Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 12:20 PM EDT

PDB ID	:	3LLA
Title	:	Crystal Structure of the Alpha-kinase Domain of Myosin Heavy Chain Kinase A Complex with AMPPCP
Authors	:	Ye, Q.; Jia, Z.
Deposited on	:	2010-01-28
Resolution	:	2.11 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:

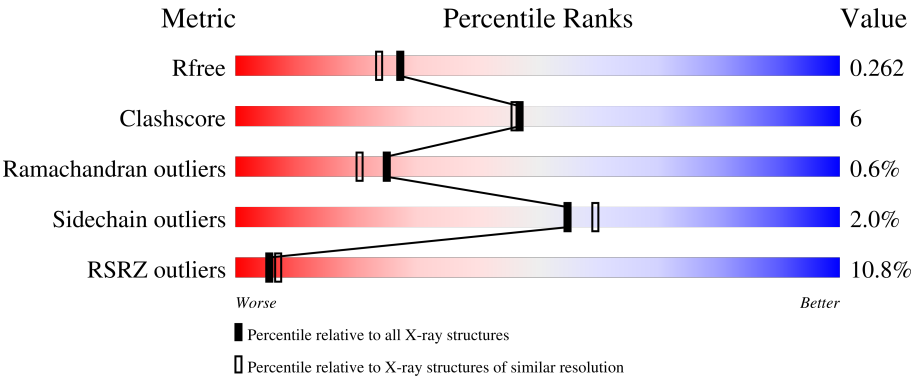
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	307	9% 73% 9% · 17%
1	B	307	9% 70% 10% •• 17%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4475 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 Myosin heavy chain kinase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2024	1297	339	376	12			
1	B	254	Total	C	N	O	S	0	0	0
			2010	1288	337	373	12			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	535	MET	-	expression tag	UNP P42527
A	536	GLY	-	expression tag	UNP P42527
A	537	GLY	-	expression tag	UNP P42527
A	538	HIS	-	expression tag	UNP P42527
A	539	HIS	-	expression tag	UNP P42527
A	540	HIS	-	expression tag	UNP P42527
A	541	HIS	-	expression tag	UNP P42527
A	542	HIS	-	expression tag	UNP P42527
A	543	HIS	-	expression tag	UNP P42527
A	544	GLY	-	expression tag	UNP P42527
A	545	GLU	-	expression tag	UNP P42527
A	546	ASN	-	expression tag	UNP P42527
A	547	LEU	-	expression tag	UNP P42527
A	548	TYR	-	expression tag	UNP P42527
A	549	PHE	-	expression tag	UNP P42527
A	550	GLN	-	expression tag	UNP P42527
A	551	GLY	-	expression tag	UNP P42527
B	535	MET	-	expression tag	UNP P42527
B	536	GLY	-	expression tag	UNP P42527
B	537	GLY	-	expression tag	UNP P42527
B	538	HIS	-	expression tag	UNP P42527
B	539	HIS	-	expression tag	UNP P42527
B	540	HIS	-	expression tag	UNP P42527
B	541	HIS	-	expression tag	UNP P42527
B	542	HIS	-	expression tag	UNP P42527

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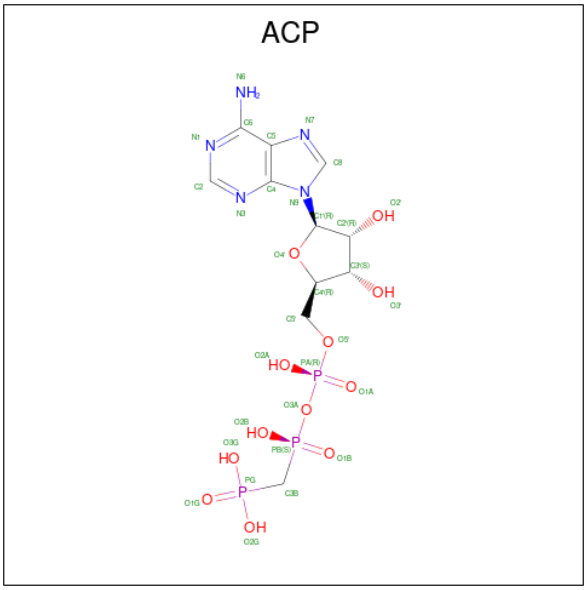
Chain	Residue	Modelled	Actual	Comment	Reference
B	543	HIS	-	expression tag	UNP P42527
B	544	GLY	-	expression tag	UNP P42527
B	545	GLU	-	expression tag	UNP P42527
B	546	ASN	-	expression tag	UNP P42527
B	547	LEU	-	expression tag	UNP P42527
B	548	TYR	-	expression tag	UNP P42527
B	549	PHE	-	expression tag	UNP P42527
B	550	GLN	-	expression tag	UNP P42527
B	551	GLY	-	expression tag	UNP P42527

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

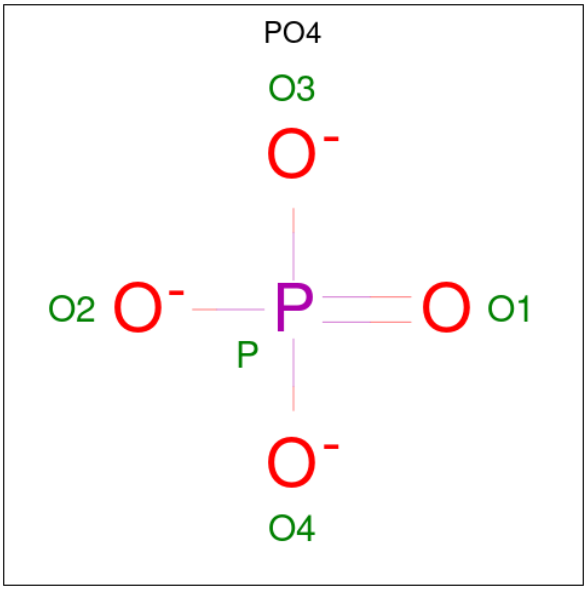
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

- 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 C N O P 31 11 5 12 3	0	0
3	B	1	Total C N O P 31 11 5 12 3	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0

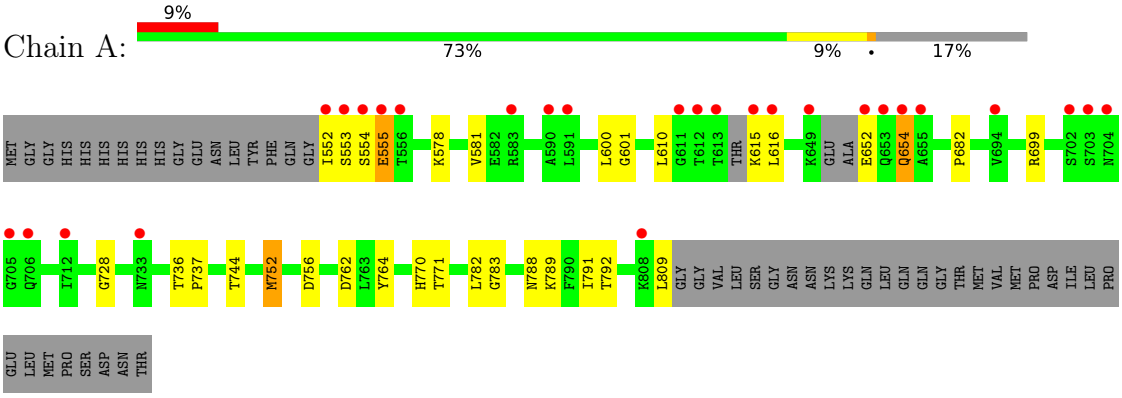
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	201	Total O 201 201	0	0
5	B	166	Total O 166 166	0	0

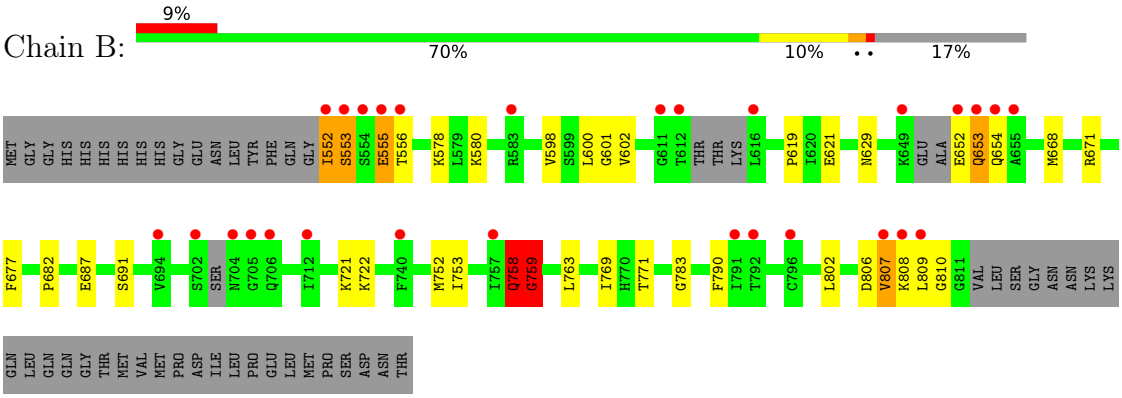
3 Residue-property plots (i)

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: Myosin heavy chain kinase A



• Molecule 1: Myosin heavy chain kinase A



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	83.08Å 109.81Å 79.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.90 – 2.11 23.90 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.5 (23.90-2.11) 99.5 (23.90-2.11)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.15 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.213 , 0.263 0.212 , 0.262	Depositor DCC
R_{free} test set	2135 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4475	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PO4, 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	0.54	0/2066	0.60	0/2786
1	B	0.54	0/2051	0.70	2/2764 (0.1%)
All	All	0.54	0/4117	0.65	2/5550 (0.0%)

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	B	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	759	GLY	N-CA-C	-11.20	85.09	113.10
1	B	758	GLN	C-N-CA	6.51	135.97	122.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	758	GLN	Peptide
1	B	759	GLY	Peptide

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	2024	0	2045	27	0
1	B	2010	0	2026	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	14	0	0
3	B	31	0	14	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	201	0	0	3	0
5	B	166	0	0	4	0
All	All	4475	0	4099	51	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 (51) 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:744:THR:HB	1:A:752:MET:HE1	1.42	0.99
1:A:554:SER:HA	1:A:555:GLU:HB2	1.46	0.98
1:A:744:THR:HB	1:A:752:MET:CE	2.09	0.82
1:A:770:HIS:HD2	1:A:782:LEU:H	1.37	0.71
1:A:552:ILE:HG22	1:A:601:GLY:HA3	1.73	0.69
1:B:668:MET:HE1	1:B:691:SER:H	1.58	0.68
1:B:552:ILE:O	1:B:553:SER:HB2	1.94	0.68
1:A:770:HIS:CD2	1:A:782:LEU:H	2.11	0.67
1:B:629:ASN:HB3	5:B:338:HOH:O	1.95	0.66
1:B:806:ASP:C	1:B:808:LYS:H	2.03	0.61
1:B:668:MET:CE	1:B:691:SER:H	2.13	0.61
1:A:554:SER:HA	1:A:555:GLU:CB	2.20	0.60
1:B:759:GLY:HA2	5:B:86:HOH:O	2.04	0.56
1:A:771:THR:O	1:A:783:GLY:HA2	2.05	0.56
1:B:771:THR:O	1:B:783:GLY:HA2	2.06	0.55
1:A:578:LYS:HB3	1:A:600:LEU:HB2	1.88	0.55
1:B:555:GLU:HA	1:B:555:GLU:OE2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:PRO:HB2	5:A:87:HOH:O	2.07	0.54
1:A:736:THR:HB	1:A:737:PRO:HD3	1.90	0.54
1:B:653:GLN:O	1:B:654:GLN:HB2	2.09	0.53
1:A:554:SER:HB3	1:A:555:GLU:O	2.10	0.52
1:A:581:VAL:HG11	1:A:699:ARG:NH2	2.25	0.51
1:A:554:SER:CA	1:A:555:GLU:HB2	2.29	0.50
1:A:581:VAL:HG11	1:A:699:ARG:HH22	1.78	0.48
1:B:677:PHE:CE2	1:B:682:PRO:HG3	2.49	0.47
1:A:615:LYS:O	1:A:616:LEU:HB3	2.15	0.47
1:A:552:ILE:CG2	1:A:601:GLY:HA3	2.41	0.46
1:A:762:ASP:HA	1:A:764:TYR:CZ	2.51	0.46
1:B:753:ILE:HD11	1:B:790:PHE:CD2	2.51	0.46
1:A:652:GLU:HG2	1:A:654:GLN:H	1.81	0.46
1:A:610:LEU:HB2	5:A:309:HOH:O	2.16	0.45
1:B:721:LYS:H	1:B:759:GLY:HA3	1.80	0.45
1:B:553:SER:H	1:B:601:GLY:HA3	1.80	0.45
1:B:552:ILE:HG22	1:B:602:VAL:O	2.16	0.45
1:B:806:ASP:C	1:B:808:LYS:N	2.70	0.45
1:B:578:LYS:HB3	1:B:600:LEU:HB2	1.99	0.45
1:B:671:ARG:NH2	5:B:58:HOH:O	2.49	0.45
1:B:752:MET:HE3	1:B:769:ILE:HD13	1.99	0.44
1:A:762:ASP:OD1	1:A:764:TYR:OH	2.23	0.44
1:B:687:GLU:HB3	1:B:763:LEU:HD23	2.00	0.44
1:B:809:LEU:HG	5:B:170:HOH:O	2.17	0.44
1:A:728:GLY:HA3	1:A:789:LYS:HG3	2.00	0.43
1:B:580:LYS:HE2	1:B:598:VAL:CG1	2.48	0.43
1:A:552:ILE:CG2	1:A:553:SER:N	2.81	0.43
1:A:581:VAL:HG12	5:A:97:HOH:O	2.18	0.42
1:B:619:PRO:HB2	1:B:621:GLU:OE2	2.20	0.42
1:A:788:ASN:O	1:A:792:THR:HG23	2.20	0.41
1:B:807:VAL:C	1:B:810:GLY:H	2.23	0.41
1:A:791:ILE:HD12	1:A:809:LEU:HD22	2.02	0.41
1:A:654:GLN:HA	1:A:654:GLN:HE21	1.86	0.41
1:B:722:LYS:HA	1:B:758:GLN:HB3	2.04	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	249/307 (81%)	240 (96%)	8 (3%)	1 (0%)	34 32
1	B	246/307 (80%)	237 (96%)	7 (3%)	2 (1%)	19 14
All	All	495/614 (81%)	477 (96%)	15 (3%)	3 (1%)	25 20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	553	SER
1	B	807	VAL
1	A	555	GLU

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	227/270 (84%)	224 (99%)	3 (1%)	69 74
1	B	224/270 (83%)	218 (97%)	6 (3%)	44 47
All	All	451/540 (84%)	442 (98%)	9 (2%)	55 59

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

Mol	Chain	Res	Type
1	A	654	GLN
1	A	752	MET
1	A	756	ASP

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Mol	Chain	Res	Type
1	B	552	ILE
1	B	555	GLU
1	B	556	THR
1	B	652	GLU
1	B	653	GLN
1	B	802	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	607	ASN
1	A	629	ASN
1	A	654	GLN
1	A	770	HIS
1	B	607	ASN
1	B	629	ASN
1	B	768	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	A	1304	-	27,33,33	1.34	4 (14%)	32,52,52	1.45	5 (15%)
4	PO4	A	5954	-	4,4,4	0.80	0	6,6,6	0.70	0
4	PO4	B	5953	-	4,4,4	1.06	0	6,6,6	0.56	0
3	ACP	B	1303	-	27,33,33	1.15	3 (11%)	32,52,52	1.38	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
3	ACP	A	1304	-	-	0/15/38/38	0/3/3/3
3	ACP	B	1303	-	-	1/15/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1304	ACP	C5-C4	3.04	1.49	1.40
3	A	1304	ACP	O4'-C1'	2.77	1.44	1.41
3	A	1304	ACP	PB-O3A	2.47	1.61	1.58
3	B	1303	ACP	C5-C4	2.45	1.47	1.40
3	A	1304	ACP	C2-N3	2.13	1.35	1.32
3	B	1303	ACP	PB-O3A	2.06	1.60	1.58
3	B	1303	ACP	PB-O2B	-2.05	1.51	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1303	ACP	PB-O3A-PA	-3.79	120.54	132.56
3	A	1304	ACP	N3-C2-N1	-3.70	122.89	128.68
3	A	1304	ACP	PB-O3A-PA	-3.08	122.78	132.56
3	B	1303	ACP	N3-C2-N1	-3.06	123.90	128.68
3	A	1304	ACP	O1G-PG-C3B	-2.82	105.16	111.24
3	B	1303	ACP	O1G-PG-C3B	-2.82	105.17	111.24
3	B	1303	ACP	C4-C5-N7	-2.70	106.58	109.40
3	A	1304	ACP	C4-C5-N7	-2.47	106.82	109.40
3	A	1304	ACP	C2-N1-C6	2.28	122.65	118.75

There are no chirality outliers.

All (1) torsion outliers are listed below:

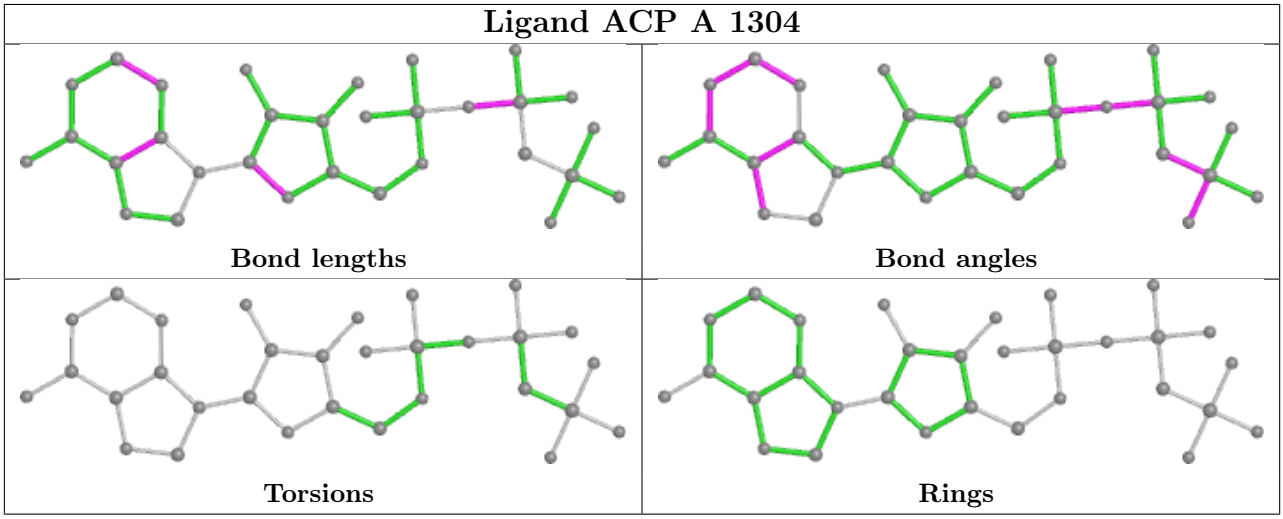
Mol	Chain	Res	Type	Atoms
3	B	1303	ACP	C4'-C5'-O5'-PA

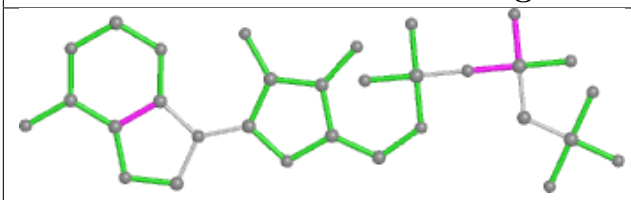
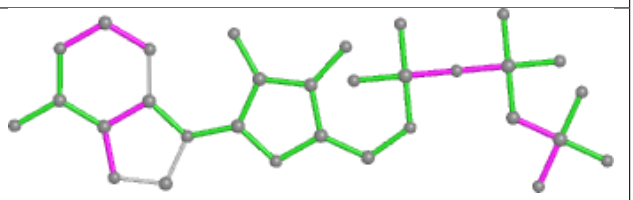
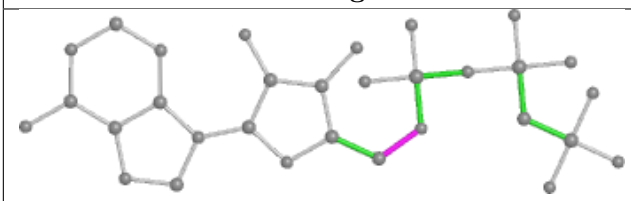
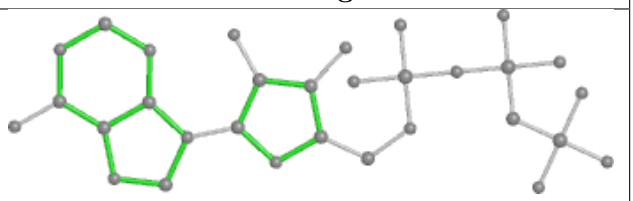
There are no ring outliers.

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 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 A 1304



Ligand ACP B 1303	
 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, 95^{th} 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	255/307 (83%)	0.38	27 (10%)	6	7	13, 26, 49, 63	0
1	B	254/307 (82%)	0.50	28 (11%)	5	7	14, 29, 52, 65	0
All	All	509/614 (82%)	0.44	55 (10%)	5	7	13, 28, 51, 65	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	552	ILE	7.4
1	B	653	GLN	6.7
1	B	809	LEU	6.7
1	B	704	ASN	6.6
1	B	705	GLY	6.3
1	A	703	SER	5.2
1	B	555	GLU	5.2
1	A	613	THR	5.0
1	B	702	SER	4.7
1	B	654	GLN	4.7
1	A	653	GLN	4.6
1	A	654	GLN	4.4
1	A	615	LYS	4.4
1	B	808	LYS	4.3
1	B	796	CYS	4.3
1	A	553	SER	4.1
1	A	702	SER	4.1
1	A	612	THR	4.1
1	A	554	SER	3.9
1	B	556	THR	3.4
1	B	611	GLY	3.4
1	B	706	GLN	3.4
1	B	583	ARG	3.3
1	A	704	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	649	LYS	3.2
1	A	555	GLU	3.2
1	B	553	SER	3.2
1	A	590	ALA	3.2
1	A	611	GLY	3.1
1	B	712	ILE	3.1
1	A	552	ILE	3.1
1	A	591	LEU	3.1
1	A	583	ARG	3.0
1	A	649	LYS	2.9
1	B	616	LEU	2.9
1	B	655	ALA	2.8
1	A	556	THR	2.7
1	B	612	THR	2.7
1	A	706	GLN	2.6
1	B	694	VAL	2.6
1	A	694	VAL	2.6
1	A	733	ASN	2.5
1	A	712	ILE	2.5
1	B	792	THR	2.3
1	A	616	LEU	2.2
1	A	808	LYS	2.2
1	B	652	GLU	2.2
1	B	757	ILE	2.2
1	B	791	ILE	2.1
1	B	740	PHE	2.1
1	A	652	GLU	2.1
1	B	807	VAL	2.1
1	A	705	GLY	2.0
1	B	554	SER	2.0
1	A	655	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

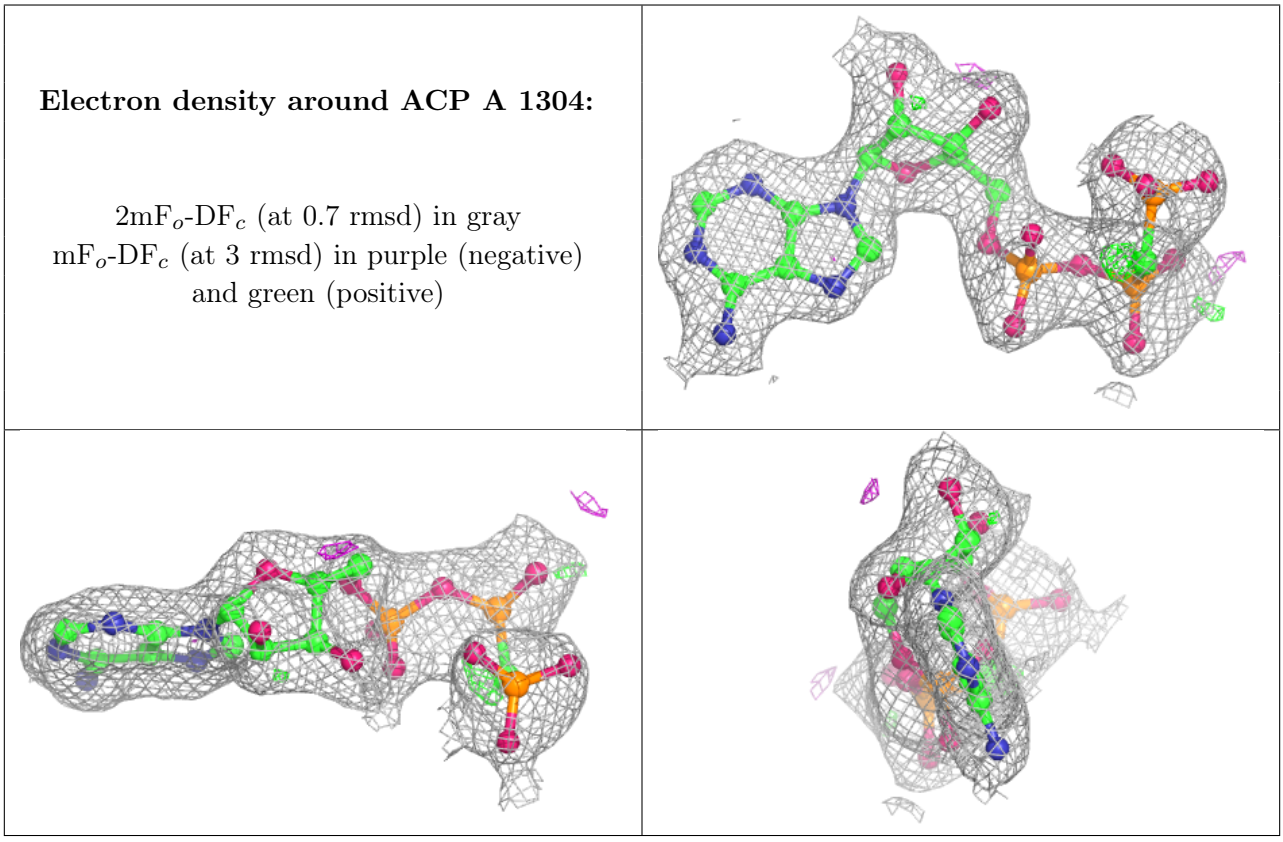
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	A	1304	31/31	0.94	0.10	22,33,49,50	0
3	ACP	B	1303	31/31	0.94	0.11	28,35,48,49	0
4	PO4	A	5954	5/5	0.94	0.12	33,36,37,38	0
2	ZN	B	2001	1/1	0.99	0.06	23,23,23,23	0
2	ZN	A	2002	1/1	0.99	0.05	23,23,23,23	0
4	PO4	B	5953	5/5	0.99	0.06	30,31,31,31	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.

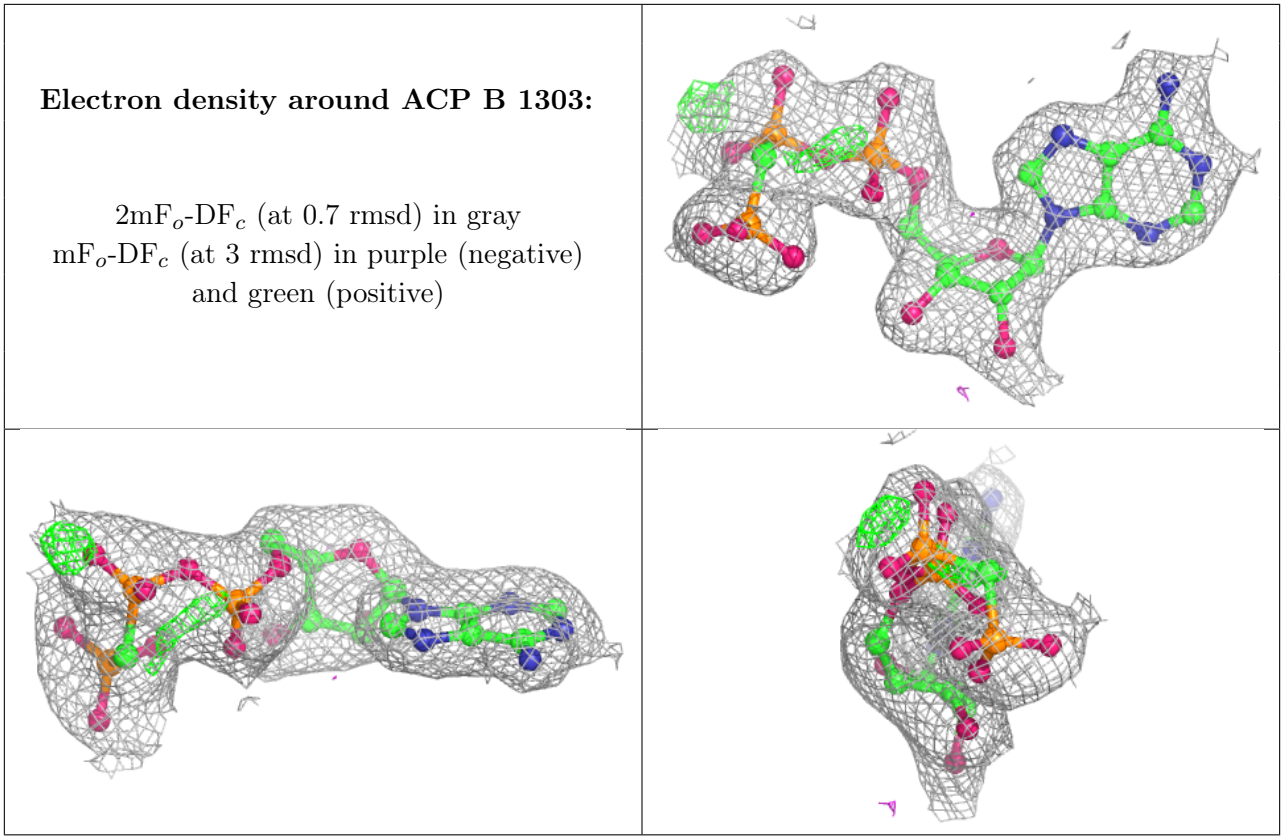
Electron density around ACP A 1304:

$2mF_o$-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 B 1303:

$2mF_o$-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.