



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:17 pm BST

PDB ID : 1IHU  
Title : CRYSTAL STRUCTURE OF THE ESCHERICHIA COLI ARSENITE-TRANSLOCATING ATPASE IN COMPLEX WITH MG-ADP-ALF3  
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Deposited on : 2001-04-20  
Resolution : 2.15 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

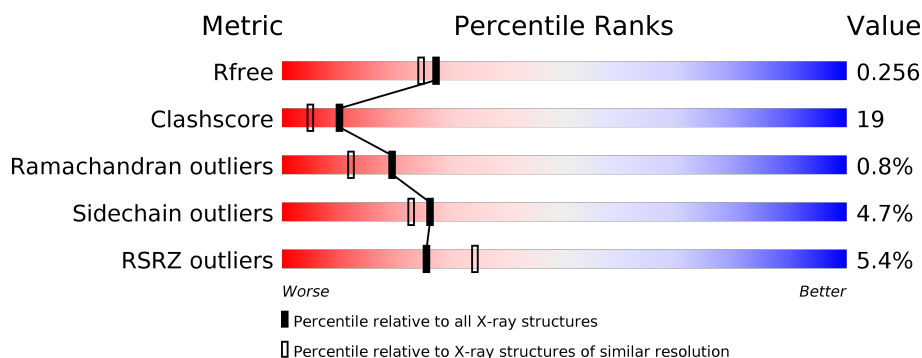
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	589	

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
7	TAS	A	701	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4389 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 ARSENICAL PUMP-DRIVING ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	0	0
			4122	2596	727	784	15			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASN	ILE	SEE REMARK 999	UNP P08690
A	584	HIS	-	EXPRESSION TAG	UNP P08690
A	585	HIS	-	EXPRESSION TAG	UNP P08690
A	586	HIS	-	EXPRESSION TAG	UNP P08690
A	587	HIS	-	EXPRESSION TAG	UNP P08690
A	588	HIS	-	EXPRESSION TAG	UNP P08690
A	589	HIS	-	EXPRESSION TAG	UNP P08690

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

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

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	Cd	0	0
			8	8		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

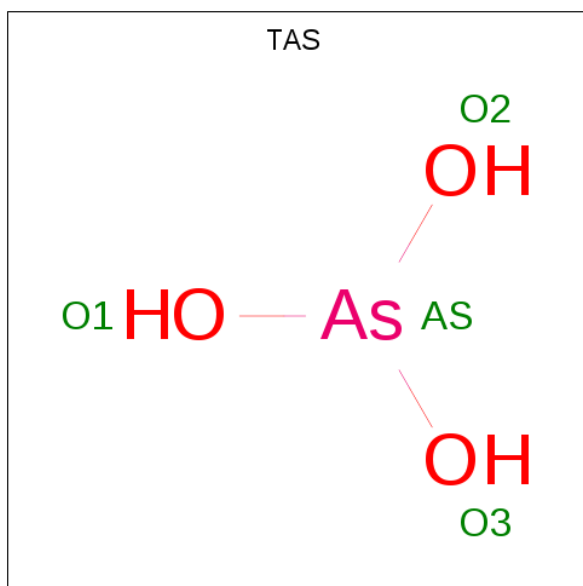
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cl	0	0
			3	3		

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

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- The diagram illustrates the AF3 molecule. A central Aluminum (Al) atom is shown in pink. It is bonded to three Fluorine (F) atoms, which are shown in green. The bonds are labeled F1, F2, and F3. The F1 bond is horizontal to the left, the F2 bond is diagonal up and to the right, and the F3 bond is diagonal down and to the right. The Al atom is labeled 'AL' to its right. The title 'AF3' is at the top center.

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

- Molecule 7 is TRIHYDROXYARSENITE(III) (three-letter code: TAS) (formula:  $\text{AsH}_3\text{O}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	As	O	0	0
			4	1	3		

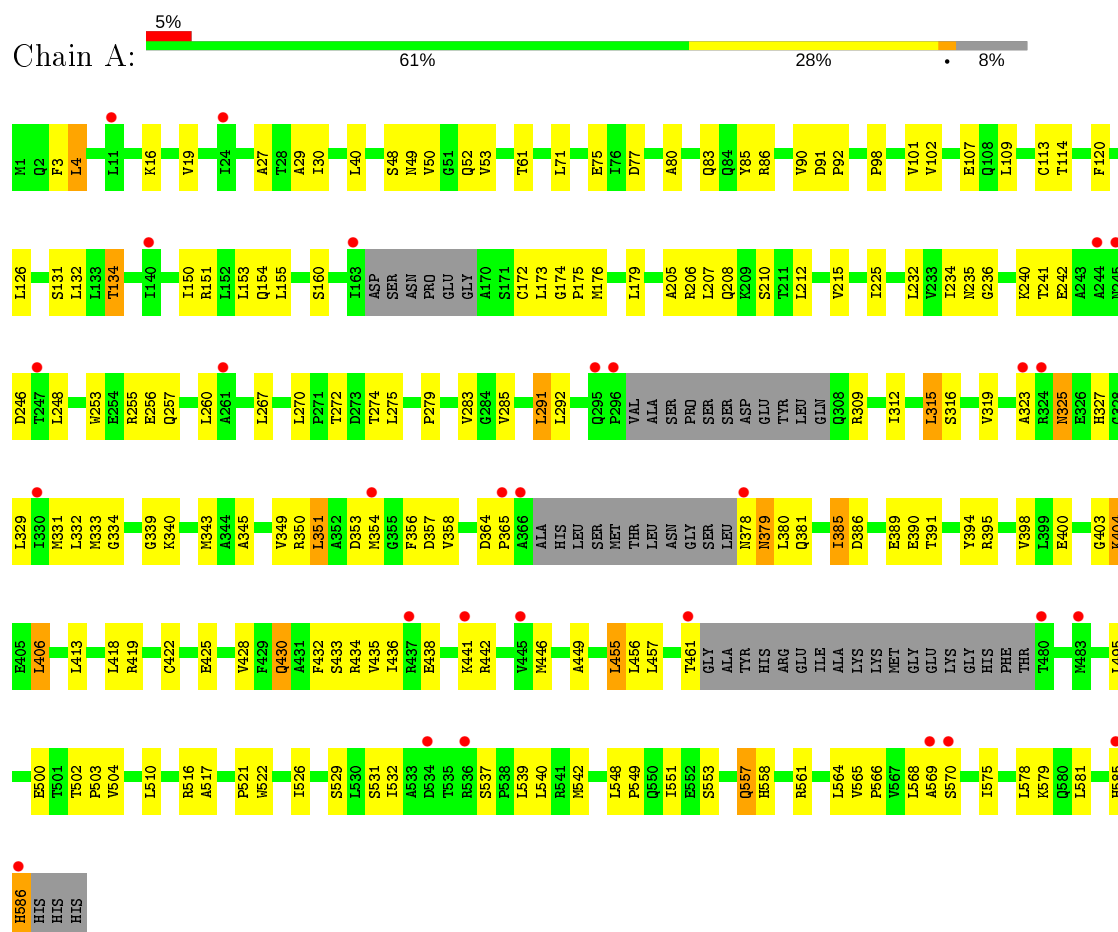
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	192	Total	O	0	0
			192	192		

### 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: ARSENICAL PUMP-DRIVING ATPASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.90Å 75.94Å 222.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.15 – 2.15 25.15 – 2.14	Depositor EDS
% Data completeness (in resolution range)	94.1 (25.15-2.15) 93.8 (25.15-2.14)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.13Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.215 , 0.262 0.208 , 0.256	Depositor DCC
$R_{free}$ test set	2621 reflections (7.65%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 60.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4389	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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: MG, ADP, CL, TAS, CD, 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	0.41	0/4189	0.67	0/5694

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4122	0	4198	159	0
2	A	2	0	0	0	0
3	A	8	0	0	0	0
4	A	3	0	0	1	0
5	A	54	0	24	3	0
6	A	4	0	0	0	0
7	A	4	0	0	0	0
8	A	192	0	0	4	0
All	All	4389	0	4222	159	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 19.

All (159) 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:27:ALA:HB1	1:A:292:LEU:HD21	1.41	0.98
1:A:329:LEU:HD11	1:A:446:MET:HE2	1.53	0.89
1:A:381:GLN:NE2	1:A:442:ARG:HH22	1.73	0.86
1:A:381:GLN:HE21	1:A:442:ARG:NH1	1.80	0.79
1:A:114:THR:OG1	1:A:175:PRO:HG3	1.83	0.78
1:A:434:ARG:HG3	1:A:435:VAL:HG13	1.66	0.76
1:A:385:ILE:HD13	1:A:390:GLU:HG3	1.69	0.75
1:A:283:VAL:O	1:A:283:VAL:HG22	1.87	0.74
1:A:381:GLN:HE22	1:A:442:ARG:HH22	1.32	0.74
1:A:329:LEU:HD11	1:A:446:MET:CE	2.18	0.73
1:A:537:SER:OG	1:A:540:LEU:HD23	1.88	0.73
1:A:30:ILE:HD13	1:A:285:VAL:HG13	1.71	0.73
1:A:381:GLN:HE21	1:A:442:ARG:HH12	1.34	0.72
1:A:381:GLN:NE2	1:A:442:ARG:NH2	2.38	0.71
1:A:107:GLU:OE1	1:A:516:ARG:NH2	2.23	0.71
1:A:315:LEU:O	1:A:319:VAL:HG23	1.92	0.70
1:A:50:VAL:O	1:A:53:VAL:HG22	1.90	0.70
1:A:526:ILE:HB	1:A:564:LEU:HD23	1.73	0.70
1:A:422:CYS:O	1:A:425:GLU:HG2	1.91	0.69
1:A:345:ALA:HB1	1:A:578:LEU:HD21	1.73	0.69
1:A:205:ALA:HB2	1:A:215:VAL:HG21	1.74	0.69
1:A:275:LEU:HD13	1:A:291:LEU:HD22	1.75	0.68
1:A:3:PHE:CE1	1:A:4:LEU:HD13	2.29	0.68
1:A:430:GLN:HE21	1:A:430:GLN:HA	1.60	0.67
1:A:441:LYS:N	1:A:441:LYS:HD2	2.10	0.67
1:A:248:LEU:HD12	1:A:569:ALA:HB2	1.77	0.66
1:A:354:MET:HG3	1:A:356:PHE:CD2	2.31	0.66
1:A:131:SER:O	1:A:134:THR:HB	1.96	0.65
1:A:430:GLN:CA	1:A:430:GLN:HE21	2.10	0.65
1:A:208:GLN:OE1	1:A:210:SER:HB3	1.96	0.65
1:A:357:ASP:OD2	1:A:442:ARG:HD3	1.97	0.65
1:A:395:ARG:HH12	1:A:419:ARG:HD3	1.61	0.64
1:A:345:ALA:O	1:A:349:VAL:HG23	1.99	0.63
1:A:113:CYS:HB3	4:A:599:CL:CL	2.36	0.63
1:A:502:THR:HB	1:A:503:PRO:HD3	1.80	0.62
1:A:329:LEU:HD22	1:A:436:ILE:HG23	1.81	0.62
1:A:495:LEU:HD13	1:A:521:PRO:HB3	1.81	0.62
1:A:172:CYS:O	1:A:175:PRO:HD2	2.00	0.61
1:A:381:GLN:HE21	1:A:442:ARG:CZ	2.13	0.61
1:A:267:LEU:HA	1:A:270:LEU:HD13	1.83	0.60
1:A:385:ILE:C	1:A:385:ILE:HD12	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:MET:HG2	1:A:446:MET:HE3	1.84	0.59
1:A:354:MET:CE	1:A:356:PHE:HE2	2.15	0.58
1:A:83:GLN:HG3	1:A:86:ARG:NH2	2.18	0.57
1:A:398:VAL:HG11	1:A:418:LEU:CD2	2.33	0.57
1:A:235:ASN:HD21	5:A:590:ADP:HN61	1.52	0.57
1:A:279:PRO:HB2	1:A:542:MET:HG2	1.86	0.57
1:A:27:ALA:HB1	1:A:292:LEU:CD2	2.27	0.57
1:A:385:ILE:HD13	1:A:390:GLU:CG	2.36	0.56
1:A:404:LYS:HA	1:A:404:LYS:HZ2	1.71	0.56
1:A:398:VAL:HG11	1:A:418:LEU:HD21	1.87	0.56
1:A:85:TYR:HE2	1:A:175:PRO:O	1.89	0.55
1:A:207:LEU:HD13	1:A:256:GLU:HB3	1.87	0.55
1:A:381:GLN:NE2	1:A:442:ARG:HH12	2.02	0.55
1:A:234:ILE:HB	1:A:274:THR:HG22	1.88	0.55
1:A:548:LEU:HB2	1:A:549:PRO:HD3	1.87	0.55
1:A:585:HIS:ND1	1:A:586:HIS:N	2.55	0.54
1:A:120:PHE:CD1	1:A:153:LEU:HD13	2.43	0.54
1:A:207:LEU:HG	1:A:234:ILE:HG21	1.90	0.53
1:A:260:LEU:C	1:A:260:LEU:HD13	2.28	0.53
1:A:283:VAL:O	1:A:283:VAL:CG2	2.55	0.53
1:A:225:ILE:O	1:A:225:ILE:HG22	2.08	0.53
1:A:456:LEU:HD21	1:A:517:ALA:HA	1.90	0.53
1:A:438:GLU:OE1	1:A:442:ARG:NH2	2.42	0.52
1:A:16:LYS:HG2	1:A:19:VAL:HG13	1.91	0.52
1:A:386:ASP:O	1:A:389:GLU:HG2	2.08	0.52
1:A:391:THR:O	1:A:395:ARG:HG3	2.09	0.52
1:A:386:ASP:HB3	1:A:389:GLU:HG2	1.91	0.52
1:A:351:LEU:O	1:A:354:MET:HG2	2.10	0.51
1:A:432:PHE:O	1:A:436:ILE:HG13	2.11	0.51
1:A:255:ARG:HD3	1:A:570:SER:HA	1.93	0.51
1:A:586:HIS:CD2	1:A:586:HIS:C	2.84	0.51
1:A:568:LEU:HG	1:A:581:LEU:HD23	1.94	0.50
1:A:98:PRO:HG2	1:A:101:VAL:CG2	2.42	0.50
1:A:242:GLU:HG2	1:A:539:LEU:HB3	1.93	0.49
1:A:260:LEU:HD13	1:A:260:LEU:O	2.12	0.49
1:A:353:ASP:OD1	1:A:579:LYS:HE2	2.12	0.49
1:A:235:ASN:HD22	1:A:275:LEU:HB2	1.78	0.49
1:A:333:MET:HG2	1:A:449:ALA:HB3	1.94	0.49
1:A:323:ALA:CB	1:A:354:MET:HE2	2.43	0.49
1:A:385:ILE:HD11	1:A:428:VAL:HG22	1.95	0.49
1:A:155:LEU:HD13	1:A:413:LEU:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASN:O	1:A:379:ASN:OD1	2.31	0.48
1:A:255:ARG:HD3	1:A:570:SER:CA	2.43	0.48
1:A:364:ASP:HB2	8:A:880:HOH:O	2.14	0.48
1:A:292:LEU:HD22	1:A:292:LEU:N	2.29	0.48
1:A:532:ILE:HG12	1:A:532:ILE:O	2.14	0.48
1:A:516:ARG:HD2	8:A:790:HOH:O	2.13	0.48
1:A:225:ILE:O	1:A:225:ILE:CG2	2.61	0.48
1:A:394:TYR:O	1:A:398:VAL:HG12	2.13	0.48
1:A:240:LYS:HA	1:A:253:TRP:CD1	2.48	0.47
1:A:354:MET:HE3	1:A:356:PHE:HE2	1.78	0.47
1:A:248:LEU:CD1	1:A:569:ALA:HB2	2.44	0.47
1:A:339:GLY:HA2	5:A:591:ADP:O2A	2.13	0.47
1:A:575:ILE:O	1:A:579:LYS:HG3	2.14	0.47
1:A:568:LEU:O	1:A:569:ALA:HB3	2.14	0.47
1:A:319:VAL:CG1	1:A:351:LEU:HD13	2.45	0.47
1:A:235:ASN:ND2	5:A:590:ADP:HN61	2.13	0.47
1:A:334:GLY:N	1:A:340:LYS:HD3	2.30	0.47
1:A:86:ARG:HD3	1:A:109:LEU:O	2.14	0.47
1:A:16:LYS:CG	1:A:19:VAL:HG13	2.44	0.47
1:A:275:LEU:HD13	1:A:291:LEU:CD2	2.44	0.47
1:A:309:ARG:HG2	1:A:531:SER:O	2.15	0.46
1:A:208:GLN:O	1:A:212:LEU:HD23	2.15	0.46
1:A:16:LYS:O	1:A:19:VAL:HG22	2.15	0.46
1:A:553:SER:O	1:A:557:GLN:HB3	2.16	0.46
1:A:312:ILE:CD1	1:A:551:ILE:CG2	2.93	0.46
1:A:91:ASP:HB2	1:A:92:PRO:HD3	1.96	0.46
1:A:325:ASN:N	1:A:325:ASN:OD1	2.47	0.45
1:A:207:LEU:CD1	1:A:256:GLU:HB3	2.46	0.45
1:A:312:ILE:HD11	1:A:551:ILE:CG2	2.46	0.45
1:A:174:GLY:N	1:A:175:PRO:CD	2.80	0.45
1:A:316:SER:OG	1:A:350:ARG:NH2	2.49	0.45
1:A:529:SER:HB3	1:A:532:ILE:HG22	1.98	0.45
1:A:354:MET:HG3	1:A:356:PHE:CE2	2.51	0.45
1:A:173:LEU:O	1:A:176:MET:HG2	2.17	0.45
1:A:558:HIS:HD2	8:A:778:HOH:O	1.99	0.45
1:A:241:THR:HG23	1:A:242:GLU:H	1.82	0.44
1:A:441:LYS:N	1:A:441:LYS:CD	2.78	0.44
1:A:235:ASN:ND2	1:A:236:GLY:H	2.15	0.44
1:A:179:LEU:HD23	1:A:179:LEU:HA	1.85	0.44
1:A:403:GLY:O	1:A:406:LEU:HB2	2.18	0.44
1:A:565:VAL:HG13	1:A:566:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:VAL:HG21	1:A:578:LEU:HD23	2.00	0.44
1:A:16:LYS:HG2	1:A:19:VAL:CG1	2.48	0.44
1:A:400:GLU:O	1:A:404:LYS:HD2	2.18	0.44
1:A:568:LEU:HG	1:A:581:LEU:CD2	2.48	0.43
1:A:90:VAL:HG13	1:A:102:VAL:HG13	2.00	0.43
1:A:292:LEU:HD22	1:A:292:LEU:H	1.83	0.43
1:A:500:GLU:O	1:A:504:VAL:HG23	2.19	0.43
1:A:29:ALA:HB1	1:A:71:LEU:HD13	1.99	0.43
1:A:77:ASP:HB3	1:A:80:ALA:HB3	2.00	0.43
1:A:48:SER:HA	8:A:868:HOH:O	2.18	0.43
1:A:270:LEU:N	1:A:270:LEU:HD12	2.34	0.43
1:A:433:SER:HA	1:A:436:ILE:HD12	2.00	0.43
1:A:83:GLN:HG3	1:A:86:ARG:HH22	1.84	0.43
1:A:532:ILE:HG23	1:A:566:PRO:HB3	2.00	0.42
1:A:332:LEU:CD2	1:A:343:MET:HB2	2.49	0.42
1:A:422:CYS:HA	1:A:425:GLU:HG2	2.01	0.42
1:A:430:GLN:CA	1:A:430:GLN:NE2	2.81	0.42
1:A:49:ASN:O	1:A:52:GLN:HB3	2.20	0.42
1:A:151:ARG:HA	1:A:154:GLN:HG2	2.01	0.42
1:A:232:LEU:O	1:A:272:THR:HA	2.19	0.42
1:A:150:ILE:HG21	1:A:225:ILE:HG21	2.02	0.42
1:A:241:THR:HG23	1:A:242:GLU:N	2.33	0.42
1:A:358:VAL:O	1:A:380:LEU:HA	2.20	0.42
1:A:455:LEU:HD12	1:A:455:LEU:HA	1.87	0.41
1:A:381:GLN:HE21	1:A:442:ARG:NH2	2.07	0.41
1:A:529:SER:HB3	1:A:532:ILE:CG2	2.50	0.41
1:A:279:PRO:O	1:A:542:MET:HG3	2.20	0.41
1:A:364:ASP:HA	1:A:365:PRO:HD2	1.96	0.41
1:A:48:SER:HB3	1:A:75:GLU:OE2	2.20	0.41
1:A:206:ARG:O	1:A:212:LEU:CD2	2.69	0.41
1:A:441:LYS:H	1:A:441:LYS:HD2	1.84	0.41
1:A:4:LEU:HD12	1:A:4:LEU:HA	1.89	0.41
1:A:522:TRP:CD1	1:A:561:ARG:NH2	2.88	0.41
1:A:400:GLU:O	1:A:404:LYS:CD	2.69	0.40
1:A:332:LEU:HD23	1:A:343:MET:HB2	2.04	0.40
1:A:564:LEU:HD23	1:A:564:LEU:HA	1.93	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	530/589 (90%)	502 (95%)	24 (4%)	4 (1%)	19	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	SER
1	A	557	GLN
1	A	379	ASN
1	A	246	ASP

### 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	447/487 (92%)	426 (95%)	21 (5%)	26	23

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	40	LEU
1	A	61	THR
1	A	126	LEU
1	A	132	LEU
1	A	134	THR
1	A	257	GLN

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Mol	Chain	Res	Type
1	A	291	LEU
1	A	315	LEU
1	A	325	ASN
1	A	327	HIS
1	A	351	LEU
1	A	385	ILE
1	A	404	LYS
1	A	406	LEU
1	A	430	GLN
1	A	455	LEU
1	A	457	LEU
1	A	461	THR
1	A	510	LEU
1	A	586	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	52	GLN
1	A	106	ASN
1	A	138	HIS
1	A	154	GLN
1	A	229	ASN
1	A	235	ASN
1	A	245	ASN
1	A	262	ASN
1	A	381	GLN
1	A	430	GLN
1	A	509	ASN
1	A	586	HIS

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 13 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
7	TAS	A	701	-	0,3,3	0.00	-	0,3,3	0.00	-
6	AF3	A	700	8,2,5	0,3,3	0.00	-	-		
5	ADP	A	590	2	24,29,29	1.33	4 (16%)	29,45,45	4.19	15 (51%)
5	ADP	A	591	2,6	24,29,29	1.29	3 (12%)	29,45,45	4.16	12 (41%)

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
5	ADP	A	590	2	-	2/12/32/32	0/3/3/3
5	ADP	A	591	2,6	-	3/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	591	ADP	C8-N7	-3.85	1.27	1.34
5	A	590	ADP	C8-N7	-3.40	1.28	1.34
5	A	590	ADP	C2'-C3'	2.57	1.60	1.53
5	A	590	ADP	PA-O2A	-2.16	1.45	1.55
5	A	591	ADP	PA-O2A	-2.10	1.45	1.55
5	A	591	ADP	C2'-C3'	2.10	1.59	1.53
5	A	590	ADP	C2-N3	2.00	1.35	1.32

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	591	ADP	O4'-C1'-C2'	-13.13	87.73	106.93
5	A	590	ADP	O4'-C1'-C2'	-11.97	89.43	106.93
5	A	590	ADP	C3'-C2'-C1'	8.63	113.97	100.98
5	A	591	ADP	C3'-C2'-C1'	8.12	113.20	100.98
5	A	590	ADP	PA-O5'-C5'	7.90	168.03	121.68
5	A	591	ADP	PA-O5'-C5'	7.80	167.41	121.68
5	A	591	ADP	C5'-C4'-C3'	7.63	143.78	115.18
5	A	591	ADP	N3-C2-N1	-6.44	118.61	128.68
5	A	590	ADP	C5'-C4'-C3'	6.37	139.06	115.18
5	A	590	ADP	N3-C2-N1	-6.24	118.93	128.68
5	A	590	ADP	O4'-C4'-C5'	-6.23	88.88	109.37
5	A	591	ADP	O4'-C4'-C5'	-5.55	91.12	109.37
5	A	590	ADP	O2A-PA-O1A	4.32	133.61	112.24
5	A	591	ADP	O4'-C4'-C3'	-4.14	96.93	105.11
5	A	590	ADP	O4'-C4'-C3'	-3.90	97.40	105.11
5	A	590	ADP	C5-C6-N6	3.32	125.39	120.35
5	A	590	ADP	C4-C5-N7	-3.30	105.96	109.40
5	A	590	ADP	C1'-N9-C4	-3.25	120.93	126.64
5	A	591	ADP	C1'-N9-C4	-3.18	121.05	126.64
5	A	591	ADP	O2A-PA-O1A	2.93	126.72	112.24
5	A	591	ADP	C2-N1-C6	2.89	123.70	118.75
5	A	590	ADP	O2'-C2'-C1'	2.89	121.52	110.85
5	A	590	ADP	O5'-PA-O1A	-2.76	98.28	109.07
5	A	590	ADP	N6-C6-N1	-2.40	113.58	118.57
5	A	591	ADP	O2'-C2'-C1'	2.38	119.63	110.85
5	A	591	ADP	O2B-PB-O3A	-2.06	97.72	104.64
5	A	590	ADP	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	591	ADP	O4'-C4'-C5'-O5'
5	A	590	ADP	O4'-C4'-C5'-O5'
5	A	591	ADP	C3'-C4'-C5'-O5'
5	A	590	ADP	C3'-C4'-C5'-O5'
5	A	591	ADP	PB-O3A-PA-O2A

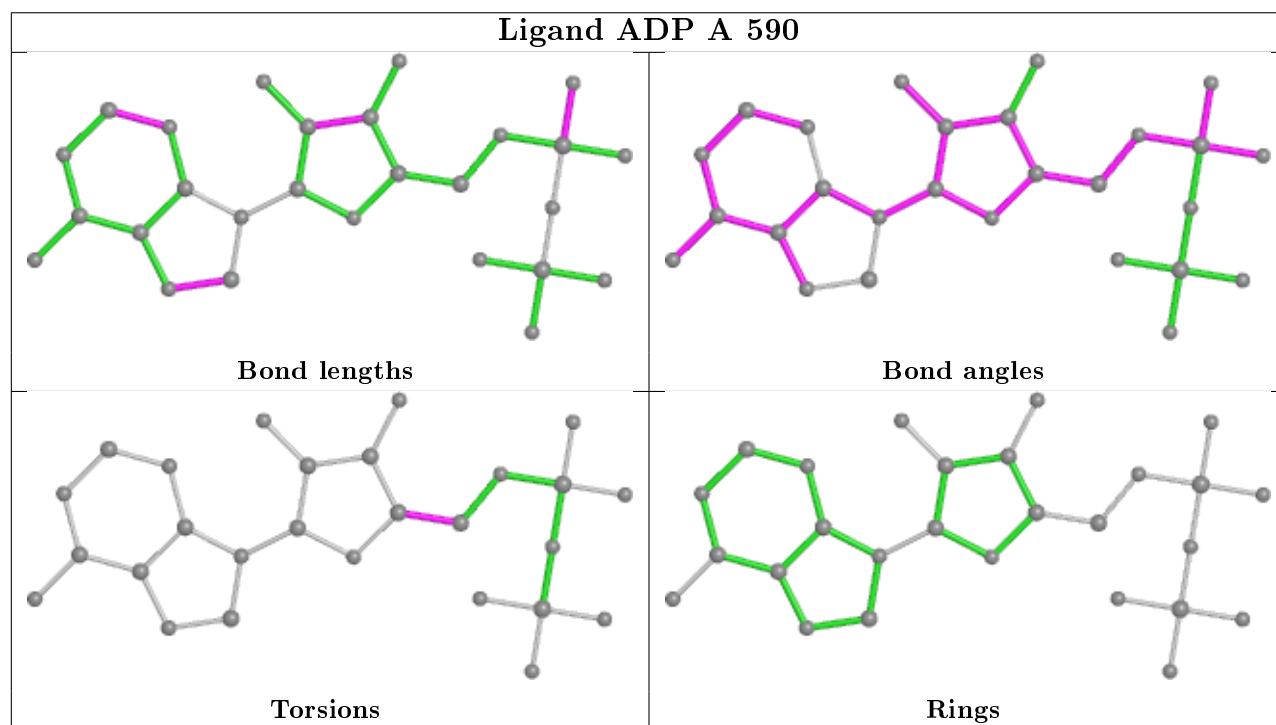
There are no ring outliers.

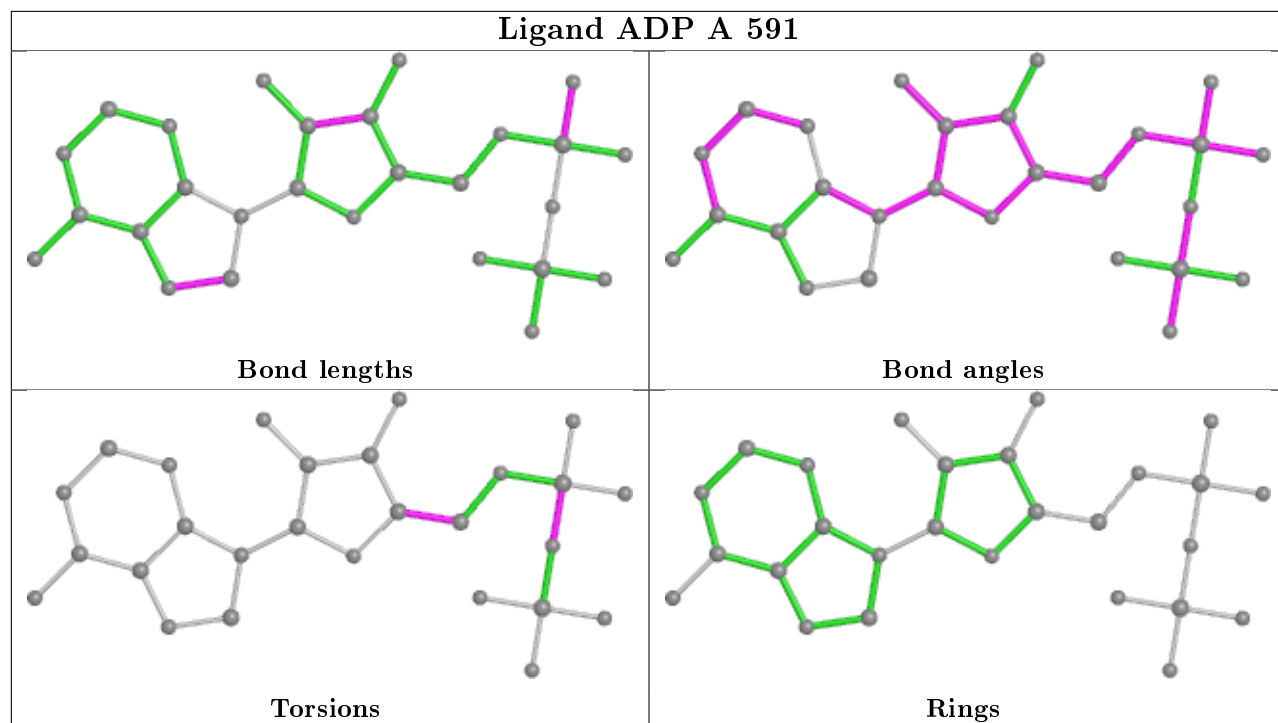
2 monomers are involved in 3 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	590	ADP	2	0
5	A	591	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 [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, 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	540/589 (91%)	0.22	29 (5%) 25 34	22, 39, 69, 83	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	ASN	5.5
1	A	244	ALA	4.8
1	A	296	PRO	4.4
1	A	365	PRO	4.1
1	A	366	ALA	4.1
1	A	585	HIS	4.0
1	A	461	THR	3.9
1	A	445	VAL	3.9
1	A	569	ALA	3.8
1	A	295	GLN	3.7
1	A	483	MET	3.4
1	A	536	ARG	3.3
1	A	586	HIS	3.2
1	A	570	SER	3.2
1	A	437	ARG	3.2
1	A	378	ASN	3.1
1	A	261	ALA	3.0
1	A	480	THR	2.9
1	A	140	ILE	2.9
1	A	324	ARG	2.7
1	A	163	ILE	2.6
1	A	247	THR	2.6
1	A	330	ILE	2.4
1	A	534	ASP	2.4
1	A	24	ILE	2.3
1	A	441	LYS	2.3
1	A	323	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	354	MET	2.0
1	A	11	LEU	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.

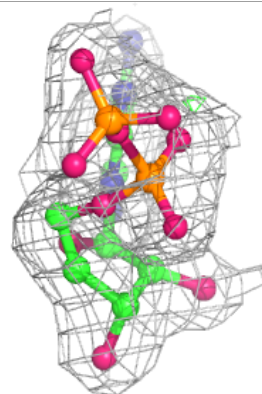
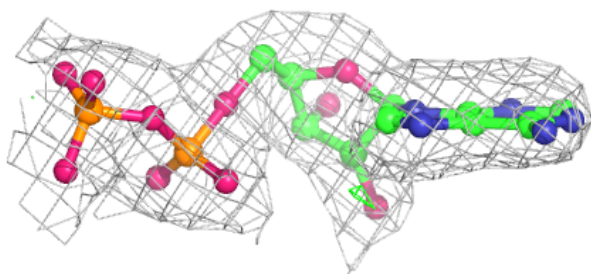
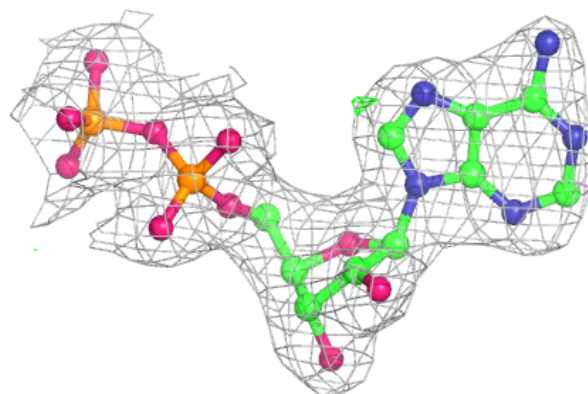
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	TAS	A	701	4/4	0.78	0.43	56,58,60,73	4
3	CD	A	603	1/1	0.94	0.04	79,79,79,79	0
3	CD	A	604	1/1	0.94	0.04	52,52,52,52	1
2	MG	A	593	1/1	0.95	0.11	28,28,28,28	0
6	AF3	A	700	4/4	0.96	0.07	49,57,59,64	0
4	CL	A	599	1/1	0.97	0.08	61,61,61,61	0
3	CD	A	601	1/1	0.98	0.08	57,57,57,57	0
5	ADP	A	591	27/27	0.98	0.09	30,37,47,51	0
5	ADP	A	590	27/27	0.98	0.11	25,36,42,43	0
2	MG	A	592	1/1	0.99	0.11	13,13,13,13	0
3	CD	A	602	1/1	0.99	0.07	55,55,55,55	0
4	CL	A	597	1/1	0.99	0.05	27,27,27,27	0
3	CD	A	600	1/1	0.99	0.03	54,54,54,54	0
3	CD	A	594	1/1	0.99	0.09	32,32,32,32	0
4	CL	A	598	1/1	0.99	0.08	27,27,27,27	0
3	CD	A	596	1/1	1.00	0.09	30,30,30,30	0
3	CD	A	595	1/1	1.00	0.10	28,28,28,28	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.

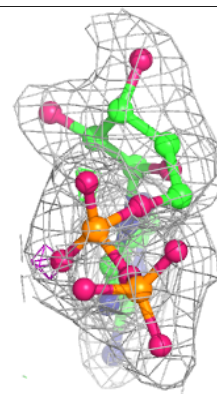
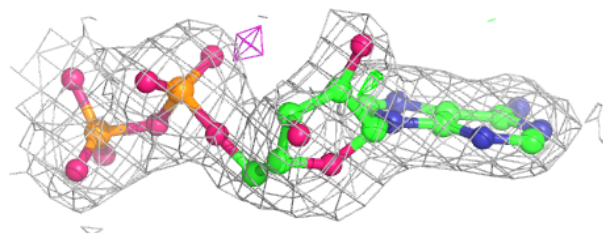
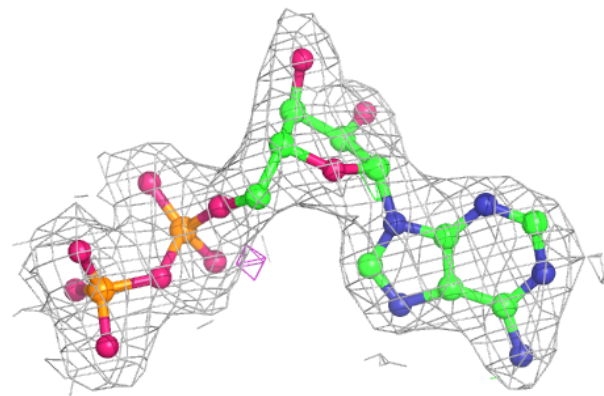
**Electron density around ADP A 591:**

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



**Electron density around ADP A 590:**

$2mF_o-DF_c$  (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.