: DNA translocase FtsK

Chain D:



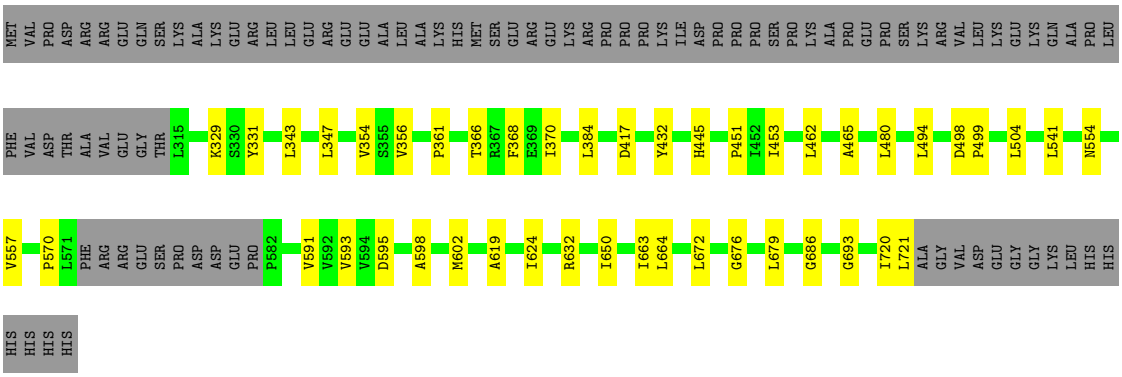
• Molecule 1: DNA translocase FtsK

Chain E:



• Molecule 1: DNA translocase FtsK

Chain F:



• Molecule 2: dsDNA substrate

Chain G: 93% 7%

• Molecule 2: dsDNA substrate

Chain H: 93% 7%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53289	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 ($e^-/Å^2$)	42.95	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.30	0/3058	0.54	0/4149
1	B	0.29	0/3042	0.55	2/4126 (0.0%)
1	C	0.31	0/3090	0.53	1/4191 (0.0%)
1	D	0.31	0/3069	0.53	1/4163 (0.0%)
1	E	0.33	1/3073 (0.0%)	0.53	0/4168
1	F	0.33	0/3081	0.54	2/4179 (0.0%)
2	G	0.60	0/299	1.10	0/459
2	H	0.61	0/297	1.10	0/456
All	All	0.32	1/19009 (0.0%)	0.57	6/25891 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	514	LEU	C-N	-5.16	1.22	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	456	LEU	CA-CB-CG	6.01	129.12	115.30
1	B	384	LEU	CA-CB-CG	5.74	128.49	115.30
1	F	384	LEU	CA-CB-CG	5.65	128.29	115.30
1	F	686	GLY	C-N-CA	5.16	134.60	121.70
1	C	456	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3014	0	3140	34	0
1	B	2991	0	3116	31	0
1	C	3038	0	3165	24	0
1	D	3018	0	3148	31	0
1	E	3021	0	3148	24	0
1	F	3029	0	3159	24	0
2	G	267	0	150	0	0
2	H	266	0	151	0	0
3	A	27	0	12	2	0
3	B	27	0	12	2	0
3	C	27	0	12	0	0
3	D	27	0	12	1	0
3	E	27	0	12	2	0
3	F	27	0	12	0	0
All	All	18806	0	19249	164	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 4.

The worst 5 of 164 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:593:VAL:HG12	1:B:627:ILE:HB	1.78	0.64
1:E:456:LEU:HD11	1:E:627:ILE:HD11	1.80	0.63
1:D:720:ILE:HG23	1:D:721:LEU:HG	1.81	0.61
1:B:465:ALA:HB1	1:B:633:PRO:HB3	1.83	0.59
1:B:418:ARG:HH12	1:B:676:GLY:HA3	1.68	0.59

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	391/491 (80%)	368 (94%)	23 (6%)	0	100	100
1	B	388/491 (79%)	358 (92%)	30 (8%)	0	100	100
1	C	394/491 (80%)	377 (96%)	17 (4%)	0	100	100
1	D	392/491 (80%)	370 (94%)	22 (6%)	0	100	100
1	E	392/491 (80%)	372 (95%)	20 (5%)	0	100	100
1	F	393/491 (80%)	369 (94%)	24 (6%)	0	100	100
All	All	2350/2946 (80%)	2214 (94%)	136 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	334/419 (80%)	333 (100%)	1 (0%)	92	95
1	B	331/419 (79%)	330 (100%)	1 (0%)	92	95
1	C	336/419 (80%)	332 (99%)	4 (1%)	71	84
1	D	334/419 (80%)	333 (100%)	1 (0%)	92	95
1	E	335/419 (80%)	335 (100%)	0	100	100
1	F	336/419 (80%)	335 (100%)	1 (0%)	92	95
All	All	2006/2514 (80%)	1998 (100%)	8 (0%)	91	94

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	329	LYS
1	D	540	ARG
1	C	450	ARG
1	C	384	LEU
1	C	632	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	666	GLN
1	F	692	HIS
1	A	625	HIS
1	D	675	HIS
1	E	435	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
3	ADP	F	801	-	24,29,29	0.97	1 (4%)	29,45,45	1.47	4 (13%)
3	ADP	A	801	-	24,29,29	0.93	1 (4%)	29,45,45	1.46	4 (13%)
3	ADP	B	801	-	24,29,29	0.96	1 (4%)	29,45,45	1.37	3 (10%)
3	ADP	D	801	-	24,29,29	0.94	1 (4%)	29,45,45	1.45	4 (13%)
3	ADP	E	801	-	24,29,29	0.95	1 (4%)	29,45,45	1.55	4 (13%)
3	ADP	C	801	-	24,29,29	0.97	1 (4%)	29,45,45	1.48	5 (17%)

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
3	ADP	F	801	-	-	4/12/32/32	0/3/3/3
3	ADP	A	801	-	-	1/12/32/32	0/3/3/3
3	ADP	B	801	-	-	2/12/32/32	0/3/3/3
3	ADP	D	801	-	-	0/12/32/32	0/3/3/3
3	ADP	E	801	-	-	1/12/32/32	0/3/3/3
3	ADP	C	801	-	-	4/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	ADP	C5-C4	2.42	1.47	1.40
3	C	801	ADP	C5-C4	2.38	1.47	1.40
3	A	801	ADP	C5-C4	2.34	1.47	1.40
3	F	801	ADP	C5-C4	2.32	1.47	1.40
3	D	801	ADP	C5-C4	2.31	1.47	1.40

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	801	ADP	PA-O3A-PB	-4.20	118.41	132.83
3	F	801	ADP	PA-O3A-PB	-4.00	119.11	132.83
3	D	801	ADP	PA-O3A-PB	-3.82	119.71	132.83
3	A	801	ADP	PA-O3A-PB	-3.79	119.83	132.83
3	C	801	ADP	PA-O3A-PB	-3.57	120.57	132.83

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

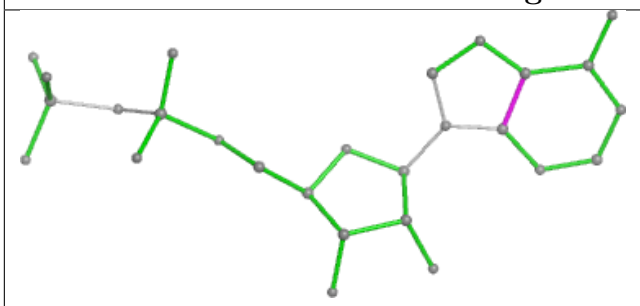
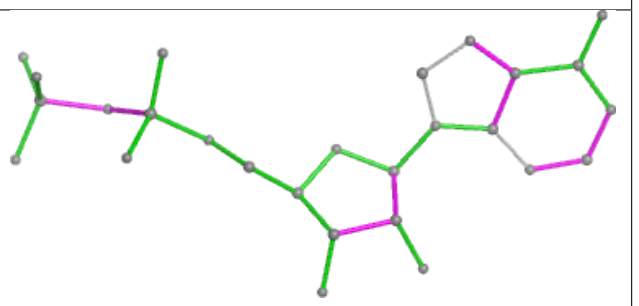
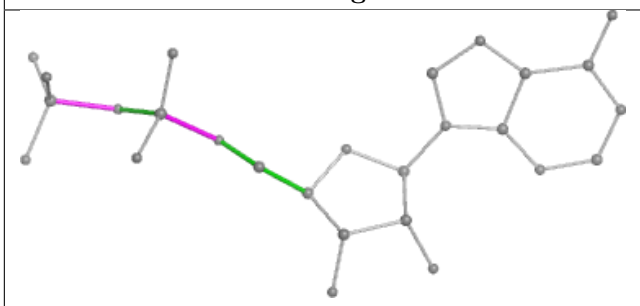
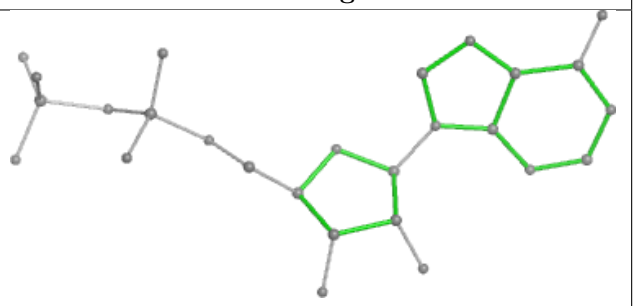
Mol	Chain	Res	Type	Atoms
3	B	801	ADP	C5'-O5'-PA-O1A
3	C	801	ADP	C5'-O5'-PA-O3A
3	C	801	ADP	C3'-C4'-C5'-O5'
3	C	801	ADP	O4'-C4'-C5'-O5'
3	F	801	ADP	PA-O3A-PB-O2B

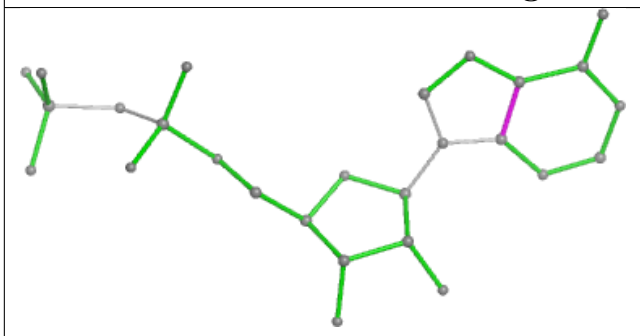
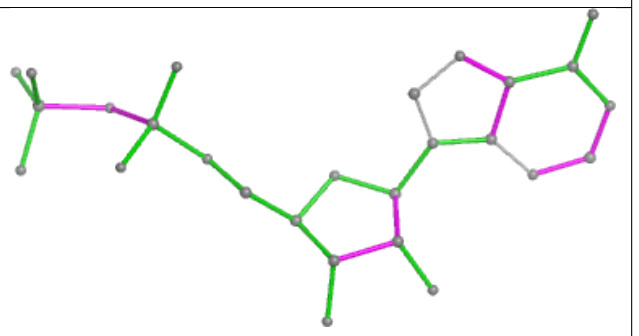
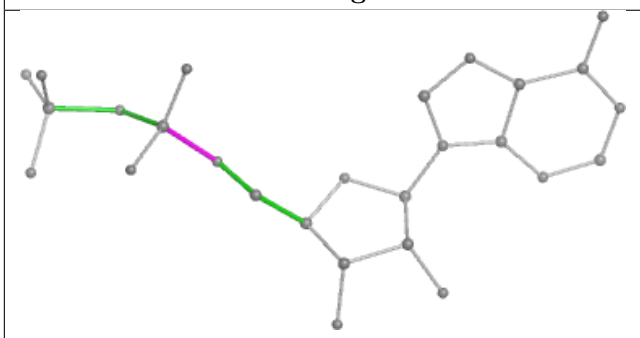
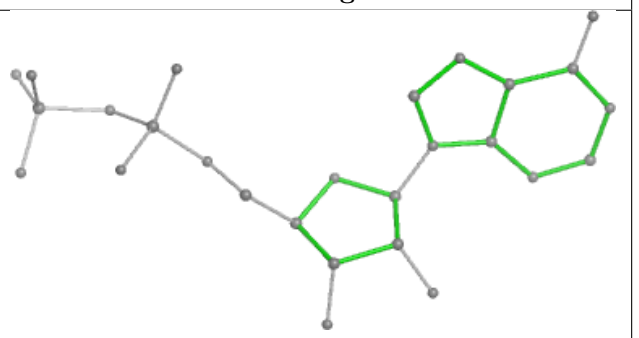
There are no ring outliers.

4 monomers are involved in 7 short contacts:

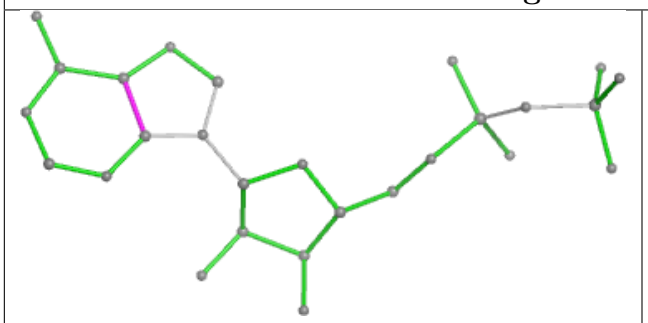
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	ADP	2	0
3	B	801	ADP	2	0
3	D	801	ADP	1	0
3	E	801	ADP	2	0

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 then 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.

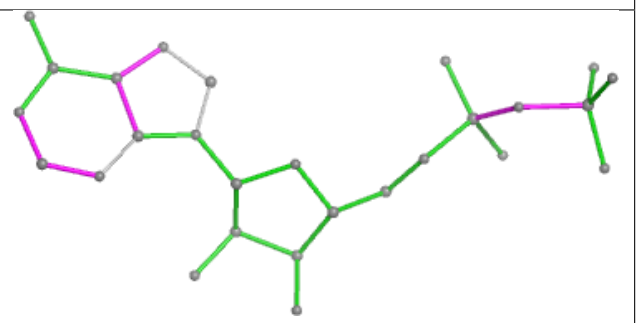
Ligand ADP F 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

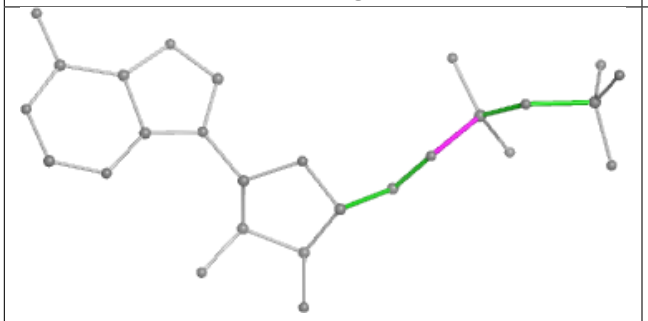
Ligand ADP B 801



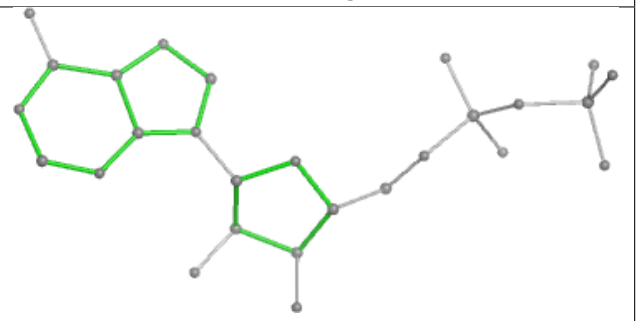
Bond lengths



Bond angles

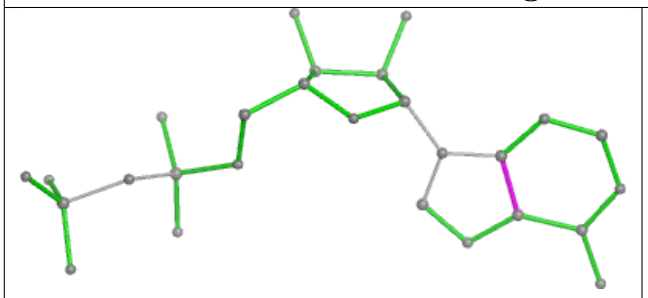


Torsions

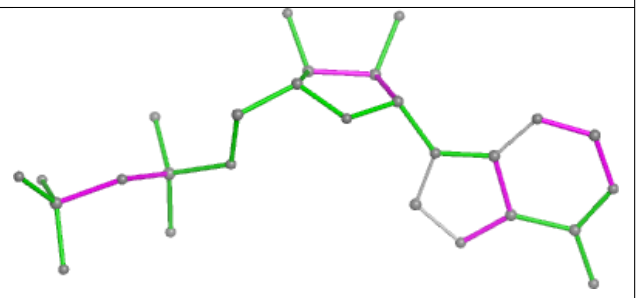


Rings

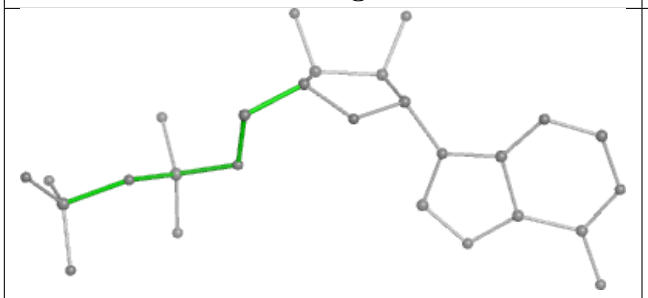
Ligand ADP D 801



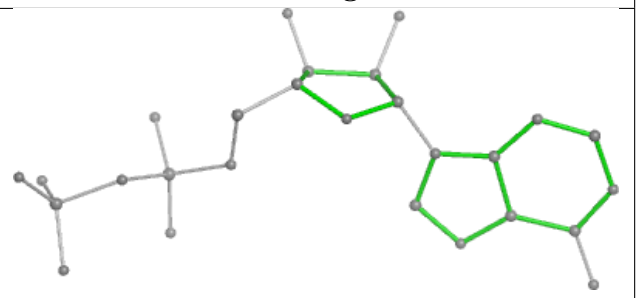
Bond lengths



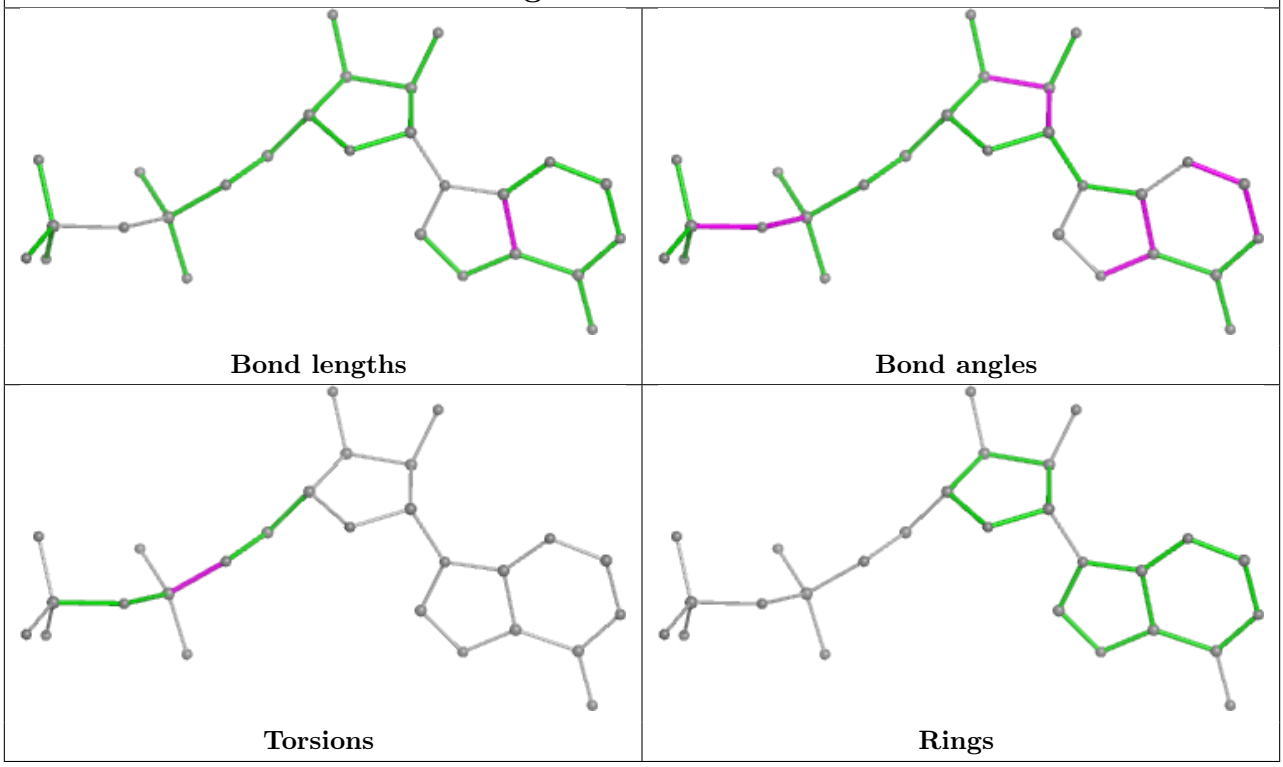
Bond angles

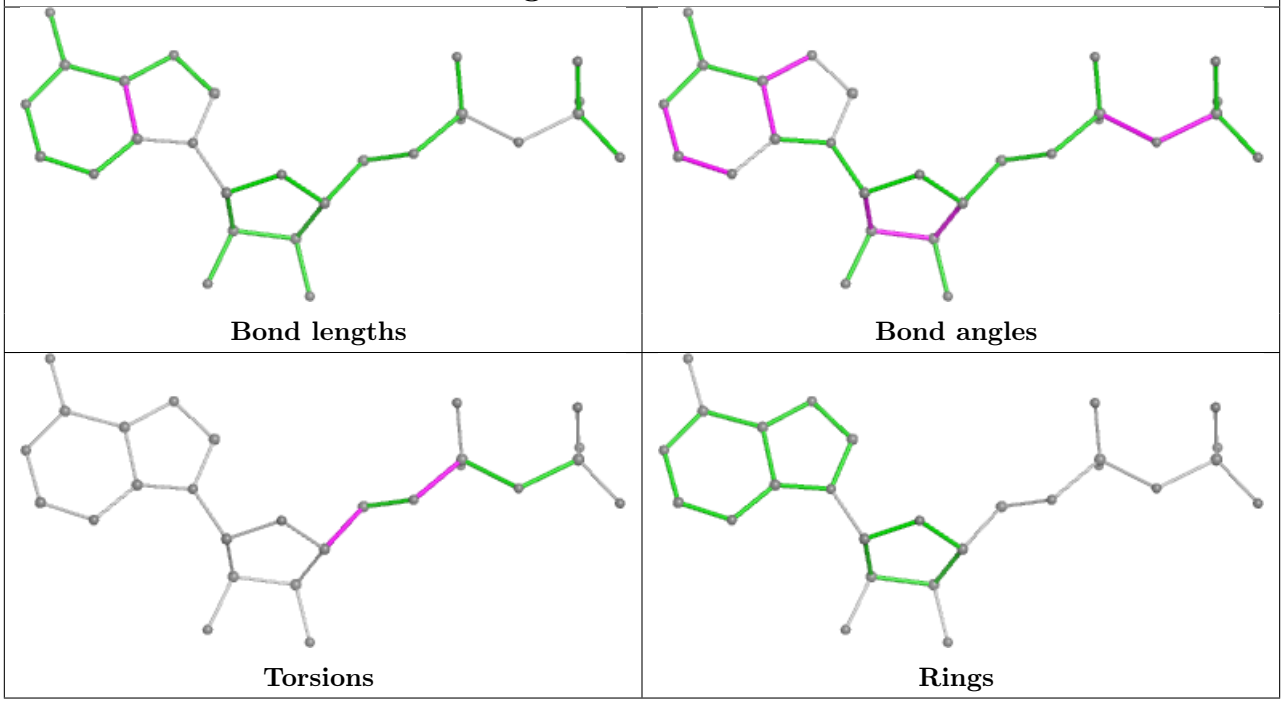


Torsions



Rings

Ligand ADP E 801	
 Bond lengths	Bond angles
Torsions	Rings

Ligand ADP C 801	
 Bond lengths	Bond angles
Torsions	Rings

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.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10402. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

This section was not generated.