WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2025 – 05:13 pm BST

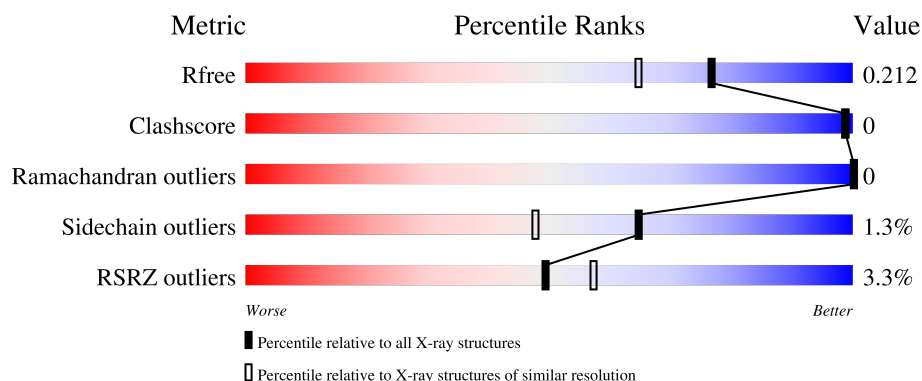|		
PDB ID	:	9FXD / pdb_00009fxd
Title	:	Structure of indole-3-acetic acid-amido synthetase GH3.6 from A.thaliana in complex with AMP and aspartate
Authors	:	Kopecny, D.; Briozzo, P.
Deposited on	:	2024-07-01
Resolution	:	1.74 Å(reported)

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 1.74 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	Percentile Ranks	Value
Rfree		0.212
Clashscore		0
Ramachandran outliers		0
Sidechain outliers		1.3%
RSRZ outliers		3.3%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1043 (1.74-1.74)
Clashscore	180529	1119 (1.74-1.74)
Ramachandran outliers	177936	1112 (1.74-1.74)
Sidechain outliers	177891	1112 (1.74-1.74)
RSRZ outliers	164620	1043 (1.74-1.74)

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 <=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	620	2% ▐ 93% · 6%
1	B	620	4% ▐ 91% · 6%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 19235 atoms, of which 9203 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 Indole-3-acetic acid-amido synthetase GH3.6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	584	Total	C	H	N	O	S	0	0	0
			9220	2953	4580	766	895	26			
1	B	584	Total	C	H	N	O	S	0	2	0
			9245	2960	4593	768	897	27			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q9LSQ4
A	-6	HIS	-	expression tag	UNP Q9LSQ4
A	-5	HIS	-	expression tag	UNP Q9LSQ4
A	-4	HIS	-	expression tag	UNP Q9LSQ4
A	-3	HIS	-	expression tag	UNP Q9LSQ4
A	-2	HIS	-	expression tag	UNP Q9LSQ4
A	-1	HIS	-	expression tag	UNP Q9LSQ4
A	0	ALA	-	expression tag	UNP Q9LSQ4
B	-7	MET	-	initiating methionine	UNP Q9LSQ4
B	-6	HIS	-	expression tag	UNP Q9LSQ4
B	-5	HIS	-	expression tag	UNP Q9LSQ4
B	-4	HIS	-	expression tag	UNP Q9LSQ4
B	-3	HIS	-	expression tag	UNP Q9LSQ4
B	-2	HIS	-	expression tag	UNP Q9LSQ4
B	-1	HIS	-	expression tag	UNP Q9LSQ4
B	0	ALA	-	expression tag	UNP Q9LSQ4

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		
2	B	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		

- Molecule 3 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$) (labeled as "Ligand of Interest" by depositor).
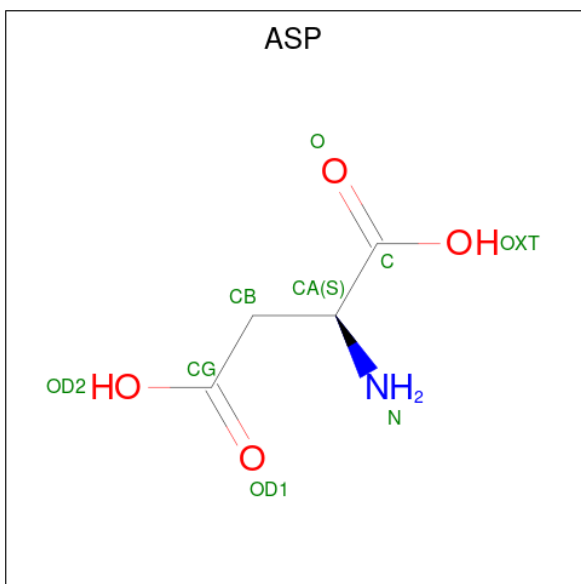
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			12	4	3	1	4		

Continued on next page...

Continued from previous page...

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 12	C 4	H 3	N 1	O 4	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	335	Total 335	O 335	0	0
4	B	341	Total 341	O 341	0	0

3 Residue-property plots ⓘ

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Indole-3-acetic acid-amido synthetase GH3.6
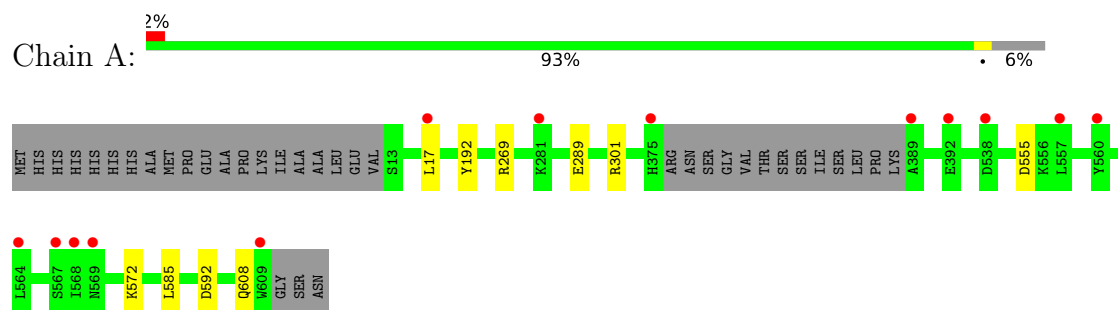
• Molecule 1: Indole-3-acetic acid-amido synthetase GH3.6
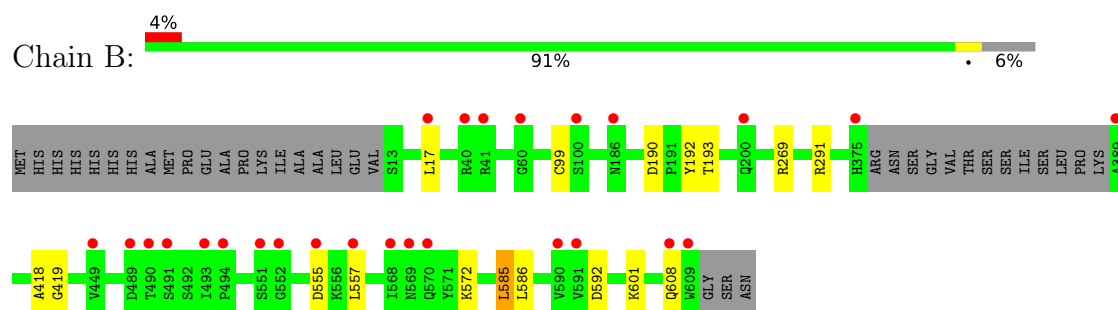
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	197.89Å　　197.89Å　　65.28Å 90.00°　　　90.00°　　　120.00°	Depositor
Resolution (Å)	25.30　–　1.74 25.30　–　1.74	Depositor EDS
% Data completeness (in resolution range)	64.3 (25.30-1.74) 64.2 (25.30-1.74)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 1.74Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.198　,　0.222 0.187　,　0.212	Depositor DCC
R_{free} test set	4781 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	24.7	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 36.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19235	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.46	0/4746	0.65	0/6442
1	B	0.48	0/4761	0.65	1/6462 (0.0%)
All	All	0.47	0/9507	0.65	1/12904 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	585	LEU	CB-CG-CD2	5.25	119.92	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4640	4580	4580	3	0
1	B	4652	4593	4592	5	0
2	A	23	12	12	0	0
2	B	23	12	12	0	0
3	A	9	3	3	0	0
3	B	9	3	3	0	0
4	A	335	0	0	0	0
4	B	341	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10032	9203	9202	8	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 0.

All (8) 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:557:LEU:HD11	1:B:586:LEU:HD21	1.83	0.60
1:A:17:LEU:HD12	1:A:192:TYR:CE2	2.47	0.50
1:B:17:LEU:HD23	1:B:192:TYR:CE2	2.46	0.49
1:B:190:ASP:HB3	1:B:193:THR:OG1	2.13	0.48
1:B:99[B]:CYS:SG	1:B:419:GLY:N	2.89	0.46
1:A:17:LEU:HD12	1:A:192:TYR:HE2	1.82	0.45
1:A:289:GLU:OE1	1:A:301:ARG:NH2	2.47	0.44
1:B:99[B]:CYS:SG	1:B:418:ALA:C	3.00	0.40

There are no symmetry-related clashes.

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	A	580/620 (94%)	573 (99%)	7 (1%)	0	100	100
1	B	582/620 (94%)	576 (99%)	6 (1%)	0	100	100
All	All	1162/1240 (94%)	1149 (99%)	13 (1%)	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 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	528/559 (94%)	522 (99%)	6 (1%)	70	55
1	B	530/559 (95%)	522 (98%)	8 (2%)	60	42
All	All	1058/1118 (95%)	1044 (99%)	14 (1%)	65	48

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	ARG
1	A	555	ASP
1	A	572	LYS
1	A	585	LEU
1	A	592	ASP
1	A	608	GLN
1	B	269	ARG
1	B	291	ARG
1	B	555	ASP
1	B	572	LYS
1	B	585	LEU
1	B	592	ASP
1	B	601	LYS
1	B	608	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no oligosaccharides in this entry.

5.6　Ligand geometry ⓘ

4 ligands are modelled in this entry.

There are no bond length outliers.
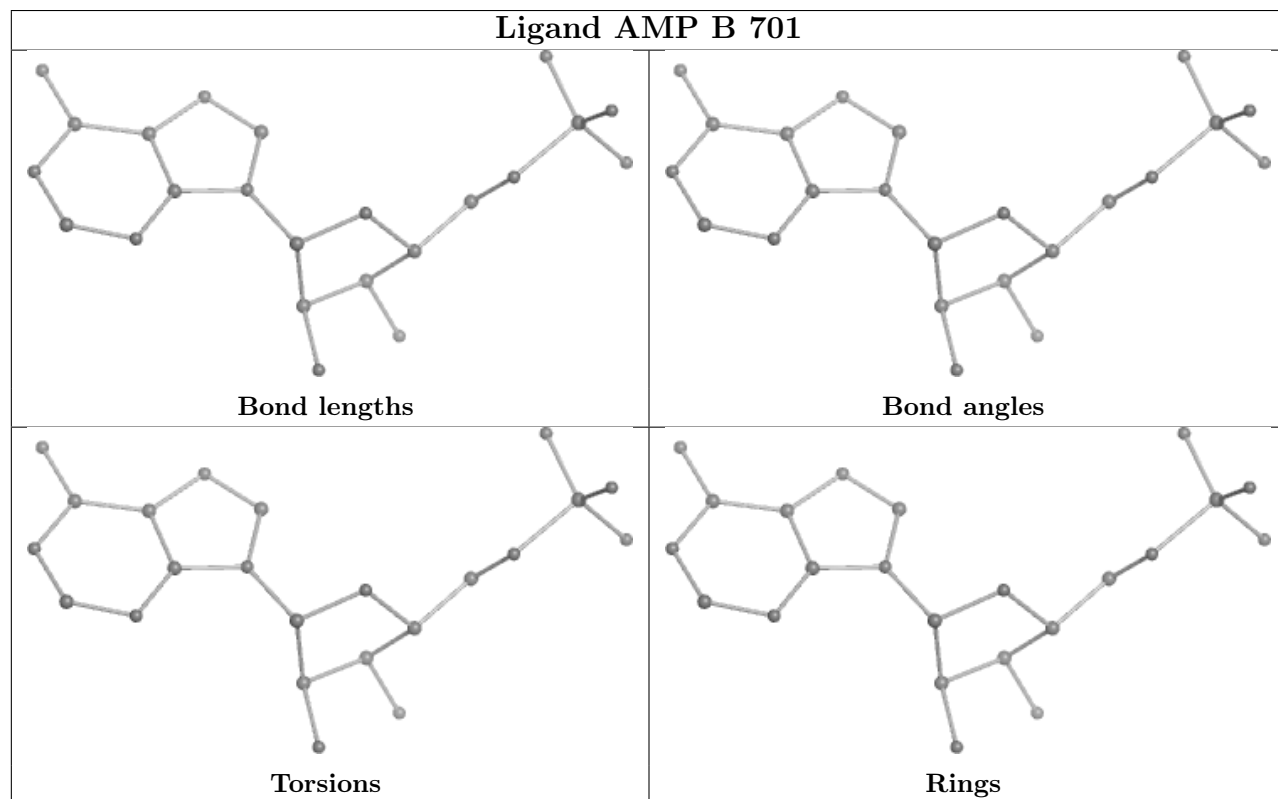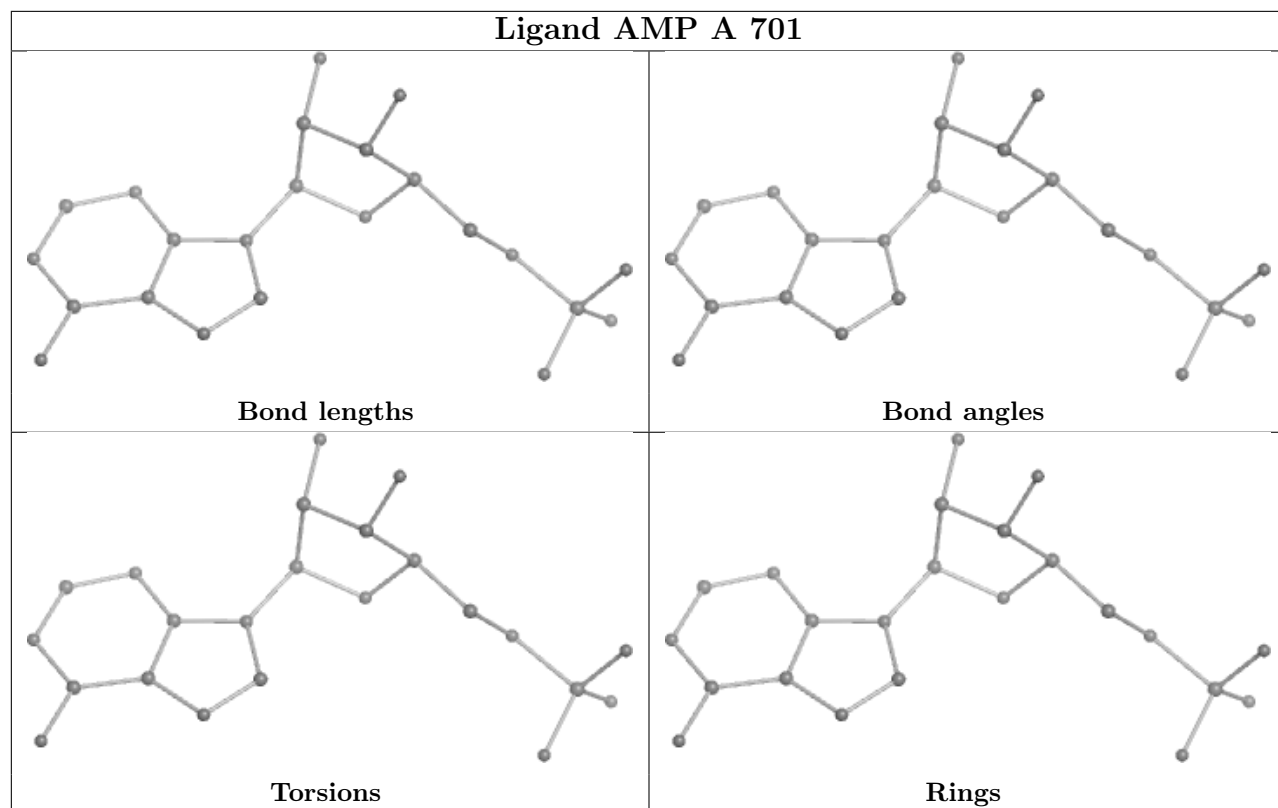
There are no bond angle outliers.

There are no chirality outliers.
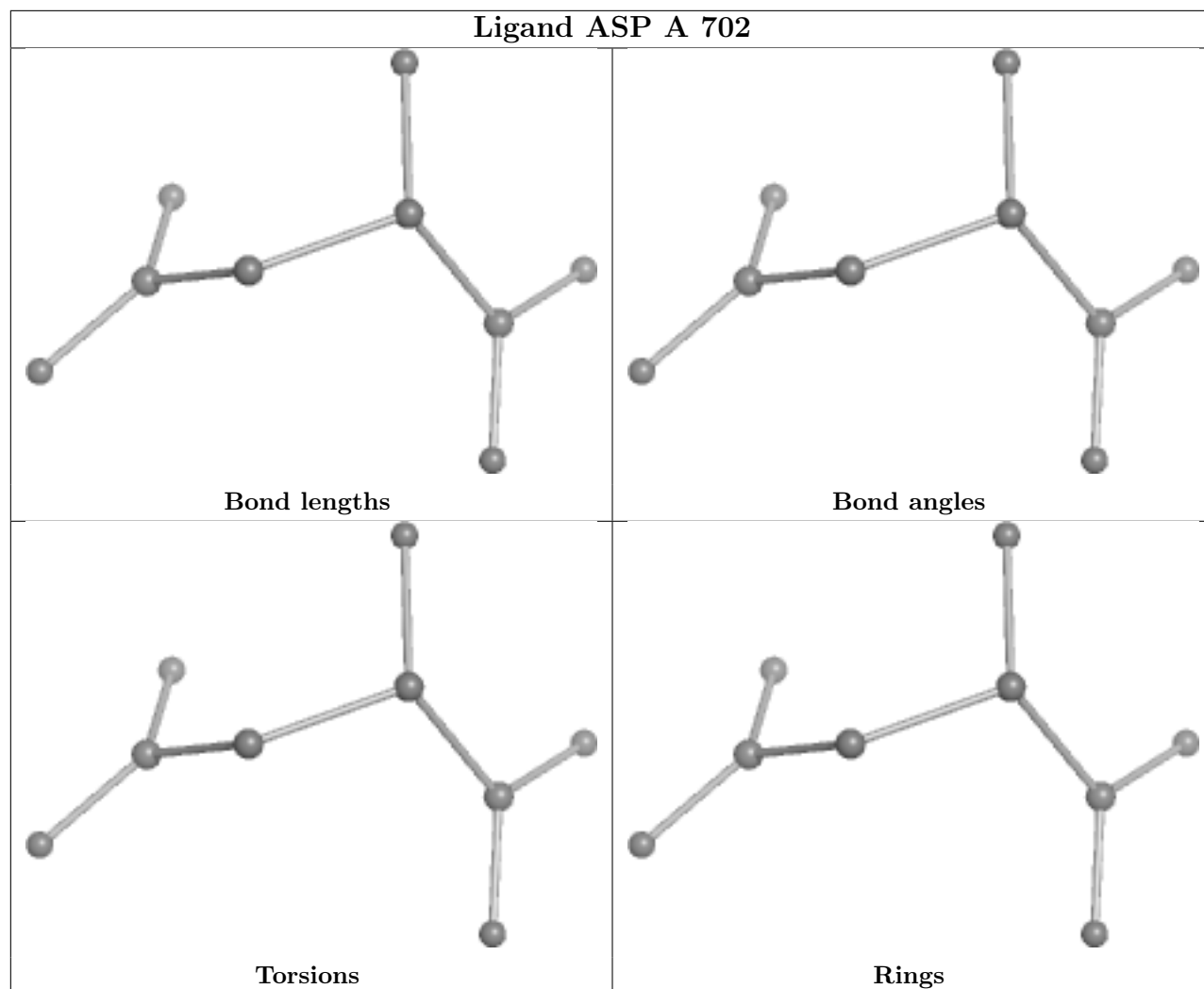
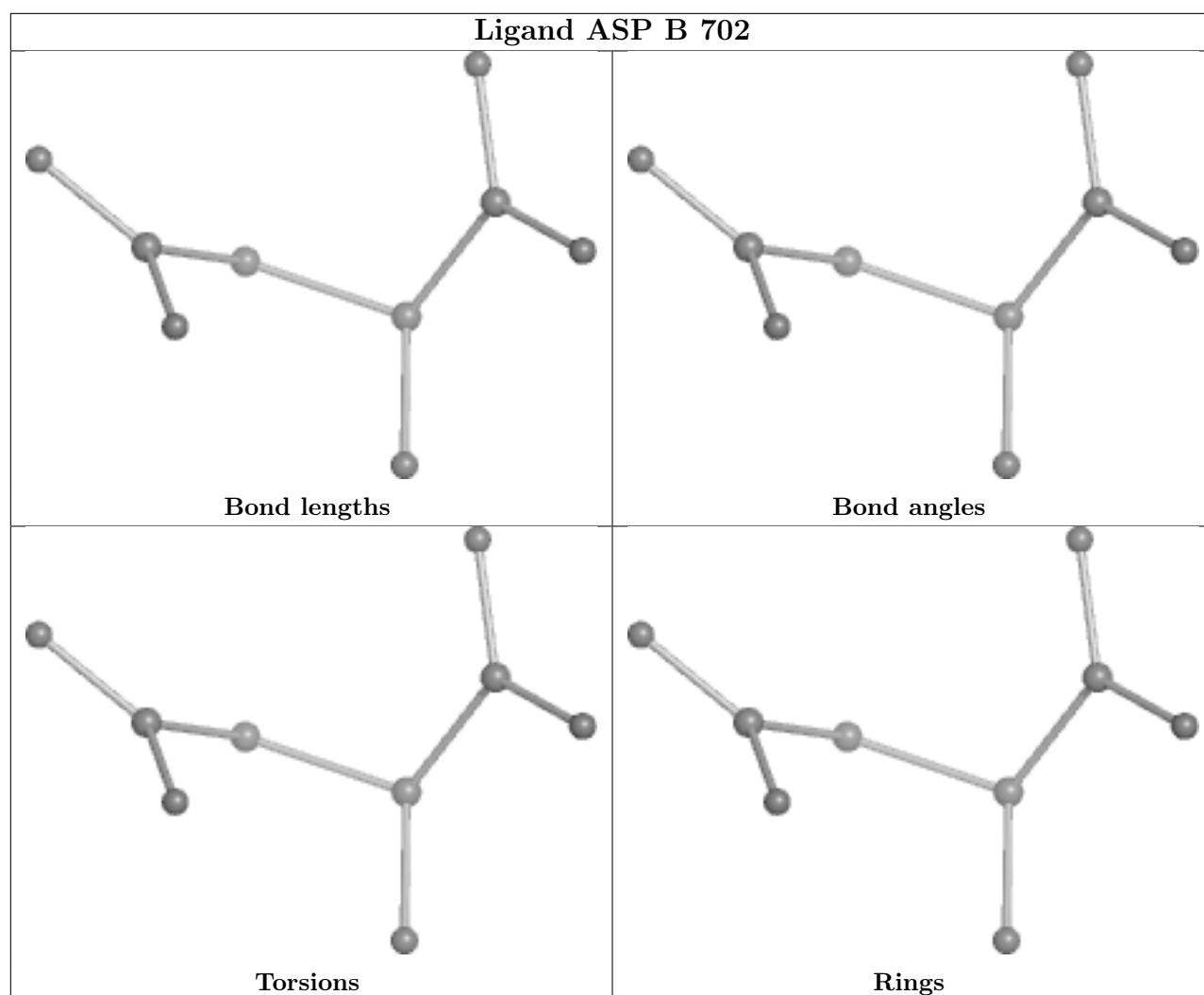There are no torsion outliers.

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 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 AMP A 701

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP B 701

Bond lengths

Bond angles

Torsions

Rings

Ligand ASP A 702

Bond lengths

Bond angles

Torsions

Rings

Ligand ASP B 702

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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	584/620 (94%)	-0.04	13 (2%)	62	68	16, 30, 51, 67	0
1	B	584/620 (94%)	0.06	26 (4%)	39	46	16, 32, 53, 68	2 (0%)
All	All	1168/1240 (94%)	0.01	39 (3%)	49	57	16, 31, 52, 68	2 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	568	ILE	4.1
1	B	389	ALA	4.0
1	A	17	LEU	3.8
1	B	609	TRP	3.6
1	A	375	HIS	3.6
1	B	375	HIS	3.5
1	B	608	GLN	3.3
1	A	568	ILE	3.2
1	A	538	ASP	3.0
1	A	557	LEU	2.9
1	A	609	TRP	2.8
1	B	557	LEU	2.8
1	B	17	LEU	2.7
1	B	491	SER	2.7
1	B	493	ILE	2.5
1	A	389	ALA	2.5
1	B	200[A]	GLN	2.5
1	B	552	GLY	2.5
1	A	569	ASN	2.5
1	A	281	LYS	2.4
1	B	60	GLY	2.4
1	B	591	VAL	2.4
1	A	564	LEU	2.3
1	B	186	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	590	VAL	2.3
1	B	40	ARG	2.2
1	B	569	ASN	2.2
1	B	41	ARG	2.1
1	B	489	ASP	2.1
1	A	560	TYR	2.1
1	A	567	SER	2.1
1	B	490	THR	2.1
1	A	392	GLU	2.1
1	B	551	SER	2.1
1	B	555	ASP	2.1
1	B	449	VAL	2.1
1	B	494	PRO	2.0
1	B	570	GLN	2.0
1	B	100	SER	2.0

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 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
3	ASP	B	702	9/9	0.90	0.10	28,32,42,42	0
3	ASP	A	702	9/9	0.94	0.07	28,31,40,42	0
2	AMP	B	701	23/23	0.97	0.05	20,21,23,23	0
2	AMP	A	701	23/23	0.99	0.03	16,18,19,19	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.
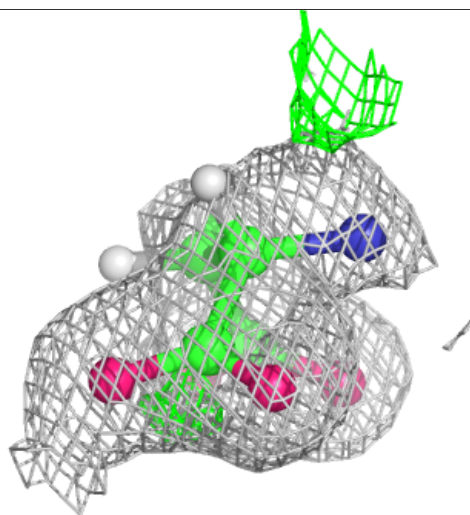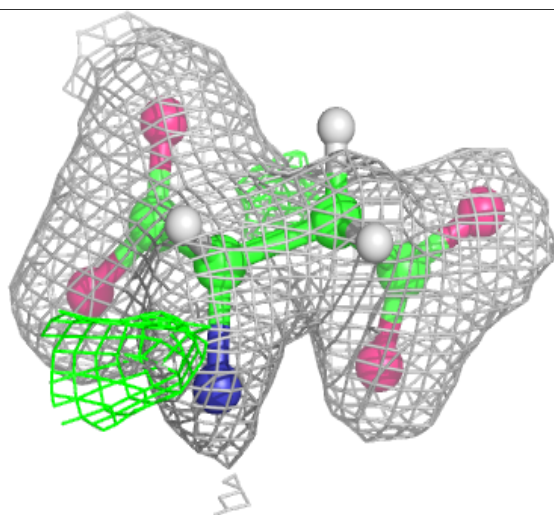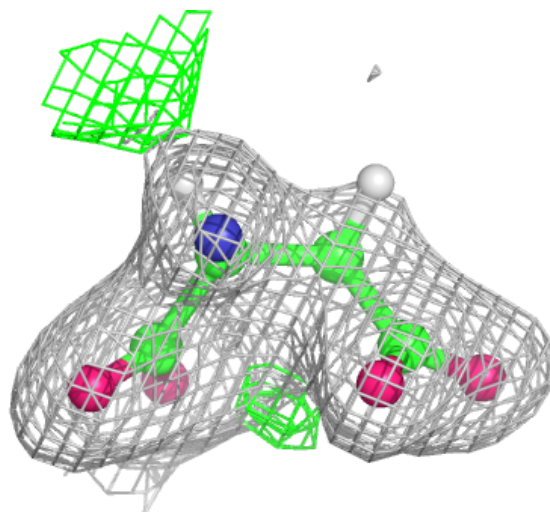
Electron density around ASP B 702:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
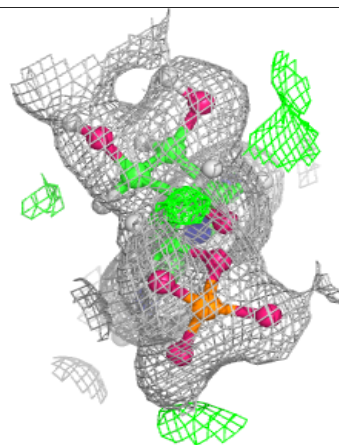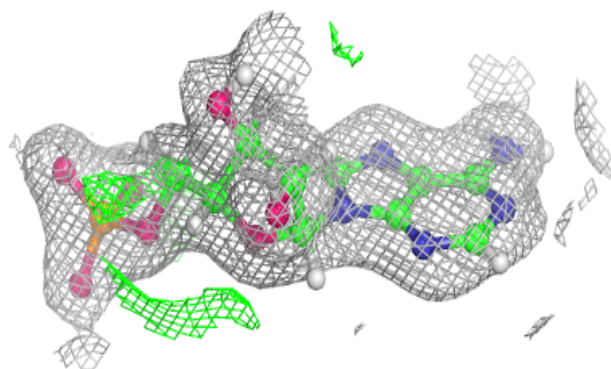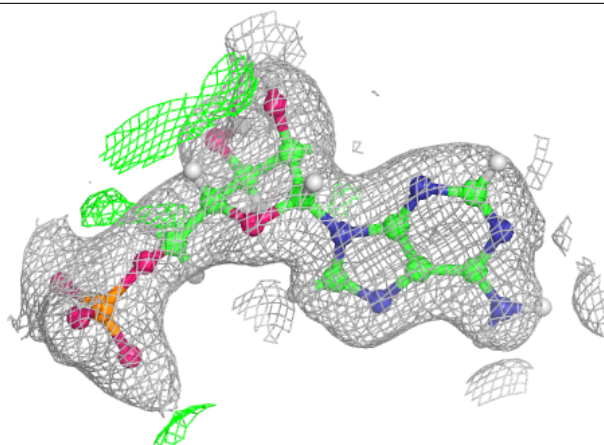and green (positive)
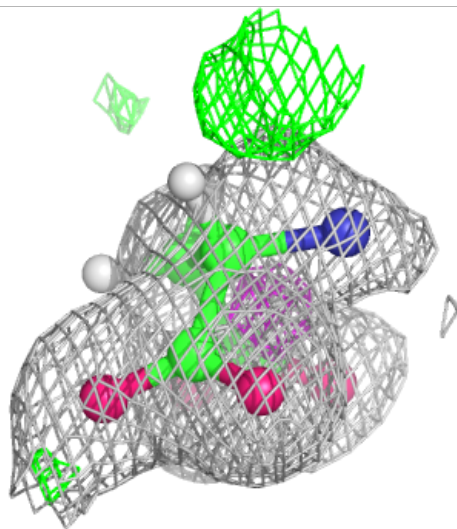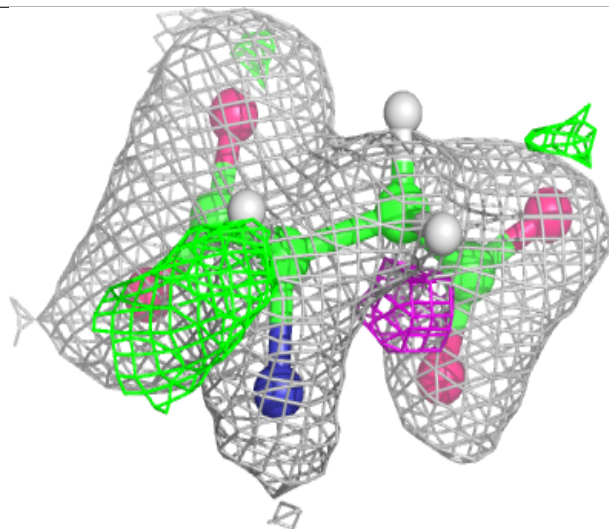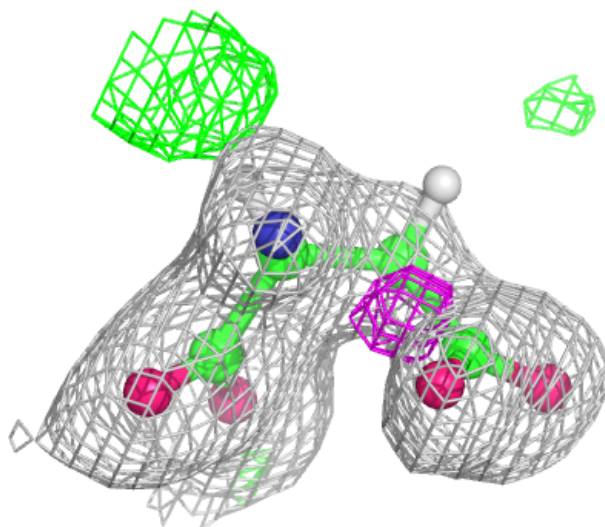
Electron density around ASP A 702:

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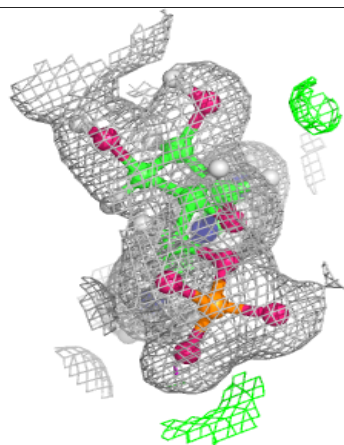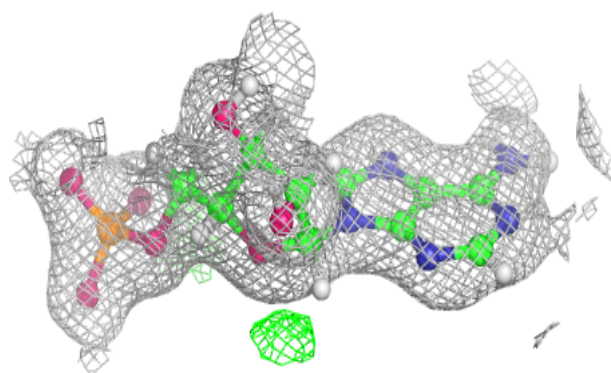$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around AMP B 701:

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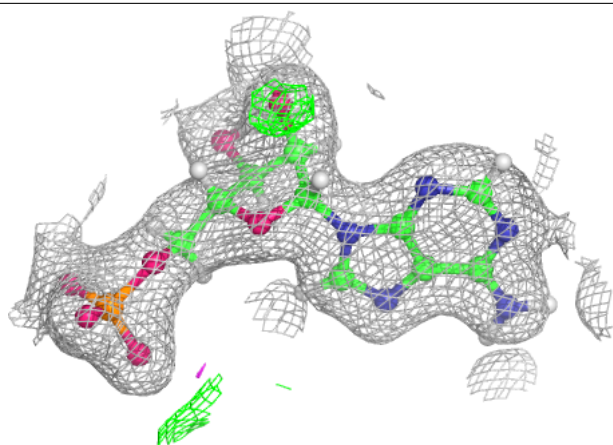$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around AMP A 701:

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 ⓘ

There are no such residues in this entry.