WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2024 – 10:17 AM JST

PDB ID	:	5X40
Title	:	Structure of a CbiO dimer bound with AMPPCP
Authors	:	Bao, Z.; Qi, X.; Wang, J.; Zhang, P.
Deposited on	:	2017-02-09
Resolution	:	1.45 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
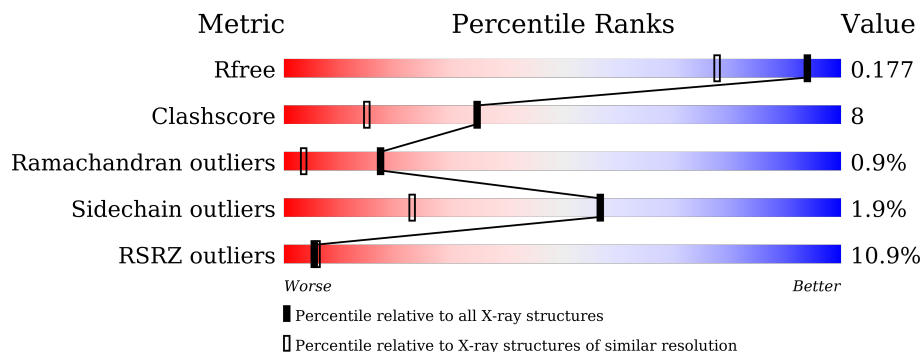http://www.wwpdb.org/validation/2017/FAQs#types.

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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 1.45 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.177
Clashscore		8
Ramachandran outliers		0.9%
Sidechain outliers		1.9%
RSRZ outliers		10.9%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	292	9% ... 87% ... 7% · · ·
1	B	292	12% ... 85% ... 9% · ·

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4766 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 Cobalt ABC transporter ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2069	1301	381	382	5			
1	B	280	Total	C	N	O	S	0	0	0
			2069	1301	381	382	5			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).
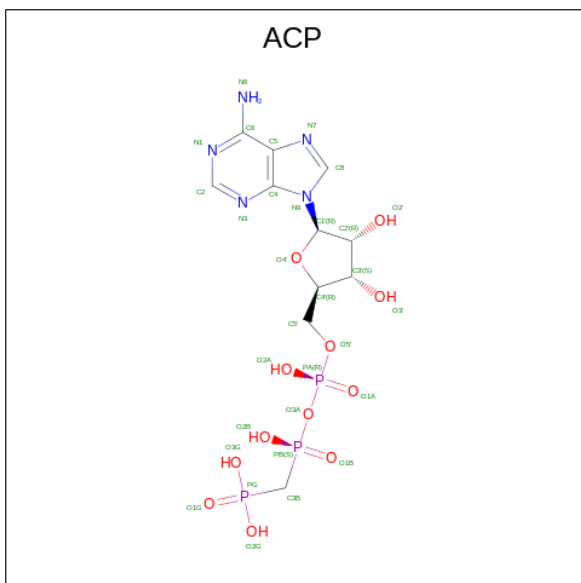
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 11	N 5	O 12	P 3	0	0
3	B	1	Total 31	C 11	N 5	O 12	P 3	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	277	Total 277	O 277	0	0
4	B	287	Total 287	O 287	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A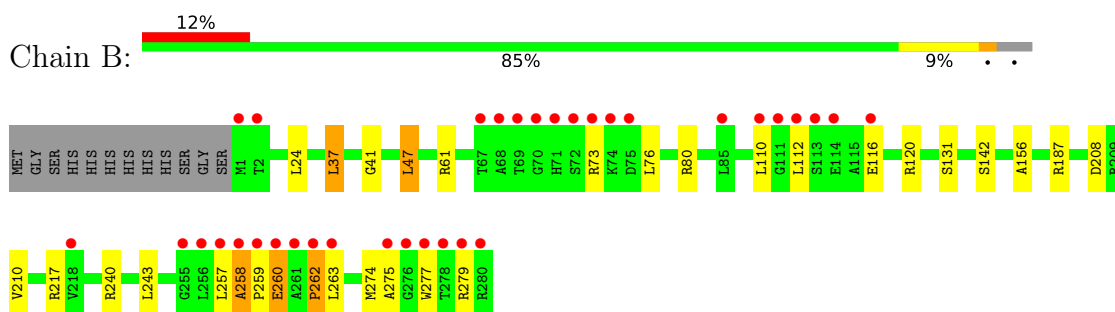 red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cobalt ABC transporter ATP-binding protein

Chain A:

• Molecule 1: Cobalt ABC transporter ATP-binding protein

Chain B:
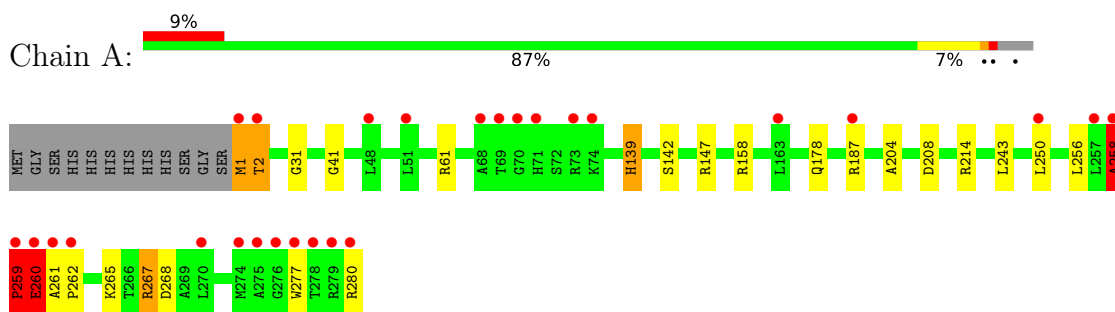
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.34Å 74.40Å 106.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.66 – 1.45 29.67 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.66-1.45) 99.9 (29.67-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 1.45Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.157 , 0.177 0.159 , 0.177	Depositor DCC
R_{free} test set	1991 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å^2)	17.6	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4766	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, 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	2/2098 (0.1%)	0.62	2/2850 (0.1%)
1	B	0.39	1/2098 (0.0%)	0.64	1/2850 (0.0%)
All	All	0.41	3/4196 (0.1%)	0.63	3/5700 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	PRO	N-CD	5.51	1.55	1.47
1	B	262	PRO	N-CD	5.14	1.55	1.47
1	A	262	PRO	N-CD	5.03	1.54	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	LEU	CA-CB-CG	-6.43	100.51	115.30
1	A	2	THR	C-N-CD	5.63	140.22	128.40
1	A	258	ALA	C-N-CD	5.53	140.01	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	HIS	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2069	0	2159	31	0
1	B	2069	0	2158	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	14	5	0
3	B	31	0	14	5	0
4	A	277	0	0	8	2
4	B	287	0	0	7	2
All	All	4766	0	4345	71	2

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 8.

All (71) 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:258:ALA:HB3	1:B:259:PRO:CA	1.69	1.21
1:B:258:ALA:CB	1:B:259:PRO:CA	2.18	1.21
1:B:73:ARG:NH1	4:B:401:HOH:O	1.63	1.20
1:B:258:ALA:HB1	1:B:259:PRO:C	1.61	1.19
1:B:258:ALA:CB	1:B:259:PRO:HA	1.68	1.16
1:B:258:ALA:CB	1:B:259:PRO:C	2.21	1.09
1:A:41:GLY:H	3:A:302:ACP:H3B1	1.22	1.03
1:B:41:GLY:H	3:B:302:ACP:H3B1	1.34	0.90
1:B:258:ALA:HB3	1:B:259:PRO:HA	0.89	0.87
1:A:187:ARG:NH2	4:A:404:HOH:O	2.09	0.85
1:B:258:ALA:HB1	1:B:259:PRO:O	1.81	0.81
1:A:178:GLN:OE1	4:A:402:HOH:O	1.99	0.81
1:B:110:LEU:O	4:B:402:HOH:O	2.00	0.80
1:A:259:PRO:O	1:A:260:GLU:HB2	1.82	0.79
3:A:302:ACP:H3B2	1:B:142:SER:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ARG:NH1	4:A:403:HOH:O	2.06	0.75
1:A:142:SER:HB2	3:B:302:ACP:H3B2	1.69	0.73
1:A:258:ALA:HB3	1:A:261:ALA:HB3	1.72	0.71
1:A:41:GLY:H	3:A:302:ACP:C3B	2.03	0.70
1:B:120:ARG:HH11	1:B:120:ARG:HG2	1.57	0.69
1:B:41:GLY:H	3:B:302:ACP:C3B	2.08	0.66
1:B:187:ARG:NH1	1:B:208:ASP:OD2	2.27	0.66
1:A:31:GLY:O	1:A:187:ARG:NE	2.23	0.66
1:B:24:LEU:HD22	1:B:47:LEU:HD13	1.78	0.66
1:B:37:LEU:HD23	1:B:210:VAL:HG13	1.80	0.63
1:A:41:GLY:N	3:A:302:ACP:H3B1	2.05	0.63
1:A:158:ARG:NH1	4:A:407:HOH:O	2.32	0.61
1:B:258:ALA:HB3	1:B:259:PRO:C	2.07	0.61
1:A:147:ARG:NH1	4:A:409:HOH:O	2.33	0.61
1:B:258:ALA:HB1	1:B:259:PRO:CA	2.06	0.61
1:A:280:ARG:NH1	1:B:277:TRP:O	2.33	0.61
1:B:112:LEU:HD11	1:B:120:ARG:HE	1.68	0.59
1:B:76:LEU:HB3	1:B:80:ARG:NH1	2.18	0.58
1:B:259:PRO:O	1:B:260:GLU:HB2	2.04	0.57
1:B:61:ARG:NH1	4:B:403:HOH:O	2.09	0.57
1:B:131:SER:OG	4:B:404:HOH:O	2.18	0.57
3:A:302:ACP:H3B2	1:B:142:SER:CB	2.35	0.57
1:B:120:ARG:HD3	1:B:156:ALA:O	2.05	0.57
1:B:41:GLY:N	3:B:302:ACP:H3B1	2.13	0.55
1:B:187:ARG:HH22	1:B:208:ASP:CG	2.11	0.54
1:B:187:ARG:HH12	1:B:208:ASP:CG	2.11	0.54
1:A:258:ALA:O	1:A:260:GLU:N	2.41	0.54
1:A:258:ALA:HB3	1:A:261:ALA:CB	2.39	0.53
1:A:1:MET:HG3	1:A:2:THR:N	2.22	0.53
1:B:279:ARG:NH1	4:B:407:HOH:O	2.29	0.53
1:A:259:PRO:O	1:A:260:GLU:CB	2.56	0.53
1:B:187:ARG:NH2	1:B:208:ASP:OD2	2.41	0.53
1:A:280:ARG:NH1	1:B:275:ALA:O	2.42	0.52
1:A:142:SER:CB	3:B:302:ACP:H3B2	2.38	0.50
1:B:76:LEU:HB3	1:B:80:ARG:HH12	1.77	0.50
1:B:217:ARG:NH1	4:B:411:HOH:O	2.43	0.49
1:A:267:ARG:NH1	1:A:268:ASP:OD1	2.45	0.49
1:B:259:PRO:O	1:B:260:GLU:CB	2.61	0.48
1:A:187:ARG:NH1	1:A:208:ASP:OD2	2.46	0.48
1:A:61:ARG:NH1	4:A:405:HOH:O	2.24	0.47
1:B:120:ARG:HH11	1:B:120:ARG:CG	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ARG:HD2	1:B:240:ARG:NE	2.30	0.46
1:A:243:LEU:HG	1:B:243:LEU:HD23	1.98	0.45
1:B:258:ALA:CB	1:B:260:GLU:N	2.76	0.45
1:B:217:ARG:NH2	4:B:412:HOH:O	2.49	0.45
1:B:187:ARG:CZ	1:B:208:ASP:OD2	2.65	0.44
1:A:256:LEU:HB3	1:A:277:TRP:CE2	2.52	0.43
1:A:204:ALA:O	1:A:265:LYS:HD3	2.19	0.42
1:A:178:GLN:CD	4:A:402:HOH:O	2.50	0.42
1:B:257:LEU:O	1:B:258:ALA:C	2.58	0.42
1:B:257:LEU:O	1:B:259:PRO:HA	2.20	0.42
1:B:47:LEU:O	1:B:47:LEU:HG	2.04	0.41
1:A:258:ALA:CB	1:A:261:ALA:CB	2.98	0.41
1:A:250:LEU:HG	1:B:274:MET:SD	2.61	0.41
1:A:1:MET:HA	1:A:1:MET:HE2	2.02	0.40
1:A:2:THR:HG21	4:A:487:HOH:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:640:HOH:O	4:B:642:HOH:O[4_555]	1.81	0.39
4:A:634:HOH:O	4:B:593:HOH:O[4_455]	2.19	0.01

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	278/292 (95%)	274 (99%)	1 (0%)	3 (1%)	14	2
1	B	278/292 (95%)	275 (99%)	1 (0%)	2 (1%)	22	5
All	All	556/584 (95%)	549 (99%)	2 (0%)	5 (1%)	17	3

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	258	ALA
1	B	260	GLU
1	A	260	GLU
1	A	259	PRO
1	A	258	ALA

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	209/219 (95%)	205 (98%)	4 (2%)	57	23
1	B	209/219 (95%)	205 (98%)	4 (2%)	57	23
All	All	418/438 (95%)	410 (98%)	8 (2%)	57	23

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	139	HIS
1	A	260	GLU
1	A	267	ARG
1	B	37	LEU
1	B	116	GLU
1	B	262	PRO
1	B	263	LEU

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are 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	$\#|Z| > 2$
3	ACP	B	302	2	27,33,33	1.24	3 (11%)	32,52,52	1.37	4 (12%)
3	ACP	A	302	2	27,33,33	1.29	2 (7%)	32,52,52	1.00	3 (9%)

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	ACP	B	302	2	-	1/15/38/38	0/3/3/3
3	ACP	A	302	2	-	0/15/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	ACP	PG-O1G	4.53	1.59	1.50
3	B	302	ACP	PG-O1G	3.94	1.58	1.50
3	A	302	ACP	PG-O3G	-3.34	1.47	1.54
3	B	302	ACP	PB-O3A	-2.53	1.55	1.58
3	B	302	ACP	PG-O2G	-2.19	1.49	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	302	ACP	O2G-PG-C3B	5.01	118.56	106.40
3	B	302	ACP	O3G-PG-C3B	-4.00	96.70	106.40
3	A	302	ACP	C5-C6-N6	2.30	123.85	120.35
3	B	302	ACP	C5-C6-N6	2.29	123.83	120.35
3	B	302	ACP	O1G-PG-C3B	-2.18	106.54	111.24
3	A	302	ACP	O1G-PG-C3B	-2.17	106.57	111.24
3	A	302	ACP	O3G-PG-O2G	2.12	114.28	108.08

There are no chirality outliers.
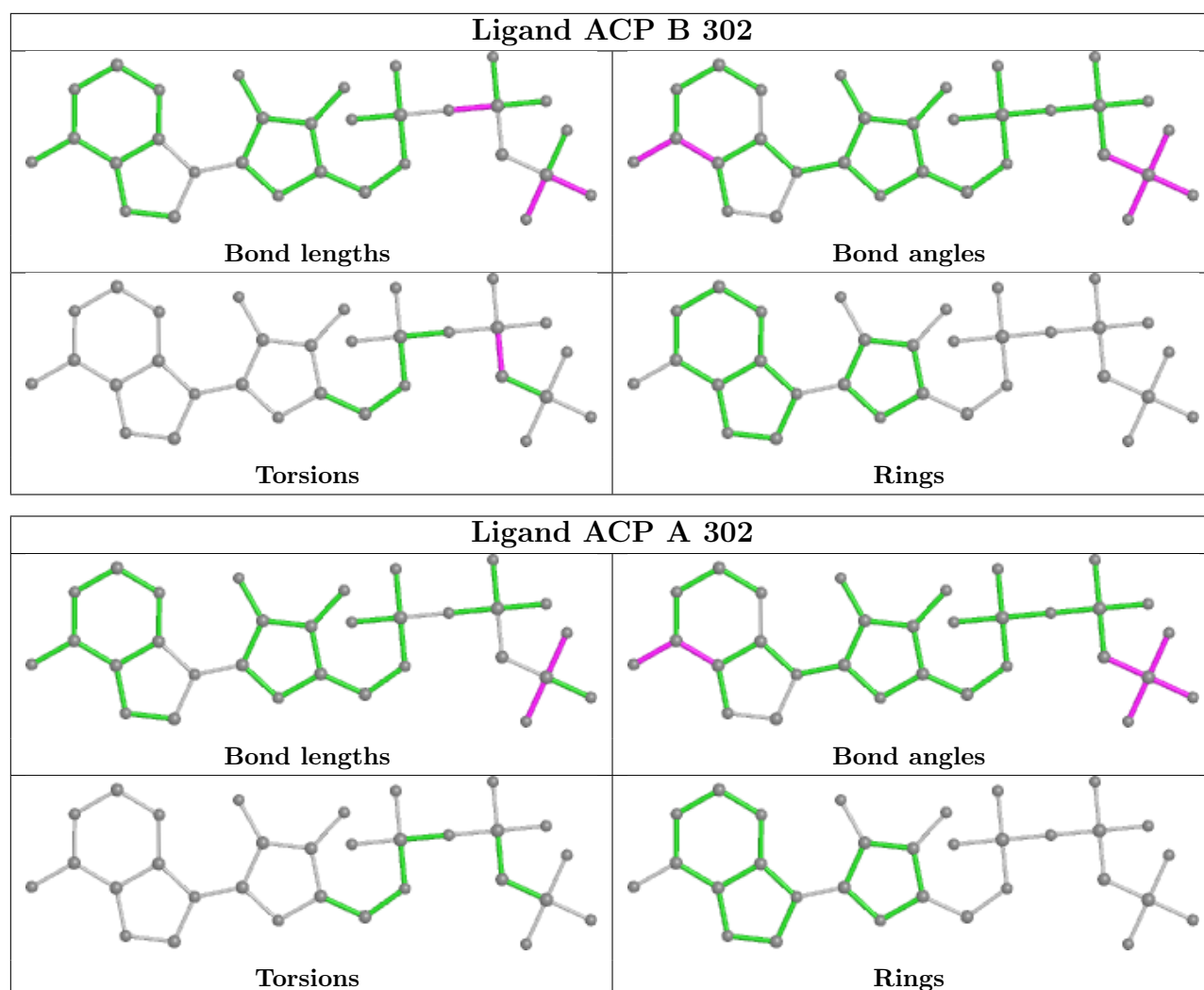
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	ACP	PG-C3B-PB-O1B

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	ACP	5	0
3	A	302	ACP	5	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ACP B 302

Bond lengths

Bond angles

Torsions

Rings

Ligand ACP A 302

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	280/292 (95%)	0.68	27 (9%)	8	9	13, 22, 47, 78	0
1	B	280/292 (95%)	0.84	34 (12%)	4	4	13, 21, 50, 87	0
All	All	560/584 (95%)	0.76	61 (10%)	5	6	13, 22, 50, 87	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	261	ALA	13.2
1	B	258	ALA	13.0
1	A	1	MET	12.4
1	A	258	ALA	11.7
1	B	259	PRO	11.5
1	B	1	MET	11.2
1	A	259	PRO	10.3
1	A	260	GLU	8.5
1	A	261	ALA	8.4
1	B	260	GLU	7.4
1	A	262	PRO	7.3
1	B	71	HIS	6.2
1	B	111	GLY	6.2
1	B	73	ARG	5.7
1	B	279	ARG	5.7
1	A	257	LEU	5.5
1	B	257	LEU	5.4
1	B	110	LEU	5.3
1	B	70	GLY	5.3
1	B	72	SER	5.0
1	B	275	ALA	5.0
1	A	71	HIS	4.9
1	B	113	SER	4.5
1	B	280	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	262	PRO	4.3
1	B	2	THR	4.3
1	B	255	GLY	4.2
1	A	280	ARG	4.2
1	A	2	THR	3.9
1	B	74	LYS	3.7
1	B	69	THR	3.7
1	A	275	ALA	3.4
1	B	256	LEU	3.4
1	B	277	TRP	3.3
1	B	278	THR	3.3
1	B	68	ALA	3.3
1	A	74	LYS	3.2
1	A	73	ARG	3.2
1	B	67	THR	3.0
1	A	277	TRP	3.0
1	B	114	GLU	2.9
1	A	276	GLY	2.8
1	A	48	LEU	2.7
1	A	279	ARG	2.7
1	B	263	LEU	2.4
1	A	68	ALA	2.4
1	B	112	LEU	2.4
1	A	70	GLY	2.3
1	A	250	LEU	2.3
1	A	270	LEU	2.3
1	B	218	VAL	2.3
1	A	51	LEU	2.2
1	B	116	GLU	2.2
1	A	278	THR	2.2
1	B	85	LEU	2.2
1	A	187	ARG	2.1
1	B	75	ASP	2.1
1	A	274	MET	2.1
1	A	163	LEU	2.1
1	B	276	GLY	2.1
1	A	69	THR	2.1

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

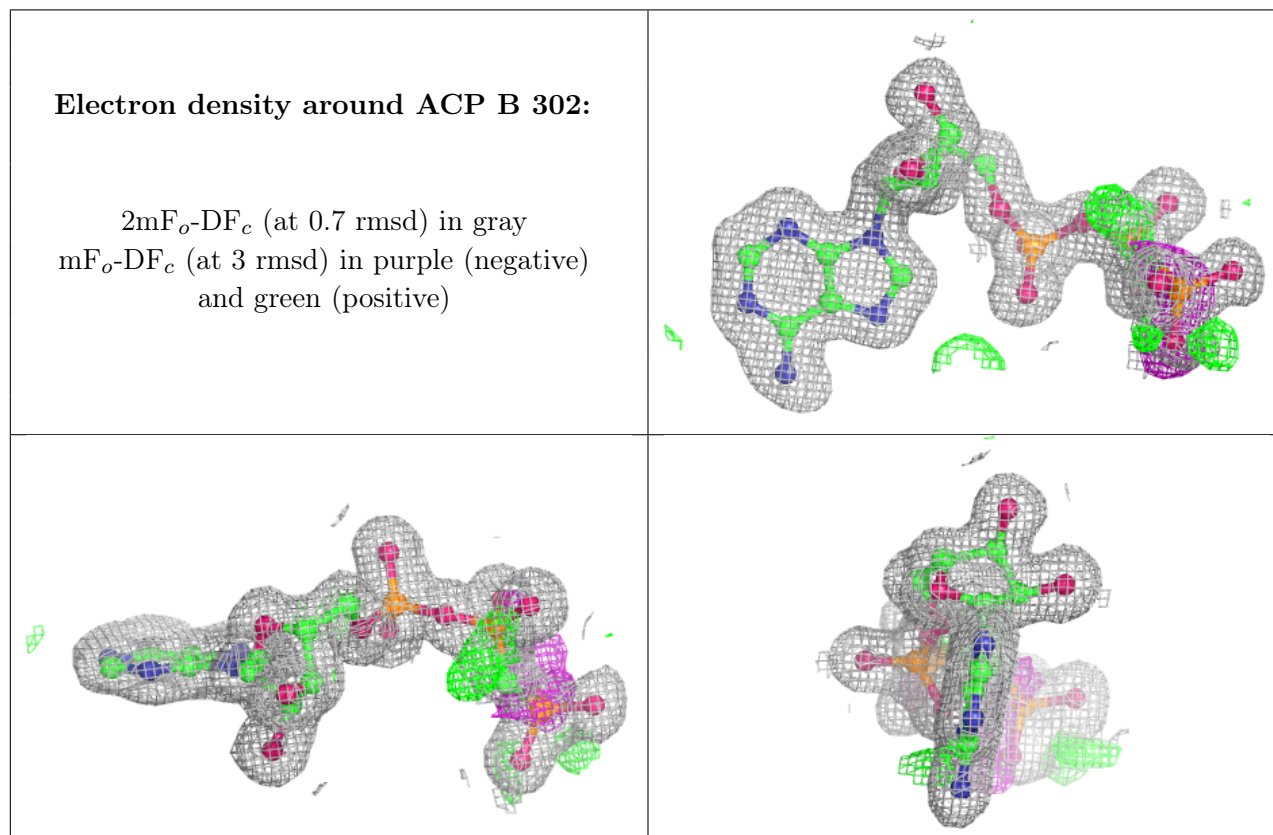There are no non-standard protein/DNA/RNA residues in this entry.

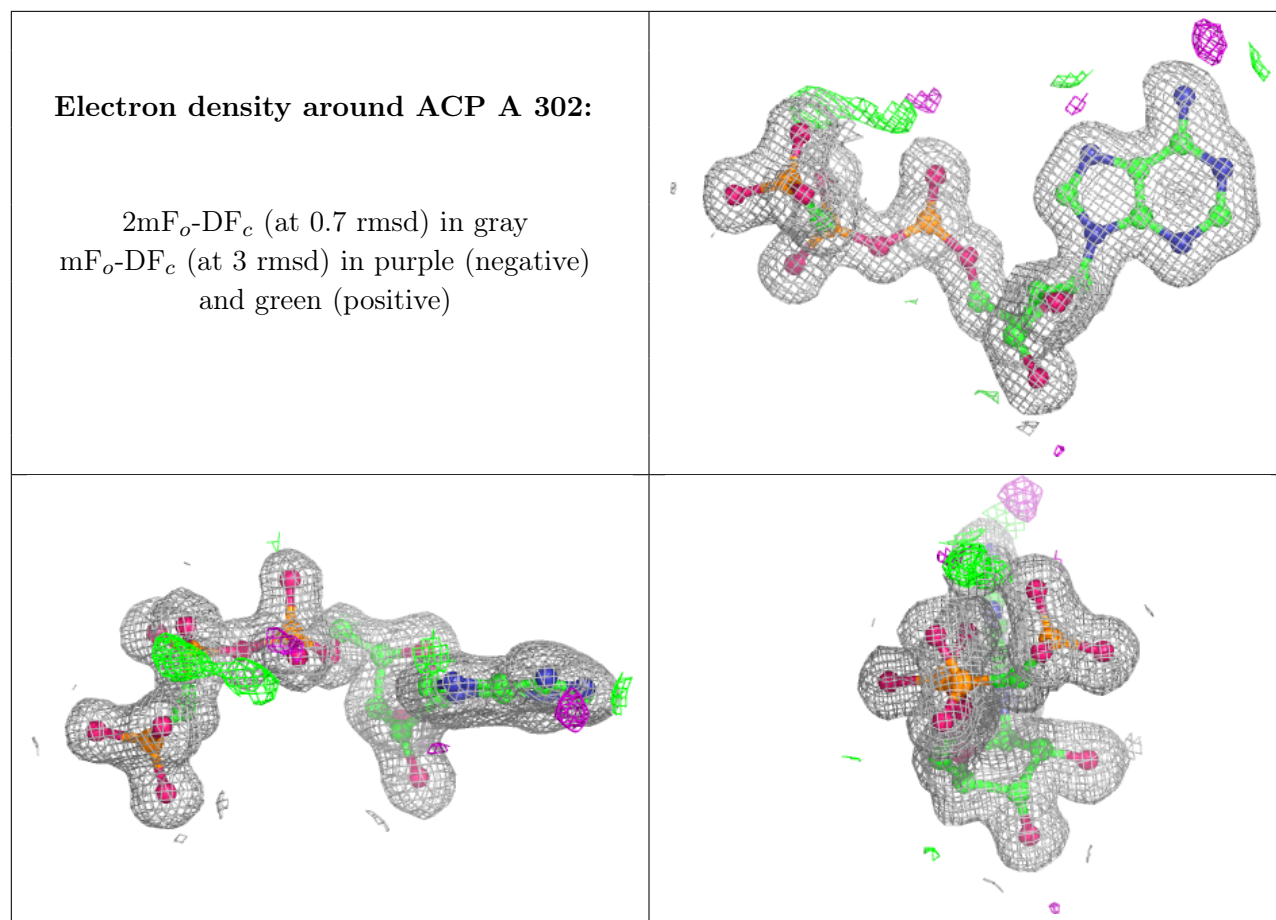## 6.3 Carbohydrates (i)

There are no monosaccharides 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
2	MG	B	301	1/1	0.85	0.26	51,51,51,51	0
2	MG	A	301	1/1	0.91	0.17	27,27,27,27	0
3	ACP	B	302	31/31	0.97	0.08	12,16,21,25	0
3	ACP	A	302	31/31	0.98	0.07	7,16,23,25	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 302:

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

Electron density around ACP A 302:

$2mF_o$-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.