



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 07:11 am BST

PDB ID : 4FRZ
Title : Arabidopsis KCBP motor domain dimerized via regulatory domain
Authors : Vinogradova, M.
Deposited on : 2012-06-26
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

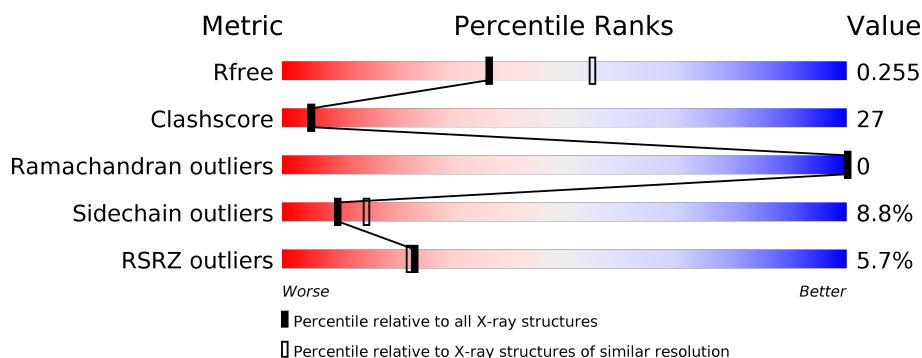
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	386	
1	B	386	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IMD	A	1304	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5831 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 calmodulin-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2840	1776	501	550	13			
1	B	349	Total	C	N	O	S	0	0	0
			2805	1761	492	540	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1131	ASN	CYS	ENGINEERED MUTATION	UNP Q9FHN8
B	1131	ASN	CYS	ENGINEERED MUTATION	UNP Q9FHN8

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

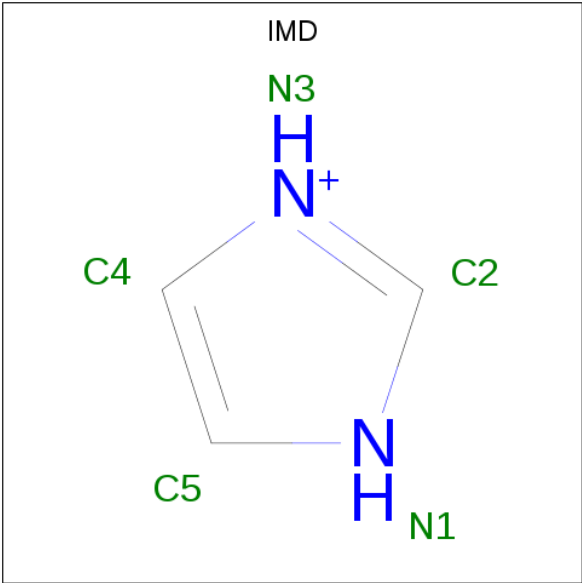
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

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



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

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	A	1	Total	C	N	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

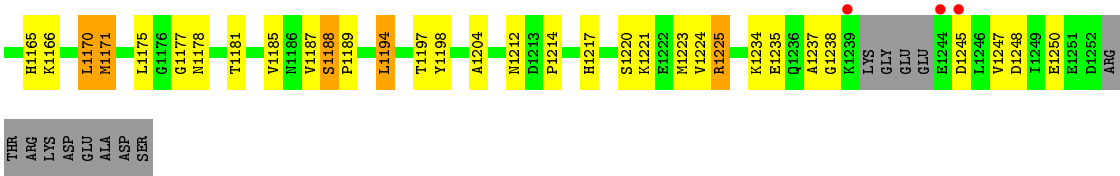
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total	O	0	0
			54	54		
6	B	44	Total	O	0	0
			44	44		

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 ($\text{RSRZ} > 2$). 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.

- [illegible]

- Chain B:
-
- 4% 56% 30% 10%
- ARG K377 E384 E385 M386 K387 I390 R391 V392 R397 P398 K902 E906 R907 Q910 M911 L912 H922 P923 W924 K925 D926 D927 R928 R929 K930 Q931 R932 R936 N940 R941 Q944 D945 D946 I947 F948 E949 D950 T951 K952 Y953 L954 A958 V959 F967 F978 H983 N986 T994 K995 L1001 R1007 F1008 S1009 F1010 M1011 L1012 V1017 E1018 L1019 Y1020 Q1021 D1022 T1023 L1024 Y1025 L1026 L1027 L1028 L1029 P1030 K1031 L1032 A1033 R1034 R1035 L1036 K1037 L1038 E1039 I1040 K1041 K1042 V1050 E1051 A1052 N1053 L1056 T1057 P1058 T1060 S1069 L1081 E1082 L1083 L1084 R1085 E1088 Q1103 T1104 Q1105 S1106 R1109 G1110 V1115 D1116 L1117 A1118 E1121 R1122 VAL LYS LYS SER GLY SER ALA GLY ASN GLN LEU LYS GLU GLN SER I1139 N1140 L1143 L1146 L1148



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.71Å 75.07Å 120.60Å 90.00° 91.45° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40 24.50 – 2.39	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.40) 91.6 (24.50-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , (Not available) 0.220 , 0.255	Depositor DCC
R_{free} test set	2948 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5831	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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, IMD, ADP, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	1/2881 (0.0%)	0.78	3/3869 (0.1%)
1	B	0.54	0/2846	0.79	2/3822 (0.1%)
All	All	0.54	1/5727 (0.0%)	0.78	5/7691 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	924	TRP	C-N	5.68	1.47	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	923	PRO	N-CA-CB	5.86	110.33	103.30
1	A	1229	LEU	CA-CB-CG	-5.77	102.02	115.30
1	B	1033	ALA	CB-CA-C	5.59	118.49	110.10
1	A	928	LYS	N-CA-C	-5.54	96.03	111.00
1	A	923	PRO	N-CA-CB	5.03	109.34	103.30

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	2840	0	2862	153	0
1	B	2805	0	2826	157	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	15	0	15	9	0
4	B	5	0	5	0	0
5	A	4	0	6	0	0
5	B	8	0	12	3	0
6	A	54	0	0	2	0
6	B	44	0	0	4	0
All	All	5831	0	5750	307	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 27.

The worst 5 of 307 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:1234:LYS:HD3	1:A:1241:GLY:CA	1.38	1.48
1:A:1234:LYS:CD	1:A:1241:GLY:HA2	1.43	1.43
1:B:1024:LEU:HD22	1:B:1038:LEU:CD1	1.73	1.19
1:A:1047:MET:CE	4:A:1304:IMD:H4	1.78	1.13
1:B:1024:LEU:CD2	1:B:1038:LEU:CD1	2.32	1.06

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	352/386 (91%)	339 (96%)	13 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	341/386 (88%)	330 (97%)	11 (3%)	0	100	100
All	All	693/772 (90%)	669 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	319/346 (92%)	286 (90%)	33 (10%)	7	10
1	B	315/346 (91%)	292 (93%)	23 (7%)	14	22
All	All	634/692 (92%)	578 (91%)	56 (9%)	10	15

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1174	SER
1	A	1244	GLU
1	B	1188	SER
1	A	1194	LEU
1	A	1228	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1157	ASN
1	A	1193	ASN
1	B	1103	GLN
1	A	1103	GLN
1	B	1157	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	IMD	B	1303	-	3,5,5	0.35	0	4,5,5	0.60	0
4	IMD	A	1303	-	3,5,5	0.42	0	4,5,5	0.59	0
3	ADP	B	1302	2	24,29,29	1.06	1 (4%)	29,45,45	1.59	5 (17%)
5	EDO	B	1304	-	3,3,3	0.46	0	2,2,2	0.10	0
5	EDO	A	1306	-	3,3,3	0.86	0	2,2,2	0.38	0
5	EDO	B	1305	-	3,3,3	0.38	0	2,2,2	0.37	0
3	ADP	A	1302	2	24,29,29	1.06	2 (8%)	29,45,45	1.51	5 (17%)
4	IMD	A	1305	-	3,5,5	0.44	0	4,5,5	0.60	0
4	IMD	A	1304	-	3,5,5	0.75	0	4,5,5	0.47	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
4	IMD	B	1303	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IMD	A	1303	-	-	-	0/1/1/1
3	ADP	B	1302	2	-	2/12/32/32	0/3/3/3
5	EDO	B	1304	-	-	0/1/1/1	-
5	EDO	A	1306	-	-	0/1/1/1	-
5	EDO	B	1305	-	-	0/1/1/1	-
3	ADP	A	1302	2	-	2/12/32/32	0/3/3/3
4	IMD	A	1305	-	-	-	0/1/1/1
4	IMD	A	1304	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	ADP	C2-N1	3.47	1.40	1.33
3	B	1302	ADP	C2-N1	3.40	1.40	1.33
3	A	1302	ADP	C2-N3	2.08	1.35	1.32

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1302	ADP	C5-C6-N6	3.97	126.39	120.35
3	A	1302	ADP	C5-C6-N6	3.58	125.79	120.35
3	B	1302	ADP	C3'-C2'-C1'	3.51	106.26	100.98
3	B	1302	ADP	N3-C2-N1	-3.44	123.31	128.68
3	A	1302	ADP	N3-C2-N1	-3.35	123.45	128.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1302	ADP	PA-O3A-PB-O3B
3	A	1302	ADP	PA-O3A-PB-O3B
3	B	1302	ADP	PA-O3A-PB-O2B
3	A	1302	ADP	PA-O3A-PB-O2B

There are no ring outliers.

5 monomers are involved in 12 short contacts:

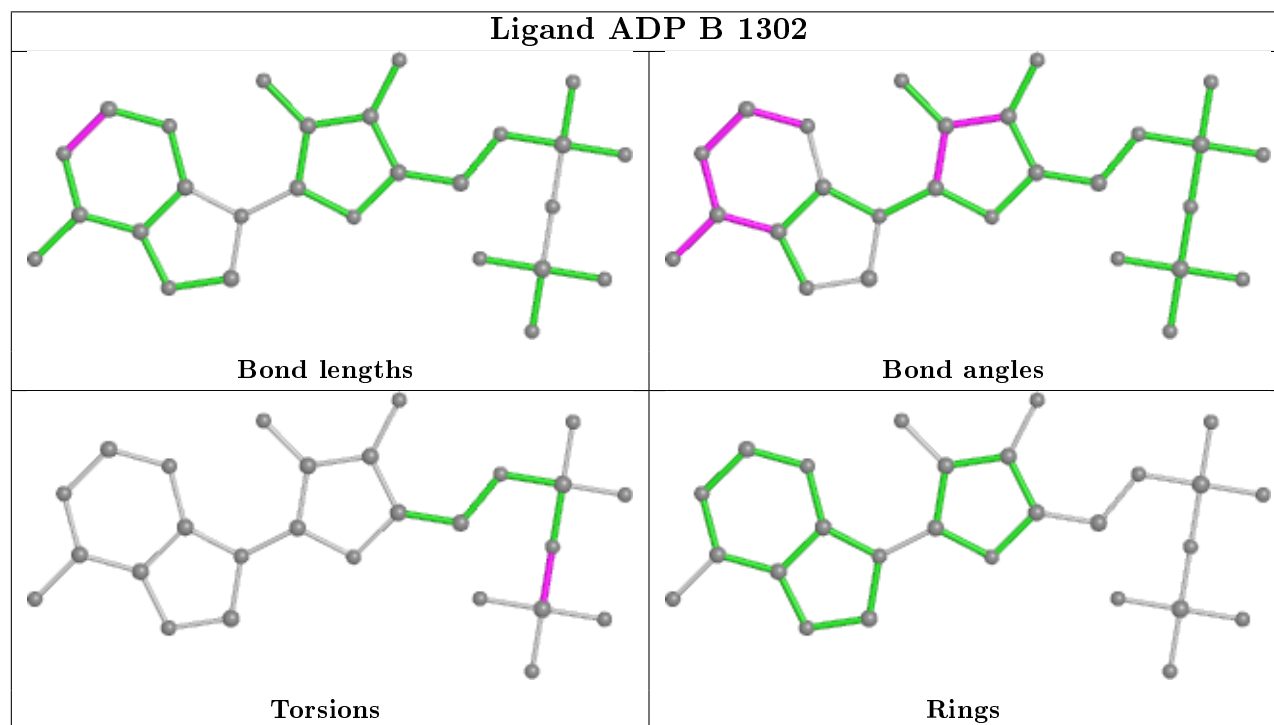
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1303	IMD	1	0
5	B	1304	EDO	2	0

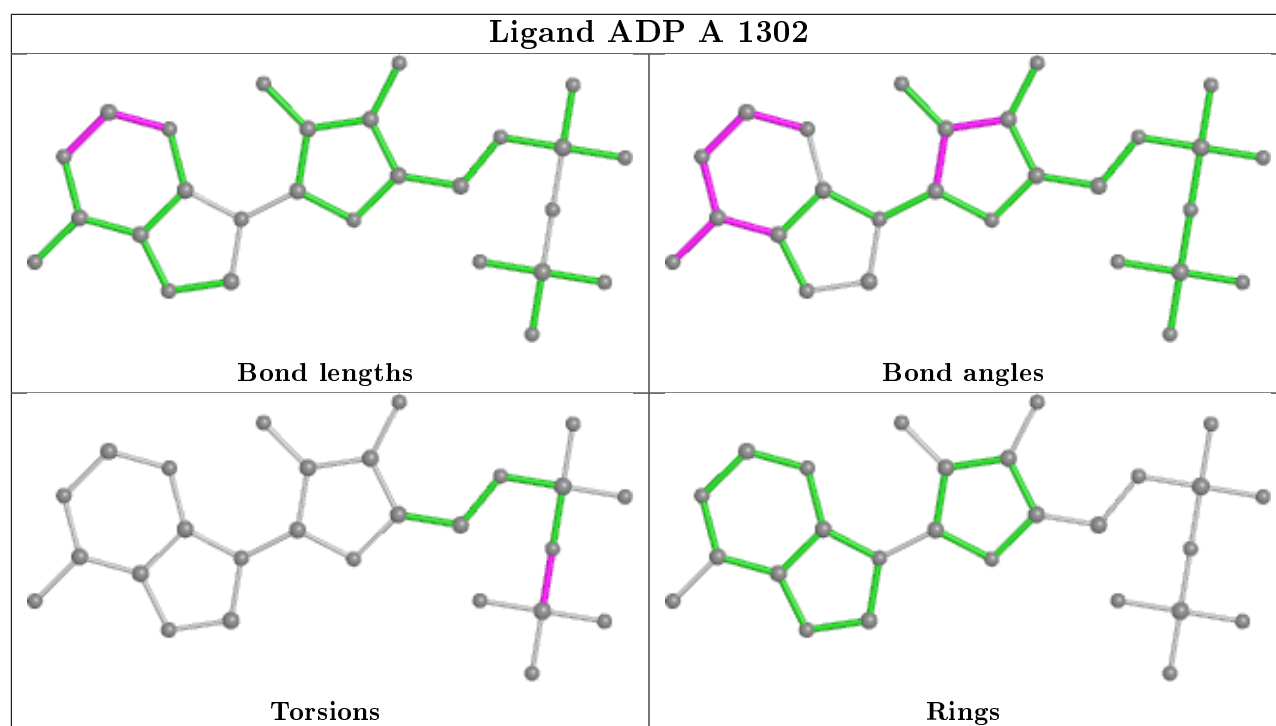
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1305	EDO	1	0
4	A	1305	IMD	2	0
4	A	1304	IMD	6	0

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 [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(Å ²)	Q<0.9
1	A	356/386 (92%)	0.09	24 (6%) 17 16	9, 34, 70, 85	0
1	B	349/386 (90%)	0.01	16 (4%) 32 31	13, 33, 62, 84	0
All	All	705/772 (91%)	0.05	40 (5%) 23 22	9, 34, 67, 85	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1241	GLY	11.8
1	B	1033	ALA	6.0
1	A	1139	ILE	5.0
1	A	1123	VAL	4.8
1	A	1242	GLU	4.6

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](#)

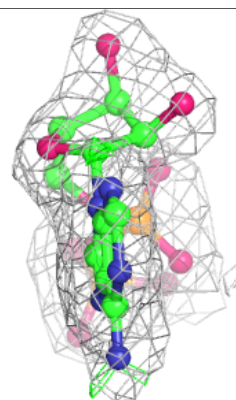
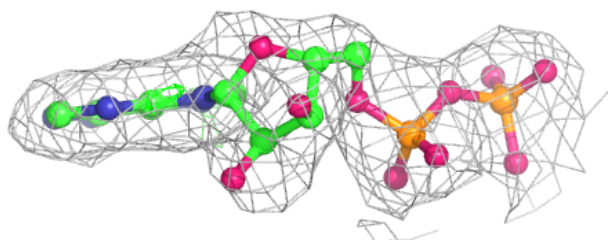
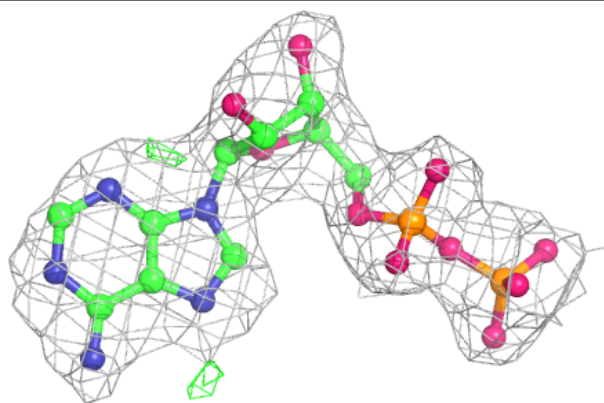
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	IMD	A	1304	5/5	0.83	0.24	57,58,61,62	0
5	EDO	B	1304	4/4	0.84	0.21	44,47,49,52	0
2	MG	A	1301	1/1	0.86	0.12	25,25,25,25	0
5	EDO	A	1306	4/4	0.89	0.19	43,47,51,53	0
5	EDO	B	1305	4/4	0.90	0.22	32,35,44,46	0
4	IMD	A	1305	5/5	0.91	0.20	65,66,66,69	0
4	IMD	A	1303	5/5	0.91	0.24	53,54,57,58	0
2	MG	B	1301	1/1	0.95	0.11	30,30,30,30	0
3	ADP	A	1302	27/27	0.97	0.12	21,29,35,40	0
3	ADP	B	1302	27/27	0.97	0.12	21,37,46,51	0
4	IMD	B	1303	5/5	0.97	0.15	35,35,38,39	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.

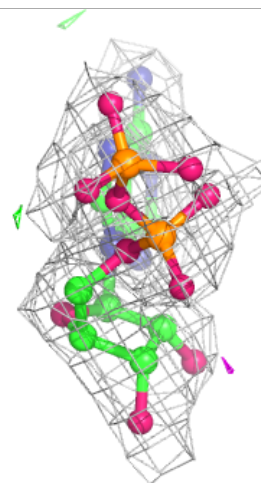
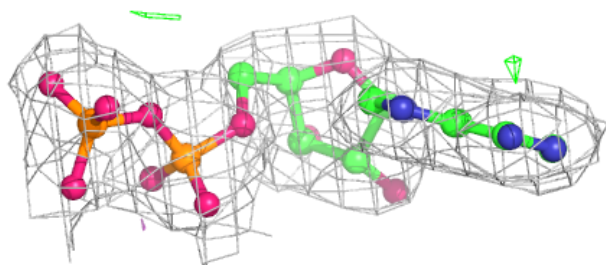
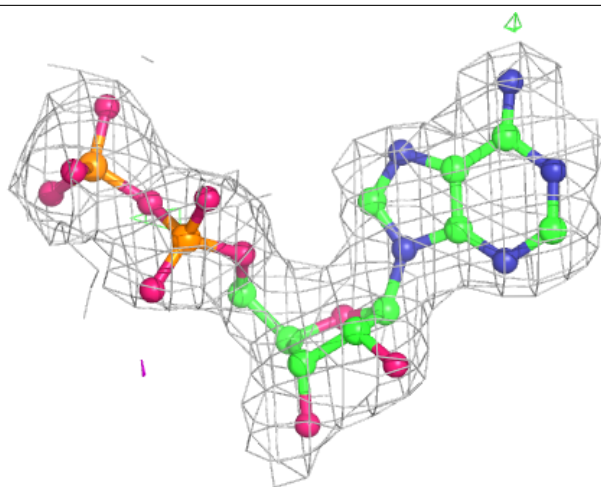
Electron density around ADP A 1302:

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 B 1302:

$2mF_o-DF_c$ (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.