



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 11:56 pm BST

PDB ID : 4XVU
Title : Structure of Get3 bound to the transmembrane domain of Nyv1
Authors : Mateja, A.; Paduch, M.; Chang, H.-Y.; Szydlowska, A.; Kossiakoff, A.A.;
Hegde, R.S.; Keenan, R.J.
Deposited on : 2015-01-28
Resolution : 2.35 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

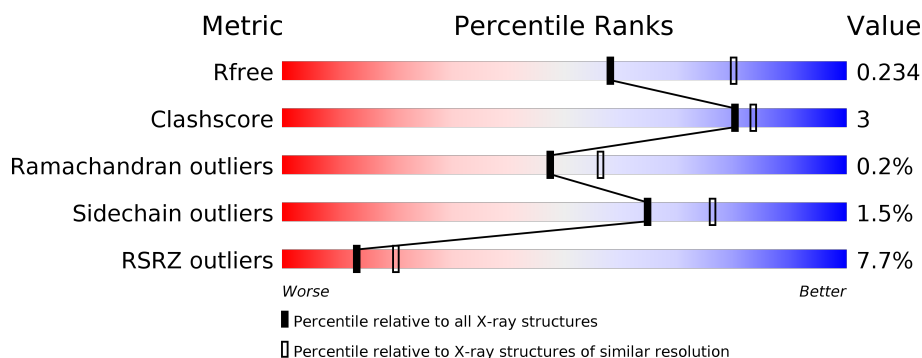
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on 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	A	354	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>5%</div> <div>15%</div> </div> </div>
1	B	354	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>6%</div> <div>14%</div> </div> </div>
1	G	354	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>13%</div> </div> </div>
1	H	354	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>12%</div> </div> </div>
2	C	230	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div></div> </div> </div>
2	E	230	<div> <div>4%</div> <div> <div></div> <div>94%</div> <div></div> <div></div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	230	<div><div></div><div>12%</div><div>83%</div><div>7%</div><div>10%</div></div>
2	K	230	<div><div></div><div>17%</div><div>80%</div><div>11%</div><div>6%</div></div>
3	D	217	<div><div></div><div>%</div><div>95%</div><div></div></div>
3	F	217	<div><div></div><div></div><div>93%</div><div>6%</div></div>
3	J	217	<div><div></div><div>22%</div><div>91%</div><div>8%</div></div>
3	L	217	<div><div></div><div>15%</div><div>90%</div><div>9%</div></div>
4	a	37	<div><div></div><div>68%</div><div>32%</div></div>
4	g	37	<div><div></div><div>32%</div><div>68%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 46586 atoms, of which 22641 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 ATPase GET3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	301	Total	C	H	N	O	S	0	2	0
			4764	1512	2373	397	464	18			
1	B	304	Total	C	H	N	O	S	0	1	0
			4794	1521	2387	399	469	18			
1	G	307	Total	C	H	N	O	S	0	0	0
			4835	1535	2408	403	473	16			
1	H	311	Total	C	H	N	O	S	0	0	0
			4887	1549	2436	408	477	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ASN	ASP	engineered mutation	UNP Q12154
B	57	ASN	ASP	engineered mutation	UNP Q12154
G	57	ASN	ASP	engineered mutation	UNP Q12154
H	57	ASN	ASP	engineered mutation	UNP Q12154

- Molecule 2 is a protein called Antibody heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	222	Total	C	H	N	O	S	0	0	0
			3289	1050	1625	282	326	6			
2	E	222	Total	C	H	N	O	S	0	0	0
			3289	1050	1625	282	326	6			
2	I	207	Total	C	H	N	O	S	0	0	0
			3097	996	1529	265	301	6			
2	K	216	Total	C	H	N	O	S	0	0	0
			3213	1029	1587	275	316	6			

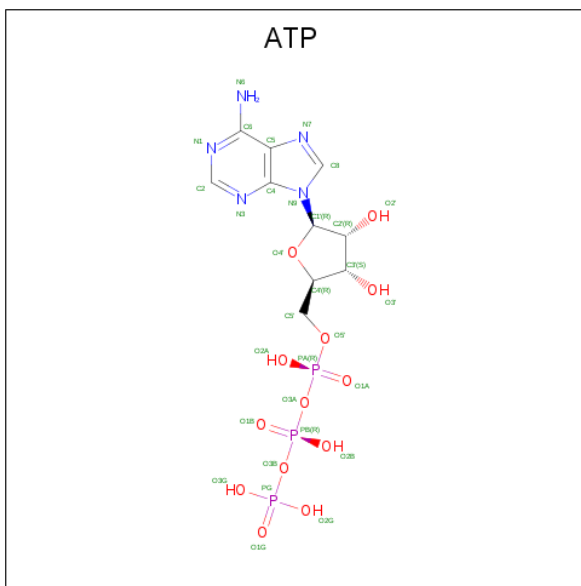
- Molecule 3 is a protein called Antibody light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	216	Total 3269	C 1038	H 1611	N 276	O 338	S 6	0	0	0
3	F	216	Total 3269	C 1038	H 1611	N 276	O 338	S 6	0	0	0
3	J	215	Total 3257	C 1034	H 1607	N 275	O 335	S 6	0	0	0
3	L	216	Total 3269	C 1038	H 1611	N 276	O 338	S 6	0	0	0

- Molecule 4 is a protein called Nyv1 TMD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	g	12	Total 119	C 36	H 59	N 12	O 12	0	0	0
4	a	25	Total 252	C 75	H 127	N 25	O 25	0	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total 42	C 10	H 11	N 5	O 13	P 3	0	0
5	B	1	Total 42	C 10	H 11	N 5	O 13	P 3	0	0
5	G	1	Total 42	C 10	H 11	N 5	O 13	P 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	H	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	Mg	0	0
			1	1		
6	G	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Zn	0	0
			1	1		
7	A	1	Total	Zn	0	0
			1	1		

- Molecule 8 is water.

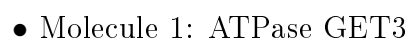
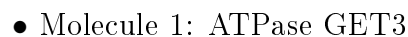
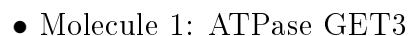
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	57	Total	O	0	0
			57	57		
8	B	85	Total	O	0	0
			85	85		
8	C	62	Total	O	0	0
			62	62		
8	D	77	Total	O	0	0
			77	77		
8	E	52	Total	O	0	0
			52	52		
8	F	93	Total	O	0	0
			93	93		
8	G	107	Total	O	0	0
			107	107		
8	H	85	Total	O	0	0
			85	85		

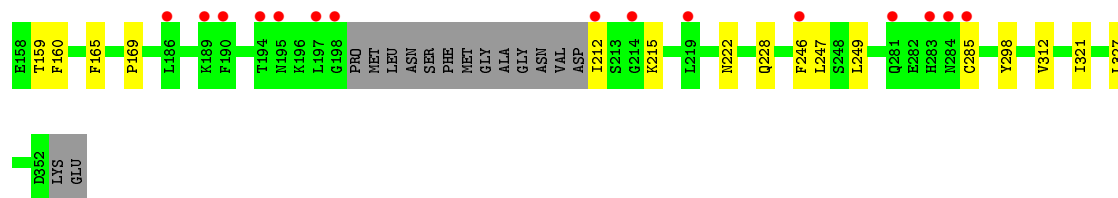
Continued on next page...

Continued from previous page...

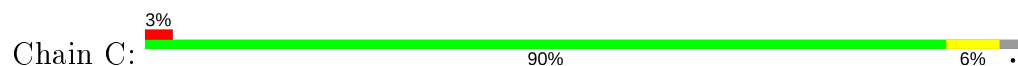
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	42	Total 42	O 42	0	0
8	J	45	Total 45	O 45	0	0
8	K	61	Total 61	O 61	0	0
8	L	42	Total 42	O 42	0	0

- Molecule 1: ATPase GET3





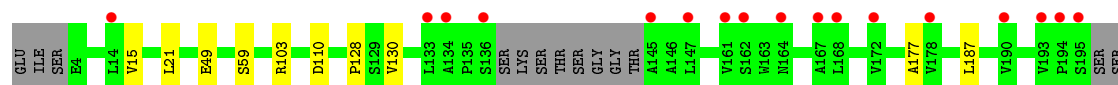
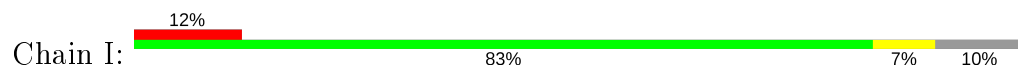
- Molecule 2: Antibody heavy chain



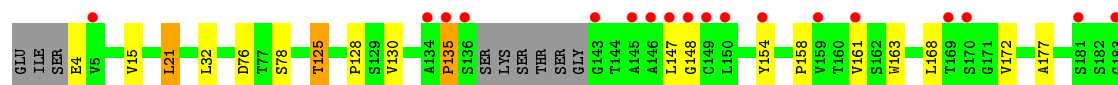
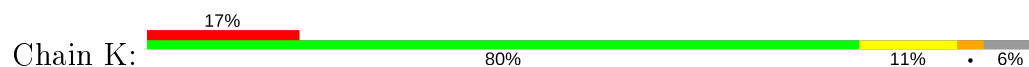
- Molecule 2: Antibody heavy chain



- Molecule 2: Antibody heavy chain



- Molecule 2: Antibody heavy chain

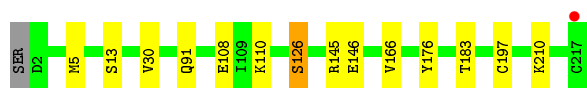


- Molecule 3: Antibody light chain




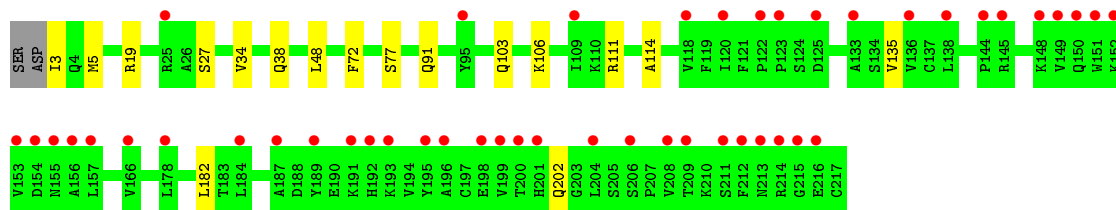
- Molecule 3: Antibody light chain

Chain F:  93% 6%




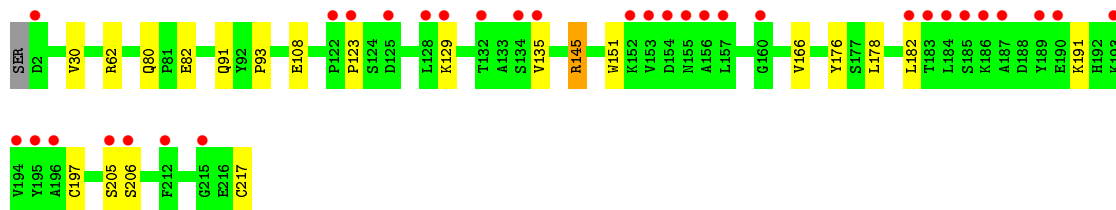
- Molecule 3: Antibody light chain

Chain J:  22% 91% 8%



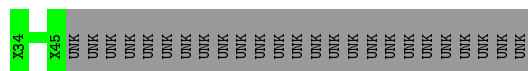
- Molecule 3: Antibody light chain

Chain L:  15% 90% 9%



- Molecule 4: Nyv1 TMD

Chain g:  32% 68%



- Molecule 4: Nyv1 TMD

Chain a:  68% 32%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.44Å 109.23Å 111.35Å 63.05° 77.74° 70.17°	Depositor
Resolution (Å)	69.38 – 2.35 69.38 – 2.35	Depositor EDS
% Data completeness (in resolution range)	94.6 (69.38-2.35) 91.0 (69.38-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.197 , 0.234 0.199 , 0.234	Depositor DCC
R_{free} test set	6209 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	46586	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: MG, ZN, ATP

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	0.28	0/2437	0.42	0/3287
1	B	0.27	0/2449	0.44	0/3302
1	G	0.29	0/2467	0.43	0/3327
1	H	0.27	0/2490	0.42	0/3356
2	C	0.30	0/1706	0.52	0/2326
2	E	0.29	0/1706	0.52	0/2326
2	I	0.27	0/1608	0.49	0/2191
2	K	0.31	0/1667	0.58	0/2273
3	D	0.29	0/1694	0.49	0/2299
3	F	0.33	0/1694	0.56	0/2299
3	J	0.27	0/1686	0.49	0/2288
3	L	0.30	0/1694	0.55	1/2299 (0.0%)
All	All	0.29	0/23298	0.49	1/31573 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	145	ARG	NE-CZ-NH1	7.12	123.86	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	146	GLU	Sidechain

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	2391	2373	2364	12	0
1	B	2407	2387	2387	14	0
1	G	2427	2408	2411	15	1
1	H	2451	2436	2436	18	0
2	C	1664	1625	1625	9	0
2	E	1664	1625	1625	2	0
2	I	1568	1529	1529	9	0
2	K	1626	1587	1587	18	0
3	D	1658	1611	1611	5	0
3	F	1658	1611	1611	7	1
3	J	1650	1607	1607	10	0
3	L	1658	1611	1612	16	0
4	a	125	127	28	0	0
4	g	60	59	14	0	0
5	A	31	11	12	0	0
5	B	31	11	12	0	0
5	G	31	11	12	0	0
5	H	31	12	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	1	0	0	0	0
7	G	1	0	0	0	0
8	A	57	0	0	1	0
8	B	85	0	0	1	0
8	C	62	0	0	1	0
8	D	77	0	0	1	0
8	E	52	0	0	1	0
8	F	93	0	0	2	0
8	G	107	0	0	6	0
8	H	85	0	0	6	0
8	I	42	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	45	0	0	2	0
8	K	61	0	0	3	0
8	L	42	0	0	5	0
All	All	23945	22641	22495	123	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 3.

The worst 5 of 123 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:G:69:LYS:O	1:G:75:ARG:NH1	2.21	0.74
3:J:3:ILE:N	3:J:27:SER:HG	1.91	0.69
2:C:139:SER:HA	3:D:119:PHE:HD1	1.60	0.66
1:H:95:LYS:HA	1:H:98:ASN:HB3	1.78	0.66
2:C:130:VAL:HG21	2:C:207:VAL:HG11	1.77	0.65

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)
3:F:210:LYS:NZ	1:G:154:GLN:O[1_645]	2.16	0.04

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 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	A	295/354 (83%)	287 (97%)	6 (2%)	2 (1%)	22	23
1	B	297/354 (84%)	287 (97%)	9 (3%)	1 (0%)	41	47
1	G	301/354 (85%)	293 (97%)	6 (2%)	2 (1%)	22	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	303/354 (86%)	288 (95%)	14 (5%)	1 (0%)	41	47
2	C	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
2	E	220/230 (96%)	214 (97%)	6 (3%)	0	100	100
2	I	201/230 (87%)	196 (98%)	5 (2%)	0	100	100
2	K	212/230 (92%)	202 (95%)	9 (4%)	1 (0%)	29	32
3	D	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
3	F	214/217 (99%)	210 (98%)	4 (2%)	0	100	100
3	J	213/217 (98%)	208 (98%)	5 (2%)	0	100	100
3	L	214/217 (99%)	207 (97%)	7 (3%)	0	100	100
All	All	2904/3204 (91%)	2818 (97%)	79 (3%)	7 (0%)	47	56

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	THR
1	B	170	THR
1	G	170	THR
1	A	285	CYS
1	G	285	CYS

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	A	273/309 (88%)	270 (99%)	3 (1%)	73	84
1	B	274/309 (89%)	267 (97%)	7 (3%)	46	56
1	G	275/309 (89%)	270 (98%)	5 (2%)	59	70
1	H	277/309 (90%)	272 (98%)	5 (2%)	59	70
2	C	185/193 (96%)	183 (99%)	2 (1%)	73	84
2	E	185/193 (96%)	183 (99%)	2 (1%)	73	84
2	I	173/193 (90%)	172 (99%)	1 (1%)	86	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	180/193 (93%)	171 (95%)	9 (5%)	24	28
3	D	191/192 (100%)	190 (100%)	1 (0%)	88	94
3	F	191/192 (100%)	189 (99%)	2 (1%)	76	85
3	J	190/192 (99%)	189 (100%)	1 (0%)	88	94
3	L	191/192 (100%)	190 (100%)	1 (0%)	88	94
All	All	2585/2776 (93%)	2546 (98%)	39 (2%)	65	76

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	94	LEU
1	G	266	VAL
2	K	212	SER
1	G	211	ASP
1	G	212	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	310	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
5	ATP	A	401	6	26,33,33	2.28	10 (38%)	31,52,52	1.79	7 (22%)
5	ATP	G	401	6	26,33,33	2.31	9 (34%)	31,52,52	1.88	8 (25%)
5	ATP	B	401	6	26,33,33	2.25	9 (34%)	31,52,52	1.89	7 (22%)
5	ATP	H	401	6	26,33,33	2.28	9 (34%)	31,52,52	1.75	6 (19%)

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
5	ATP	A	401	6	-	0/18/38/38	0/3/3/3
5	ATP	G	401	6	-	0/18/38/38	0/3/3/3
5	ATP	B	401	6	-	0/18/38/38	0/3/3/3
5	ATP	H	401	6	-	0/18/38/38	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	401	ATP	C2-N1	-5.36	1.23	1.33
5	A	401	ATP	C2-N1	-5.22	1.24	1.33
5	H	401	ATP	C2-N1	-5.13	1.24	1.33
5	B	401	ATP	C2-N1	-5.07	1.24	1.33
5	G	401	ATP	C4-N3	4.30	1.41	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	ATP	C2-N1-C6	5.63	128.39	118.75
5	G	401	ATP	C2-N1-C6	5.59	128.32	118.75
5	A	401	ATP	C2-N1-C6	5.46	128.09	118.75
5	H	401	ATP	C2-N1-C6	5.28	127.78	118.75
5	G	401	ATP	N3-C2-N1	-4.01	122.42	128.68

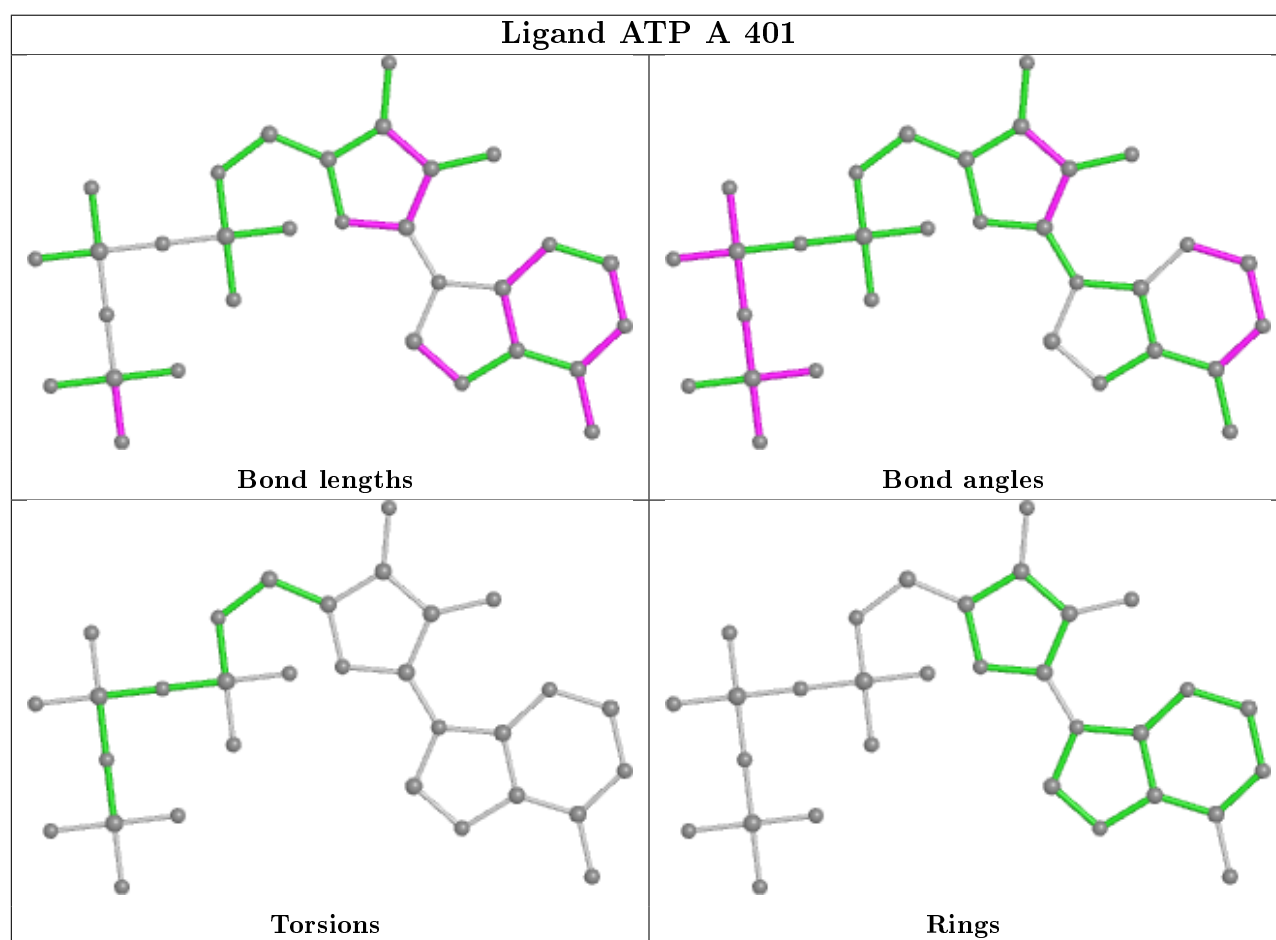
There are no chirality outliers.

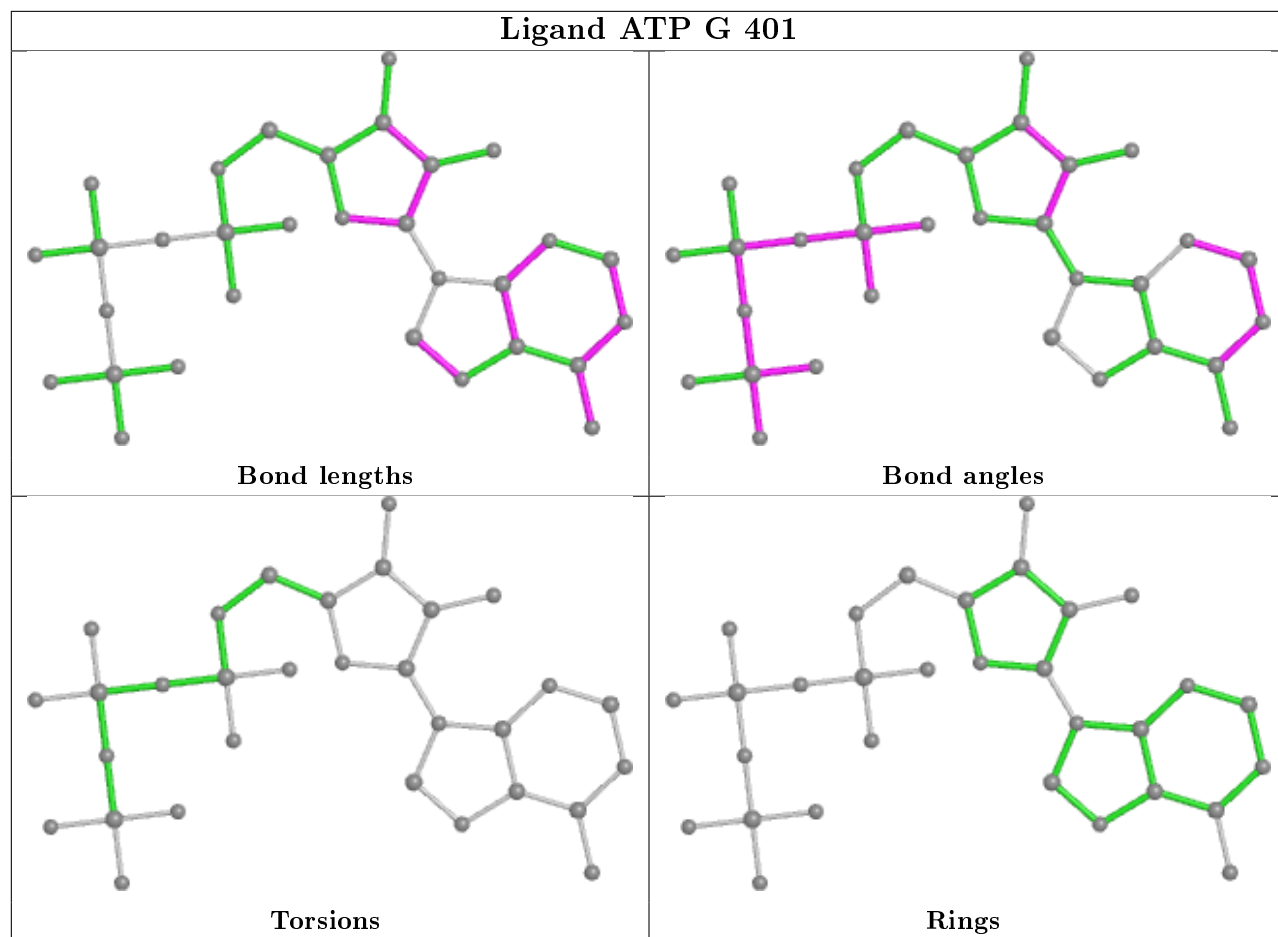
There are no torsion outliers.

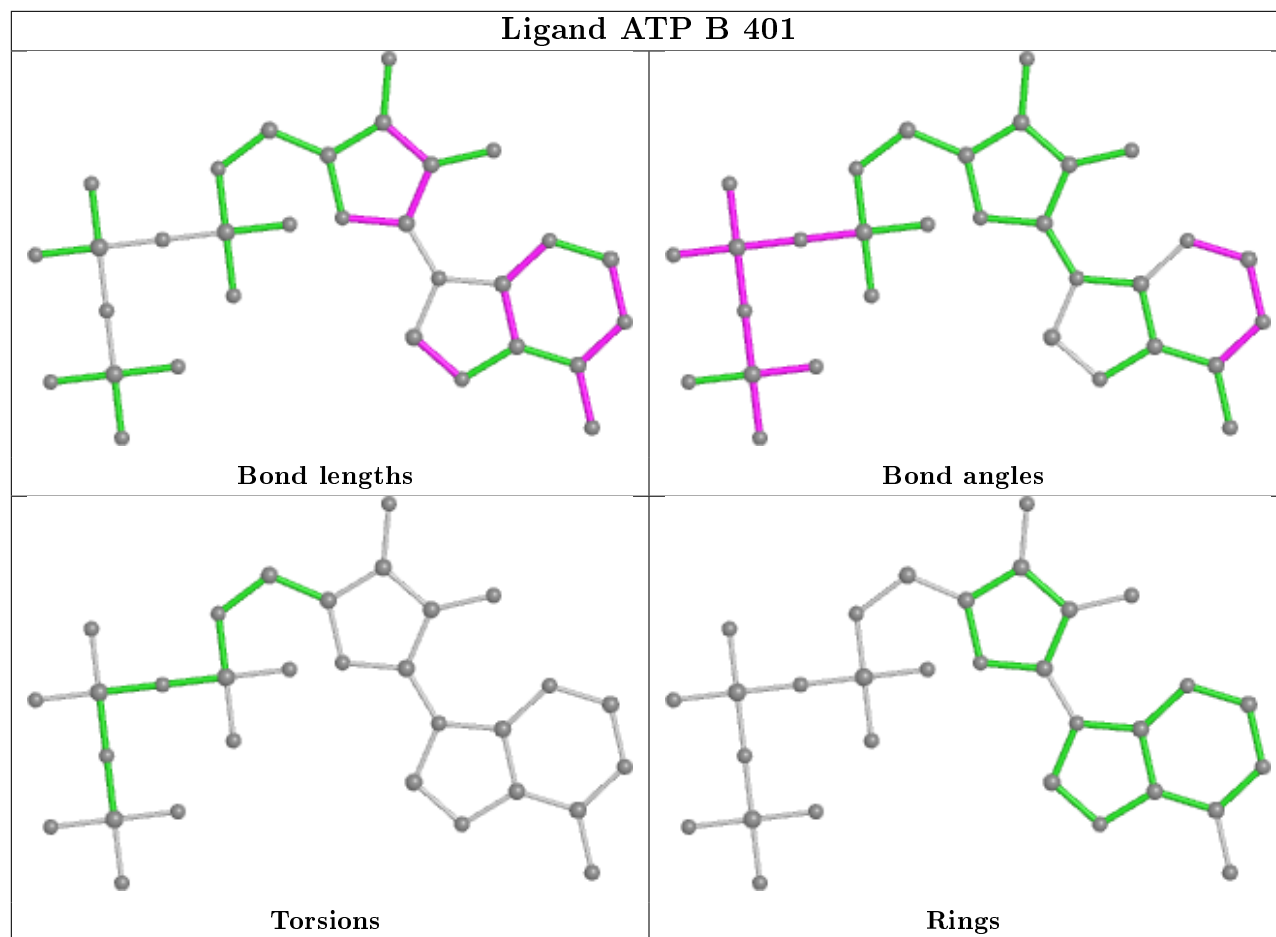
There are no ring outliers.

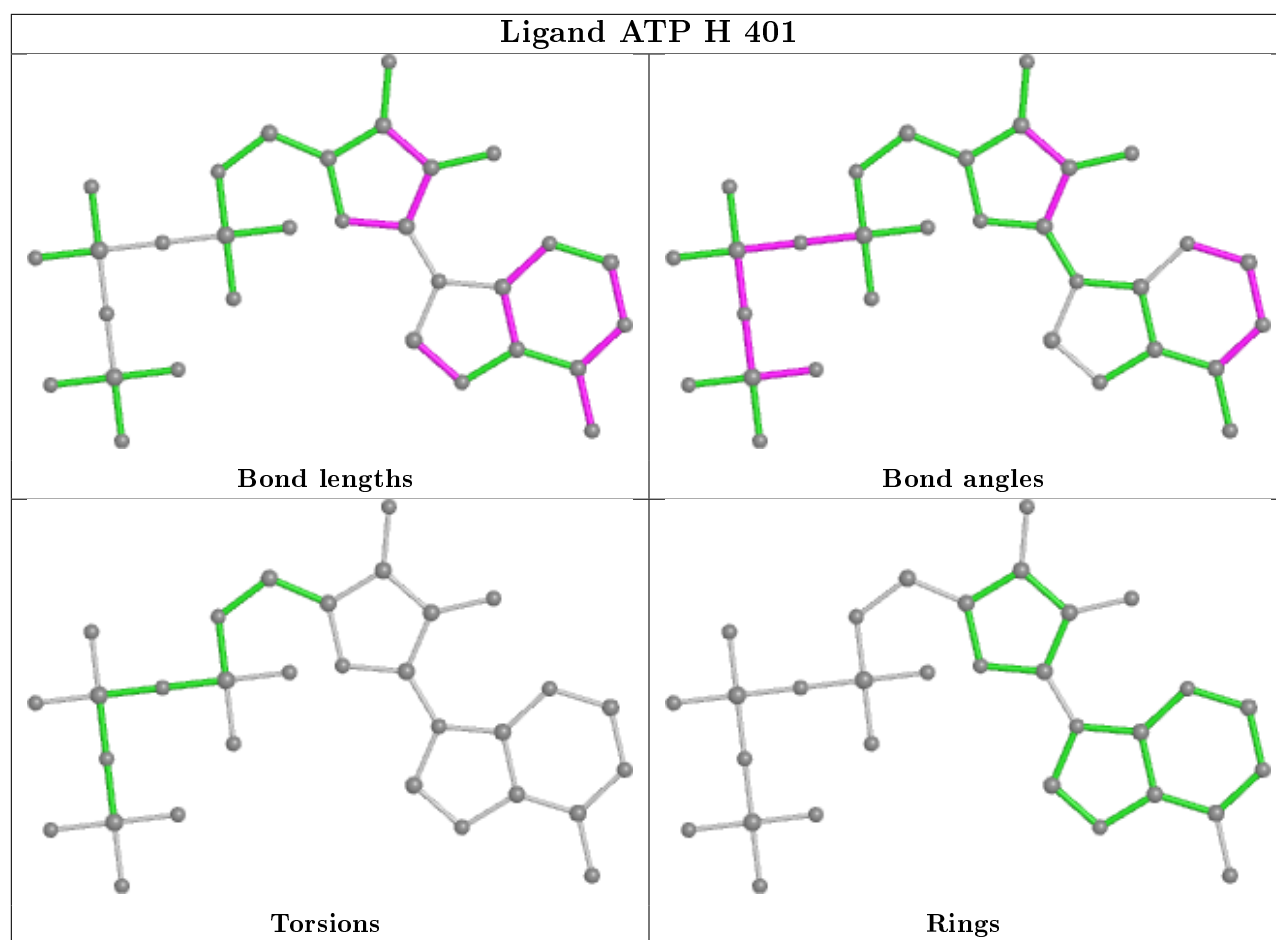
No monomer is involved in short contacts.

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.









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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	A	301/354 (85%)	0.32	16 (5%) 26 38	30, 54, 128, 154	0
1	B	304/354 (85%)	0.23	13 (4%) 35 47	27, 44, 129, 182	0
1	G	307/354 (86%)	0.19	15 (4%) 29 42	27, 43, 111, 166	0
1	H	311/354 (87%)	0.36	21 (6%) 17 25	34, 51, 135, 172	0
2	C	222/230 (96%)	0.19	7 (3%) 47 59	28, 41, 94, 131	0
2	E	222/230 (96%)	0.16	9 (4%) 37 49	28, 43, 84, 151	0
2	I	207/230 (90%)	0.57	27 (13%) 3 5	35, 65, 126, 211	0
2	K	216/230 (93%)	0.87	38 (17%) 1 2	30, 63, 144, 184	0
3	D	216/217 (99%)	0.03	2 (0%) 84 90	28, 47, 73, 114	0
3	F	216/217 (99%)	-0.03	1 (0%) 91 95	28, 42, 77, 159	0
3	J	215/217 (99%)	1.07	47 (21%) 0 1	33, 80, 162, 200	0
3	L	216/217 (99%)	0.65	32 (14%) 2 3	31, 60, 141, 175	0
4	a	0/37	-	-	-	-
4	g	0/37	-	-	-	-
All	All	2953/3278 (90%)	0.37	228 (7%) 13 20	27, 49, 132, 211	0

The worst 5 of 228 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	209	THR	10.6
2	K	143	GLY	10.0
3	J	216	GLU	8.9
3	J	211	SER	8.9
1	H	194	THR	8.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

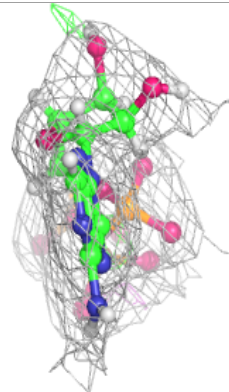
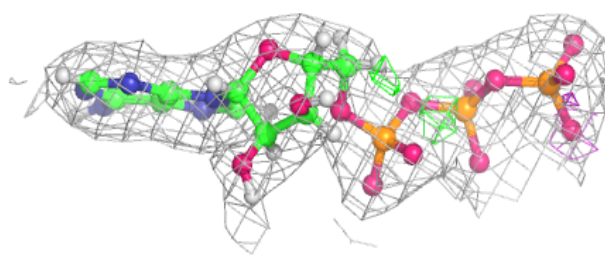
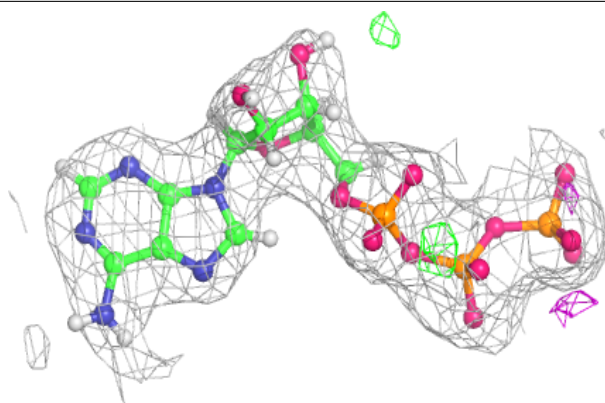
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	B	402	1/1	0.96	0.14	35,35,35,35	0
6	MG	H	402	1/1	0.97	0.12	37,37,37,37	0
5	ATP	H	401	31/31	0.97	0.13	35,38,46,47	0
5	ATP	B	401	31/31	0.97	0.14	25,34,41,43	0
5	ATP	G	401	31/31	0.97	0.14	36,43,60,68	0
7	ZN	A	403	1/1	0.97	0.15	55,55,55,55	0
6	MG	A	402	1/1	0.98	0.10	31,31,31,31	0
5	ATP	A	401	31/31	0.98	0.13	32,39,46,48	0
7	ZN	G	403	1/1	0.99	0.15	56,56,56,56	0
6	MG	G	402	1/1	0.99	0.10	42,42,42,42	0

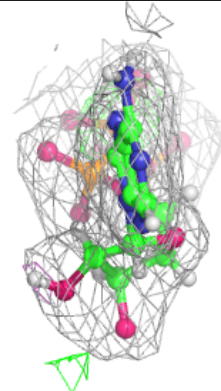
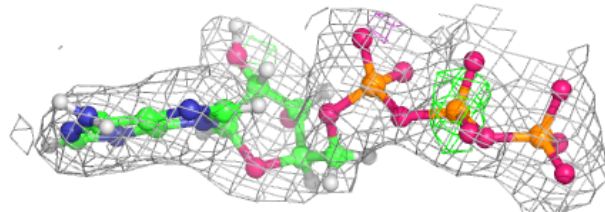
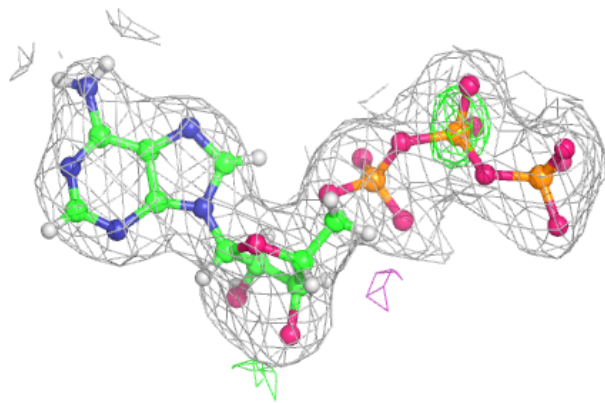
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP H 401:

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

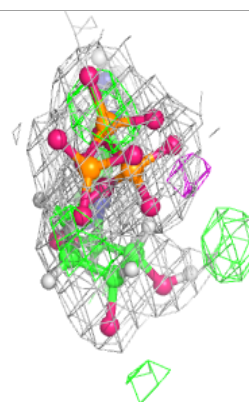
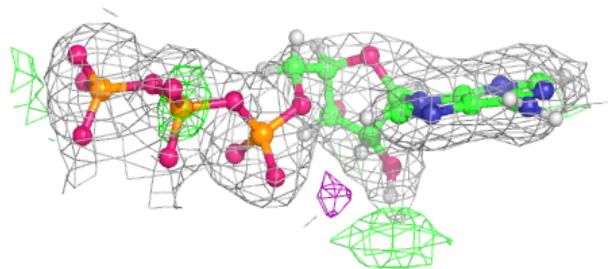
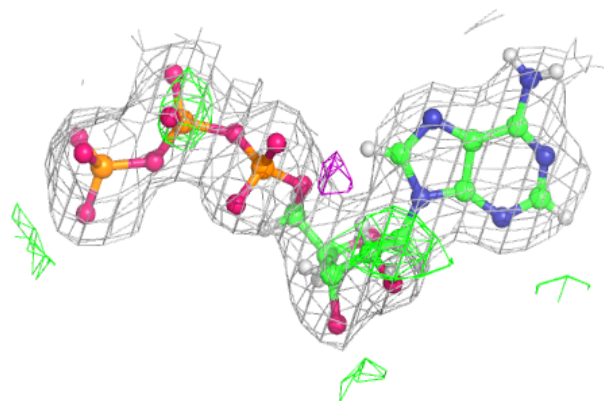
**Electron density around ATP B 401:**

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

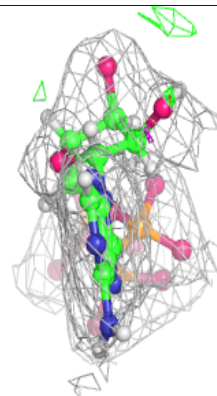
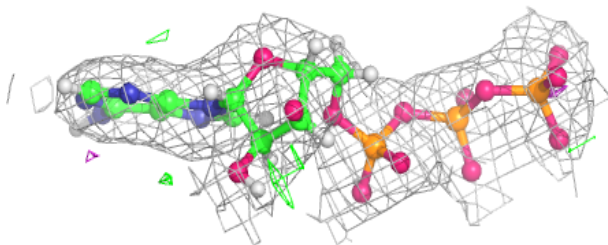
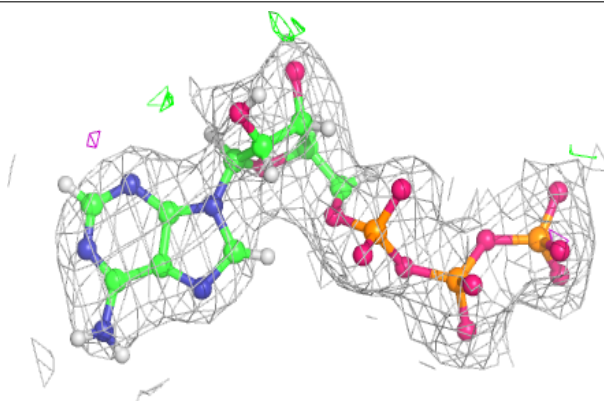


Electron density around ATP G 401:

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

**Electron density around ATP A 401:**

$2mF_o-DF_c$ (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.