



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2022 – 06:42 pm GMT

PDB ID : 7Q92
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

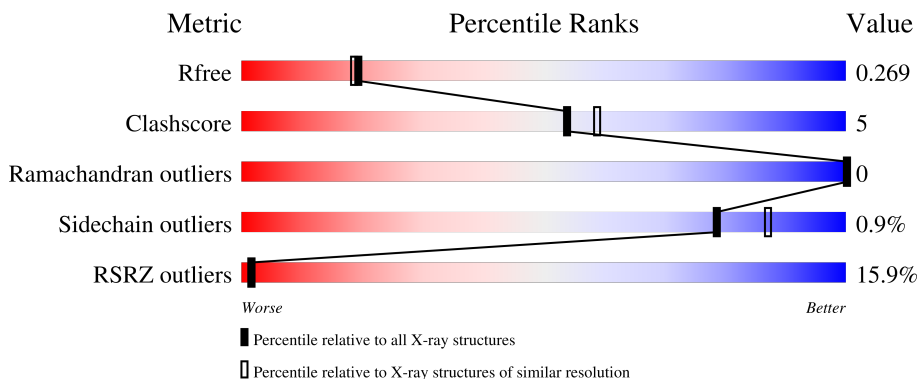
1 Overall quality at a glance

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}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (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	 8% (Poor fit), 74% (0-3 outliers), 12% (1 outlier), 14% (2+ outliers)
1	B	336	 17% (Poor fit), 73% (0-3 outliers), 13% (1 outlier), 14% (2+ outliers)
1	C	336	 18% (Poor fit), 74% (0-3 outliers), 13% (1 outlier), 13% (2+ outliers)
1	D	336	 11% (Poor fit), 77% (0-3 outliers), 10% (1 outlier), 14% (2+ outliers)

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
3	K	D	403	-	-	-	X
3	K	D	404	-	-	-	X
3	K	D	406	-	-	-	X

2 Entry composition [i](#)

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

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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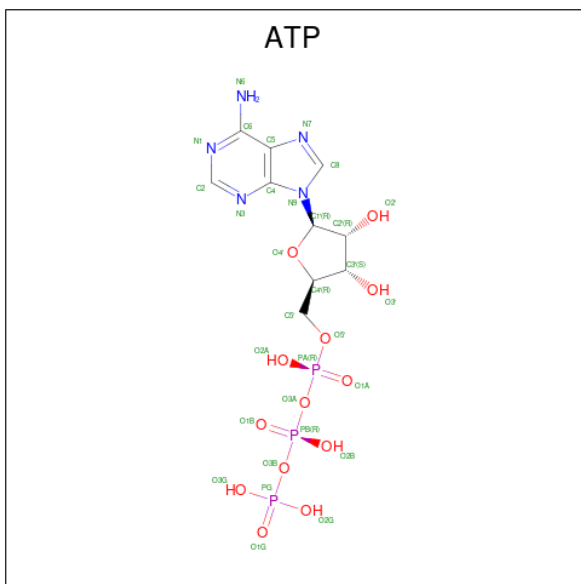
Chain	Residue	Modelled	Actual	Comment	Reference
C	32	ASP	-	expression tag	UNP A9CG24
C	33	HIS	-	expression tag	UNP A9CG24
C	34	PRO	-	expression tag	UNP A9CG24
C	35	PHE	-	expression tag	UNP A9CG24
C	36	THR	-	expression tag	UNP A9CG24
C	37	VAL	-	expression tag	UNP A9CG24
D	1	MSE	-	initiating methionine	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 (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
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 (three-letter code: K) (formula: K).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

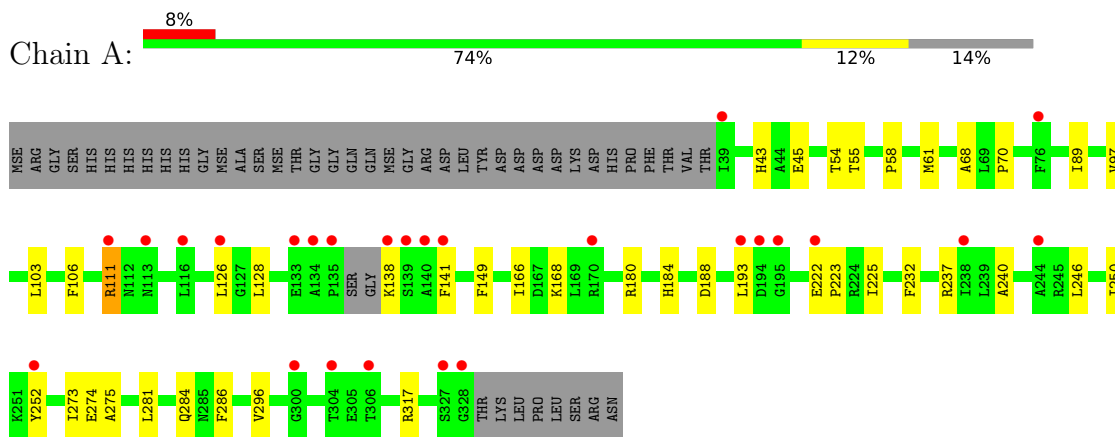
- Molecule 5 is water.

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

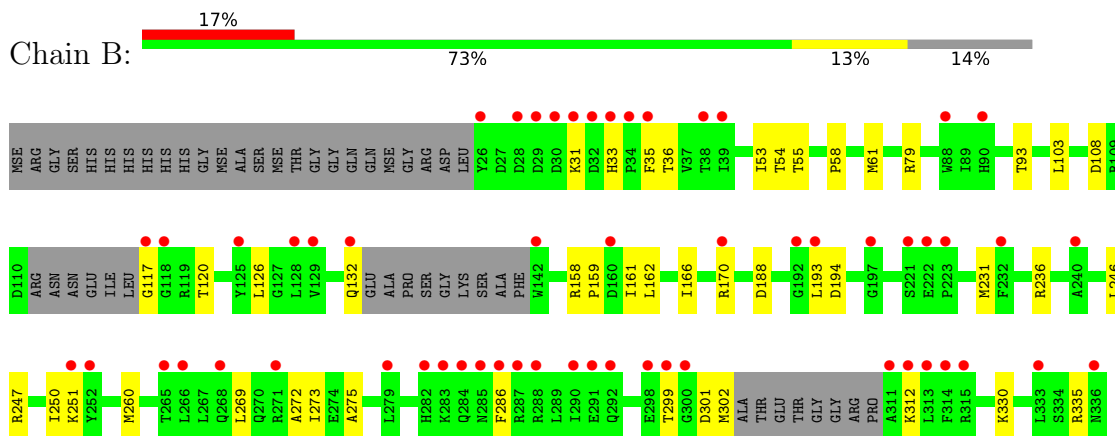
3 Residue-property plots [i](#)

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.

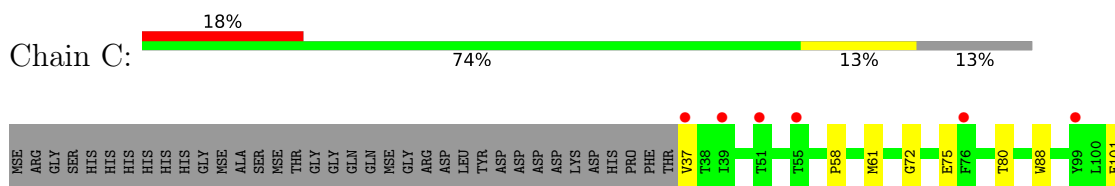
- Molecule 1: NADQ transcription factor

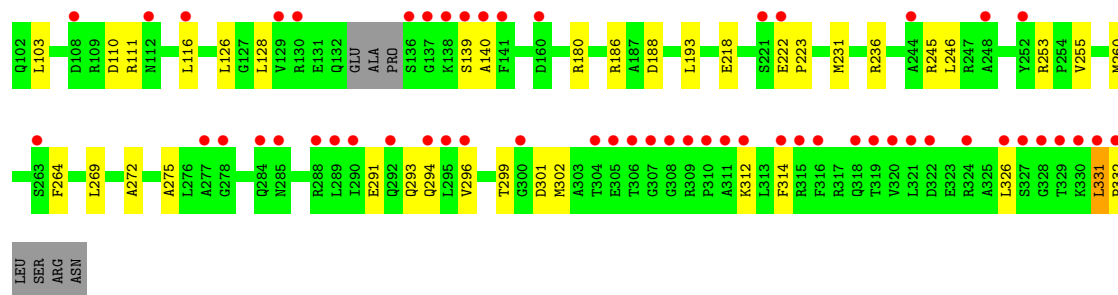


- Molecule 1: NADQ transcription factor

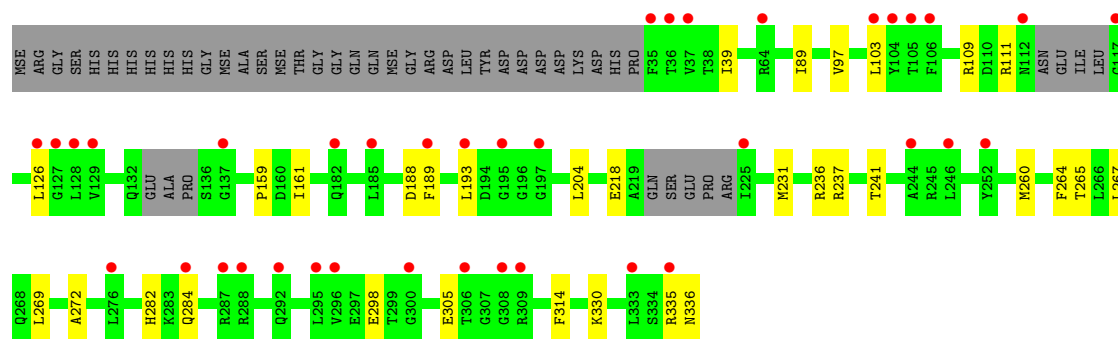
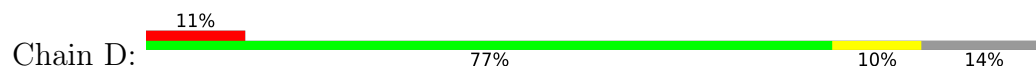


- Molecule 1: NADQ transcription factor





- 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)	Xtrriage
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 (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtrriage
Anisotropy	0.165	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, K, 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	0.24	0/2380	0.51	0/3212
1	B	0.24	0/2396	0.51	0/3233
1	C	0.24	0/2414	0.52	0/3258
1	D	0.24	0/2388	0.51	0/3219
All	All	0.24	0/9578	0.51	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

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	20	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	98	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 (98) 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:D:265:THR:OG1	1:D:305:GLU:OE2	2.28	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%)	233 (98%)	4 (2%)	60	72
1	B	242/270 (90%)	240 (99%)	2 (1%)	81	89
1	C	242/270 (90%)	240 (99%)	2 (1%)	81	89
1	D	239/270 (88%)	238 (100%)	1 (0%)	91	95
All	All	960/1080 (89%)	951 (99%)	9 (1%)	78	87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ARG
1	A	138	LYS

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Mol	Chain	Res	Type
1	A	141	PHE
1	A	252	TYR
1	B	132	GLN
1	B	335	ARG
1	C	111	ARG
1	C	296	VAL
1	D	335	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	-	26,33,33	0.59	0	31,52,52	0.76	1 (3%)
2	ATP	C	501	-	26,33,33	0.60	0	31,52,52	0.76	1 (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
2	ATP	A	501	-	-	4/18/38/38	0/3/3/3
2	ATP	C	501	-	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	ATP	C5-C6-N6	2.25	123.78	120.35
2	A	501	ATP	C5-C6-N6	2.25	123.76	120.35

There are no chirality outliers.

All (8) 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	A	501	ATP	PB-O3B-PG-O2G
2	C	501	ATP	PB-O3A-PA-O2A
2	A	501	ATP	PB-O3B-PG-O1G

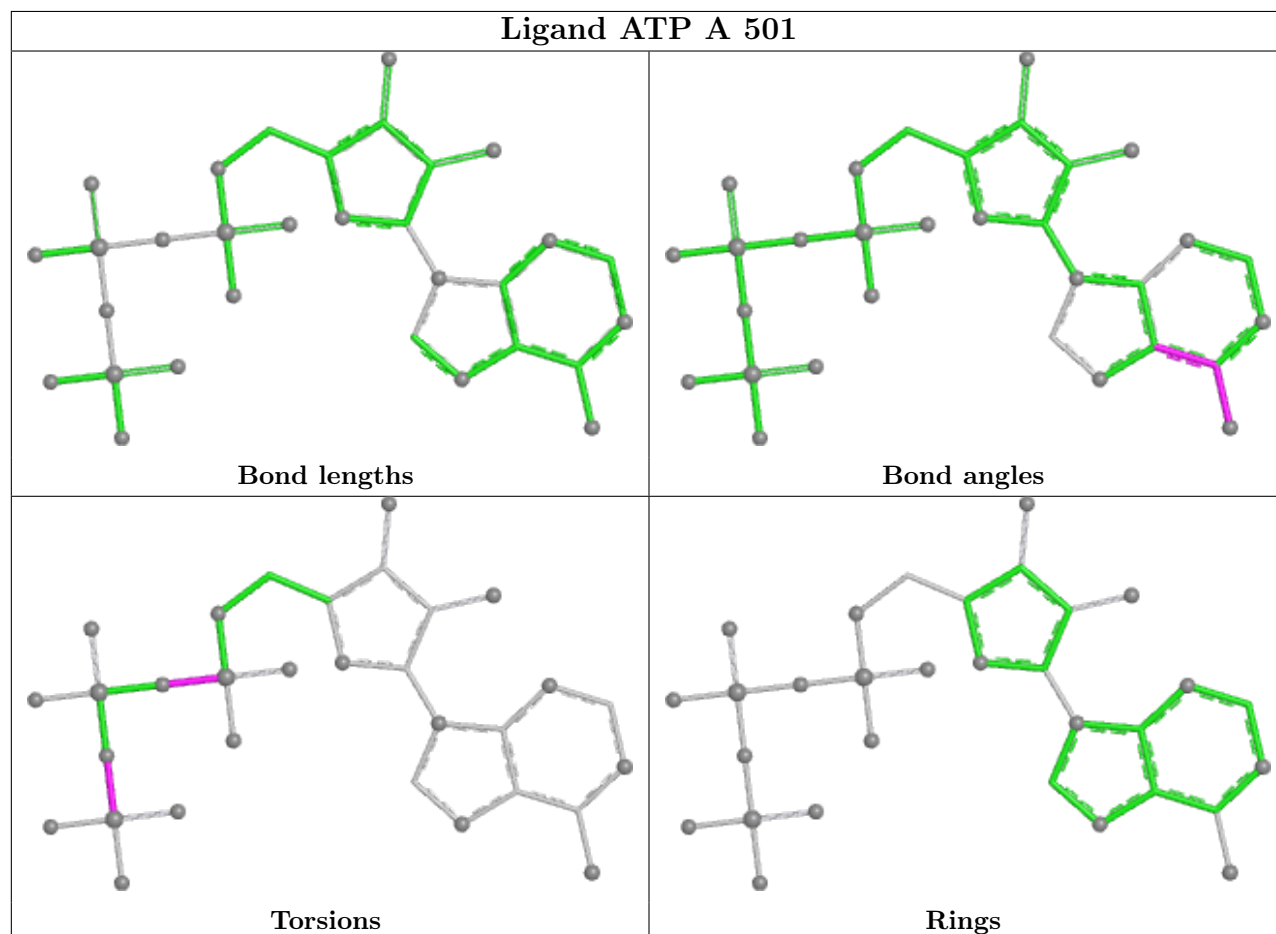
There are no ring outliers.

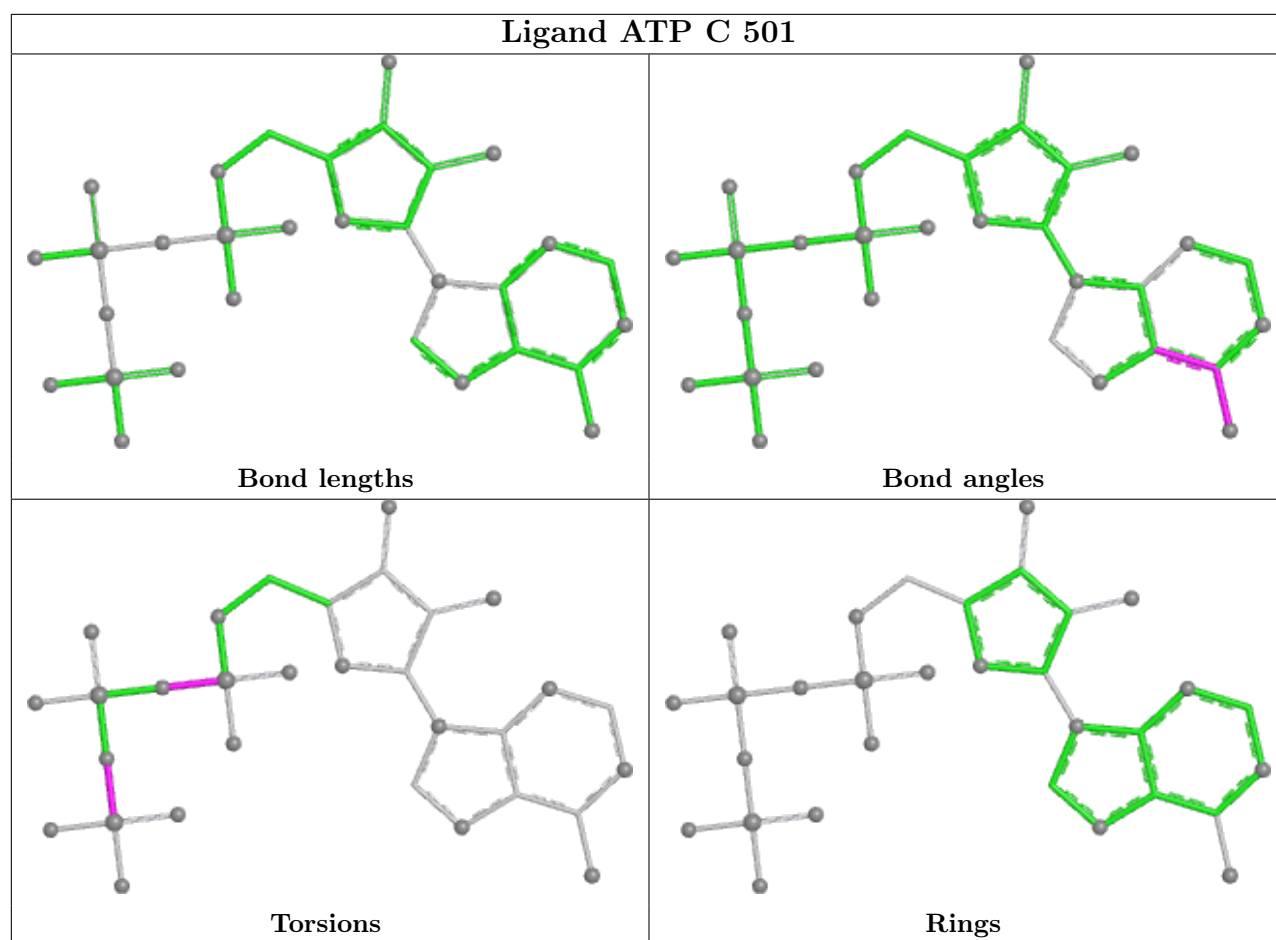
2 monomers are involved in 2 short contacts:

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%)	0.75	26 (9%) 9 9	25, 38, 66, 89	0
1	B	284/336 (84%)	1.25	57 (20%) 1 1	23, 42, 77, 111	0
1	C	289/336 (86%)	1.29	61 (21%) 1 0	22, 38, 91, 109	0
1	D	286/336 (85%)	0.94	38 (13%) 3 3	26, 42, 63, 77	0
All	All	1143/1344 (85%)	1.06	182 (15%) 1 2	22, 40, 77, 111	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	328	GLY	9.8
1	C	306	THR	9.7
1	C	329	THR	8.0
1	C	308	GLY	7.0
1	B	31	LYS	7.0
1	C	332	PRO	6.7
1	C	295	LEU	6.6
1	B	32	ASP	6.6
1	B	30	ASP	6.3
1	C	309	ARG	6.2
1	B	222	GLU	6.0
1	B	282	HIS	5.6
1	B	290	ILE	5.4
1	C	327	SER	5.1
1	D	127	GLY	5.1
1	B	193	LEU	4.9
1	C	137	GLY	4.7
1	D	35	PHE	4.7
1	A	111	ARG	4.7
1	B	29	ASP	4.6
1	B	291	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	296	VAL	4.6
1	B	28	ASP	4.5
1	A	138	LYS	4.4
1	D	284	GLN	4.4
1	C	37	VAL	4.4
1	A	139	SER	4.3
1	B	252	TYR	4.3
1	B	286	PHE	4.2
1	C	139	SER	4.2
1	D	126	LEU	4.1
1	C	310	PRO	4.1
1	C	305	GLU	4.1
1	B	312	LYS	4.1
1	D	128	LEU	4.0
1	C	322	ASP	4.0
1	D	112	ASN	4.0
1	A	135	PRO	3.9
1	B	33	HIS	3.9
1	B	299	THR	3.9
1	D	105	THR	3.9
1	C	136	SER	3.9
1	D	252	TYR	3.9
1	B	284	GLN	3.9
1	A	141	PHE	3.9
1	B	35	PHE	3.9
1	A	328	GLY	3.8
1	A	327	SER	3.8
1	B	232	PHE	3.8
1	C	140	ALA	3.8
1	B	311	ALA	3.7
1	A	134	ALA	3.6
1	A	140	ALA	3.6
1	B	170	ARG	3.6
1	D	64	ARG	3.6
1	C	331	LEU	3.6
1	D	117	GLY	3.6
1	C	39	ILE	3.6
1	B	288	ARG	3.5
1	B	118	GLY	3.5
1	B	287	ARG	3.5
1	A	222	GLU	3.5
1	C	307	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	55	THR	3.4
1	D	300	GLY	3.4
1	B	313	LEU	3.4
1	C	141	PHE	3.4
1	C	316	PHE	3.4
1	C	290	ILE	3.4
1	D	37	VAL	3.4
1	A	306	THR	3.3
1	C	324	ARG	3.3
1	B	221	SER	3.3
1	B	39	ILE	3.3
1	C	138	LYS	3.2
1	D	306	THR	3.2
1	B	34	PRO	3.2
1	B	314	PHE	3.2
1	B	333	LEU	3.2
1	D	193	LEU	3.2
1	C	129	VAL	3.2
1	D	225	ILE	3.2
1	C	285	ASN	3.2
1	B	266	LEU	3.1
1	C	311	ALA	3.1
1	D	104	TYR	3.1
1	C	321	LEU	3.1
1	C	252	TYR	3.1
1	B	26	TYR	3.0
1	B	129	VAL	3.0
1	B	192	GLY	3.0
1	B	223	PRO	3.0
1	C	278	GLY	2.9
1	B	300	GLY	2.9
1	C	284	GLN	2.9
1	B	336	ASN	2.9
1	C	300	GLY	2.9
1	D	288	ARG	2.9
1	C	294	GLN	2.9
1	C	130	ARG	2.9
1	C	326	LEU	2.9
1	C	248	ALA	2.8
1	C	222	GLU	2.8
1	B	160	ASP	2.8
1	C	318	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	304	THR	2.8
1	C	319	THR	2.8
1	D	197	GLY	2.8
1	D	103	LEU	2.8
1	A	300	GLY	2.7
1	D	182	GLN	2.7
1	D	309	ARG	2.7
1	D	185	LEU	2.7
1	C	108	ASP	2.7
1	B	285	ASN	2.7
1	D	296	VAL	2.7
1	A	194	ASP	2.7
1	A	126	LEU	2.7
1	C	99	TYR	2.6
1	C	314	PHE	2.6
1	B	298	GLU	2.6
1	B	315	ARG	2.6
1	D	189	PHE	2.6
1	A	252	TYR	2.6
1	A	116	LEU	2.6
1	C	330	LYS	2.5
1	D	137	GLY	2.5
1	C	160	ASP	2.5
1	D	276	LEU	2.5
1	B	142	TRP	2.5
1	D	36	THR	2.5
1	A	193	LEU	2.4
1	B	271	ARG	2.4
1	B	128	LEU	2.4
1	A	170	ARG	2.4
1	B	283	LYS	2.4
1	B	132	GLN	2.4
1	C	244	ALA	2.4
1	B	292	GLN	2.4
1	C	51	THR	2.4
1	B	88	TRP	2.4
1	C	76	PHE	2.3
1	D	292	GLN	2.3
1	A	195	GLY	2.3
1	B	117	GLY	2.3
1	B	279	LEU	2.3
1	A	304	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	129	VAL	2.3
1	B	38	THR	2.3
1	C	312	LYS	2.3
1	A	76	PHE	2.2
1	D	106	PHE	2.2
1	A	113	ASN	2.2
1	B	197	GLY	2.2
1	D	195	GLY	2.2
1	C	277	ALA	2.2
1	C	221	SER	2.2
1	A	133	GLU	2.2
1	C	288	ARG	2.2
1	D	308	GLY	2.2
1	C	263	SER	2.2
1	C	116	LEU	2.1
1	D	295	LEU	2.1
1	D	333	LEU	2.1
1	C	112	ASN	2.1
1	B	251	LYS	2.1
1	B	125	TYR	2.1
1	B	268	GLN	2.1
1	B	265	THR	2.1
1	C	315	ARG	2.1
1	A	244	ALA	2.1
1	D	246	LEU	2.1
1	D	244	ALA	2.1
1	B	90	HIS	2.1
1	C	292	GLN	2.1
1	D	335	ARG	2.0
1	A	39	ILE	2.0
1	C	289	LEU	2.0
1	B	240	ALA	2.0
1	C	320	VAL	2.0
1	A	238	ILE	2.0
1	D	287	ARG	2.0

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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

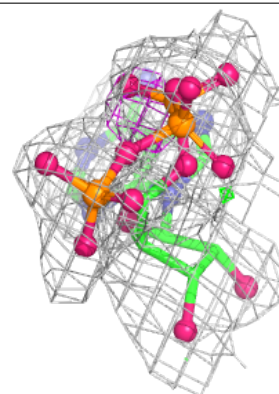
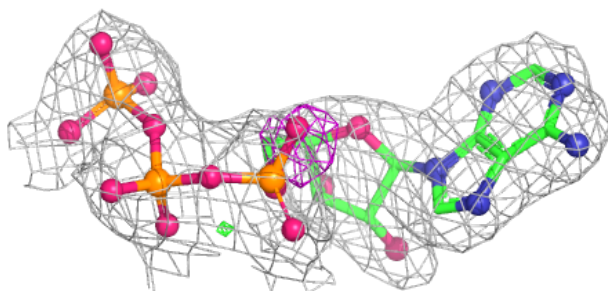
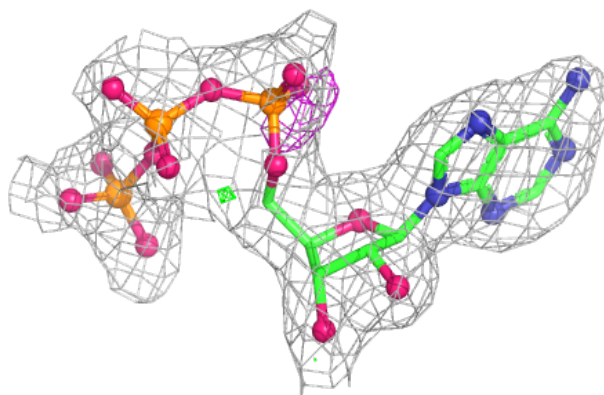
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	-0.12	1.73	108,108,108,108	0
3	K	A	502	1/1	0.28	0.34	84,84,84,84	0
3	K	D	405	1/1	0.44	0.30	86,86,86,86	0
3	K	D	403	1/1	0.56	0.45	99,99,99,99	0
3	K	C	509	1/1	0.60	1.46	70,70,70,70	0
3	K	C	502	1/1	0.69	0.13	92,92,92,92	0
3	K	D	406	1/1	0.73	0.41	77,77,77,77	0
3	K	D	402	1/1	0.84	0.13	52,52,52,52	0
3	K	C	510	1/1	0.85	0.21	59,59,59,59	0
3	K	C	503	1/1	0.86	0.87	85,85,85,85	0
3	K	B	402	1/1	0.86	0.24	58,58,58,58	0
4	NA	D	408	1/1	0.88	0.19	47,47,47,47	0
3	K	D	407	1/1	0.89	0.15	61,61,61,61	0
3	K	C	508	1/1	0.92	0.18	65,65,65,65	0
3	K	C	505	1/1	0.93	0.30	58,58,58,58	0
3	K	C	507	1/1	0.93	0.08	60,60,60,60	0
3	K	B	401	1/1	0.93	0.14	50,50,50,50	0
2	ATP	A	501	31/31	0.93	0.17	35,51,68,76	0
2	ATP	C	501	31/31	0.95	0.13	28,36,46,51	0
3	K	C	504	1/1	0.95	0.10	54,54,54,54	0
4	NA	A	503	1/1	0.96	0.13	32,32,32,32	0
3	K	C	506	1/1	0.97	0.10	59,59,59,59	0
3	K	D	401	1/1	0.98	0.07	51,51,51,51	0

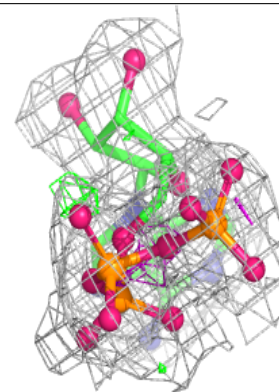
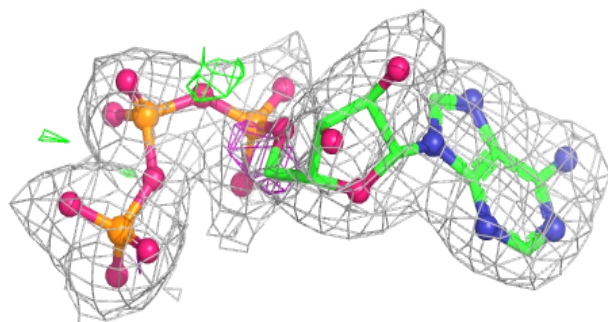
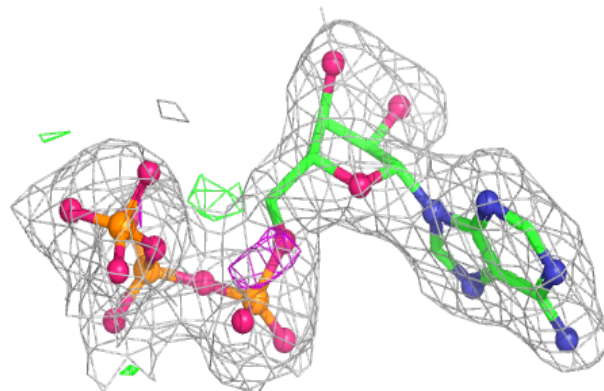
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP A 501:

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

**Electron density around ATP C 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 [i](#)

There are no such residues in this entry.