



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:20 pm BST

PDB ID : 5XJA
Title : The Crystal Structure of the Minimal Core Domain of the Microtubule Depolymerizer KIF2C Complexed with ADP-Mg-AlF_x
Authors : Ogawa, T.; Jiang, X.; Hirokawa, N.
Deposited on : 2017-04-30
Resolution : 3.43 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

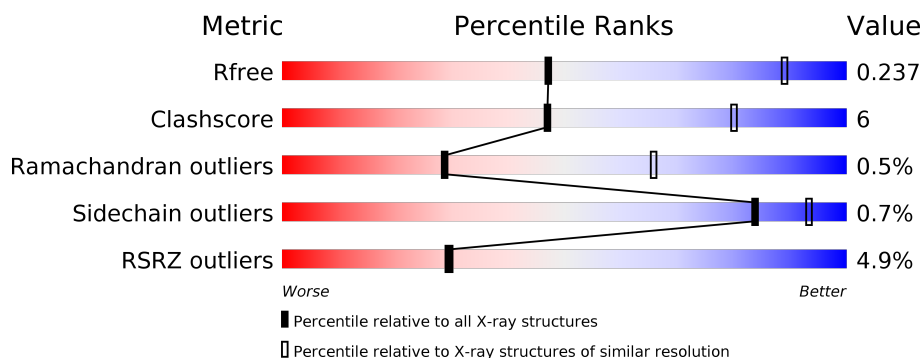
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.43 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	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)

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	426	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>7%</div> <div>21%</div> </div> </div>
1	B	426	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>9%</div> <div>22%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5338 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 Kinesin-like protein KIF2C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2650	1673	465	491	21			
1	B	332	Total	C	N	O	S	0	0	0
			2617	1653	459	484	21			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	MET	-	initiating methionine	UNP Q922S8
A	168	ALA	-	expression tag	UNP Q922S8
A	169	SER	-	expression tag	UNP Q922S8
A	170	MET	-	expression tag	UNP Q922S8
A	171	THR	-	expression tag	UNP Q922S8
A	172	GLY	-	expression tag	UNP Q922S8
A	173	GLY	-	expression tag	UNP Q922S8
A	174	GLN	-	expression tag	UNP Q922S8
A	175	GLN	-	expression tag	UNP Q922S8
A	176	MET	-	expression tag	UNP Q922S8
A	177	GLY	-	expression tag	UNP Q922S8
A	178	ARG	-	expression tag	UNP Q922S8
A	179	ASP	-	expression tag	UNP Q922S8
A	180	PRO	-	expression tag	UNP Q922S8
A	181	ASN	-	expression tag	UNP Q922S8
A	182	SER	-	expression tag	UNP Q922S8
A	586	HIS	-	expression tag	UNP Q922S8
A	587	HIS	-	expression tag	UNP Q922S8
A	588	HIS	-	expression tag	UNP Q922S8
A	589	HIS	-	expression tag	UNP Q922S8
A	590	HIS	-	expression tag	UNP Q922S8
A	591	HIS	-	expression tag	UNP Q922S8
A	592	HIS	-	expression tag	UNP Q922S8
B	167	MET	-	initiating methionine	UNP Q922S8
B	168	ALA	-	expression tag	UNP Q922S8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	169	SER	-	expression tag	UNP Q922S8
B	170	MET	-	expression tag	UNP Q922S8
B	171	THR	-	expression tag	UNP Q922S8
B	172	GLY	-	expression tag	UNP Q922S8
B	173	GLY	-	expression tag	UNP Q922S8
B	174	GLN	-	expression tag	UNP Q922S8
B	175	GLN	-	expression tag	UNP Q922S8
B	176	MET	-	expression tag	UNP Q922S8
B	177	GLY	-	expression tag	UNP Q922S8
B	178	ARG	-	expression tag	UNP Q922S8
B	179	ASP	-	expression tag	UNP Q922S8
B	180	PRO	-	expression tag	UNP Q922S8
B	181	ASN	-	expression tag	UNP Q922S8
B	182	SER	-	expression tag	UNP Q922S8
B	586	HIS	-	expression tag	UNP Q922S8
B	587	HIS	-	expression tag	UNP Q922S8
B	588	HIS	-	expression tag	UNP Q922S8
B	589	HIS	-	expression tag	UNP Q922S8
B	590	HIS	-	expression tag	UNP Q922S8
B	591	HIS	-	expression tag	UNP Q922S8
B	592	HIS	-	expression tag	UNP Q922S8

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

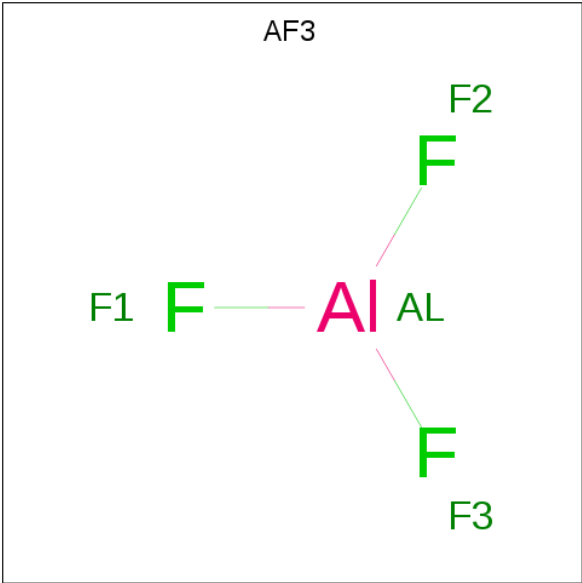
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Al	F	0	0
			4	1	3		
4	B	1	Total	Al	F	0	0
			4	1	3		

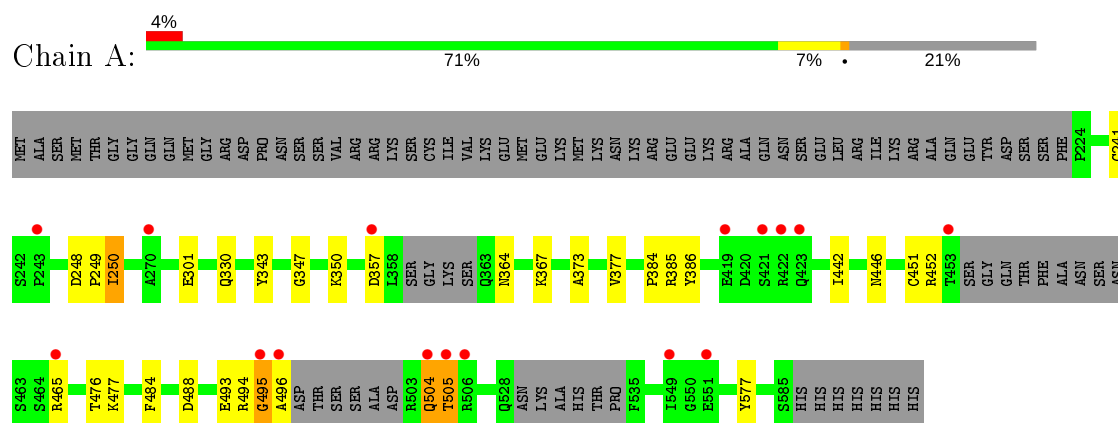
- Molecule 5 is water.

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

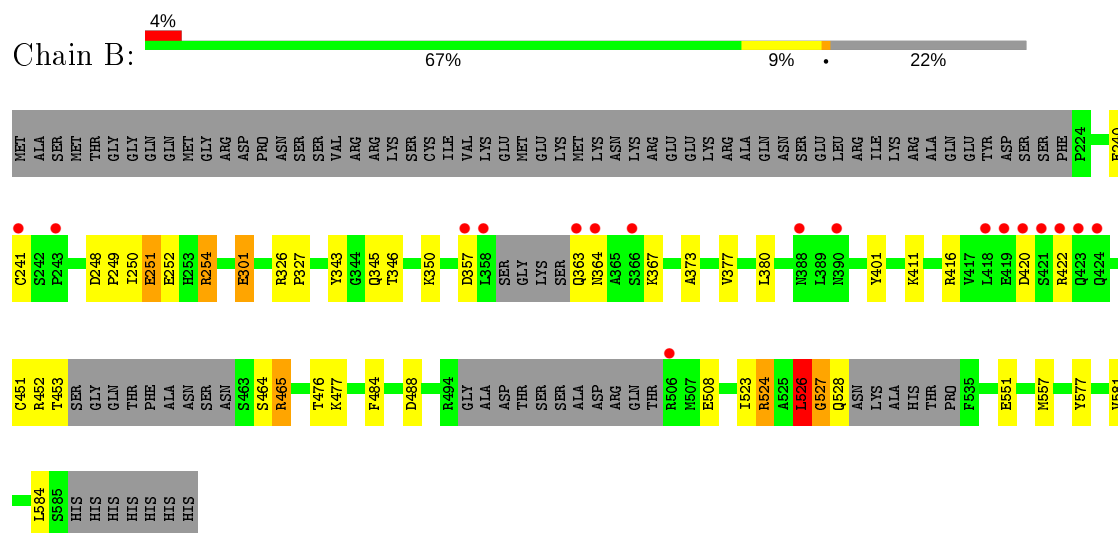
3 Residue-property plots [i](#)

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: Kinesin-like protein KIF2C



• Molecule 1: Kinesin-like protein KIF2C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.10 Å 166.99 Å 74.99 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.43 29.88 – 3.43	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-3.43) 100.0 (29.88-3.43)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.47 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.198 , 0.230 0.201 , 0.237	Depositor DCC
R_{free} test set	846 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5338	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, AF3

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	0.76	3/2688 (0.1%)	1.00	8/3611 (0.2%)
1	B	0.72	2/2655 (0.1%)	0.95	8/3566 (0.2%)
All	All	0.74	5/5343 (0.1%)	0.98	16/7177 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	504	GLN	C-O	6.96	1.36	1.23
1	A	465	ARG	CZ-NH1	5.88	1.40	1.33
1	A	465	ARG	CZ-NH2	5.64	1.40	1.33
1	B	465	ARG	CZ-NH2	5.30	1.40	1.33
1	B	465	ARG	CZ-NH1	5.13	1.39	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	THR	CB-CA-C	-12.64	77.48	111.60
1	A	505	THR	N-CA-C	8.64	134.34	111.00
1	B	252	GLU	N-CA-C	8.35	133.53	111.00
1	A	504	GLN	CB-CA-C	-8.25	93.90	110.40
1	B	488	ASP	CB-CG-OD1	8.24	125.72	118.30
1	A	495	GLY	N-CA-C	-7.98	93.14	113.10
1	A	488	ASP	CB-CG-OD1	7.54	125.08	118.30
1	A	505	THR	C-N-CA	6.33	137.53	121.70
1	B	254	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	B	524	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	B	464	SER	CB-CA-C	-5.52	99.61	110.10
1	A	241	CYS	N-CA-C	5.47	125.77	111.00
1	B	527	GLY	N-CA-C	-5.37	99.67	113.10
1	A	488	ASP	CB-CG-OD2	-5.34	113.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	GLU	CB-CA-C	-5.17	100.07	110.40
1	B	416	ARG	NE-CZ-NH1	5.11	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2650	0	2673	39	1
1	B	2617	0	2638	33	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	2	0
3	B	27	0	12	1	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	4	0	0	0	0
5	B	3	0	0	0	0
All	All	5338	0	5335	66	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 6.

All (66) 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:505:THR:HG22	1:A:505:THR:O	1.33	1.10
1:A:504:GLN:O	1:A:505:THR:OG1	1.74	1.05
1:A:505:THR:CG2	1:A:505:THR:O	2.09	0.97
1:A:249:PRO:CB	1:A:250:ILE:HD12	2.04	0.86
1:A:357:ASP:HB2	1:A:367:LYS:HD3	1.57	0.86
1:A:250:ILE:HG23	1:B:380:LEU:CD1	2.09	0.82
1:A:249:PRO:HG2	1:A:250:ILE:HD12	1.63	0.81
1:A:249:PRO:CG	1:A:250:ILE:HD12	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:PRO:HB2	1:A:250:ILE:HD12	1.63	0.79
1:A:494:ARG:C	1:A:496:ALA:H	1.86	0.78
1:A:249:PRO:HG2	1:A:250:ILE:CD1	2.14	0.78
1:A:249:PRO:C	1:A:250:ILE:HD12	2.04	0.77
1:B:251:GLU:O	1:B:251:GLU:HG3	1.85	0.76
1:B:452:ARG:O	1:B:453:THR:OG1	2.09	0.70
1:A:248:ASP:OD1	1:A:249:PRO:HD2	1.91	0.70
1:A:250:ILE:O	1:A:250:ILE:HG22	1.92	0.70
1:A:249:PRO:HB2	1:A:250:ILE:CD1	2.24	0.68
1:B:364:ASN:HD22	1:B:367:LYS:HB2	1.59	0.68
1:B:364:ASN:ND2	1:B:367:LYS:HB2	2.12	0.64
1:B:357:ASP:O	1:B:363:GLN:N	2.32	0.62
1:A:350:LYS:N	3:A:602:ADP:O2B	2.32	0.62
1:A:493:GLU:O	1:A:493:GLU:HG2	2.00	0.61
1:A:367:LYS:HG2	1:A:367:LYS:O	2.00	0.61
1:A:250:ILE:HG23	1:B:380:LEU:HD13	1.84	0.60
1:A:384:PRO:HG2	1:B:254:ARG:NH1	2.17	0.59
1:A:504:GLN:C	1:A:505:THR:HG1	2.01	0.59
1:A:494:ARG:C	1:A:496:ALA:N	2.50	0.58
1:B:254:ARG:NH2	1:B:551:GLU:O	2.35	0.57
1:B:420:ASP:OD1	1:B:422:ARG:N	2.38	0.56
1:B:527:GLY:O	1:B:528:GLN:CB	2.52	0.56
1:B:527:GLY:O	1:B:584:LEU:HD21	2.07	0.55
1:B:357:ASP:HB3	1:B:364:ASN:HB3	1.88	0.55
1:A:504:GLN:O	1:A:505:THR:CB	2.55	0.54
1:A:495:GLY:O	1:A:496:ALA:HB3	2.09	0.53
1:A:452:ARG:O	1:A:452:ARG:HG2	2.10	0.51
1:B:557:MET:HE3	1:B:581:VAL:HG11	1.93	0.51
1:A:330:GLN:OE1	1:B:249:PRO:HB2	2.11	0.50
1:A:249:PRO:O	1:A:250:ILE:HD12	2.10	0.49
1:B:326:ARG:HB3	1:B:327:PRO:HD3	1.94	0.49
1:B:465:ARG:HD3	1:B:508:GLU:OE2	2.13	0.49
1:A:250:ILE:HA	1:B:380:LEU:HD11	1.95	0.48
1:A:347:GLY:N	3:A:602:ADP:O3B	2.47	0.48
1:B:350:LYS:NZ	3:B:602:ADP:O1B	2.41	0.47
1:B:411:LYS:HA	1:B:451:CYS:SG	2.55	0.47
1:A:343:TYR:CZ	1:A:577:TYR:CD2	3.04	0.46
1:A:442:ILE:O	1:A:446:ASN:ND2	2.49	0.45
1:A:250:ILE:HG23	1:B:380:LEU:HD11	1.92	0.45
1:B:373:ALA:O	1:B:377:VAL:HG23	2.17	0.45
1:B:401:TYR:C	1:B:401:TYR:CD2	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ASP:CG	1:B:248:ASP:O	2.54	0.44
1:A:364:ASN:ND2	1:A:367:LYS:HB2	2.32	0.44
1:B:345:GLN:HG2	1:B:346:THR:O	2.18	0.44
1:A:373:ALA:O	1:A:377:VAL:HG23	2.17	0.43
1:A:249:PRO:O	1:A:250:ILE:HB	2.18	0.42
1:A:476:THR:HG23	1:A:477:LYS:N	2.34	0.42
1:B:523:ILE:O	1:B:526:LEU:HB3	2.20	0.42
1:B:343:TYR:CZ	1:B:577:TYR:CD2	3.07	0.42
1:B:526:LEU:HB3	1:B:527:GLY:H	1.75	0.42
1:A:451:CYS:O	1:A:451:CYS:SG	2.78	0.41
1:B:240:GLU:HG3	1:B:241:CYS:N	2.35	0.41
1:B:524:ARG:O	1:B:584:LEU:HD23	2.20	0.41
1:B:357:ASP:HB3	1:B:364:ASN:CB	2.51	0.41
1:B:251:GLU:O	1:B:251:GLU:CG	2.64	0.41
1:A:249:PRO:CG	1:A:250:ILE:CD1	2.85	0.41
1:A:385:ARG:HD2	1:A:386:TYR:CE1	2.55	0.41
1:B:476:THR:HG23	1:B:477:LYS:N	2.36	0.41

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)
1:A:301:GLU:OE2	1:A:301:GLU:OE2[2_655]	1.47	0.73
1:B:301:GLU:OE2	1:B:301:GLU:OE2[2_655]	1.95	0.25

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	327/426 (77%)	294 (90%)	32 (10%)	1 (0%)	41	75
1	B	322/426 (76%)	293 (91%)	27 (8%)	2 (1%)	25	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	649/852 (76%)	587 (90%)	59 (9%)	3 (0%)	29 66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	250	ILE
1	B	526	LEU
1	A	250	ILE

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	290/374 (78%)	289 (100%)	1 (0%)	92 98
1	B	287/374 (77%)	284 (99%)	3 (1%)	76 89
All	All	577/748 (77%)	573 (99%)	4 (1%)	84 93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	484	PHE
1	B	301	GLU
1	B	484	PHE
1	B	526	LEU

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

Mol	Chain	Res	Type
1	A	253	HIS
1	A	364	ASN
1	A	390	ASN
1	A	402	ASN
1	A	471	GLN
1	B	364	ASN

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Mol	Chain	Res	Type
1	B	467	HIS

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 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	$\# Z > 2$
4	AF3	B	603	-	0,3,3	0.00	-	-		
4	AF3	A	603	-	0,3,3	0.00	-	-		
3	ADP	B	602	2	24,29,29	1.06	2 (8%)	29,45,45	1.99	9 (31%)
3	ADP	A	602	2	24,29,29	1.07	1 (4%)	29,45,45	1.32	2 (6%)

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	ADP	B	602	2	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	602	2	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	ADP	C5-C4	2.42	1.47	1.40
3	A	602	ADP	C5-C4	2.40	1.47	1.40
3	B	602	ADP	O4'-C1'	2.10	1.44	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	ADP	PA-O3A-PB	-4.91	115.97	132.83
3	B	602	ADP	O3B-PB-O2B	3.90	122.53	107.64
3	B	602	ADP	N3-C2-N1	-3.85	122.66	128.68
3	B	602	ADP	C5'-C4'-C3'	-2.98	104.02	115.18
3	B	602	ADP	O2A-PA-O1A	2.94	126.77	112.24
3	A	602	ADP	N3-C2-N1	-2.87	124.20	128.68
3	B	602	ADP	O5'-PA-O1A	-2.80	98.11	109.07
3	A	602	ADP	N6-C6-N1	2.78	124.34	118.57
3	B	602	ADP	O2'-C2'-C1'	2.39	119.68	110.85
3	B	602	ADP	C2-N1-C6	2.35	122.77	118.75
3	B	602	ADP	PA-O5'-C5'	-2.29	108.25	121.68

There are no chirality outliers.

There are no torsion outliers.

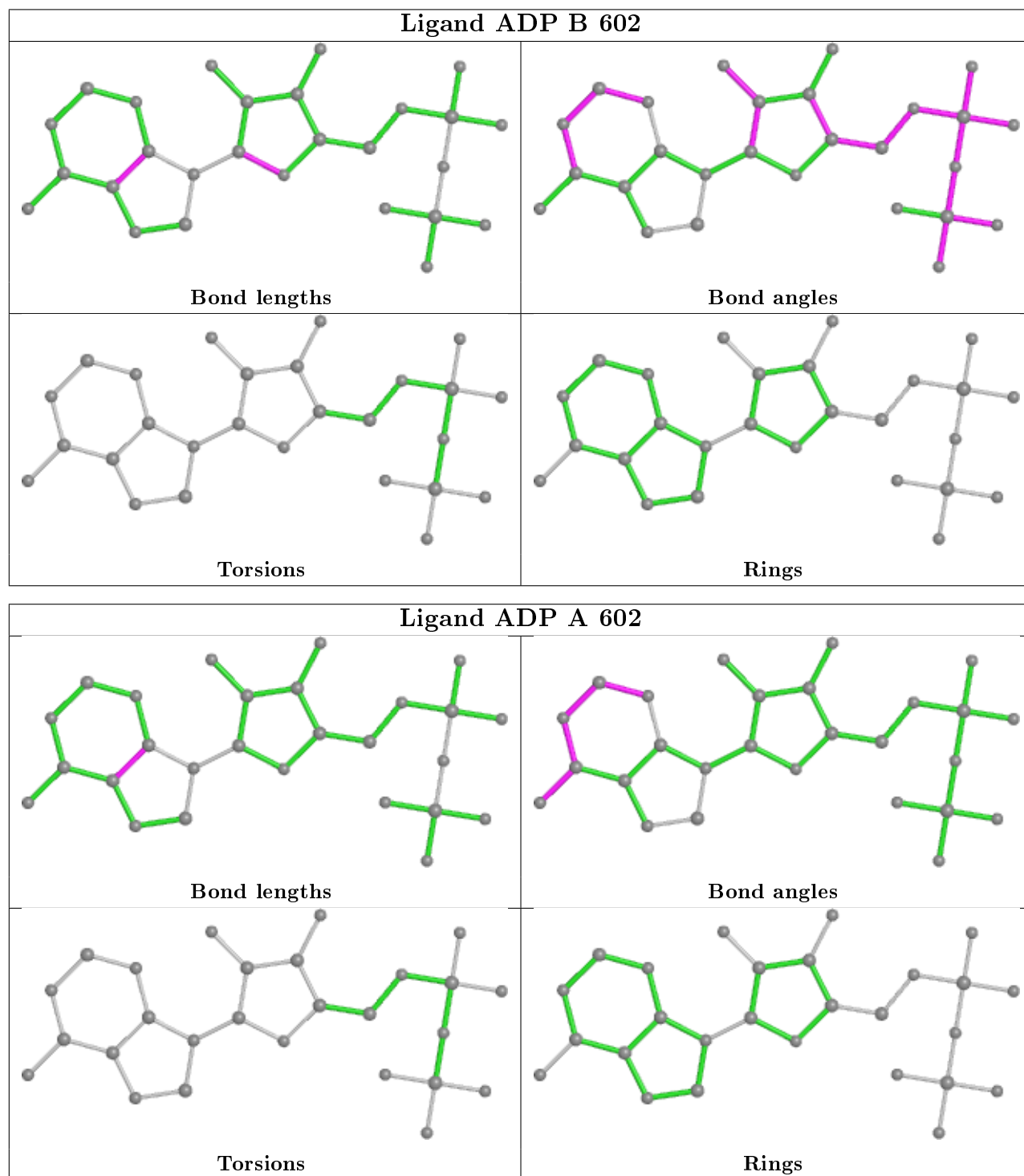
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	ADP	1	0
3	A	602	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 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	337/426 (79%)	-0.03	16 (4%) 31 31	30, 61, 108, 136	0
1	B	332/426 (77%)	-0.03	17 (5%) 28 28	35, 64, 110, 140	0
All	All	669/852 (78%)	-0.03	33 (4%) 29 30	30, 63, 110, 140	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	SER	5.3
1	B	364	ASN	4.3
1	A	504	GLN	3.5
1	A	505	THR	3.3
1	A	421	SER	3.3
1	B	423	GLN	3.1
1	B	388	ASN	3.0
1	B	358	LEU	3.0
1	A	495	GLY	2.9
1	A	549	ILE	2.8
1	A	357	ASP	2.8
1	A	243	PRO	2.8
1	A	423	GLN	2.8
1	B	506	ARG	2.7
1	B	418	LEU	2.7
1	B	363	GLN	2.6
1	B	420	ASP	2.6
1	B	241	CYS	2.4
1	B	366	SER	2.4
1	A	453	THR	2.4
1	B	357	ASP	2.4
1	A	270	ALA	2.3
1	A	506	ARG	2.3
1	A	496	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	551	GLU	2.2
1	B	424	GLN	2.1
1	B	243	PRO	2.1
1	A	419	GLU	2.1
1	A	465	ARG	2.1
1	B	390	ASN	2.1
1	A	422	ARG	2.1
1	B	419	GLU	2.0
1	B	422	ARG	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](#)

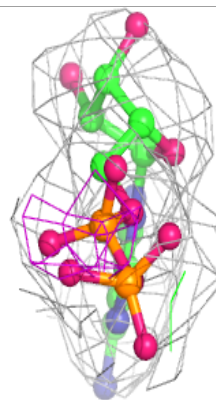
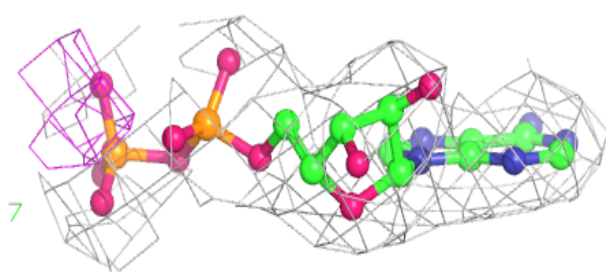
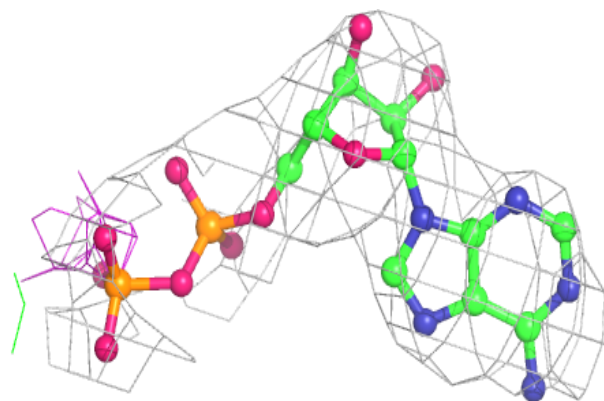
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	AF3	B	603	4/4	0.94	0.23	33,34,34,35	0
4	AF3	A	603	4/4	0.94	0.24	32,32,34,36	0
3	ADP	B	602	27/27	0.97	0.13	39,47,64,72	0
2	MG	A	601	1/1	0.97	0.12	123,123,123,123	0
3	ADP	A	602	27/27	0.97	0.12	46,53,58,66	0
2	MG	B	601	1/1	0.98	0.11	58,58,58,58	0

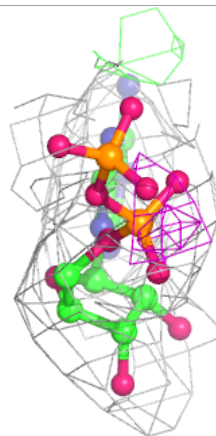
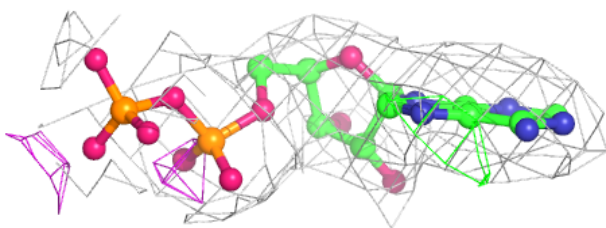
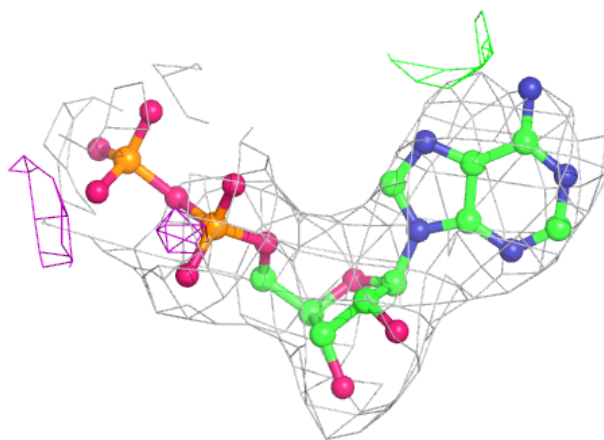
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP B 602:

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

**Electron density around ADP A 602:**

$2mF_o-DF_c$ (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.