



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2024 – 03:36 PM EDT

PDB ID : 4QFS
Title : Structure of AMPK in complex with Br2-A769662core activator and STAU-ROSPORINE inhibitor
Authors : Calabrese, M.F.; Kurumbail, R.G.
Deposited on : 2014-05-21
Resolution : 3.55 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

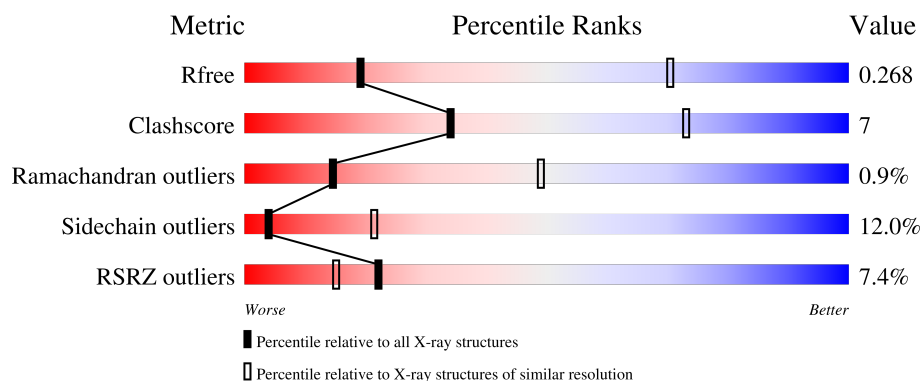
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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}	164625	1261 (3.62-3.50)
Clashscore	180529	1351 (3.62-3.50)
Ramachandran outliers	177936	1336 (3.62-3.50)
Sidechain outliers	177891	1337 (3.62-3.50)
RSRZ outliers	164620	1260 (3.62-3.50)

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	A	503	<div> <div>2%</div> <div>52% 18% • 28%</div> </div>
2	B	204	<div> <div>%</div> <div>53% 22% • 23%</div> </div>
3	C	330	<div> <div>14%</div> <div>68% 12% • 19%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6128 atoms, of which 26 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 5'-AMP-activated protein kinase catalytic subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	P	S	0	0	0
			2854	1826	493	516	1	18			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P54645
A	517	ALA	-	SEE REMARK 999	UNP P54645
A	518	SER	-	SEE REMARK 999	UNP P54645
A	519	GLY	-	SEE REMARK 999	UNP P54645
A	520	GLY	-	SEE REMARK 999	UNP P54645
A	521	PRO	-	SEE REMARK 999	UNP P54645
A	522	GLY	-	SEE REMARK 999	UNP P54645
A	523	GLY	-	SEE REMARK 999	UNP P54645
A	524	SER	-	SEE REMARK 999	UNP P54645

- Molecule 2 is a protein called 5'-AMP-activated protein kinase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	158	Total	C	N	O	S	0	0	0
			1214	790	203	218	3			

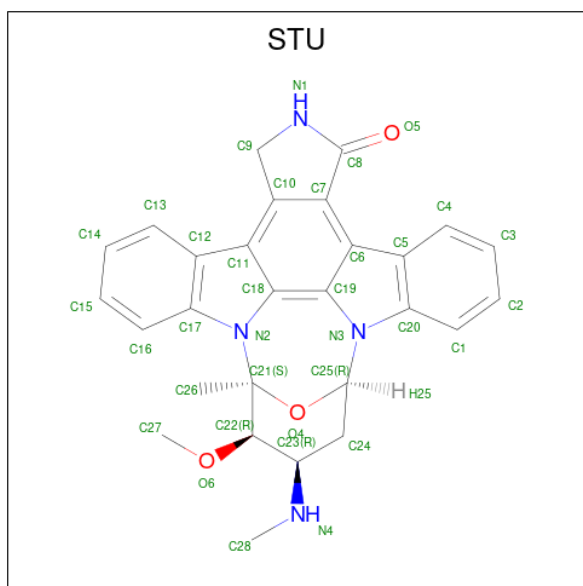
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MET	-	expression tag	UNP P80386
B	108	ASP	SER	engineered mutation	UNP P80386

- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

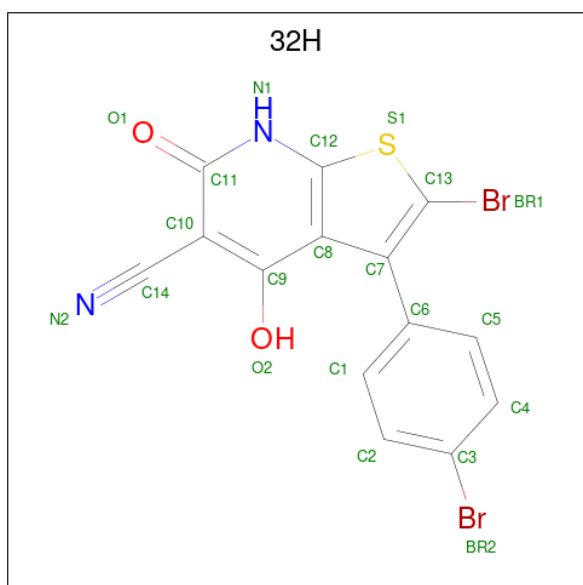
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	267	Total	C	N	O	S	0	0	0
			1940	1249	322	363	6			

- Molecule 4 is STAUROSPORINE (three-letter code: STU) (formula: $C_{28}H_{26}N_4O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			61	28	26	4	3		

- Molecule 5 is 2-bromo-3-(4-bromophenyl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile (three-letter code: 32H) (formula: $C_{14}H_6Br_2N_2O_2S$).

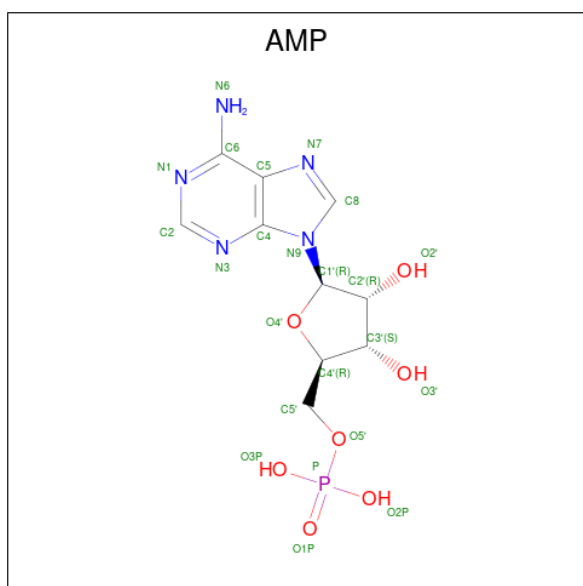


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	Br	C	N	O	S	
			21	2	14	2	2	1	
								0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

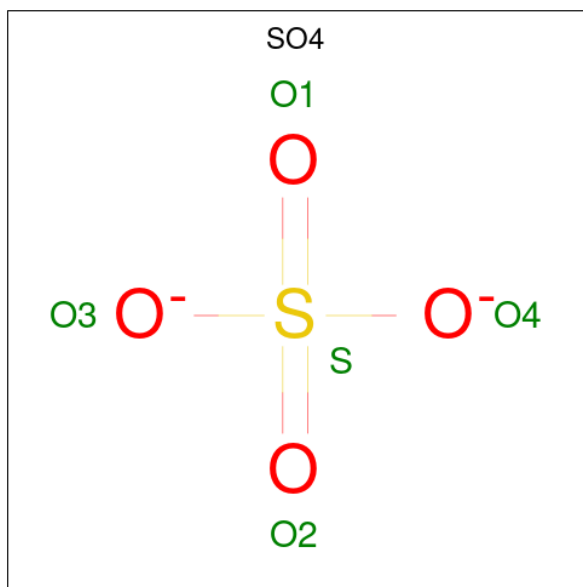
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	Cl		
			4	4	0	0
6	B	1	Total	Cl		
			1	1	0	0

- Molecule 7 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).

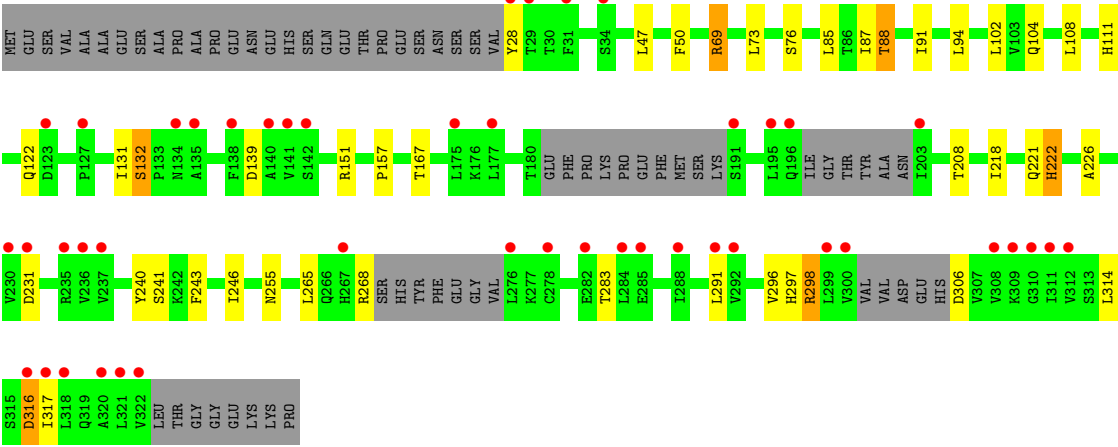


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P		
			23	10	5	7	1	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.88Å 123.88Å 401.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.59 – 3.55 29.59 – 3.55	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.59-3.55) 89.8 (29.59-3.55)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 3.55Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.5, BUSTER 2.11.5	Depositor
R, R_{free}	0.226 , 0.269 0.222 , 0.268	Depositor DCC
R_{free} test set	1048 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	76.6	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 130.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6128	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: 32H, TPO, CL, SO4, STU, AMP

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	0.50	0/2905	0.76	2/3933 (0.1%)
2	B	0.49	0/1248	0.73	0/1711
3	C	0.47	0/1976	0.68	0/2710
All	All	0.49	0/6129	0.73	2/8354 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	GLY	N-CA-C	-6.69	96.37	113.10
1	A	55	LEU	N-CA-C	-5.21	96.92	111.00

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	2854	0	2797	53	0
2	B	1214	0	1170	23	0
3	C	1940	0	1775	16	0
4	A	35	26	26	4	0
5	A	21	0	5	3	0
6	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	C	23	0	12	1	0
8	C	10	0	0	0	0
All	All	6102	26	5785	89	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 7.

The worst 5 of 89 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:A:455:ASP:HB2	1:A:458:THR:HG22	1.58	0.84
4:A:601:STU:H261	4:A:601:STU:H16	1.60	0.80
2:B:79:PRO:HA	2:B:117:ASP:HA	1.68	0.74
1:A:185:ILE:HD11	1:A:227:CYS:SG	2.31	0.71
3:C:87:ILE:HG23	3:C:246:ILE:HG23	1.72	0.71

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 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	355/503 (71%)	333 (94%)	20 (6%)	2 (1%)	22	56
2	B	152/204 (74%)	137 (90%)	12 (8%)	3 (2%)	6	34
3	C	257/330 (78%)	242 (94%)	13 (5%)	2 (1%)	16	51
All	All	764/1037 (74%)	712 (93%)	45 (6%)	7 (1%)	14	49

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	GLY
1	A	139	ASP
3	C	122	GLN
3	C	231	ASP
2	B	246	ASP

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	306/448 (68%)	274 (90%)	32 (10%)	5	26
2	B	130/185 (70%)	110 (85%)	20 (15%)	2	14
3	C	189/299 (63%)	166 (88%)	23 (12%)	4	20
All	All	625/932 (67%)	550 (88%)	75 (12%)	4	21

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	94	LEU
3	C	283	THR
3	C	104	GLN
3	C	167	THR
1	A	271	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	232	ASN
3	C	104	GLN
3	C	247	ASN
2	B	110	ASN
1	A	218	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	TPO	A	172	1	8,10,11	1.67	1 (12%)	10,14,16	1.99	3 (30%)

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
1	TPO	A	172	1	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	TPO	P-OG1	-4.08	1.52	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TPO	P-OG1-CB	-4.04	112.36	123.33
1	A	172	TPO	O3P-P-O2P	2.83	118.42	107.80
1	A	172	TPO	OG1-P-O1P	-2.02	102.14	109.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	172	TPO	CB-OG1-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\# Z > 2$
4	STU	A	601	-	34,42,42	2.74	11 (32%)	32,68,68	2.46	16 (50%)
8	SO4	C	403	-	4,4,4	0.39	0	6,6,6	0.22	0
7	AMP	C	401	-	21,25,25	0.65	0	23,38,38	0.81	1 (4%)
8	SO4	C	402	-	4,4,4	0.39	0	6,6,6	0.26	0
5	32H	A	602	-	22,23,23	0.81	1 (4%)	18,34,34	0.60	0

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
7	AMP	C	401	-	-	2/6/26/26	0/3/3/3
4	STU	A	601	-	-	1/4/42/42	-
5	32H	A	602	-	-	0/4/6/6	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	STU	C7-C10	9.34	1.46	1.37
4	A	601	STU	C9-C10	-5.25	1.46	1.50
4	A	601	STU	C12-C17	4.58	1.48	1.41
4	A	601	STU	C5-C20	4.51	1.48	1.41
4	A	601	STU	C11-C18	3.97	1.47	1.42

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	STU	C28-N4-C23	5.56	121.03	114.39
4	A	601	STU	C10-C7-C8	-4.55	104.32	108.13
4	A	601	STU	C16-C17-N2	4.51	137.74	132.29
4	A	601	STU	C7-C10-C11	-4.14	116.58	122.32
4	A	601	STU	C7-C8-N1	3.96	110.15	106.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	401	AMP	C5'-O5'-P-O1P
7	C	401	AMP	C5'-O5'-P-O3P
4	A	601	STU	C24-C23-N4-C28

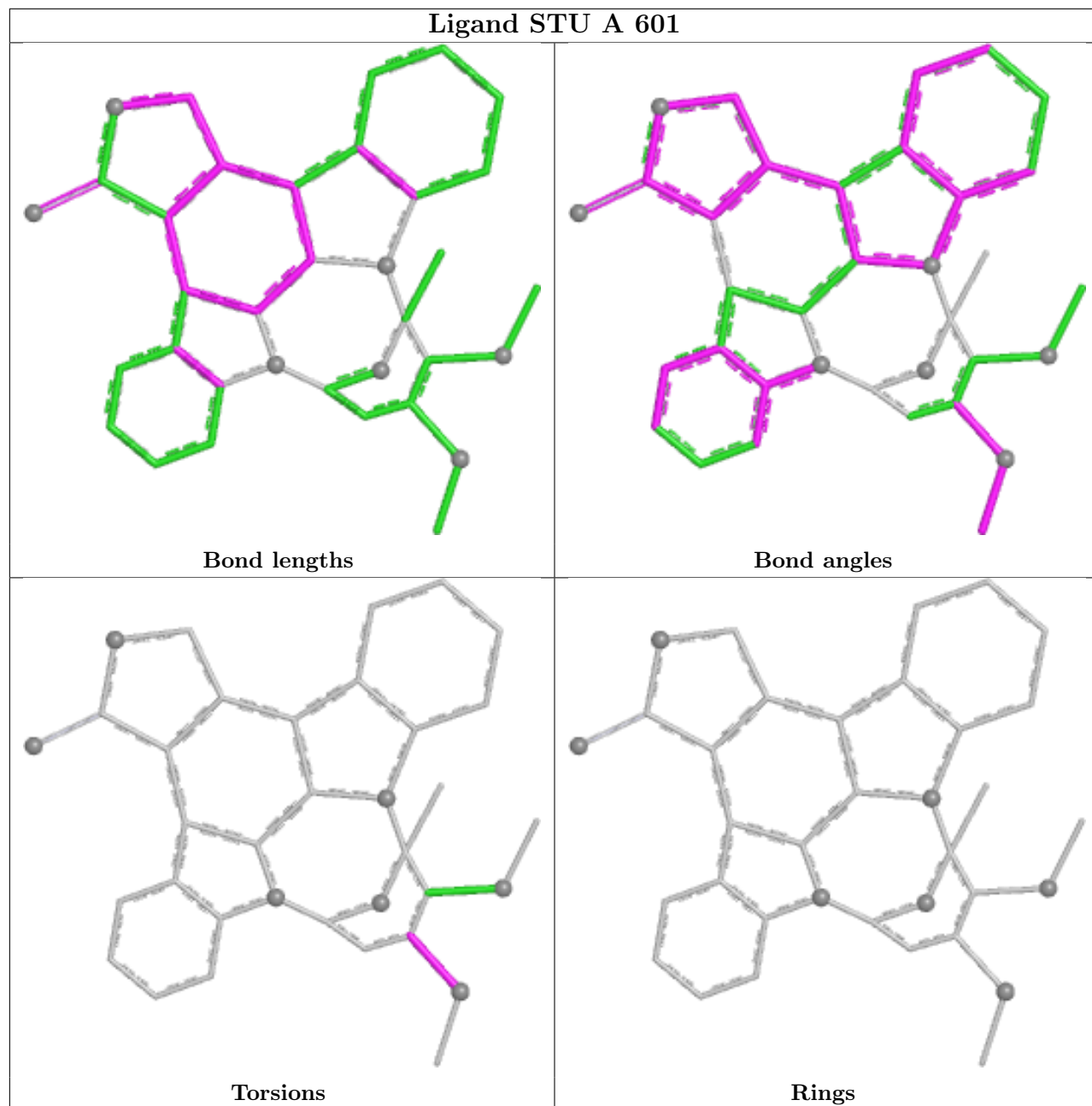
There are no ring outliers.

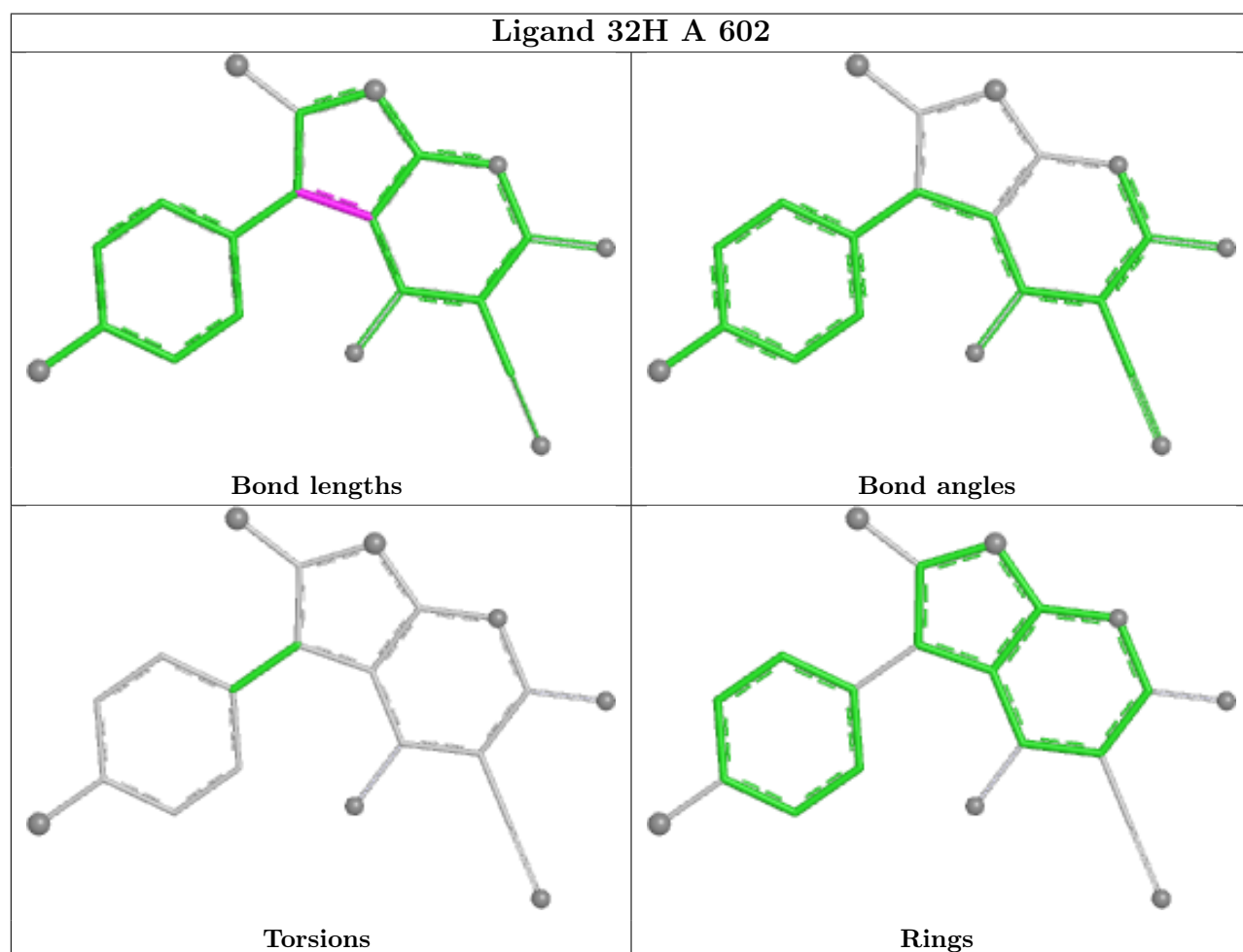
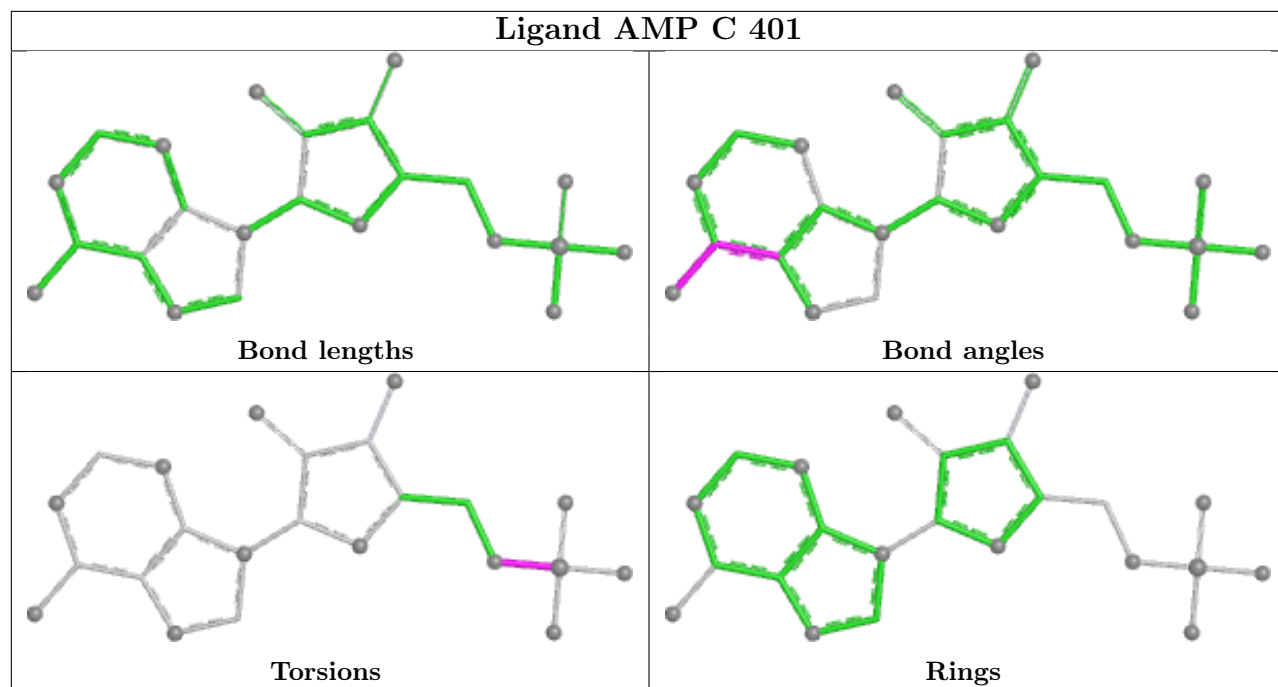
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	STU	4	0
7	C	401	AMP	1	0
5	A	602	32H	3	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.





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	A	361/503 (71%)	-0.21	10 (2%) 55 34	44, 72, 170, 275	0
2	B	158/204 (77%)	-0.05	3 (1%) 66 44	54, 85, 123, 137	0
3	C	267/330 (80%)	0.67	45 (16%) 5 5	63, 114, 234, 264	0
All	All	786/1037 (75%)	0.12	58 (7%) 22 15	44, 90, 230, 275	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	310	GLY	6.3
3	C	236	VAL	6.1
3	C	311	ILE	5.3
3	C	237	VAL	5.2
3	C	312	VAL	5.2

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

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
1	TPO	A	172	11/12	0.97	0.07	73,75,79,81	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

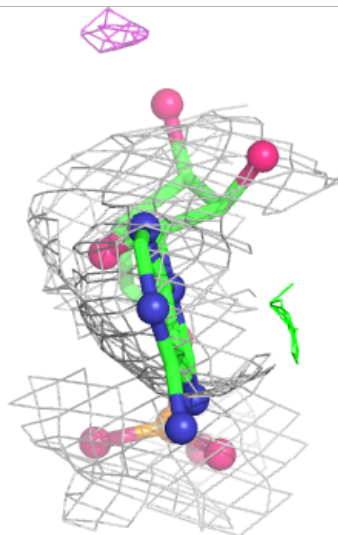
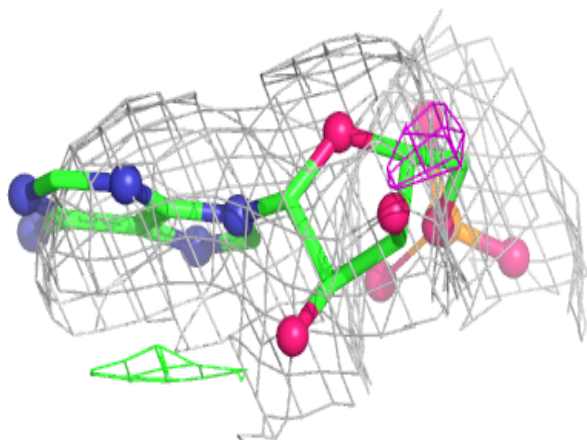
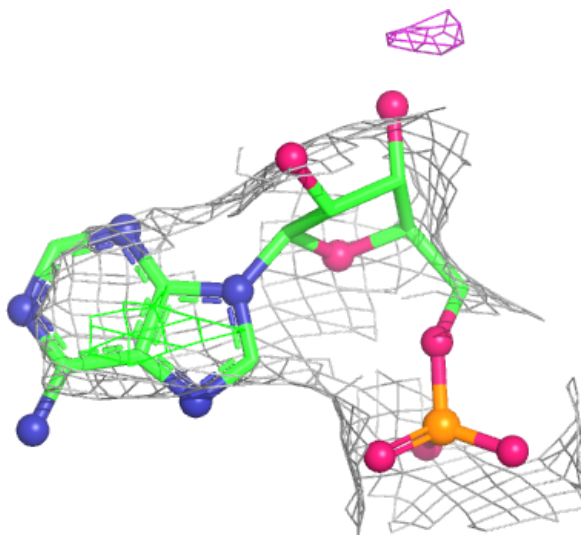
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	SO4	C	403	5/5	0.65	0.13	142,142,142,143	0
8	SO4	C	402	5/5	0.73	0.18	143,144,145,145	0
7	AMP	C	401	23/23	0.83	0.13	134,145,184,206	0
6	CL	A	604	1/1	0.93	0.18	117,117,117,117	0
4	STU	A	601	35/35	0.95	0.13	52,59,65,67	0
6	CL	B	301	1/1	0.96	0.10	89,89,89,89	0
5	32H	A	602	21/21	0.97	0.12	91,99,111,168	0
6	CL	A	605	1/1	0.98	0.16	50,50,50,50	0
6	CL	A	606	1/1	0.98	0.06	56,56,56,56	0
6	CL	A	603	1/1	0.98	0.05	69,69,69,69	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.

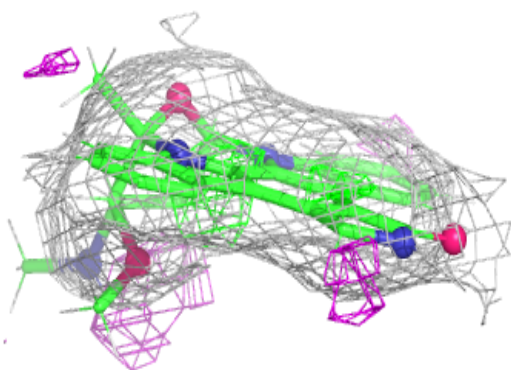
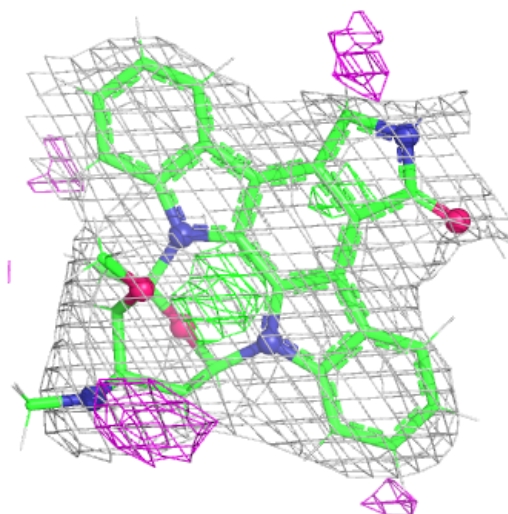
Electron density around AMP C 401:

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



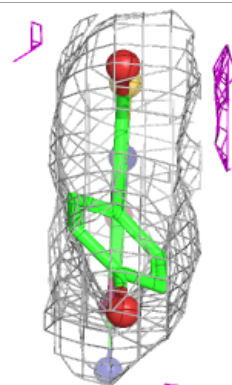
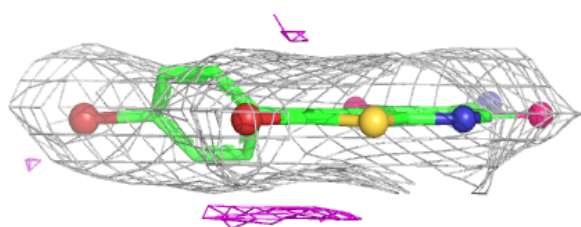
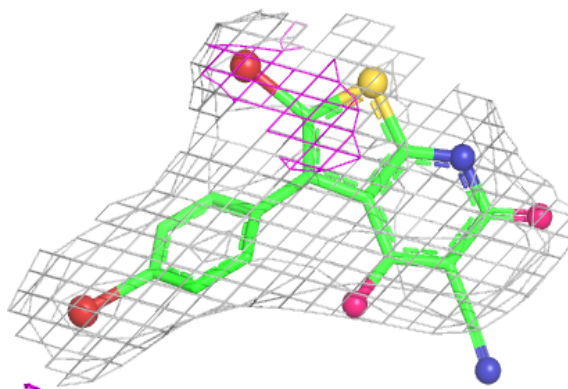
Electron density around STU A 601:

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



Electron density around 32H A 602:

$2mF_o - DF_c$ (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.