



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:07 PM UTC

PDB ID : 4EAH / pdb_00004eah
Title : Crystal structure of the formin homology 2 domain of FMNL3 bound to actin
Authors : Thompson, M.E.; Heimsath, E.G.; Gauvin, T.J.; Higgs, H.N.; Kull, F.J.
Deposited on : 2012-03-22
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

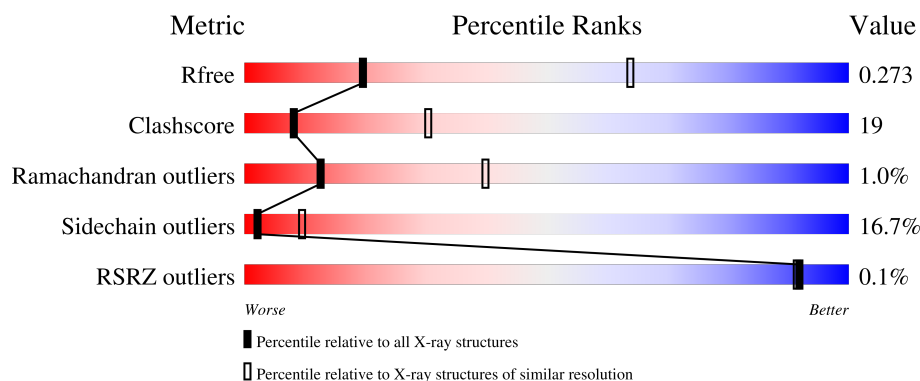
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	377	<div> <div>51%</div> <div>34%</div> <div>8%</div> <div>6%</div> </div>
1	F	377	<div> <div>51%</div> <div>36%</div> <div>8%</div> <div>6%</div> </div>
1	G	377	<div> <div>50%</div> <div>36%</div> <div>8%</div> <div>6%</div> </div>
1	H	377	<div> <div>49%</div> <div>38%</div> <div>8%</div> <div>6%</div> </div>
2	A	402	<div> <div>50%</div> <div>31%</div> <div>6%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	402	
2	C	402	
2	E	402	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	B	1001	-	-	X	-
3	ACT	D	401	-	-	X	-
3	ACT	G	401	-	-	X	-
3	ACT	H	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22892 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	356	Total	C	N	O	S	121	0	0
			2785	1766	468	533	18			
1	H	356	Total	C	N	O	S	123	0	0
			2785	1766	468	533	18			
1	G	356	Total	C	N	O	S	132	0	0
			2785	1766	468	533	18			
1	F	356	Total	C	N	O	S	65	0	0
			2785	1766	468	533	18			

- Molecule 2 is a protein called Formin-like protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	357	Total	C	N	O	S	265	0	0
			2895	1848	502	533	12			
2	E	357	Total	C	N	O	S	272	0	0
			2895	1848	502	533	12			
2	C	357	Total	C	N	O	S	252	0	0
			2895	1848	502	533	12			
2	B	357	Total	C	N	O	S	260	0	0
			2895	1848	502	533	12			

There are 8 discrepancies between the modelled and reference sequences:

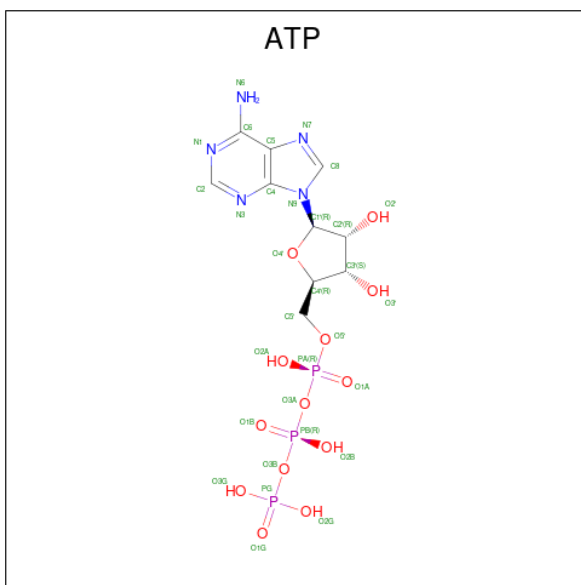
Chain	Residue	Modelled	Actual	Comment	Reference
A	553	GLY	-	expression tag	UNP Q6ZPF4
A	554	SER	-	expression tag	UNP Q6ZPF4
E	553	GLY	-	expression tag	UNP Q6ZPF4
E	554	SER	-	expression tag	UNP Q6ZPF4
C	553	GLY	-	expression tag	UNP Q6ZPF4
C	554	SER	-	expression tag	UNP Q6ZPF4
B	553	GLY	-	expression tag	UNP Q6ZPF4
B	554	SER	-	expression tag	UNP Q6ZPF4

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



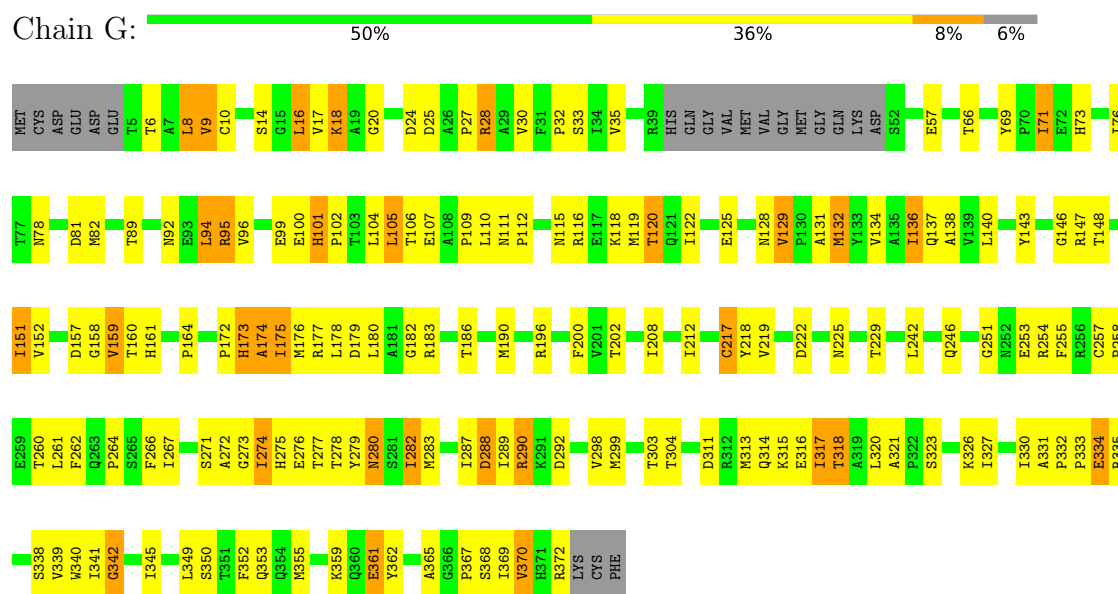
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

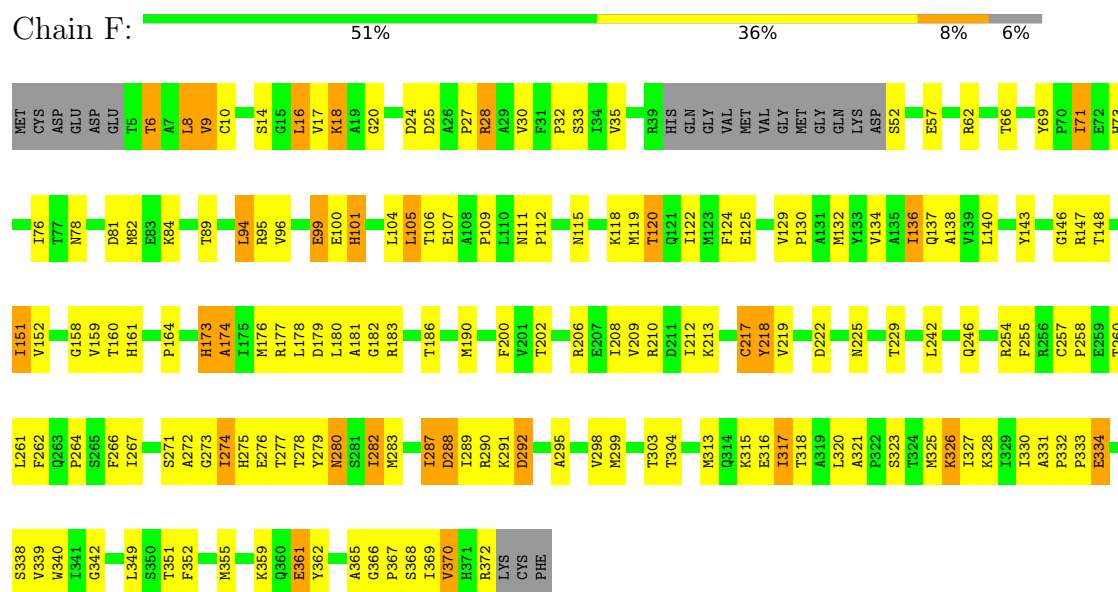


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	H	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	G	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	F	1	Total 31	C 10	N 5	O 13	P 3	0	0

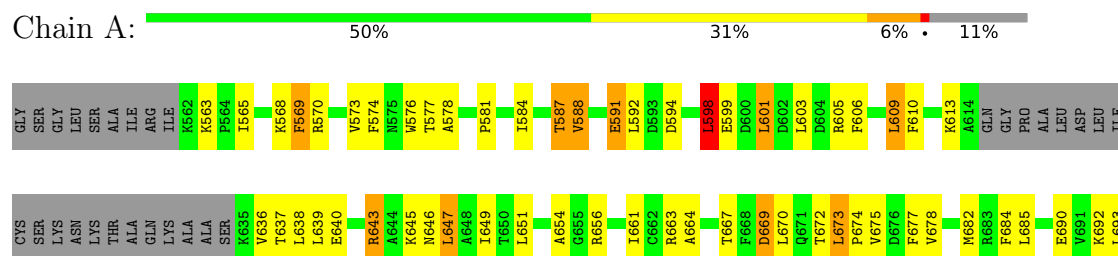
• Molecule 1: Actin, alpha skeletal muscle

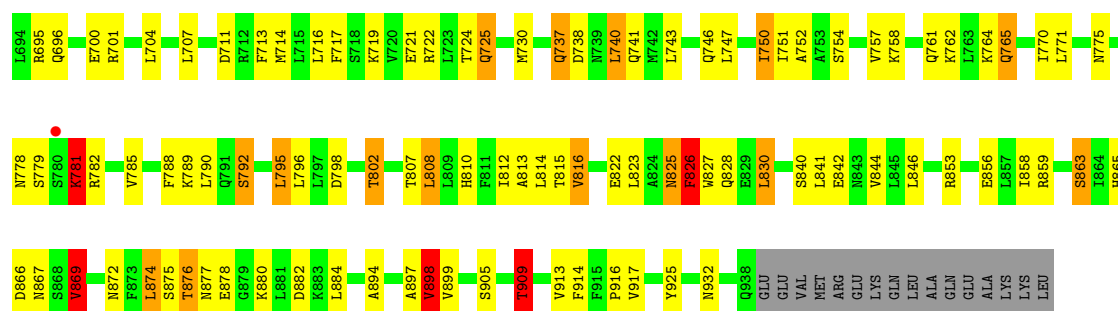


• Molecule 1: Actin, alpha skeletal muscle



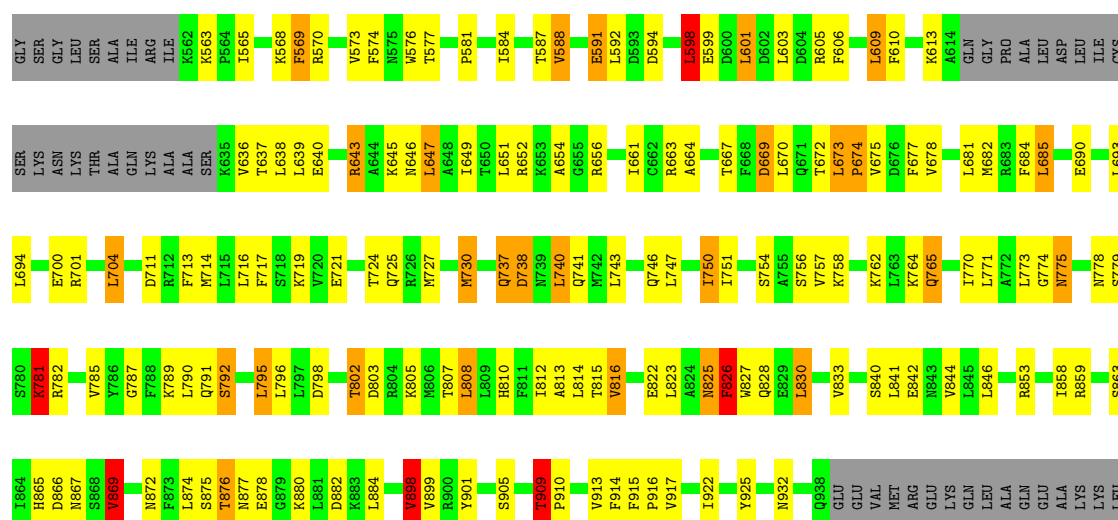
• Molecule 2: Formin-like protein 3





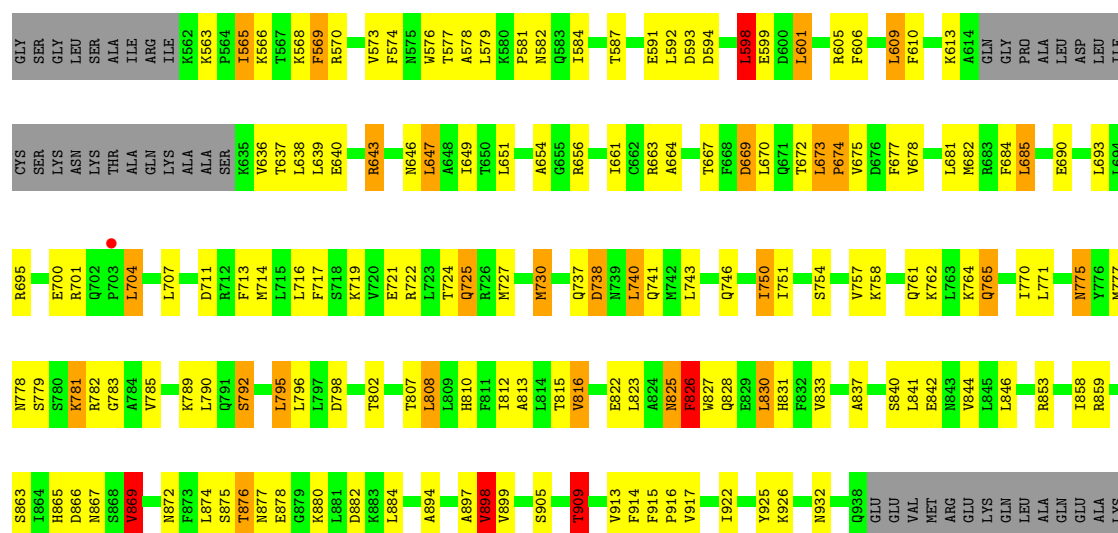
• Molecule 2: Formin-like protein 3

Chain E: 49% 32% 7% 11%



• Molecule 2: Formin-like protein 3

Chain C: 49% 32% 6% 11%



LYS
LYS
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.98Å 126.05Å 129.62Å 90.00° 93.17° 90.00°	Depositor
Resolution (Å)	19.82 – 3.40 19.82 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.82-3.40) 99.2 (19.82-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 3.44Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.230 , 0.277 0.226 , 0.273	Depositor DCC
R_{free} test set	2894 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	98.3	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.037 for l,k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22892	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: ATP, ACT

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	D	0.67	0/2845	1.11	16/3858 (0.4%)
1	F	0.64	0/2845	1.10	16/3858 (0.4%)
1	G	0.62	0/2845	1.09	14/3858 (0.4%)
1	H	0.62	0/2845	1.10	10/3858 (0.3%)
2	A	0.64	0/2942	1.09	11/3956 (0.3%)
2	B	0.62	0/2942	1.09	14/3956 (0.4%)
2	C	0.64	0/2942	1.09	15/3956 (0.4%)
2	E	0.62	0/2942	1.09	13/3956 (0.3%)
All	All	0.63	0/23148	1.10	109/31256 (0.3%)

There are no bond length outliers.

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	331	ALA	CA-C-N	9.02	126.24	119.66
1	F	331	ALA	C-N-CA	9.02	126.24	119.66
2	E	569	PHE	N-CA-C	8.40	123.76	113.17
2	B	569	PHE	N-CA-C	8.37	123.72	113.17
2	C	569	PHE	N-CA-C	8.34	123.67	113.17

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	D	2785	0	2758	102	1
1	F	2785	0	2758	100	1
1	G	2785	0	2758	112	0
1	H	2785	0	2758	115	0
2	A	2895	0	2971	106	0
2	B	2895	0	2971	115	0
2	C	2895	0	2971	107	0
2	E	2895	0	2971	109	0
3	A	12	0	9	1	0
3	B	4	0	3	2	0
3	C	8	0	6	2	0
3	D	4	0	3	2	0
3	E	4	0	3	1	0
3	F	8	0	6	1	0
3	G	4	0	3	2	0
3	H	4	0	3	2	0
4	D	31	0	12	5	0
4	F	31	0	12	1	0
4	G	31	0	12	3	0
4	H	31	0	12	2	0
All	All	22892	0	23000	815	1

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 19.

The worst 5 of 815 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:H:147:ARG:HH12	1:H:330:ILE:HG12	1.29	0.94
1:H:261:LEU:HB3	1:H:274:ILE:HD11	1.54	0.90
1:D:261:LEU:HB3	1:D:274:ILE:HD11	1.55	0.89
1:D:147:ARG:HH12	1:D:330:ILE:HG12	1.36	0.88
1:G:261:LEU:HB3	1:G:274:ILE:HD11	1.55	0.88

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:SER:OG	1:F:62:ARG:O[1_554]	2.11	0.09

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 X-ray entries followed by that with respect to entries of similar resolution.

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	D	352/377 (93%)	326 (93%)	25 (7%)	1 (0%)	36	65
1	F	352/377 (93%)	324 (92%)	27 (8%)	1 (0%)	36	65
1	G	352/377 (93%)	324 (92%)	27 (8%)	1 (0%)	36	65
1	H	352/377 (93%)	325 (92%)	26 (7%)	1 (0%)	36	65
2	A	353/402 (88%)	310 (88%)	37 (10%)	6 (2%)	7	28
2	B	353/402 (88%)	313 (89%)	34 (10%)	6 (2%)	7	28
2	C	353/402 (88%)	313 (89%)	34 (10%)	6 (2%)	7	28
2	E	353/402 (88%)	310 (88%)	38 (11%)	5 (1%)	9	31
All	All	2820/3116 (90%)	2545 (90%)	248 (9%)	27 (1%)	12	40

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	869	VAL
2	E	869	VAL
2	C	869	VAL
2	B	869	VAL
2	A	598	LEU

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 X-ray entries followed by that with respect to entries of similar resolution.

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	D	302/320 (94%)	253 (84%)	49 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	302/320 (94%)	253 (84%)	49 (16%)	2	10
1	G	302/320 (94%)	253 (84%)	49 (16%)	2	10
1	H	302/320 (94%)	254 (84%)	48 (16%)	2	10
2	A	316/351 (90%)	263 (83%)	53 (17%)	2	9
2	B	316/351 (90%)	261 (83%)	55 (17%)	2	8
2	C	316/351 (90%)	262 (83%)	54 (17%)	2	9
2	E	316/351 (90%)	261 (83%)	55 (17%)	2	8
All	All	2472/2684 (92%)	2060 (83%)	412 (17%)	2	9

5 of 412 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	700	GLU
1	H	159	VAL
1	F	303	THR
2	B	740	LEU
2	B	869	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	137	GLN
1	F	137	GLN
1	F	263	GLN
1	F	252	ASN
2	C	746	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	ACT	E	1001	-	3,3,3	0.85	0	3,3,3	1.56	1 (33%)
3	ACT	F	401	-	3,3,3	0.76	0	3,3,3	1.41	0
3	ACT	B	1001	-	3,3,3	0.78	0	3,3,3	1.38	0
3	ACT	H	401	-	3,3,3	0.80	0	3,3,3	1.50	0
4	ATP	G	402	-	32,33,33	1.56	5 (15%)	48,52,52	1.62	9 (18%)
3	ACT	C	1002	-	3,3,3	0.88	0	3,3,3	1.35	0
3	ACT	C	1001	-	3,3,3	0.82	0	3,3,3	1.25	0
4	ATP	H	402	-	32,33,33	1.72	8 (25%)	48,52,52	1.68	10 (20%)
4	ATP	F	403	-	32,33,33	1.63	8 (25%)	48,52,52	1.73	11 (22%)
3	ACT	A	1002	-	3,3,3	0.88	0	3,3,3	1.43	0
4	ATP	D	402	-	32,33,33	1.69	7 (21%)	48,52,52	1.74	12 (25%)
3	ACT	F	402	-	3,3,3	0.73	0	3,3,3	1.34	0
3	ACT	A	1003	-	3,3,3	0.89	0	3,3,3	1.53	1 (33%)
3	ACT	A	1001	-	3,3,3	0.81	0	3,3,3	0.87	0
3	ACT	G	401	-	3,3,3	0.84	0	3,3,3	1.34	0
3	ACT	D	401	-	3,3,3	0.64	0	3,3,3	1.70	1 (33%)

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	ATP	D	402	-	-	8/22/38/38	0/3/3/3
4	ATP	G	402	-	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	H	402	-	-	5/22/38/38	0/3/3/3
4	ATP	F	403	-	-	0/22/38/38	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	402	ATP	C5-C4	5.34	1.48	1.39
4	G	402	ATP	C5-C4	5.02	1.48	1.39
4	D	402	ATP	PB-O3A	4.27	1.64	1.59
4	F	403	ATP	C5-C4	4.20	1.46	1.39
4	F	403	ATP	PB-O3B	4.15	1.64	1.59

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	402	ATP	C5-C4-N3	-5.47	119.18	126.72
4	G	402	ATP	C5-C4-N3	-5.27	119.46	126.72
4	F	403	ATP	C5-C4-N3	-4.98	119.86	126.72
4	D	402	ATP	C5-C4-N3	-4.60	120.38	126.72
4	H	402	ATP	N3-C4-N9	4.46	134.75	127.17

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	402	ATP	C5'-O5'-PA-O1A
4	H	402	ATP	C5'-O5'-PA-O2A
4	H	402	ATP	C5'-O5'-PA-O3A
4	D	402	ATP	PG-O3B-PB-O3A
4	D	402	ATP	PA-O3A-PB-O1B

There are no ring outliers.

13 monomers are involved in 24 short contacts:

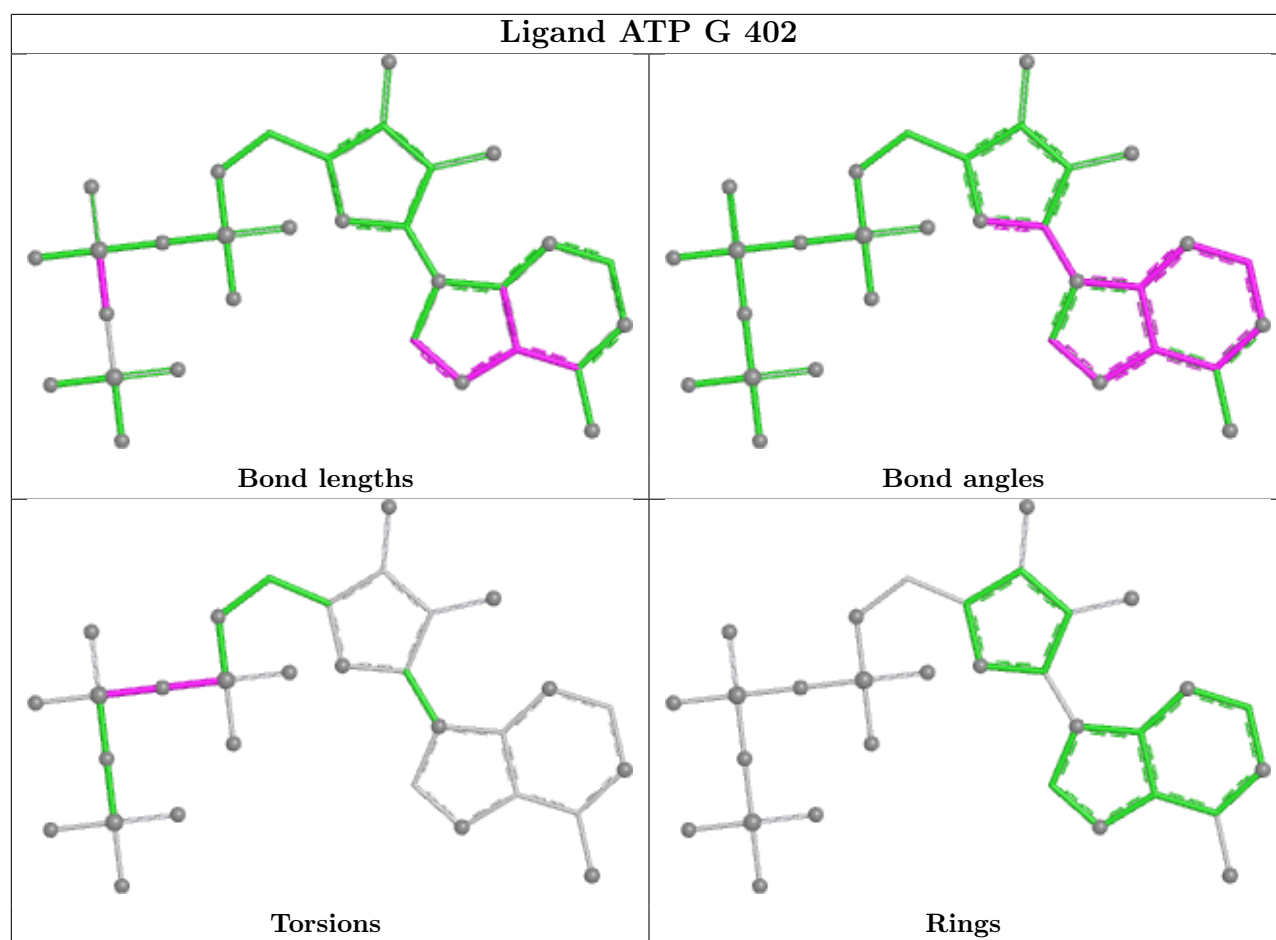
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1001	ACT	1	0
3	B	1001	ACT	2	0
3	H	401	ACT	2	0
4	G	402	ATP	3	0
3	C	1002	ACT	1	0
3	C	1001	ACT	1	0

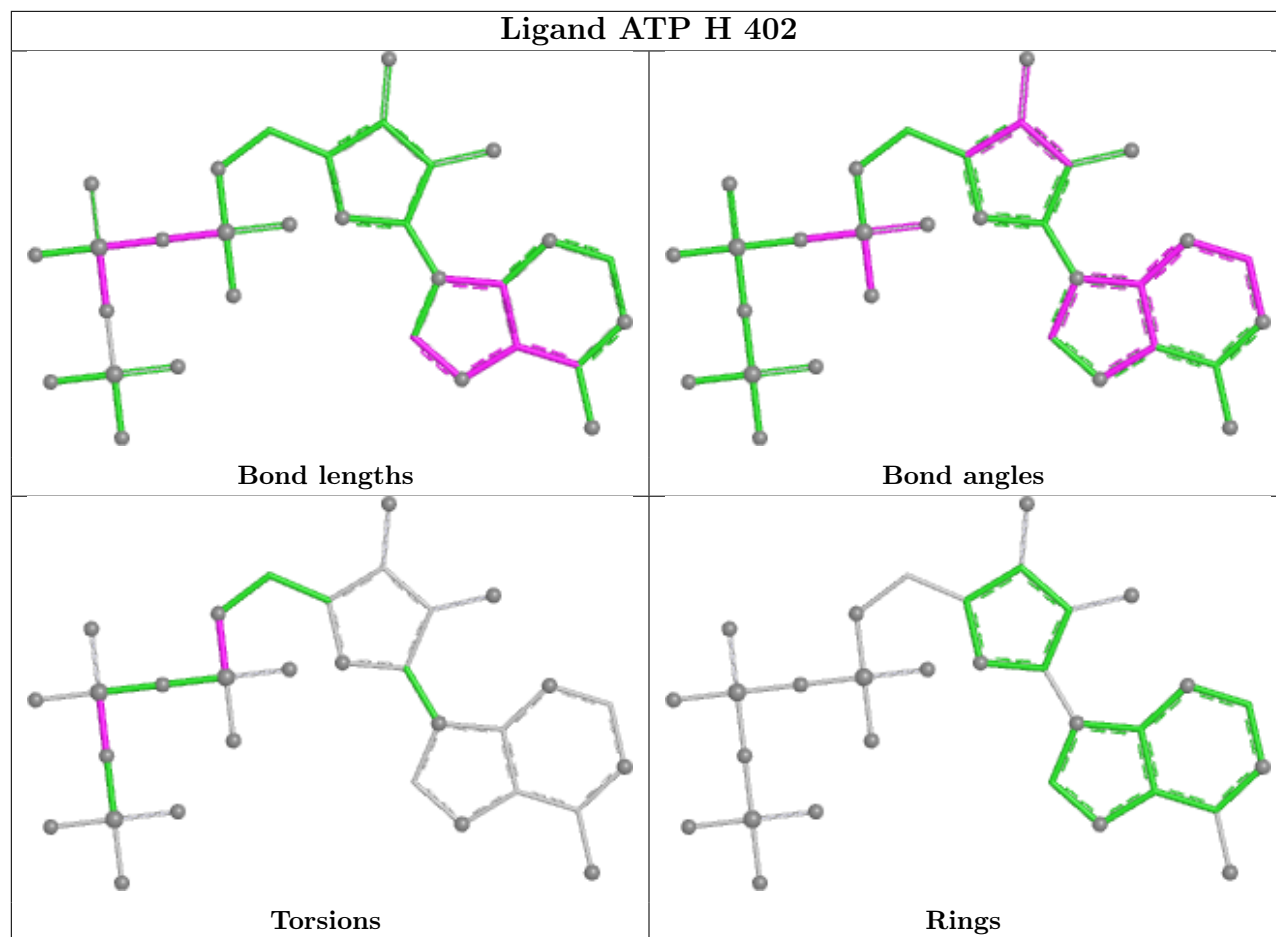
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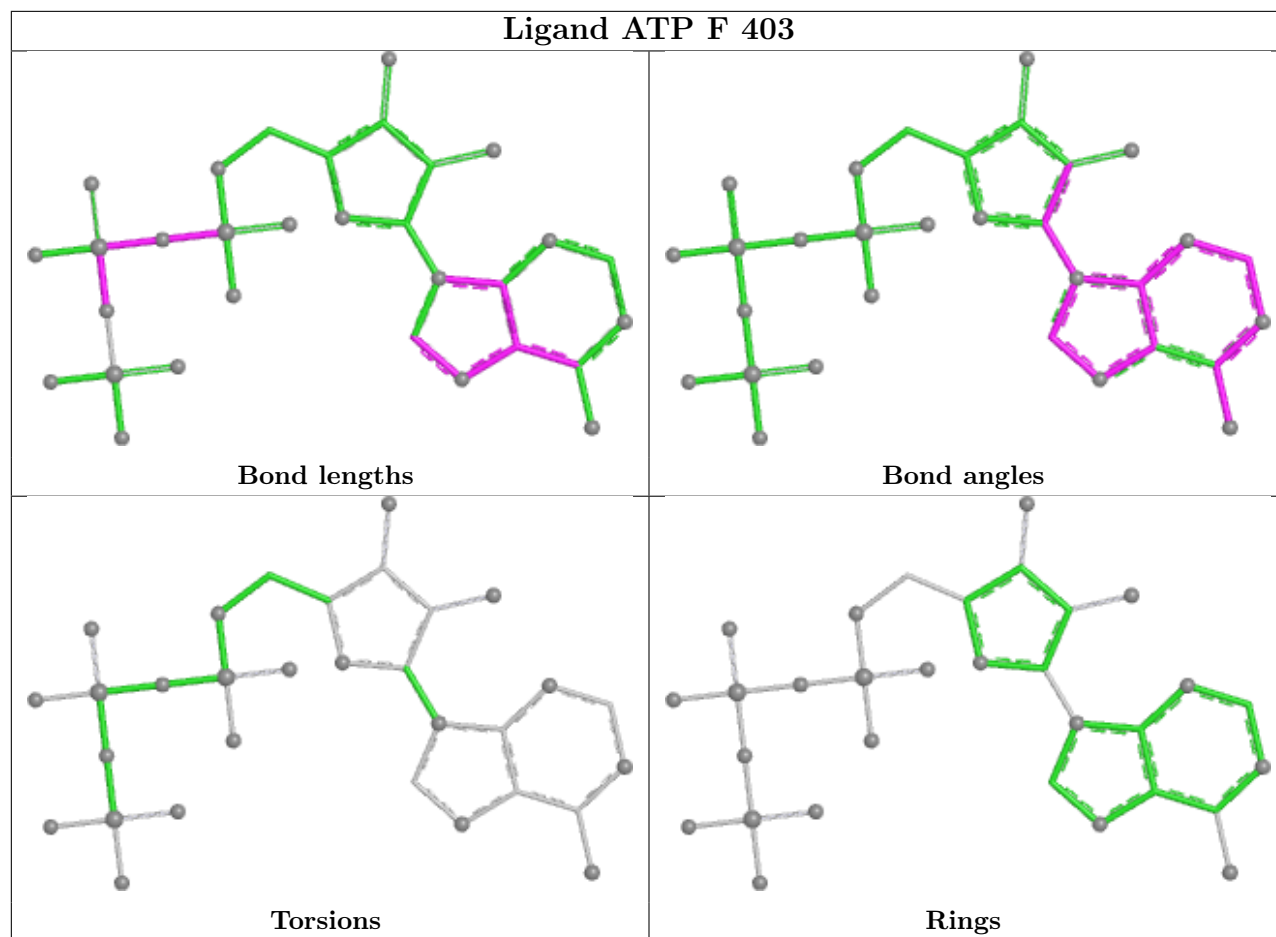
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	402	ATP	2	0
4	F	403	ATP	1	0
4	D	402	ATP	5	0
3	F	402	ACT	1	0
3	A	1003	ACT	1	0
3	G	401	ACT	2	0
3	D	401	ACT	2	0

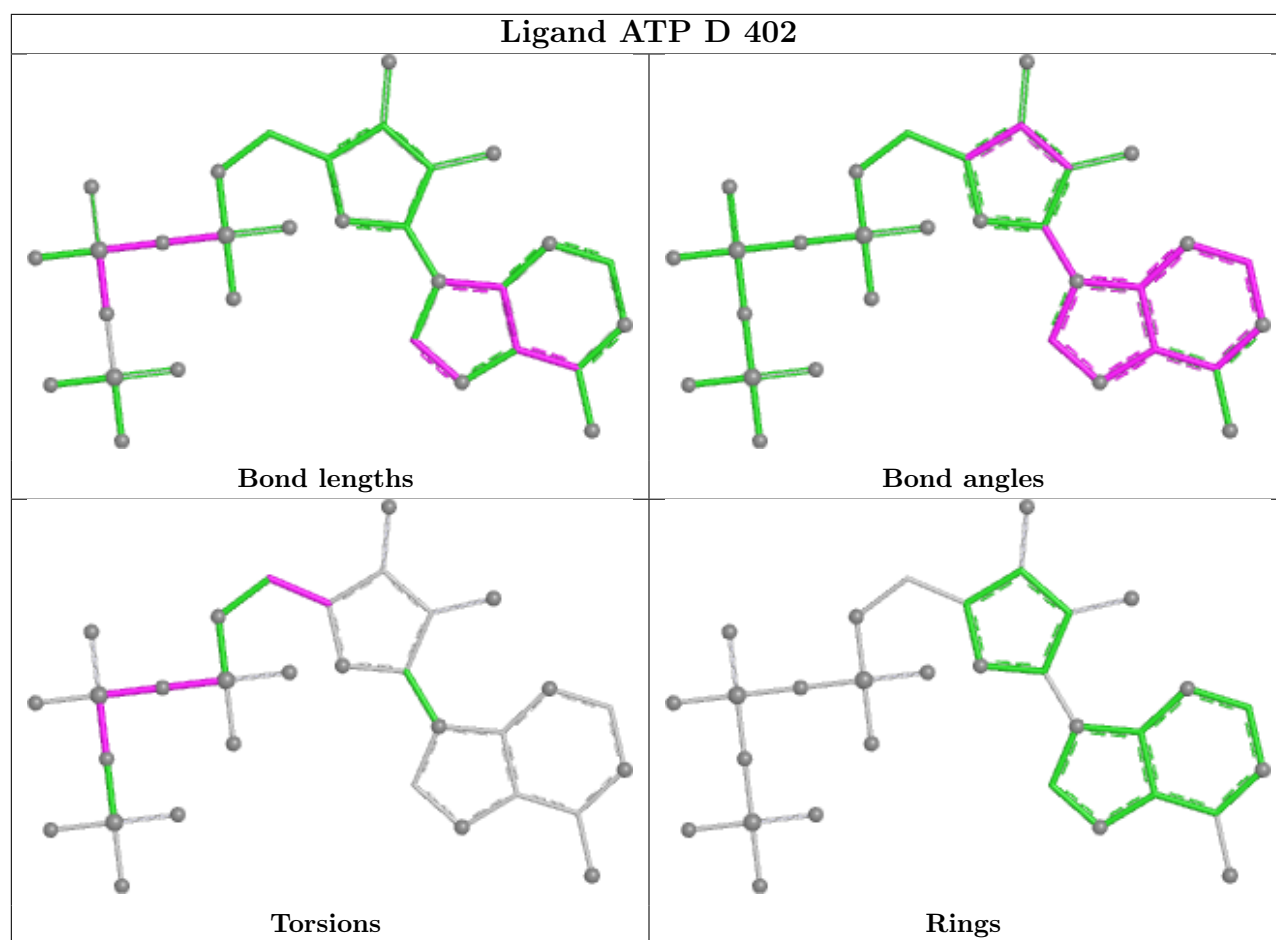
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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 ATP F 403





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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	D	356/377 (94%)	-0.15	2 (0%) 85 75	49, 91, 151, 191	33 (9%)
1	F	356/377 (94%)	-0.19	0 100 100	49, 93, 161, 190	15 (4%)
1	G	356/377 (94%)	-0.32	0 100 100	38, 93, 158, 192	33 (9%)
1	H	356/377 (94%)	-0.17	0 100 100	43, 94, 159, 194	28 (7%)
2	A	357/402 (88%)	-0.22	1 (0%) 90 84	38, 95, 135, 158	61 (17%)
2	B	357/402 (88%)	-0.31	0 100 100	40, 96, 133, 159	59 (16%)
2	C	357/402 (88%)	-0.24	1 (0%) 90 84	39, 96, 137, 156	56 (15%)
2	E	357/402 (88%)	-0.30	0 100 100	40, 95, 139, 159	62 (17%)
All	All	2852/3116 (91%)	-0.24	4 (0%) 92 91	38, 94, 144, 194	347 (12%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	780	SER	3.3
1	D	242	LEU	2.7
1	D	199	SER	2.4
2	C	703	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

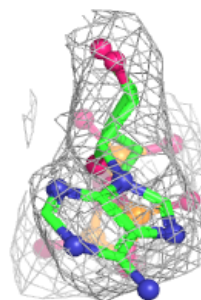
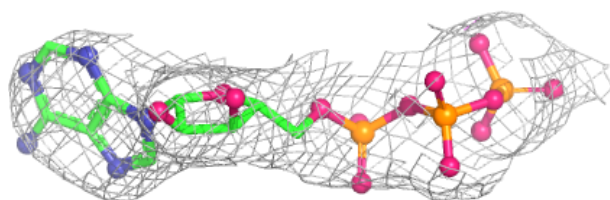
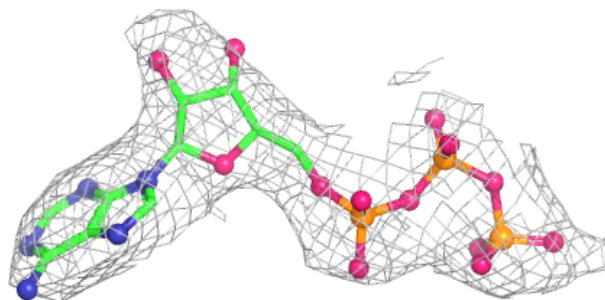
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ACT	A	1003	4/4	0.74	0.20	81,83,97,104	0
3	ACT	B	1001	4/4	0.85	0.14	75,94,95,97	0
3	ACT	E	1001	4/4	0.86	0.17	73,103,103,103	0
3	ACT	F	402	4/4	0.86	0.14	78,80,106,107	0
3	ACT	A	1001	4/4	0.87	0.14	72,74,83,89	0
3	ACT	F	401	4/4	0.90	0.14	88,111,123,124	0
3	ACT	C	1001	4/4	0.93	0.18	75,88,90,100	0
3	ACT	A	1002	4/4	0.93	0.12	80,96,99,103	0
4	ATP	H	402	31/31	0.93	0.07	85,109,122,133	0
3	ACT	D	401	4/4	0.94	0.12	62,66,91,110	0
4	ATP	D	402	31/31	0.95	0.08	53,86,104,106	0
3	ACT	G	401	4/4	0.95	0.08	84,88,105,122	0
3	ACT	H	401	4/4	0.96	0.07	70,89,100,122	0
3	ACT	C	1002	4/4	0.96	0.11	69,89,92,102	0
4	ATP	G	402	31/31	0.96	0.07	73,104,119,122	0
4	ATP	F	403	31/31	0.96	0.08	70,91,110,116	0

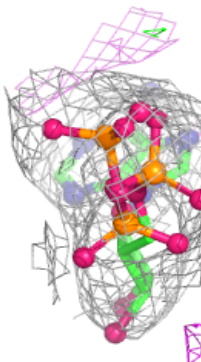
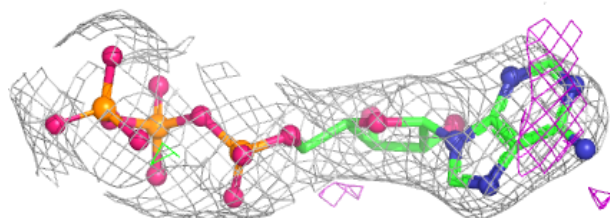
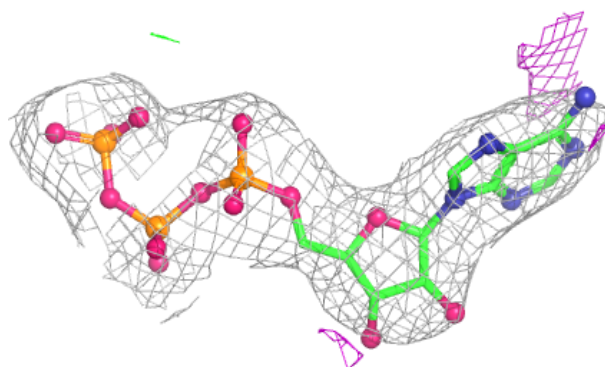
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP H 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

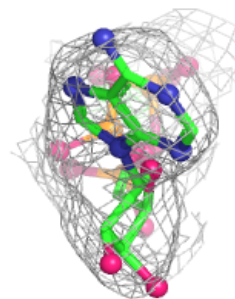
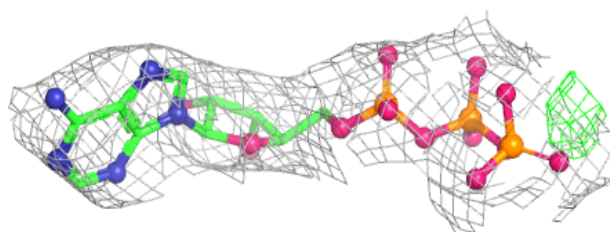
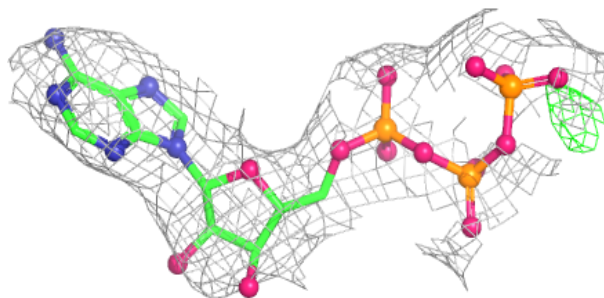
**Electron density around ATP D 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

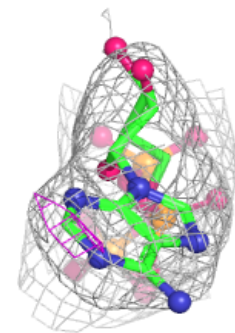
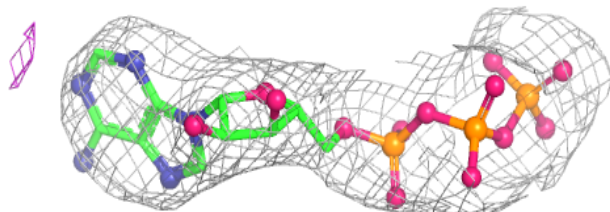
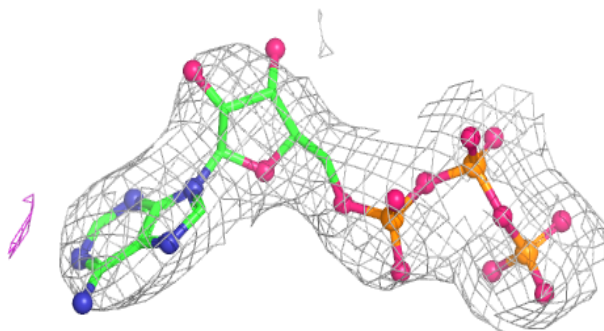


Electron density around ATP G 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ATP F 403:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.