



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:56 AM EDT

PDB ID : 1IHU / pdb_00001ihu
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

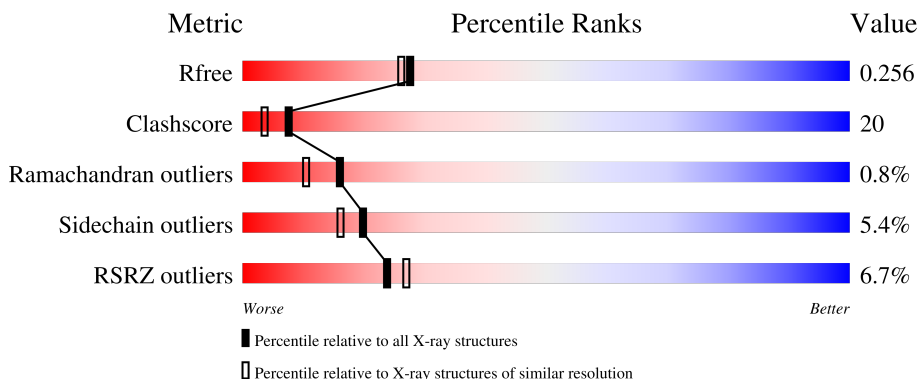
1 Overall quality at a glance

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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	589	6% 59% 30% • 8%

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 (CCD ID: MG) (formula: Mg).

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

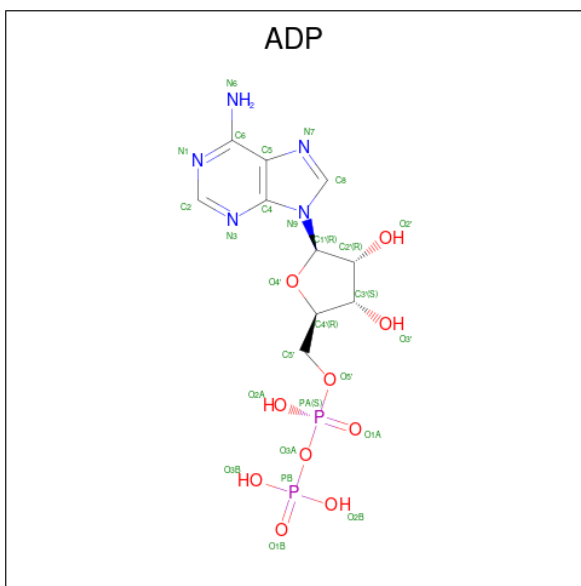
- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

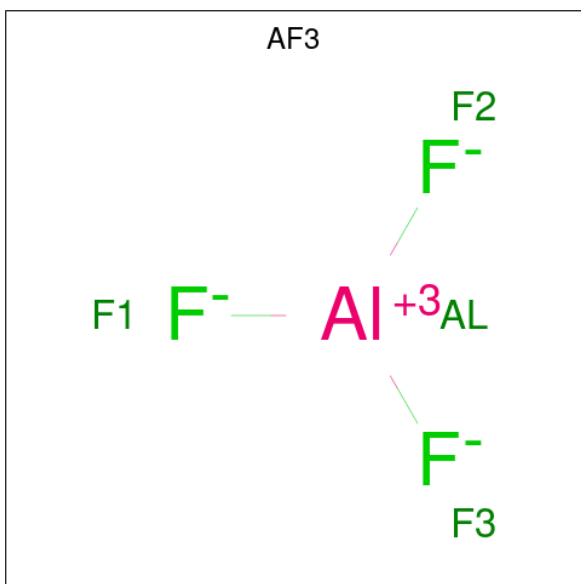
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cl	0	0
			3	3		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



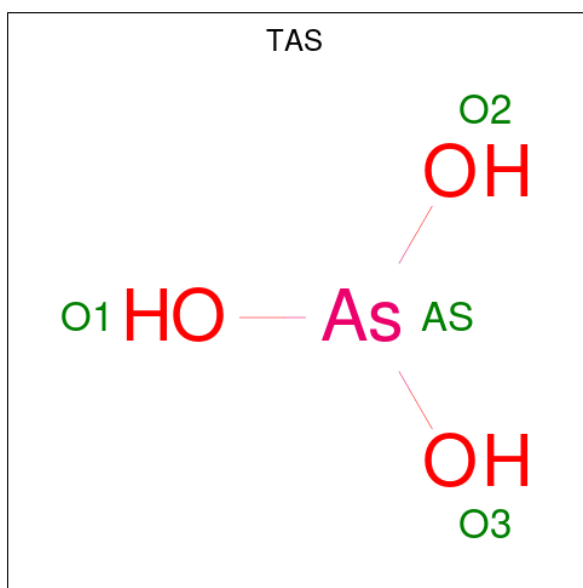
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



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

- Molecule 7 is TRIHYDROXYARSENITE(III) (CCD ID: TAS) (formula: AsH_3O_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, DNA and oligosaccharide 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, α , β , γ	73.90Å 75.94Å 222.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.15 – 2.15 25.15 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.1 (25.15-2.15) 94.0 (25.15-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.13Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.262 0.209 , 0.256	Depositor DCC
R_{free} test set	2621 reflections (7.65%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MG, TAS, AF3, ADP, CD

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	0.52	0/4189	0.99	12/5694 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	ARG	N-CA-C	7.75	117.25	108.25
1	A	567	VAL	N-CA-C	-7.04	100.49	109.30
1	A	45	ASP	CA-C-N	6.98	127.56	119.47
1	A	45	ASP	C-N-CA	6.98	127.56	119.47
1	A	99	ASP	N-CA-C	5.90	118.47	111.33
1	A	39	VAL	N-CA-C	5.76	116.77	108.48
1	A	487	ASP	CA-C-N	5.50	125.32	119.28
1	A	487	ASP	C-N-CA	5.50	125.32	119.28
1	A	199	THR	N-CA-C	5.16	117.85	109.24
1	A	584	HIS	N-CA-C	5.15	118.06	110.59
1	A	181	LYS	N-CA-C	5.05	117.91	110.59
1	A	452	GLY	N-CA-C	-5.04	106.68	112.73

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	4122	0	4198	170	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	170	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 20.

All (170) 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:329:LEU:HD11	1:A:446:MET:HE2	1.35	1.02
1:A:27:ALA:HB1	1:A:292:LEU:HD21	1.41	0.98
1:A:354:MET:HE2	1:A:356:PHE:HE2	1.24	0.98
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: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:107:GLU:OE1	1:A:516:ARG:NH2	2.23	0.71
1:A:381:GLN:NE2	1:A:442:ARG:NH2	2.38	0.71
1:A:50:VAL:O	1:A:53:VAL:HG22	1.90	0.70
1:A:315:LEU:O	1:A:319:VAL:HG23	1.92	0.70
1:A:354:MET:HE2	1:A:356:PHE:CE2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:HD11	1:A:446:MET:CE	2.18	0.66
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:HE21	1:A:430:GLN:CA	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:385:ILE:HD12	1:A:385:ILE:C	2.22	0.64
1:A:331:MET:HE3	1:A:446:MET:HE3	1.78	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:331:MET:HE3	1:A:446:MET:CE	2.31	0.60
1:A:260:LEU:C	1:A:260:LEU:HD13	2.28	0.58
1:A:331:MET:HG2	1:A:446:MET:HE3	1.86	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:27:ALA:HB1	1:A:292:LEU:CD2	2.27	0.57
1:A:279:PRO:HB2	1:A:542:MET:HG2	1.86	0.57
1:A:385:ILE:HD13	1:A:390:GLU:CG	2.36	0.56
1:A:404:LYS:HZ2	1:A:404:LYS:HA	1.71	0.56
1:A:522:TRP:CD1	1:A:561:ARG:HH21	2.23	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:586:HIS:CD2	1:A:586:HIS:C	2.84	0.55
1:A:381:GLN:NE2	1:A:442:ARG:HH12	2.02	0.55
1:A:331:MET:HE2	1:A:449:ALA:HB2	1.87	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:114:THR:HG1	1:A:175:PRO:HG3	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:VAL:O	1:A:283:VAL:CG2	2.55	0.53
1:A:225:ILE:HG22	1:A:225:ILE:O	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:255:ARG:HD3	1:A:570:SER:HA	1.93	0.51
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:98:PRO:HG2	1:A:101:VAL:CG2	2.42	0.50
1:A:568:LEU:HG	1:A:581:LEU:HD23	1.94	0.50
1:A:542:MET:HE1	1:A:545:GLN:OE1	2.11	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:155:LEU:HD13	1:A:413:LEU:HA	1.95	0.49
1:A:385:ILE:HD11	1:A:428:VAL:HG22	1.95	0.49
1:A:255:ARG:HD3	1:A:570:SER:CA	2.43	0.48
1:A:378:ASN:O	1:A:379:ASN:OD1	2.31	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: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:86:ARG:HD3	1:A:109:LEU:O	2.14	0.47
1:A:235:ASN:ND2	5:A:590:ADP:HN61	2.13	0.47
1:A:319:VAL:CG1	1:A:351:LEU:HD13	2.45	0.47
1:A:334:GLY:N	1:A:340:LYS:HD3	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:A:325:ASN:N	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:329:LEU:CD1	1:A:446:MET:HE2	2.26	0.44
1:A:349:VAL:HG21	1:A:578:LEU:HD23	2.00	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
1:A:333:MET:HE1	1:A:514:LEU:HD21	1.98	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:59:GLY:C	1:A:61:THR:H	2.26	0.43
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: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: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:48:SER:HA	8:A:868:HOH:O	2.18	0.43
1:A:270:LEU:HD12	1:A:270:LEU:N	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:49:ASN:O	1:A:52:GLN:HB3	2.20	0.42
1:A:430:GLN:CA	1:A:430:GLN:NE2	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:240:LYS:O	1:A:241:THR:C	2.62	0.42
1:A:378:ASN:C	1:A:380:LEU:N	2.77	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:HD2	1:A:441:LYS:H	1.84	0.41
1:A:4:LEU:HD12	1:A:4:LEU:HA	1.89	0.41
1:A:417:ASP:C	1:A:419:ARG:H	2.29	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%)	16	10

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%)	423 (95%)	24 (5%)	20	16

All (24) 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
1	A	291	LEU
1	A	315	LEU
1	A	325	ASN
1	A	351	LEU
1	A	385	ILE
1	A	398	VAL
1	A	399	LEU
1	A	404	LYS
1	A	406	LEU
1	A	419	ARG
1	A	430	GLN
1	A	455	LEU
1	A	457	LEU
1	A	461	THR
1	A	510	LEU
1	A	552	GLU

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Mol	Chain	Res	Type
1	A	586	HIS

Sometimes 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	108	GLN
1	A	138	HIS
1	A	154	GLN
1	A	185	GLN
1	A	229	ASN
1	A	235	ASN
1	A	262	ASN
1	A	278	GLN
1	A	381	GLN
1	A	430	GLN
1	A	509	ASN
1	A	580	GLN
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 oligosaccharides 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$
5	ADP	A	591	6,2	28,29,29	1.47	5 (17%)	43,45,45	3.58	19 (44%)
5	ADP	A	590	2	28,29,29	1.44	6 (21%)	43,45,45	3.75	23 (53%)
6	AF3	A	700	5,8	0,3,3	-	-	-	-	-
7	TAS	A	701	-	0,3,3	-	-	0,3,3	-	-

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
5	ADP	A	591	6,2	-	3/16/32/32	0/3/3/3
5	ADP	A	590	2	-	3/16/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	591	ADP	PA-O3A	4.41	1.64	1.59
5	A	590	ADP	PA-O3A	3.32	1.63	1.59
5	A	590	ADP	C8-N9	-3.05	1.32	1.37
5	A	591	ADP	C8-N9	-2.79	1.32	1.37
5	A	590	ADP	C2'-C3'	2.58	1.60	1.53
5	A	591	ADP	C1'-N9	2.48	1.53	1.46
5	A	590	ADP	C1'-N9	2.47	1.53	1.46
5	A	590	ADP	C5-C6	2.30	1.47	1.41
5	A	590	ADP	PA-O2A	-2.20	1.45	1.55
5	A	591	ADP	PA-O2A	-2.14	1.45	1.55
5	A	591	ADP	C2'-C3'	2.11	1.59	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	590	ADP	C4'-O4'-C1'	9.48	130.40	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	591	ADP	C4'-O4'-C1'	9.04	129.42	109.47
5	A	591	ADP	O4'-C1'-C2'	-8.82	87.73	106.62
5	A	590	ADP	PA-O5'-C5'	8.15	168.03	121.35
5	A	591	ADP	PA-O5'-C5'	8.04	167.41	121.35
5	A	590	ADP	O4'-C1'-C2'	-8.03	89.43	106.62
5	A	591	ADP	C5'-C4'-C3'	7.94	143.78	115.21
5	A	590	ADP	C5'-C4'-C3'	6.62	139.06	115.21
5	A	590	ADP	C3'-C2'-C1'	6.61	113.97	101.46
5	A	591	ADP	N3-C2-N1	-6.59	118.61	128.58
5	A	590	ADP	O4'-C4'-C5'	-6.39	88.88	109.33
5	A	590	ADP	N3-C2-N1	-6.38	118.93	128.58
5	A	591	ADP	C3'-C2'-C1'	6.21	113.20	101.46
5	A	591	ADP	O4'-C4'-C5'	-5.69	91.12	109.33
5	A	590	ADP	C6-C5-N7	5.23	142.18	132.09
5	A	590	ADP	O2A-PA-O1A	4.55	133.61	112.44
5	A	591	ADP	C6-C5-C4	-4.17	111.48	117.18
5	A	591	ADP	O4'-C4'-C3'	-4.14	96.93	105.15
5	A	590	ADP	O2A-PA-O3A	-4.11	96.16	107.27
5	A	590	ADP	C4-C5-N7	-4.04	105.96	110.58
5	A	590	ADP	C2'-C1'-N9	3.91	123.02	113.30
5	A	590	ADP	O4'-C4'-C3'	-3.90	97.40	105.15
5	A	590	ADP	C6-C5-C4	-3.90	111.86	117.18
5	A	591	ADP	C6-C5-N7	3.72	139.27	132.09
5	A	591	ADP	C2'-C1'-N9	3.57	122.17	113.30
5	A	590	ADP	C2-N3-C4	3.42	120.17	111.83
5	A	591	ADP	O2A-PA-O3A	-3.38	98.14	107.27
5	A	590	ADP	O2'-C2'-C1'	3.31	121.52	110.10
5	A	591	ADP	O2A-PA-O1A	3.07	126.72	112.44
5	A	591	ADP	C2-N1-C6	3.02	123.70	118.73
5	A	591	ADP	O2'-C2'-C1'	2.77	119.63	110.10
5	A	591	ADP	C2-N3-C4	2.69	118.40	111.83
5	A	590	ADP	O5'-PA-O1A	-2.69	98.28	108.94
5	A	590	ADP	O3A-PA-O1A	2.61	118.55	110.70
5	A	590	ADP	C4-N9-C1'	-2.44	120.93	126.63
5	A	590	ADP	C5-N7-C8	2.39	107.20	103.45
5	A	591	ADP	C4-N9-C1'	-2.39	121.05	126.63
5	A	591	ADP	O3A-PA-O1A	2.18	117.26	110.70
5	A	590	ADP	N6-C6-N1	-2.15	113.58	118.38
5	A	590	ADP	C1'-N9-C8	2.15	131.86	127.09
5	A	590	ADP	C2-N1-C6	2.11	122.19	118.73
5	A	591	ADP	O2B-PB-O3A	-2.06	97.72	104.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

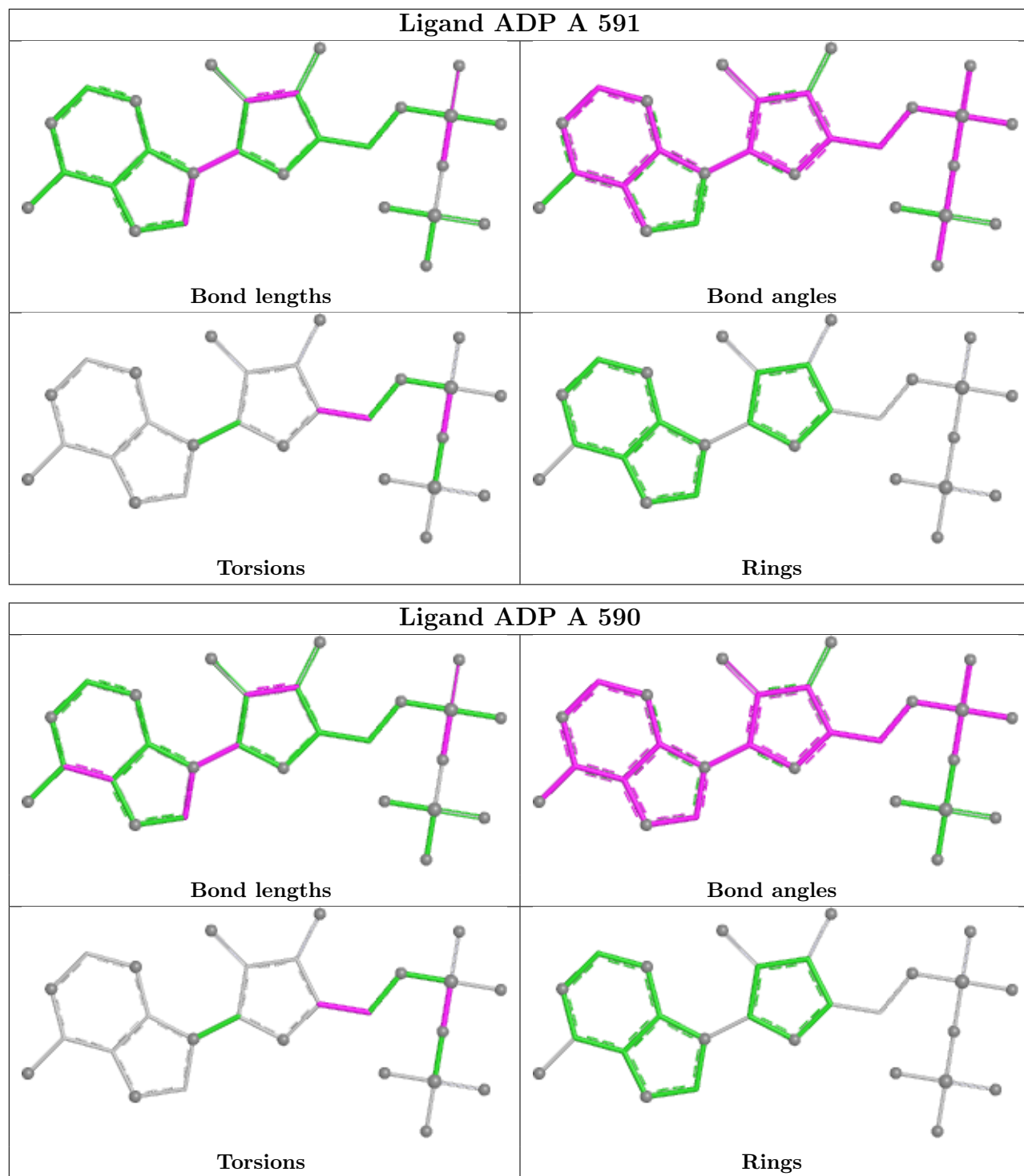
Mol	Chain	Res	Type	Atoms
5	A	590	ADP	O4'-C4'-C5'-O5'
5	A	591	ADP	O4'-C4'-C5'-O5'
5	A	591	ADP	C3'-C4'-C5'-O5'
5	A	590	ADP	C3'-C4'-C5'-O5'
5	A	591	ADP	PB-O3A-PA-O2A
5	A	590	ADP	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	591	ADP	1	0
5	A	590	ADP	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	540/589 (91%)	0.31	36 (6%) 24 27	22, 39, 69, 83	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	585	HIS	4.7
1	A	163	ILE	4.7
1	A	569	ALA	3.8
1	A	586	HIS	3.8
1	A	323	ALA	3.6
1	A	354	MET	3.4
1	A	293	SER	3.1
1	A	436	ILE	3.0
1	A	296	PRO	3.0
1	A	356	PHE	3.0
1	A	480	THR	2.9
1	A	568	LEU	2.8
1	A	325	ASN	2.8
1	A	570	SER	2.8
1	A	366	ALA	2.8
1	A	378	ASN	2.6
1	A	575	ILE	2.6
1	A	365	PRO	2.6
1	A	481	PRO	2.6
1	A	432	PHE	2.6
1	A	461	THR	2.6
1	A	170	ALA	2.5
1	A	162	PHE	2.5
1	A	243	ALA	2.5
1	A	532	ILE	2.4
1	A	244	ALA	2.3
1	A	247	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	324	ARG	2.2
1	A	572	PRO	2.2
1	A	250	ALA	2.2
1	A	309	ARG	2.2
1	A	284	GLY	2.2
1	A	533	ALA	2.2
1	A	435	VAL	2.1
1	A	434	ARG	2.0
1	A	540	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

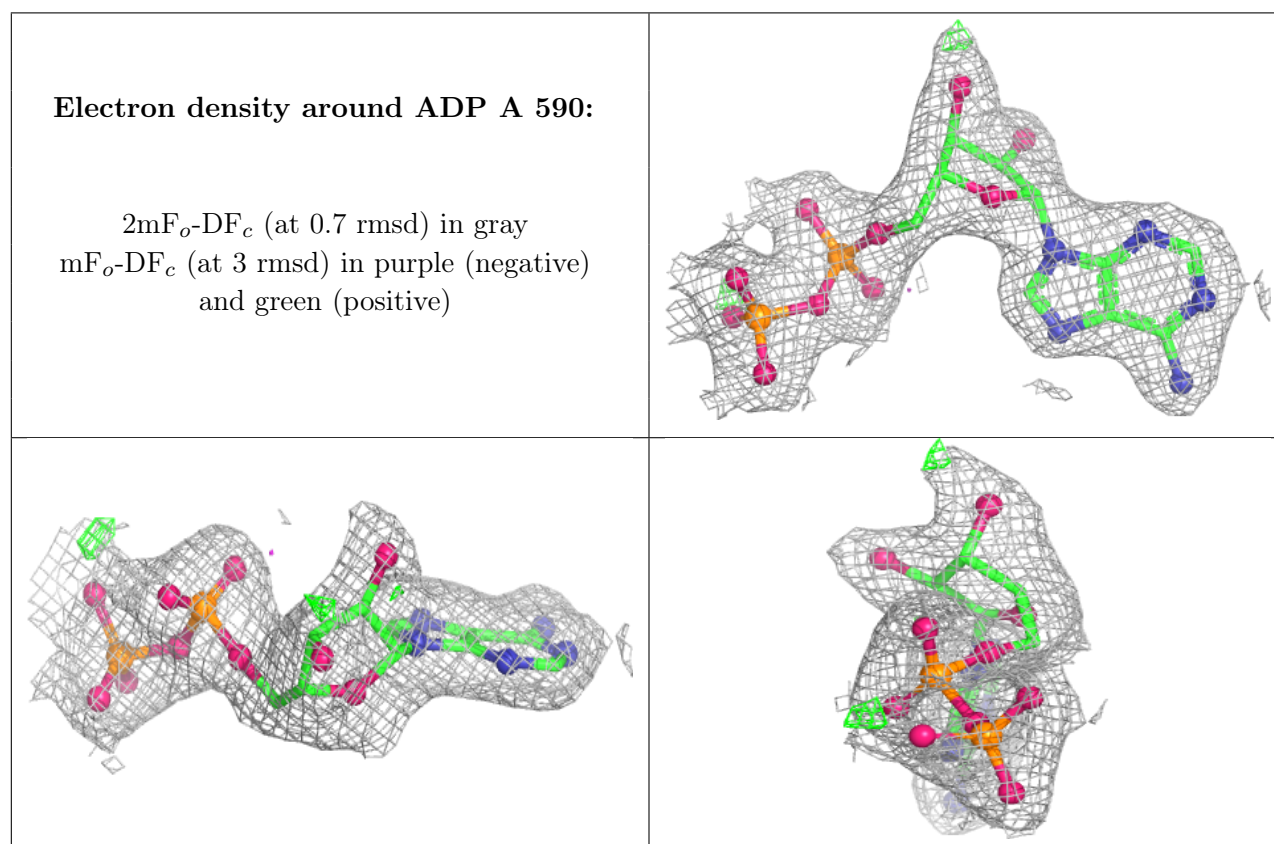
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TAS	A	701	4/4	0.75	0.24	56,58,60,73	4
6	AF3	A	700	4/4	0.94	0.08	49,57,59,64	0
3	CD	A	603	1/1	0.96	0.05	79,79,79,79	0
3	CD	A	604	1/1	0.97	0.05	52,52,52,52	1
5	ADP	A	590	27/27	0.97	0.06	25,36,42,43	0
5	ADP	A	591	27/27	0.97	0.07	30,37,47,51	0
3	CD	A	601	1/1	0.97	0.07	57,57,57,57	0
3	CD	A	600	1/1	0.97	0.05	54,54,54,54	0
4	CL	A	599	1/1	0.98	0.09	61,61,61,61	0
3	CD	A	602	1/1	0.99	0.04	55,55,55,55	0
2	MG	A	592	1/1	0.99	0.03	13,13,13,13	0
2	MG	A	593	1/1	0.99	0.07	28,28,28,28	0
4	CL	A	597	1/1	0.99	0.04	27,27,27,27	0
4	CL	A	598	1/1	0.99	0.04	27,27,27,27	0

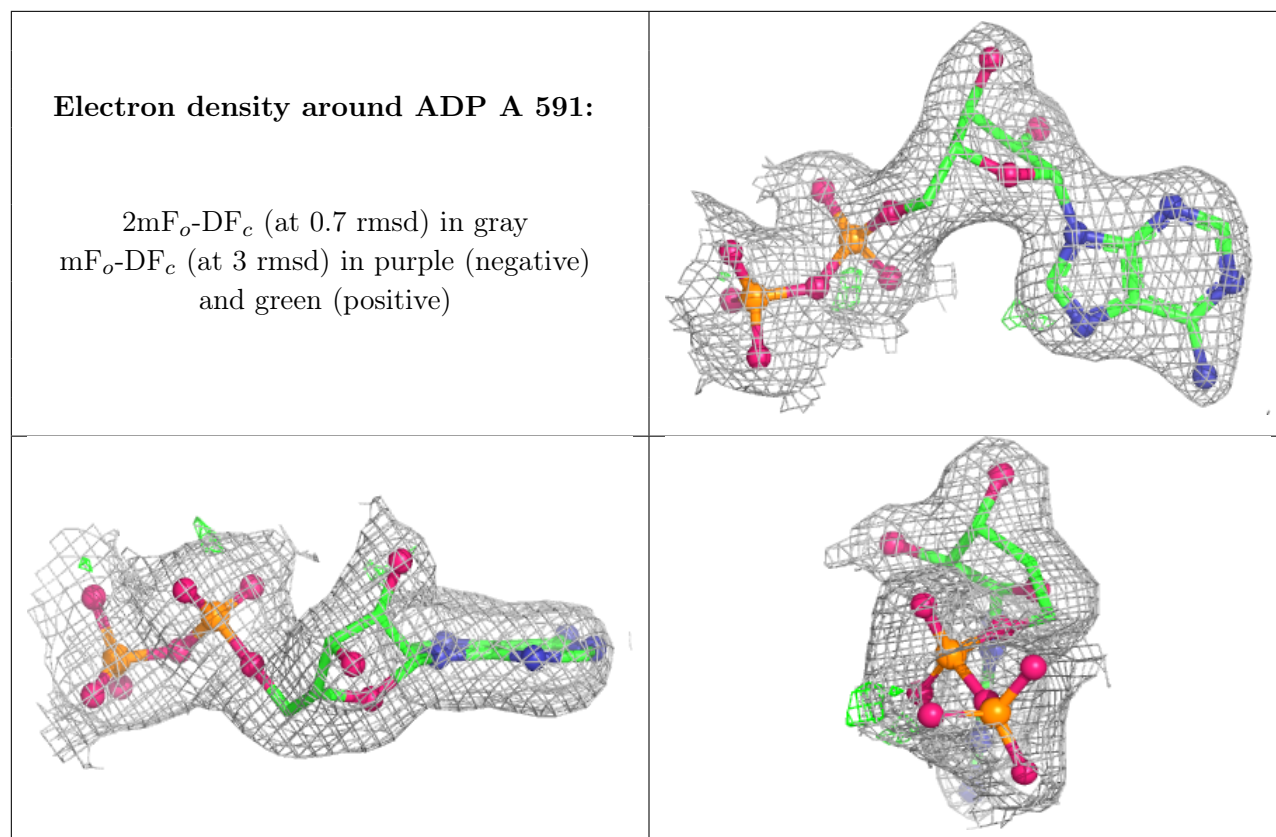
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CD	A	595	1/1	1.00	0.02	28,28,28,28	0
3	CD	A	596	1/1	1.00	0.01	30,30,30,30	0
3	CD	A	594	1/1	1.00	0.01	32,32,32,32	0

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.