



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:22 PM UTC

PDB ID : 3ETH / pdb_00003eth
Title : Crystal structure of E. coli Purk in complex with MgATP
Authors : Holden, H.M.; Thoden, J.B.
Deposited on : 2008-10-08
Resolution : 1.60 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)
Xtrriage (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

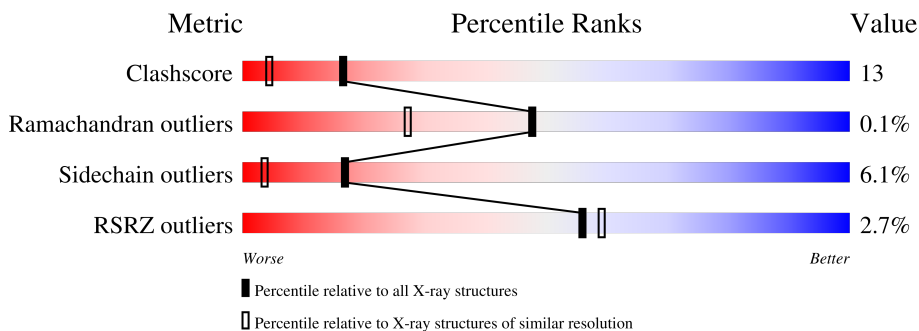
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

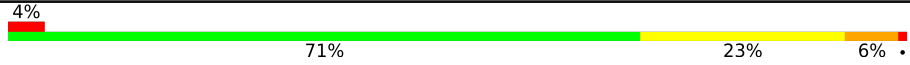
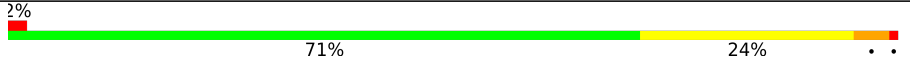
The reported resolution of this entry is 1.60 Å.

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))
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	355	 4% 71% 23% 6%
1	B	355	 2% 71% 24% 3%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6346 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.

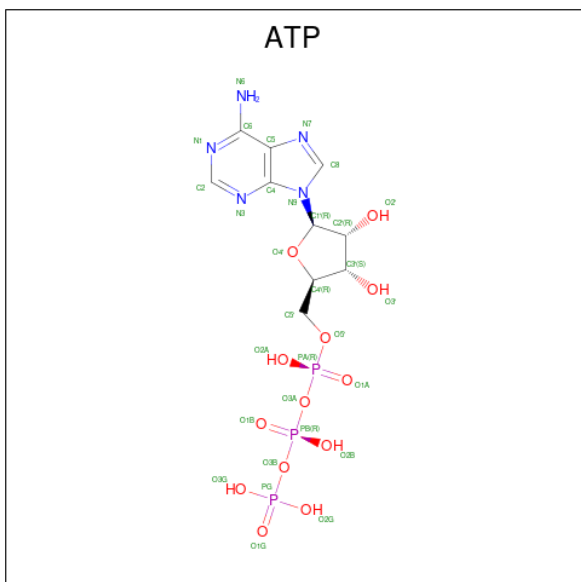
- Molecule 1 is a protein called Phosphoribosylaminoimidazole carboxylase ATPase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	355	2802	1782	498	511	11	0	4	0
1	B	355	2788	1774	495	508	11	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	GLU	engineered mutation	UNP P09029
A	205	ARG	GLN	engineered mutation	UNP P09029
B	61	GLN	GLU	engineered mutation	UNP P09029
B	205	ARG	GLN	engineered mutation	UNP P09029

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



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

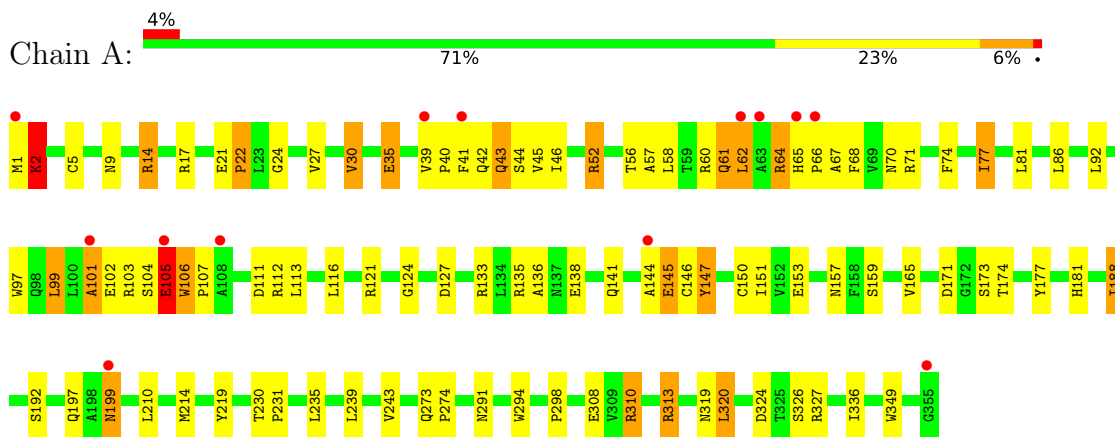
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	375	375	375	0	0
4	B	315	315	315	0	0

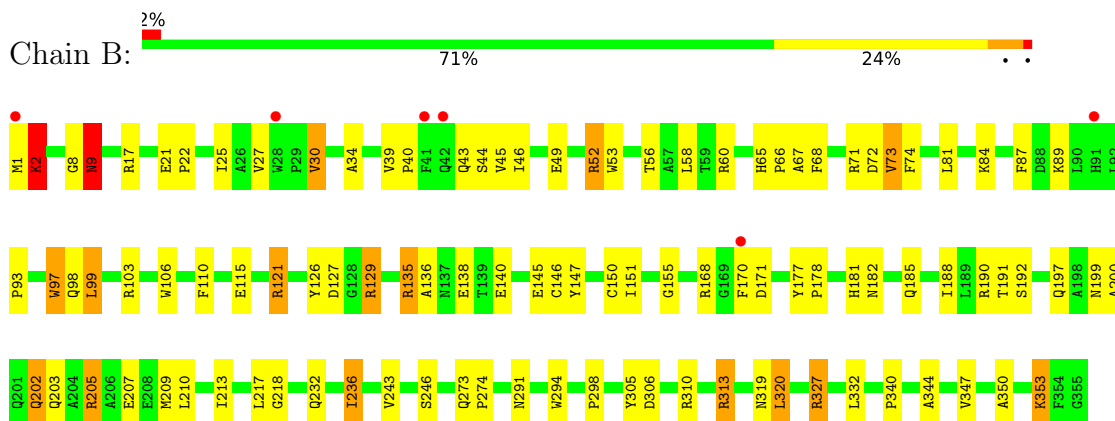
3 Residue-property plots

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: Phosphoribosylaminoimidazole carboxylase ATPase subunit



- Molecule 1: Phosphoribosylaminoimidazole carboxylase ATPase subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.10Å 57.11Å 59.22Å 77.46° 82.39° 77.26°	Depositor
Resolution (Å)	30.00 – 1.60 30.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.8 (30.00-1.60) 93.8 (30.00-1.60)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.60Å)	Xtrriage
Refinement program	TNT	Depositor
R, R_{free}	0.175 , 0.228 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtrriage
Anisotropy	0.704	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 85.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.014 for -l,-k,-h	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6346	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% 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, 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	0.90	1/2888 (0.0%)	1.62	43/3934 (1.1%)
1	B	0.88	0/2862	1.64	36/3900 (0.9%)
All	All	0.89	1/5750 (0.0%)	1.63	79/7834 (1.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	336	ILE	CA-CB	9.96	1.59	1.54

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	LYS	N-CA-C	10.86	124.79	109.15
1	B	115	GLU	N-CA-C	10.64	124.20	111.33
1	A	111	ASP	N-CA-C	-9.43	100.95	111.14
1	A	99	LEU	N-CA-C	-9.04	97.76	110.50
1	A	101	ALA	N-CA-C	8.72	122.42	111.69
1	B	236	ILE	CB-CA-C	-8.72	100.10	110.91
1	A	113	LEU	N-CA-C	8.13	123.20	113.28
1	A	298	PRO	N-CA-C	8.06	124.31	113.84
1	B	39	VAL	N-CA-C	7.94	116.55	107.89
1	B	39	VAL	CB-CA-C	-7.80	102.02	110.37
1	A	67	ALA	N-CA-C	7.74	122.15	111.55
1	B	178	PRO	N-CA-C	-7.63	99.97	111.41
1	A	177	TYR	N-CA-C	-7.57	101.23	110.31
1	A	199	ASN	N-CA-C	-7.51	98.77	109.96
1	A	45	VAL	CB-CA-C	-7.45	101.68	110.91
1	B	313	ARG	NE-CZ-NH1	-7.41	114.09	121.50
1	B	155	GLY	N-CA-C	-7.41	100.66	111.03
1	B	232	GLN	N-CA-C	-7.23	104.20	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	TRP	CA-C-O	7.09	124.85	118.33
1	A	14	ARG	NE-CZ-NH1	-6.87	114.63	121.50
1	A	9	ASN	N-CA-C	6.78	120.86	112.59
1	B	200	ALA	N-CA-C	6.70	118.58	111.28
1	A	159	SER	N-CA-C	-6.61	105.04	113.23
1	B	106	TRP	N-CA-C	6.52	121.62	112.75
1	A	14	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	B	99	LEU	N-CA-C	-6.48	100.69	110.28
1	A	57	ALA	N-CA-C	-6.40	104.31	111.28
1	A	2	LYS	CB-CA-C	-6.37	97.74	110.42
1	B	135	ARG	N-CA-C	-6.33	101.09	110.46
1	A	105	GLU	N-CA-C	6.20	120.69	113.18
1	B	72	ASP	N-CA-C	6.16	120.80	113.16
1	B	217	LEU	N-CA-C	6.16	120.63	113.18
1	A	44	SER	N-CA-C	6.10	119.49	109.85
1	B	243	VAL	N-CA-C	-6.08	100.17	109.78
1	A	97	TRP	N-CA-CB	-6.08	101.49	110.97
1	B	327	ARG	NE-CZ-NH2	-6.05	113.75	119.20
1	B	44	SER	N-CA-C	6.00	118.07	109.14
1	A	145	GLU	CB-CA-C	-5.97	100.53	110.68
1	A	92	LEU	N-CA-C	5.95	117.16	109.72
1	B	129	ARG	N-CA-C	-5.92	101.51	110.28
1	B	146	CYS	N-CA-C	5.77	118.35	111.71
1	B	151	ILE	N-CA-C	-5.76	101.12	109.29
1	B	298	PRO	N-CA-C	5.76	121.32	113.84
1	B	191	THR	CB-CA-C	-5.74	99.65	110.16
1	A	153	GLU	CB-CA-C	-5.74	98.02	109.79
1	A	22	PRO	N-CA-C	-5.73	106.70	113.86
1	A	30	VAL	CB-CA-C	-5.67	102.73	110.77
1	B	168	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	A	45	VAL	N-CA-C	-5.64	100.46	108.58
1	A	62	LEU	O-C-N	5.60	128.06	122.12
1	A	112	ARG	N-CA-C	5.58	117.17	111.14
1	B	213	ILE	N-CA-C	5.56	115.76	110.42
1	A	151	ILE	N-CA-C	-5.52	101.84	109.46
1	B	9	ASN	N-CA-C	5.48	118.97	112.72
1	B	45	VAL	N-CA-C	-5.48	100.69	108.58
1	A	173[A]	SER	CA-C-N	-5.46	114.01	122.59
1	A	173[A]	SER	C-N-CA	-5.46	114.01	122.59
1	A	173[B]	SER	CA-C-N	-5.46	114.01	122.59
1	A	173[B]	SER	C-N-CA	-5.46	114.01	122.59
1	B	73	VAL	N-CA-C	-5.45	105.80	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	TRP	N-CA-C	-5.43	105.36	111.28
1	A	74	PHE	N-CA-C	5.40	120.27	113.25
1	A	144	ALA	CA-C-N	5.33	127.69	120.38
1	A	144	ALA	C-N-CA	5.33	127.69	120.38
1	A	243	VAL	N-CA-C	-5.30	101.40	109.78
1	A	147	TYR	CB-CA-C	5.28	118.13	109.90
1	B	170	PHE	CA-C-N	-5.27	114.72	122.83
1	B	170	PHE	C-N-CA	-5.27	114.72	122.83
1	B	177	TYR	N-CA-C	-5.26	103.51	110.40
1	A	174	THR	CB-CA-C	-5.23	99.08	109.79
1	A	136	ALA	N-CA-C	5.16	117.57	111.33
1	B	327	ARG	CG-CD-NE	-5.13	100.71	112.00
1	B	97	TRP	N-CA-CB	-5.09	103.20	111.24
1	B	147	TYR	CB-CA-C	5.06	117.79	109.90
1	A	165	VAL	N-CA-C	-5.05	101.21	108.53
1	A	124	GLY	N-CA-C	5.03	122.05	115.36
1	B	344	ALA	N-CA-C	5.02	116.75	111.28
1	B	218	GLY	N-CA-C	-5.02	106.15	114.48
1	A	35	GLU	N-CA-C	-5.01	102.27	109.24

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	2802	0	2779	89	0
1	B	2788	0	2767	56	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	375	0	0	10	0
4	B	315	0	0	5	0
All	All	6346	0	5570	145	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 13.

All (145) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LYS:NZ	1:A:2:LYS:H	1.39	1.20
1:A:199:ASN:HB3	4:A:770:HOH:O	1.47	1.14
1:A:2:LYS:HZ3	1:A:2:LYS:N	1.61	0.98
1:A:310:ARG:HG3	1:A:313:ARG:HD3	1.47	0.93
1:A:2:LYS:H	1:A:2:LYS:HZ3	0.97	0.92
1:A:1:MET:HG3	1:A:24:GLY:O	1.71	0.90
1:A:146:CYS:HB3	1:A:150:CYS:SG	2.12	0.89
1:A:308:GLU:HB3	1:A:313:ARG:HH12	1.37	0.87
1:B:127:ASP:HB3	1:B:188:ILE:HG12	1.56	0.85
1:A:2:LYS:NZ	1:A:2:LYS:N	2.20	0.84
1:A:310:ARG:HD2	1:A:313:ARG:HD2	1.62	0.79
1:A:310:ARG:CG	1:A:313:ARG:HH11	2.00	0.74
1:A:310:ARG:CD	1:A:313:ARG:HD2	2.17	0.74
1:A:101:ALA:N	1:A:105:GLU:OE2	2.23	0.71
1:B:21:GLU:HB3	1:B:22:PRO:HD3	1.71	0.71
1:A:320:LEU:N	1:A:320:LEU:HD12	2.05	0.71
1:A:65:HIS:O	1:A:71:ARG:NH2	2.19	0.70
1:A:86:LEU:HA	4:A:524:HOH:O	1.93	0.69
1:A:273:GLN:NE2	4:A:467:HOH:O	2.28	0.67
1:B:52:ARG:HG3	4:B:445:HOH:O	1.93	0.67
1:A:135[A]:ARG:HD2	4:A:769:HOH:O	1.95	0.66
1:B:203:GLN:O	1:B:207:GLU:HG3	1.96	0.66
1:B:135:ARG:N	1:B:138:GLU:OE2	2.21	0.65
1:A:102:GLU:N	1:A:105:GLU:OE2	2.28	0.64
1:A:319:ASN:C	1:A:320:LEU:HD12	2.22	0.64
1:A:310:ARG:HG3	1:A:313:ARG:CD	2.26	0.63
1:A:52:ARG:N	1:A:52:ARG:HD2	2.14	0.62
1:A:116:LEU:HD11	1:A:133:ARG:HG2	1.81	0.61
1:B:52:ARG:HD2	1:B:53:TRP:N	2.15	0.61
1:B:52:ARG:HD2	1:B:52:ARG:C	2.26	0.60
1:A:77:ILE:CD1	1:A:239:LEU:HD12	2.31	0.60
1:A:230:THR:HG21	1:A:235:LEU:HD13	1.82	0.60
1:A:138:GLU:HB3	1:A:141:GLN:OE1	2.02	0.60
1:A:1:MET:HE1	4:A:629:HOH:O	2.02	0.60
1:A:320:LEU:N	1:A:320:LEU:CD1	2.65	0.60
1:B:197:GLN:HG2	4:B:694:HOH:O	2.01	0.59
1:A:42:GLN:OE1	1:A:43:GLN:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ARG:HG2	1:B:17:ARG:HH11	1.67	0.58
1:B:273:GLN:NE2	4:B:551:HOH:O	2.36	0.58
1:A:135[A]:ARG:NH1	4:A:769:HOH:O	2.35	0.57
1:A:46:ILE:HB	1:A:68:PHE:HA	1.86	0.57
1:A:310:ARG:HG2	1:A:313:ARG:HH11	1.69	0.57
1:A:308:GLU:HB3	1:A:313:ARG:NH1	2.14	0.57
1:A:1:MET:HG2	1:A:1:MET:O	2.03	0.57
1:A:65:HIS:ND1	1:A:66:PRO:HD2	2.20	0.56
1:B:110:PHE:CE1	1:B:136:ALA:HA	2.40	0.56
1:B:2:LYS:CB	1:B:25:ILE:HG12	2.36	0.55
1:A:1:MET:O	1:A:2:LYS:C	2.49	0.54
1:B:2:LYS:HB2	1:B:25:ILE:HA	1.89	0.54
1:B:84:LYS:HE3	1:B:97:TRP:CD1	2.43	0.54
1:B:40:PRO:HB3	1:B:43:GLN:HE21	1.73	0.54
1:A:65:HIS:CG	1:A:66:PRO:HD2	2.43	0.54
1:A:230:THR:CG2	1:A:235:LEU:HD13	2.39	0.53
1:A:2:LYS:NZ	1:A:2:LYS:CB	2.73	0.52
1:A:35:GLU:O	1:A:39:VAL:HG23	2.09	0.52
1:A:17:ARG:HA	1:A:27:VAL:HB	1.92	0.52
1:A:77:ILE:HD11	1:A:239:LEU:HD12	1.92	0.51
1:B:1:MET:SD	1:B:2:LYS:N	2.83	0.51
1:B:310:ARG:HE	1:B:313:ARG:HD2	1.76	0.51
1:A:101:ALA:CA	1:A:105:GLU:OE2	2.58	0.51
1:A:310:ARG:CG	1:A:313:ARG:HD3	2.32	0.50
1:A:310:ARG:CD	1:A:313:ARG:CD	2.88	0.50
1:A:324:ASP:CG	1:A:326:SER:HG	2.19	0.50
1:A:105:GLU:HA	4:A:530:HOH:O	2.11	0.50
1:A:2:LYS:H	1:A:2:LYS:HZ2	1.46	0.49
1:A:77:ILE:HD13	1:A:239:LEU:HD12	1.93	0.49
1:A:102:GLU:HA	1:A:147:TYR:HB3	1.94	0.49
1:A:52:ARG:HD2	1:A:52:ARG:H	1.77	0.49
1:A:106:TRP:N	1:A:107:PRO:CD	2.75	0.49
1:B:17:ARG:HA	1:B:27:VAL:HB	1.95	0.49
1:B:93:PRO:HD2	1:B:209:MET:SD	2.53	0.49
1:A:135[B]:ARG:HD2	4:A:769:HOH:O	2.13	0.48
1:A:68:PHE:HD2	1:A:71:ARG:HD3	1.78	0.48
1:B:73:VAL:O	1:B:74:PHE:C	2.56	0.47
1:B:121:ARG:HD2	1:B:150:CYS:SG	2.54	0.47
1:A:40:PRO:HA	1:A:43:GLN:HE22	1.80	0.47
1:B:2:LYS:HB2	1:B:25:ILE:HG12	1.97	0.47
1:A:70:ASN:ND2	1:A:219:TYR:CE1	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:TYR:CZ	1:B:129:ARG:NE	2.83	0.46
1:A:127:ASP:CG	1:A:188:ILE:HD12	2.41	0.46
1:B:17:ARG:HG2	1:B:17:ARG:NH1	2.31	0.46
1:B:291:ASN:HB3	1:B:294:TRP:CE2	2.51	0.46
1:A:308:GLU:H	1:A:313:ARG:HH22	1.64	0.46
1:A:308:GLU:O	1:A:313:ARG:NH1	2.49	0.46
1:A:308:GLU:H	1:A:313:ARG:NH2	2.13	0.46
1:B:30:VAL:HG23	1:B:34:ALA:HB3	1.98	0.46
1:A:171:ASP:OD1	1:A:171:ASP:C	2.55	0.46
1:B:319:ASN:C	1:B:320:LEU:HD12	2.41	0.46
1:B:171:ASP:OD1	1:B:171:ASP:C	2.59	0.45
1:B:8:GLY:O	4:B:451:HOH:O	2.21	0.45
1:A:39:VAL:HB	1:A:41:PHE:HD2	1.81	0.45
1:B:87:PHE:CZ	1:B:236:ILE:HG21	2.51	0.45
1:B:310:ARG:HH21	1:B:313:ARG:HD2	1.81	0.45
1:B:2:LYS:HB2	1:B:25:ILE:HG23	1.98	0.45
1:B:2:LYS:CG	1:B:25:ILE:HG12	2.47	0.45
1:A:291:ASN:HB3	1:A:294:TRP:CE2	2.51	0.45
1:B:273:GLN:NE2	1:B:274:PRO:HD2	2.31	0.45
1:A:17:ARG:HG2	1:A:17:ARG:HH11	1.82	0.44
1:B:98:GLN:HG3	1:B:99:LEU:O	2.17	0.44
1:B:205:ARG:CZ	1:B:205:ARG:CB	2.95	0.44
1:A:230:THR:HB	1:A:231:PRO:HD2	1.99	0.44
1:B:121:ARG:HD2	1:B:121:ARG:HA	1.43	0.44
1:A:2:LYS:HZ3	1:A:2:LYS:CB	2.30	0.44
1:A:5:CYS:HB2	1:A:46:ILE:HD13	1.99	0.44
1:B:305:TYR:O	1:B:306:ASP:HB3	2.18	0.44
1:A:70:ASN:O	1:A:71:ARG:C	2.59	0.44
1:B:181:HIS:O	1:B:192:SER:HA	2.18	0.43
1:B:34:ALA:O	1:B:58:LEU:HB2	2.19	0.43
1:B:199:ASN:OD1	1:B:202:GLN:N	2.44	0.43
1:A:21:GLU:HB3	1:A:22:PRO:HD3	2.00	0.43
1:A:81:LEU:HD13	1:A:99:LEU:HD13	2.00	0.43
1:A:121:ARG:HD2	1:A:150:CYS:SG	2.58	0.43
1:A:77:ILE:HD13	1:A:77:ILE:HG23	1.81	0.43
1:B:273:GLN:OE1	4:B:550:HOH:O	2.21	0.43
1:A:65:HIS:CE1	1:A:66:PRO:HD2	2.54	0.42
1:B:66:PRO:HA	1:B:71:ARG:HH21	1.83	0.42
1:B:185:GLN:HE21	1:B:190:ARG:HG3	1.83	0.42
1:A:61:GLN:O	1:A:64:ARG:HG3	2.19	0.42
1:A:1:MET:O	1:A:2:LYS:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ASN:OD1	4:A:681:HOH:O	2.21	0.42
1:A:310:ARG:CG	1:A:313:ARG:CD	2.94	0.42
1:B:350:ALA:O	1:B:353:LYS:HB2	2.19	0.42
1:A:210:LEU:HG	1:A:214:MET:HE2	2.00	0.42
1:A:30:VAL:HG23	1:A:30:VAL:O	2.19	0.42
1:A:39:VAL:HB	1:A:41:PHE:CD2	2.54	0.42
1:A:121:ARG:HD2	1:A:121:ARG:HA	1.60	0.41
1:A:39:VAL:HA	1:A:40:PRO:HD3	1.89	0.41
1:B:56:THR:O	1:B:60:ARG:HG3	2.20	0.41
1:B:126:TYR:O	1:B:129:ARG:HD3	2.21	0.41
1:B:353:LYS:HD2	1:B:353:LYS:HA	1.63	0.41
1:A:56:THR:O	1:A:60:ARG:HG3	2.21	0.41
1:B:81:LEU:HD12	1:B:97:TRP:HZ3	1.85	0.41
1:B:40:PRO:HB3	1:B:43:GLN:NE2	2.36	0.41
1:A:273:GLN:NE2	1:A:274:PRO:HD2	2.35	0.41
1:A:308:GLU:O	1:A:313:ARG:CZ	2.69	0.41
1:A:52:ARG:HH11	1:A:52:ARG:HD3	1.74	0.40
1:A:68:PHE:CD2	1:A:71:ARG:HB2	2.55	0.40
1:B:46:ILE:HB	1:B:68:PHE:HA	2.02	0.40
1:B:65:HIS:CE1	1:B:67:ALA:HB3	2.56	0.40
1:B:89:LYS:O	1:B:89:LYS:CG	2.68	0.40
1:B:182:ASN:HD21	1:B:246:SER:HB2	1.86	0.40
1:B:9:ASN:HD22	1:B:9:ASN:HA	1.49	0.40
1:A:181:HIS:O	1:A:192:SER:HA	2.20	0.40
1:A:313:ARG:NH2	4:A:622:HOH:O	2.53	0.40
1:B:332:LEU:HB3	1:B:347:VAL:HG13	2.04	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	357/355 (101%)	352 (99%)	4 (1%)	1 (0%)	36	20
1	B	354/355 (100%)	351 (99%)	3 (1%)	0	100	100
All	All	711/710 (100%)	703 (99%)	7 (1%)	1 (0%)	48	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LYS

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	300/296 (101%)	280 (93%)	20 (7%)	15	3
1	B	297/296 (100%)	281 (95%)	16 (5%)	20	4
All	All	597/592 (101%)	561 (94%)	36 (6%)	17	4

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	14	ARG
1	A	43	GLN
1	A	52	ARG
1	A	58	LEU
1	A	61	GLN
1	A	62	LEU
1	A	64	ARG
1	A	77	ILE
1	A	103	ARG
1	A	104	SER
1	A	105	GLU
1	A	145	GLU
1	A	157	ASN
1	A	188	ILE

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Mol	Chain	Res	Type
1	A	197	GLN
1	A	310	ARG
1	A	313	ARG
1	A	320	LEU
1	A	327	ARG
1	B	2	LYS
1	B	9	ASN
1	B	30	VAL
1	B	49	GLU
1	B	52	ARG
1	B	103	ARG
1	B	121	ARG
1	B	140	GLU
1	B	145	GLU
1	B	202	GLN
1	B	205	ARG
1	B	210	LEU
1	B	320	LEU
1	B	327	ARG
1	B	340	PRO
1	B	353	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	61	GLN
1	A	91	HIS
1	A	202	GLN
1	A	215	GLN
1	A	273	GLN
1	A	278	ASN
1	B	9	ASN
1	B	61	GLN
1	B	85	GLN
1	B	182	ASN
1	B	185	GLN
1	B	197	GLN
1	B	201	GLN
1	B	273	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 6 ligands modelled in this entry, 4 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	400	3	32,33,33	1.08	1 (3%)	48,52,52	1.71	14 (29%)
2	ATP	B	400	3	32,33,33	1.15	3 (9%)	48,52,52	1.66	9 (18%)

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	400	3	-	4/22/38/38	0/3/3/3
2	ATP	B	400	3	-	4/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	ATP	C6-N6	-2.87	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	ATP	PB-O3B	-2.60	1.56	1.59
2	B	400	ATP	C6-N6	-2.59	1.27	1.34
2	B	400	ATP	C8-N7	2.00	1.35	1.31

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	ATP	N3-C2-N1	-4.66	121.52	128.58
2	B	400	ATP	C2-N1-C6	4.60	126.28	118.73
2	A	400	ATP	C2-N1-C6	4.49	126.11	118.73
2	A	400	ATP	O2G-PG-O3B	3.94	117.86	104.64
2	B	400	ATP	O2B-PB-O3B	3.13	115.74	107.27
2	A	400	ATP	O4'-C4'-C3'	-3.07	99.06	105.15
2	A	400	ATP	C5-C6-N1	-3.05	109.76	117.51
2	A	400	ATP	O3A-PA-O1A	-3.04	101.55	110.70
2	A	400	ATP	O2A-PA-O5'	3.00	121.17	107.57
2	B	400	ATP	C2'-C3'-C4'	-2.74	97.31	102.61
2	A	400	ATP	N9-C8-N7	-2.63	110.21	113.94
2	B	400	ATP	O5'-C5'-C4'	-2.60	100.14	108.99
2	A	400	ATP	O2'-C2'-C1'	-2.40	101.85	110.10
2	B	400	ATP	O4'-C4'-C5'	2.37	116.93	109.33
2	A	400	ATP	C5-N7-C8	2.34	107.12	103.45
2	A	400	ATP	O3B-PG-O1G	-2.33	98.77	111.04
2	B	400	ATP	N9-C8-N7	-2.31	110.65	113.94
2	A	400	ATP	N3-C2-N1	-2.31	125.08	128.58
2	A	400	ATP	C6-C5-C4	2.28	120.29	117.18
2	B	400	ATP	C5-C6-N1	-2.24	111.84	117.51
2	A	400	ATP	C4-N9-C8	2.15	108.00	105.74
2	A	400	ATP	N6-C6-N1	2.12	123.09	118.38
2	B	400	ATP	C5-N7-C8	2.02	106.63	103.45

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	ATP	PB-O3B-PG-O2G
2	B	400	ATP	PB-O3B-PG-O2G
2	A	400	ATP	PB-O3A-PA-O2A
2	A	400	ATP	PB-O3B-PG-O3G
2	B	400	ATP	PB-O3B-PG-O3G
2	B	400	ATP	PB-O3B-PG-O1G
2	A	400	ATP	PB-O3A-PA-O1A

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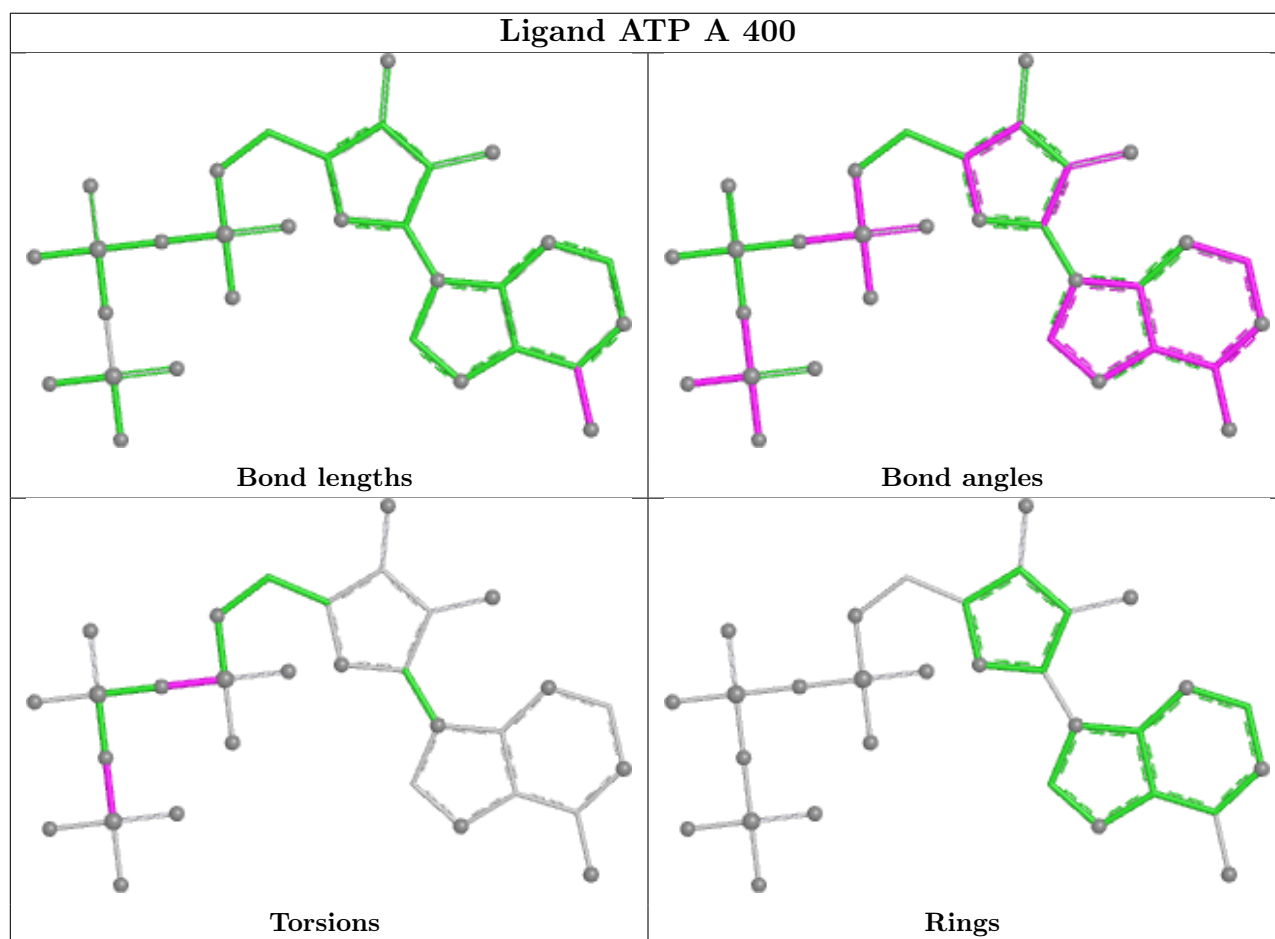
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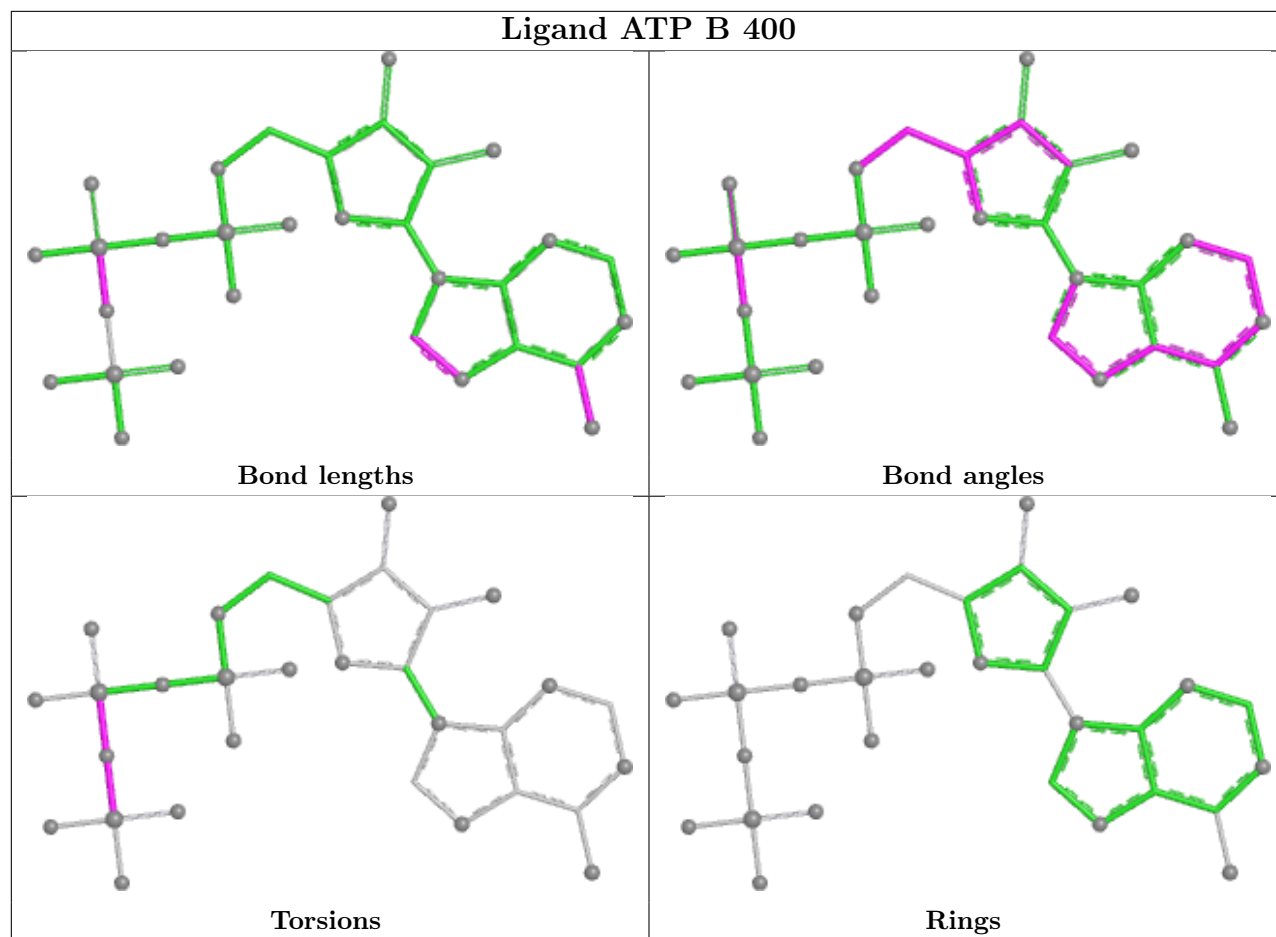
Mol	Chain	Res	Type	Atoms
2	B	400	ATP	PG-O3B-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	355/355 (100%)	-0.01	13 (3%) 45 47	12, 21, 56, 84	4 (1%)
1	B	355/355 (100%)	-0.08	6 (1%) 69 72	10, 22, 52, 86	1 (0%)
All	All	710/710 (100%)	-0.04	19 (2%) 56 59	10, 21, 54, 86	5 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	63	ALA	4.5
1	B	41	PHE	3.7
1	A	41	PHE	3.6
1	A	1	MET	3.5
1	A	199	ASN	2.8
1	A	39	VAL	2.7
1	B	42	GLN	2.6
1	A	108	ALA	2.6
1	A	144	ALA	2.4
1	B	28	TRP	2.4
1	B	170	PHE	2.3
1	A	105	GLU	2.3
1	A	62	LEU	2.2
1	A	66	PRO	2.1
1	A	101	ALA	2.1
1	A	65	HIS	2.0
1	B	91	HIS	2.0
1	A	355	GLY	2.0
1	B	1	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

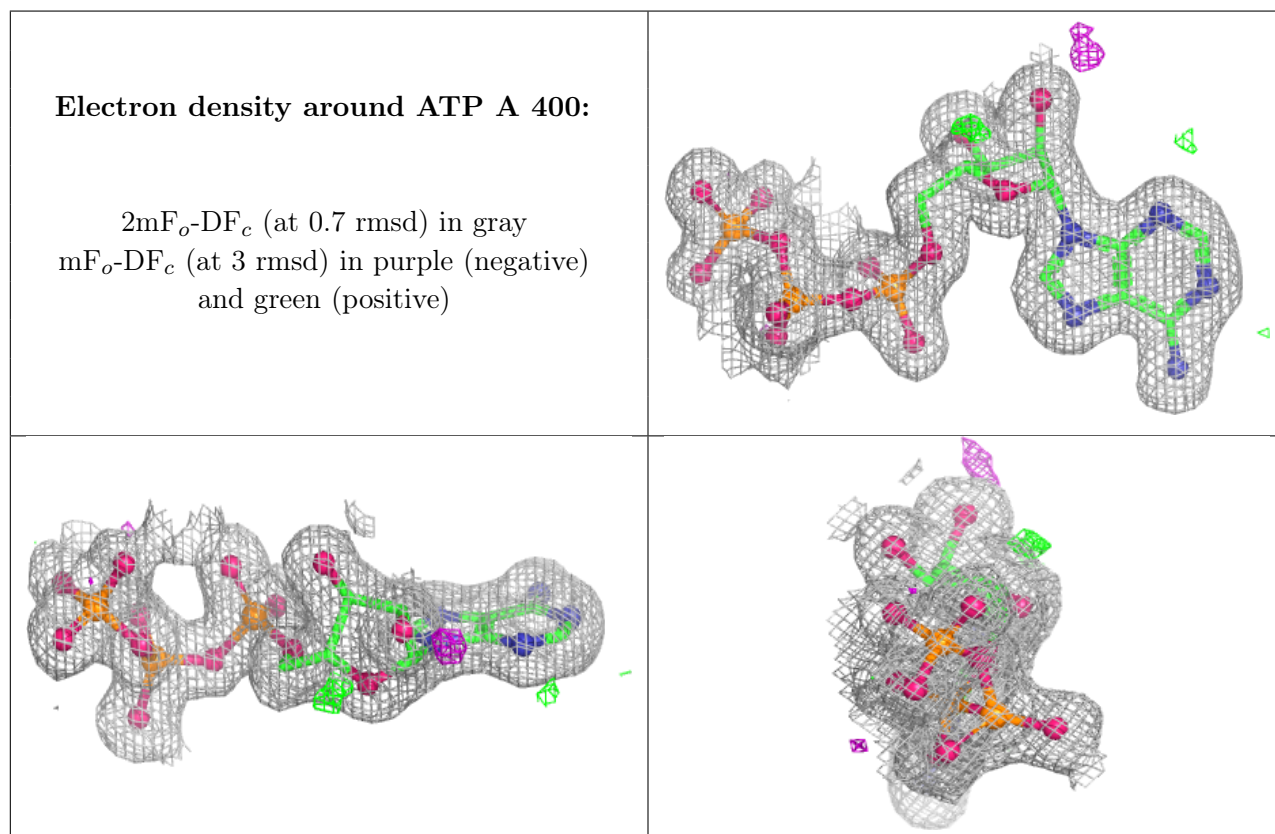
There are no oligosaccharides in this entry.

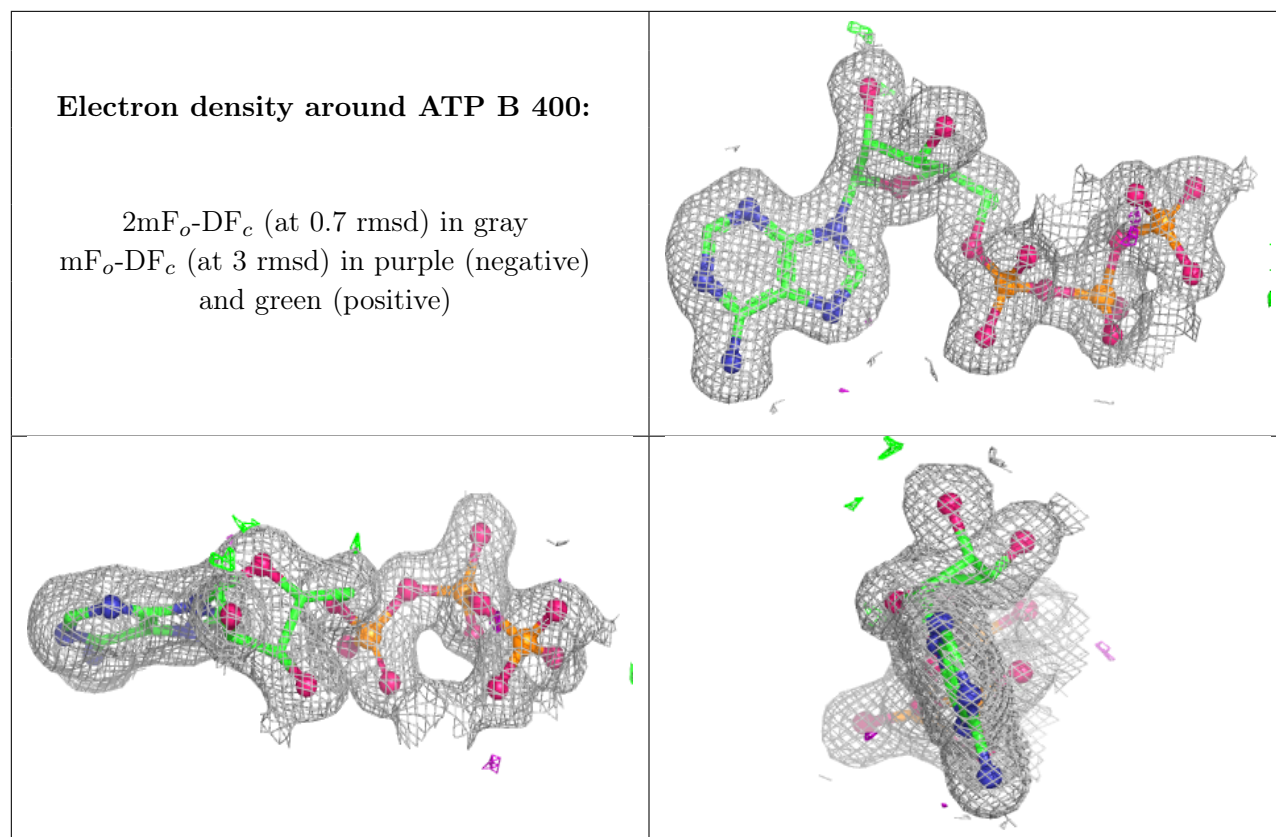
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ATP	A	400	31/31	0.98	0.04	13,20,25,29	0
2	ATP	B	400	31/31	0.98	0.04	15,19,24,31	0
3	MG	A	401	1/1	0.98	0.04	17,17,17,17	0
3	MG	A	402	1/1	0.98	0.04	16,16,16,16	0
3	MG	B	402	1/1	0.99	0.03	19,19,19,19	0
3	MG	B	401	1/1	1.00	0.02	17,17,17,17	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.