



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:59 am BST

PDB ID : 1F48  
Title : CRYSTAL STRUCTURE OF THE ESCHERICHIA COLI ARSENITE-TRANSLOCATING ATPASE  
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Deposited on : 2000-06-07  
Resolution : 2.30 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

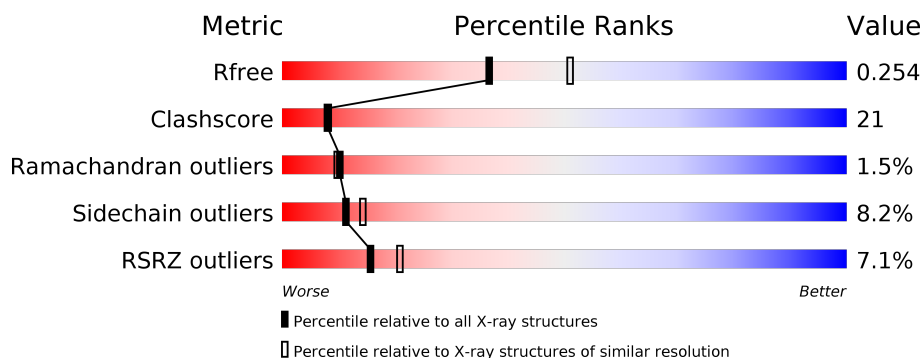
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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
2	SB	A	594	-	-	X	-
2	SB	A	595	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SB	A	596	-	-	X	-
6	SBO	A	701	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4467 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 ARSENITE-TRANSLOCATING ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4178	2629	737	797	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 ANTIMONY (III) ION (three-letter code: SB) (formula: Sb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Sb	0	0
			3	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

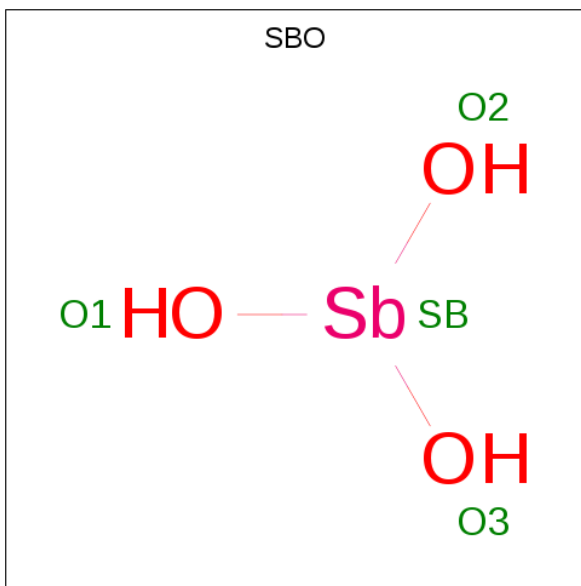
- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	Cd	0	0
			6	6		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

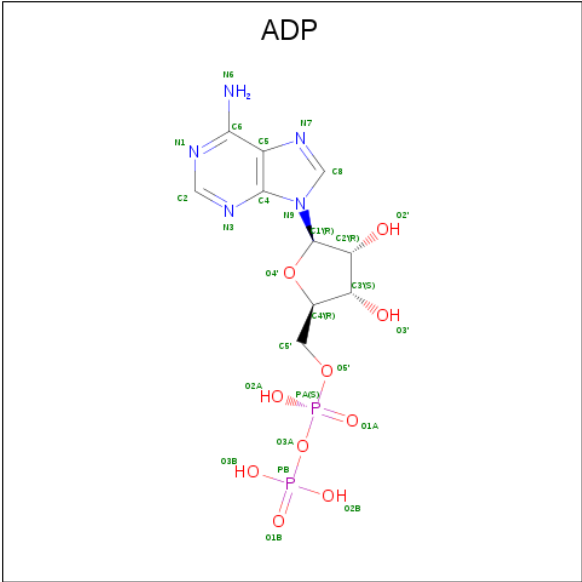
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Cl	0	0
			3	3		

- Molecule 6 is TRIHYDROXYANTIMONITE(III) (three-letter code: SBO) (formula: H<sub>3</sub>O<sub>3</sub>Sb).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	Sb	0	0
			4	3	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	217	Total	O	0	0
			217	217		

### 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: ARSENITE-TRANSLOCATING ATPASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.52Å 75.72Å 222.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.37 – 2.30 26.37 – 2.29	Depositor EDS
% Data completeness (in resolution range)	94.4 (26.37-2.30) 93.7 (26.37-2.29)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.206 , 0.263 0.193 , 0.254	Depositor DCC
$R_{free}$ test set	2623 reflections (9.44%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4467	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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, CD, SB, SBO

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	0.53	0/4248	0.78	4/5777 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	419	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	516	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	171	SER	N-CA-C	5.29	125.30	111.00
1	A	516	ARG	NE-CZ-NH1	5.05	122.82	120.30

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	4178	0	4247	176	1
2	A	3	0	0	14	0
3	A	2	0	0	0	0
4	A	6	0	0	0	0
5	A	3	0	0	2	0
6	A	4	0	0	4	0
7	A	54	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	217	0	0	7	1
All	All	4467	0	4271	182	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (182) 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:148:HIS:NE2	2:A:596:SB:SB	2.38	1.35
1:A:453:HIS:NE2	2:A:595:SB:SB	2.41	1.33
1:A:172:CYS:SG	2:A:594:SB:SB	2.69	1.30
2:A:595:SB:SB	5:A:598:CL:CL	2.68	1.29
1:A:420:SER:OG	2:A:596:SB:SB	2.34	1.25
2:A:595:SB:SB	5:A:597:CL:CL	2.82	1.14
2:A:596:SB:SB	8:A:788:HOH:O	2.55	1.04
1:A:367:ALA:HB3	1:A:384:ARG:HH12	1.20	1.04
1:A:385:ILE:HD11	1:A:428:VAL:HG13	1.49	0.95
2:A:595:SB:SB	8:A:720:HOH:O	2.62	0.95
1:A:329:LEU:HD11	1:A:446:MET:HE3	1.48	0.94
1:A:27:ALA:HB1	1:A:292:LEU:HD21	1.54	0.89
1:A:404:LYS:HA	1:A:404:LYS:HE3	1.57	0.87
1:A:381:GLN:NE2	1:A:442:ARG:HH22	1.78	0.82
1:A:368:HIS:ND1	1:A:369:LEU:N	2.30	0.80
1:A:79:GLN:O	1:A:83:GLN:HG3	1.82	0.79
1:A:30:ILE:HD13	1:A:285:VAL:HG13	1.65	0.79
1:A:329:LEU:HD11	1:A:446:MET:CE	2.13	0.79
1:A:369:LEU:HD21	1:A:382:VAL:HG21	1.64	0.78
2:A:594:SB:SB	8:A:717:HOH:O	2.82	0.78
1:A:157:GLY:O	1:A:161:SER:HB2	1.86	0.76
1:A:367:ALA:HB3	1:A:384:ARG:NH1	2.01	0.74
1:A:114:THR:OG1	1:A:175:PRO:HG3	1.87	0.74
1:A:351:LEU:O	1:A:354:MET:HG2	1.90	0.72
1:A:353:ASP:OD1	1:A:579:LYS:HE2	1.90	0.72
1:A:386:ASP:HB3	1:A:389:GLU:HG2	1.73	0.71
1:A:391:THR:O	1:A:395:ARG:HG3	1.91	0.70
1:A:235:ASN:HD22	1:A:275:LEU:HB2	1.56	0.70
1:A:537:SER:OG	1:A:540:LEU:HD23	1.91	0.69
1:A:502:THR:HB	1:A:503:PRO:HD3	1.74	0.69
1:A:148:HIS:CD2	2:A:596:SB:SB	3.27	0.68
1:A:238:LEU:HD22	1:A:239:PRO:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD13	1:A:256:GLU:HB3	1.76	0.67
1:A:128:THR:HG22	1:A:188:TYR:HD1	1.59	0.67
1:A:329:LEU:HD22	1:A:436:ILE:HG23	1.78	0.66
2:A:594:SB:SB	2:A:595:SB:SB	3.74	0.66
1:A:345:ALA:O	1:A:349:VAL:HG23	1.97	0.65
1:A:381:GLN:HE21	1:A:442:ARG:NH2	1.94	0.64
1:A:248:LEU:HD12	1:A:569:ALA:HB2	1.80	0.64
1:A:404:LYS:CA	1:A:404:LYS:HE3	2.28	0.64
1:A:441:LYS:HG3	8:A:895:HOH:O	1.98	0.63
1:A:3:PHE:CE1	1:A:4:LEU:HD13	2.33	0.63
1:A:354:MET:HG3	1:A:356:PHE:CD2	2.34	0.62
1:A:543:ARG:NH2	6:A:701:SBO:SB	3.12	0.62
1:A:369:LEU:HG	1:A:384:ARG:HH22	1.64	0.62
1:A:368:HIS:CG	1:A:369:LEU:N	2.67	0.62
1:A:436:ILE:HG12	1:A:446:MET:CE	2.30	0.62
1:A:207:LEU:HD11	1:A:260:LEU:HD23	1.80	0.62
1:A:319:VAL:CG1	1:A:351:LEU:HD13	2.30	0.61
1:A:430:GLN:CA	1:A:430:GLN:HE21	2.13	0.61
1:A:312:ILE:CD1	1:A:551:ILE:CG2	2.80	0.60
1:A:163:ILE:O	1:A:164:ASP:C	2.40	0.60
1:A:436:ILE:CD1	1:A:446:MET:HE1	2.32	0.60
1:A:260:LEU:HD13	1:A:260:LEU:O	2.02	0.59
1:A:83:GLN:HB3	8:A:828:HOH:O	2.01	0.59
1:A:107:GLU:OE1	1:A:516:ARG:NH2	2.35	0.59
1:A:16:LYS:HG2	1:A:19:VAL:HG13	1.83	0.59
1:A:532:ILE:HG12	1:A:532:ILE:O	2.03	0.59
1:A:240:LYS:HA	1:A:253:TRP:CD1	2.38	0.59
1:A:381:GLN:NE2	1:A:442:ARG:NH2	2.48	0.59
1:A:585:HIS:CG	1:A:586:HIS:H	2.21	0.59
1:A:131:SER:O	1:A:134:THR:HB	2.03	0.58
1:A:172:CYS:O	1:A:175:PRO:HD2	2.03	0.58
1:A:529:SER:O	1:A:566:PRO:HA	2.03	0.58
1:A:432:PHE:O	1:A:436:ILE:HG13	2.03	0.58
1:A:532:ILE:HD12	1:A:564:LEU:HB3	1.86	0.58
1:A:205:ALA:HB2	1:A:215:VAL:HG21	1.85	0.58
1:A:381:GLN:HE21	1:A:442:ARG:HH22	1.46	0.58
1:A:367:ALA:CB	1:A:384:ARG:HH12	2.06	0.58
1:A:453:HIS:CE1	2:A:595:SB:SB	3.31	0.58
1:A:316:SER:OG	1:A:350:ARG:NH2	2.38	0.57
1:A:354:MET:HE2	1:A:356:PHE:HE2	1.68	0.56
1:A:235:ASN:HD21	7:A:590:ADP:HN61	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:O	1:A:319:VAL:HG23	2.05	0.56
1:A:20:GLY:HA2	7:A:590:ADP:O1A	2.05	0.56
1:A:345:ALA:HB1	1:A:578:LEU:HD21	1.87	0.56
1:A:568:LEU:HG	1:A:581:LEU:HD23	1.87	0.56
1:A:568:LEU:O	1:A:569:ALA:HB3	2.05	0.56
1:A:314:SER:OG	1:A:316:SER:HB2	2.06	0.56
1:A:166:ASN:HD22	1:A:402:LYS:HE2	1.71	0.56
1:A:225:ILE:O	1:A:225:ILE:HG22	2.05	0.55
1:A:163:ILE:HD12	1:A:173:LEU:HD13	1.88	0.55
1:A:207:LEU:HG	1:A:234:ILE:HG21	1.87	0.55
1:A:170:ALA:HB1	1:A:394:TYR:OH	2.06	0.55
1:A:349:VAL:HG21	1:A:578:LEU:HD23	1.87	0.55
1:A:85:TYR:HE2	1:A:175:PRO:O	1.89	0.54
1:A:248:LEU:CD1	1:A:569:ALA:HB2	2.37	0.54
1:A:394:TYR:O	1:A:398:VAL:HG12	2.07	0.54
1:A:167:PRO:HD2	1:A:402:LYS:HE3	1.90	0.53
1:A:434:ARG:CG	1:A:435:VAL:HG13	2.39	0.53
1:A:354:MET:HG3	1:A:356:PHE:CE2	2.45	0.52
1:A:357:ASP:OD2	1:A:442:ARG:HD3	2.10	0.52
1:A:77:ASP:HB3	1:A:80:ALA:HB3	1.92	0.52
1:A:236:GLY:O	1:A:277:LEU:HB2	2.09	0.52
1:A:436:ILE:HG12	1:A:446:MET:HE1	1.91	0.52
1:A:225:ILE:O	1:A:225:ILE:CG2	2.57	0.51
1:A:128:THR:HG22	1:A:188:TYR:CD1	2.42	0.51
1:A:174:GLY:N	1:A:175:PRO:CD	2.73	0.51
1:A:526:ILE:HB	1:A:564:LEU:HD23	1.93	0.51
1:A:292:LEU:HD22	1:A:292:LEU:N	2.25	0.51
1:A:16:LYS:HG2	1:A:19:VAL:CG1	2.40	0.51
1:A:163:ILE:HD12	1:A:173:LEU:CD1	2.41	0.51
1:A:339:GLY:HA2	7:A:591:ADP:O1A	2.10	0.51
1:A:312:ILE:HD11	1:A:551:ILE:HG22	1.92	0.51
1:A:332:LEU:CD2	1:A:343:MET:HB2	2.41	0.50
1:A:436:ILE:HG12	1:A:446:MET:HE2	1.93	0.50
1:A:86:ARG:HD3	1:A:109:LEU:O	2.11	0.50
1:A:542:MET:O	1:A:546:GLN:HG2	2.10	0.50
1:A:120:PHE:CD1	1:A:153:LEU:HD13	2.47	0.50
1:A:532:ILE:HG23	1:A:566:PRO:HB3	1.94	0.50
1:A:543:ARG:HH21	6:A:701:SBO:SB	2.74	0.50
1:A:50:VAL:O	1:A:53:VAL:HG22	2.12	0.49
1:A:317:ALA:O	1:A:320:ASP:HB2	2.12	0.49
1:A:169:GLY:C	1:A:171:SER:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PRO:HG2	1:A:267:LEU:HD12	1.93	0.49
1:A:26:CYS:HB3	1:A:288:LEU:HD13	1.95	0.49
1:A:453:HIS:CD2	2:A:595:SB:SB	3.40	0.49
1:A:430:GLN:HE21	1:A:430:GLN:HA	1.75	0.48
1:A:430:GLN:O	1:A:433:SER:HB2	2.13	0.48
1:A:568:LEU:C	1:A:569:ALA:O	2.50	0.48
1:A:235:ASN:ND2	1:A:275:LEU:HB2	2.25	0.48
1:A:527:ASN:OD1	1:A:528:ASN:N	2.41	0.48
1:A:312:ILE:HD11	1:A:551:ILE:CG2	2.44	0.48
1:A:134:THR:HG22	1:A:135:ARG:HG2	1.95	0.48
1:A:292:LEU:HD22	1:A:292:LEU:H	1.78	0.48
1:A:434:ARG:O	1:A:437:ARG:HG2	2.14	0.47
1:A:258:GLU:HG2	1:A:262:ASN:HD22	1.79	0.47
1:A:401:THR:HG22	1:A:402:LYS:N	2.29	0.47
1:A:318:LEU:HD22	1:A:522:TRP:CZ3	2.50	0.47
1:A:151:ARG:HA	1:A:154:GLN:HG2	1.97	0.47
1:A:245:ASN:O	1:A:245:ASN:OD1	2.32	0.46
1:A:7:ILE:HG22	1:A:8:PRO:O	2.15	0.46
1:A:434:ARG:HG3	1:A:435:VAL:HG13	1.98	0.46
1:A:244:ALA:O	1:A:245:ASN:HB3	2.16	0.46
1:A:206:ARG:NH1	6:A:701:SBO:O3	2.49	0.46
1:A:19:VAL:HG11	8:A:795:HOH:O	2.15	0.46
1:A:235:ASN:ND2	1:A:236:GLY:H	2.14	0.46
1:A:275:LEU:HD13	1:A:291:LEU:HD22	1.98	0.45
1:A:361:THR:HG21	1:A:435:VAL:HG21	1.98	0.45
1:A:482:MET:HE3	1:A:517:ALA:O	2.16	0.45
1:A:369:LEU:CD2	1:A:382:VAL:HG21	2.40	0.45
1:A:418:LEU:O	1:A:423:THR:HG21	2.16	0.45
1:A:568:LEU:HD23	1:A:568:LEU:HA	1.80	0.45
1:A:180:GLU:HA	8:A:734:HOH:O	2.16	0.45
1:A:529:SER:HB3	1:A:532:ILE:HG22	1.98	0.45
1:A:548:LEU:HB2	1:A:549:PRO:HD3	1.98	0.44
1:A:420:SER:HB3	2:A:594:SB:SB	2.97	0.44
1:A:91:ASP:N	1:A:92:PRO:CD	2.81	0.44
1:A:404:LYS:HA	1:A:404:LYS:CE	2.40	0.44
1:A:432:PHE:CD1	1:A:446:MET:SD	3.11	0.44
1:A:282:MET:SD	1:A:282:MET:N	2.84	0.44
1:A:318:LEU:O	1:A:322:ILE:HG13	2.18	0.44
1:A:441:LYS:N	1:A:441:LYS:HD2	2.32	0.44
1:A:20:GLY:O	1:A:24:ILE:HG13	2.18	0.43
1:A:216:ALA:HA	1:A:267:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:ARG:O	1:A:546:GLN:HB2	2.18	0.43
1:A:565:VAL:HG13	1:A:566:PRO:HD2	2.00	0.43
1:A:333:MET:HG2	1:A:449:ALA:HB3	2.00	0.43
1:A:436:ILE:HG22	1:A:436:ILE:O	2.18	0.43
1:A:524:TRP:CG	1:A:559:ALA:HB2	2.54	0.43
1:A:369:LEU:HG	1:A:384:ARG:NH2	2.32	0.43
1:A:332:LEU:HD23	1:A:343:MET:HB2	2.00	0.43
1:A:354:MET:CE	1:A:356:PHE:HE2	2.30	0.43
1:A:564:LEU:HA	1:A:564:LEU:HD23	1.86	0.43
1:A:480:THR:HA	1:A:481:PRO:HD2	1.86	0.42
1:A:436:ILE:CG1	1:A:446:MET:HE1	2.50	0.42
1:A:456:LEU:HD21	1:A:517:ALA:HA	2.00	0.42
1:A:179:LEU:HD23	1:A:179:LEU:HA	1.80	0.42
1:A:90:VAL:HG13	1:A:102:VAL:HG13	2.02	0.42
1:A:404:LYS:N	1:A:404:LYS:HD2	2.35	0.42
1:A:434:ARG:HG2	1:A:435:VAL:HG13	2.02	0.42
1:A:255:ARG:NH1	1:A:570:SER:O	2.49	0.42
1:A:206:ARG:HH22	6:A:701:SBO:SB	2.82	0.41
1:A:318:LEU:HD12	1:A:563:ALA:HB2	2.02	0.41
1:A:240:LYS:HB2	1:A:253:TRP:NE1	2.35	0.41
1:A:403:GLY:HA2	1:A:406:LEU:HD22	2.02	0.41
1:A:404:LYS:O	1:A:405:GLU:HB2	2.20	0.41
1:A:585:HIS:ND1	1:A:586:HIS:N	2.61	0.41
1:A:562:VAL:HG12	1:A:563:ALA:N	2.36	0.41
1:A:312:ILE:HA	1:A:313:PRO:HD3	1.89	0.40
1:A:164:ASP:O	1:A:165:SER:C	2.60	0.40
1:A:240:LYS:O	1:A:241:THR:C	2.58	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LYS:NZ	1:A:240:LYS:NZ[2_655]	2.13	0.07
8:A:860:HOH:O	8:A:860:HOH:O[2_655]	2.16	0.04

## 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	540/589 (92%)	505 (94%)	27 (5%)	8 (2%)	10	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	SER
1	A	164	ASP
1	A	379	ASN
1	A	575	ILE
1	A	166	ASN
1	A	366	ALA
1	A	570	SER
1	A	167	PRO

### 5.3.2 Protein sidechains [i](#)

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	453/487 (93%)	416 (92%)	37 (8%)	11	14

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	40	LEU
1	A	53	VAL

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Mol	Chain	Res	Type
1	A	84	GLN
1	A	104	SER
1	A	126	LEU
1	A	132	LEU
1	A	134	THR
1	A	210	SER
1	A	212	LEU
1	A	229	ASN
1	A	241	THR
1	A	257	GLN
1	A	260	LEU
1	A	291	LEU
1	A	315	LEU
1	A	327	HIS
1	A	350	ARG
1	A	351	LEU
1	A	357	ASP
1	A	368	HIS
1	A	399	LEU
1	A	401	THR
1	A	404	LYS
1	A	406	LEU
1	A	414	LEU
1	A	419	ARG
1	A	430	GLN
1	A	455	LEU
1	A	489	GLU
1	A	495	LEU
1	A	503	PRO
1	A	510	LEU
1	A	534	ASP
1	A	564	LEU
1	A	566	PRO
1	A	585	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	52	GLN
1	A	83	GLN
1	A	138	HIS

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Mol	Chain	Res	Type
1	A	166	ASN
1	A	213	GLN
1	A	229	ASN
1	A	235	ASN
1	A	262	ASN
1	A	327	HIS
1	A	378	ASN
1	A	381	GLN
1	A	430	GLN
1	A	486	GLN
1	A	509	ASN
1	A	586	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 14 are monoatomic - leaving 3 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
6	SBO	A	701	-	0,3,3	0.00	-	-		
7	ADP	A	590	3	24,29,29	1.58	4 (16%)	29,45,45	3.89	15 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	ADP	A	591	3	24,29,29	1.44	4 (16%)	29,45,45	4.09	14 (48%)

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
7	ADP	A	590	3	-	4/12/32/32	0/3/3/3
7	ADP	A	591	3	-	4/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	591	ADP	C8-N7	-3.99	1.27	1.34
7	A	590	ADP	C8-N7	-3.79	1.27	1.34
7	A	590	ADP	C2-N3	2.66	1.36	1.32
7	A	591	ADP	O4'-C1'	2.60	1.44	1.41
7	A	591	ADP	C2-N3	2.37	1.35	1.32
7	A	590	ADP	PA-O1A	-2.35	1.42	1.50
7	A	590	ADP	C2'-C3'	2.29	1.59	1.53
7	A	591	ADP	C2'-C3'	2.23	1.59	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	590	ADP	O4'-C1'-C2'	-11.30	90.42	106.93
7	A	591	ADP	O4'-C1'-C2'	-10.50	91.59	106.93
7	A	590	ADP	C3'-C2'-C1'	8.30	113.48	100.98
7	A	591	ADP	PA-O5'-C5'	7.83	167.59	121.68
7	A	590	ADP	PA-O5'-C5'	7.73	167.01	121.68
7	A	591	ADP	C5'-C4'-C3'	7.52	143.38	115.18
7	A	591	ADP	C3'-C2'-C1'	7.52	112.31	100.98
7	A	591	ADP	O4'-C4'-C5'	-7.22	85.60	109.37
7	A	591	ADP	PA-O3A-PB	6.32	154.52	132.83
7	A	590	ADP	N3-C2-N1	-6.21	118.97	128.68
7	A	590	ADP	C5'-C4'-C3'	5.67	136.44	115.18
7	A	591	ADP	N3-C2-N1	-4.91	121.00	128.68
7	A	590	ADP	C4-C5-N7	-3.84	105.40	109.40
7	A	590	ADP	O2A-PA-O1A	3.69	130.46	112.24
7	A	590	ADP	O2'-C2'-C1'	3.30	123.03	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	591	ADP	O2A-PA-O1A	3.24	128.26	112.24
7	A	590	ADP	O4'-C4'-C5'	-3.22	98.79	109.37
7	A	591	ADP	C1'-N9-C4	-3.21	121.01	126.64
7	A	590	ADP	O4'-C4'-C3'	-3.19	98.80	105.11
7	A	591	ADP	O2'-C2'-C1'	3.17	122.55	110.85
7	A	590	ADP	C1'-N9-C4	-3.03	121.31	126.64
7	A	591	ADP	O3A-PB-O1B	-2.94	94.87	111.19
7	A	591	ADP	O4'-C4'-C3'	-2.92	99.34	105.11
7	A	590	ADP	C5-C6-N6	2.64	124.37	120.35
7	A	590	ADP	O5'-PA-O1A	-2.56	99.06	109.07
7	A	591	ADP	C2-N1-C6	2.52	123.06	118.75
7	A	590	ADP	O3A-PB-O1B	-2.39	97.92	111.19
7	A	591	ADP	O5'-C5'-C4'	-2.36	100.86	108.99
7	A	590	ADP	O3B-PB-O2B	2.22	116.11	107.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	590	ADP	C3'-C4'-C5'-O5'
7	A	591	ADP	O4'-C4'-C5'-O5'
7	A	590	ADP	O4'-C4'-C5'-O5'
7	A	591	ADP	PB-O3A-PA-O1A
7	A	590	ADP	PB-O3A-PA-O1A
7	A	591	ADP	PB-O3A-PA-O2A
7	A	591	ADP	C3'-C4'-C5'-O5'
7	A	590	ADP	PB-O3A-PA-O2A

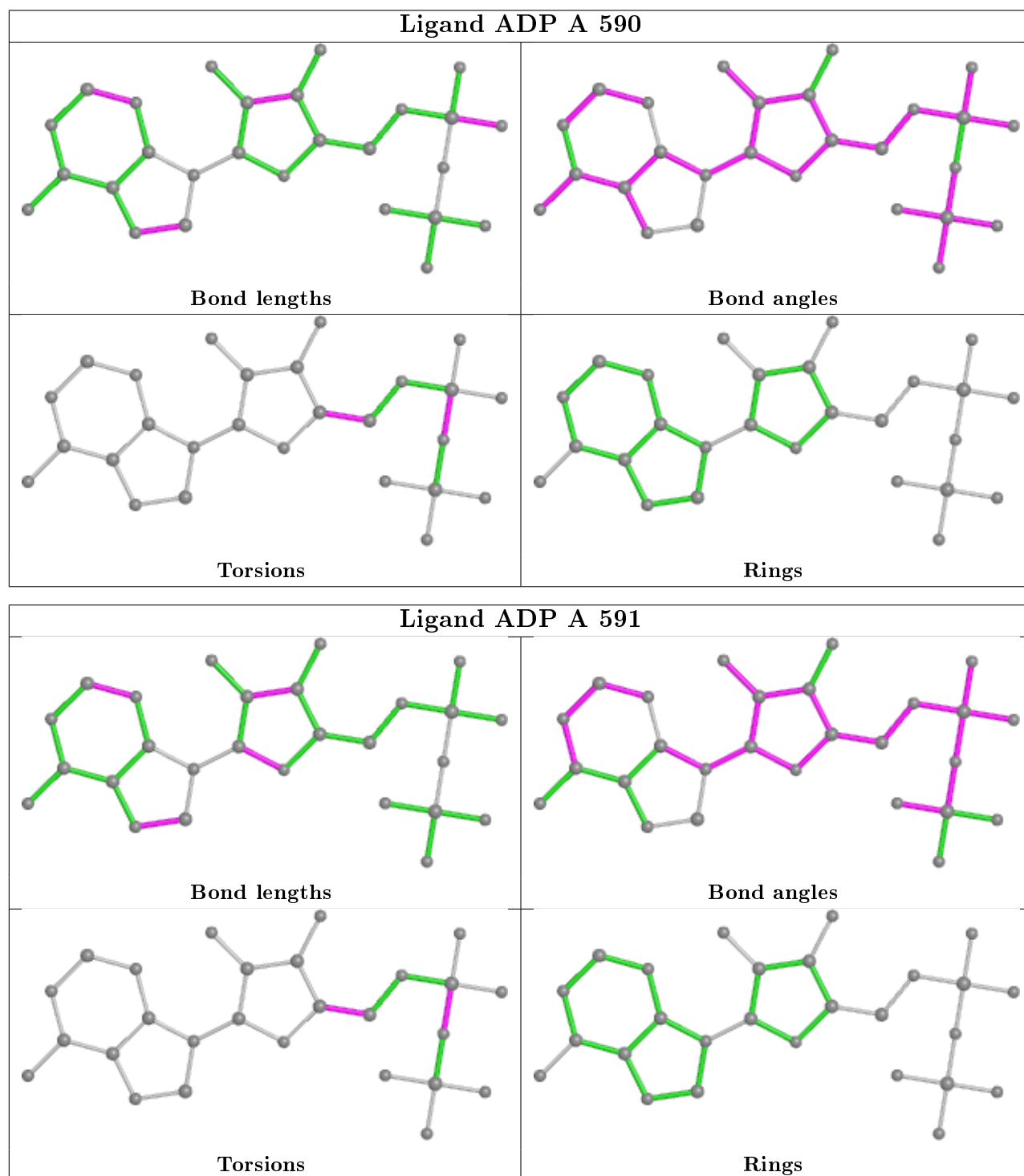
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	701	SBO	4	0
7	A	590	ADP	2	0
7	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

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	548/589 (93%)	0.18	39 (7%) 16 21	27, 46, 82, 127	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	165	SER	8.0
1	A	170	ALA	5.2
1	A	585	HIS	4.3
1	A	166	ASN	4.3
1	A	295	GLN	4.2
1	A	244	ALA	4.2
1	A	536	ARG	3.9
1	A	245	ASN	3.9
1	A	445	VAL	3.9
1	A	167	PRO	3.5
1	A	168	GLU	3.4
1	A	437	ARG	3.4
1	A	164	ASP	3.3
1	A	296	PRO	3.2
1	A	480	THR	3.2
1	A	461	THR	3.1
1	A	441	LYS	3.0
1	A	169	GLY	2.8
1	A	369	LEU	2.7
1	A	534	ASP	2.7
1	A	69	PRO	2.6
1	A	541	ARG	2.4
1	A	261	ALA	2.4
1	A	140	ILE	2.4
1	A	163	ILE	2.4
1	A	586	HIS	2.4
1	A	432	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	260	LEU	2.3
1	A	247	THR	2.2
1	A	368	HIS	2.2
1	A	570	SER	2.2
1	A	243	ALA	2.2
1	A	330	ILE	2.1
1	A	555	LYS	2.1
1	A	366	ALA	2.1
1	A	293	SER	2.1
1	A	324	ARG	2.1
1	A	331	MET	2.1
1	A	569	ALA	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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.

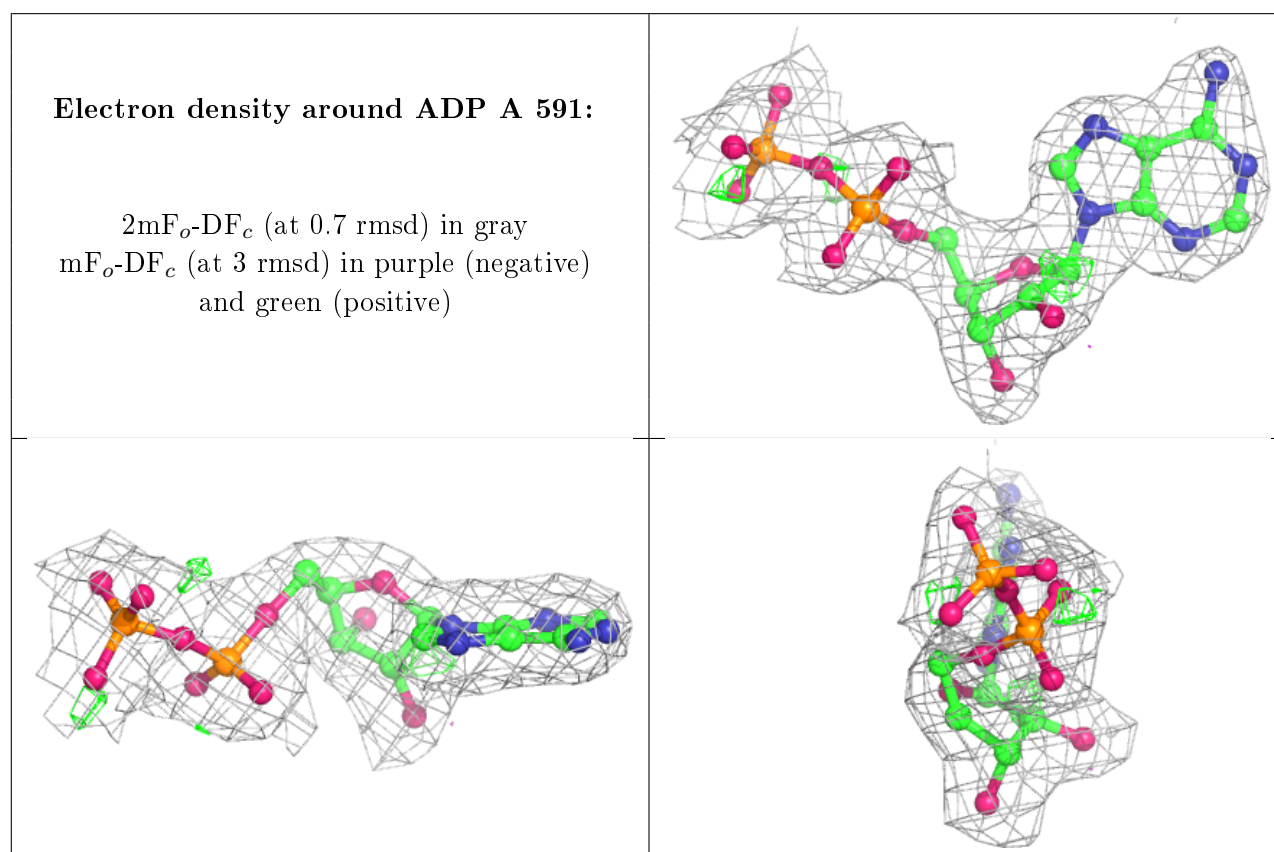
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CD	A	605	1/1	0.59	0.18	120,120,120,120	1
6	SBO	A	701	4/4	0.83	0.39	73,75,78,93	4
4	CD	A	604	1/1	0.93	0.07	58,58,58,58	1
3	MG	A	592	1/1	0.95	0.14	32,32,32,32	0
5	CL	A	598	1/1	0.97	0.09	31,31,31,31	0
7	ADP	A	591	27/27	0.97	0.10	31,41,50,52	0
4	CD	A	603	1/1	0.97	0.17	68,68,68,68	1
3	MG	A	593	1/1	0.97	0.17	34,34,34,34	0
7	ADP	A	590	27/27	0.98	0.13	30,40,45,46	0
4	CD	A	601	1/1	0.98	0.11	66,66,66,66	0
5	CL	A	599	1/1	0.99	0.09	54,54,54,54	0

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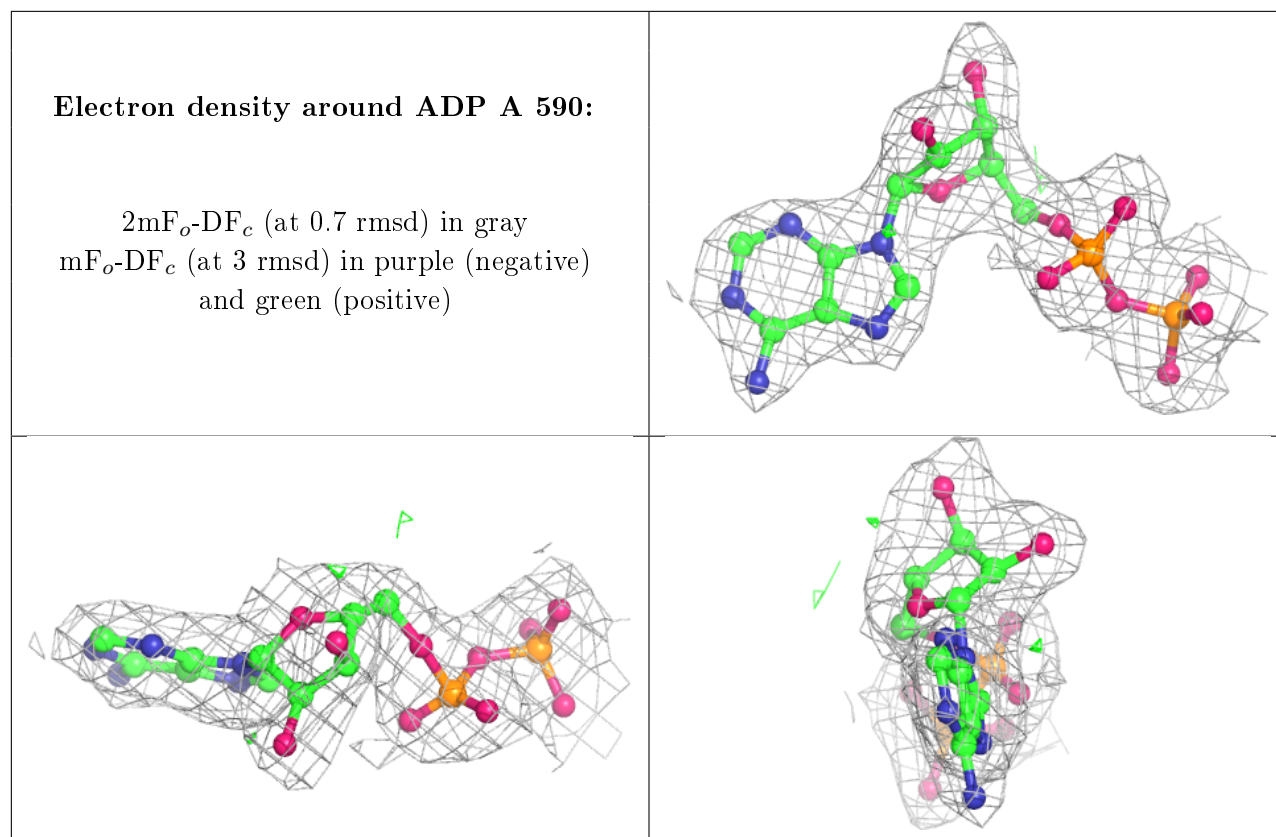
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CD	A	600	1/1	0.99	0.05	69,69,69,69	0
5	CL	A	597	1/1	1.00	0.06	32,32,32,32	0
2	SB	A	594	1/1	1.00	0.09	40,40,40,40	0
2	SB	A	595	1/1	1.00	0.10	36,36,36,36	0
2	SB	A	596	1/1	1.00	0.10	39,39,39,39	0
4	CD	A	602	1/1	1.00	0.08	62,62,62,62	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.