



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:36 PM UTC

PDB ID : 9FU5 / pdb\_00009fu5  
Title : 25-hydroxy steroid kinase + AMP  
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Deposited on : 2024-06-26  
Resolution : 1.50 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

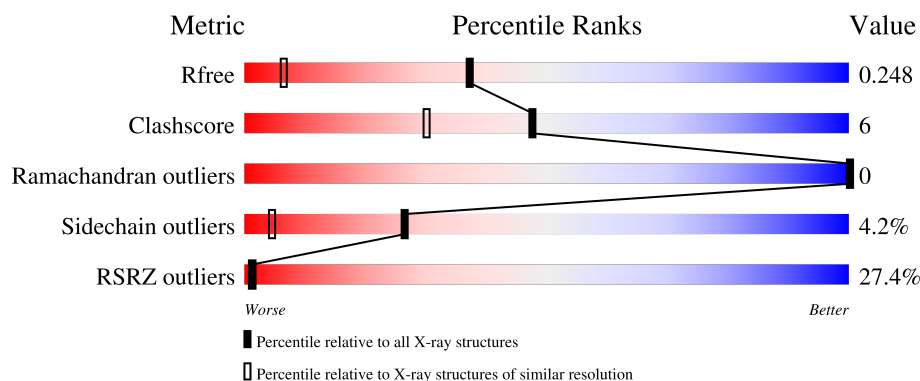
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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  $\geq 3$ , 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	379	<div> <div>27%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

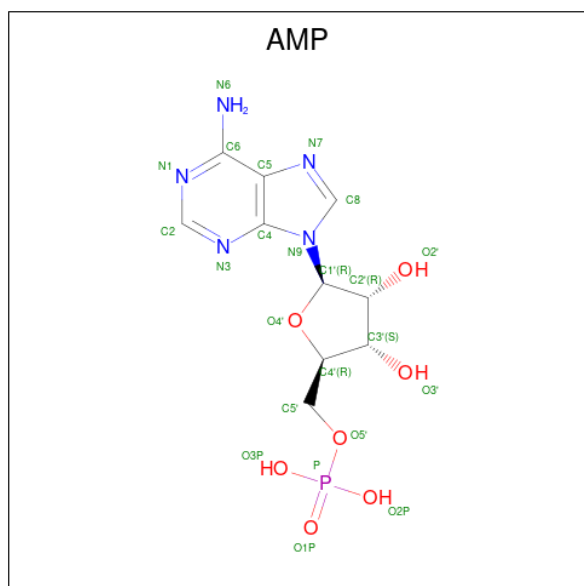
There are 4 unique types of molecules in this entry. The entry contains 6060 atoms, of which 2911 are hydrogens and 0 are deuteriums.

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 Aminoglycoside phosphotransferase-like protein.

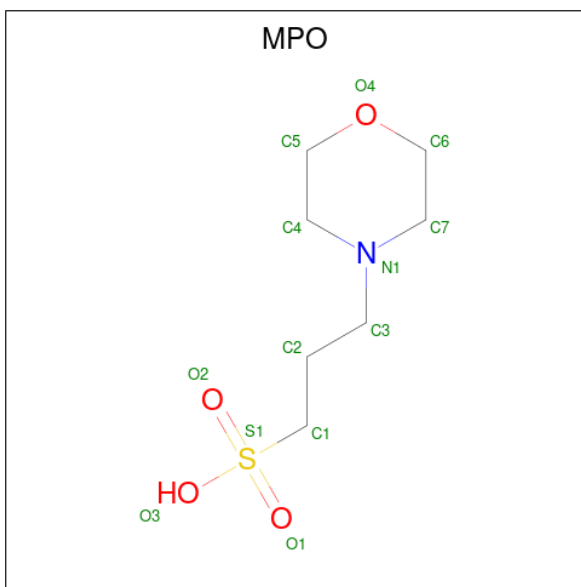
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	369	5867	1914	2885	507	541	20	0	3	0

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



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

- Molecule 3 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula:  $C_7H_{15}NO_4S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			27	7	14	1	4	1		

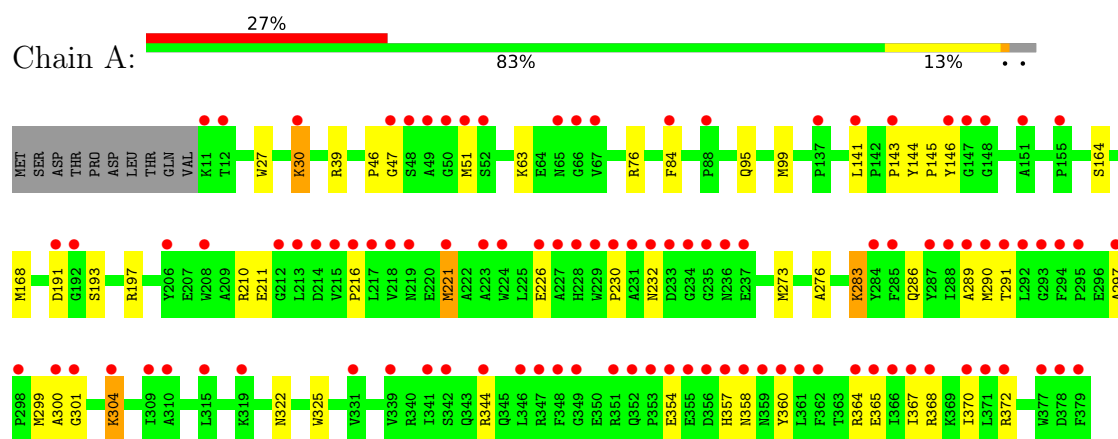
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	128	Total	O	0	3
			131	131		

### 3 Residue-property plots [i](#)

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: Aminoglycoside phosphotransferase-like protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.05Å 68.05Å 185.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.76 – 1.50 45.76 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.76-1.50) 99.9 (45.76-1.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 1.50Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.223 , 0.245 0.227 , 0.248	Depositor DCC
$R_{free}$ test set	3510 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MPO, 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	3/3075 (0.1%)	0.74	4/4173 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	ARG	C-O	-8.91	1.12	1.24
1	A	46	PRO	C-O	-6.83	1.15	1.23
1	A	276	ALA	C-O	-5.03	1.18	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	TYR	CB-CA-C	-7.78	98.66	110.88
1	A	47	GLY	CA-C-N	6.35	133.66	121.54
1	A	47	GLY	C-N-CA	6.35	133.66	121.54
1	A	47	GLY	N-CA-C	6.27	122.19	112.60

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	2982	2885	2880	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	23	12	12	0	0
3	A	13	14	15	0	0
4	A	131	0	0	3	0
All	All	3149	2911	2907	33	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 6.

All (33) 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:232:ASN:O	1:A:232:ASN:ND2	2.35	0.59
1:A:290:MET:HE3	1:A:297:ALA:HB2	1.85	0.58
1:A:221:MET:HG2	1:A:367:ILE:HG23	1.86	0.58
1:A:368:ARG:HB2	1:A:372:ARG:NH1	2.21	0.55
1:A:221:MET:HE1	1:A:370:ILE:HG21	1.89	0.55
1:A:226:GLU:HG3	4:A:606:HOH:O	2.06	0.54
1:A:230:PRO:HB3	1:A:322:ASN:OD1	2.07	0.54
1:A:99[A]:MET:HE3	4:A:594:HOH:O	2.10	0.51
1:A:230:PRO:HD3	1:A:325:TRP:CE2	2.46	0.50
1:A:146:TYR:CE1	1:A:289:ALA:HB2	2.47	0.49
1:A:297:ALA:HB3	1:A:300:ALA:HB2	1.94	0.48
1:A:39:ARG:CZ	1:A:39:ARG:HB3	2.44	0.47
1:A:144:TYR:CG	1:A:145:PRO:HD3	2.50	0.47
1:A:286:GLN:NE2	1:A:299:MET:O	2.48	0.46
1:A:27:TRP:CD1	1:A:30:LYS:NZ	2.84	0.46
1:A:84:PHE:CE2	1:A:344:ARG:HA	2.51	0.45
1:A:193:SER:O	1:A:197:ARG:HG3	2.16	0.45
1:A:283:LYS:HE2	1:A:286:GLN:OE1	2.16	0.45
1:A:51:MET:HE1	1:A:344:ARG:NH1	2.32	0.45
1:A:221:MET:CE	1:A:370:ILE:HG21	2.46	0.45
1:A:39:ARG:HG2	4:A:572:HOH:O	2.18	0.44
1:A:372:ARG:HG3	1:A:372:ARG:HH11	1.82	0.44
1:A:364:ARG:O	1:A:368:ARG:HG2	2.18	0.44
1:A:95:GLN:O	1:A:99[A]:MET:HG3	2.18	0.43
1:A:143:PRO:C	1:A:145:PRO:HD2	2.44	0.43
1:A:357:HIS:ND1	1:A:357:HIS:N	2.66	0.43
1:A:164:SER:O	1:A:168:MET:HG2	2.19	0.42
1:A:39:ARG:HB3	1:A:39:ARG:NH2	2.35	0.42
1:A:301:GLY:HA2	1:A:304:LYS:HD2	2.01	0.41
1:A:144:TYR:CD2	1:A:145:PRO:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:TYR:CD1	1:A:146:TYR:N	2.87	0.41
1:A:216:PRO:HG2	1:A:358:ASN:ND2	2.36	0.41
1:A:144:TYR:N	1:A:145:PRO:CD	2.84	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	370/379 (98%)	365 (99%)	5 (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	310/318 (98%)	297 (96%)	13 (4%)	26	4

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	63	LYS
1	A	76	ARG

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Mol	Chain	Res	Type
1	A	141	LEU
1	A	191	ASP
1	A	211	GLU
1	A	221	MET
1	A	273	MET
1	A	283	LYS
1	A	291	THR
1	A	304	LYS
1	A	354	GLU
1	A	365	GLU

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

Mol	Chain	Res	Type
1	A	232	ASN

### 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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MPO	A	402	-	13,13,13	1.46	3 (23%)	17,17,17	2.36	7 (41%)
2	AMP	A	401	-	25,25,25	2.60	9 (36%)	37,38,38	3.32	16 (43%)

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
3	MPO	A	402	-	-	2/7/15/15	0/1/1/1
2	AMP	A	401	-	-	0/10/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	AMP	C5-N7	7.03	1.51	1.39
2	A	401	AMP	C8-N9	-5.72	1.27	1.37
2	A	401	AMP	C4-N9	-4.62	1.28	1.37
2	A	401	AMP	C6-N6	3.96	1.44	1.34
3	A	402	MPO	C1-S1	3.56	1.82	1.77
2	A	401	AMP	C8-N7	3.00	1.37	1.31
2	A	401	AMP	C5-C4	2.88	1.44	1.39
3	A	402	MPO	O2-S1	2.46	1.52	1.45
2	A	401	AMP	O4'-C1'	2.46	1.47	1.42
2	A	401	AMP	P-O2P	-2.20	1.46	1.54
2	A	401	AMP	P-O3P	-2.16	1.46	1.54
3	A	402	MPO	O1-S1	2.15	1.51	1.45

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	AMP	C4-N9-C8	13.83	120.26	105.74
2	A	401	AMP	C4-C5-N7	-5.63	104.14	110.58
2	A	401	AMP	N3-C4-N9	5.04	135.73	127.17
2	A	401	AMP	N9-C8-N7	-4.82	107.10	113.94
2	A	401	AMP	C5-C4-N3	-4.62	120.36	126.72
2	A	401	AMP	C3'-C2'-C1'	4.08	109.18	101.46
3	A	402	MPO	O2-S1-C1	3.94	112.69	106.73
3	A	402	MPO	O2-S1-O1	-3.82	101.40	113.82
2	A	401	AMP	C1'-N9-C8	-3.81	118.63	127.09
3	A	402	MPO	O4-C5-C4	3.80	119.96	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	AMP	C6-C5-N7	3.48	138.79	132.09
3	A	402	MPO	C6-O4-C5	3.27	120.45	109.88
3	A	402	MPO	C7-N1-C4	3.18	115.69	108.84
3	A	402	MPO	O1-S1-C1	3.03	111.31	106.73
2	A	401	AMP	N3-C2-N1	-2.80	124.35	128.58
3	A	402	MPO	C6-C7-N1	2.79	114.35	110.12
2	A	401	AMP	O3P-P-O5'	2.77	113.89	106.67
2	A	401	AMP	O2P-P-O5'	2.71	113.74	106.67
2	A	401	AMP	C2-N3-C4	2.71	118.44	111.83
2	A	401	AMP	O5'-P-O1P	2.51	113.21	106.44
2	A	401	AMP	C4-N9-C1'	-2.38	121.06	126.63
2	A	401	AMP	O4'-C1'-C2'	-2.10	102.13	106.62
2	A	401	AMP	C2'-C1'-N9	2.07	118.45	113.30

There are no chirality outliers.

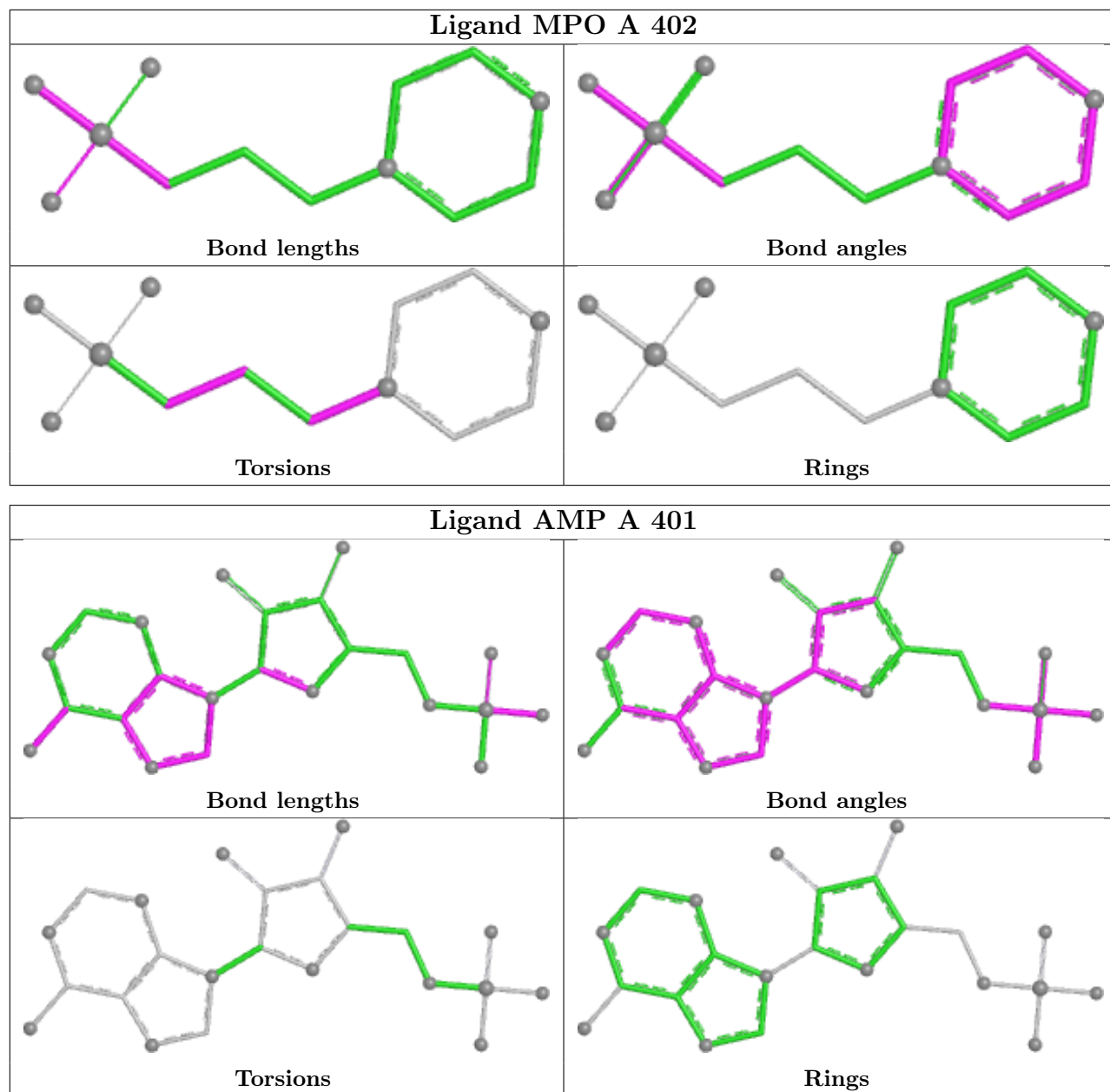
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	MPO	S1-C1-C2-C3
3	A	402	MPO	C2-C3-N1-C4

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	369/379 (97%)	1.29	101 (27%) <b>1</b> <b>1</b>	17, 52, 102, 146	2 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	TYR	7.9
1	A	218	VAL	5.8
1	A	353	PRO	5.8
1	A	292	LEU	5.3
1	A	47	GLY	5.3
1	A	362	PHE	5.0
1	A	379	PHE	4.9
1	A	84	PHE	4.8
1	A	291	THR	4.8
1	A	12	THR	4.6
1	A	230	PRO	4.6
1	A	294	PHE	4.5
1	A	348	PHE	4.4
1	A	216	PRO	4.4
1	A	347	ARG	4.4
1	A	295	PRO	4.3
1	A	231	ALA	4.3
1	A	213	LEU	4.3
1	A	346	LEU	4.2
1	A	355	GLU	4.0
1	A	293	GLY	4.0
1	A	357	HIS	3.8
1	A	217	LEU	3.7
1	A	359	ASN	3.7
1	A	366	ILE	3.7
1	A	361	LEU	3.6
1	A	141	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	288	ILE	3.6
1	A	290	MET	3.6
1	A	65	ASN	3.5
1	A	358	ASN	3.4
1	A	49	ALA	3.4
1	A	223	ALA	3.4
1	A	289	ALA	3.3
1	A	367	ILE	3.3
1	A	137	PRO	3.2
1	A	227	ALA	3.2
1	A	365	GLU	3.2
1	A	229	TRP	3.2
1	A	215	VAL	3.2
1	A	192	GLY	3.2
1	A	235	GLY	3.1
1	A	151	ALA	3.0
1	A	67	VAL	3.0
1	A	354	GLU	3.0
1	A	356	ASP	3.0
1	A	370	ILE	2.9
1	A	287	TYR	2.9
1	A	351	ARG	2.9
1	A	319	LYS	2.9
1	A	191	ASP	2.9
1	A	232	ASN	2.9
1	A	146	TYR	2.9
1	A	50	GLY	2.9
1	A	48	SER	2.9
1	A	341	ILE	2.8
1	A	224	TRP	2.8
1	A	371	LEU	2.8
1	A	297	ALA	2.8
1	A	364	ARG	2.8
1	A	221	MET	2.7
1	A	52	SER	2.7
1	A	352	GLN	2.7
1	A	234	GLY	2.7
1	A	372	ARG	2.7
1	A	236	ASN	2.6
1	A	301	GLY	2.6
1	A	237	GLU	2.6
1	A	226	GLU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	228	HIS	2.5
1	A	298	PRO	2.5
1	A	331	VAL	2.5
1	A	143	PRO	2.4
1	A	155	PRO	2.4
1	A	377	TRP	2.4
1	A	349	GLY	2.4
1	A	309	ILE	2.4
1	A	219	ASN	2.4
1	A	300	ALA	2.3
1	A	233	ASP	2.3
1	A	30	LYS	2.3
1	A	88	PRO	2.3
1	A	339	VAL	2.3
1	A	214	ASP	2.3
1	A	284	TYR	2.3
1	A	148	GLY	2.3
1	A	208	TRP	2.3
1	A	368	ARG	2.2
1	A	11	LYS	2.2
1	A	66	GLY	2.2
1	A	344	ARG	2.2
1	A	285	PHE	2.2
1	A	147	GLY	2.1
1	A	342	SER	2.1
1	A	310	ALA	2.1
1	A	315	LEU	2.1
1	A	212	GLY	2.1
1	A	51	MET	2.0
1	A	304	LYS	2.0
1	A	378	ASP	2.0
1	A	206	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

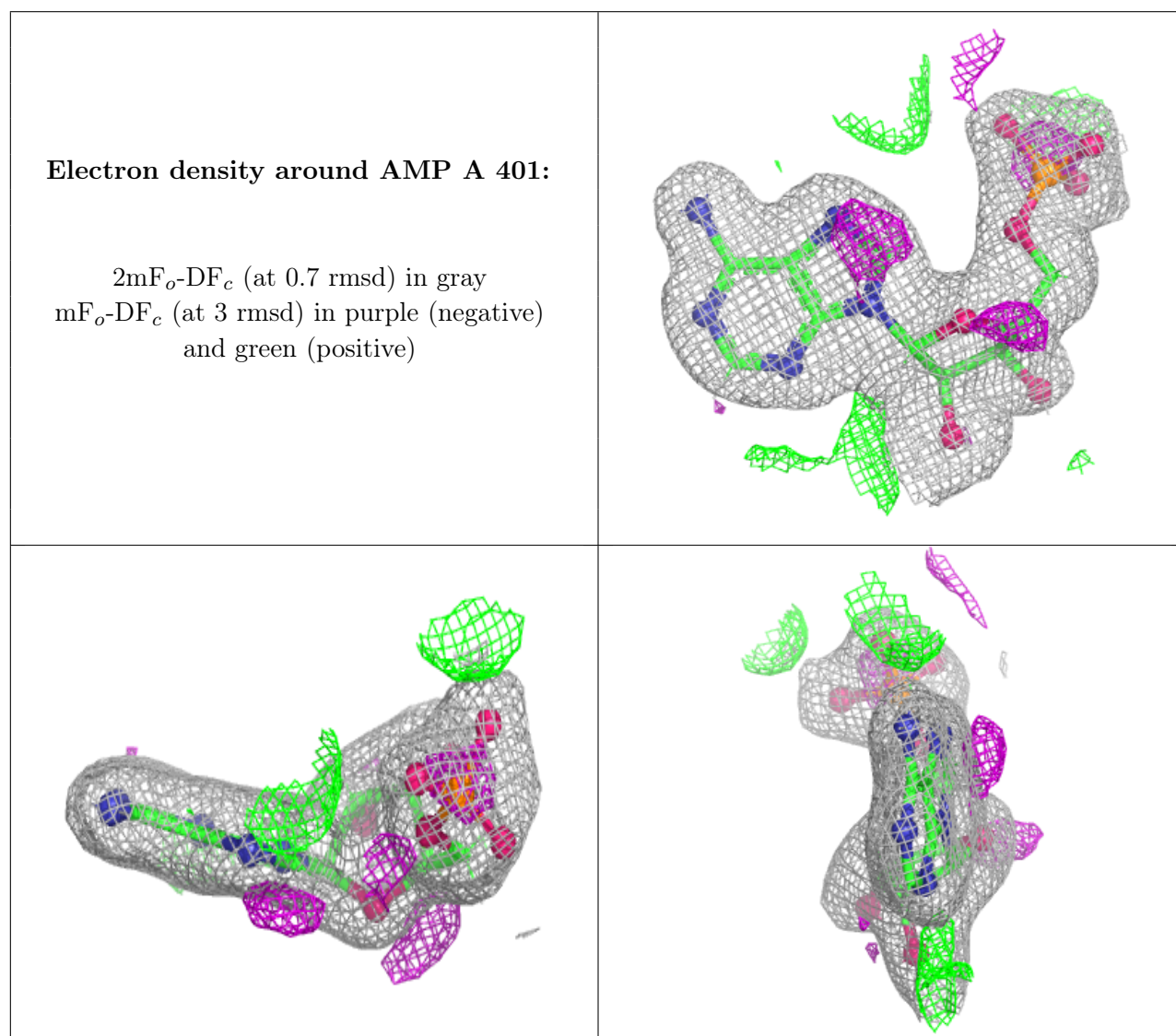


## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

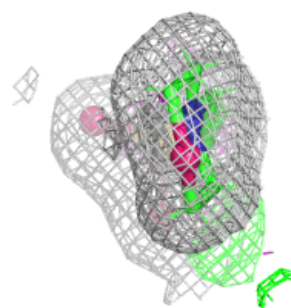
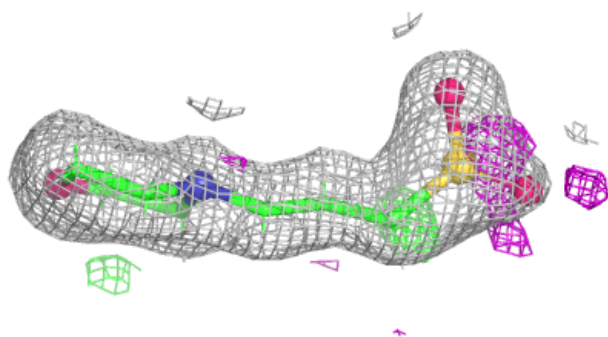
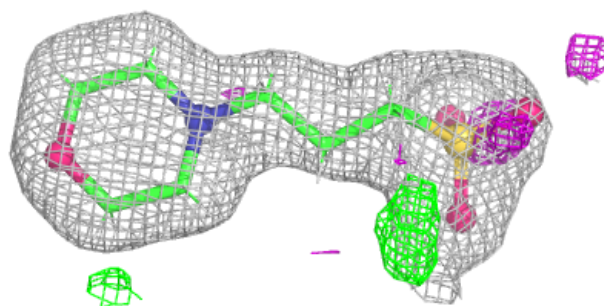
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	AMP	A	401	23/23	0.90	0.11	29,41,56,67	0
3	MPO	A	402	13/13	0.92	0.11	28,35,49,61	0

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 MPO 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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.