



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 08:01 AM EDT

PDB ID : 3A1E  
Title : Crystal structure of the P- and N-domains of His462Gln mutant CopA, a copper-transporting P-type ATPase, bound with AMPPCP-Mg  
Authors : Tsuda, T.; Toyoshima, C.  
Deposited on : 2009-03-31  
Resolution : 1.95 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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

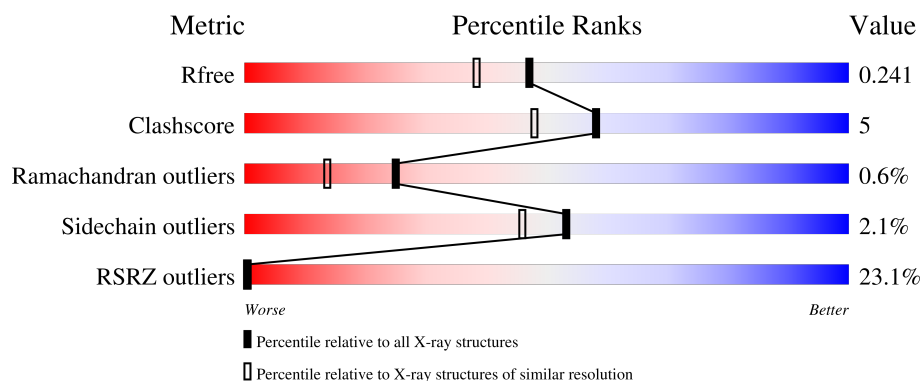
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	287	<div> <div>15%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>
1	B	287	<div> <div>28%</div> <div>80%</div> <div>12%</div> <div>• 5%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4411 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.

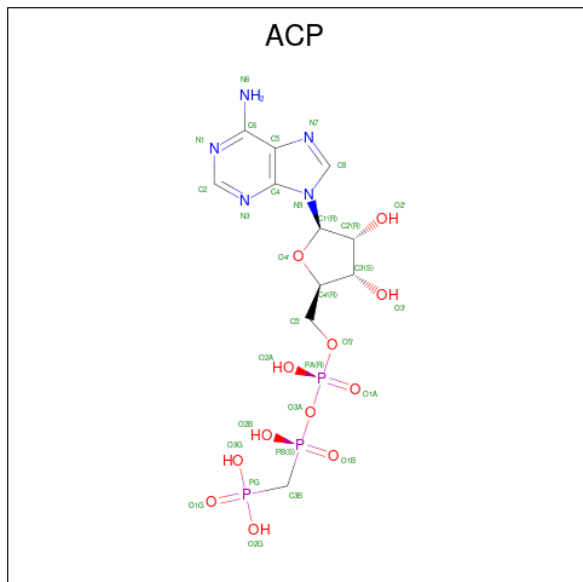
- Molecule 1 is a protein called Probable copper-exporting P-type ATPase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2003	1254	349	397	3			
1	B	272	Total	C	N	O	S	0	0	0
			2028	1268	353	403	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	MET	-	expression tag	UNP O29777
A	388	GLY	-	expression tag	UNP O29777
A	389	HIS	-	expression tag	UNP O29777
A	390	HIS	-	expression tag	UNP O29777
A	391	HIS	-	expression tag	UNP O29777
A	392	HIS	-	expression tag	UNP O29777
A	393	HIS	-	expression tag	UNP O29777
A	394	HIS	-	expression tag	UNP O29777
A	395	GLY	-	expression tag	UNP O29777
A	396	SER	-	expression tag	UNP O29777
A	397	ARG	-	expression tag	UNP O29777
A	462	GLN	HIS	engineered mutation	UNP O29777
B	387	MET	-	expression tag	UNP O29777
B	388	GLY	-	expression tag	UNP O29777
B	389	HIS	-	expression tag	UNP O29777
B	390	HIS	-	expression tag	UNP O29777
B	391	HIS	-	expression tag	UNP O29777
B	392	HIS	-	expression tag	UNP O29777
B	393	HIS	-	expression tag	UNP O29777
B	394	HIS	-	expression tag	UNP O29777
B	395	GLY	-	expression tag	UNP O29777
B	396	SER	-	expression tag	UNP O29777
B	397	ARG	-	expression tag	UNP O29777
B	462	GLN	HIS	engineered mutation	UNP O29777

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

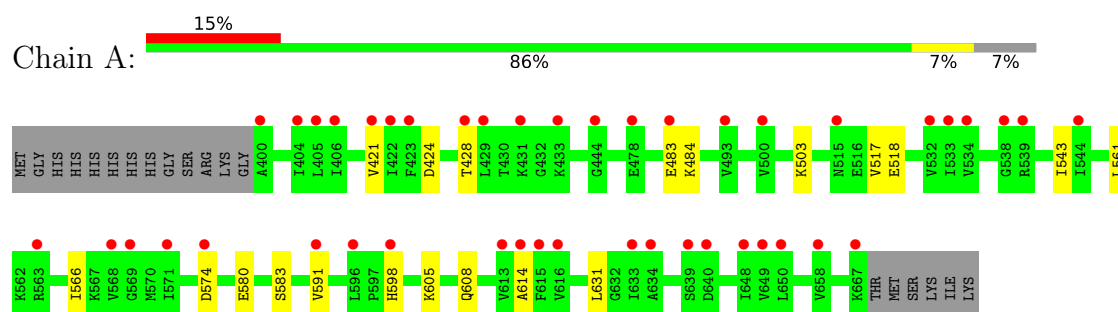
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	204	Total	O	0	0
			204	204		
4	B	113	Total	O	0	0
			113	113		

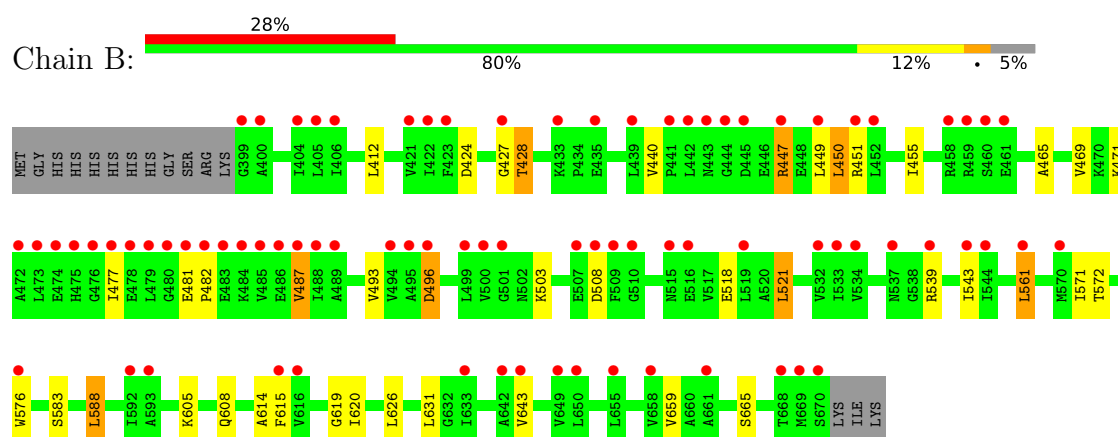
### 3 Residue-property plots [i](#)

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: Probable copper-exporting P-type ATPase A



- Molecule 1: Probable copper-exporting P-type ATPase A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.53Å 90.53Å 191.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 27.42 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.95) 99.9 (27.42-1.95)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.208 , 0.245 0.206 , 0.241	Depositor DCC
$R_{free}$ test set	2964 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4411	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: MG, ACP

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	0.52	0/2016	0.64	0/2722
1	B	0.63	3/2041 (0.1%)	0.65	2/2755 (0.1%)
All	All	0.58	3/4057 (0.1%)	0.64	2/5477 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	447	ARG	CZ-NH1	9.78	1.45	1.33
1	B	447	ARG	NE-CZ	6.21	1.41	1.33
1	B	496	ASP	C-O	-5.66	1.12	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	447	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	B	447	ARG	NE-CZ-NH2	-7.39	116.61	120.30

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	2003	0	2091	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2028	0	2116	27	0
2	A	31	0	14	0	0
2	B	31	0	14	1	0
3	A	1	0	0	0	0
4	A	204	0	0	1	0
4	B	113	0	0	1	0
All	All	4411	0	4235	40	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 5.

All (40) 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:427:GLY:O	1:B:428:THR:OG1	1.84	0.92
1:B:447:ARG:HG2	1:B:477:ILE:HD11	1.68	0.73
1:A:605:LYS:HA	1:A:608:GLN:HE21	1.53	0.72
1:A:583:SER:HB2	1:A:591:VAL:HG21	1.70	0.72
1:B:427:GLY:C	1:B:428:THR:HG1	1.91	0.71
1:A:574:ASP:HB3	4:A:1132:HOH:O	1.95	0.66
1:B:619:GLY:HA2	1:B:626:LEU:HD11	1.79	0.64
1:B:561:LEU:HD13	1:B:659:VAL:HG22	1.82	0.61
1:A:503:LYS:HB3	1:A:503:LYS:NZ	2.17	0.59
1:B:605:LYS:HA	1:B:608:GLN:HE21	1.70	0.55
1:A:580:GLU:HG3	1:B:576:TRP:CZ3	2.42	0.54
1:B:465:ALA:O	1:B:469:VAL:HG23	2.08	0.54
1:A:583:SER:HB2	1:A:591:VAL:CG2	2.37	0.54
1:A:483:GLU:HG2	1:A:484:LYS:HG3	1.90	0.53
1:B:619:GLY:HA2	1:B:626:LEU:CD1	2.38	0.52
1:B:440:VAL:HB	1:B:543:ILE:HG12	1.91	0.52
1:B:424:ASP:O	1:B:428:THR:HB	2.10	0.52
1:B:428:THR:N	4:B:1360:HOH:O	2.42	0.51
1:B:451:ARG:O	1:B:455:ILE:HG12	2.11	0.50
1:B:583:SER:HA	1:B:588:LEU:HD22	1.91	0.50
1:A:421:VAL:HG23	1:A:566:ILE:HG21	1.92	0.50
1:B:503:LYS:HD2	1:B:518:GLU:OE1	2.13	0.49
1:A:503:LYS:NZ	1:A:503:LYS:CB	2.78	0.47
1:A:424:ASP:O	1:A:428:THR:HB	2.14	0.47
1:A:503:LYS:HB3	1:A:503:LYS:HZ3	1.79	0.47
1:B:571:ILE:HG21	1:B:615:PHE:HE1	1.80	0.47
1:B:620:ILE:HD11	1:B:643:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:ALA:HA	1:B:631:LEU:O	2.17	0.44
1:B:451:ARG:HB2	1:B:477:ILE:HD12	1.99	0.43
1:A:614:ALA:HA	1:A:631:LEU:O	2.20	0.42
1:B:450:LEU:HD11	1:B:471:LYS:HG3	2.02	0.42
1:B:447:ARG:NH1	1:B:477:ILE:HD13	2.33	0.42
1:A:503:LYS:HE2	1:A:518:GLU:OE2	2.20	0.42
1:B:521:LEU:HD13	1:B:543:ILE:HG21	2.02	0.42
1:B:572:THR:HA	2:B:997:ACP:O3G	2.20	0.42
1:B:412:LEU:O	1:B:665:SER:HB2	2.20	0.41
1:B:487:VAL:HG22	1:B:493:VAL:HG12	2.03	0.41
1:A:517:VAL:HG13	1:A:543:ILE:HD11	2.02	0.40
1:B:481:GLU:HA	1:B:482:PRO:HD3	1.97	0.40
1:B:451:ARG:HA	1:B:477:ILE:HG21	2.02	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	266/287 (93%)	263 (99%)	3 (1%)	0	100	100
1	B	270/287 (94%)	262 (97%)	5 (2%)	3 (1%)	14	5
All	All	536/574 (93%)	525 (98%)	8 (2%)	3 (1%)	25	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	428	THR
1	B	496	ASP
1	B	487	VAL

### 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	212/228 (93%)	210 (99%)	2 (1%)	78	77
1	B	215/228 (94%)	208 (97%)	7 (3%)	38	26
All	All	427/456 (94%)	418 (98%)	9 (2%)	53	46

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

Mol	Chain	Res	Type
1	A	561	LEU
1	A	598	HIS
1	B	449	LEU
1	B	450	LEU
1	B	508	ASP
1	B	521	LEU
1	B	539	ARG
1	B	561	LEU
1	B	588	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	587	ASN
1	A	598	HIS
1	A	608	GLN
1	A	628	GLN
1	B	515	ASN
1	B	608	GLN
1	B	628	GLN
1	B	663	GLN

### 5.3.3 RNA

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	ACP	A	997	3	27,33,33	1.19	4 (14%)	32,52,52	1.52	6 (18%)
2	ACP	B	997	-	27,33,33	1.33	5 (18%)	32,52,52	1.30	5 (15%)

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	ACP	A	997	3	-	0/15/38/38	0/3/3/3
2	ACP	B	997	-	-	2/15/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	997	ACP	PB-O3A	3.29	1.62	1.58
2	B	997	ACP	C5-C4	2.78	1.48	1.40
2	A	997	ACP	C5-C4	2.66	1.48	1.40
2	A	997	ACP	PB-O2B	-2.32	1.50	1.56
2	B	997	ACP	PB-O2B	-2.17	1.51	1.56
2	B	997	ACP	C2-N3	2.09	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	997	ACP	O4'-C1'	2.07	1.44	1.41
2	A	997	ACP	PG-O3G	-2.05	1.50	1.54
2	A	997	ACP	C2-N3	2.05	1.35	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	997	ACP	N3-C2-N1	-3.47	123.25	128.68
2	A	997	ACP	PA-O3A-PB	-3.43	121.67	132.56
2	B	997	ACP	N3-C2-N1	-3.38	123.39	128.68
2	A	997	ACP	O2B-PB-O1B	3.09	120.38	110.07
2	A	997	ACP	O3G-PG-O2G	3.07	117.04	108.08
2	B	997	ACP	C4-C5-N7	-2.52	106.77	109.40
2	A	997	ACP	C4-C5-N7	-2.41	106.89	109.40
2	B	997	ACP	O1G-PG-C3B	-2.40	106.08	111.24
2	B	997	ACP	O2B-PB-O1B	2.19	117.40	110.07
2	A	997	ACP	O2A-PA-O1A	2.14	122.80	112.24
2	B	997	ACP	C2-N1-C6	2.01	122.20	118.75

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	997	ACP	PG-C3B-PB-O1B
2	B	997	ACP	C5'-O5'-PA-O1A

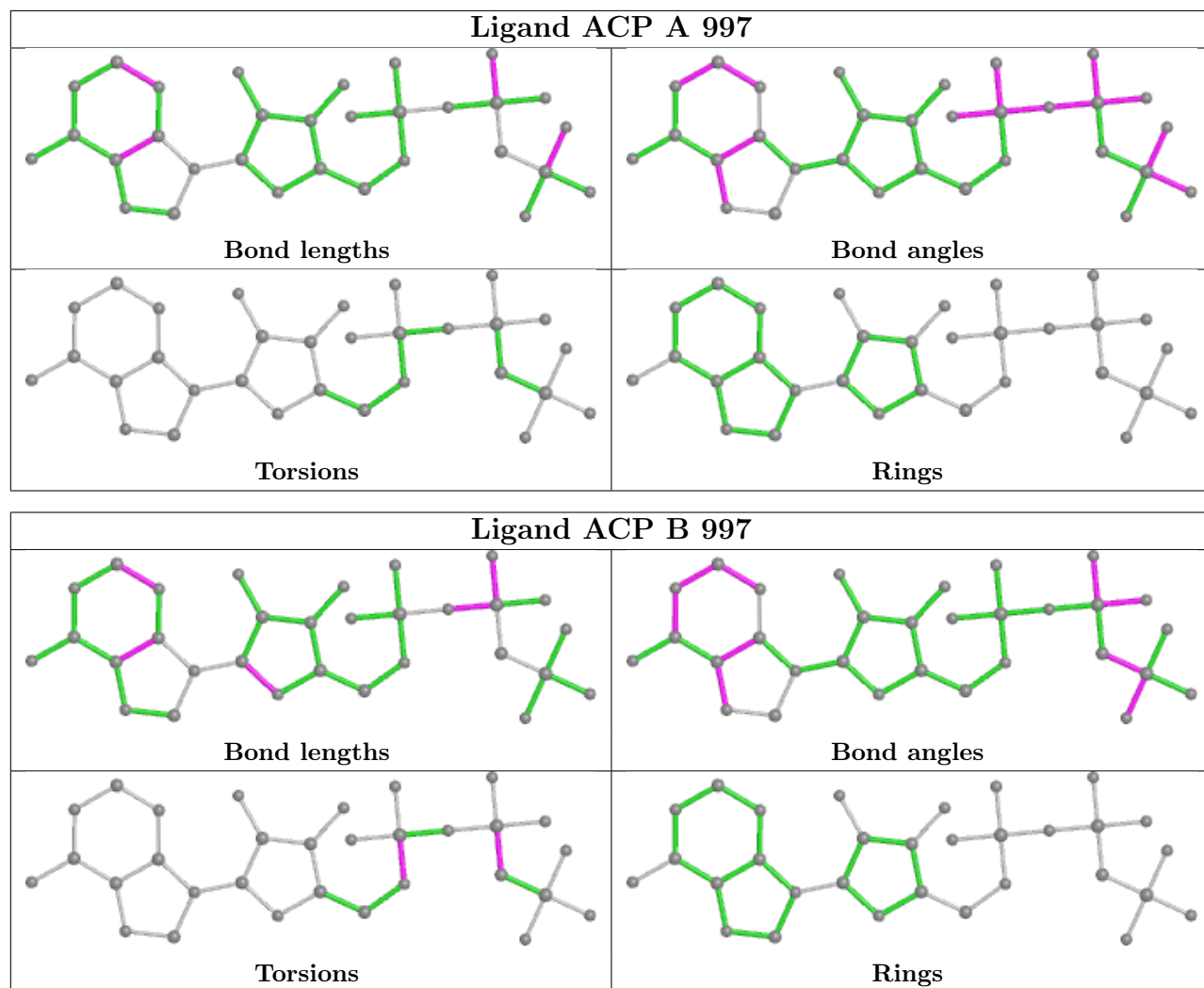
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	997	ACP	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, 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	268/287 (93%)	0.85	44 (16%) <b>1</b> <b>2</b>	31, 44, 55, 67	0
1	B	272/287 (94%)	1.43	81 (29%) <b>0</b> <b>0</b>	33, 49, 77, 86	0
All	All	540/574 (94%)	1.14	125 (23%) <b>0</b> <b>0</b>	31, 45, 75, 86	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	GLY	8.2
1	B	643	VAL	8.2
1	B	477	ILE	8.1
1	B	482	PRO	7.1
1	B	473	LEU	6.3
1	B	481	GLU	6.3
1	A	667	LYS	6.2
1	B	459	ARG	5.7
1	B	485	VAL	5.4
1	B	479	LEU	5.3
1	B	480	GLY	5.2
1	B	442	LEU	5.0
1	B	496	ASP	4.9
1	B	488	ILE	4.7
1	A	422	ILE	4.5
1	B	501	GLY	4.4
1	B	443	ASN	4.3
1	B	484	LYS	4.2
1	B	668	THR	4.2
1	B	642	ALA	4.1
1	B	658	VAL	4.1
1	B	486	GLU	4.1
1	B	478	GLU	4.0
1	B	458	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	539	ARG	4.0
1	B	444	GLY	4.0
1	B	487	VAL	4.0
1	A	658	VAL	3.9
1	B	534	VAL	3.9
1	A	633	ILE	3.8
1	B	515	ASN	3.8
1	A	404	ILE	3.8
1	B	406	ILE	3.8
1	A	616	VAL	3.8
1	A	423	PHE	3.7
1	B	476	GLY	3.6
1	B	495	ALA	3.6
1	B	616	VAL	3.6
1	B	533	ILE	3.6
1	B	670	SER	3.5
1	B	461	GLU	3.4
1	B	472	ALA	3.4
1	B	532	VAL	3.4
1	B	423	PHE	3.4
1	A	421	VAL	3.3
1	B	447	ARG	3.2
1	B	537	ASN	3.2
1	B	451	ARG	3.2
1	A	532	VAL	3.2
1	A	478	GLU	3.2
1	A	639	SER	3.2
1	A	596	LEU	3.1
1	B	489	ALA	3.1
1	B	441	PRO	3.1
1	A	444	GLY	3.1
1	B	449	LEU	3.0
1	B	499	LEU	3.0
1	A	433	LYS	3.0
1	B	633	ILE	3.0
1	A	539	ARG	2.9
1	B	422	ILE	2.9
1	B	421	VAL	2.9
1	A	613	VAL	2.9
1	B	544	ILE	2.9
1	B	494	VAL	2.9
1	A	533	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	571	ILE	2.9
1	A	614	ALA	2.9
1	B	483	GLU	2.8
1	B	516	GLU	2.8
1	B	650	LEU	2.8
1	B	509	PHE	2.8
1	A	500	VAL	2.8
1	B	445	ASP	2.7
1	B	592	ILE	2.7
1	A	598	HIS	2.7
1	A	563	ARG	2.7
1	A	431	LYS	2.6
1	B	427	GLY	2.6
1	B	500	VAL	2.6
1	B	404	ILE	2.6
1	B	519	LEU	2.5
1	B	474	GLU	2.5
1	A	650	LEU	2.5
1	B	405	LEU	2.5
1	B	475	HIS	2.5
1	A	428	THR	2.5
1	B	661	ALA	2.5
1	B	510	GLY	2.5
1	B	669	MET	2.5
1	A	574	ASP	2.5
1	B	439	LEU	2.5
1	B	615	PHE	2.5
1	A	591	VAL	2.4
1	B	460	SER	2.4
1	A	544	ILE	2.4
1	B	576	TRP	2.4
1	A	534	VAL	2.4
1	B	593	ALA	2.3
1	A	649	VAL	2.3
1	B	433	LYS	2.3
1	B	452	LEU	2.3
1	A	493	VAL	2.3
1	A	538	GLY	2.3
1	B	655	LEU	2.3
1	A	615	PHE	2.2
1	A	405	LEU	2.2
1	B	561	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	515	ASN	2.2
1	A	400	ALA	2.2
1	A	568	VAL	2.2
1	A	406	ILE	2.2
1	A	429	LEU	2.2
1	A	483	GLU	2.2
1	B	507	GLU	2.2
1	A	640	ASP	2.1
1	B	508	ASP	2.1
1	B	649	VAL	2.1
1	B	570	MET	2.1
1	A	648	ILE	2.1
1	B	435	GLU	2.1
1	B	400	ALA	2.1
1	B	543	ILE	2.1
1	A	634	ALA	2.0
1	A	569	GLY	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.

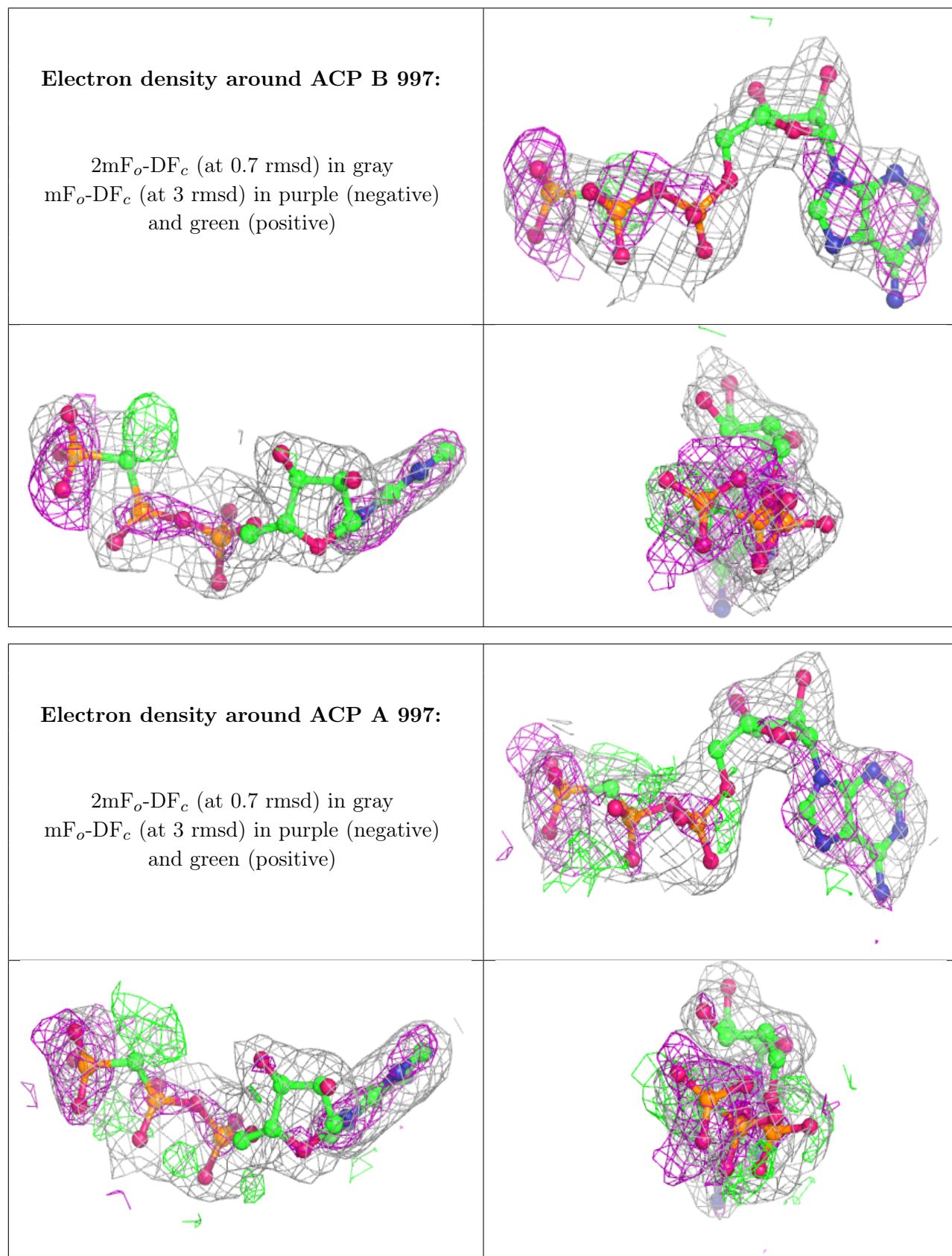
## 6.4 Ligands ⓘ

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, 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
3	MG	A	998	1/1	0.53	0.30	79,79,79,79	0
2	ACP	B	997	31/31	0.89	0.20	67,70,78,78	0
2	ACP	A	997	31/31	0.92	0.12	46,49,62,65	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.