



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:25 PM UTC

PDB ID : 7Q92 / pdb_00007q92
Title : Crystal Structure of Agrobacterium tumefaciens NADQ, ATP complex.
Authors : Cianci, M.; Minazzato, G.; Heroux, A.; Raffaelli, N.; Sorci, L.; Gasparrini, M.
Deposited on : 2021-11-11
Resolution : 2.18 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

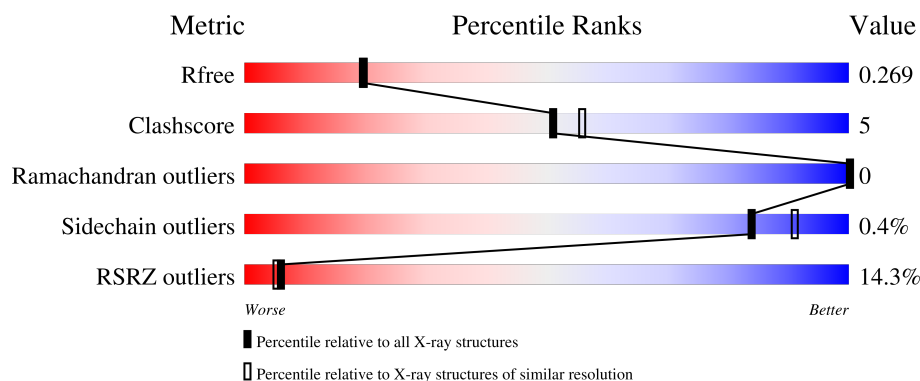
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	336	7% 74% 11% 14%
1	B	336	12% 73% 13% 14%
1	C	336	20% 74% 13% 13%
1	D	336	10% 77% 9% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	K	C	509	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9832 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 NADQ transcription factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	Se	0	0	0
			2330	1474	427	425	4			
1	B	288	Total	C	N	O	Se	0	0	0
			2346	1486	426	430	4			
1	C	293	Total	C	N	O	Se	0	0	0
			2364	1496	433	431	4			
1	D	290	Total	C	N	O	Se	0	0	0
			2340	1483	429	424	4			

There are 148 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP A9CG24
A	2	ARG	-	expression tag	UNP A9CG24
A	3	GLY	-	expression tag	UNP A9CG24
A	4	SER	-	expression tag	UNP A9CG24
A	5	HIS	-	expression tag	UNP A9CG24
A	6	HIS	-	expression tag	UNP A9CG24
A	7	HIS	-	expression tag	UNP A9CG24
A	8	HIS	-	expression tag	UNP A9CG24
A	9	HIS	-	expression tag	UNP A9CG24
A	10	HIS	-	expression tag	UNP A9CG24
A	11	GLY	-	expression tag	UNP A9CG24
A	12	MSE	-	expression tag	UNP A9CG24
A	13	ALA	-	expression tag	UNP A9CG24
A	14	SER	-	expression tag	UNP A9CG24
A	15	MSE	-	expression tag	UNP A9CG24
A	16	THR	-	expression tag	UNP A9CG24
A	17	GLY	-	expression tag	UNP A9CG24
A	18	GLY	-	expression tag	UNP A9CG24
A	19	GLN	-	expression tag	UNP A9CG24
A	20	GLN	-	expression tag	UNP A9CG24
A	21	MSE	-	expression tag	UNP A9CG24

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP A9CG24
A	23	ARG	-	expression tag	UNP A9CG24
A	24	ASP	-	expression tag	UNP A9CG24
A	25	LEU	-	expression tag	UNP A9CG24
A	26	TYR	-	expression tag	UNP A9CG24
A	27	ASP	-	expression tag	UNP A9CG24
A	28	ASP	-	expression tag	UNP A9CG24
A	29	ASP	-	expression tag	UNP A9CG24
A	30	ASP	-	expression tag	UNP A9CG24
A	31	LYS	-	expression tag	UNP A9CG24
A	32	ASP	-	expression tag	UNP A9CG24
A	33	HIS	-	expression tag	UNP A9CG24
A	34	PRO	-	expression tag	UNP A9CG24
A	35	PHE	-	expression tag	UNP A9CG24
A	36	THR	-	expression tag	UNP A9CG24
A	37	VAL	-	expression tag	UNP A9CG24
B	1	MSE	-	initiating methionine	UNP A9CG24
B	2	ARG	-	expression tag	UNP A9CG24
B	3	GLY	-	expression tag	UNP A9CG24
B	4	SER	-	expression tag	UNP A9CG24
B	5	HIS	-	expression tag	UNP A9CG24
B	6	HIS	-	expression tag	UNP A9CG24
B	7	HIS	-	expression tag	UNP A9CG24
B	8	HIS	-	expression tag	UNP A9CG24
B	9	HIS	-	expression tag	UNP A9CG24
B	10	HIS	-	expression tag	UNP A9CG24
B	11	GLY	-	expression tag	UNP A9CG24
B	12	MSE	-	expression tag	UNP A9CG24
B	13	ALA	-	expression tag	UNP A9CG24
B	14	SER	-	expression tag	UNP A9CG24
B	15	MSE	-	expression tag	UNP A9CG24
B	16	THR	-	expression tag	UNP A9CG24
B	17	GLY	-	expression tag	UNP A9CG24
B	18	GLY	-	expression tag	UNP A9CG24
B	19	GLN	-	expression tag	UNP A9CG24
B	20	GLN	-	expression tag	UNP A9CG24
B	21	MSE	-	expression tag	UNP A9CG24
B	22	GLY	-	expression tag	UNP A9CG24
B	23	ARG	-	expression tag	UNP A9CG24
B	24	ASP	-	expression tag	UNP A9CG24
B	25	LEU	-	expression tag	UNP A9CG24
B	26	TYR	-	expression tag	UNP A9CG24

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	ASP	-	expression tag	UNP A9CG24
B	28	ASP	-	expression tag	UNP A9CG24
B	29	ASP	-	expression tag	UNP A9CG24
B	30	ASP	-	expression tag	UNP A9CG24
B	31	LYS	-	expression tag	UNP A9CG24
B	32	ASP	-	expression tag	UNP A9CG24
B	33	HIS	-	expression tag	UNP A9CG24
B	34	PRO	-	expression tag	UNP A9CG24
B	35	PHE	-	expression tag	UNP A9CG24
B	36	THR	-	expression tag	UNP A9CG24
B	37	VAL	-	expression tag	UNP A9CG24
C	1	MSE	-	initiating methionine	UNP A9CG24
C	2	ARG	-	expression tag	UNP A9CG24
C	3	GLY	-	expression tag	UNP A9CG24
C	4	SER	-	expression tag	UNP A9CG24
C	5	HIS	-	expression tag	UNP A9CG24
C	6	HIS	-	expression tag	UNP A9CG24
C	7	HIS	-	expression tag	UNP A9CG24
C	8	HIS	-	expression tag	UNP A9CG24
C	9	HIS	-	expression tag	UNP A9CG24
C	10	HIS	-	expression tag	UNP A9CG24
C	11	GLY	-	expression tag	UNP A9CG24
C	12	MSE	-	expression tag	UNP A9CG24
C	13	ALA	-	expression tag	UNP A9CG24
C	14	SER	-	expression tag	UNP A9CG24
C	15	MSE	-	expression tag	UNP A9CG24
C	16	THR	-	expression tag	UNP A9CG24
C	17	GLY	-	expression tag	UNP A9CG24
C	18	GLY	-	expression tag	UNP A9CG24
C	19	GLN	-	expression tag	UNP A9CG24
C	20	GLN	-	expression tag	UNP A9CG24
C	21	MSE	-	expression tag	UNP A9CG24
C	22	GLY	-	expression tag	UNP A9CG24
C	23	ARG	-	expression tag	UNP A9CG24
C	24	ASP	-	expression tag	UNP A9CG24
C	25	LEU	-	expression tag	UNP A9CG24
C	26	TYR	-	expression tag	UNP A9CG24
C	27	ASP	-	expression tag	UNP A9CG24
C	28	ASP	-	expression tag	UNP A9CG24
C	29	ASP	-	expression tag	UNP A9CG24
C	30	ASP	-	expression tag	UNP A9CG24
C	31	LYS	-	expression tag	UNP A9CG24

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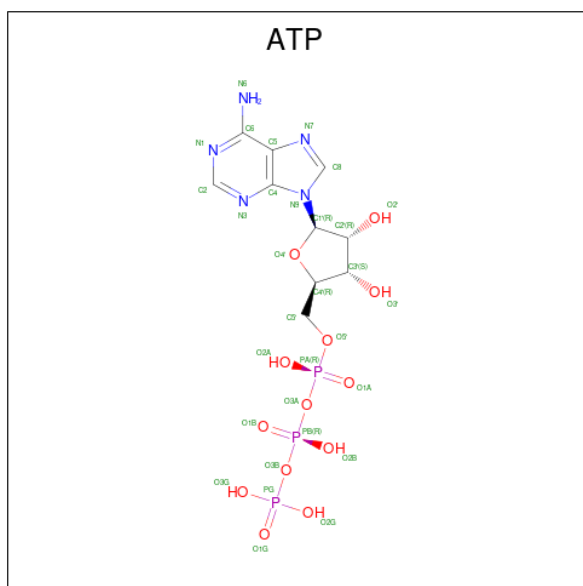
Chain	Residue	Modelled	Actual	Comment	Reference
C	32	ASP	-	expression tag	UNP A9CG24
C	33	HIS	-	expression tag	UNP A9CG24
C	34	PRO	-	expression tag	UNP A9CG24
C	35	PHE	-	expression tag	UNP A9CG24
C	36	THR	-	expression tag	UNP A9CG24
C	37	VAL	-	expression tag	UNP A9CG24
D	1	MSE	-	initiating methionine	UNP A9CG24
D	2	ARG	-	expression tag	UNP A9CG24
D	3	GLY	-	expression tag	UNP A9CG24
D	4	SER	-	expression tag	UNP A9CG24
D	5	HIS	-	expression tag	UNP A9CG24
D	6	HIS	-	expression tag	UNP A9CG24
D	7	HIS	-	expression tag	UNP A9CG24
D	8	HIS	-	expression tag	UNP A9CG24
D	9	HIS	-	expression tag	UNP A9CG24
D	10	HIS	-	expression tag	UNP A9CG24
D	11	GLY	-	expression tag	UNP A9CG24
D	12	MSE	-	expression tag	UNP A9CG24
D	13	ALA	-	expression tag	UNP A9CG24
D	14	SER	-	expression tag	UNP A9CG24
D	15	MSE	-	expression tag	UNP A9CG24
D	16	THR	-	expression tag	UNP A9CG24
D	17	GLY	-	expression tag	UNP A9CG24
D	18	GLY	-	expression tag	UNP A9CG24
D	19	GLN	-	expression tag	UNP A9CG24
D	20	GLN	-	expression tag	UNP A9CG24
D	21	MSE	-	expression tag	UNP A9CG24
D	22	GLY	-	expression tag	UNP A9CG24
D	23	ARG	-	expression tag	UNP A9CG24
D	24	ASP	-	expression tag	UNP A9CG24
D	25	LEU	-	expression tag	UNP A9CG24
D	26	TYR	-	expression tag	UNP A9CG24
D	27	ASP	-	expression tag	UNP A9CG24
D	28	ASP	-	expression tag	UNP A9CG24
D	29	ASP	-	expression tag	UNP A9CG24
D	30	ASP	-	expression tag	UNP A9CG24
D	31	LYS	-	expression tag	UNP A9CG24
D	32	ASP	-	expression tag	UNP A9CG24
D	33	HIS	-	expression tag	UNP A9CG24
D	34	PRO	-	expression tag	UNP A9CG24
D	35	PHE	-	expression tag	UNP A9CG24
D	36	THR	-	expression tag	UNP A9CG24

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Chain	Residue	Modelled	Actual	Comment	Reference
D	37	VAL	-	expression tag	UNP A9CG24

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

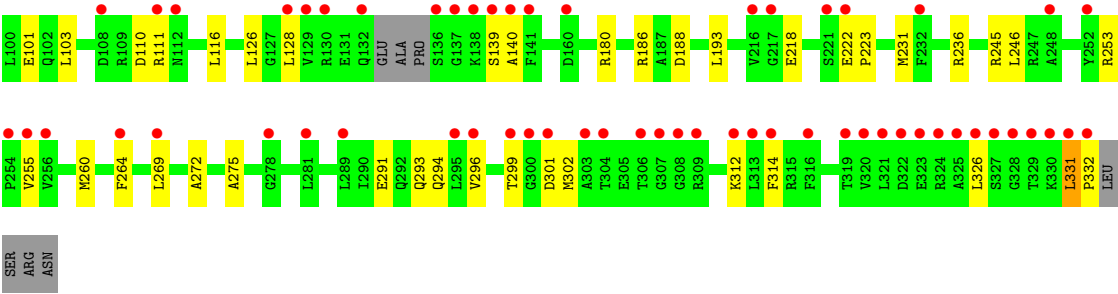
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	B	2	Total	K	0	0
			2	2		
3	C	9	Total	K	0	0
			9	9		
3	D	7	Total	K	0	0
			7	7		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

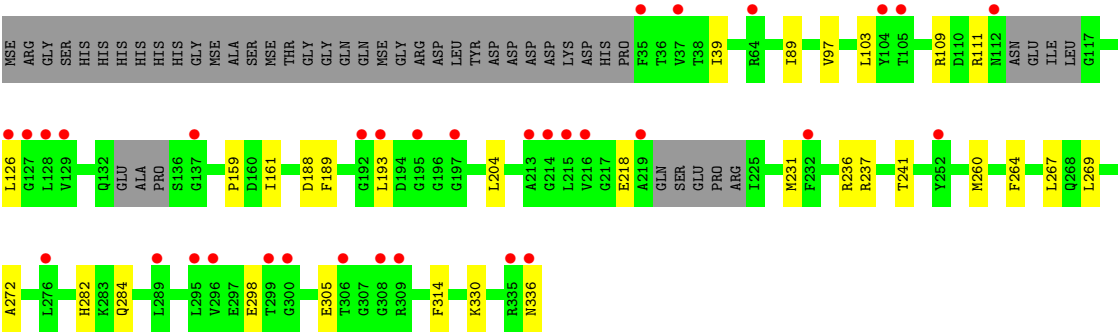
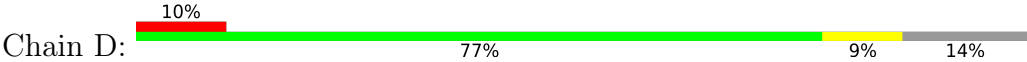
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Na 1	0	0
4	D	1	Total 1	Na 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	96	Total 96	O 96	0	0
5	B	82	Total 82	O 82	0	0
5	C	107	Total 107	O 107	0	0
5	D	84	Total 84	O 84	0	0



● Molecule 1: NADQ transcription factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.92Å 132.57Å 86.85Å 90.00° 100.16° 90.00°	Depositor
Resolution (Å)	51.84 – 2.18 51.84 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.5 (51.84-2.18) 99.5 (51.84-2.18)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.230 , 0.269 0.230 , 0.269	Depositor DCC
R_{free} test set	3386 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9832	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, K, NA

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	0.08	0/2380	0.24	0/3212
1	B	0.09	0/2396	0.24	0/3233
1	C	0.09	0/2414	0.27	0/3258
1	D	0.08	0/2388	0.22	0/3219
All	All	0.08	0/9578	0.24	0/12922

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	331	LEU	Peptide

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	2330	0	2279	25	0
1	B	2346	0	2282	26	0
1	C	2364	0	2322	33	0
1	D	2340	0	2295	19	0
2	A	31	0	12	1	0
2	C	31	0	12	1	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	9	0	0	0	0
3	D	7	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	96	0	0	0	0
5	B	82	0	0	1	0
5	C	107	0	0	4	0
5	D	84	0	0	0	0
All	All	9832	0	9202	97	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (97) 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:B:108:ASP:O	1:B:117:GLY:N	2.22	0.72
1:C:260:MSE:HE3	1:C:269:LEU:HD12	1.71	0.71
1:C:332:PRO:HG2	1:D:237:ARG:HH12	1.56	0.70
1:B:58:PRO:HD3	1:B:275:ALA:HB1	1.75	0.68
1:C:103:LEU:O	1:D:336:ASN:ND2	2.27	0.67
1:B:260:MSE:HE1	1:B:272:ALA:HB3	1.77	0.66
1:B:53:ILE:HD13	1:B:272:ALA:HB1	1.77	0.65
1:C:260:MSE:HE1	1:C:272:ALA:HB3	1.79	0.65
1:C:302:MSE:HE1	1:C:312:LYS:HG2	1.80	0.64
1:A:296:VAL:O	1:A:317:ARG:NH2	2.28	0.64
1:D:260:MSE:HE3	1:D:269:LEU:HD12	1.79	0.62
1:C:218:GLU:OE1	1:C:236:ARG:NH2	2.32	0.62
1:C:58:PRO:HD3	1:C:275:ALA:HB1	1.80	0.62
1:A:126:LEU:HD21	1:A:246:LEU:HG	1.82	0.61
1:A:58:PRO:HD3	1:A:275:ALA:HB1	1.82	0.60
1:C:331:LEU:HB3	1:C:332:PRO:HD2	1.83	0.58
1:C:116:LEU:HD11	1:D:39:ILE:HG21	1.85	0.58
1:A:188:ASP:HA	1:A:193:LEU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:LEU:HD13	1:D:189:PHE:HB2	1.85	0.58
1:C:291:GLU:O	1:C:294:GLN:NE2	2.36	0.58
1:A:237:ARG:NH2	2:A:501:ATP:O1A	2.36	0.57
1:D:204:LEU:HD22	1:D:241:THR:HG22	1.87	0.57
1:A:281:LEU:HD22	1:A:286:PHE:HB2	1.87	0.57
1:A:54:THR:HG22	1:A:55:THR:HG23	1.87	0.57
1:D:267:LEU:HB3	1:D:305:GLU:OE2	2.07	0.55
1:B:299:THR:HG23	1:B:301:ASP:H	1.73	0.54
1:B:170:ARG:NH1	1:B:194:ASP:OD1	2.40	0.54
1:D:260:MSE:HE1	1:D:272:ALA:HB3	1.90	0.54
1:B:159:PRO:HB2	1:B:161:ILE:HG22	1.90	0.53
1:C:222:GLU:HB2	1:C:223:PRO:HD3	1.90	0.53
1:C:331:LEU:HB3	1:C:332:PRO:CD	2.39	0.53
1:A:61:MSE:HE3	1:A:70:PRO:HG2	1.90	0.53
1:C:186:ARG:NH1	5:C:609:HOH:O	2.39	0.53
1:B:250:ILE:HD12	1:B:273:ILE:HG23	1.89	0.53
1:A:168:LYS:HE2	1:A:225:ILE:HD13	1.91	0.53
1:B:247:ARG:O	1:B:251:LYS:HG2	2.09	0.52
1:B:302:MSE:HE1	1:B:312:LYS:HG2	1.91	0.52
1:C:264:PHE:O	1:C:314:PHE:N	2.37	0.51
1:B:158:ARG:HH21	1:B:162:LEU:HB3	1.76	0.51
1:B:61:MSE:SE	1:B:93:THR:HG21	2.60	0.51
1:A:166:ILE:HD13	1:A:193:LEU:HD21	1.93	0.50
1:C:126:LEU:HD21	1:C:246:LEU:HG	1.93	0.50
1:B:188:ASP:OD1	1:B:194:ASP:N	2.26	0.49
1:C:37:VAL:N	5:C:613:HOH:O	2.44	0.49
1:C:80:THR:HB	1:C:332:PRO:HA	1.94	0.49
1:D:298:GLU:HG2	1:D:314:PHE:CE2	2.48	0.49
1:A:111:ARG:HH11	1:A:111:ARG:HB2	1.78	0.49
1:B:108:ASP:HB3	1:B:120:THR:HB	1.95	0.49
1:B:166:ILE:HG23	1:B:193:LEU:HG	1.94	0.48
1:C:188:ASP:HA	1:C:193:LEU:H	1.77	0.48
1:A:43:HIS:NE2	1:A:45:GLU:OE2	2.42	0.48
1:C:61:MSE:HG3	1:C:140:ALA:HB1	1.95	0.48
1:C:80:THR:HG22	1:C:332:PRO:HD3	1.95	0.48
1:B:126:LEU:HD21	1:B:246:LEU:HG	1.95	0.48
1:A:68:ALA:HB2	1:A:232:PHE:HB3	1.96	0.47
2:C:501:ATP:O2A	1:D:330:LYS:NZ	2.47	0.47
1:D:231:MSE:HG3	1:D:236:ARG:HG3	1.97	0.47
1:B:54:THR:HG22	1:B:55:THR:HG23	1.97	0.47
1:B:269:LEU:HG	1:B:286:PHE:HZ	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:ILE:HG21	1:D:97:VAL:HG21	1.97	0.46
1:C:231:MSE:HB2	1:C:236:ARG:HG3	1.97	0.46
1:A:274:GLU:HG3	1:A:281:LEU:HD12	1.96	0.46
1:B:33:HIS:HB3	1:B:36:THR:HB	1.98	0.46
1:A:284:GLN:NE2	1:C:75:GLU:OE1	2.49	0.45
1:B:103:LEU:HD21	1:B:126:LEU:HB2	1.98	0.45
1:C:253:ARG:NH1	1:C:293:GLN:OE1	2.50	0.45
1:B:33:HIS:CE1	1:B:35:PHE:HB2	2.51	0.45
1:B:260:MSE:HE3	1:B:269:LEU:HA	1.98	0.45
1:B:31:LYS:HD2	1:B:31:LYS:HA	1.84	0.44
1:C:110:ASP:N	5:C:622:HOH:O	2.50	0.44
1:C:180:ARG:NH2	5:C:618:HOH:O	2.49	0.44
1:A:149:PHE:CZ	1:A:240:ALA:HB2	2.52	0.44
1:A:222:GLU:HB3	1:A:223:PRO:HD3	1.99	0.44
1:D:159:PRO:HB2	1:D:161:ILE:HG22	1.99	0.43
1:C:101:GLU:OE2	1:C:245:ARG:NH1	2.50	0.43
1:C:299:THR:HG23	1:C:301:ASP:H	1.82	0.43
1:A:128:LEU:HD21	1:A:246:LEU:HD11	2.01	0.43
1:A:273:ILE:HB	1:A:281:LEU:HD11	2.00	0.43
1:A:89:ILE:HG21	1:A:97:VAL:HG21	2.01	0.43
1:D:218:GLU:OE1	1:D:236:ARG:NH2	2.46	0.43
1:C:253:ARG:HG2	1:C:255:VAL:HG23	2.00	0.43
1:A:61:MSE:HE1	1:A:89:ILE:HG23	2.02	0.42
1:A:180:ARG:HG2	1:A:184:HIS:HD2	1.84	0.42
1:B:79:ARG:NH1	5:B:508:HOH:O	2.39	0.42
1:C:103:LEU:HD21	1:C:126:LEU:HB2	2.00	0.42
1:D:188:ASP:HA	1:D:193:LEU:H	1.84	0.42
1:C:72:GLY:HA3	1:C:88:TRP:CG	2.54	0.42
1:C:139:SER:OG	1:C:140:ALA:N	2.52	0.42
1:D:264:PHE:O	1:D:314:PHE:N	2.43	0.42
1:A:106:PHE:HE1	1:B:330:LYS:HE3	1.85	0.41
1:C:128:LEU:HD21	1:C:246:LEU:HD11	2.01	0.41
1:B:231:MSE:HG3	1:B:236:ARG:HG3	2.02	0.41
1:A:250:ILE:HD12	1:A:273:ILE:HG23	2.02	0.41
1:A:103:LEU:HD21	1:A:126:LEU:HB2	2.03	0.40
1:D:103:LEU:HD21	1:D:126:LEU:HB2	2.03	0.40
1:D:282:HIS:CE1	1:D:284:GLN:HB2	2.57	0.40
1:D:109:ARG:O	1:D:111:ARG:NH1	2.54	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	284/336 (84%)	270 (95%)	14 (5%)	0	100	100
1	B	280/336 (83%)	263 (94%)	17 (6%)	0	100	100
1	C	289/336 (86%)	274 (95%)	15 (5%)	0	100	100
1	D	282/336 (84%)	272 (96%)	10 (4%)	0	100	100
All	All	1135/1344 (84%)	1079 (95%)	56 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	237/270 (88%)	236 (100%)	1 (0%)	84	91
1	B	242/270 (90%)	241 (100%)	1 (0%)	84	91
1	C	242/270 (90%)	240 (99%)	2 (1%)	73	83
1	D	239/270 (88%)	239 (100%)	0	100	100
All	All	960/1080 (89%)	956 (100%)	4 (0%)	84	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ARG
1	B	132	GLN

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Mol	Chain	Res	Type
1	C	111	ARG
1	C	296	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	294	GLN
1	B	43	HIS
1	B	132	GLN
1	D	132	GLN
1	D	294	GLN

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 23 ligands modelled in this entry, 21 are monoatomic - leaving 2 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	$\# Z > 2$
2	ATP	A	501	-	32,33,33	0.28	0	48,52,52	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	C	501	-	32,33,33	0.31	0	48,52,52	0.32	0

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	A	501	-	-	7/22/38/38	0/3/3/3
2	ATP	C	501	-	-	8/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

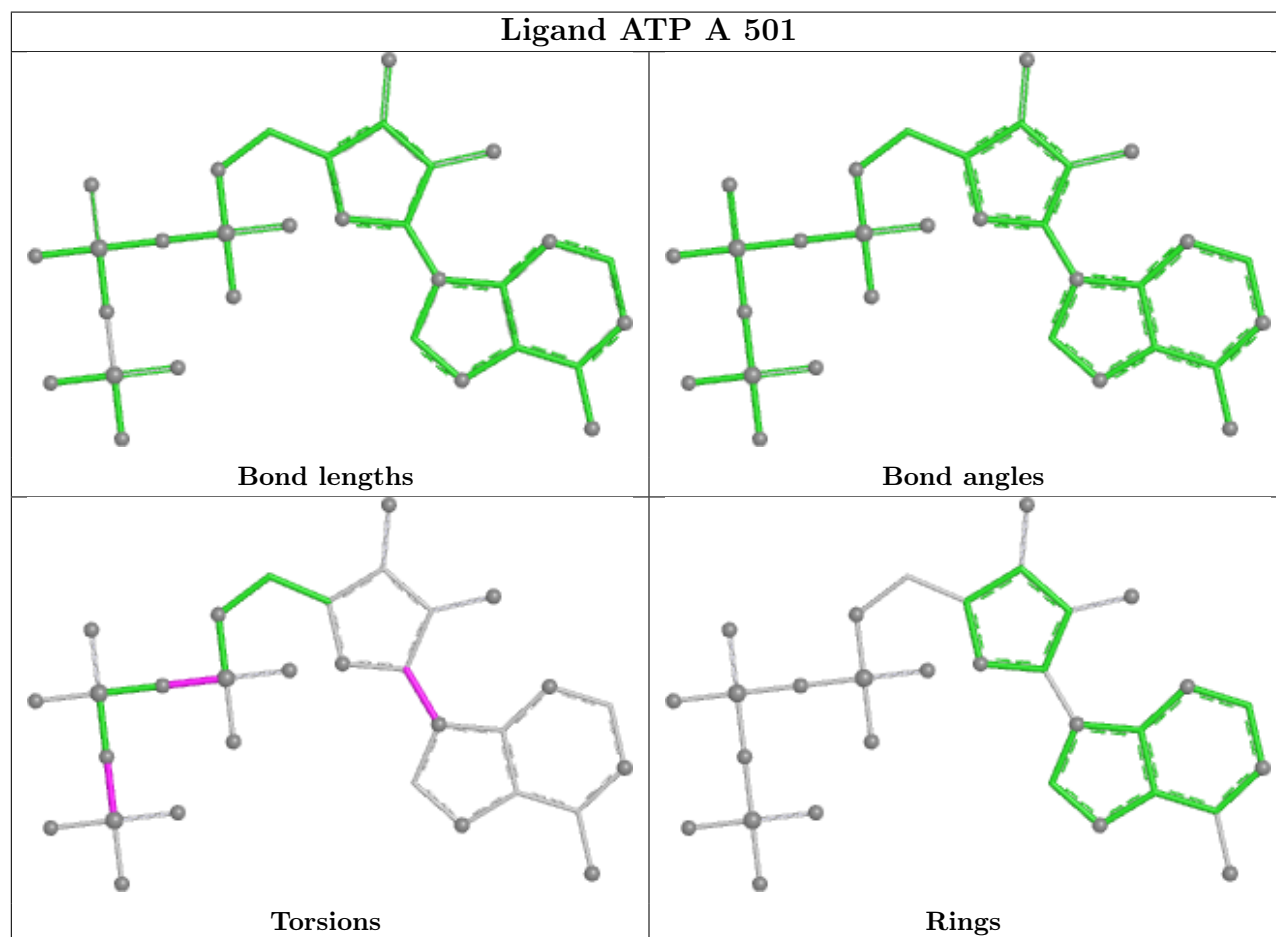
Mol	Chain	Res	Type	Atoms
2	A	501	ATP	PB-O3B-PG-O3G
2	A	501	ATP	PB-O3A-PA-O5'
2	C	501	ATP	PB-O3B-PG-O2G
2	C	501	ATP	PB-O3B-PG-O3G
2	C	501	ATP	PB-O3A-PA-O1A
2	C	501	ATP	C2'-C1'-N9-C8
2	A	501	ATP	C2'-C1'-N9-C8
2	A	501	ATP	C2'-C1'-N9-C4
2	C	501	ATP	C2'-C1'-N9-C4
2	C	501	ATP	O4'-C1'-N9-C8
2	A	501	ATP	PB-O3B-PG-O2G
2	C	501	ATP	PB-O3A-PA-O2A
2	A	501	ATP	O4'-C1'-N9-C8
2	A	501	ATP	PB-O3B-PG-O1G
2	C	501	ATP	PA-O3A-PB-O2B

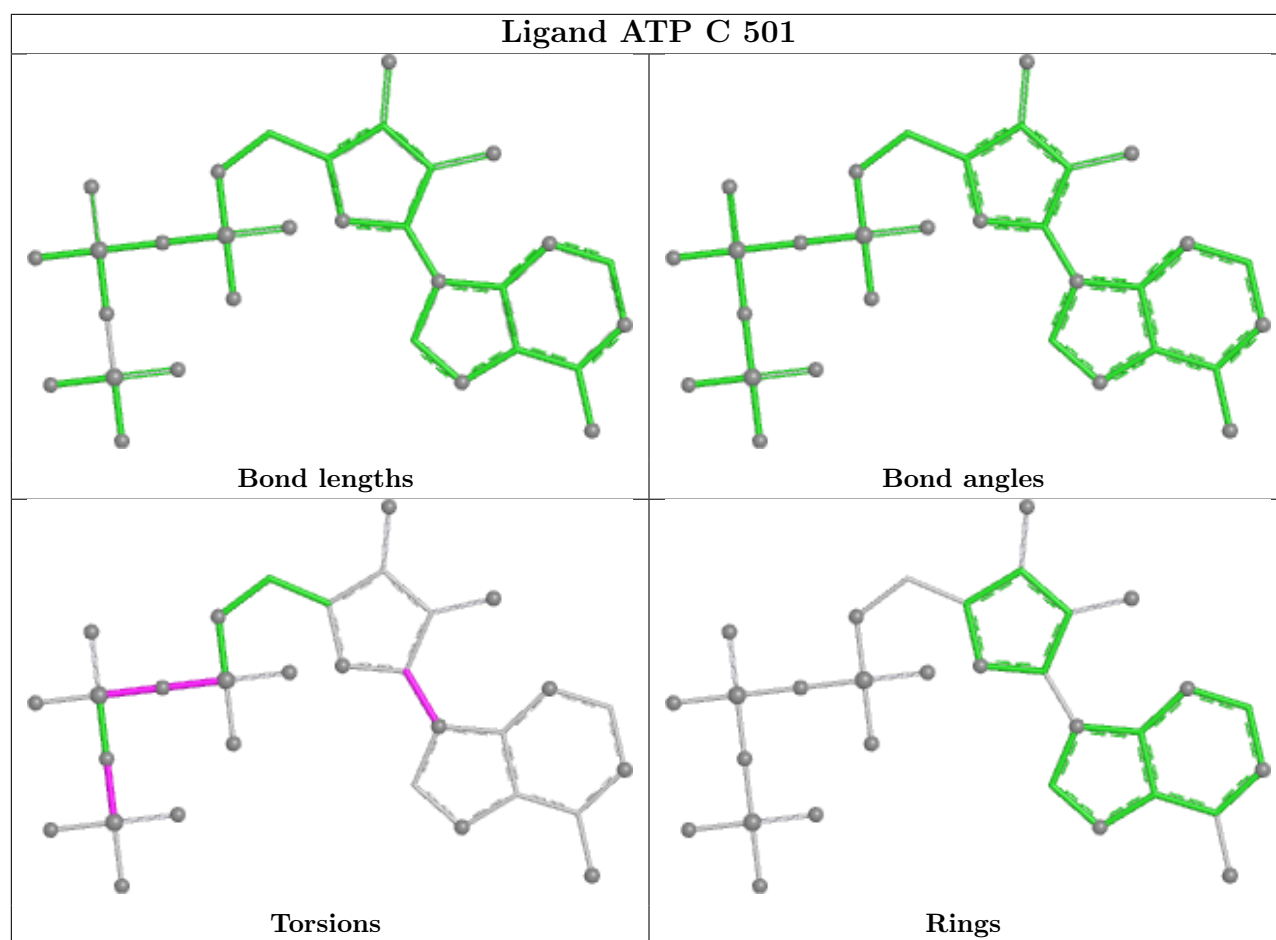
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ATP	1	0
2	C	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 ⓘ

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	284/336 (84%)	0.73	23 (8%) 18 17	25, 38, 66, 89	0
1	B	284/336 (84%)	1.08	41 (14%) 6 5	23, 42, 77, 111	0
1	C	289/336 (86%)	1.10	66 (22%) 2 2	22, 38, 91, 109	0
1	D	286/336 (85%)	0.97	33 (11%) 9 8	26, 42, 63, 77	0
All	All	1143/1344 (85%)	0.97	163 (14%) 6 5	22, 40, 77, 111	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	332	PRO	6.6
1	B	26	TYR	5.7
1	D	127	GLY	5.4
1	C	306	THR	5.0
1	C	295	LEU	4.9
1	C	328	GLY	4.9
1	C	329	THR	4.9
1	C	140	ALA	4.6
1	B	27	ASP	4.4
1	A	141	PHE	4.4
1	C	129	VAL	4.4
1	D	128	LEU	4.2
1	A	134	ALA	4.1
1	B	129	VAL	4.1
1	D	213	ALA	4.0
1	D	126	LEU	4.0
1	A	223	PRO	4.0
1	C	37	VAL	4.0
1	C	325	ALA	3.9
1	D	129	VAL	3.8
1	C	303	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	108	ASP	3.8
1	B	301	ASP	3.8
1	D	105	THR	3.7
1	D	252	TYR	3.7
1	A	113	ASN	3.6
1	A	328	GLY	3.6
1	B	232	PHE	3.6
1	A	135	PRO	3.6
1	C	320	VAL	3.5
1	B	132	GLN	3.5
1	B	299	THR	3.5
1	C	55	THR	3.4
1	A	111	ARG	3.4
1	C	331	LEU	3.4
1	B	222	GLU	3.3
1	C	313	LEU	3.3
1	B	279	LEU	3.2
1	B	336	ASN	3.2
1	C	252	TYR	3.2
1	A	194	ASP	3.1
1	C	138	LYS	3.1
1	A	195	GLY	3.1
1	B	32	ASP	3.1
1	A	39	ILE	3.1
1	C	327	SER	3.1
1	C	132	GLN	3.1
1	C	130	ARG	3.0
1	A	115	ILE	3.0
1	D	300	GLY	3.0
1	B	31	LYS	3.0
1	B	35	PHE	3.0
1	C	141	PHE	3.0
1	C	319	THR	3.0
1	B	193	LEU	2.9
1	B	128	LEU	2.9
1	B	192	GLY	2.9
1	C	278	GLY	2.9
1	C	330	LYS	2.9
1	C	296	VAL	2.9
1	B	300	GLY	2.9
1	C	321	LEU	2.9
1	C	139	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	282	HIS	2.8
1	C	281	LEU	2.8
1	D	193	LEU	2.8
1	C	248	ALA	2.8
1	C	316	PHE	2.7
1	D	232	PHE	2.7
1	C	304	THR	2.7
1	B	30	ASP	2.7
1	C	254	PRO	2.7
1	D	112	ASN	2.7
1	B	52	ALA	2.7
1	C	264	PHE	2.7
1	B	333	LEU	2.7
1	D	215	LEU	2.7
1	A	327	SER	2.7
1	B	221	SER	2.7
1	B	272	ALA	2.6
1	C	76	PHE	2.6
1	C	221	SER	2.6
1	D	64	ARG	2.6
1	B	160	ASP	2.6
1	C	39	ILE	2.6
1	A	140	ALA	2.6
1	B	142	TRP	2.6
1	B	252	TYR	2.5
1	C	307	GLY	2.5
1	C	299	THR	2.5
1	C	322	ASP	2.5
1	C	53	ILE	2.5
1	B	170	ARG	2.5
1	C	160	ASP	2.5
1	C	301	ASP	2.5
1	A	139	SER	2.5
1	B	289	LEU	2.5
1	C	289	LEU	2.5
1	D	289	LEU	2.5
1	C	300	GLY	2.5
1	D	336	ASN	2.5
1	B	223	PRO	2.4
1	B	313	LEU	2.4
1	A	307	GLY	2.4
1	C	308	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	214	GLY	2.4
1	D	308	GLY	2.4
1	D	37	VAL	2.4
1	D	219	ALA	2.4
1	D	35	PHE	2.4
1	B	28	ASP	2.4
1	D	306	THR	2.4
1	C	137	GLY	2.4
1	D	137	GLY	2.4
1	D	197	GLY	2.4
1	B	290	ILE	2.4
1	C	326	LEU	2.3
1	A	196	GLY	2.3
1	D	195	GLY	2.3
1	C	232	PHE	2.3
1	C	312	LYS	2.3
1	D	335	ARG	2.3
1	D	296	VAL	2.3
1	A	138	LYS	2.3
1	A	225	ILE	2.3
1	A	112	ASN	2.3
1	C	256	VAL	2.3
1	D	216	VAL	2.3
1	C	324	ARG	2.3
1	B	311	ALA	2.3
1	B	117	GLY	2.3
1	C	314	PHE	2.2
1	B	281	LEU	2.2
1	D	295	LEU	2.2
1	B	39	ILE	2.2
1	C	54	THR	2.2
1	A	326	LEU	2.2
1	D	192	GLY	2.2
1	A	116	LEU	2.2
1	D	276	LEU	2.2
1	B	119	ARG	2.2
1	C	99	TYR	2.2
1	D	104	TYR	2.2
1	C	222	GLU	2.1
1	B	118	GLY	2.1
1	C	255	VAL	2.1
1	A	317	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	112	ASN	2.1
1	D	299	THR	2.1
1	B	130	ARG	2.1
1	C	111	ARG	2.1
1	C	217	GLY	2.1
1	B	191	PHE	2.1
1	B	267	LEU	2.1
1	C	128	LEU	2.1
1	C	269	LEU	2.1
1	C	323	GLU	2.1
1	A	252	TYR	2.1
1	C	216	VAL	2.1
1	C	95	HIS	2.0
1	C	136	SER	2.0
1	C	309	ARG	2.0
1	D	309	ARG	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.

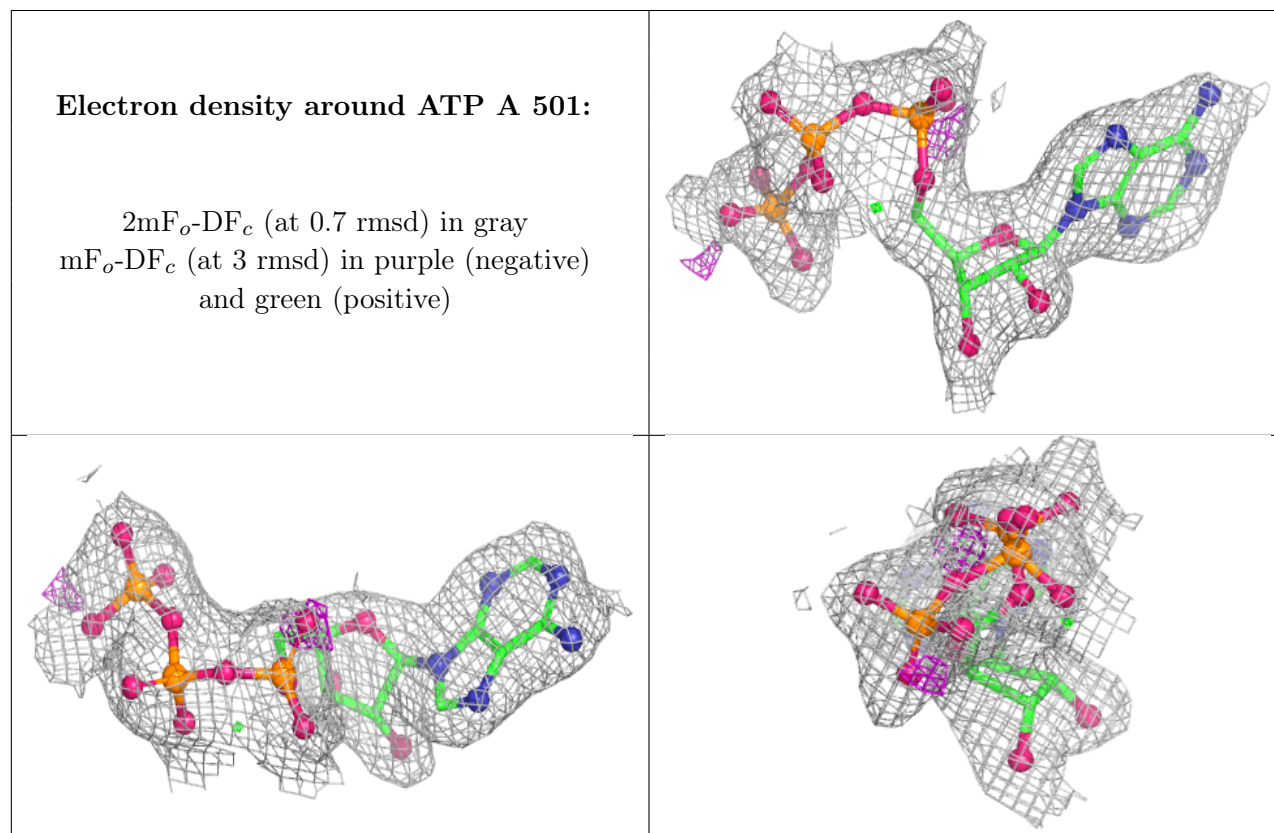
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	K	D	404	1/1	0.40	0.28	108,108,108,108	0
3	K	C	509	1/1	0.44	0.47	70,70,70,70	0
3	K	D	405	1/1	0.58	0.26	86,86,86,86	0
3	K	A	502	1/1	0.60	0.22	84,84,84,84	0
3	K	D	403	1/1	0.67	0.13	99,99,99,99	0
3	K	C	503	1/1	0.72	0.32	85,85,85,85	0
3	K	D	406	1/1	0.72	0.25	77,77,77,77	0

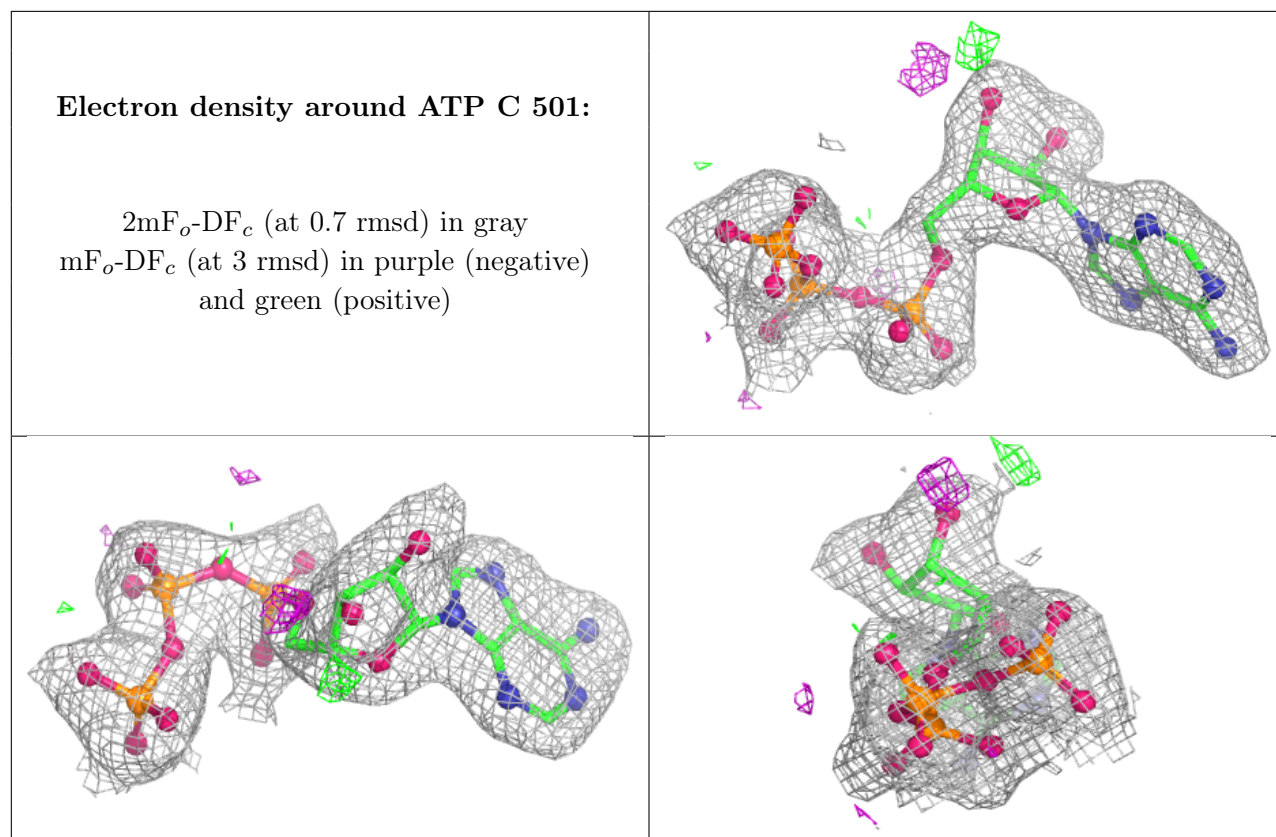
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	K	C	502	1/1	0.80	0.15	92,92,92,92	0
4	NA	D	408	1/1	0.86	0.21	47,47,47,47	0
3	K	C	510	1/1	0.87	0.35	59,59,59,59	0
2	ATP	A	501	31/31	0.89	0.12	35,51,68,76	0
3	K	D	407	1/1	0.90	0.12	61,61,61,61	0
3	K	B	402	1/1	0.90	0.23	58,58,58,58	0
3	K	C	505	1/1	0.91	0.23	58,58,58,58	0
3	K	C	507	1/1	0.92	0.13	60,60,60,60	0
3	K	C	504	1/1	0.93	0.08	54,54,54,54	0
3	K	D	402	1/1	0.93	0.15	52,52,52,52	0
3	K	C	508	1/1	0.93	0.09	65,65,65,65	0
3	K	B	401	1/1	0.93	0.21	50,50,50,50	0
4	NA	A	503	1/1	0.94	0.10	32,32,32,32	0
2	ATP	C	501	31/31	0.94	0.08	28,36,46,51	0
3	K	C	506	1/1	0.95	0.09	59,59,59,59	0
3	K	D	401	1/1	0.95	0.07	51,51,51,51	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 ⓘ

There are no such residues in this entry.