



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 08:52 AM EDT

PDB ID : 4CTA  
Title : Competence or damage-inducible protein CinA from *Thermus thermophilus*  
Authors : Derrick, J.; Karuppiah, V.  
Deposited on : 2014-03-12  
Resolution : 2.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

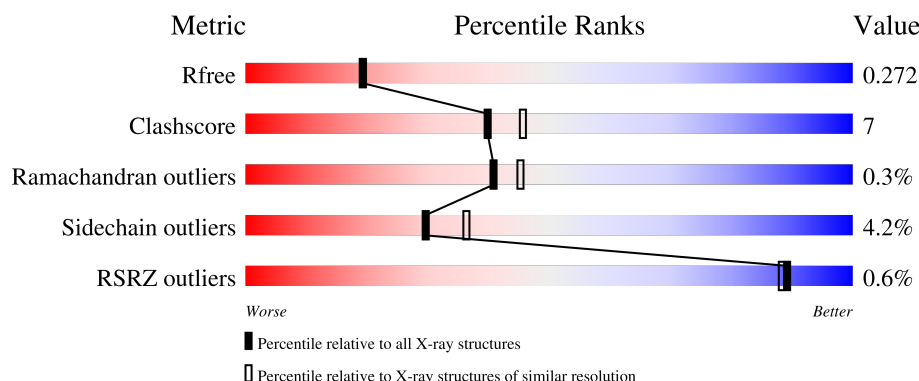
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	394	
2	B	394	

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
4	GOL	A	405	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6300 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 CINA-LIKE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3030	1915	546	561	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	GLU	GLY	conflict	UNP Q5SHB0
A	204	GLU	VAL	conflict	UNP Q5SHB0

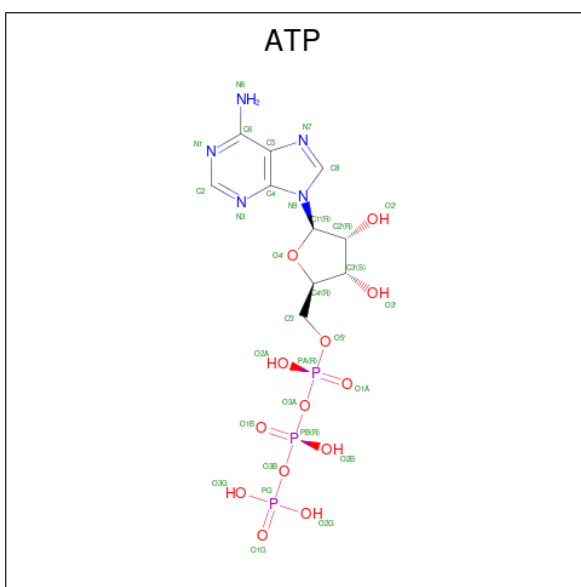
- Molecule 2 is a protein called CINA-LIKE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S	0	0	0
			3028	1915	546	559	8			

There is a discrepancy between the modelled and reference sequences:

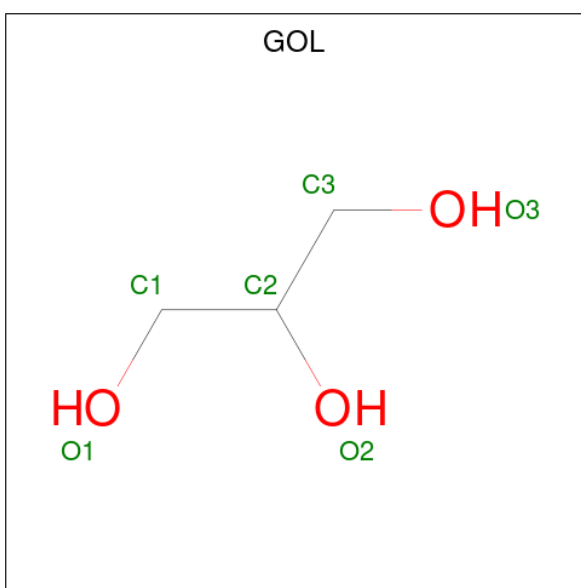
Chain	Residue	Modelled	Actual	Comment	Reference
B	201	GLU	GLY	conflict	UNP Q5SHB0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



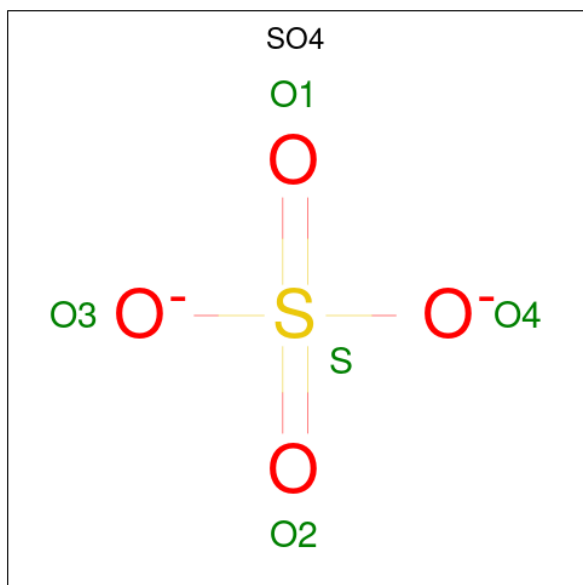
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	B	1	Total	Na	0	0
			1	1		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 1	Mg 1	0	0

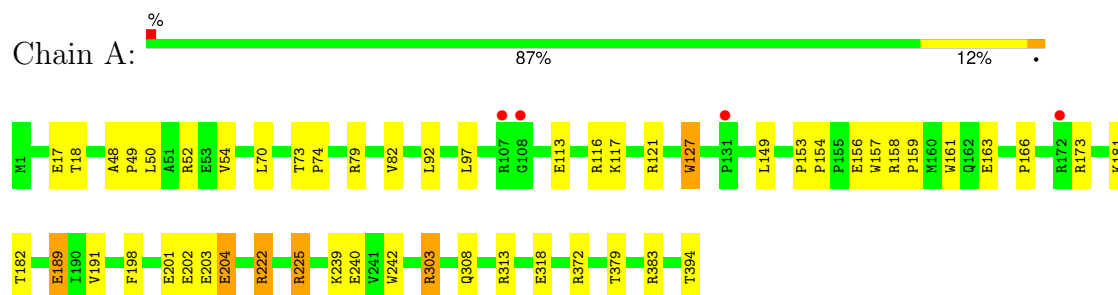
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	62	Total 62	O 62	0	0
8	B	70	Total 70	O 70	0	0

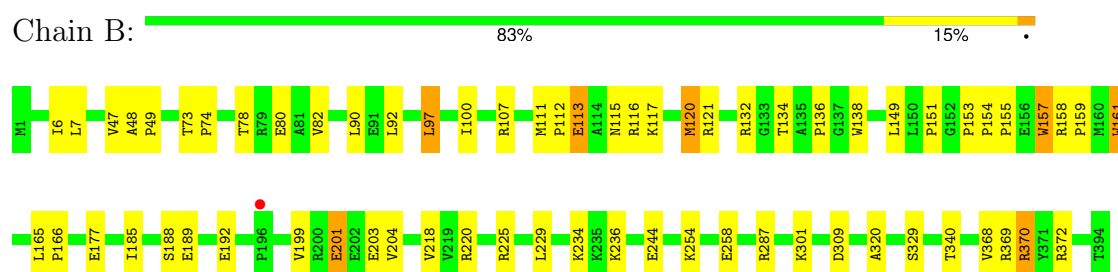
### 3 Residue-property plots

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: CINA-LIKE PROTEIN



#### • Molecule 2: CINA-LIKE PROTEIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.59Å 93.77Å 131.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.89 – 2.21 65.89 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.9 (65.89-2.21) 98.9 (65.89-2.21)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.220 , 0.274 0.221 , 0.272	Depositor DCC
$R_{free}$ test set	2350 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 31.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6300	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ATP, GOL, NA, MG

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	0.92	4/3089 (0.1%)	0.91	0/4191
2	B	0.92	2/3087 (0.1%)	0.86	1/4189 (0.0%)
All	All	0.92	6/6176 (0.1%)	0.88	1/8380 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	TRP	CD2-CE2	6.52	1.49	1.41
1	A	157	TRP	CD2-CE2	5.98	1.48	1.41
1	A	161	TRP	CD2-CE2	5.34	1.47	1.41
1	A	189	GLU	CG-CD	5.22	1.59	1.51
2	B	157	TRP	CD2-CE2	5.18	1.47	1.41
2	B	161	TRP	CD2-CE2	5.16	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	370	ARG	NE-CZ-NH1	6.04	123.32	120.30

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	3030	0	3094	43	0
2	B	3028	0	3098	46	0
3	A	31	0	12	5	0
3	B	31	0	12	3	0
4	A	18	0	24	6	0
4	B	12	0	16	0	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	1	0	0	0	0
8	A	62	0	0	3	0
8	B	70	0	0	2	0
All	All	6300	0	6256	91	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 7.

All (91) 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)
3:A:400:ATP:H8	3:A:400:ATP:H5'1	1.13	1.13
1:A:204:GLU:OE2	1:A:225:ARG:HB2	1.63	0.97
1:A:203:GLU:OE2	1:A:222:ARG:NH1	1.98	0.96
1:A:113:GLU:O	1:A:116:ARG:HG3	1.70	0.92
1:A:303:ARG:HG3	1:A:303:ARG:HH11	1.36	0.91
3:A:400:ATP:H5'1	3:A:400:ATP:C8	2.05	0.91
3:A:400:ATP:H8	3:A:400:ATP:C5'	1.85	0.90
2:B:225:ARG:HH11	2:B:225:ARG:HG3	1.41	0.85
1:A:82:VAL:HG21	1:A:149:LEU:HD11	1.58	0.83
1:A:52:ARG:HD2	8:A:2015:HOH:O	1.82	0.79
2:B:301:LYS:HE2	8:B:2040:HOH:O	1.87	0.75
1:A:308:GLN:HB3	8:A:2044:HOH:O	1.87	0.73
1:A:203:GLU:OE2	1:A:222:ARG:CZ	2.38	0.71
2:B:92:LEU:HD13	2:B:120:MET:CE	2.21	0.70
2:B:153:PRO:HD3	3:B:400:ATP:H5'2	1.75	0.68
2:B:225:ARG:HG3	2:B:225:ARG:NH1	2.07	0.68
1:A:204:GLU:OE2	1:A:225:ARG:CB	2.39	0.67
1:A:73:THR:CG2	1:A:74:PRO:HD2	2.24	0.66
3:A:400:ATP:C8	3:A:400:ATP:C5'	2.71	0.65
1:A:204:GLU:OE1	1:A:204:GLU:HA	1.97	0.65
2:B:134:THR:O	2:B:136:PRO:HD3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:LYS:HD2	2:B:244:GLU:OE2	1.99	0.63
1:A:198:PHE:CE1	2:B:74:PRO:HD2	2.34	0.62
1:A:383:ARG:HH12	4:A:405:GOL:H32	1.64	0.62
1:A:73:THR:HG22	1:A:74:PRO:HD2	1.82	0.61
1:A:303:ARG:HG3	1:A:303:ARG:NH1	2.11	0.61
1:A:203:GLU:HG2	1:A:222:ARG:HG3	1.81	0.61
1:A:48:ALA:HB3	1:A:49:PRO:HD3	1.83	0.59
2:B:90:LEU:HB3	2:B:120:MET:HG2	1.84	0.59
2:B:82:VAL:HG21	2:B:149:LEU:HD21	1.86	0.58
1:A:383:ARG:HH12	4:A:405:GOL:C3	2.17	0.56
1:A:121:ARG:HB3	1:A:127:TRP:CZ2	2.41	0.55
2:B:201:GLU:OE1	2:B:225:ARG:NH2	2.40	0.55
1:A:50:LEU:O	1:A:54:VAL:HG23	2.07	0.54
1:A:383:ARG:NH2	4:A:405:GOL:H31	2.23	0.54
2:B:203:GLU:CB	2:B:225:ARG:HH12	2.20	0.53
2:B:48:ALA:HB3	2:B:49:PRO:HD3	1.89	0.53
2:B:113:GLU:OE1	2:B:116:ARG:HD3	2.10	0.52
2:B:113:GLU:O	2:B:116:ARG:HG3	2.10	0.51
2:B:203:GLU:HB2	2:B:225:ARG:HH12	1.76	0.51
1:A:18:THR:HG21	3:A:400:ATP:H2'	1.92	0.51
2:B:254:LYS:NZ	2:B:287:ARG:HH21	2.09	0.51
1:A:379:THR:O	1:A:383:ARG:HG2	2.11	0.51
2:B:204:VAL:HG21	2:B:229:LEU:HD23	1.92	0.51
2:B:158:ARG:HB2	2:B:159:PRO:HD3	1.92	0.51
2:B:254:LYS:O	2:B:258:GLU:HG3	2.11	0.51
2:B:7:LEU:HD12	2:B:7:LEU:N	2.26	0.50
1:A:383:ARG:HH22	4:A:405:GOL:H31	1.77	0.50
2:B:189:GLU:OE1	2:B:189:GLU:N	2.32	0.50
1:A:73:THR:HG23	1:A:74:PRO:HD2	1.93	0.49
2:B:203:GLU:HA	2:B:203:GLU:OE1	2.11	0.49
2:B:100:ILE:HG21	2:B:111:MET:HE3	1.94	0.49
2:B:165:LEU:HB3	2:B:166:PRO:HD3	1.94	0.49
1:A:73:THR:HG22	1:A:74:PRO:CD	2.42	0.49
1:A:70:LEU:O	1:A:79:ARG:NH2	2.43	0.48
1:A:204:GLU:OE1	1:A:204:GLU:CA	2.59	0.48
2:B:153:PRO:HD3	3:B:400:ATP:C5'	2.42	0.48
2:B:151:PRO:HD2	2:B:157:TRP:HB3	1.96	0.47
2:B:111:MET:HE3	2:B:115:ASN:HB3	1.97	0.47
2:B:154:PRO:HB2	2:B:155:PRO:HD3	1.97	0.47
2:B:368:VAL:O	2:B:369:ARG:NH1	2.47	0.47
2:B:177:GLU:HG2	2:B:220:ARG:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:TRP:CZ2	2:B:165:LEU:HD13	2.50	0.46
1:A:163:GLU:O	1:A:166:PRO:HD2	2.16	0.46
2:B:218:VAL:HG11	2:B:220:ARG:HH11	1.80	0.46
1:A:158:ARG:HB2	1:A:159:PRO:HD3	1.98	0.45
1:A:182:THR:HA	1:A:240:GLU:O	2.15	0.45
1:A:372:ARG:HB2	2:B:107:ARG:HG2	1.98	0.45
1:A:73:THR:CG2	1:A:74:PRO:CD	2.94	0.44
2:B:47:VAL:HG23	8:B:2011:HOH:O	2.17	0.44
2:B:320:ALA:HB2	2:B:340:THR:HG22	1.99	0.44
1:A:181:LYS:HB3	1:A:242:TRP:CZ2	2.53	0.44
2:B:92:LEU:CD1	2:B:120:MET:HE2	2.48	0.44
2:B:121:ARG:HA	2:B:138:TRP:CZ2	2.53	0.43
2:B:111:MET:HA	2:B:112:PRO:HD3	1.86	0.43
2:B:111:MET:HE3	2:B:115:ASN:CB	2.49	0.43
2:B:6:ILE:C	2:B:7:LEU:HD12	2.39	0.43
2:B:254:LYS:HZ2	2:B:287:ARG:HH21	1.66	0.43
1:A:153:PRO:HA	1:A:154:PRO:HD3	1.94	0.43
1:A:191:VAL:CG2	2:B:73:THR:HG22	2.49	0.43
1:A:52:ARG:NH1	8:A:2016:HOH:O	2.52	0.42
1:A:383:ARG:NH1	4:A:405:GOL:C3	2.81	0.42
2:B:78:THR:O	2:B:82:VAL:HG23	2.20	0.41
1:A:201:GLU:OE2	1:A:225:ARG:NH1	2.54	0.41
3:B:400:ATP:H5'1	3:B:400:ATP:C8	2.55	0.41
1:A:156:GLU:O	1:A:159:PRO:HD2	2.21	0.41
1:A:173:ARG:O	1:A:173:ARG:HG3	2.21	0.41
1:A:92:LEU:HD11	1:A:97:LEU:HD22	2.02	0.41
1:A:383:ARG:NH1	4:A:405:GOL:H32	2.35	0.40
2:B:92:LEU:CD1	2:B:120:MET:CE	2.94	0.40
2:B:97:LEU:HD23	2:B:97:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/394 (100%)	374 (95%)	18 (5%)	0	100	100
2	B	392/394 (100%)	376 (96%)	14 (4%)	2 (0%)	29	30
All	All	784/788 (100%)	750 (96%)	32 (4%)	2 (0%)	41	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	309	ASP
2	B	185	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/308 (100%)	296 (96%)	12 (4%)	32	40
2	B	308/308 (100%)	294 (96%)	14 (4%)	27	33
All	All	616/616 (100%)	590 (96%)	26 (4%)	30	36

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	117	LYS
1	A	189	GLU
1	A	202	GLU
1	A	204	GLU
1	A	222	ARG
1	A	225	ARG
1	A	239	LYS
1	A	303	ARG
1	A	313	ARG
1	A	318	GLU
1	A	394	THR
2	B	80	GLU
2	B	97	LEU

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Mol	Chain	Res	Type
2	B	113	GLU
2	B	117	LYS
2	B	120	MET
2	B	132	ARG
2	B	188	SER
2	B	192	GLU
2	B	199	VAL
2	B	201	GLU
2	B	236	LYS
2	B	329	SER
2	B	370	ARG
2	B	372	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 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	A	403	-	4,4,4	0.77	0	6,6,6	0.54	0
3	ATP	A	400	-	28,33,33	2.55	6 (21%)	34,52,52	1.57	8 (23%)
4	GOL	B	403	-	5,5,5	0.37	0	5,5,5	1.22	1 (20%)
3	ATP	B	400	7	28,33,33	1.62	4 (14%)	34,52,52	2.14	9 (26%)
4	GOL	A	401	-	5,5,5	0.92	0	5,5,5	0.65	0
5	SO4	A	402	-	4,4,4	0.50	0	6,6,6	0.89	0
5	SO4	B	402	-	4,4,4	0.38	0	6,6,6	0.83	0
4	GOL	A	404	-	5,5,5	1.01	0	5,5,5	1.02	0
4	GOL	B	404	-	5,5,5	0.85	0	5,5,5	0.67	0
4	GOL	A	405	-	5,5,5	1.25	1 (20%)	5,5,5	1.25	1 (20%)

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
3	ATP	A	400	-	-	4/18/38/38	0/3/3/3
4	GOL	B	403	-	-	2/4/4/4	-
3	ATP	B	400	7	-	4/18/38/38	0/3/3/3
4	GOL	A	401	-	-	0/4/4/4	-
4	GOL	A	404	-	-	2/4/4/4	-
4	GOL	B	404	-	-	0/4/4/4	-
4	GOL	A	405	-	-	0/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	ATP	PB-O3B	9.10	1.69	1.59
3	A	400	ATP	PB-O3A	5.91	1.65	1.59
3	B	400	ATP	PA-O3A	5.37	1.65	1.59
3	A	400	ATP	PA-O3A	5.05	1.64	1.59
3	B	400	ATP	PB-O3A	3.72	1.63	1.59
3	A	400	ATP	C2-N3	3.33	1.37	1.32
3	A	400	ATP	O4'-C1'	2.94	1.44	1.40
4	A	405	GOL	O3-C3	2.29	1.52	1.42
3	A	400	ATP	C2-N1	2.25	1.37	1.33
3	B	400	ATP	C2-N3	2.14	1.35	1.32
3	B	400	ATP	PB-O3B	2.10	1.61	1.59



All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	400	ATP	C4'-O4'-C1'	5.68	115.13	109.92
3	B	400	ATP	O4'-C4'-C5'	-5.19	92.70	109.33
3	B	400	ATP	N3-C2-N1	-4.23	122.93	128.67
3	A	400	ATP	N3-C2-N1	-4.20	122.97	128.67
3	B	400	ATP	O3G-PG-O3B	-3.77	91.99	104.64
3	B	400	ATP	O2A-PA-O3A	3.47	116.64	107.27
3	B	400	ATP	O3A-PA-O1A	-3.00	101.68	110.70
3	A	400	ATP	O4'-C1'-N9	2.94	112.64	108.75
3	A	400	ATP	O3'-C3'-C2'	2.74	120.61	111.82
4	A	405	GOL	O3-C3-C2	2.44	121.37	110.38
3	B	400	ATP	O2B-PB-O3B	2.39	113.72	107.27
4	B	403	GOL	O1-C1-C2	-2.27	100.17	110.38
3	A	400	ATP	N6-C6-N1	2.24	123.12	118.33
3	B	400	ATP	O2'-C2'-C3'	-2.20	104.77	111.82
3	B	400	ATP	O4'-C1'-N9	-2.16	105.88	108.75
3	A	400	ATP	O2B-PB-O3B	2.16	113.10	107.27
3	A	400	ATP	O2'-C2'-C3'	2.05	118.38	111.82
3	A	400	ATP	O2A-PA-O3A	2.04	112.78	107.27
3	A	400	ATP	C5'-C4'-C3'	-2.02	107.96	115.21

There are no chirality outliers.

All (12) torsion outliers are listed below:

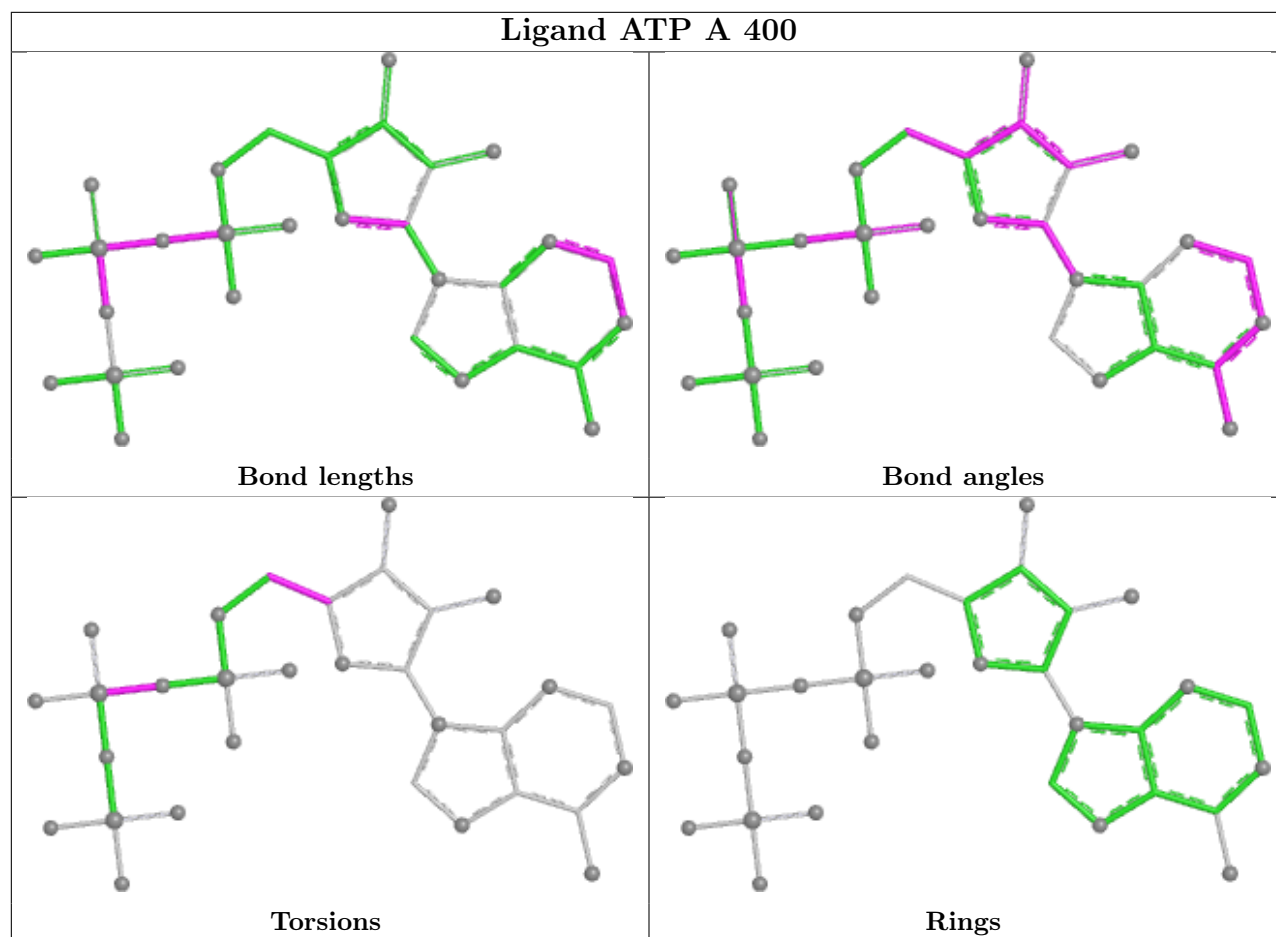
Mol	Chain	Res	Type	Atoms
3	B	400	ATP	C5'-O5'-PA-O2A
3	B	400	ATP	C5'-O5'-PA-O3A
4	A	404	GOL	C1-C2-C3-O3
4	B	403	GOL	O1-C1-C2-C3
3	B	400	ATP	O4'-C4'-C5'-O5'
3	A	400	ATP	C3'-C4'-C5'-O5'
4	B	403	GOL	O1-C1-C2-O2
3	A	400	ATP	O4'-C4'-C5'-O5'
4	A	404	GOL	O2-C2-C3-O3
3	B	400	ATP	C5'-O5'-PA-O1A
3	A	400	ATP	PA-O3A-PB-O1B
3	A	400	ATP	PA-O3A-PB-O2B

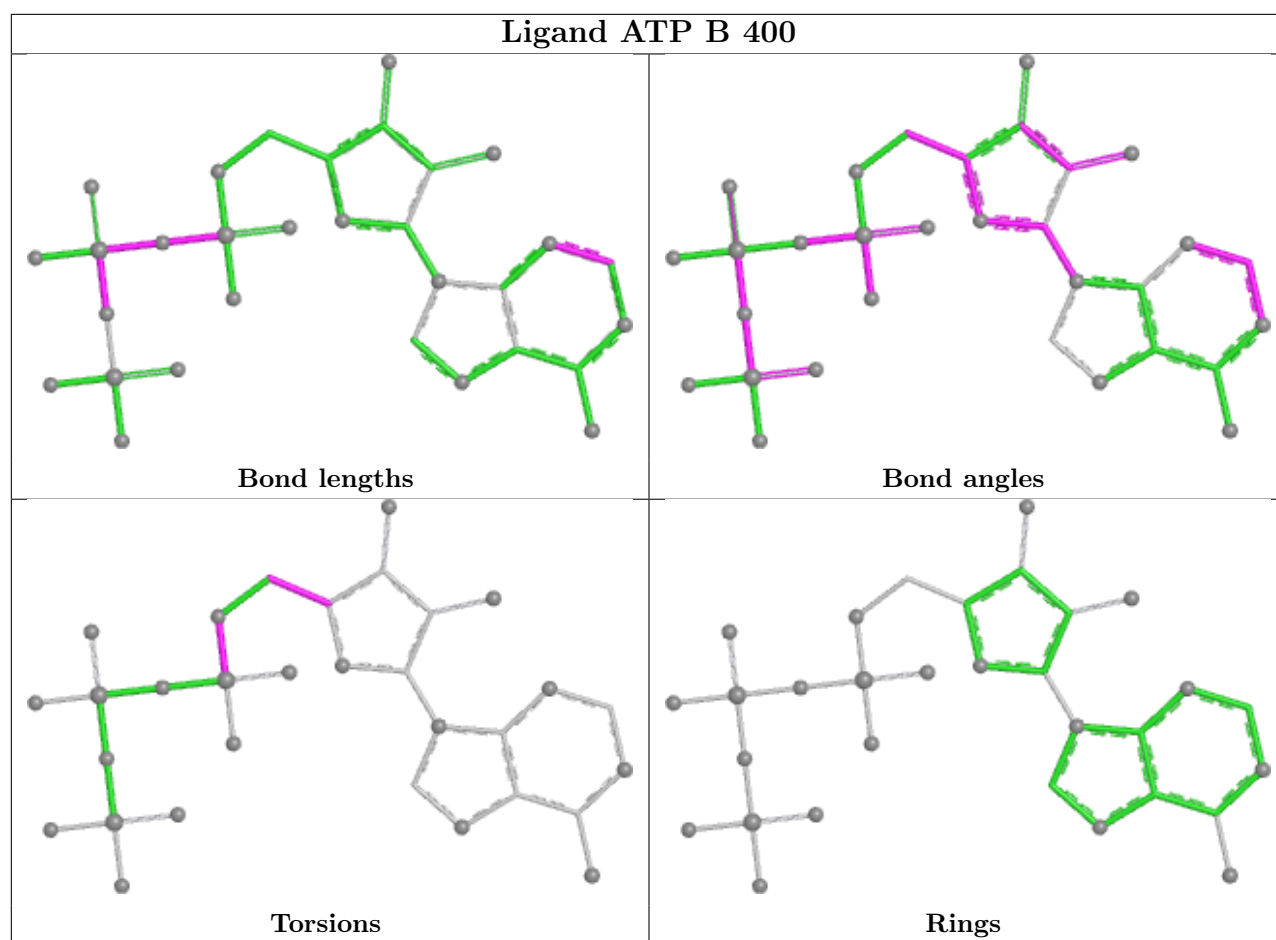
There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	ATP	5	0
3	B	400	ATP	3	0
4	A	405	GOL	6	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	394/394 (100%)	0.10	4 (1%) 82 81	16, 33, 58, 78	0
2	B	394/394 (100%)	0.03	1 (0%) 94 93	17, 31, 61, 84	0
All	All	788/788 (100%)	0.06	5 (0%) 89 88	16, 32, 59, 84	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	PRO	4.3
1	A	108	GLY	2.8
1	A	107	ARG	2.8
1	A	172	ARG	2.2
2	B	196	PRO	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](#)

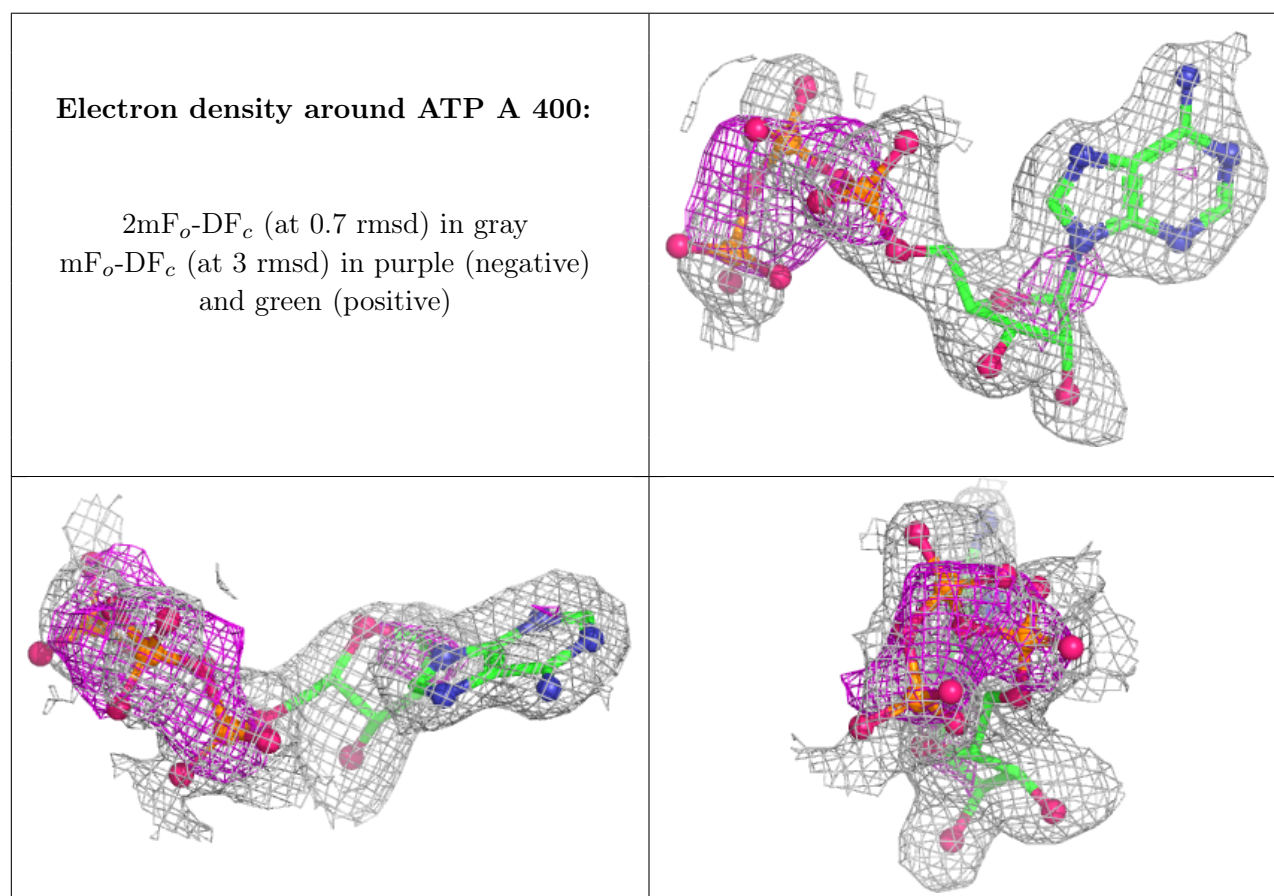
There are no monosaccharides in this entry.

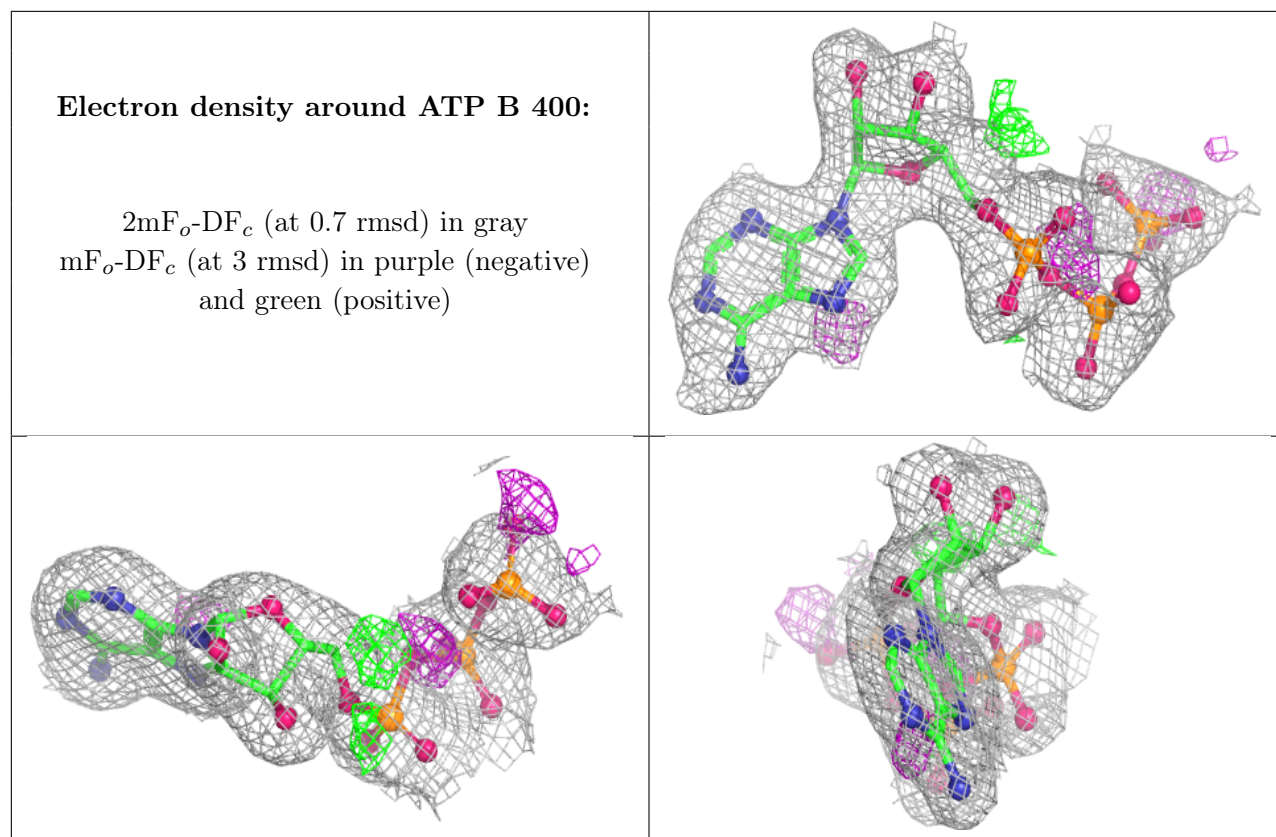
### 6.4 Ligands [i](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	404	6/6	0.79	0.16	39,42,46,49	0
3	ATP	A	400	31/31	0.80	0.28	33,50,69,76	0
4	GOL	A	405	6/6	0.82	0.20	28,32,36,38	0
4	GOL	A	401	6/6	0.87	0.15	33,35,39,39	0
4	GOL	B	404	6/6	0.93	0.16	29,36,41,42	0
4	GOL	B	403	6/6	0.94	0.13	32,35,36,36	0
6	NA	B	405	1/1	0.94	0.11	31,31,31,31	0
3	ATP	B	400	31/31	0.96	0.13	19,22,31,34	0
7	MG	B	401	1/1	0.96	0.05	26,26,26,26	0
5	SO4	A	403	5/5	0.97	0.21	49,50,54,55	0
6	NA	A	406	1/1	0.99	0.25	18,18,18,18	0
5	SO4	A	402	5/5	0.99	0.14	19,23,26,29	0
5	SO4	B	402	5/5	0.99	0.16	26,27,29,30	0

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.