



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:08 AM UTC

PDB ID : 4MO5 / pdb_00004mo5
Title : Crystal structure of AnmK bound to AMPPCP and anhMurNAc
Authors : Bacik, J.P.; Mark, B.L.
Deposited on : 2013-09-11
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

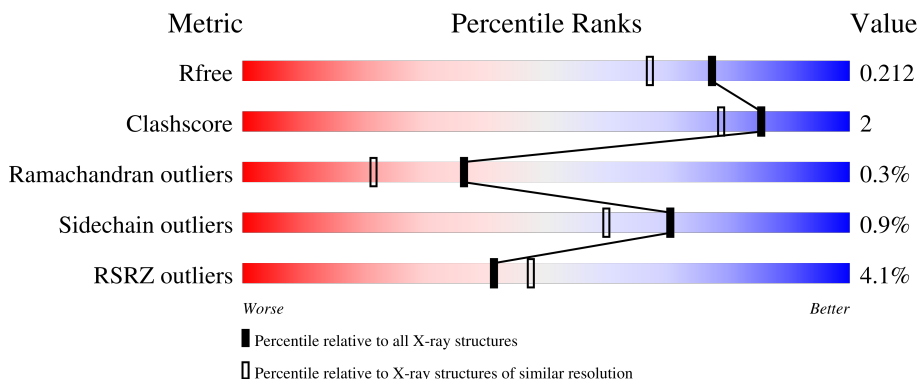
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	371	 6% 86% 7% 7%
1	B	371	 6% 89% 6% 6%
1	C	371	 2% 90% 5% 5%
1	D	371	 % 90% 5% 5%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 11637 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 Anhydro-N-acetylmuramic acid kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	345	2562	1619	456	472	15	0	0	0
1	B	350	2581	1636	462	468	15	0	0	0
1	C	351	2619	1658	468	478	15	0	0	0
1	D	352	2639	1669	470	485	15	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

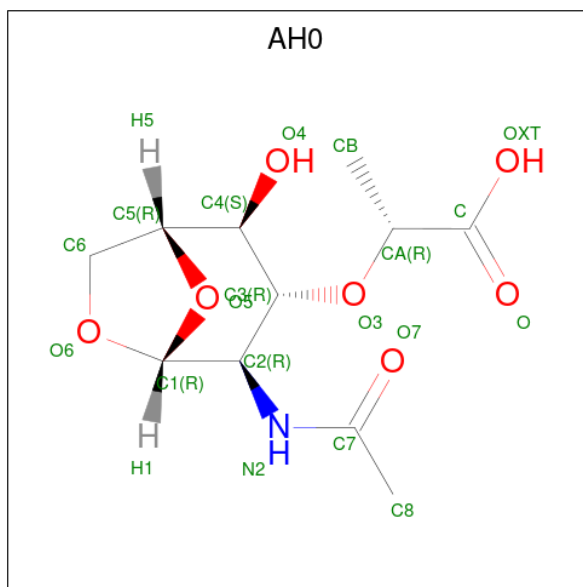
Chain	Residue	Modelled	Actual	Comment	Reference
A	364	GLY	-	expression tag	UNP Q9I5Q5
A	365	SER	-	expression tag	UNP Q9I5Q5
A	366	HIS	-	expression tag	UNP Q9I5Q5
A	367	HIS	-	expression tag	UNP Q9I5Q5
A	368	HIS	-	expression tag	UNP Q9I5Q5
A	369	HIS	-	expression tag	UNP Q9I5Q5
A	370	HIS	-	expression tag	UNP Q9I5Q5
A	371	HIS	-	expression tag	UNP Q9I5Q5
B	364	GLY	-	expression tag	UNP Q9I5Q5
B	365	SER	-	expression tag	UNP Q9I5Q5
B	366	HIS	-	expression tag	UNP Q9I5Q5
B	367	HIS	-	expression tag	UNP Q9I5Q5
B	368	HIS	-	expression tag	UNP Q9I5Q5
B	369	HIS	-	expression tag	UNP Q9I5Q5
B	370	HIS	-	expression tag	UNP Q9I5Q5
B	371	HIS	-	expression tag	UNP Q9I5Q5
C	364	GLY	-	expression tag	UNP Q9I5Q5
C	365	SER	-	expression tag	UNP Q9I5Q5
C	366	HIS	-	expression tag	UNP Q9I5Q5
C	367	HIS	-	expression tag	UNP Q9I5Q5
C	368	HIS	-	expression tag	UNP Q9I5Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	369	HIS	-	expression tag	UNP Q9I5Q5
C	370	HIS	-	expression tag	UNP Q9I5Q5
C	371	HIS	-	expression tag	UNP Q9I5Q5
D	364	GLY	-	expression tag	UNP Q9I5Q5
D	365	SER	-	expression tag	UNP Q9I5Q5
D	366	HIS	-	expression tag	UNP Q9I5Q5
D	367	HIS	-	expression tag	UNP Q9I5Q5
D	368	HIS	-	expression tag	UNP Q9I5Q5
D	369	HIS	-	expression tag	UNP Q9I5Q5
D	370	HIS	-	expression tag	UNP Q9I5Q5
D	371	HIS	-	expression tag	UNP Q9I5Q5

- Molecule 2 is 2-(2-ACETYLAMINO-4-HYDROXY-6,8-DIOXA-BICYCLO[3.2.1]OCT-3-YLOXY)-PROPIONIC ACID (CCD ID: AH0) (formula: C₁₁H₁₇NO₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
2	A	1	19	11	1	7	0	0
2	B	1	19	11	1	7	0	0
2	C	1	19	11	1	7	0	0
2	D	1	19	11	1	7	0	0

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).

HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.30Å 70.41Å 90.97Å 106.43° 104.43° 98.25°	Depositor
Resolution (Å)	44.81 – 1.75 44.81 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.5 (44.81-1.75) 92.7 (44.81-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.75Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.174 , 0.210 0.177 , 0.212	Depositor DCC
R_{free} test set	6692 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtrriage
Anisotropy	0.107	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11637	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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: ACP, AH0, MG

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	0.43	0/2621	0.80	1/3570 (0.0%)
1	B	0.48	0/2643	0.79	0/3605
1	C	0.44	0/2682	0.78	0/3656
1	D	0.47	1/2702 (0.0%)	0.75	0/3681
All	All	0.46	1/10648 (0.0%)	0.78	1/14512 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	110	ILE	C-O	-5.15	1.18	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ARG	N-CA-C	5.85	117.66	111.28

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	2562	0	2490	14	0
1	B	2581	0	2515	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2619	0	2552	11	0
1	D	2639	0	2572	9	0
2	A	19	0	16	1	0
2	B	19	0	16	0	0
2	C	19	0	16	0	0
2	D	19	0	16	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	31	0	14	0	0
4	D	1	0	0	0	0
5	A	225	0	0	2	0
5	B	198	0	0	2	0
5	C	266	0	0	1	0
5	D	358	0	0	1	0
All	All	11637	0	10243	45	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 2.

All (45) 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:C:169:VAL:HG21	1:C:277:LEU:HD11	1.66	0.78
1:A:44:ASP:OD2	1:A:65:ARG:NH2	2.22	0.69
1:C:311:ARG:NH2	1:C:317:GLU:OE1	2.31	0.64
1:D:169:VAL:HG21	1:D:277:LEU:HD11	1.84	0.59
1:C:44:ASP:OD2	1:C:65:ARG:NH2	2.28	0.56
1:D:41:LEU:HD13	1:D:65:ARG:HG2	1.89	0.54
1:B:16:MET:HE3	1:B:69:LEU:HD23	1.91	0.53
1:B:82:GLN:HG2	1:C:65:ARG:HD3	1.90	0.53
1:A:168:ASN:ND2	5:A:669:HOH:O	2.41	0.53
1:D:111:GLY:O	1:D:112:ASN:C	2.52	0.53
1:C:271:ARG:NH1	5:C:721:HOH:O	2.29	0.52
1:A:55:GLU:HB3	1:B:56:ILE:HG12	1.93	0.51
1:A:156:THR:HG22	1:A:158:ARG:HG3	1.93	0.51
1:D:295:PHE:CZ	1:D:322:PRO:HG2	2.46	0.50
1:C:153:ASP:O	1:C:154:ASP:CB	2.60	0.49
1:A:171:LEU:HD22	1:A:281:GLN:HG2	1.96	0.47
1:D:16:MET:HE3	1:D:69:LEU:HD23	1.97	0.46
1:A:154:ASP:HA	1:A:175:GLY:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HD11	1:A:181:PHE:HE1	1.81	0.45
2:A:401:AH0:HA	2:A:401:AH0:H4	1.84	0.45
1:C:184:GLY:HA2	1:C:227:PHE:CE2	2.52	0.45
1:B:82:GLN:CG	1:C:65:ARG:HD3	2.47	0.45
1:B:254:PRO:O	1:B:255:ALA:C	2.61	0.44
1:A:325:MET:HG2	5:A:539:HOH:O	2.16	0.44
1:B:61:GLU:HG2	5:B:692:HOH:O	2.18	0.44
1:D:7:LEU:HD13	1:D:70:ALA:HB1	1.99	0.44
1:D:189:LEU:HD21	1:D:241:PHE:HB3	2.00	0.44
1:C:169:VAL:O	1:C:180:GLY:HA2	2.19	0.43
1:B:16:MET:HE2	1:B:66:TRP:NE1	2.33	0.43
1:A:63:GLU:OE1	1:B:130:ARG:NH2	2.52	0.43
1:A:209:ALA:HB2	1:A:262:GLN:HG3	1.99	0.43
1:D:38:PRO:HG2	5:D:836:HOH:O	2.19	0.43
1:A:281:GLN:HA	1:A:282:PRO:HD2	1.82	0.43
1:A:16:MET:HE2	1:A:66:TRP:CE2	2.54	0.43
1:B:35:LEU:HD22	1:B:69:LEU:HD11	2.00	0.42
1:B:65:ARG:HD2	5:B:685:HOH:O	2.18	0.42
1:D:256:LEU:HD12	1:D:257:PRO:HD2	2.01	0.42
1:A:141:PRO:HD2	1:A:348:VAL:HG12	2.02	0.42
1:C:49:CYS:HA	1:C:98:ILE:O	2.20	0.41
1:C:35:LEU:HD12	1:C:35:LEU:HA	1.85	0.41
1:B:256:LEU:HB2	1:B:261:ILE:HD11	2.03	0.41
1:B:29:LEU:HD23	1:B:321:PRO:HG2	2.03	0.41
1:B:101:GLU:OE1	1:B:104:ARG:HD3	2.21	0.41
1:B:35:LEU:CD2	1:B:69:LEU:HD11	2.50	0.40
1:A:321:PRO:HA	1:A:322:PRO:HD2	1.91	0.40

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	339/371 (91%)	330 (97%)	8 (2%)	1 (0%)	36	21
1	B	346/371 (93%)	341 (99%)	4 (1%)	1 (0%)	36	21
1	C	347/371 (94%)	342 (99%)	4 (1%)	1 (0%)	36	21
1	D	348/371 (94%)	343 (99%)	4 (1%)	1 (0%)	36	21
All	All	1380/1484 (93%)	1356 (98%)	20 (1%)	4 (0%)	36	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	112	ASN
1	A	112	ASN
1	B	112	ASN
1	C	112	ASN

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	256/287 (89%)	253 (99%)	3 (1%)	63	49
1	B	255/287 (89%)	252 (99%)	3 (1%)	63	49
1	C	262/287 (91%)	261 (100%)	1 (0%)	84	80
1	D	265/287 (92%)	263 (99%)	2 (1%)	73	64
All	All	1038/1148 (90%)	1029 (99%)	9 (1%)	70	60

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	183	CYS
1	A	345	CYS
1	B	3	ARG
1	B	83	MET
1	B	277	LEU
1	C	277	LEU

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Mol	Chain	Res	Type
1	D	46	LEU
1	D	65	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	105	HIS
1	A	109	GLN
1	A	187	ASN
1	A	196	HIS
1	A	249	HIS
1	B	162	ASN
1	B	168	ASN
1	B	201	HIS
1	C	105	HIS
1	C	187	ASN
1	C	195	HIS
1	D	105	HIS
1	D	109	GLN
1	D	187	ASN
1	D	196	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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
2	AH0	D	401	-	20,20,20	0.19	0	25,29,29	0.49	0
3	ACP	C	402	-	29,29,33	0.61	1 (3%)	41,45,52	0.63	1 (2%)
2	AH0	A	401	-	20,20,20	0.16	0	25,29,29	0.43	0
3	ACP	B	402	-	29,29,33	0.79	1 (3%)	41,45,52	0.69	0
2	AH0	B	401	-	20,20,20	0.18	0	25,29,29	0.44	0
2	AH0	C	401	-	20,20,20	0.22	0	25,29,29	0.73	1 (4%)
3	ACP	A	402	-	29,29,33	0.58	0	41,45,52	0.62	1 (2%)
3	ACP	D	402	4	31,33,33	0.82	1 (3%)	47,52,52	0.70	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
2	AH0	D	401	-	-	0/12/37/37	0/3/2/2
3	ACP	C	402	-	-	1/13/32/38	0/3/3/3
2	AH0	A	401	-	-	1/12/37/37	0/3/2/2
3	ACP	B	402	-	-	2/13/32/38	0/3/3/3
2	AH0	B	401	-	-	1/12/37/37	0/3/2/2
2	AH0	C	401	-	-	1/12/37/37	0/3/2/2
3	ACP	A	402	-	-	0/13/32/38	0/3/3/3
3	ACP	D	402	4	-	4/19/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	ACP	PA-O3A	-4.14	1.55	1.59
3	B	402	ACP	PA-O3A	-3.49	1.55	1.59
3	C	402	ACP	PA-O3A	-2.52	1.56	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	AH0	O3-C3-C4	2.87	114.53	107.23
3	A	402	ACP	O3A-PA-O1A	2.43	118.00	110.70
3	C	402	ACP	O3A-PA-O1A	2.39	117.90	110.70

There are no chirality outliers.

All (10) torsion outliers are listed below:

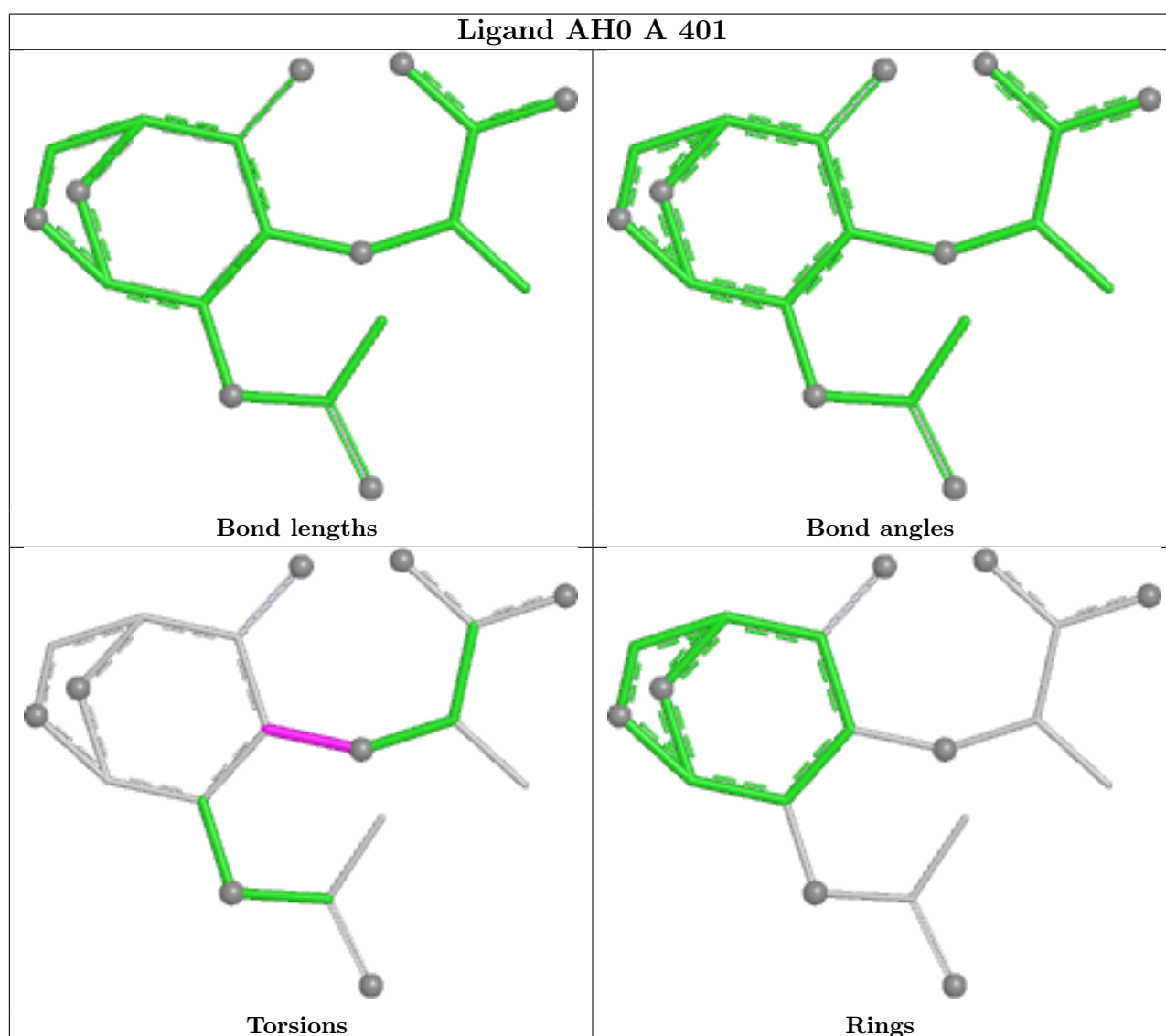
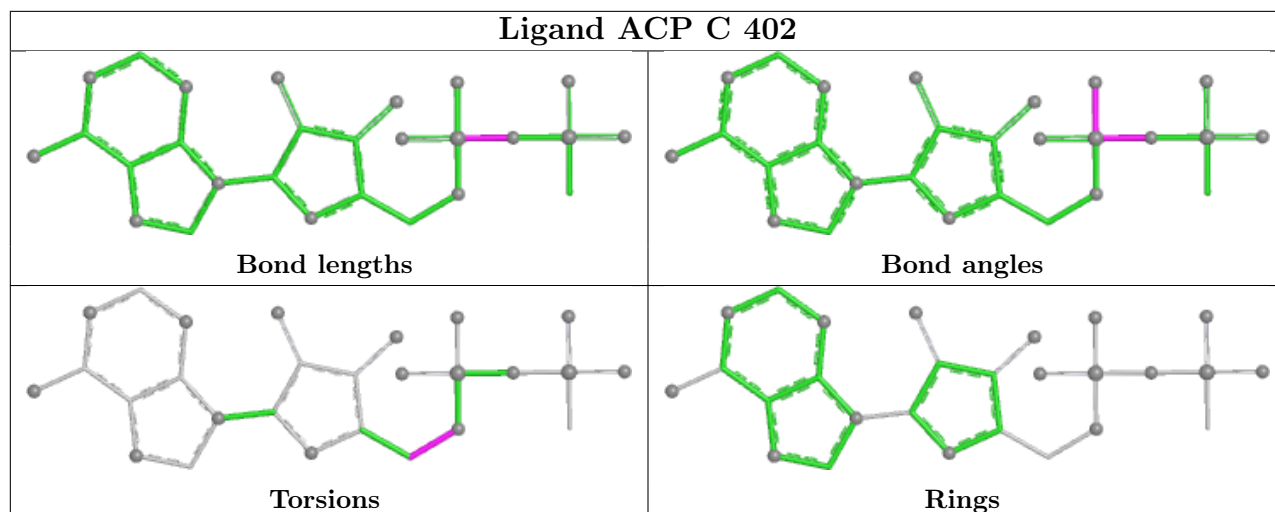
Mol	Chain	Res	Type	Atoms
2	A	401	AH0	C4-C3-O3-CA
2	B	401	AH0	C4-C3-O3-CA
2	C	401	AH0	C4-C3-O3-CA
3	D	402	ACP	PB-C3B-PG-O1G
3	D	402	ACP	PB-C3B-PG-O2G
3	D	402	ACP	PB-C3B-PG-O3G
3	B	402	ACP	C3'-C4'-C5'-O5'
3	C	402	ACP	C4'-C5'-O5'-PA
3	D	402	ACP	C4'-C5'-O5'-PA
3	B	402	ACP	O4'-C4'-C5'-O5'

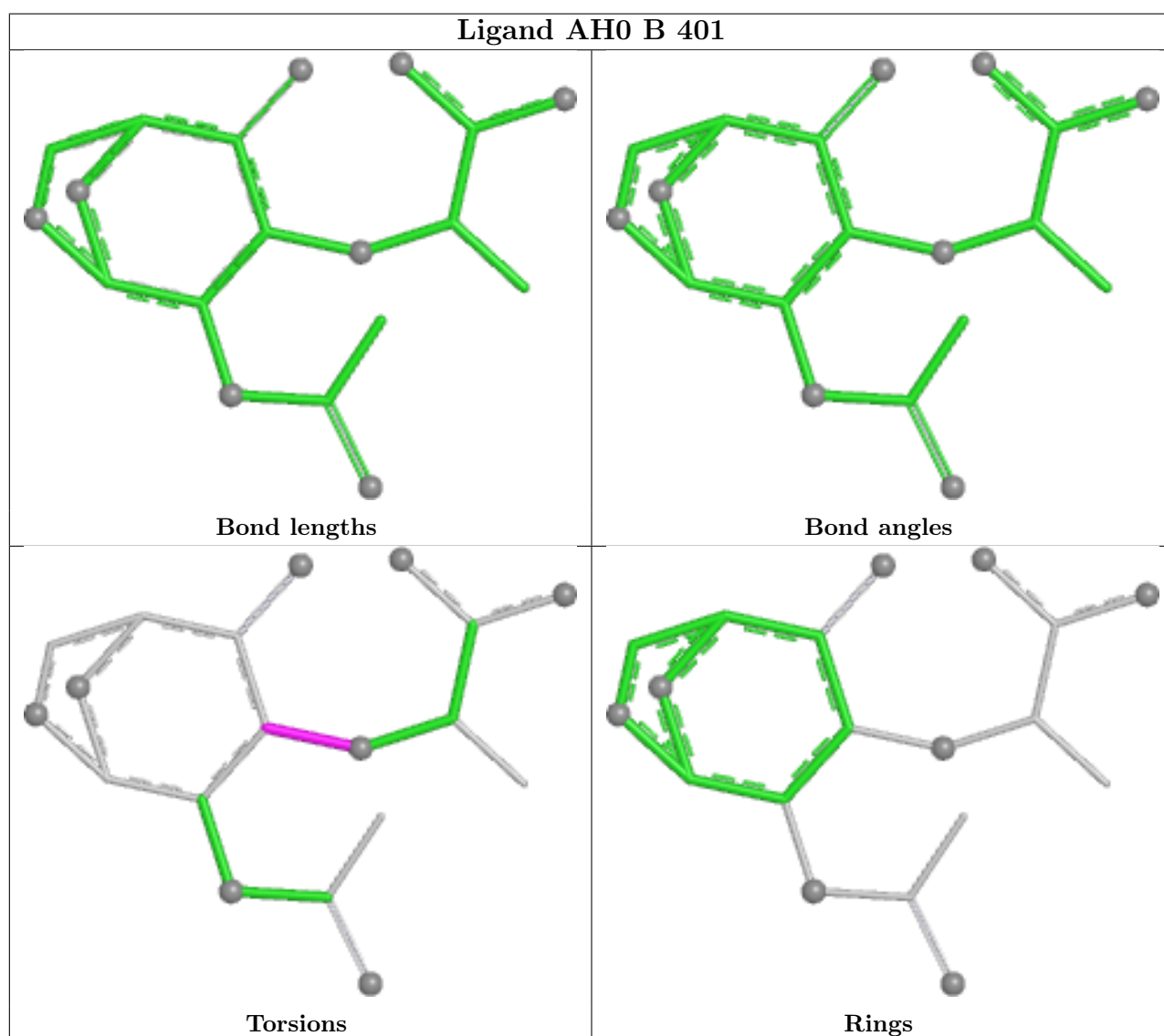
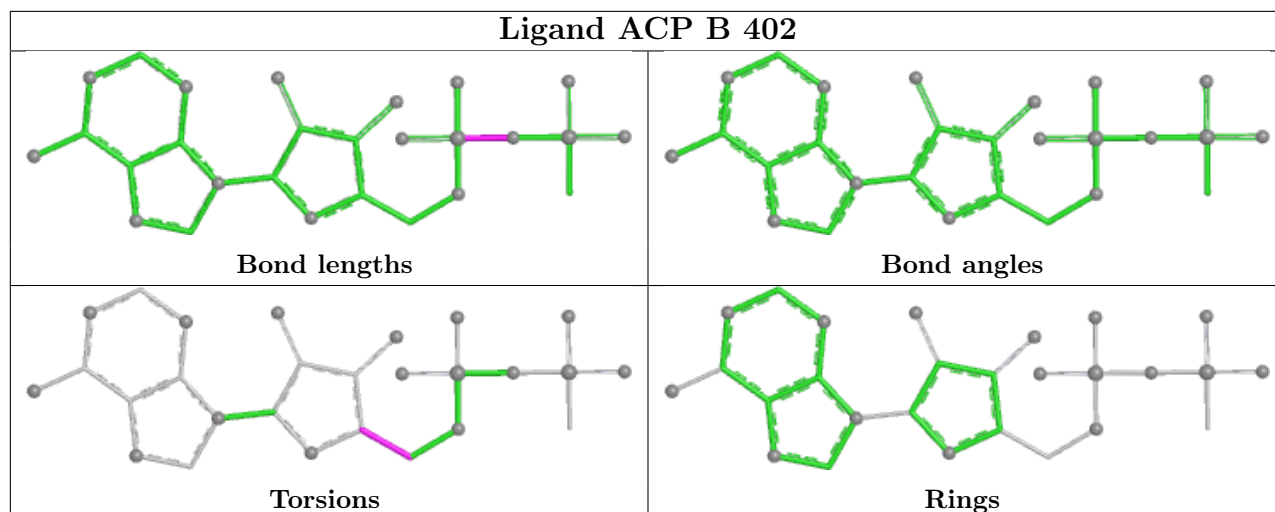
There are no ring outliers.

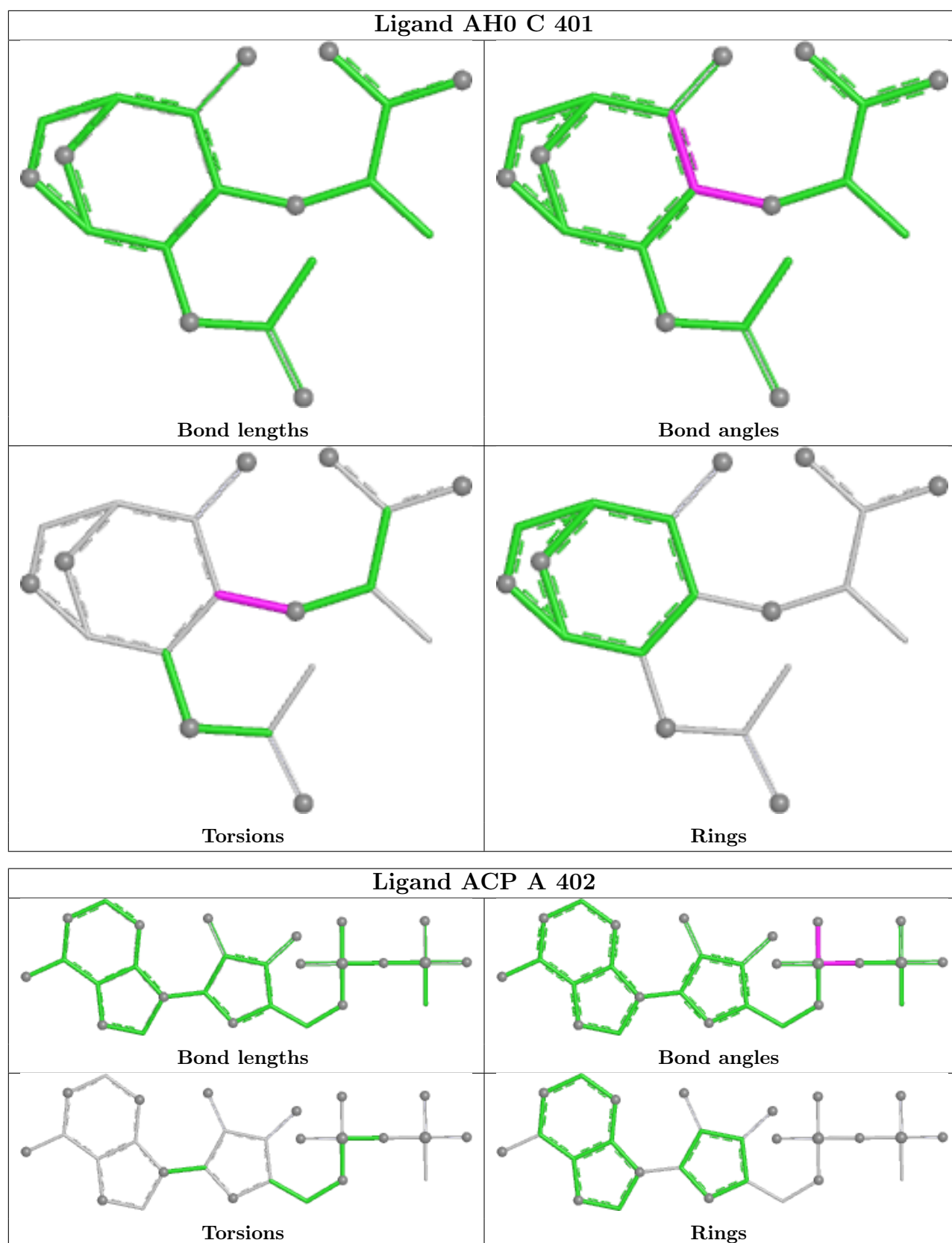
1 monomer is involved in 1 short contact:

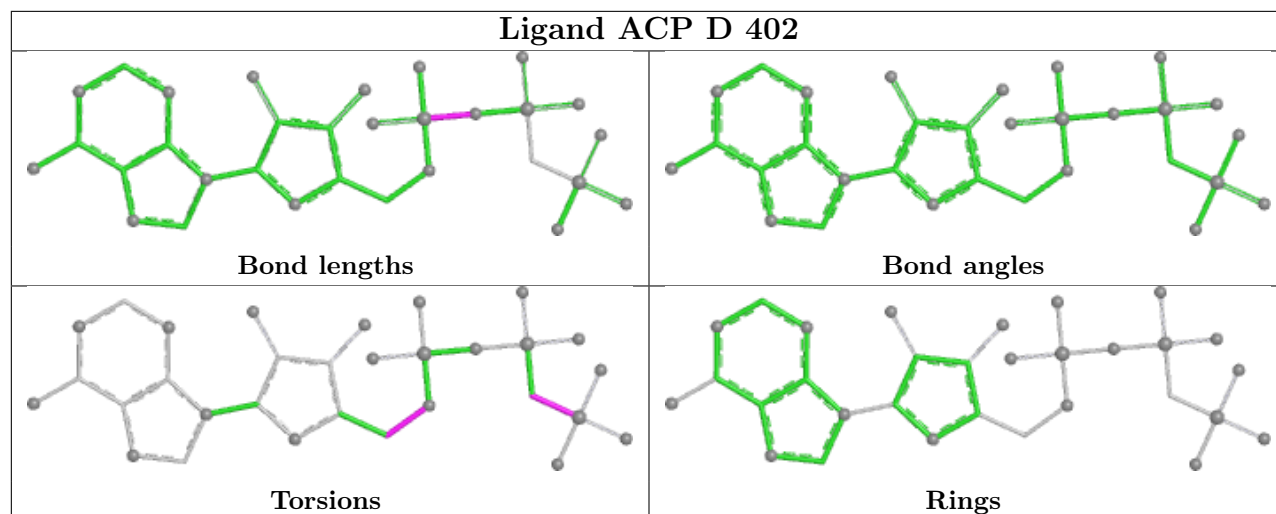
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	AH0	1	0

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

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	345/371 (92%)	0.28	24 (6%) 22 26	16, 30, 66, 93	0
1	B	350/371 (94%)	0.31	21 (6%) 27 31	15, 31, 66, 80	0
1	C	351/371 (94%)	0.11	7 (1%) 65 71	14, 28, 51, 64	0
1	D	352/371 (94%)	-0.16	5 (1%) 73 80	13, 23, 41, 63	0
All	All	1398/1484 (94%)	0.13	57 (4%) 41 47	13, 28, 58, 93	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	318	TYR	4.4
1	D	227	PHE	4.3
1	D	228	PHE	4.2
1	A	251	ALA	4.0
1	C	166	PHE	3.6
1	C	227	PHE	3.5
1	B	251	ALA	3.5
1	C	318	TYR	3.2
1	A	154	ASP	3.2
1	A	247	GLN	3.2
1	A	242	ASN	3.1
1	A	246	LEU	3.1
1	D	241	PHE	3.0
1	A	252	ARG	3.0
1	A	224	ALA	2.9
1	B	224	ALA	2.9
1	A	258	ALA	2.9
1	C	228	PHE	2.9
1	A	253	HIS	2.9
1	A	245	TRP	2.8
1	A	241	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	199	GLY	2.8
1	A	153	ASP	2.8
1	B	245	TRP	2.7
1	A	250	LEU	2.7
1	A	184	GLY	2.7
1	B	243	LEU	2.6
1	A	156	THR	2.6
1	A	193	TRP	2.6
1	A	175	GLY	2.6
1	A	244	PRO	2.6
1	A	155	ASP	2.5
1	C	153	ASP	2.4
1	B	193	TRP	2.4
1	B	241	PHE	2.4
1	B	178	VAL	2.4
1	A	243	LEU	2.4
1	B	181	PHE	2.4
1	C	154	ASP	2.4
1	A	366	HIS	2.4
1	D	226	GLU	2.3
1	B	194	ILE	2.3
1	A	259	ALA	2.3
1	B	201	HIS	2.3
1	B	318	TYR	2.3
1	B	175	GLY	2.3
1	C	175	GLY	2.3
1	A	217	ALA	2.3
1	B	183	CYS	2.2
1	B	35	LEU	2.1
1	B	11	THR	2.1
1	B	195	HIS	2.1
1	B	205	ASP	2.1
1	A	220	ALA	2.0
1	B	25	ASP	2.0
1	B	154	ASP	2.0
1	B	192	ALA	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

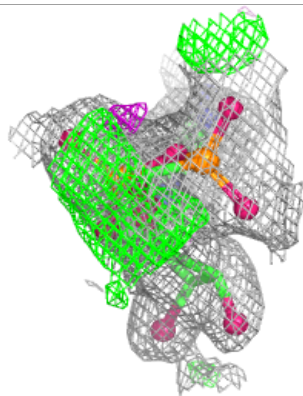
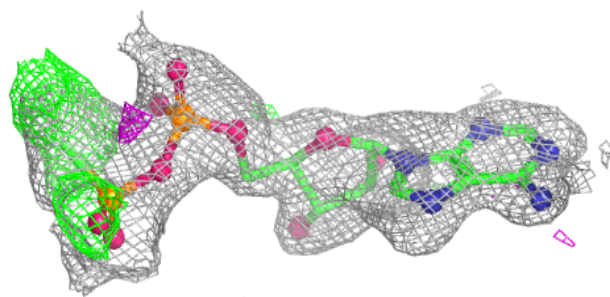
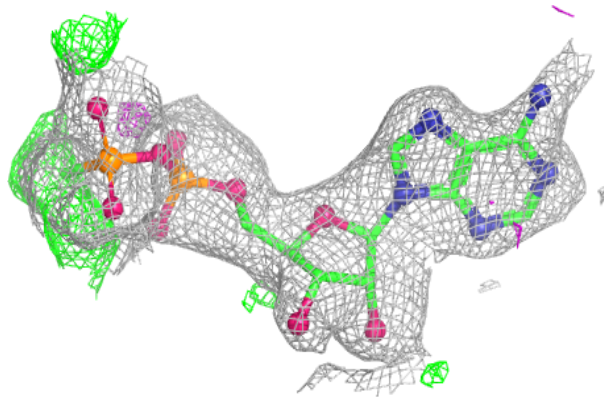
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ACP	B	402	27/31	0.77	0.14	37,51,85,97	0
3	ACP	A	402	27/31	0.88	0.10	28,39,64,68	0
3	ACP	C	402	27/31	0.88	0.10	23,29,57,103	0
2	AH0	A	401	19/19	0.93	0.08	22,27,35,35	0
3	ACP	D	402	31/31	0.94	0.08	22,28,62,66	0
2	AH0	D	401	19/19	0.95	0.06	18,22,26,28	0
4	MG	D	403	1/1	0.96	0.06	12,12,12,12	1
2	AH0	B	401	19/19	0.97	0.05	17,24,30,30	0
2	AH0	C	401	19/19	0.98	0.04	19,22,30,31	0

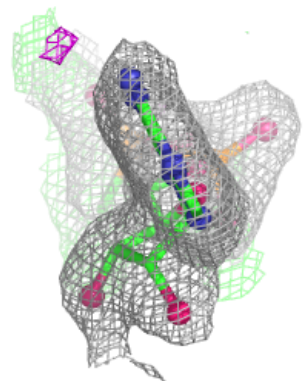
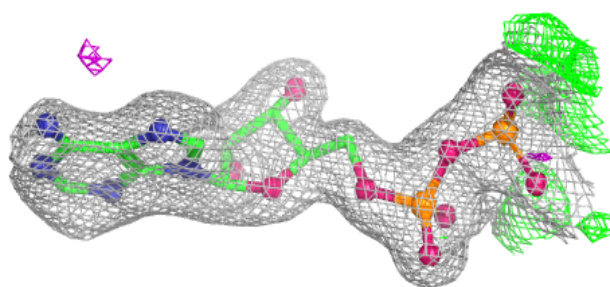
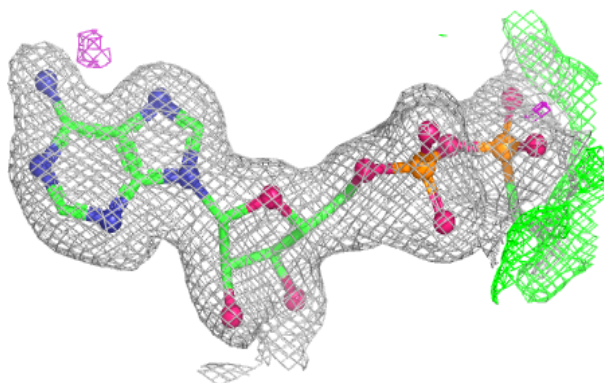
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP B 402:

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

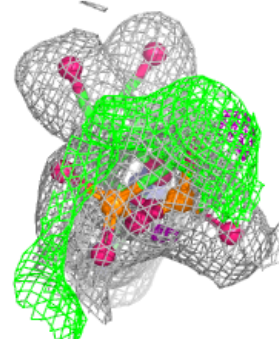
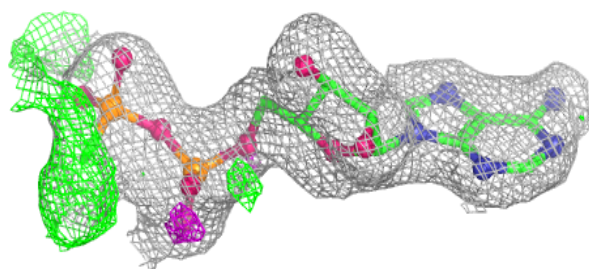
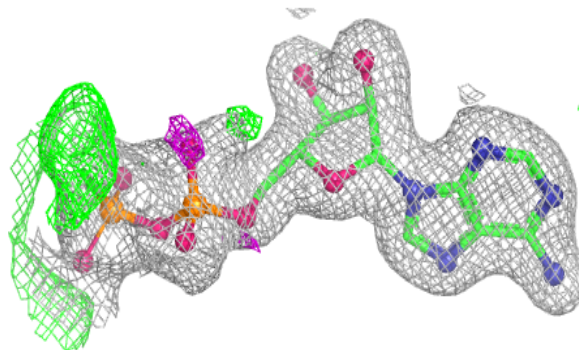
**Electron density around ACP A 402:**

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

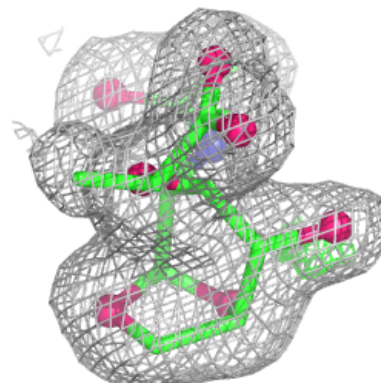
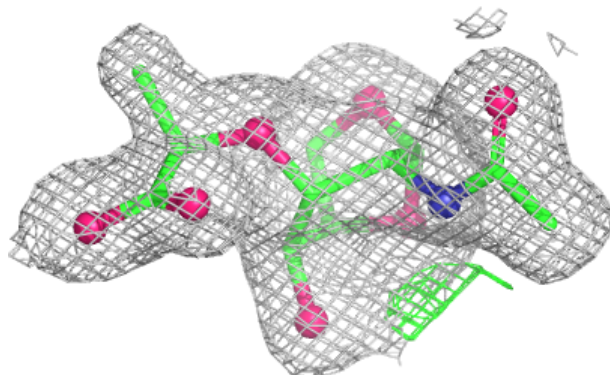
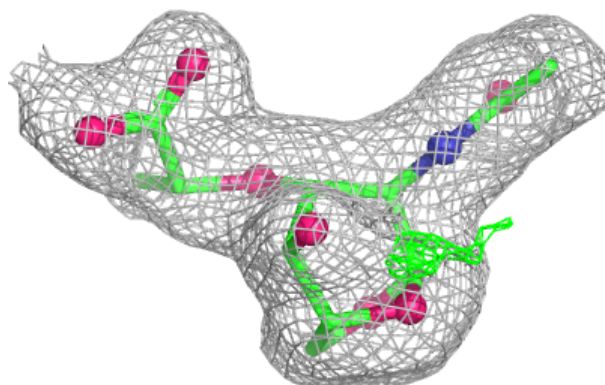


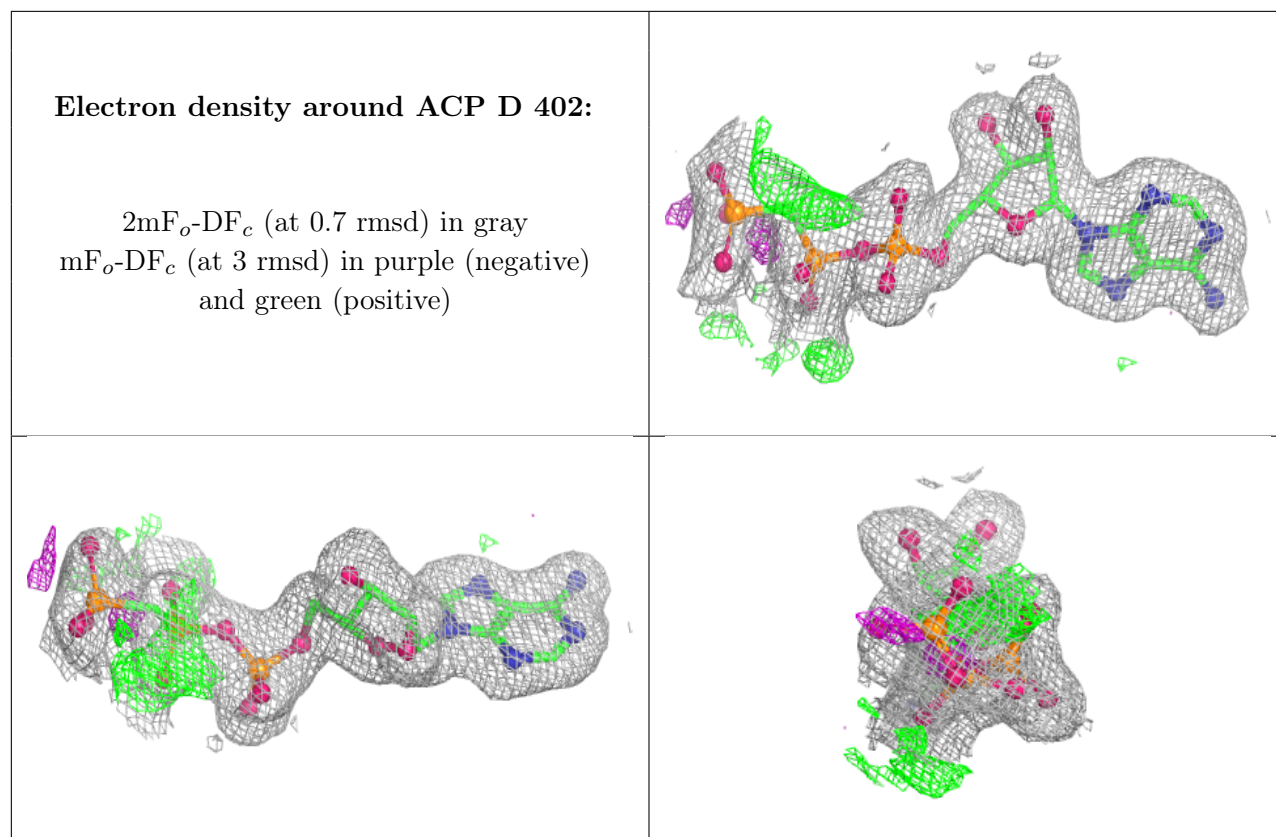
Electron density around ACP C 402:

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

**Electron density around AH0 A 401:**

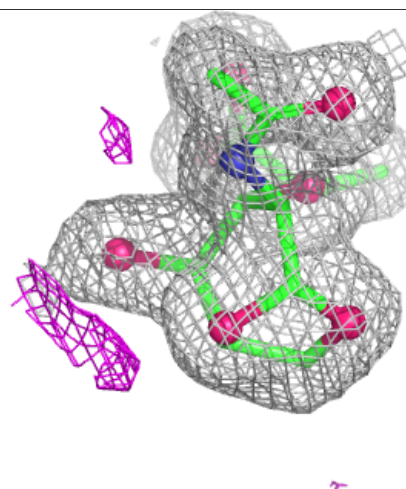
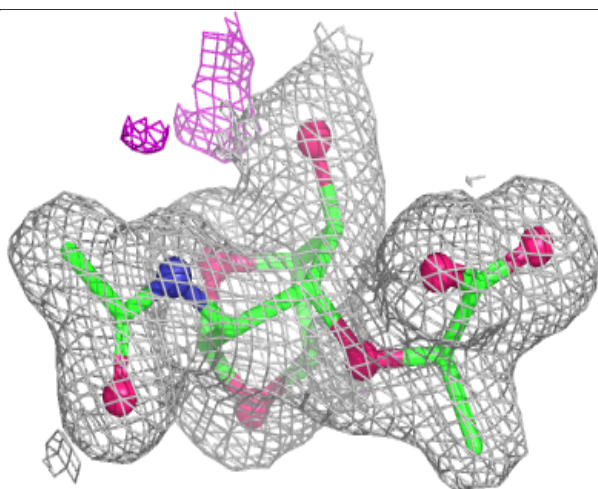
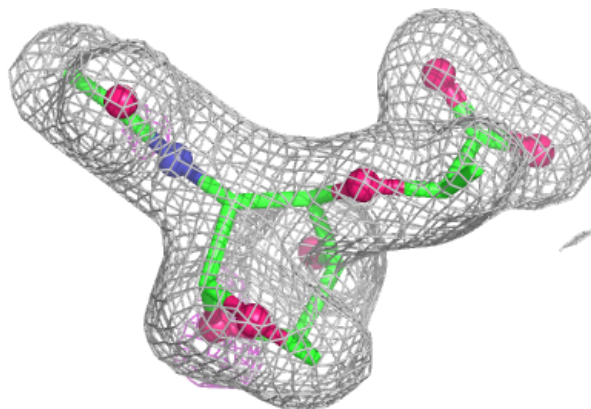
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

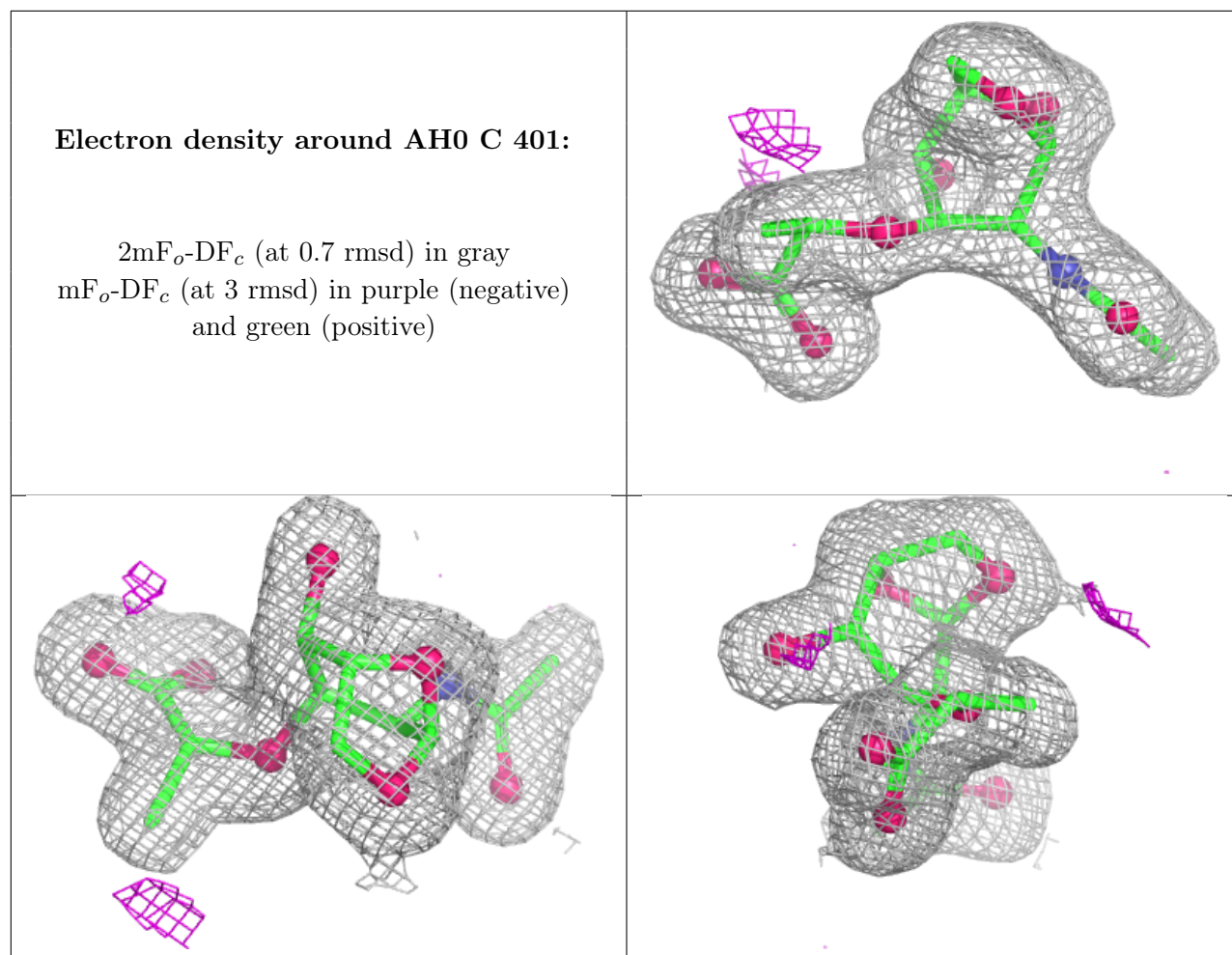




Electron density around AH0 B 401:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.