Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2020 – 10:31 PM BST

PDB ID	:	4IFC
Title	:	Crystal Structure of ADP-bound Human PRPF4B kinase domain
Authors	:	Mechin, I.; Haas, K.; Chen, X.; Zhang, Y.; McLean, L.
Deposited on	:	2012-12-14
Resolution	:	2.13 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
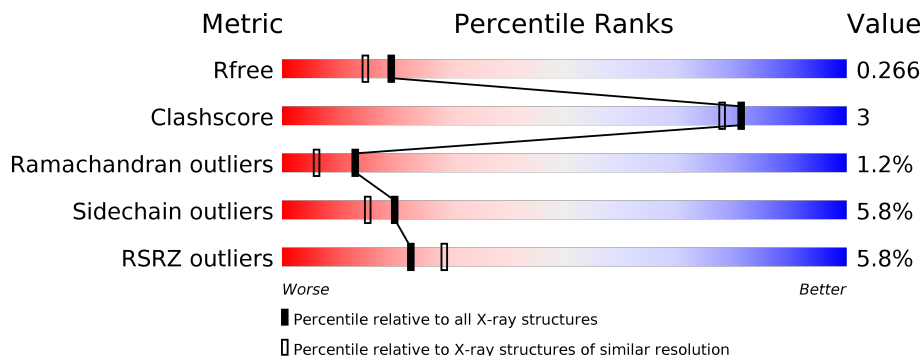with specific help available everywhere you see the (i) symbol.

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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 2.13 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		0.266
Clashscore		3
Ramachandran outliers		1.2%
Sidechain outliers		5.8%
RSRZ outliers		5.8%

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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 <=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	358	5% / 78% 11% · 8%
1	B	358	6% / 82% 10% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5779 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 Serine/threonine-protein kinase PRP4 homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	P	S	0	1	0
			2683	1718	468	480	1	16			
1	B	330	Total	C	N	O	P	S	0	1	0
			2694	1721	473	484	1	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	656	MET	-	EXPRESSION TAG	UNP Q13523
A	1008	HIS	-	EXPRESSION TAG	UNP Q13523
A	1009	HIS	-	EXPRESSION TAG	UNP Q13523
A	1010	HIS	-	EXPRESSION TAG	UNP Q13523
A	1011	HIS	-	EXPRESSION TAG	UNP Q13523
A	1012	HIS	-	EXPRESSION TAG	UNP Q13523
A	1013	HIS	-	EXPRESSION TAG	UNP Q13523
B	656	MET	-	EXPRESSION TAG	UNP Q13523
B	1008	HIS	-	EXPRESSION TAG	UNP Q13523
B	1009	HIS	-	EXPRESSION TAG	UNP Q13523
B	1010	HIS	-	EXPRESSION TAG	UNP Q13523
B	1011	HIS	-	EXPRESSION TAG	UNP Q13523
B	1012	HIS	-	EXPRESSION TAG	UNP Q13523
B	1013	HIS	-	EXPRESSION TAG	UNP Q13523

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 5	O 4	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	185	Total 185	O 185	0	0
4	B	148	Total 148	O 148	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: Serine/threonine-protein kinase PRP4 homolog
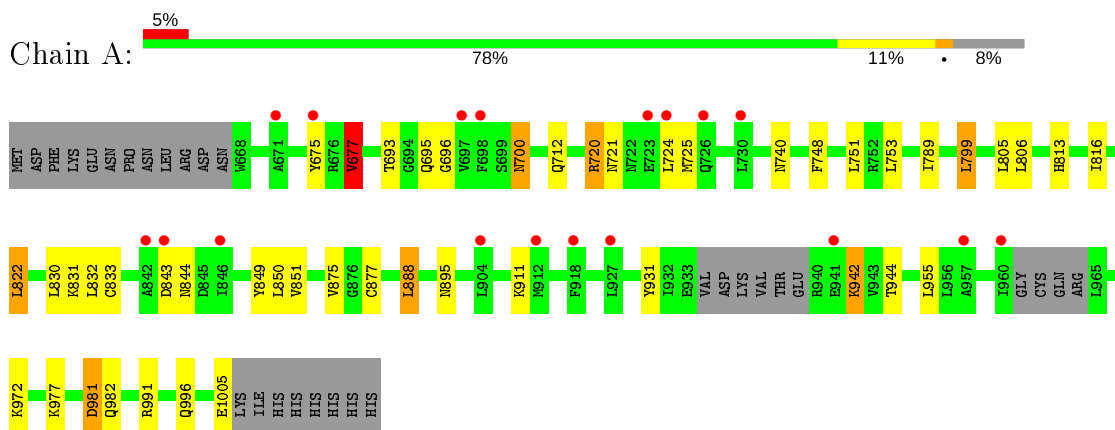
- Molecule 1: Serine/threonine-protein kinase PRP4 homolog
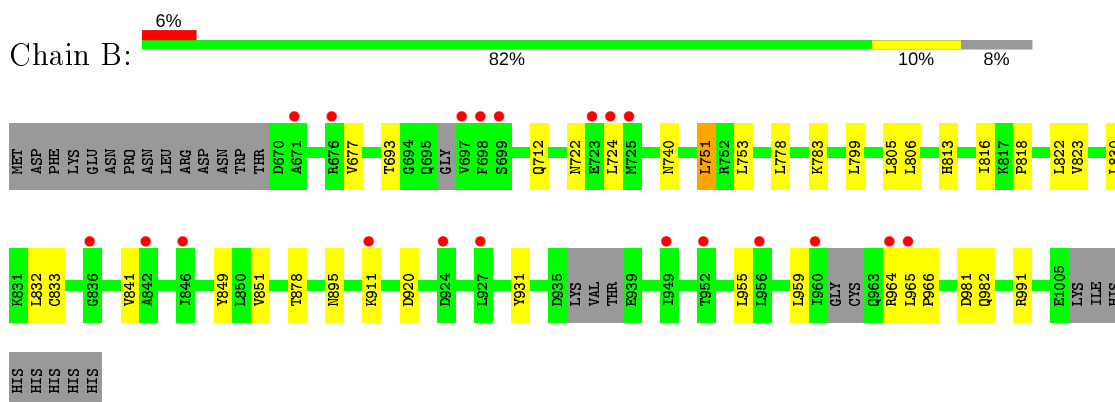
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	52.32Å 52.26Å 78.98Å 104.47° 104.63° 93.01°	Depositor
Resolution (Å)	31.04 – 2.13 31.04 – 2.13	Depositor EDS
% Data completeness (in resolution range)	97.1 (31.04-2.13) 97.3 (31.04-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.14Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.9.1, BUSTER 2.9.1	Depositor
R, R_{free}	0.243 , 0.256 0.250 , 0.266	Depositor DCC
R_{free} test set	2127 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.4	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.449 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5779	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% 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: SO4, ADP, PTR

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	0.39	0/2719	0.61	1/3655 (0.0%)
1	B	0.38	0/2726	0.59	1/3662 (0.0%)
All	All	0.38	0/5445	0.60	2/7317 (0.0%)

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	981	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	981	ASP	CB-CG-OD2	5.17	122.95	118.30

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	2683	0	2728	17	0
1	B	2694	0	2742	11	0
2	A	27	0	12	2	0
2	B	27	0	12	1	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
4	A	185	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	148	0	0	0	0
All	All	5779	0	5494	28	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 3.

All (28) 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:965:LEU:HB3	1:B:966:PRO:HD2	1.55	0.89
1:B:822:LEU:HD11	2:B:1101:ADP:H2'	1.70	0.72
1:B:740:ASN:HD21	1:B:753:LEU:H	1.51	0.58
1:A:720:ARG:HD2	1:A:725:MET:HG3	1.86	0.57
1:B:965:LEU:HB3	1:B:966:PRO:CD	2.33	0.55
1:A:740:ASN:HD21	1:A:753:LEU:H	1.57	0.53
1:A:751:LEU:HD22	1:A:833[B]:CYS:HB2	1.90	0.52
1:B:751:LEU:HG	1:B:833:CYS:SG	2.51	0.51
1:A:675:TYR:HB3	1:A:700:ASN:HD21	1.76	0.50
1:A:977:LYS:HE3	1:A:981:ASP:OD2	2.12	0.50
1:A:675:TYR:HD2	1:A:677:VAL:HG12	1.78	0.47
1:B:955:LEU:O	1:B:959:LEU:HB2	2.14	0.47
1:A:877:CYS:HA	1:A:888:LEU:HD12	1.95	0.47
1:B:806:LEU:HD21	1:B:813:HIS:HB2	1.98	0.45
1:B:816:ILE:HG12	1:B:832[A]:LEU:HD11	1.99	0.45
1:A:822:LEU:HD11	2:A:1101:ADP:H2'	1.99	0.44
1:A:972:LYS:HZ3	1:A:1005:GLU:HA	1.82	0.44
1:B:895:ASN:HD21	1:B:931:TYR:HA	1.83	0.44
1:A:799:LEU:HD23	1:A:875:VAL:HG22	2.00	0.43
1:A:789:ILE:HG12	1:A:972:LYS:HB3	2.01	0.43
1:A:693:THR:HG21	2:A:1101:ADP:H1'	2.01	0.43
1:A:816:ILE:HG12	1:A:832:LEU:HD11	2.01	0.43
1:A:806:LEU:HD21	1:A:813:HIS:HB2	2.01	0.42
1:A:895:ASN:HD21	1:A:931:TYR:HA	1.85	0.42
1:A:695:GLN:HA	1:A:696:GLY:HA2	1.79	0.42
1:B:818:PRO:HD3	1:B:878:THR:HG22	2.02	0.41
1:A:748:PHE:HB3	1:A:805:LEU:HB2	2.03	0.41
1:B:778:LEU:HA	1:B:778:LEU:HD12	1.99	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	322/358 (90%)	296 (92%)	21 (6%)	5 (2%)	9	3
1	B	322/358 (90%)	304 (94%)	15 (5%)	3 (1%)	17	10
All	All	644/716 (90%)	600 (93%)	36 (6%)	8 (1%)	13	6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	677	VAL
1	A	721	ASN
1	A	851	VAL
1	A	942	LYS
1	B	677	VAL
1	B	851	VAL
1	B	964	ARG
1	A	844	ASN

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	293/323 (91%)	274 (94%)	19 (6%)	17	11
1	B	294/323 (91%)	279 (95%)	15 (5%)	24	19
All	All	587/646 (91%)	553 (94%)	34 (6%)	20	15

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	677	VAL
1	A	700	ASN
1	A	712	GLN
1	A	720	ARG
1	A	724	LEU
1	A	799	LEU
1	A	822	LEU
1	A	830	LEU
1	A	831	LYS
1	A	843	ASP
1	A	850	LEU
1	A	888	LEU
1	A	911	LYS
1	A	942	LYS
1	A	944	THR
1	A	955	LEU
1	A	982	GLN
1	A	991	ARG
1	A	996	GLN
1	B	693	THR
1	B	712	GLN
1	B	722	ASN
1	B	724	LEU
1	B	751	LEU
1	B	783	LYS
1	B	799	LEU
1	B	805	LEU
1	B	823	VAL
1	B	830	LEU
1	B	841	VAL
1	B	911	LYS
1	B	920	ASP
1	B	982	GLN
1	B	991	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	700	ASN
1	A	722	ASN
1	A	726	GLN
1	A	740	ASN
1	A	895	ASN

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Mol	Chain	Res	Type
1	A	996	GLN
1	B	722	ASN
1	B	740	ASN
1	B	762	HIS
1	B	895	ASN
1	B	996	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)

2 non-standard protein/DNA/RNA residues 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	#$|Z| > 2$
1	PTR	B	849	1	15,16,17	1.22	2 (13%)	19,22,24	1.18	2 (10%)
1	PTR	A	849	1	15,16,17	1.20	2 (13%)	19,22,24	1.20	2 (10%)

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
1	PTR	B	849	1	-	1/10/11/13	0/1/1/1
1	PTR	A	849	1	-	1/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	849	PTR	P-OH	-2.36	1.55	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	849	PTR	CE2-CZ	2.32	1.43	1.38
1	B	849	PTR	P-OH	-2.32	1.55	1.59
1	A	849	PTR	CE2-CZ	2.31	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	849	PTR	OH-CZ-CE2	2.20	125.77	119.23
1	B	849	PTR	O2P-P-OH	2.12	111.88	105.24
1	B	849	PTR	OH-CZ-CE2	2.09	125.46	119.23
1	A	849	PTR	O2P-P-OH	2.03	111.59	105.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	849	PTR	O-C-CA-CB
1	A	849	PTR	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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
2	ADP	B	1101	-	24,29,29	1.35	3 (12%)	29,45,45	1.41	3 (10%)
2	ADP	A	1101	-	24,29,29	1.37	3 (12%)	29,45,45	1.42	4 (13%)
3	SO4	B	1102	-	4,4,4	0.17	0	6,6,6	0.07	0
3	SO4	A	1102	-	4,4,4	0.16	0	6,6,6	0.05	0
3	SO4	B	1103	-	4,4,4	0.13	0	6,6,6	0.05	0

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	ADP	B	1101	-	-	0/12/32/32	0/3/3/3
2	ADP	A	1101	-	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	ADP	O4'-C1'	3.65	1.46	1.41
2	B	1101	ADP	O4'-C1'	3.49	1.46	1.41
2	A	1101	ADP	PA-O1A	3.13	1.62	1.50
2	B	1101	ADP	PA-O1A	3.08	1.61	1.50
2	A	1101	ADP	PB-O1B	2.66	1.59	1.50
2	B	1101	ADP	PB-O1B	2.65	1.59	1.50

All (7) bond angle outliers are listed below:

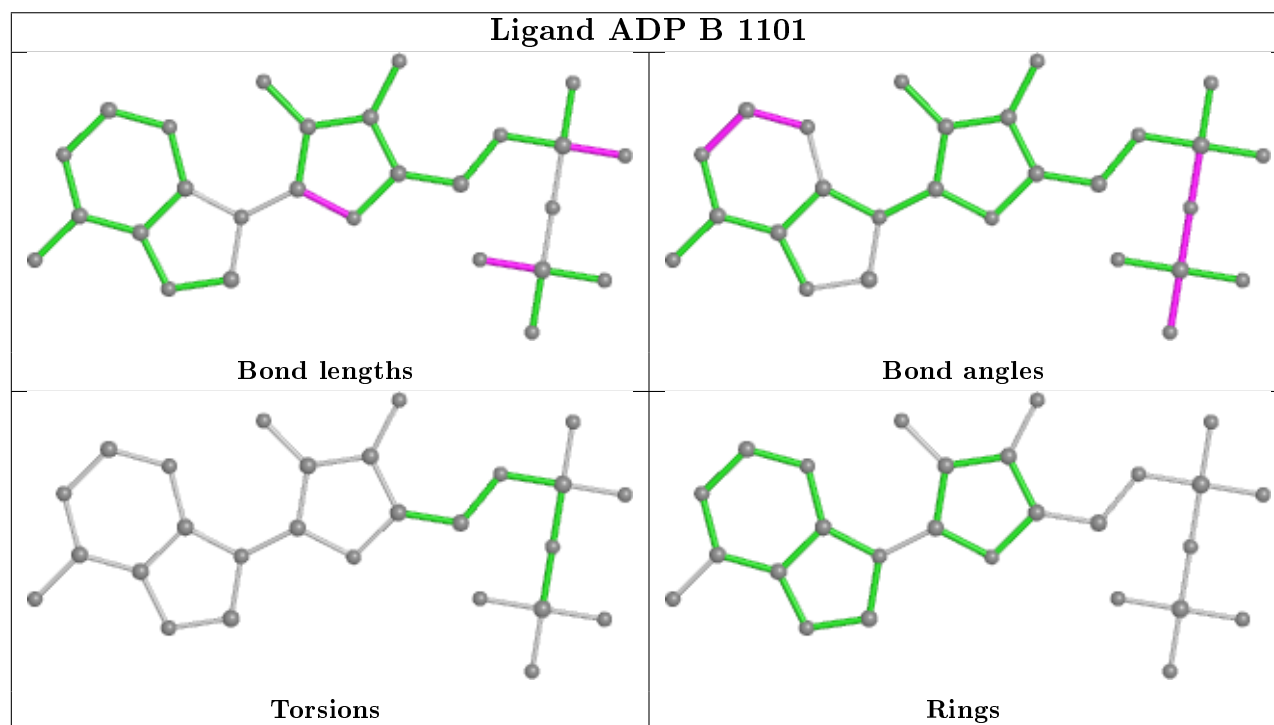| Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	ADP	N3-C2-N1	-4.70	121.33	128.68
2	A	1101	ADP	N3-C2-N1	-4.67	121.37	128.68
2	A	1101	ADP	PA-O3A-PB	-3.46	120.95	132.83
2	B	1101	ADP	PA-O3A-PB	-3.17	121.94	132.83
2	B	1101	ADP	O2B-PB-O3A	2.91	114.38	104.64
2	A	1101	ADP	O2B-PB-O3A	2.86	114.23	104.64
2	A	1101	ADP	C4-C5-N7	-2.01	107.31	109.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	ADP	1	0
2	A	1101	ADP	2	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 ADP B 1101

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 1101

Bond lengths

Bond angles

Torsions

Rings
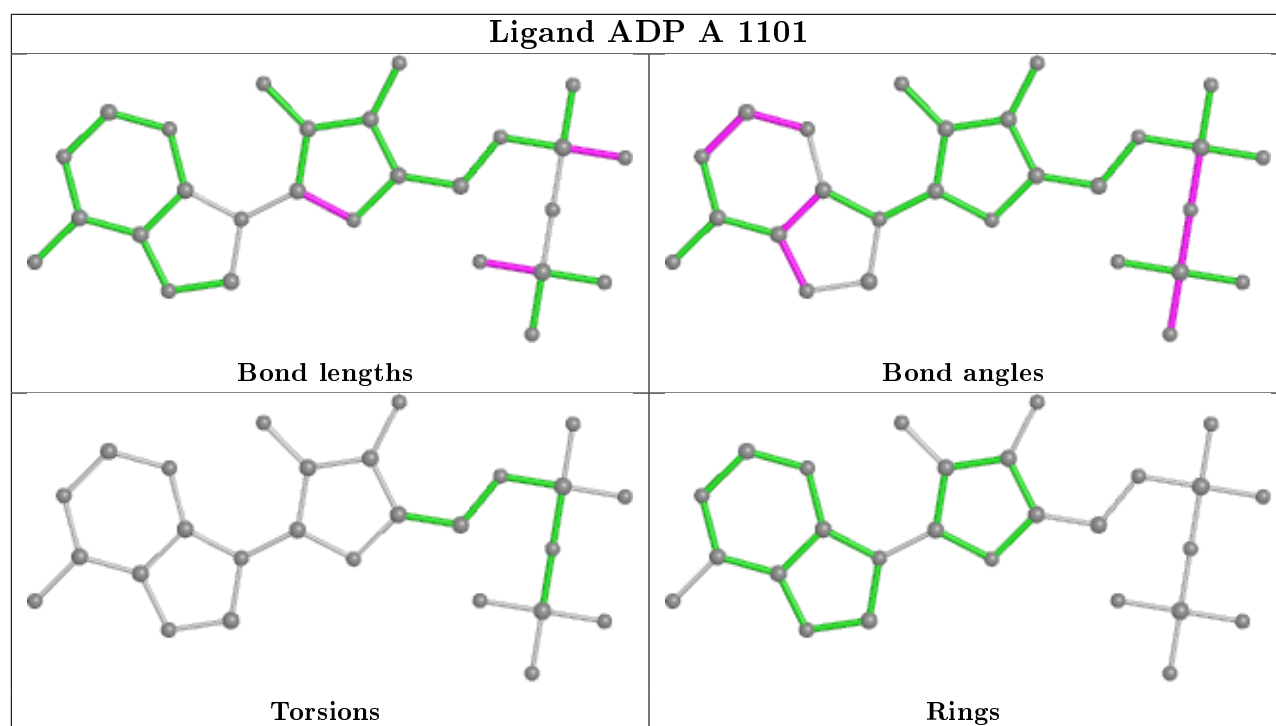
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	327/358 (91%)	0.58	18 (5%)	25	31	28, 47, 77, 95	0
1	B	329/358 (91%)	0.52	20 (6%)	21	26	28, 46, 77, 106	0
All	All	656/716 (91%)	0.55	38 (5%)	23	29	28, 47, 77, 106	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	698	PHE	6.4
1	B	952	THR	5.3
1	B	676	ARG	4.6
1	B	927	LEU	4.5
1	B	964	ARG	3.9
1	A	671	ALA	3.5
1	B	724	LEU	3.5
1	A	846	ILE	3.5
1	A	675	TYR	3.2
1	B	965	LEU	3.2
1	B	671	ALA	3.2
1	A	726	GLN	3.2
1	A	724	LEU	3.1
1	A	960	ILE	3.1
1	A	927	LEU	2.9
1	A	904	LEU	2.9
1	B	846	ILE	2.8
1	B	723	GLU	2.8
1	B	956	LEU	2.7
1	A	918	PHE	2.6
1	B	698	PHE	2.6
1	A	842	ALA	2.5
1	B	725	MET	2.5
1	B	924	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	941	GLU	2.4
1	B	842	ALA	2.4
1	A	697	VAL	2.3
1	A	957	ALA	2.3
1	B	697	VAL	2.3
1	B	960	ILE	2.3
1	A	912	MET	2.3
1	B	699	SER	2.3
1	B	836	GLY	2.3
1	B	949	ILE	2.2
1	B	911	LYS	2.2
1	A	723	GLU	2.2
1	A	843	ASP	2.2
1	A	730	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	PTR	B	849	16/17	0.65	0.22	50,55,60,60	0
1	PTR	A	849	16/17	0.65	0.21	50,55,60,60	0

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.
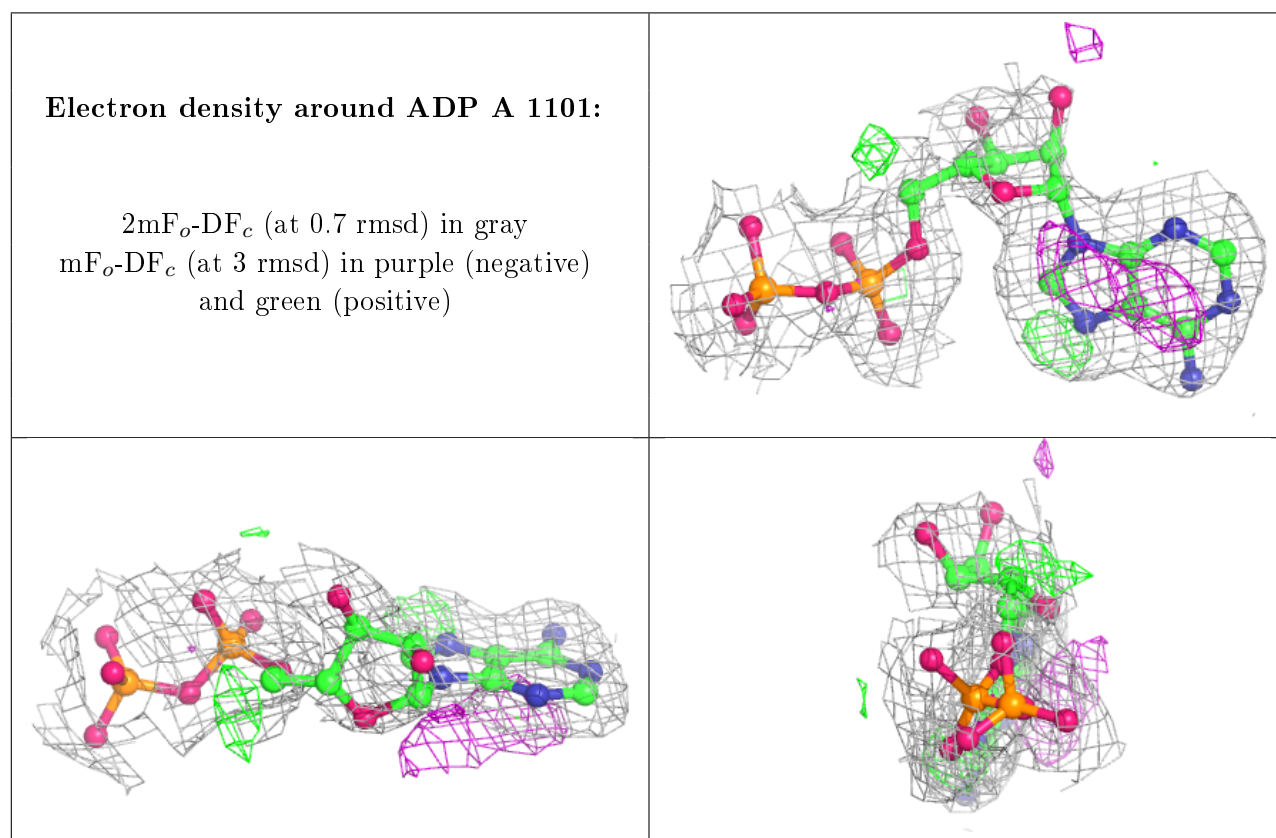
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	A	1101	27/27	0.69	0.22	66,76,82,82	0
2	ADP	B	1101	27/27	0.70	0.24	64,74,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	SO4	B	1103	5/5	0.88	0.13	81,85,86,87	0
3	SO4	B	1102	5/5	0.94	0.14	68,73,73,74	0
3	SO4	A	1102	5/5	0.95	0.13	80,84,85,86	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 ADP A 1101:

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

Electron density around ADP B 1101:

$2mF_o$-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.