Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:25 am BST

PDB ID	:	5M7P
Title	:	Crystal structure of NtrX from Brucella abortus in complex with ADP processed with the CrystalDirect automated mounting and cryo-cooling technology
Authors	:	Cornaciu, I.; Fernandez, I.; Hoffmann, G.; Carrica, M.C.; Goldbaum, F.A.; Marquez, J.A.
Deposited on	:	2016-10-28
Resolution	:	2.36 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:

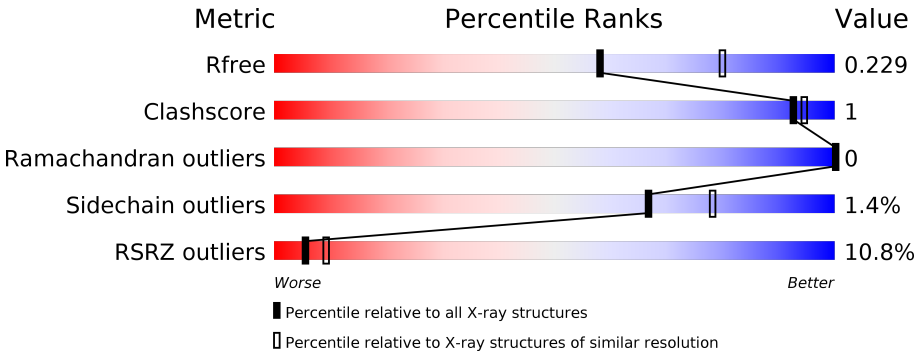
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	454	6% 93%
1	B	454	15% 91% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7042 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 Nitrogen assimilation regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3352	2103	609	628	12			
1	B	437	Total	C	N	O	S	0	0	0
			3341	2094	610	626	11			

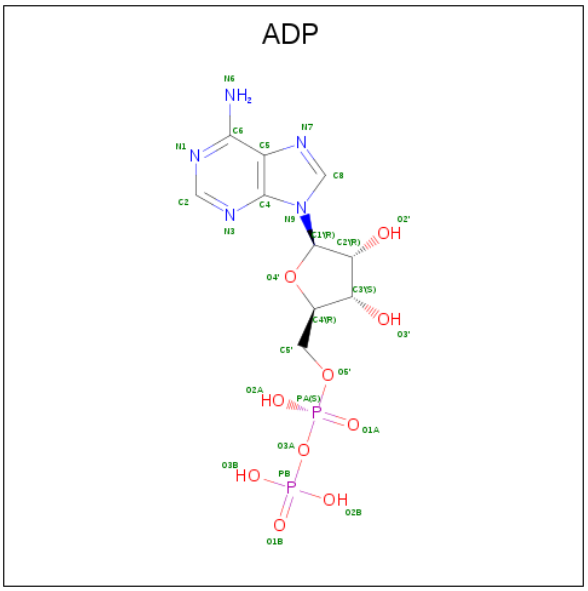
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP C4IRH0
B	0	GLY	-	expression tag	UNP C4IRH0

- 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: $C_{10}H_{15}N_5O_{10}P_2$).



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 water.

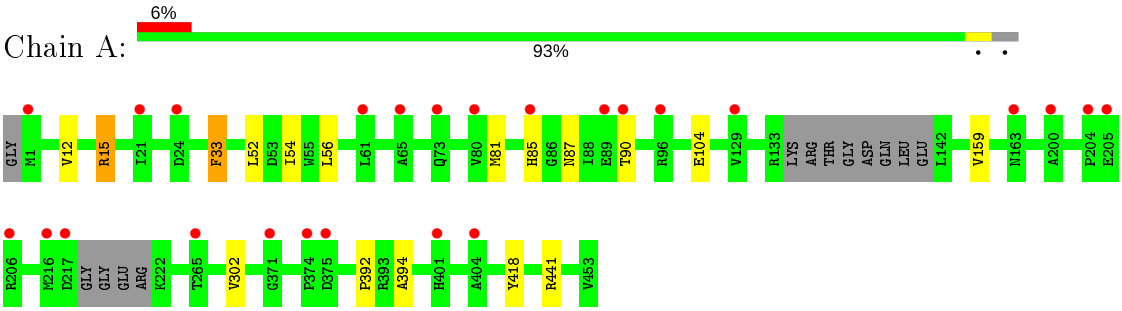
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	159	Total	O	0	0
			159	159		
4	B	134	Total	O	0	0
			134	134		

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.

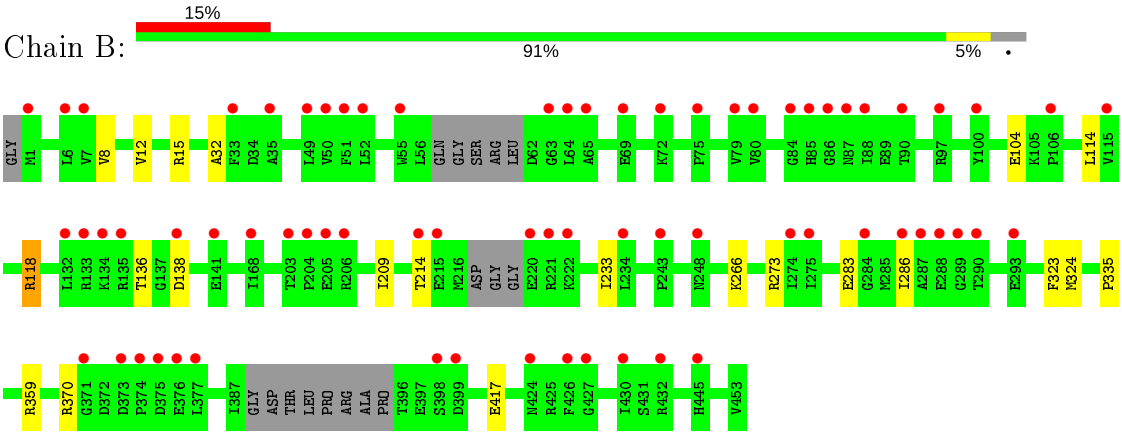
- Molecule 1: Nitrogen assimilation regulatory protein

Chain A:



- Molecule 1: Nitrogen assimilation regulatory protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	116.98Å 190.84Å 111.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.36 29.87 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.87-2.36) 99.7 (29.87-2.36)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.36Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.199 , 0.229 0.202 , 0.229	Depositor DCC
R_{free} test set	2517 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	45.4	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.016 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.025 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7042	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: MG, ADP

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	0.47	0/3398	0.65	0/4603
1	B	0.46	0/3385	0.64	0/4578
All	All	0.47	0/6783	0.64	0/9181

There are no bond length outliers.

There are no bond angle outliers.

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	3352	0	3372	10	0
1	B	3341	0	3366	11	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	159	0	0	0	0
4	B	134	0	0	0	0
All	All	7042	0	6762	20	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 1.

All (20) 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:12:VAL:HG22	1:A:15:ARG:HH12	1.58	0.69
1:A:15:ARG:HH11	1:A:33:PHE:HB3	1.65	0.61
1:A:54:ILE:HG21	1:A:90:THR:HG22	1.84	0.59
1:B:136:THR:HG22	1:B:138:ASP:HB2	1.87	0.55
1:A:394:ALA:HB1	1:B:417:GLU:HG3	1.90	0.52
1:B:323:PHE:CD1	1:B:359:ARG:HG3	2.45	0.52
1:B:283:GLU:HA	1:B:286:ILE:HD12	1.93	0.50
1:A:12:VAL:HG22	1:A:15:ARG:NH1	2.28	0.49
1:B:136:THR:CG2	1:B:138:ASP:HB2	2.43	0.48
1:B:12:VAL:HG12	1:B:15:ARG:NH2	2.31	0.46
1:A:159:VAL:HG11	1:A:302:VAL:HG11	1.98	0.46
1:A:392:PRO:HG2	1:A:418:TYR:HA	1.98	0.45
1:A:85:HIS:HA	1:A:104:GLU:OE1	2.19	0.42
1:B:8:VAL:HG22	1:B:32:ALA:HB3	2.02	0.42
1:A:12:VAL:HA	1:A:15:ARG:NH2	2.35	0.41
1:B:209:ILE:HG23	1:B:214:THR:HG23	2.02	0.41
1:B:233:ILE:HG12	1:B:273:ARG:HB3	2.03	0.41
1:B:118:ARG:HA	1:B:118:ARG:HD3	1.79	0.41
1:A:52:LEU:O	1:A:81:MET:HA	2.21	0.41
1:B:324:MET:HB3	1:B:335:PRO:HB3	2.03	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	435/454 (96%)	427 (98%)	8 (2%)	0	100	100
1	B	429/454 (94%)	422 (98%)	7 (2%)	0	100	100
All	All	864/908 (95%)	849 (98%)	15 (2%)	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	346/375 (92%)	341 (99%)	5 (1%)	67	78
1	B	346/375 (92%)	341 (99%)	5 (1%)	67	78
All	All	692/750 (92%)	682 (99%)	10 (1%)	67	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	33	PHE
1	A	56	LEU
1	A	87	ASN
1	A	441	ARG
1	B	104	GLU
1	B	114	LEU
1	B	118	ARG
1	B	266	LYS
1	B	370	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	ASN

5.3.3 RNA

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	B	502	-	24,29,29	0.72	0	29,45,45	0.88	1 (3%)
3	ADP	A	502	-	24,29,29	0.80	1 (4%)	29,45,45	0.67	1 (3%)

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	502	-	-	0/12/32/32	0/3/3/3
3	ADP	A	502	-	-	1/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	ADP	C8-N7	-2.06	1.31	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	ADP	C5-C6-N6	2.72	124.48	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	ADP	C5-C6-N6	2.01	123.41	120.35

There are no chirality outliers.

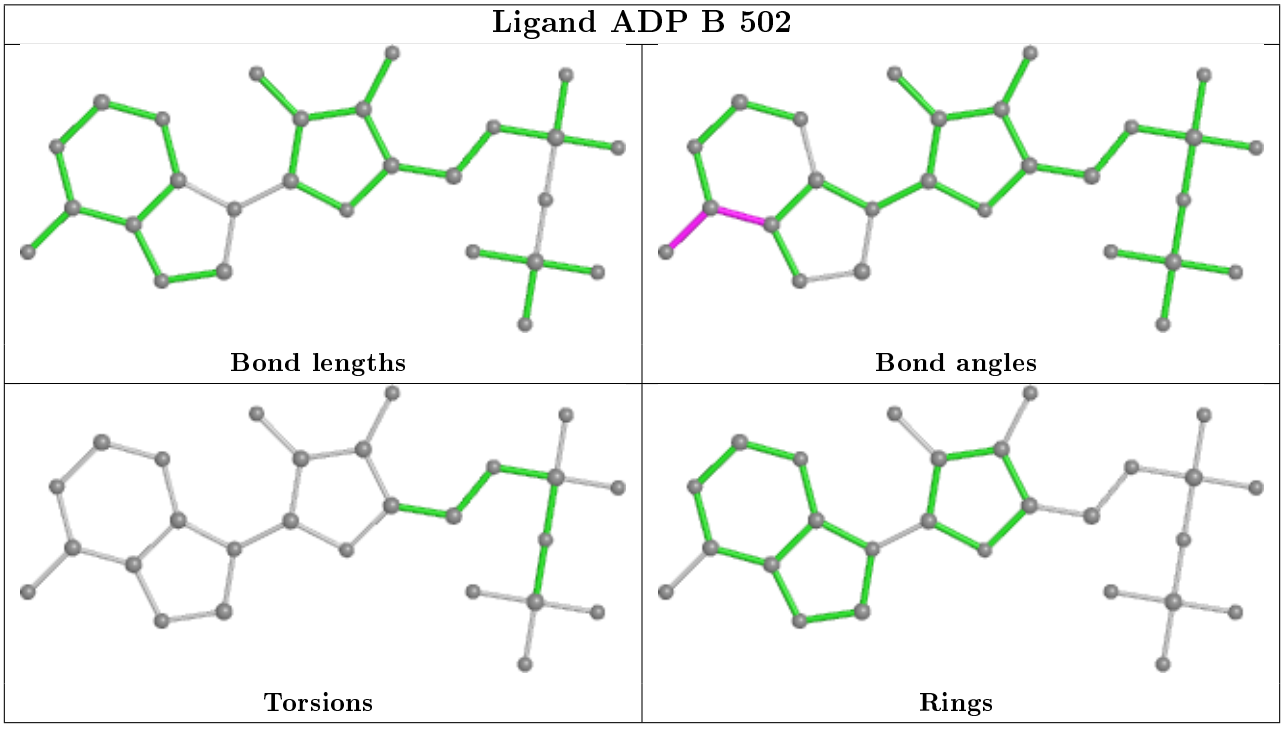
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	ADP	PA-O3A-PB-O2B

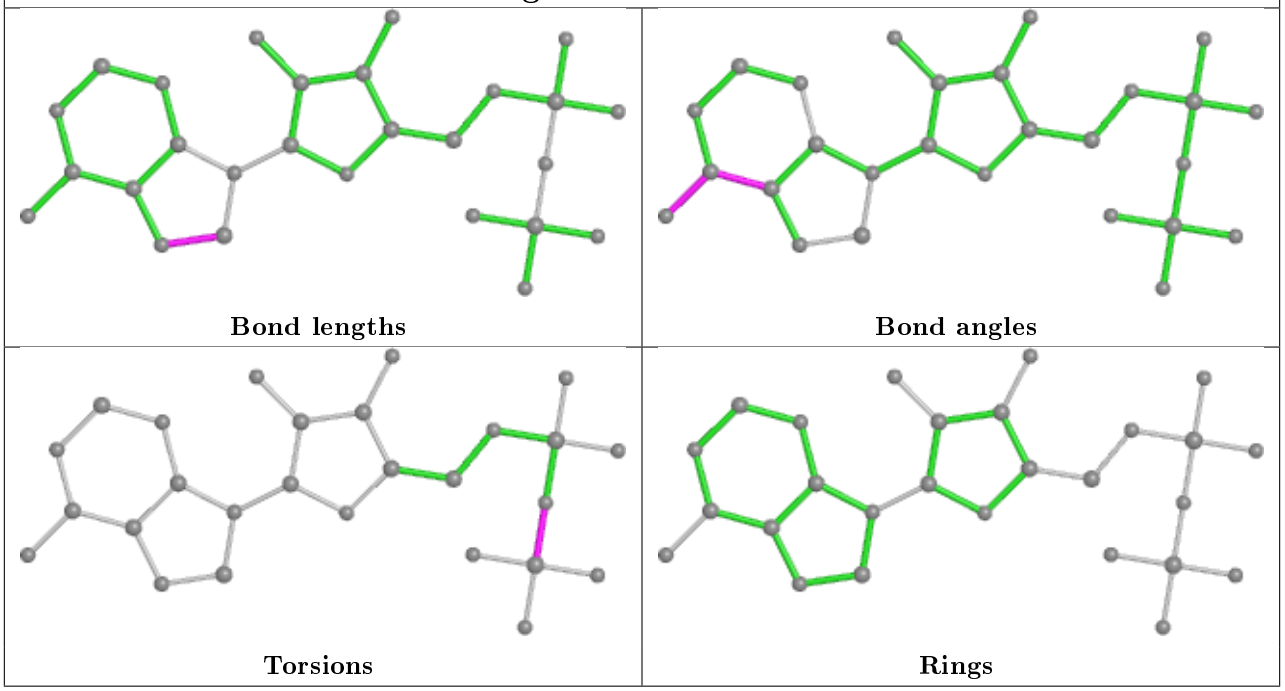
There are no ring outliers.

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 ADP A 502



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	441/454 (97%)	0.20	25 (5%) 23 34	32, 49, 75, 115	0
1	B	437/454 (96%)	0.70	70 (16%) 1 3	36, 56, 82, 97	0
All	All	878/908 (96%)	0.45	95 (10%) 5 9	32, 52, 79, 115	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	87	ASN	6.8
1	B	132	LEU	6.6
1	B	374	PRO	5.2
1	B	287	ALA	5.2
1	A	1	MET	5.2
1	A	217	ASP	5.1
1	B	204	PRO	5.1
1	B	375	ASP	5.1
1	B	86	GLY	4.7
1	A	216	MET	4.5
1	A	401	HIS	4.5
1	B	85	HIS	4.4
1	B	290	THR	4.3
1	B	1	MET	4.1
1	B	50	VAL	3.9
1	B	205	GLU	3.9
1	B	289	GLY	3.8
1	B	138	ASP	3.8
1	B	106	PRO	3.7
1	B	377	LEU	3.4
1	B	203	THR	3.4
1	B	72	LYS	3.4
1	A	89	GLU	3.4
1	B	399	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	288	GLU	3.2
1	A	374	PRO	3.2
1	A	61	LEU	3.1
1	B	80	VAL	3.1
1	B	90	THR	3.1
1	A	96	ARG	3.1
1	B	214	THR	3.1
1	A	205	GLU	3.1
1	B	293	GLU	3.0
1	A	206	ARG	3.0
1	B	51	PHE	3.0
1	B	64	LEU	3.0
1	B	275	ILE	2.9
1	B	7	VAL	2.9
1	B	33	PHE	2.9
1	B	215	GLU	2.9
1	B	168	ILE	2.9
1	B	286	ILE	2.9
1	B	426	PHE	2.8
1	B	55	TRP	2.8
1	B	141	GLU	2.8
1	A	129	VAL	2.8
1	A	24	ASP	2.7
1	A	80	VAL	2.7
1	A	90	THR	2.7
1	B	220	GLU	2.7
1	A	375	ASP	2.6
1	A	21	ILE	2.6
1	B	6	LEU	2.5
1	B	134	LYS	2.5
1	B	222	LYS	2.5
1	A	265	THR	2.5
1	B	133	ARG	2.4
1	B	221	ARG	2.4
1	B	430	ILE	2.4
1	B	284	GLY	2.4
1	B	115	VAL	2.4
1	B	135	ARG	2.4
1	B	206	ARG	2.4
1	B	371	GLY	2.4
1	B	84	GLY	2.3
1	B	88	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	73	GLN	2.3
1	A	65	ALA	2.3
1	B	49	LEU	2.3
1	A	200	ALA	2.3
1	B	97	ARG	2.3
1	B	445	HIS	2.3
1	B	424	ASN	2.3
1	B	427	GLY	2.2
1	A	163	ASN	2.2
1	B	69	GLU	2.2
1	A	204	PRO	2.2
1	B	248	ASN	2.2
1	B	243	PRO	2.2
1	B	79	VAL	2.2
1	A	371	GLY	2.2
1	B	52	LEU	2.2
1	B	398	SER	2.2
1	A	85	HIS	2.2
1	B	75	PRO	2.2
1	B	63	GLY	2.1
1	B	432	ARG	2.1
1	B	65	ALA	2.1
1	B	274	ILE	2.1
1	A	404	ALA	2.1
1	B	35	ALA	2.1
1	B	100	TYR	2.0
1	B	234	LEU	2.0
1	B	373	ASP	2.0
1	B	376	GLU	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)

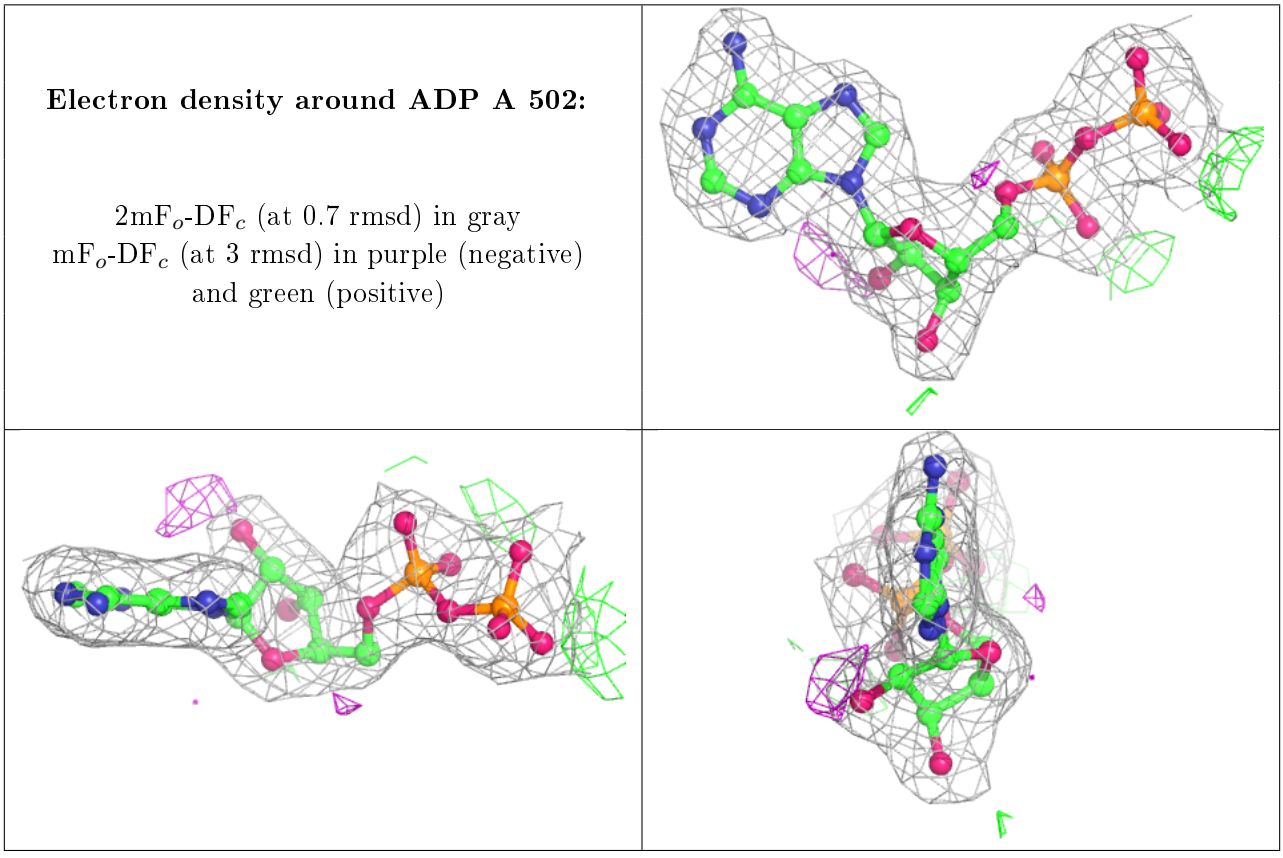
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	MG	B	501	1/1	0.70	0.19	62,62,62,62	0
2	MG	A	501	1/1	0.89	0.21	74,74,74,74	0
3	ADP	A	502	27/27	0.97	0.14	33,39,42,44	0
3	ADP	B	502	27/27	0.98	0.16	39,43,47,52	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.

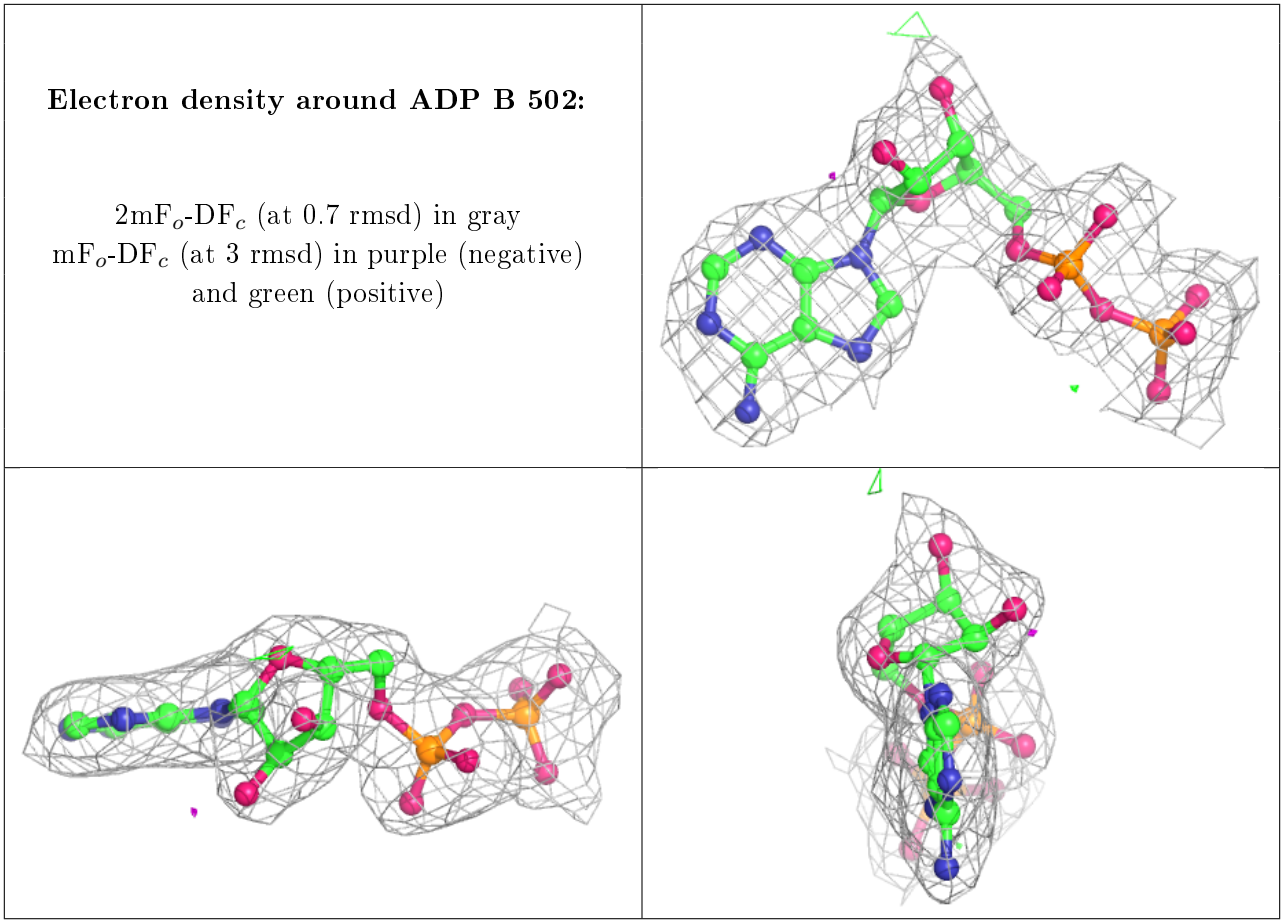
Electron density around ADP A 502:

$2mF_o$-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 502:

$2mF_o$-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.