



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:45 AM UTC

PDB ID : 4BIV / pdb_00004biv
Title : Crystal structure of CpxAHDC (trigonal form)
Authors : Mechaly, A.E.; Sassoon, N.; Betton, J.M.; Alzari, P.M.
Deposited on : 2013-04-13
Resolution : 3.40 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

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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

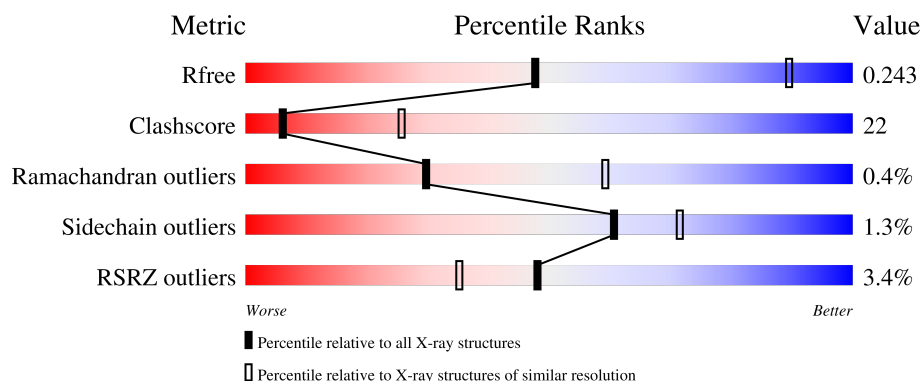
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	298	2% 58% 28% 5% 10%
1	B	298	4% 59% 29% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4292 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 SENSOR PROTEIN CPXA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	Se	0	0	0
			2115	1316	386	407	6			
1	B	269	Total	C	N	O	Se	0	0	0
			2115	1316	386	407	6			

There are 56 discrepancies between the modelled and reference sequences:

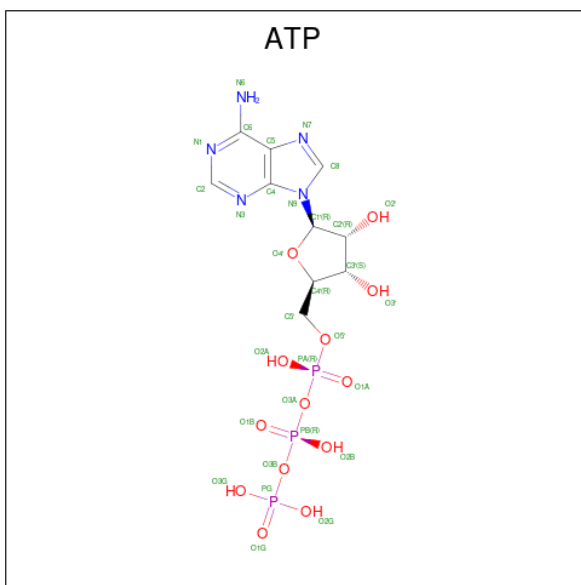
Chain	Residue	Modelled	Actual	Comment	Reference
A	160	MSE	-	expression tag	UNP P0AE82
A	161	GLY	-	expression tag	UNP P0AE82
A	162	SER	-	expression tag	UNP P0AE82
A	163	SER	-	expression tag	UNP P0AE82
A	164	HIS	-	expression tag	UNP P0AE82
A	165	HIS	-	expression tag	UNP P0AE82
A	166	HIS	-	expression tag	UNP P0AE82
A	167	HIS	-	expression tag	UNP P0AE82
A	168	HIS	-	expression tag	UNP P0AE82
A	169	HIS	-	expression tag	UNP P0AE82
A	170	SER	-	expression tag	UNP P0AE82
A	171	SER	-	expression tag	UNP P0AE82
A	172	GLY	-	expression tag	UNP P0AE82
A	173	LEU	-	expression tag	UNP P0AE82
A	174	VAL	-	expression tag	UNP P0AE82
A	175	PRO	-	expression tag	UNP P0AE82
A	176	ARG	-	expression tag	UNP P0AE82
A	177	GLY	-	expression tag	UNP P0AE82
A	178	SER	-	expression tag	UNP P0AE82
A	179	HIS	-	expression tag	UNP P0AE82
A	180	MSE	-	expression tag	UNP P0AE82
A	181	GLU	-	expression tag	UNP P0AE82
A	182	ASN	-	expression tag	UNP P0AE82
A	183	LEU	-	expression tag	UNP P0AE82
A	184	TYR	-	expression tag	UNP P0AE82

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Chain	Residue	Modelled	Actual	Comment	Reference
A	185	PHE	-	expression tag	UNP P0AE82
A	186	GLN	-	expression tag	UNP P0AE82
A	187	GLY	-	expression tag	UNP P0AE82
B	160	MSE	-	expression tag	UNP P0AE82
B	161	GLY	-	expression tag	UNP P0AE82
B	162	SER	-	expression tag	UNP P0AE82
B	163	SER	-	expression tag	UNP P0AE82
B	164	HIS	-	expression tag	UNP P0AE82
B	165	HIS	-	expression tag	UNP P0AE82
B	166	HIS	-	expression tag	UNP P0AE82
B	167	HIS	-	expression tag	UNP P0AE82
B	168	HIS	-	expression tag	UNP P0AE82
B	169	HIS	-	expression tag	UNP P0AE82
B	170	SER	-	expression tag	UNP P0AE82
B	171	SER	-	expression tag	UNP P0AE82
B	172	GLY	-	expression tag	UNP P0AE82
B	173	LEU	-	expression tag	UNP P0AE82
B	174	VAL	-	expression tag	UNP P0AE82
B	175	PRO	-	expression tag	UNP P0AE82
B	176	ARG	-	expression tag	UNP P0AE82
B	177	GLY	-	expression tag	UNP P0AE82
B	178	SER	-	expression tag	UNP P0AE82
B	179	HIS	-	expression tag	UNP P0AE82
B	180	MSE	-	expression tag	UNP P0AE82
B	181	GLU	-	expression tag	UNP P0AE82
B	182	ASN	-	expression tag	UNP P0AE82
B	183	LEU	-	expression tag	UNP P0AE82
B	184	TYR	-	expression tag	UNP P0AE82
B	185	PHE	-	expression tag	UNP P0AE82
B	186	GLN	-	expression tag	UNP P0AE82
B	187	GLY	-	expression tag	UNP P0AE82

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

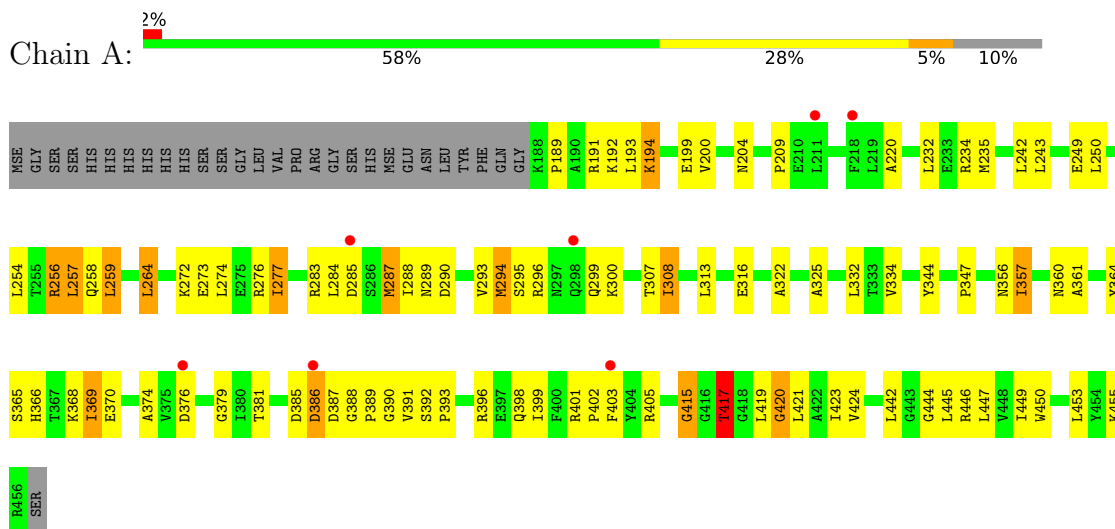


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

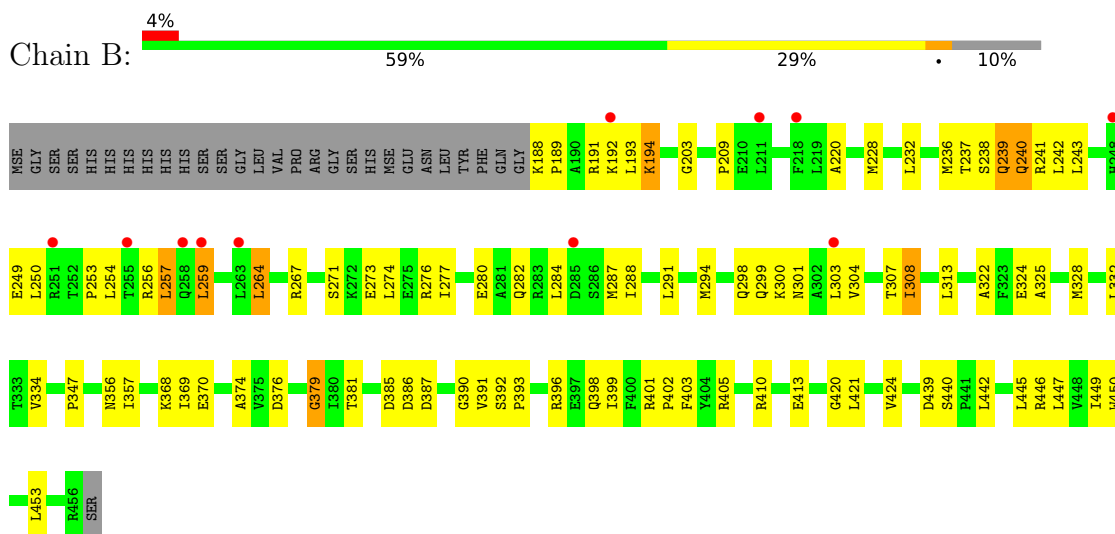
3 Residue-property plots

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: SENSOR PROTEIN CPXA



• Molecule 1: SENSOR PROTEIN CPXA



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.83Å 141.83Å 121.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.42 – 3.40 46.42 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.42-3.40) 99.9 (46.42-3.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.227 , 0.234 (Not available) , 0.243	Depositor DCC
R_{free} test set	1015 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	137.5	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 177.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4292	wwPDB-VP
Average B, all atoms (Å ²)	185.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: ATP

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	0.93	7/2145 (0.3%)	1.50	24/2892 (0.8%)
1	B	0.84	1/2145 (0.0%)	1.47	24/2892 (0.8%)
All	All	0.88	8/4290 (0.2%)	1.48	48/5784 (0.8%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	ILE	CG1-CD1	-6.61	1.25	1.51
1	A	256	ARG	C-N	6.41	1.41	1.33
1	A	287	MSE	SE-CE	-6.28	1.76	1.95
1	A	277	ILE	CG1-CD1	-6.18	1.27	1.51
1	A	308	ILE	CG1-CD1	-5.83	1.29	1.51
1	A	256	ARG	CA-C	5.72	1.60	1.52
1	B	308	ILE	CG1-CD1	-5.68	1.29	1.51
1	A	386	ASP	CA-C	-5.07	1.46	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	LEU	CA-C-N	8.02	136.85	121.54
1	B	242	LEU	C-N-CA	8.02	136.85	121.54
1	A	257	LEU	CA-C-N	7.73	130.96	120.38
1	A	257	LEU	C-N-CA	7.73	130.96	120.38
1	A	259	LEU	CA-C-N	7.31	128.05	119.94
1	A	259	LEU	C-N-CA	7.31	128.05	119.94
1	B	386	ASP	CA-C-N	7.24	130.57	120.29
1	B	386	ASP	C-N-CA	7.24	130.57	120.29
1	B	379	GLY	N-CA-C	6.95	120.67	110.38
1	A	417	THR	N-CA-C	6.77	121.31	111.02
1	B	209	PRO	CA-C-N	6.70	129.56	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	PRO	C-N-CA	6.70	129.56	120.38
1	A	209	PRO	CA-C-N	6.66	129.51	120.38
1	A	209	PRO	C-N-CA	6.66	129.51	120.38
1	B	282	GLN	CA-C-N	6.50	128.99	120.28
1	B	282	GLN	C-N-CA	6.50	128.99	120.28
1	B	259	LEU	CA-C-N	6.44	127.09	119.94
1	B	259	LEU	C-N-CA	6.44	127.09	119.94
1	B	257	LEU	CA-C-N	5.99	128.30	120.28
1	B	257	LEU	C-N-CA	5.99	128.30	120.28
1	A	376	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	264	LEU	CA-C-N	5.57	127.74	120.28
1	A	264	LEU	C-N-CA	5.57	127.74	120.28
1	B	194	LYS	CA-C-N	5.47	127.61	120.28
1	B	194	LYS	C-N-CA	5.47	127.61	120.28
1	A	455	LYS	CA-C-N	5.46	131.53	121.70
1	A	455	LYS	C-N-CA	5.46	131.53	121.70
1	A	194	LYS	CA-C-N	5.45	127.58	120.28
1	A	194	LYS	C-N-CA	5.45	127.58	120.28
1	A	294	MSE	CG-SE-CE	-5.39	87.07	98.92
1	B	264	LEU	CA-C-N	5.35	127.44	120.28
1	B	264	LEU	C-N-CA	5.35	127.44	120.28
1	A	357	ILE	CA-C-N	5.26	127.30	120.56
1	A	357	ILE	C-N-CA	5.26	127.30	120.56
1	A	316	GLU	CA-C-N	5.22	127.22	120.70
1	A	316	GLU	C-N-CA	5.22	127.22	120.70
1	A	356	ASN	CA-C-N	5.21	127.33	120.60
1	A	356	ASN	C-N-CA	5.21	127.33	120.60
1	B	376	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	239	GLN	CA-C-N	5.17	127.51	120.54
1	B	239	GLN	C-N-CA	5.17	127.51	120.54
1	A	334	VAL	CA-C-N	5.12	127.86	120.38
1	A	334	VAL	C-N-CA	5.12	127.86	120.38
1	B	334	VAL	CA-C-N	5.08	127.80	120.38
1	B	334	VAL	C-N-CA	5.08	127.80	120.38
1	A	415	GLY	N-CA-C	5.06	120.55	111.34
1	B	356	ASN	CA-C-N	5.06	127.12	120.60
1	B	356	ASN	C-N-CA	5.06	127.12	120.60

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	2115	0	2110	134	0
1	B	2115	0	2110	100	0
2	A	31	0	12	1	0
2	B	31	0	12	1	0
All	All	4292	0	4244	192	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 22.

All (192) 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:294:MSE:HE1	1:A:423:ILE:CD1	1.47	1.43
1:A:243:LEU:HD11	1:B:243:LEU:CD2	1.62	1.27
1:A:294:MSE:HE1	1:A:423:ILE:HD11	1.28	1.10
1:A:294:MSE:HG3	1:A:419:LEU:HD13	1.21	1.08
1:A:243:LEU:HD11	1:B:243:LEU:HD21	1.25	1.07
1:A:243:LEU:HD21	1:B:243:LEU:HD22	1.31	1.06
1:A:294:MSE:CG	1:A:419:LEU:HD13	1.87	1.04
1:A:294:MSE:CE	1:A:423:ILE:CD1	2.38	0.99
1:A:381:THR:HG22	1:A:450:TRP:HD1	1.27	0.99
1:B:381:THR:HG22	1:B:450:TRP:HD1	1.28	0.98
1:A:287:MSE:HE1	1:B:253:PRO:HG2	1.42	0.98
1:B:385:ASP:OD1	1:B:446:ARG:HG2	1.65	0.95
1:A:294:MSE:CE	1:A:423:ILE:HD11	1.97	0.93
1:A:361:ALA:HB1	1:A:386:ASP:OD1	1.69	0.93
1:A:294:MSE:HE1	1:A:423:ILE:CG1	1.99	0.93
1:A:332:LEU:HD23	1:A:369:ILE:HB	1.49	0.92
1:A:361:ALA:HA	1:A:386:ASP:OD2	1.69	0.91
1:B:332:LEU:HD23	1:B:369:ILE:HB	1.51	0.90
1:A:294:MSE:HE1	1:A:423:ILE:HD13	1.52	0.90
1:A:284:LEU:HA	1:A:287:MSE:HE3	1.53	0.89
1:A:294:MSE:CE	1:A:423:ILE:HG12	2.02	0.89
1:A:308:ILE:CD1	1:A:347:PRO:HG3	2.03	0.89
1:A:243:LEU:CD2	1:B:243:LEU:HD22	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ILE:CD1	1:B:347:PRO:HG3	2.04	0.87
1:A:243:LEU:CD1	1:B:243:LEU:CD2	2.52	0.85
1:A:294:MSE:CE	1:A:423:ILE:CG1	2.54	0.84
1:B:239:GLN:O	1:B:243:LEU:HG	1.78	0.83
1:B:399:ILE:CG2	1:B:421:LEU:HD12	2.11	0.80
1:A:332:LEU:CD2	1:A:369:ILE:HB	2.13	0.79
1:B:357:ILE:HG13	1:B:449:ILE:HD11	1.64	0.79
1:A:243:LEU:HD11	1:B:243:LEU:HD22	1.62	0.77
1:B:332:LEU:CD2	1:B:369:ILE:HB	2.15	0.77
1:B:385:ASP:OD1	1:B:446:ARG:CG	2.32	0.76
1:A:299:GLN:HG3	1:B:403:PHE:CZ	2.21	0.76
1:A:405:ARG:HH21	1:A:417:THR:H	1.34	0.76
1:A:381:THR:HG22	1:A:450:TRP:CD1	2.18	0.76
1:A:405:ARG:NH2	1:A:417:THR:H	1.85	0.75
1:B:276:ARG:O	1:B:280:GLU:HG2	1.88	0.74
1:A:249:GLU:HB3	1:B:287:MSE:HE1	1.68	0.74
1:B:381:THR:CG2	1:B:450:TRP:HD1	2.01	0.74
1:A:357:ILE:HG13	1:A:449:ILE:HD11	1.71	0.72
1:A:399:ILE:CG2	1:A:421:LEU:HD12	2.20	0.72
1:A:254:LEU:HD11	1:A:288:ILE:HD12	1.71	0.71
1:A:381:THR:CG2	1:A:450:TRP:HD1	2.00	0.71
1:A:295:SER:O	1:A:299:GLN:HG2	1.91	0.70
1:A:308:ILE:HD11	1:A:347:PRO:HG3	1.74	0.70
1:B:308:ILE:HD11	1:B:347:PRO:HG3	1.73	0.69
1:B:381:THR:HG22	1:B:450:TRP:CD1	2.19	0.68
1:A:258:GLN:NE2	1:A:285:ASP:OD2	2.25	0.68
1:A:294:MSE:HE2	1:A:423:ILE:HG12	1.76	0.68
1:B:322:ALA:HA	1:B:332:LEU:HD12	1.78	0.66
1:A:417:THR:HG21	1:A:419:LEU:HD12	1.77	0.66
1:A:374:ALA:HB3	1:A:381:THR:OG1	1.96	0.66
1:A:322:ALA:HA	1:A:332:LEU:HD12	1.79	0.65
1:B:374:ALA:HB3	1:B:381:THR:OG1	1.96	0.65
1:A:254:LEU:HD13	1:A:285:ASP:OD1	1.95	0.65
1:A:264:LEU:HD13	1:A:274:LEU:HD21	1.78	0.64
1:A:243:LEU:CD1	1:B:243:LEU:HD22	2.25	0.63
1:A:403:PHE:HA	1:A:417:THR:O	1.98	0.63
1:A:283:ARG:NH1	1:B:256:ARG:HH22	1.97	0.63
1:A:391:VAL:HG21	1:A:399:ILE:HD11	1.82	0.62
1:A:243:LEU:CD1	1:B:243:LEU:HD21	2.16	0.61
1:A:254:LEU:HD11	1:A:288:ILE:CD1	2.30	0.61
1:A:254:LEU:O	1:A:257:LEU:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ILE:CG2	1:A:313:LEU:HG	2.31	0.61
1:B:308:ILE:CG2	1:B:313:LEU:HG	2.31	0.61
1:B:254:LEU:HD12	1:B:288:ILE:HD12	1.84	0.60
1:A:243:LEU:HD23	1:B:291:LEU:HD11	1.82	0.60
1:A:243:LEU:CG	1:B:243:LEU:HD22	2.31	0.60
1:A:283:ARG:HH11	1:B:256:ARG:HH22	1.48	0.60
1:B:391:VAL:HG11	1:B:399:ILE:HD11	1.82	0.60
1:A:290:ASP:HB3	1:A:417:THR:CG2	2.32	0.60
1:A:325:ALA:HB2	1:A:332:LEU:HG	1.84	0.59
1:A:357:ILE:HD11	1:A:424:VAL:HG11	1.85	0.59
1:A:368:LYS:H	1:A:387:ASP:HB2	1.68	0.59
1:A:258:GLN:CD	1:A:285:ASP:OD2	2.45	0.59
1:A:264:LEU:HG	1:B:273:GLU:HB2	1.86	0.58
1:A:365:SER:CB	1:A:369:ILE:HD11	2.32	0.58
1:B:357:ILE:HD11	1:B:424:VAL:HG11	1.84	0.58
1:A:365:SER:HB3	1:A:369:ILE:HD11	1.84	0.58
1:A:420:GLY:HA2	1:A:423:ILE:HD12	1.86	0.57
1:A:200:VAL:HB	1:B:228:MSE:HE3	1.86	0.57
1:A:234:ARG:HG2	1:B:300:LYS:HZ1	1.68	0.57
1:A:290:ASP:O	1:A:294:MSE:HG2	2.04	0.57
1:A:405:ARG:NH1	1:A:415:GLY:HA3	2.21	0.56
1:A:189:PRO:HA	1:A:192:LYS:HD3	1.88	0.56
1:A:235:MSE:HE3	1:B:298:GLN:O	2.06	0.56
1:B:390:GLY:HA2	1:B:445:LEU:HG	1.87	0.55
1:A:254:LEU:HD23	1:A:257:LEU:HD12	1.87	0.55
1:A:361:ALA:CA	1:A:386:ASP:OD2	2.51	0.55
1:A:272:LYS:HD2	1:B:267:ARG:HH12	1.72	0.54
1:A:249:GLU:HB3	1:B:287:MSE:CE	2.37	0.54
1:B:189:PRO:HA	1:B:192:LYS:HD3	1.90	0.54
1:A:220:ALA:HB3	1:B:194:LYS:HE2	1.88	0.53
1:A:402:PRO:O	1:B:249:GLU:OE1	2.26	0.53
1:B:391:VAL:HG23	1:B:445:LEU:HD11	1.91	0.53
1:A:256:ARG:HA	1:A:259:LEU:HD12	1.91	0.53
1:A:289:ASN:O	1:A:293:VAL:HG23	2.09	0.53
1:A:191:ARG:HA	1:A:194:LYS:HD2	1.91	0.52
1:A:264:LEU:CD1	1:B:277:ILE:CD1	2.87	0.52
1:A:366:HIS:NE2	1:A:389:PRO:HD3	2.24	0.52
1:B:325:ALA:HB2	1:B:332:LEU:HG	1.91	0.52
1:A:385:ASP:OD1	1:A:446:ARG:HB3	2.09	0.52
1:A:273:GLU:HG3	1:A:276:ARG:HH21	1.72	0.52
1:B:368:LYS:H	1:B:387:ASP:HB2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:THR:O	1:B:308:ILE:HG13	2.10	0.52
1:B:308:ILE:HG22	1:B:313:LEU:HG	1.92	0.52
1:A:287:MSE:CE	1:B:253:PRO:HG2	2.29	0.52
1:B:391:VAL:CG2	1:B:445:LEU:HD11	2.39	0.51
1:A:357:ILE:HD13	1:A:447:LEU:HD13	1.93	0.51
1:A:194:LYS:HE2	1:B:220:ALA:HB3	1.93	0.51
1:A:307:THR:O	1:A:308:ILE:HG13	2.10	0.51
1:A:417:THR:CG2	1:A:419:LEU:HD12	2.41	0.51
1:B:191:ARG:HA	1:B:194:LYS:HD2	1.93	0.51
1:A:193:LEU:HD22	1:B:193:LEU:HD22	1.92	0.51
1:B:308:ILE:HG21	1:B:313:LEU:HG	1.93	0.51
1:A:250:LEU:HD23	1:B:284:LEU:HD23	1.93	0.50
1:A:391:VAL:HG11	1:A:399:ILE:HD11	1.93	0.50
1:A:308:ILE:HG22	1:A:313:LEU:HG	1.93	0.50
1:A:365:SER:HB3	1:A:369:ILE:CD1	2.42	0.50
1:B:399:ILE:HG21	1:B:421:LEU:HD12	1.91	0.49
1:A:390:GLY:HA2	1:A:445:LEU:HG	1.94	0.49
1:A:308:ILE:HG21	1:A:313:LEU:HG	1.93	0.49
1:A:294:MSE:SE	1:A:423:ILE:HD11	2.62	0.49
1:B:254:LEU:CD1	1:B:288:ILE:HD12	2.43	0.49
1:A:242:LEU:HD11	1:B:294:MSE:HB3	1.94	0.49
1:A:264:LEU:HD11	1:B:277:ILE:CD1	2.43	0.48
1:B:301:ASN:C	1:B:303:LEU:H	2.21	0.48
1:A:257:LEU:HG	1:B:280:GLU:CB	2.43	0.48
1:A:368:LYS:H	1:A:387:ASP:CB	2.25	0.48
1:B:391:VAL:HG21	1:B:399:ILE:HD11	1.95	0.48
1:A:283:ARG:NH1	1:B:256:ARG:NH2	2.61	0.48
1:A:290:ASP:HB3	1:A:417:THR:HG21	1.96	0.47
1:A:264:LEU:HD21	1:B:271:SER:OG	2.14	0.47
1:B:374:ALA:HB3	1:B:381:THR:HG1	1.78	0.47
1:B:256:ARG:HA	1:B:259:LEU:HD12	1.97	0.47
1:B:410:ARG:HA	1:B:413:GLU:HG3	1.97	0.47
1:A:368:LYS:O	1:A:369:ILE:HD13	2.15	0.47
1:A:369:ILE:HD12	1:A:386:ASP:OD1	2.14	0.47
1:A:294:MSE:HE2	1:A:423:ILE:CG1	2.34	0.47
1:A:366:HIS:HB2	1:A:387:ASP:OD2	2.14	0.46
1:A:254:LEU:CD1	1:A:288:ILE:HD12	2.43	0.46
1:A:391:VAL:HB	1:A:445:LEU:HD11	1.98	0.46
1:B:399:ILE:CG2	1:B:421:LEU:CD1	2.90	0.46
1:A:420:GLY:O	1:A:424:VAL:HG23	2.15	0.46
1:A:360:ASN:O	1:A:364:TYR:HD2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:ILE:HG22	1:B:421:LEU:HD12	1.96	0.46
1:A:385:ASP:OD1	1:A:446:ARG:CB	2.63	0.46
1:A:257:LEU:HG	1:B:280:GLU:HB2	1.98	0.46
1:A:296:ARG:O	1:A:300:LYS:HG2	2.17	0.45
1:A:379:GLY:HA2	1:A:453:LEU:HG	1.98	0.45
1:B:393:PRO:HA	1:B:396:ARG:HG3	1.99	0.45
1:B:357:ILE:HD13	1:B:447:LEU:HD13	1.99	0.45
1:A:204:ASN:HA	1:A:344:TYR:CE1	2.52	0.45
1:A:243:LEU:CD2	1:B:291:LEU:HD11	2.47	0.44
1:B:304:VAL:O	1:B:304:VAL:HG12	2.18	0.44
1:B:379:GLY:HA2	1:B:453:LEU:HG	1.99	0.44
1:B:405:ARG:HH21	1:B:413:GLU:HG2	1.83	0.44
1:A:365:SER:HA	1:A:388:GLY:HA3	1.99	0.44
1:B:439:ASP:O	1:B:446:ARG:NH2	2.51	0.44
1:A:193:LEU:HD13	1:B:193:LEU:HD13	2.00	0.43
1:B:445:LEU:HD12	2:B:501:ATP:C2	2.53	0.43
1:A:287:MSE:HA	1:A:403:PHE:CE1	2.54	0.43
1:A:399:ILE:CG2	1:A:421:LEU:CD1	2.94	0.43
1:A:294:MSE:HB3	1:A:294:MSE:HE3	1.76	0.43
1:A:264:LEU:HD12	1:B:277:ILE:CD1	2.49	0.43
1:A:277:ILE:CD1	1:B:264:LEU:CD1	2.96	0.43
1:B:250:LEU:O	1:B:253:PRO:HD2	2.19	0.43
1:B:237:THR:HA	1:B:240:GLN:HB3	2.01	0.43
1:A:393:PRO:HA	1:A:396:ARG:HG3	2.00	0.42
1:A:370:GLU:HG3	1:A:442:LEU:HD11	2.00	0.42
1:B:324:GLU:HG2	1:B:328:MSE:HE3	2.01	0.42
1:B:370:GLU:HG3	1:B:442:LEU:HD11	2.01	0.42
1:B:402:PRO:HB2	1:B:403:PHE:CD1	2.53	0.42
1:A:232:LEU:HD22	1:B:232:LEU:HD22	2.02	0.42
1:B:203:GLY:HA3	1:B:299:GLN:HE21	1.85	0.42
1:A:405:ARG:HE	1:A:417:THR:C	2.29	0.41
1:A:242:LEU:HD11	1:B:294:MSE:CB	2.51	0.41
1:A:365:SER:OG	1:A:369:ILE:HD11	2.20	0.41
1:B:440:SER:HA	1:B:446:ARG:HG3	2.02	0.41
1:B:264:LEU:HD13	1:B:274:LEU:HD21	2.01	0.41
1:A:277:ILE:HG23	1:B:257:LEU:HG	2.03	0.41
1:A:398:GLN:O	1:A:401:ARG:HB2	2.20	0.41
1:A:421:LEU:HG	2:A:501:ATP:O2A	2.21	0.41
1:B:368:LYS:H	1:B:387:ASP:CB	2.32	0.40
1:B:241:ARG:C	1:B:243:LEU:H	2.28	0.40
1:B:391:VAL:HB	1:B:445:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:GLN:O	1:B:401:ARG:HB2	2.22	0.40
1:A:273:GLU:OE1	1:B:264:LEU:HD23	2.22	0.40
1:B:236:MSE:C	1:B:238:SER:H	2.29	0.40
1:A:254:LEU:HA	1:A:257:LEU:HD12	2.03	0.40
1:A:388:GLY:O	1:A:444:GLY:HA2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	267/298 (90%)	248 (93%)	18 (7%)	1 (0%)	30	59
1	B	267/298 (90%)	242 (91%)	24 (9%)	1 (0%)	30	59
All	All	534/596 (90%)	490 (92%)	42 (8%)	2 (0%)	30	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	GLY
1	B	420	GLY

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	226/243 (93%)	223 (99%)	3 (1%)	61	71
1	B	226/243 (93%)	223 (99%)	3 (1%)	61	71
All	All	452/486 (93%)	446 (99%)	6 (1%)	61	71

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	GLU
1	A	392	SER
1	A	417	THR
1	B	188	LYS
1	B	240	GLN
1	B	392	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
1	A	248	HIS
1	A	258	GLN
1	A	298	GLN
1	A	346	ASN
1	B	207	GLN
1	B	282	GLN
1	B	289	ASN
1	B	298	GLN
1	B	398	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	ATP	B	501	-	32,33,33	2.29	2 (6%)	48,52,52	0.68	1 (2%)
2	ATP	A	501	-	32,33,33	2.24	2 (6%)	48,52,52	0.75	1 (2%)

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
2	ATP	B	501	-	-	2/22/38/38	0/3/3/3
2	ATP	A	501	-	-	2/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ATP	PB-O3B	-8.79	1.50	1.59
2	A	501	ATP	PA-O3A	-8.73	1.50	1.59
2	B	501	ATP	PA-O3A	-8.68	1.50	1.59
2	A	501	ATP	PB-O3B	-8.40	1.50	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	ATP	C4-N9-C8	-2.26	103.36	105.74
2	A	501	ATP	C4-C5-N7	2.19	113.09	110.58

There are no chirality outliers.

All (4) torsion outliers are listed below:

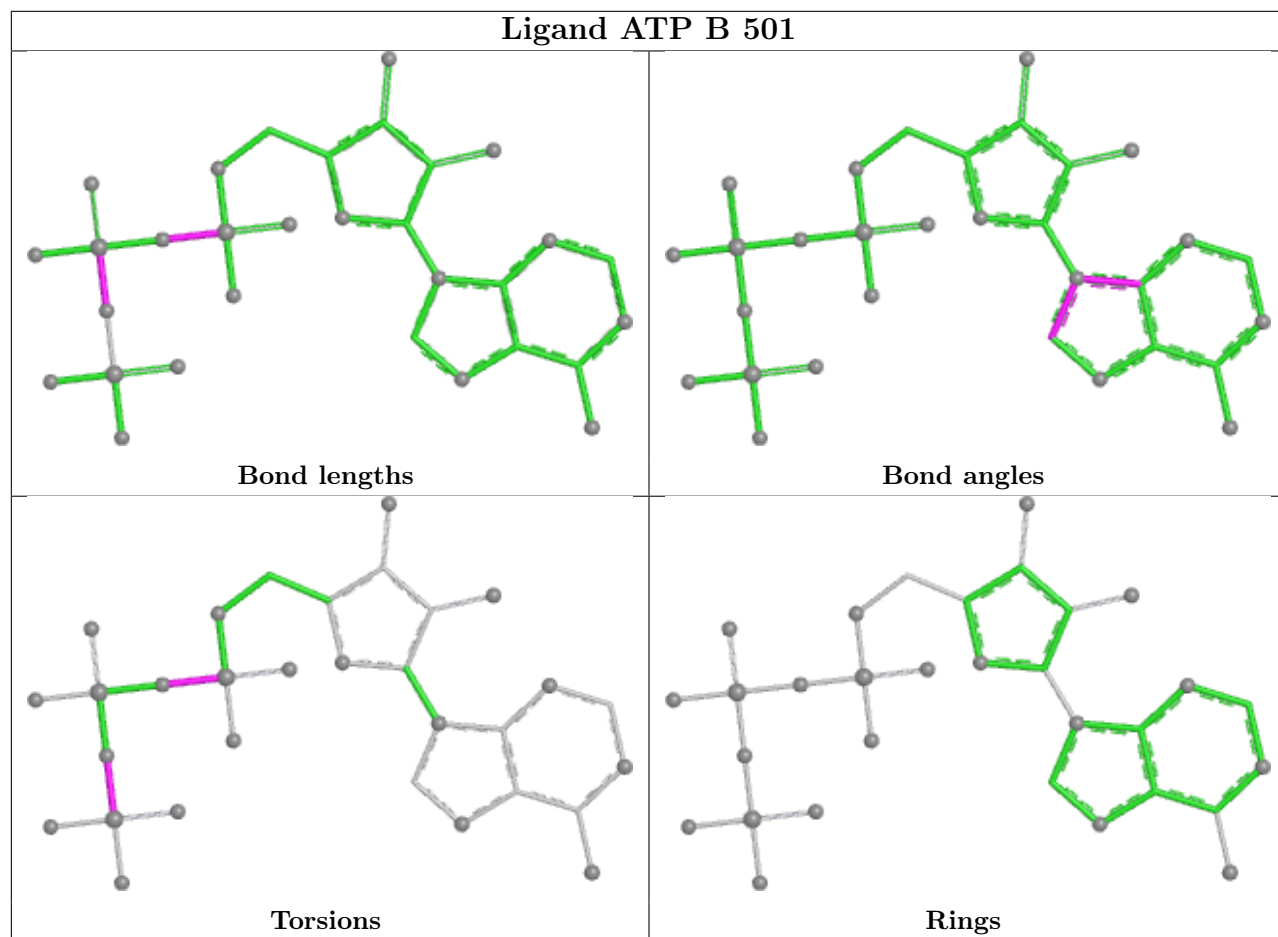
Mol	Chain	Res	Type	Atoms
2	B	501	ATP	PB-O3A-PA-O5'
2	A	501	ATP	PB-O3A-PA-O1A
2	B	501	ATP	PB-O3B-PG-O1G
2	A	501	ATP	PB-O3A-PA-O2A

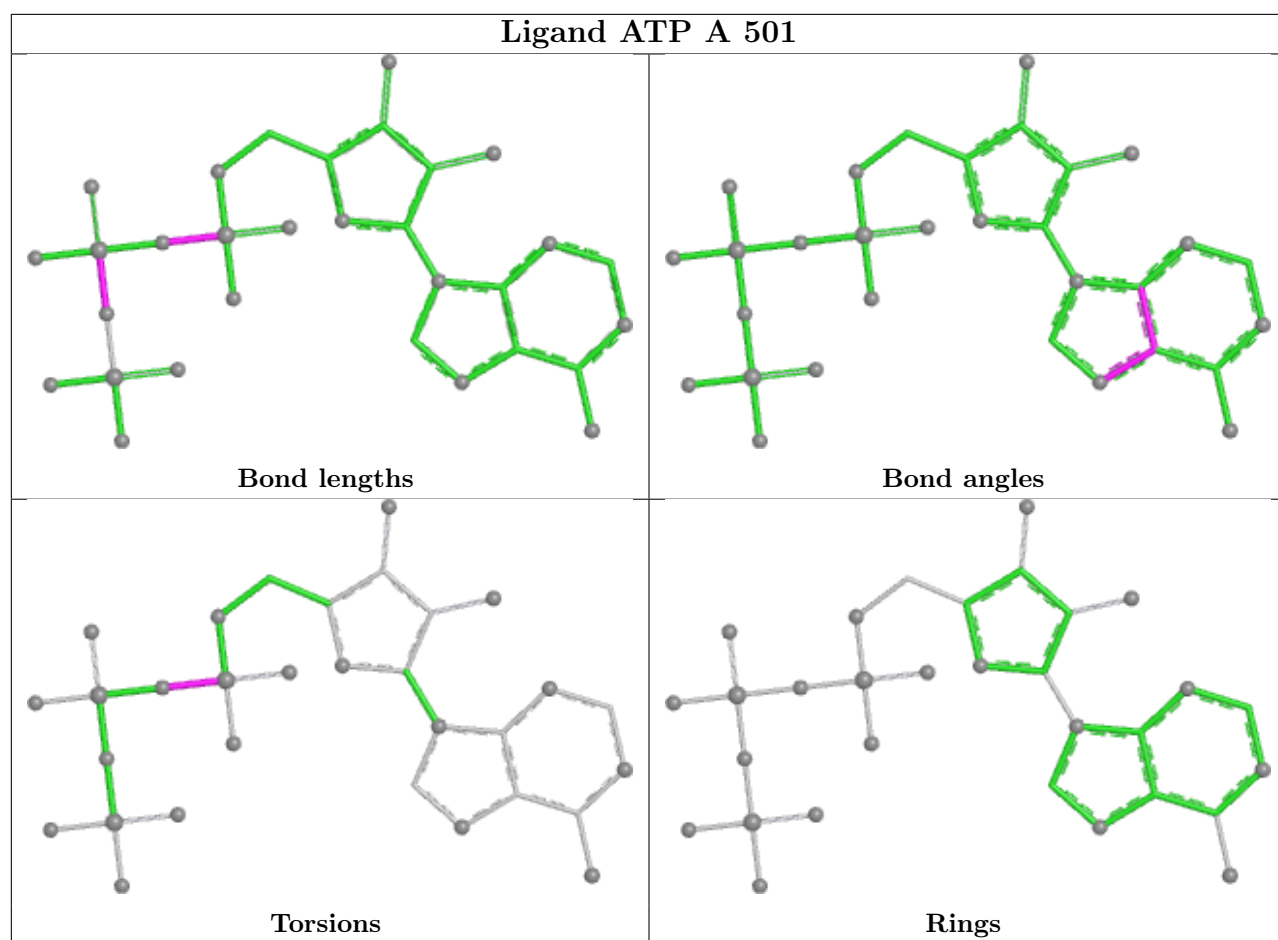
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	ATP	1	0
2	A	501	ATP	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	263/298 (88%)	0.21	7 (2%) 56 42	104, 181, 255, 273	0
1	B	263/298 (88%)	0.24	11 (4%) 40 29	112, 170, 258, 271	0
All	All	526/596 (88%)	0.22	18 (3%) 48 35	104, 175, 256, 273	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	211	LEU	4.0
1	B	255	THR	3.9
1	A	285	ASP	3.8
1	B	259	LEU	3.6
1	B	303	LEU	3.5
1	A	211	LEU	3.5
1	A	386	ASP	3.3
1	A	298	GLN	3.1
1	B	285	ASP	3.0
1	B	251	ARG	2.8
1	B	218	PHE	2.8
1	B	192	LYS	2.6
1	B	248	HIS	2.4
1	A	218	PHE	2.3
1	B	258	GLN	2.1
1	A	403	PHE	2.1
1	A	376	ASP	2.0
1	B	263	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](#)

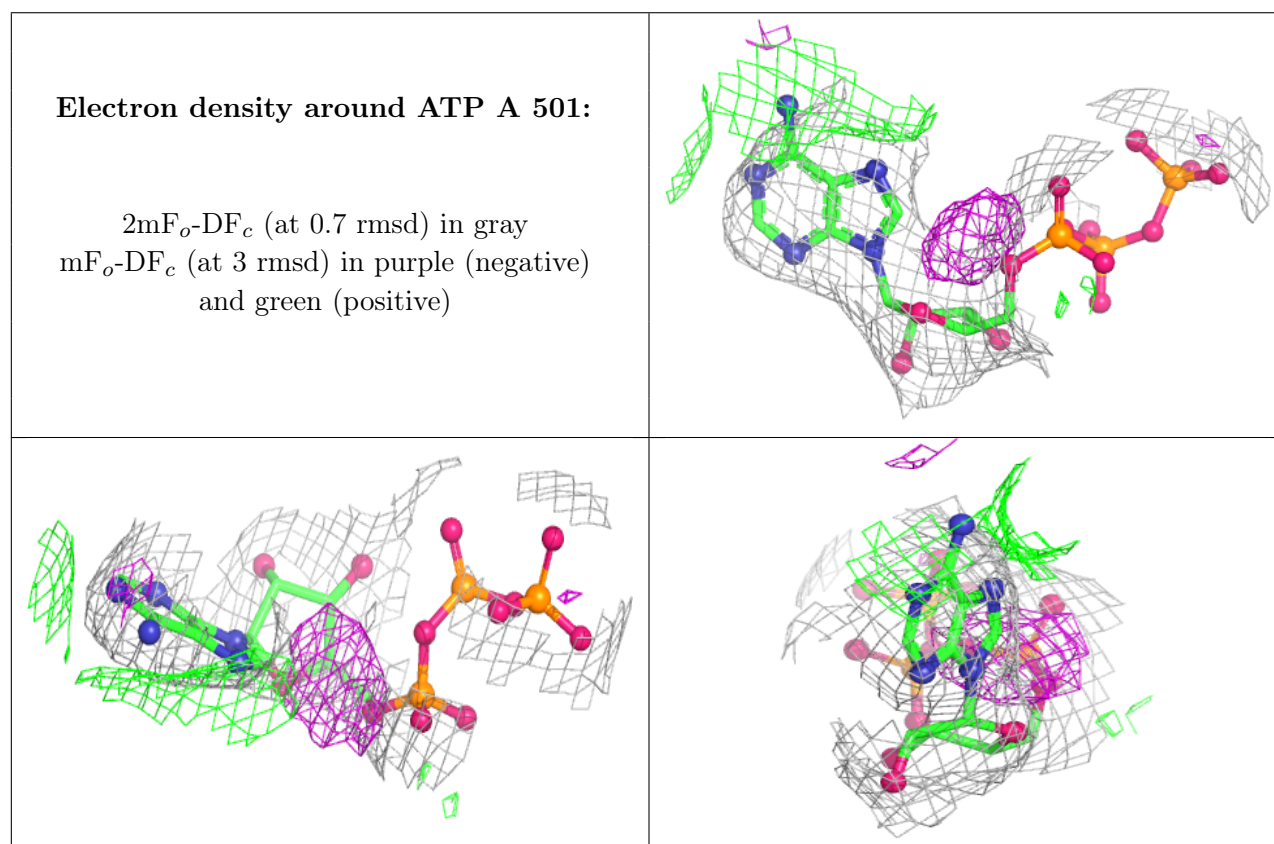
There are no oligosaccharides in this entry.

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.

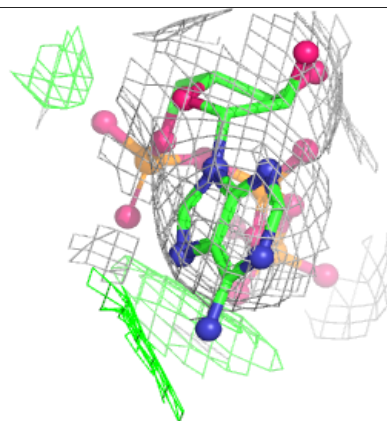
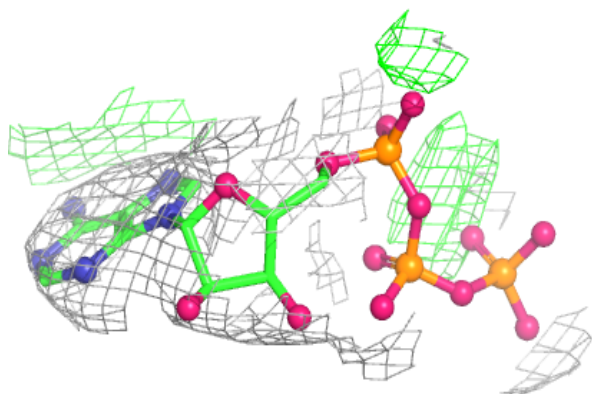
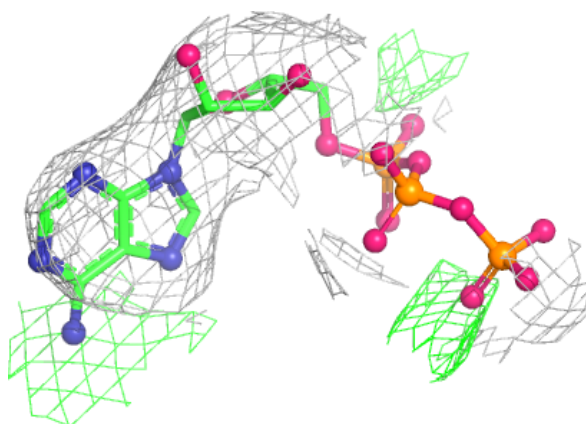
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ATP	A	501	31/31	0.92	0.10	170,181,207,210	0
2	ATP	B	501	31/31	0.96	0.07	169,175,183,183	0

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 ATP B 501:

$2mF_o-DF_c$ (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.