



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 10:44 am BST

PDB ID : 2GK6  
Title : Structural and Functional insights into the human Upf1 helicase core  
Authors : Cheng, Z.; Muhlrads, D.; Parker, R.; Song, H.  
Deposited on : 2006-03-31  
Resolution : 2.40 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](mailto: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.

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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

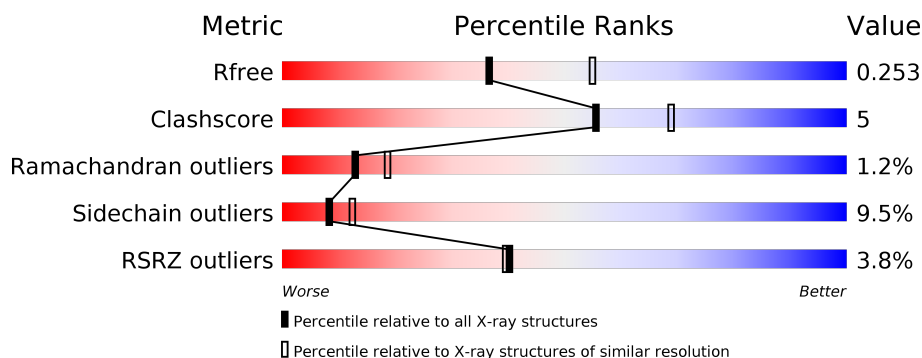
# 1 Overall quality at a glance

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  $\geq 3$ , 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	624	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>
1	B	624	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>

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
3	PO4	A	990	-	-	X	-
3	PO4	B	1990	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9795 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 Regulator of nonsense transcripts 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	0	0
			4748	3022	829	874	23			
1	B	602	Total	C	N	O	S	0	0	0
			4748	3022	829	874	23			

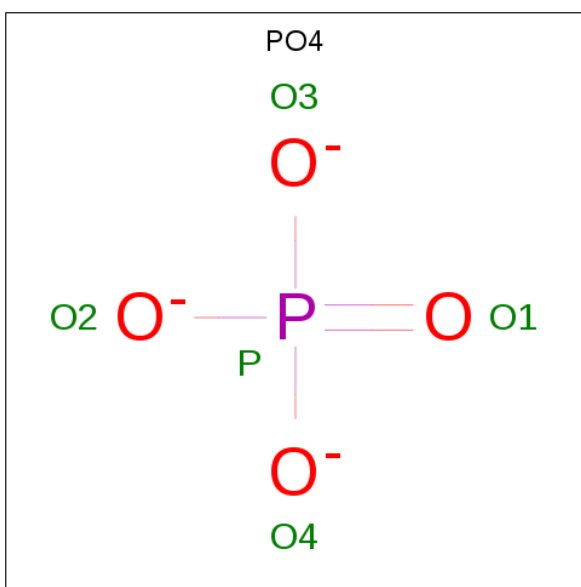
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	PRO	-	CLONING ARTIFACT	UNP Q92900
A	292	LEU	-	CLONING ARTIFACT	UNP Q92900
A	293	GLY	-	CLONING ARTIFACT	UNP Q92900
A	294	SER	-	CLONING ARTIFACT	UNP Q92900
B	291	PRO	-	CLONING ARTIFACT	UNP Q92900
B	292	LEU	-	CLONING ARTIFACT	UNP Q92900
B	293	GLY	-	CLONING ARTIFACT	UNP Q92900
B	294	SER	-	CLONING ARTIFACT	UNP Q92900

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

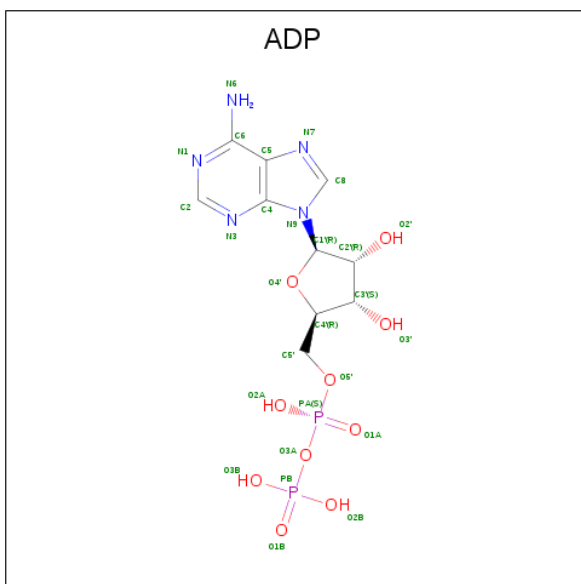
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



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

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

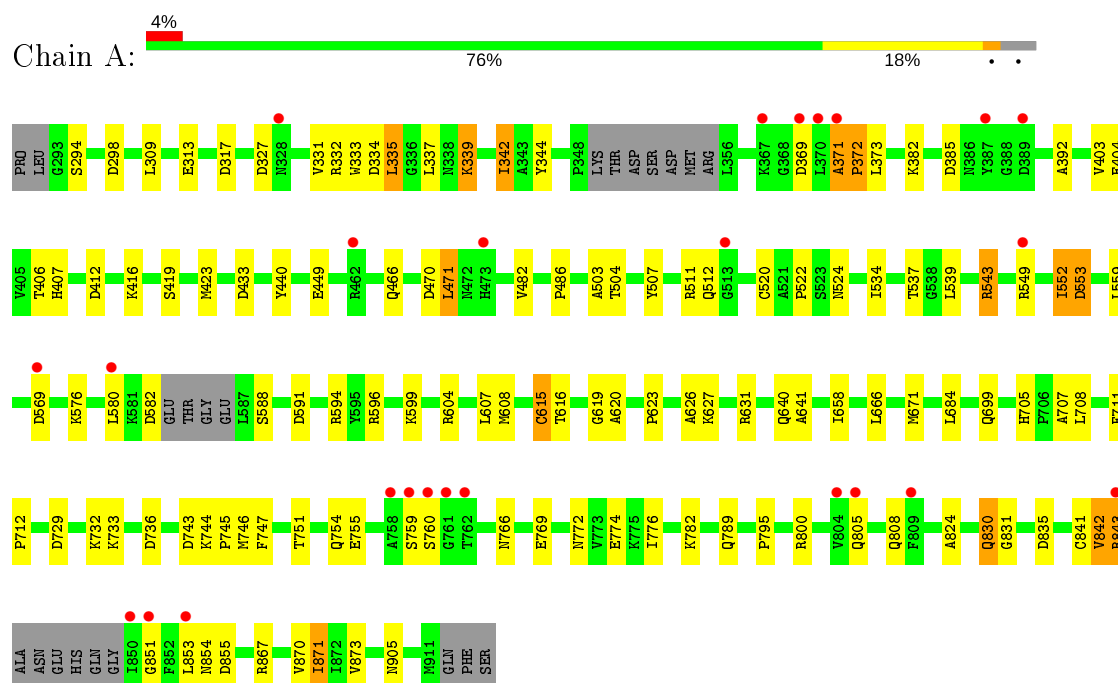
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total	O	0	0
			115	115		
5	B	118	Total	O	0	0
			118	118		

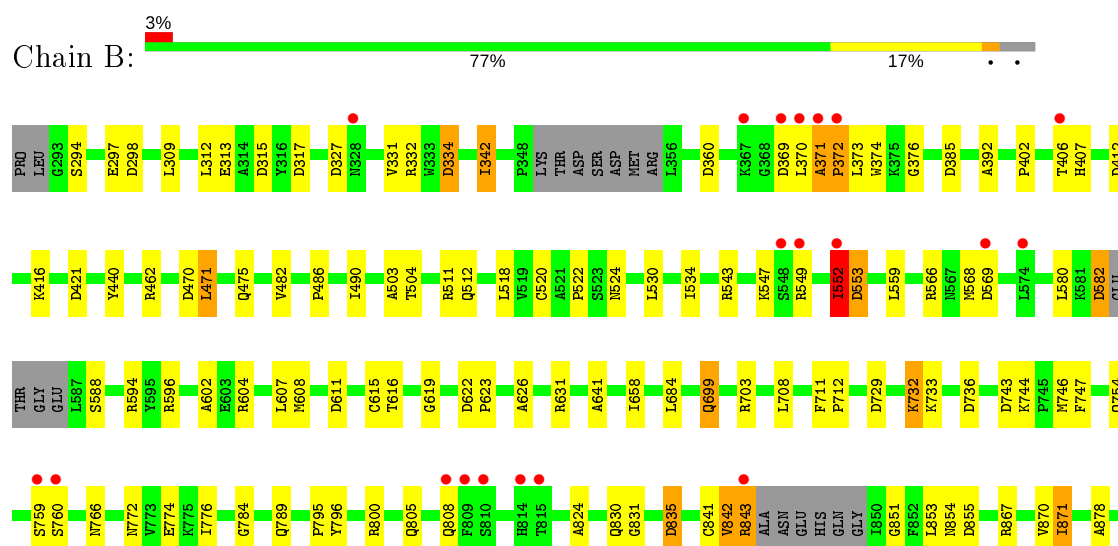
### 3 Residue-property plots [i](#)

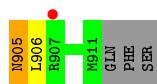
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Regulator of nonsense transcripts 1



#### • Molecule 1: Regulator of nonsense transcripts 1







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.28Å 67.84Å 87.25Å 114.41° 90.13° 110.22°	Depositor
Resolution (Å)	20.00 – 2.40 39.01 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.9 (20.00-2.40) 90.8 (39.01-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.235 , 0.272 0.239 , 0.253	Depositor DCC
$R_{free}$ test set	2171 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9795	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.37	0/4839	0.69	13/6545 (0.2%)
1	B	0.38	1/4839 (0.0%)	0.70	17/6545 (0.3%)
All	All	0.37	1/9678 (0.0%)	0.69	30/13090 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	842	VAL	C-N	7.21	1.50	1.34

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	855	ASP	CB-CG-OD2	7.25	124.82	118.30
1	A	385	ASP	CB-CG-OD2	6.82	124.43	118.30
1	A	855	ASP	CB-CG-OD2	6.71	124.34	118.30
1	B	842	VAL	O-C-N	6.55	133.18	122.70
1	A	412	ASP	CB-CG-OD2	6.24	123.92	118.30
1	B	317	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	317	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	385	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	369	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	369	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	743	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	743	ASP	CB-CG-OD2	5.56	123.31	118.30
1	B	412	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	470	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	569	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	736	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	433	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	298	ASP	CB-CG-OD2	5.21	122.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	582	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	553	ASP	CB-CG-OD2	5.17	122.96	118.30
1	B	470	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	421	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	835	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	736	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	298	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	611	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	569	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	622	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	591	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	360	ASP	CB-CG-OD2	5.00	122.80	118.30

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	4748	0	4828	46	0
1	B	4748	0	4827	51	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	2	0
3	B	5	0	0	2	0
4	A	27	0	12	1	0
4	B	27	0	12	2	0
5	A	115	0	0	1	0
5	B	118	0	0	2	0
All	All	9795	0	9679	98	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 5.

All (98) 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:524:ASN:HD22	1:A:543:ARG:HH22	1.23	0.85
1:A:708:LEU:HD22	1:A:870:VAL:HG12	1.68	0.74
1:B:524:ASN:HD22	1:B:543:ARG:HH22	1.37	0.70
1:B:843:ARG:O	1:B:853:LEU:HD21	1.92	0.70
1:B:616:THR:HG23	1:B:619:GLY:H	1.58	0.68
1:A:747:PHE:CZ	1:A:871:ILE:HD12	2.29	0.67
1:B:843:ARG:C	1:B:853:LEU:HD22	2.15	0.67
1:B:482:VAL:HG13	1:B:658:ILE:HG12	1.77	0.66
1:B:843:ARG:C	1:B:853:LEU:CD2	2.64	0.66
1:B:747:PHE:CZ	1:B:871:ILE:HD12	2.31	0.65
1:A:520:CYS:HA	1:A:615:CYS:O	1.97	0.64
1:B:708:LEU:HD22	1:B:870:VAL:HG12	1.79	0.64
1:A:482:VAL:HG13	1:A:658:ILE:HG12	1.80	0.64
1:A:616:THR:HG23	1:A:619:GLY:H	1.64	0.62
3:B:1990:PO4:O1	4:B:1820:ADP:O2B	2.19	0.60
1:B:795:PRO:HB3	1:B:851:GLY:HA3	1.84	0.59
1:A:795:PRO:HB3	1:A:851:GLY:HA3	1.84	0.58
1:A:746:MET:HA	1:A:870:VAL:O	2.03	0.58
1:B:746:MET:HA	1:B:870:VAL:O	2.04	0.57
1:B:482:VAL:HG21	1:B:490:ILE:HD11	1.87	0.57
1:B:518:LEU:HD11	1:B:615:CYS:SG	2.46	0.56
1:B:772:ASN:O	1:B:776:ILE:HG12	2.06	0.55
1:B:342:ILE:HD11	1:B:392:ALA:HB1	1.90	0.54
1:B:800:ARG:HD2	1:B:824:ALA:HA	1.89	0.54
1:B:520:CYS:HA	1:B:615:CYS:O	2.09	0.53
1:B:371:ALA:N	1:B:372:PRO:CD	2.73	0.52
1:A:342:ILE:HD11	1:A:392:ALA:HB1	1.93	0.51
1:B:331:VAL:O	1:B:406:THR:OG1	2.27	0.51
1:A:482:VAL:CG1	1:A:658:ILE:HG12	2.40	0.51
1:B:766:ASN:HB2	1:B:842:VAL:HB	1.93	0.51
1:B:482:VAL:CG1	1:B:658:ILE:HG12	2.40	0.51
1:A:331:VAL:O	1:A:406:THR:OG1	2.29	0.50
1:A:371:ALA:N	1:A:372:PRO:CD	2.74	0.50
1:A:449:GLU:HB2	5:A:236:HOH:O	2.11	0.50
1:A:772:ASN:O	1:A:776:ILE:HG12	2.11	0.50
1:B:843:ARG:O	1:B:853:LEU:CD2	2.59	0.50
1:A:522:PRO:HG3	1:A:641:ALA:HB2	1.94	0.49
3:A:990:PO4:O3	4:A:1001:ADP:O2B	2.30	0.49
1:B:374:TRP:CZ2	1:B:376:GLY:HA3	2.48	0.48
1:B:440:TYR:CE2	1:B:486:PRO:HG2	2.47	0.48
1:A:666:LEU:HD12	1:A:830:GLN:HG3	1.95	0.48
1:B:905:ASN:HD22	1:B:905:ASN:C	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1820:ADP:H1'	5:B:178:HOH:O	2.11	0.48
1:B:843:ARG:C	1:B:853:LEU:HD21	2.33	0.48
1:A:831:GLY:HA2	3:A:990:PO4:O2	2.14	0.47
1:A:471:LEU:HD21	1:A:504:THR:HG21	1.96	0.47
1:B:471:LEU:HA	1:B:475:GLN:NE2	2.29	0.47
1:B:503:ALA:HA	1:B:534:ILE:HD11	1.95	0.47
1:A:507:TYR:HA	1:A:539:LEU:HD11	1.96	0.47
1:B:471:LEU:HD21	1:B:504:THR:HG21	1.97	0.47
1:B:566:ARG:HD2	5:B:112:HOH:O	2.14	0.47
1:A:705:HIS:ND1	1:A:745:PRO:HG2	2.30	0.47
1:B:503:ALA:HA	1:B:534:ILE:CD1	2.45	0.46
1:A:800:ARG:HD2	1:A:824:ALA:HA	1.95	0.46
1:B:623:PRO:O	1:B:626:ALA:HB2	2.16	0.46
1:A:766:ASN:HB2	1:A:842:VAL:HB	1.97	0.46
1:A:769:GLU:HG2	1:A:873:VAL:HG12	1.98	0.46
1:B:703:ARG:O	1:B:867:ARG:HG2	2.16	0.46
1:B:699:GLN:HB2	1:B:699:GLN:HE21	1.55	0.46
1:A:337:LEU:HB3	1:B:784:GLY:HA3	1.97	0.46
1:B:796:TYR:CE1	1:B:842:VAL:HG22	2.51	0.46
1:A:776:ILE:HG21	1:A:871:ILE:HD13	1.98	0.45
1:B:711:PHE:HB3	1:B:712:PRO:HD3	1.97	0.45
1:B:530:LEU:O	1:B:534:ILE:HG12	2.16	0.45
1:A:331:VAL:HG12	1:A:332:ARG:N	2.31	0.45
1:A:800:ARG:HB3	1:A:800:ARG:CZ	2.47	0.45
1:A:623:PRO:O	1:A:626:ALA:HB2	2.17	0.45
1:A:419:SER:O	1:A:423:MET:HG3	2.17	0.44
1:A:332:ARG:HB2	1:A:344:TYR:HB2	1.99	0.44
1:B:371:ALA:N	1:B:372:PRO:HD3	2.33	0.43
1:B:334:ASP:HB3	1:B:342:ILE:HG22	2.00	0.43
1:B:522:PRO:HG3	1:B:641:ALA:HB2	1.99	0.43
1:A:751:THR:HG21	1:A:769:GLU:HA	2.00	0.43
1:A:776:ILE:CG2	1:A:871:ILE:HD13	2.48	0.43
1:B:568:MET:CE	1:B:602:ALA:HB1	2.48	0.43
1:A:371:ALA:N	1:A:372:PRO:HD3	2.33	0.43
1:A:711:PHE:HB3	1:A:712:PRO:HD3	2.01	0.43
1:B:843:ARG:HG3	1:B:878:ALA:HB1	2.00	0.43
1:B:374:TRP:CD2	1:B:402:PRO:HD3	2.53	0.43
1:B:789:GLN:HB3	1:B:835:ASP:HB2	2.00	0.43
1:A:337:LEU:HD11	1:B:732:LYS:HG2	2.00	0.42
1:B:552:ILE:HD13	1:B:553:ASP:H	1.85	0.42
1:B:747:PHE:CE1	1:B:871:ILE:HD12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HD22	1:A:339:LYS:HA	2.02	0.42
1:A:440:TYR:CE2	1:A:486:PRO:HG2	2.55	0.42
1:B:776:ILE:HG21	1:B:871:ILE:HD13	2.02	0.42
1:A:705:HIS:HD2	1:A:707:ALA:H	1.66	0.42
1:A:466:GLN:O	1:A:537:THR:HA	2.20	0.41
1:A:382:LYS:HB3	1:A:392:ALA:HB3	2.01	0.41
1:B:331:VAL:HG12	1:B:332:ARG:N	2.35	0.41
1:A:503:ALA:HA	1:A:534:ILE:HD11	2.02	0.41
1:A:503:ALA:HA	1:A:534:ILE:CD1	2.51	0.41
1:A:789:GLN:HB3	1:A:835:ASP:HB2	2.03	0.41
1:A:333:TRP:CB	1:A:403:VAL:HG13	2.51	0.41
1:B:370:LEU:C	1:B:372:PRO:HD2	2.42	0.40
1:A:843:ARG:O	1:A:843:ARG:NE	2.53	0.40
1:B:831:GLY:HA2	3:B:1990:PO4:O4	2.21	0.40
1:A:615:CYS:SG	1:A:620:ALA:HB2	2.61	0.40

There are no symmetry-related clashes.

## 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	594/624 (95%)	540 (91%)	47 (8%)	7 (1%)	13	19
1	B	594/624 (95%)	545 (92%)	42 (7%)	7 (1%)	13	19
All	All	1188/1248 (95%)	1085 (91%)	89 (8%)	14 (1%)	13	19

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372	PRO
1	A	759	SER
1	B	372	PRO

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Mol	Chain	Res	Type
1	B	808	GLN
1	A	808	GLN
1	B	760	SER
1	A	760	SER
1	B	371	ALA
1	B	373	LEU
1	B	759	SER
1	A	373	LEU
1	B	552	ILE
1	A	371	ALA
1	A	552	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	521/540 (96%)	467 (90%)	54 (10%)	7	10
1	B	521/540 (96%)	476 (91%)	45 (9%)	10	16
All	All	1042/1080 (96%)	943 (90%)	99 (10%)	8	12

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	294	SER
1	A	309	LEU
1	A	313	GLU
1	A	327	ASP
1	A	334	ASP
1	A	335	LEU
1	A	339	LYS
1	A	342	ILE
1	A	404	GLU
1	A	407	HIS
1	A	416	LYS
1	A	471	LEU

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Mol	Chain	Res	Type
1	A	511	ARG
1	A	512	GLN
1	A	543	ARG
1	A	549	ARG
1	A	552	ILE
1	A	553	ASP
1	A	559	LEU
1	A	576	LYS
1	A	580	LEU
1	A	582	ASP
1	A	588	SER
1	A	594	ARG
1	A	596	ARG
1	A	599	LYS
1	A	604	ARG
1	A	607	LEU
1	A	608	MET
1	A	615	CYS
1	A	627	LYS
1	A	631	ARG
1	A	640	GLN
1	A	671	MET
1	A	684	LEU
1	A	699	GLN
1	A	729	ASP
1	A	732	LYS
1	A	733	LYS
1	A	744	LYS
1	A	754	GLN
1	A	755	GLU
1	A	774	GLU
1	A	782	LYS
1	A	805	GLN
1	A	830	GLN
1	A	841	CYS
1	A	842	VAL
1	A	843	ARG
1	A	853	LEU
1	A	854	ASN
1	A	867	ARG
1	A	871	ILE
1	A	905	ASN

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Mol	Chain	Res	Type
1	B	294	SER
1	B	297	GLU
1	B	309	LEU
1	B	312	LEU
1	B	313	GLU
1	B	315	ASP
1	B	327	ASP
1	B	334	ASP
1	B	342	ILE
1	B	407	HIS
1	B	416	LYS
1	B	462	ARG
1	B	471	LEU
1	B	511	ARG
1	B	512	GLN
1	B	547	LYS
1	B	549	ARG
1	B	552	ILE
1	B	553	ASP
1	B	559	LEU
1	B	580	LEU
1	B	582	ASP
1	B	588	SER
1	B	594	ARG
1	B	596	ARG
1	B	604	ARG
1	B	607	LEU
1	B	608	MET
1	B	631	ARG
1	B	684	LEU
1	B	699	GLN
1	B	729	ASP
1	B	732	LYS
1	B	733	LYS
1	B	744	LYS
1	B	754	GLN
1	B	774	GLU
1	B	805	GLN
1	B	830	GLN
1	B	841	CYS
1	B	843	ARG
1	B	854	ASN

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Mol	Chain	Res	Type
1	B	871	ILE
1	B	905	ASN
1	B	906	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
1	A	408	ASN
1	A	475	GLN
1	A	524	ASN
1	A	536	GLN
1	A	578	GLN
1	A	665	GLN
1	A	699	GLN
1	A	714	ASN
1	A	738	GLN
1	A	772	ASN
1	A	805	GLN
1	A	860	ASN
1	A	886	ASN
1	A	905	ASN
1	B	304	ASN
1	B	408	ASN
1	B	475	GLN
1	B	524	ASN
1	B	699	GLN
1	B	738	GLN
1	B	772	ASN
1	B	805	GLN
1	B	860	ASN
1	B	905	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 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	PO4	A	990	-	4,4,4	1.23	0	6,6,6	0.57	0
3	PO4	B	1990	-	4,4,4	1.14	0	6,6,6	0.63	0
4	ADP	B	1820	2	24,29,29	1.18	2 (8%)	29,45,45	1.71	5 (17%)
4	ADP	A	1001	2	24,29,29	1.16	2 (8%)	29,45,45	1.73	5 (17%)

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	ADP	B	1820	2	-	2/12/32/32	0/3/3/3
4	ADP	A	1001	2	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1820	ADP	C2-N3	3.94	1.38	1.32
4	A	1001	ADP	C2-N3	3.87	1.38	1.32
4	B	1820	ADP	C2-N1	2.74	1.39	1.33
4	A	1001	ADP	C2-N1	2.54	1.38	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1820	ADP	N3-C2-N1	-5.68	119.80	128.68
4	A	1001	ADP	N3-C2-N1	-5.60	119.93	128.68
4	B	1820	ADP	PA-O3A-PB	-3.40	121.17	132.83
4	A	1001	ADP	PA-O3A-PB	-3.31	121.46	132.83
4	A	1001	ADP	O3'-C3'-C2'	3.09	121.82	111.82
4	B	1820	ADP	O3'-C3'-C2'	3.00	121.52	111.82
4	A	1001	ADP	C3'-C2'-C1'	2.76	105.13	100.98
4	B	1820	ADP	O4'-C4'-C5'	2.46	117.48	109.37
4	A	1001	ADP	O4'-C4'-C5'	2.38	117.22	109.37
4	B	1820	ADP	C3'-C2'-C1'	2.29	104.42	100.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

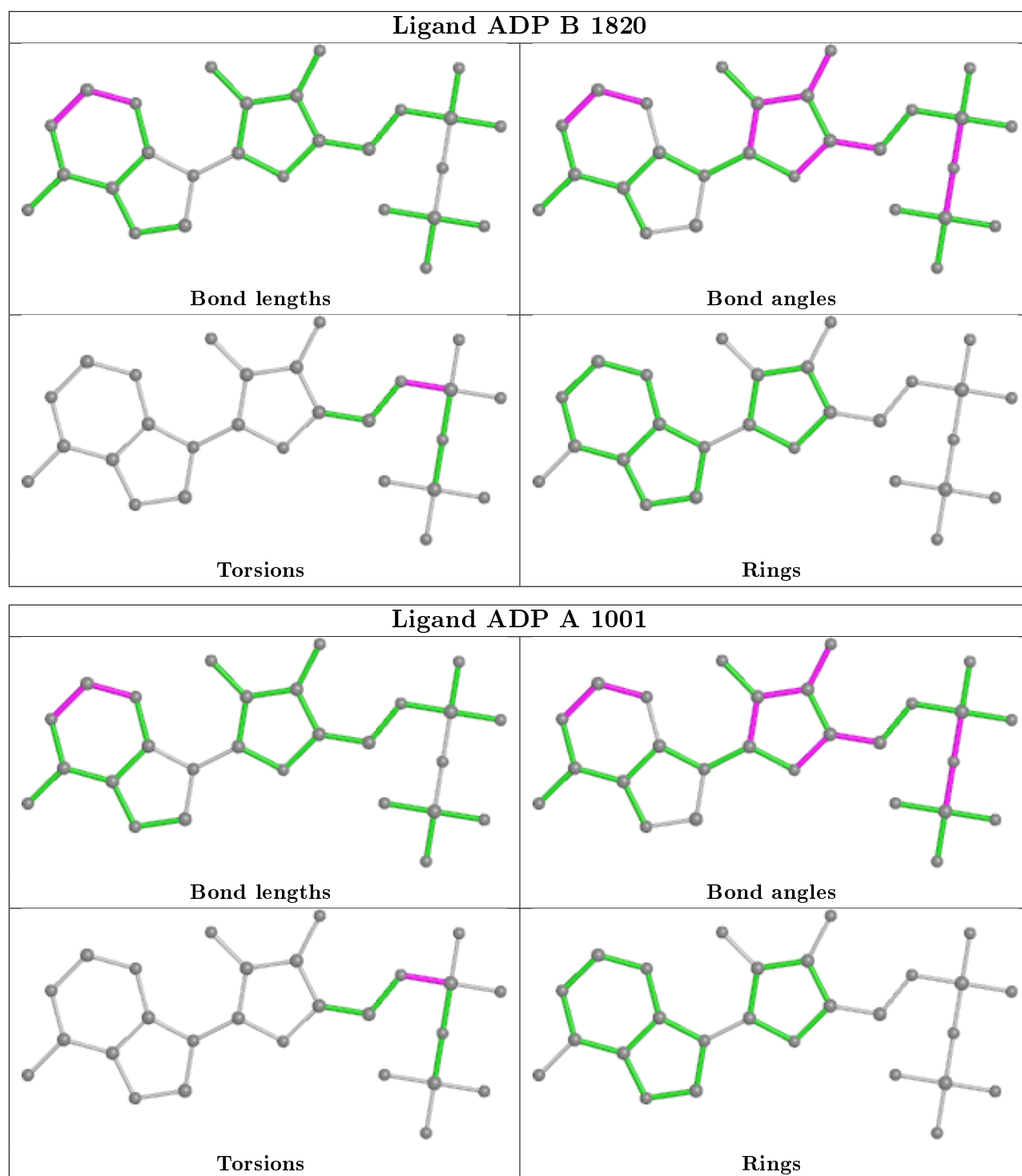
Mol	Chain	Res	Type	Atoms
4	B	1820	ADP	C5'-O5'-PA-O3A
4	A	1001	ADP	C5'-O5'-PA-O1A
4	A	1001	ADP	C5'-O5'-PA-O3A
4	B	1820	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	990	PO4	2	0
3	B	1990	PO4	2	0
4	B	1820	ADP	2	0
4	A	1001	ADP	1	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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	602/624 (96%)	-0.01	25 (4%) 36 35	12, 33, 53, 62	0
1	B	602/624 (96%)	0.00	21 (3%) 44 43	13, 33, 53, 62	0
All	All	1204/1248 (96%)	-0.00	46 (3%) 40 39	12, 33, 53, 62	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	759	SER	8.4
1	B	843	ARG	7.8
1	A	371	ALA	5.7
1	A	843	ARG	5.6
1	B	371	ALA	5.2
1	B	814	HIS	4.7
1	B	810	SER	4.6
1	A	370	LEU	4.5
1	B	552	ILE	4.4
1	A	758	ALA	4.3
1	A	580	LEU	4.2
1	A	569	ASP	4.0
1	B	809	PHE	3.9
1	B	808	GLN	3.5
1	A	387	TYR	3.4
1	B	759	SER	3.4
1	B	815	THR	3.2
1	B	370	LEU	3.2
1	B	569	ASP	3.2
1	A	369	ASP	2.9
1	A	462	ARG	2.9
1	B	907	ARG	2.9
1	A	762	THR	2.8
1	B	372	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	760	SER	2.8
1	A	549	ARG	2.7
1	A	853	LEU	2.7
1	A	761	GLY	2.6
1	A	513	GLY	2.5
1	A	804	VAL	2.4
1	B	549	ARG	2.4
1	B	574	LEU	2.4
1	A	805	GLN	2.4
1	A	851	GLY	2.3
1	A	809	PHE	2.3
1	B	548	SER	2.3
1	A	389	ASP	2.3
1	A	367	LYS	2.2
1	A	328	ASN	2.2
1	B	406	THR	2.1
1	A	760	SER	2.1
1	B	328	ASN	2.1
1	B	367	LYS	2.1
1	B	369	ASP	2.1
1	A	850	ILE	2.1
1	A	473	HIS	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	MG	A	1000	1/1	0.67	0.31	55,55,55,55	0

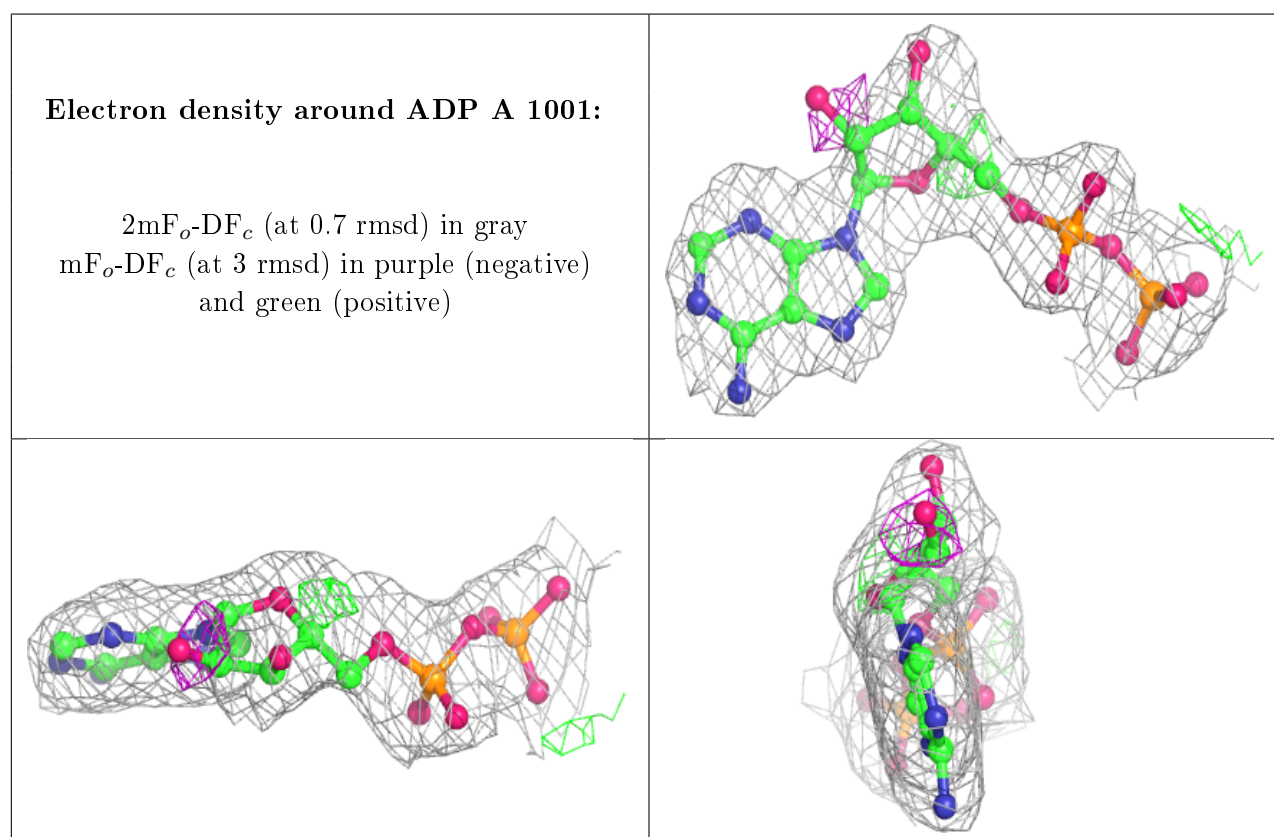
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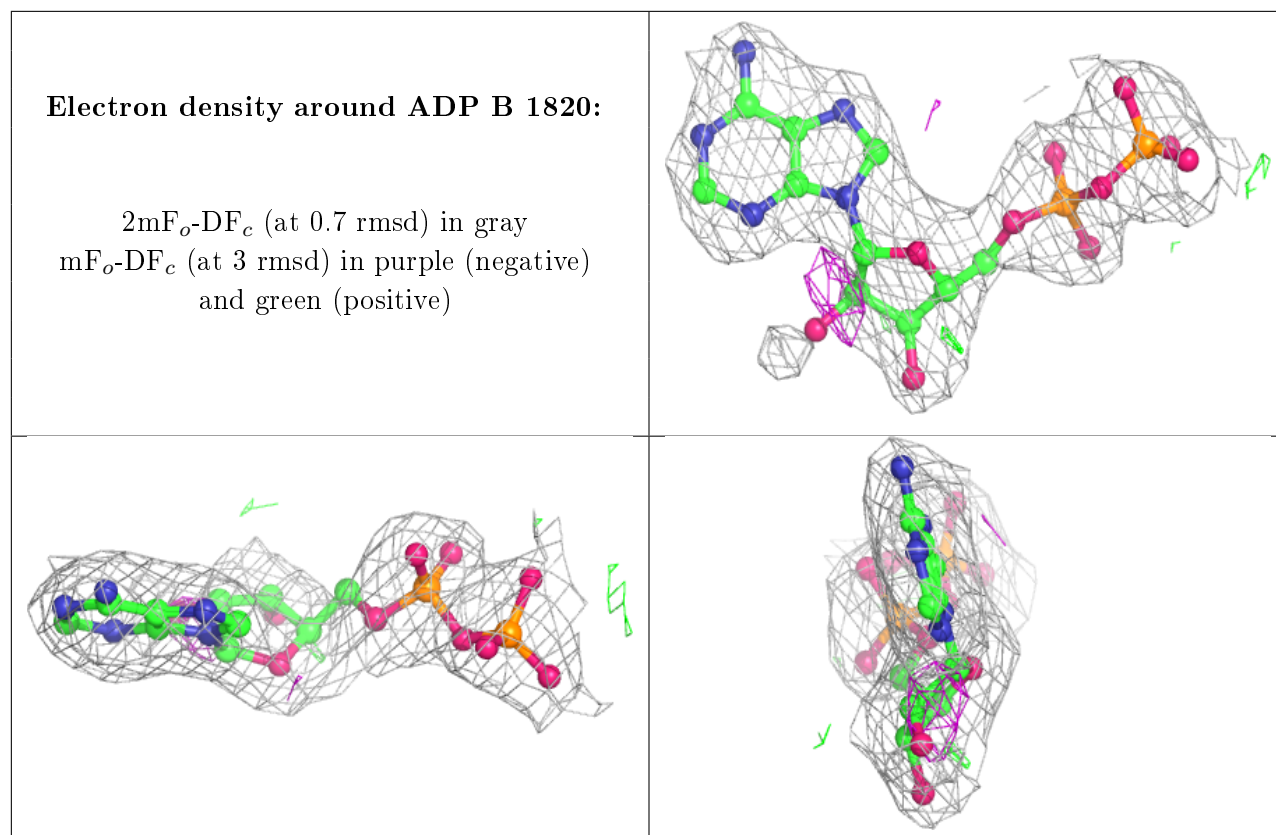


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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	2000	1/1	0.79	0.23	50,50,50,50	0
4	ADP	A	1001	27/27	0.93	0.16	41,52,54,56	0
4	ADP	B	1820	27/27	0.93	0.15	42,51,54,55	0
3	PO4	A	990	5/5	0.99	0.13	39,40,40,41	0
3	PO4	B	1990	5/5	0.99	0.12	41,41,42,42	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.