



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:54 am BST

PDB ID : 3A1C
Title : crystal structure of the P- and N-domains of CopA, a copper-transporting P-type ATPase, bound with AMPPCP-Mg
Authors : Tsuda, T.; Toyoshima, C.
Deposited on : 2009-03-31
Resolution : 1.85 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 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 : 2.11
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) : 2.11

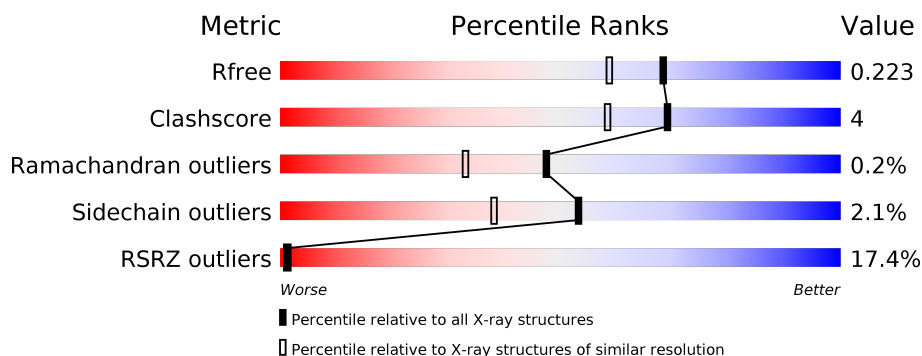
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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	287	<div> <div>9%</div> <div>83%</div> <div>9%</div> <div>7%</div> </div>
1	B	287	<div> <div>23%</div> <div>86%</div> <div>8%</div> <div>5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4573 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.

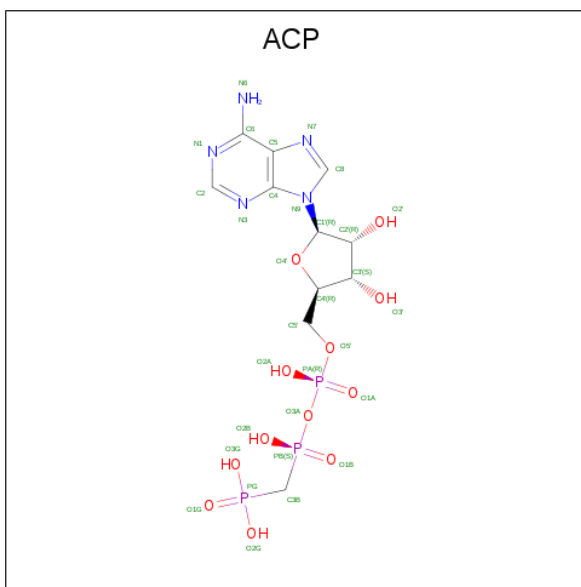
- Molecule 1 is a protein called Probable copper-exporting P-type ATPase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			1995	1249	348	395	3			
1	B	273	Total	C	N	O	S	0	0	0
			2042	1279	356	403	4			

There are 22 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
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

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

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

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

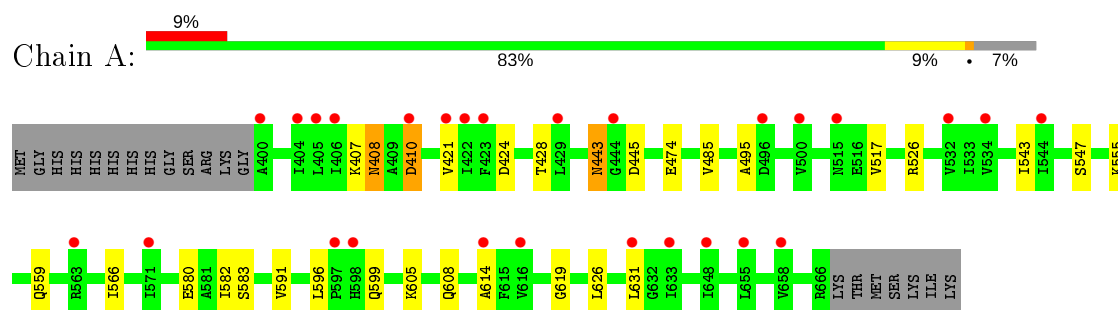
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	262	Total O 262 262	0	0
4	B	211	Total O 211 211	0	0

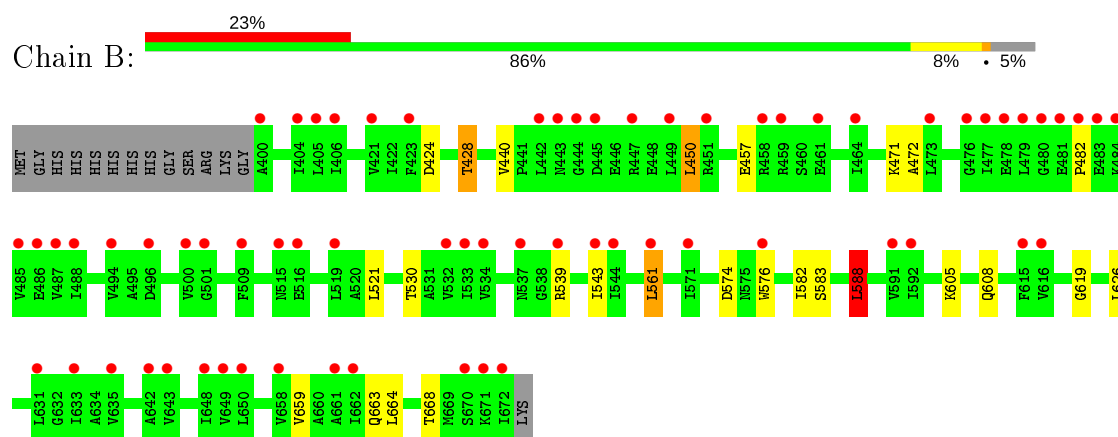
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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, α , β , γ	90.79 Å 90.79 Å 191.79 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.85 27.35 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.85) 99.7 (27.35-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 1.85 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.225 0.194 , 0.223	Depositor DCC
R_{free} test set	3501 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4573	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: 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	0.55	0/2009	0.68	2/2714 (0.1%)
1	B	0.47	0/2056	0.60	1/2775 (0.0%)
All	All	0.51	0/4065	0.64	3/5489 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	526	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	A	526	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	B	588	LEU	CB-CG-CD1	5.05	119.59	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1995	0	2078	17	0
1	B	2042	0	2136	15	0
2	A	31	0	14	0	0
2	B	31	0	14	1	0
3	A	1	0	0	0	0
4	A	262	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	211	0	0	2	0
All	All	4573	0	4242	31	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 4.

All (31) 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:664:LEU:O	1:B:668:THR:HG23	1.73	0.89
1:B:450:LEU:HD11	1:B:471:LYS:HG3	1.76	0.67
1:A:605:LYS:HA	1:A:608:GLN:HE21	1.62	0.64
1:B:605:LYS:HA	1:B:608:GLN:HE21	1.62	0.62
1:A:424:ASP:O	1:A:428:THR:HB	1.99	0.62
1:B:561:LEU:HD13	1:B:659:VAL:HG22	1.83	0.61
1:A:582:ILE:HD12	4:A:1133:HOH:O	2.03	0.59
1:B:583:SER:HA	1:B:588:LEU:HD22	1.85	0.58
1:B:424:ASP:O	1:B:428:THR:HB	2.04	0.57
1:A:474:GLU:OE1	4:A:1091:HOH:O	2.17	0.57
1:A:407:LYS:HD3	4:A:1075:HOH:O	2.08	0.52
1:A:408:ASN:ND2	1:A:410:ASP:OD1	2.42	0.52
1:A:421:VAL:HG23	1:A:566:ILE:HG21	1.93	0.49
1:A:583:SER:HB2	1:A:591:VAL:HG21	1.93	0.49
1:B:619:GLY:HA2	1:B:626:LEU:CD1	2.42	0.49
1:B:440:VAL:HB	1:B:543:ILE:HG12	1.95	0.48
1:B:530:THR:OG1	1:B:574:ASP:OD2	2.33	0.47
1:A:443:ASN:ND2	1:A:445:ASP:H	2.14	0.46
1:B:582:ILE:HD12	4:B:1428:HOH:O	2.15	0.46
1:B:663:GLN:OE1	4:B:1339:HOH:O	2.21	0.46
1:A:547:SER:HB2	4:A:1106:HOH:O	2.16	0.45
1:A:580:GLU:HG3	1:B:576:TRP:CZ3	2.52	0.45
1:A:555:LYS:O	1:A:559:GLN:HG3	2.17	0.45
1:B:619:GLY:HA2	1:B:626:LEU:HD11	1.99	0.44
1:A:596:LEU:O	1:A:599:GLN:HB2	2.18	0.43
1:A:619:GLY:HA2	1:A:626:LEU:CD1	2.50	0.42
1:A:517:VAL:HG13	1:A:543:ILE:HD11	2.01	0.42
1:A:485:VAL:HG22	1:A:495:ALA:HB2	2.03	0.41
1:B:450:LEU:HD22	1:B:472:ALA:HB2	2.02	0.41
1:A:614:ALA:HA	1:A:631:LEU:O	2.21	0.40
1:B:457:GLU:OE2	2:B:997:ACP:N1	2.54	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	265/287 (92%)	262 (99%)	3 (1%)	0	100	100
1	B	271/287 (94%)	264 (97%)	6 (2%)	1 (0%)	34	19
All	All	536/574 (93%)	526 (98%)	9 (2%)	1 (0%)	47	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	482	PRO

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	211/228 (92%)	208 (99%)	3 (1%)	67	55
1	B	217/228 (95%)	211 (97%)	6 (3%)	43	27
All	All	428/456 (94%)	419 (98%)	9 (2%)	53	38

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

Mol	Chain	Res	Type
1	A	408	ASN
1	A	410	ASP

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Mol	Chain	Res	Type
1	A	443	ASN
1	B	428	THR
1	B	450	LEU
1	B	521	LEU
1	B	539	ARG
1	B	561	LEU
1	B	588	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	408	ASN
1	A	443	ASN
1	A	587	ASN
1	A	608	GLN
1	A	628	GLN
1	B	515	ASN
1	B	608	GLN
1	B	621	ASN
1	B	628	GLN

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 carbohydrates 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	1.40	4 (14%)	32,52,52	1.49	7 (21%)
2	ACP	B	997	-	27,33,33	1.30	4 (14%)	32,52,52	1.35	4 (12%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	997	ACP	PB-O3A	3.31	1.62	1.58
2	B	997	ACP	PB-O3A	3.05	1.61	1.58
2	A	997	ACP	C5-C4	2.70	1.48	1.40
2	B	997	ACP	C5-C4	2.70	1.48	1.40
2	B	997	ACP	O4'-C1'	2.33	1.44	1.41
2	A	997	ACP	C2-N3	2.29	1.35	1.32
2	B	997	ACP	C2-N3	2.24	1.35	1.32
2	A	997	ACP	PG-O2G	-2.01	1.50	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	997	ACP	N3-C2-N1	-3.84	122.67	128.68
2	A	997	ACP	O3G-PG-O2G	3.68	118.81	108.08
2	B	997	ACP	N3-C2-N1	-3.60	123.04	128.68
2	B	997	ACP	O1G-PG-C3B	-2.98	104.81	111.24
2	A	997	ACP	PA-O3A-PB	-2.72	123.93	132.56
2	A	997	ACP	O2B-PB-O1B	2.35	117.91	110.07
2	B	997	ACP	C4-C5-N7	-2.29	107.02	109.40
2	A	997	ACP	C2-N1-C6	2.18	122.48	118.75
2	A	997	ACP	O2A-PA-O1A	2.12	122.74	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	997	ACP	C2-N1-C6	2.02	122.20	118.75
2	A	997	ACP	O2G-PG-C3B	-2.00	101.54	106.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

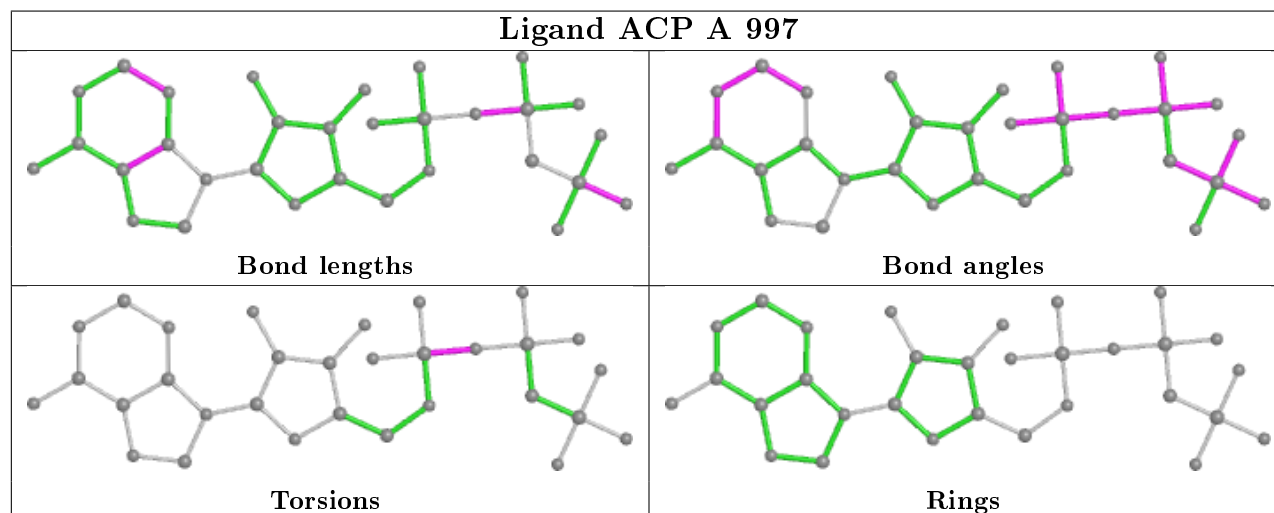
Mol	Chain	Res	Type	Atoms
2	A	997	ACP	PB-O3A-PA-O2A
2	A	997	ACP	PB-O3A-PA-O1A

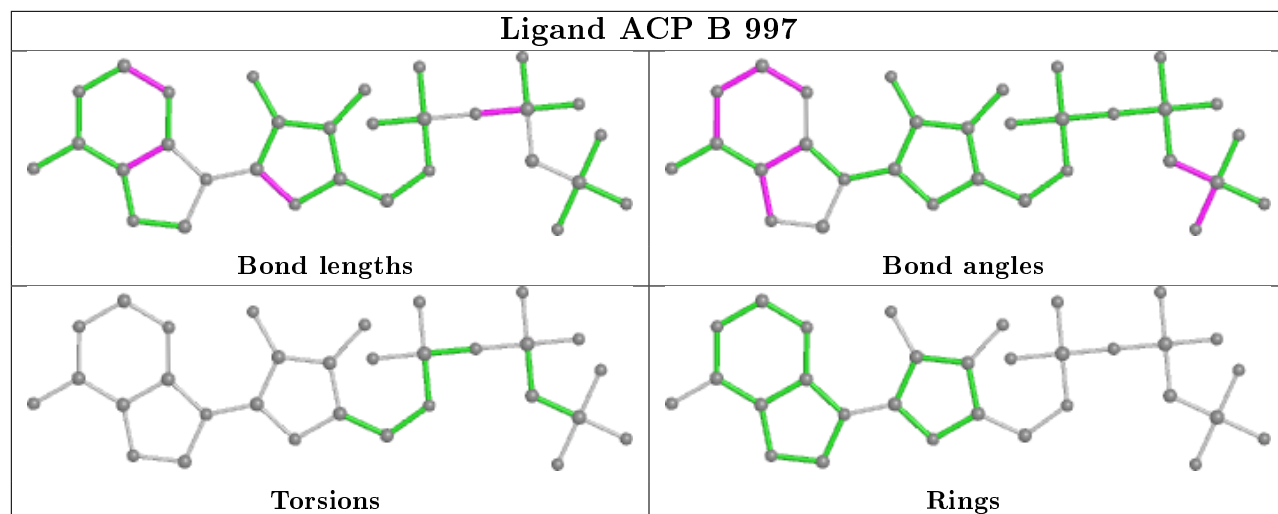
There are no ring outliers.

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, 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	267/287 (93%)	0.63	27 (10%) 7 6	28, 39, 50, 56	0
1	B	273/287 (95%)	1.11	67 (24%) 0 0	31, 44, 67, 75	0
All	All	540/574 (94%)	0.87	94 (17%) 1 1	28, 40, 63, 75	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	672	ILE	10.0
1	B	480	GLY	7.4
1	B	481	GLU	7.0
1	B	643	VAL	6.6
1	B	670	SER	6.3
1	B	482	PRO	5.3
1	B	485	VAL	5.0
1	B	443	ASN	4.6
1	B	533	ILE	4.5
1	B	532	VAL	4.5
1	B	473	LEU	4.3
1	B	459	ARG	4.2
1	B	671	LYS	4.2
1	A	616	VAL	4.1
1	B	539	ARG	4.0
1	B	484	LYS	4.0
1	B	496	ASP	4.0
1	B	478	GLU	3.9
1	B	494	VAL	3.7
1	B	519	LEU	3.6
1	A	400	ALA	3.6
1	B	509	PHE	3.5
1	B	658	VAL	3.5
1	B	444	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	500	VAL	3.4
1	B	534	VAL	3.4
1	A	658	VAL	3.3
1	B	544	ILE	3.3
1	A	423	PHE	3.2
1	A	633	ILE	3.2
1	A	563	ARG	3.2
1	A	648	ILE	3.2
1	B	479	LEU	3.1
1	B	404	ILE	3.1
1	A	444	GLY	3.1
1	B	476	GLY	3.1
1	B	442	LEU	3.1
1	A	598	HIS	3.0
1	B	483	GLU	3.0
1	B	648	ILE	2.9
1	B	421	VAL	2.9
1	B	405	LEU	2.9
1	B	423	PHE	2.9
1	A	422	ILE	2.8
1	B	650	LEU	2.8
1	B	458	ARG	2.8
1	B	616	VAL	2.7
1	A	571	ILE	2.6
1	A	597	PRO	2.6
1	A	614	ALA	2.6
1	A	404	ILE	2.6
1	A	421	VAL	2.6
1	B	661	ALA	2.5
1	A	515	ASN	2.5
1	A	410	ASP	2.5
1	B	406	ILE	2.5
1	B	543	ILE	2.5
1	B	633	ILE	2.5
1	A	532	VAL	2.5
1	A	405	LEU	2.5
1	B	592	ILE	2.5
1	A	534	VAL	2.5
1	B	615	PHE	2.5
1	B	576	TRP	2.4
1	B	451	ARG	2.4
1	B	449	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	662	ILE	2.4
1	B	486	GLU	2.4
1	B	642	ALA	2.4
1	A	406	ILE	2.4
1	B	561	LEU	2.3
1	B	591	VAL	2.3
1	B	501	GLY	2.3
1	B	631	LEU	2.3
1	B	635	VAL	2.3
1	B	464	ILE	2.3
1	B	445	ASP	2.3
1	B	477	ILE	2.2
1	A	429	LEU	2.2
1	B	516	GLU	2.2
1	A	500	VAL	2.2
1	B	487	VAL	2.2
1	A	655	LEU	2.2
1	B	537	ASN	2.2
1	A	496	ASP	2.1
1	B	649	VAL	2.1
1	B	447	ARG	2.1
1	B	571	ILE	2.1
1	B	400	ALA	2.1
1	B	461	GLU	2.1
1	A	544	ILE	2.1
1	B	488	ILE	2.0
1	A	631	LEU	2.0
1	B	515	ASN	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 carbohydrates in this entry.

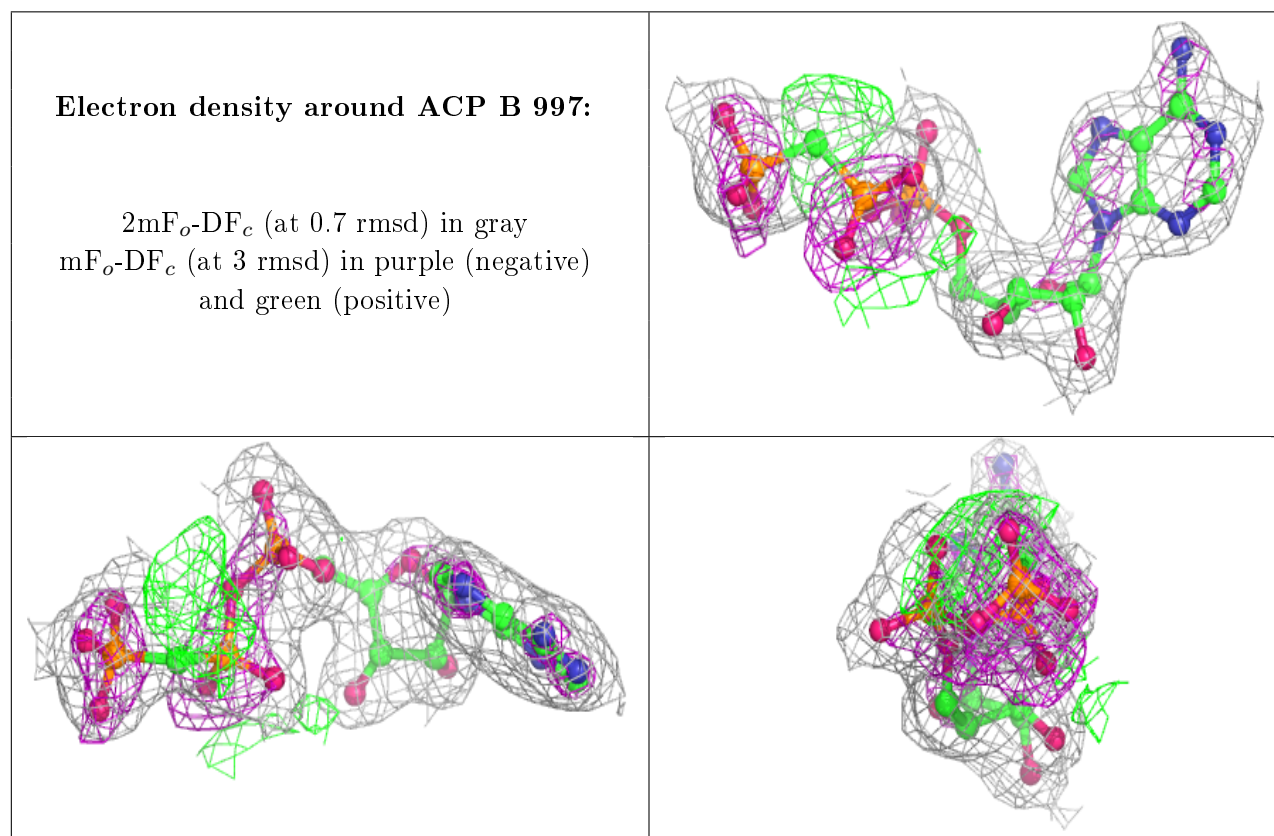
6.4 Ligands [i](#)

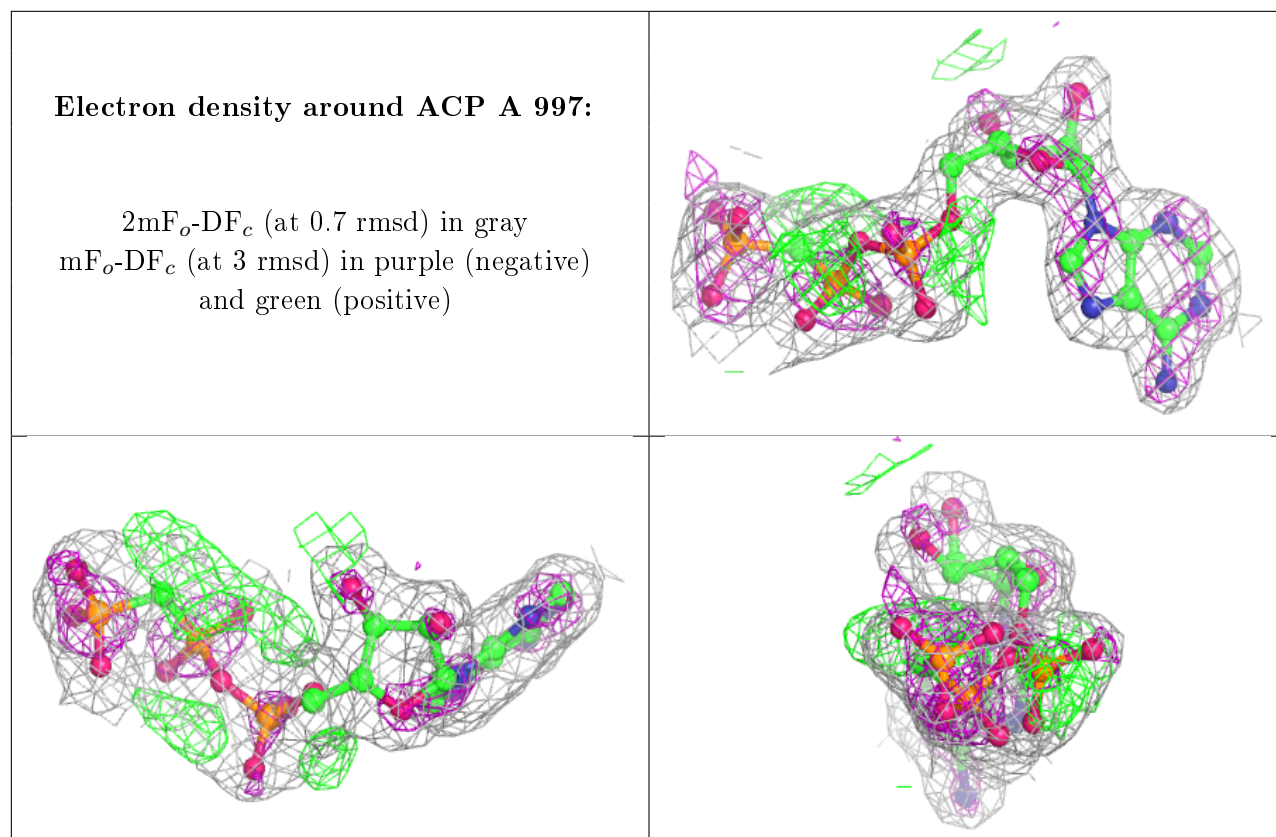
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	MG	A	998	1/1	0.76	0.13	74,74,74,74	0
2	ACP	B	997	31/31	0.94	0.12	44,49,52,54	0
2	ACP	A	997	31/31	0.94	0.10	34,38,54,56	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.