



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:00 AM UTC

PDB ID : 4G5Y / pdb_00004g5y
Title : Crystal Structure of Mycobacterium tuberculosis Pantothenate synthetase in a ternary complex with ATP and N,N-DIMETHYLTHIOPHENE-3-SULFONAMIDE
Authors : Ciulli, A.; Silvestre, H.L.; Blundell, T.L.; Abell, C.
Deposited on : 2012-07-18
Resolution : 1.80 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

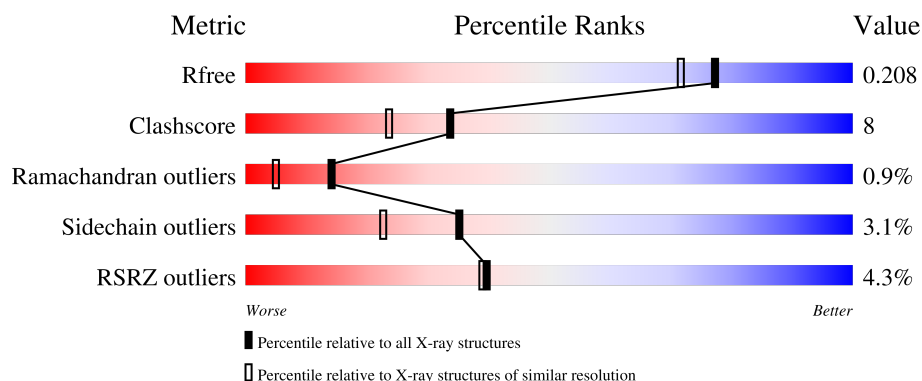
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	301	6% 81% 12% • 5%
1	B	301	2% 78% 11% • 10%

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	0OC	B	403	-	X	-	-
4	0OC	B	404	-	X	X	-
5	GOL	B	405	-	-	X	-
6	EOH	A	405	-	-	X	-
6	EOH	B	407	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4688 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.

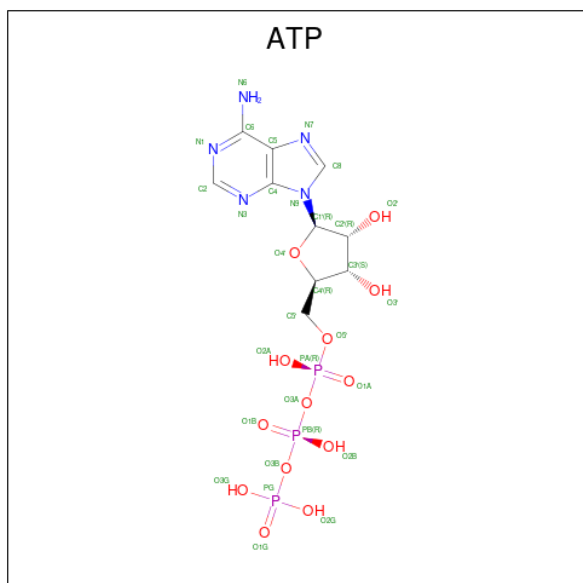
- Molecule 1 is a protein called Pantothenate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	4	0
			2134	1350	385	393	6			
1	B	272	Total	C	N	O	S	0	4	0
			2029	1287	369	368	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP P0A5R0
A	2	ALA	THR	engineered mutation	UNP P0A5R0
A	77	GLY	GLU	engineered mutation	UNP P0A5R0
B	0	ALA	-	expression tag	UNP P0A5R0
B	2	ALA	THR	engineered mutation	UNP P0A5R0
B	77	GLY	GLU	engineered mutation	UNP P0A5R0

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

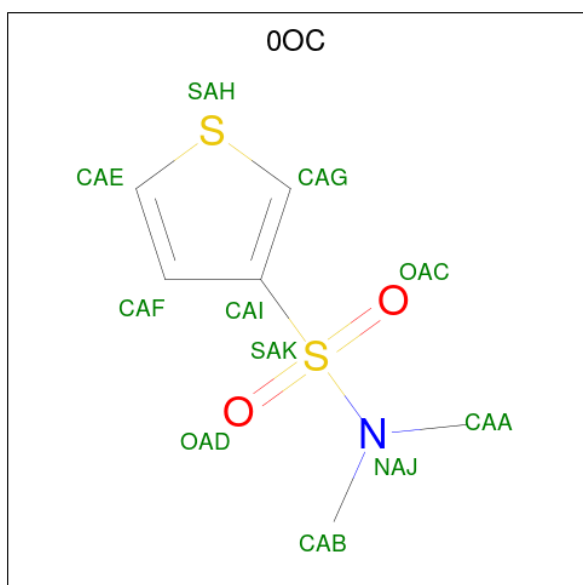


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

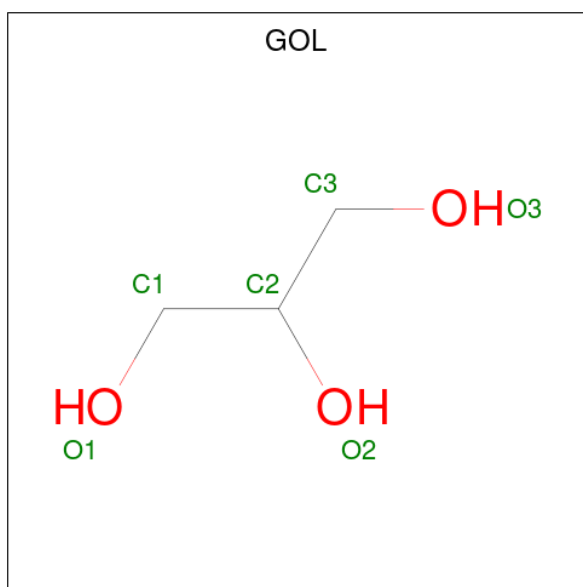
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is N,N-dimethylthiophene-3-sulfonamide (CCD ID: 0OC) (formula: C₆H₉NO₂S₂).



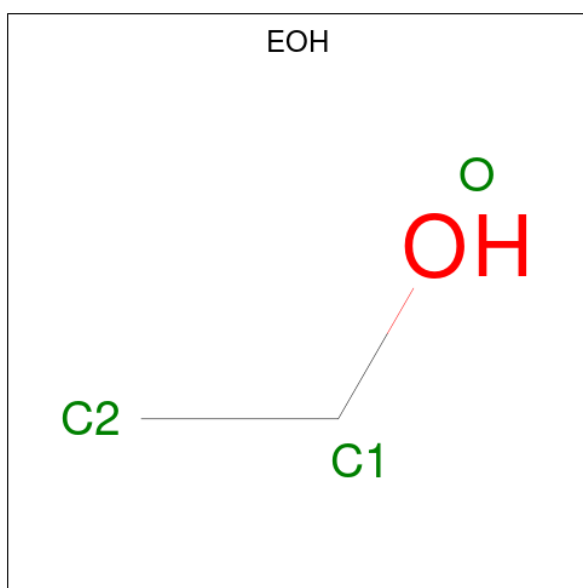
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			11	6	1	2	2		
4	B	1	Total	C	N	O	S	0	0
			11	6	1	2	2		
4	B	1	Total	C	N	O	S	0	0
			11	6	1	2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is ETHANOL (CCD ID: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	2	1		
6	A	1	Total	C	O	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			3	2	1		
6	B	1	Total	C	O	0	0
			3	2	1		

- Molecule 7 is water.

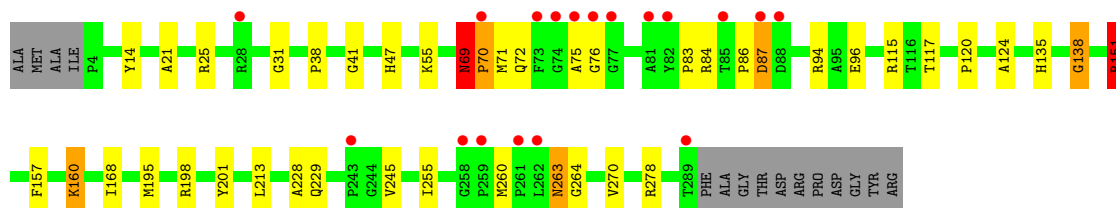
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	196	Total	O	0	0
			196	196		
7	B	208	Total	O	0	0
			208	208		

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.

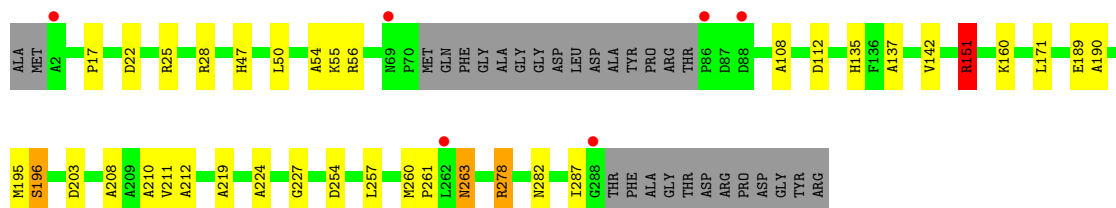
• Molecule 1: Pantothenate synthetase

Chain A: 



• Molecule 1: Pantothenate synthetase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.26Å 71.06Å 81.65Å 90.00° 99.35° 90.00°	Depositor
Resolution (Å)	37.57 – 1.80 37.57 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.57-1.80) 99.7 (37.57-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.158 , 0.208 0.158 , 0.208	Depositor DCC
R_{free} test set	2547 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4688	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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: 0OC, MG, EOH, GOL, 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	1.49	12/2179 (0.6%)	1.39	8/2975 (0.3%)
1	B	1.48	14/2072 (0.7%)	1.32	11/2828 (0.4%)
All	All	1.49	26/4251 (0.6%)	1.35	19/5803 (0.3%)

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	A	0	2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	ASN	C-O	8.46	1.35	1.24
1	B	151	ARG	CA-CB	7.47	1.57	1.52
1	B	224	ALA	N-CA	6.73	1.54	1.46
1	A	213	LEU	C-O	6.62	1.31	1.24
1	A	151	ARG	CA-CB	6.42	1.58	1.52
1	B	257	LEU	N-CA	6.09	1.54	1.46
1	B	47	HIS	ND1-CE1	5.94	1.38	1.32
1	B	135	HIS	CE1-NE2	5.79	1.38	1.32
1	A	47	HIS	CG-ND1	-5.61	1.32	1.38
1	A	228	ALA	C-O	5.54	1.30	1.24
1	B	135	HIS	CG-CD2	5.46	1.41	1.35
1	B	227	GLY	C-O	5.45	1.28	1.23
1	A	270	VAL	N-CA	5.36	1.52	1.46
1	A	135	HIS	CG-CD2	5.34	1.41	1.35
1	B	50	LEU	N-CA	5.34	1.52	1.46
1	A	38	PRO	C-O	5.30	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	137	ALA	N-CA	5.29	1.52	1.46
1	B	171	LEU	N-CA	5.27	1.52	1.46
1	B	210	ALA	N-CA	5.22	1.53	1.46
1	A	135	HIS	CD2-NE2	-5.17	1.32	1.37
1	B	195	MET	N-CA	5.12	1.52	1.46
1	A	138	GLY	N-CA	5.10	1.52	1.45
1	A	151	ARG	N-CA	5.08	1.50	1.46
1	B	282	ASN	C-O	5.08	1.29	1.23
1	B	151	ARG	C-O	5.07	1.26	1.23
1	A	14	TYR	N-CA	5.00	1.52	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ASN	CA-C-N	-8.02	109.81	119.84
1	A	69	ASN	C-N-CA	-8.02	109.81	119.84
1	A	255	ILE	N-CA-C	6.73	119.46	111.05
1	B	219	ALA	N-CA-C	-5.78	104.98	111.28
1	B	190	ALA	CA-C-N	-5.69	113.54	122.65
1	B	190	ALA	C-N-CA	-5.69	113.54	122.65
1	B	203	ASP	CA-C-N	-5.68	112.75	119.05
1	B	203	ASP	C-N-CA	-5.68	112.75	119.05
1	A	21	ALA	N-CA-C	-5.66	105.19	111.36
1	B	278	ARG	NE-CZ-NH2	-5.62	114.14	119.20
1	B	108	ALA	N-CA-C	-5.50	105.30	112.23
1	B	112	ASP	N-CA-C	-5.35	105.46	112.41
1	B	189	GLU	N-CA-C	-5.20	104.01	110.41
1	B	54	ALA	N-CA-C	-5.20	105.70	111.36
1	B	137	ALA	N-CA-C	-5.19	105.62	111.28
1	A	245	VAL	CA-C-N	-5.15	115.83	123.05
1	A	245	VAL	C-N-CA	-5.15	115.83	123.05
1	A	96	GLU	N-CA-C	-5.12	106.72	113.17
1	A	31	GLY	N-CA-C	5.06	122.30	115.32

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	69	ASN	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	2134	0	2183	23	0
1	B	2029	0	2105	36	0
2	A	31	0	12	0	0
2	B	31	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	11	0	8	0	0
4	B	22	0	18	8	0
5	A	6	0	8	0	0
5	B	6	0	8	18	0
6	A	6	0	12	2	0
6	B	6	0	12	3	0
7	A	196	0	0	6	0
7	B	208	0	0	7	0
All	All	4688	0	4378	67	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 8.

All (67) 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:196:SER:HB2	5:B:405:GOL:O1	1.25	1.27
1:B:196:SER:CB	5:B:405:GOL:O1	1.95	1.14
1:B:160:LYS:HE3	5:B:405:GOL:H31	1.34	1.09
1:A:115:ARG:O	6:A:405:EOH:H22	1.61	1.00
5:B:405:GOL:H2	7:B:504:HOH:O	1.64	0.97
4:B:404:OOC:H5	7:B:587:HOH:O	1.63	0.96
1:B:160:LYS:HD2	5:B:405:GOL:O3	1.70	0.92
1:B:208:ALA:HB1	4:B:404:OOC:H3	1.58	0.85
1:A:117:THR:OG1	6:A:405:EOH:H21	1.81	0.79
1:B:208:ALA:CB	4:B:404:OOC:H3	2.18	0.73
1:B:160:LYS:HE3	5:B:405:GOL:C3	2.15	0.73
1:A:263:ASN:CG	1:A:264:GLY:H	1.98	0.72
1:B:142[A]:VAL:HG11	4:B:403:OOC:CAF	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:405:GOL:C2	7:B:504:HOH:O	2.29	0.70
1:B:160:LYS:CD	5:B:405:GOL:O3	2.40	0.69
4:B:404:OOC:CAB	7:B:587:HOH:O	2.28	0.69
7:A:613:HOH:O	6:B:407:EOH:H23	1.93	0.68
7:A:613:HOH:O	6:B:407:EOH:C2	2.42	0.67
1:A:69:ASN:HD22	1:A:72:GLN:N	1.95	0.63
1:B:196:SER:OG	5:B:405:GOL:O1	2.15	0.63
1:B:278:ARG:HG2	1:B:278:ARG:HH21	1.64	0.63
1:B:278:ARG:HG2	1:B:278:ARG:NH2	2.14	0.62
1:B:196:SER:CB	5:B:405:GOL:HO1	2.12	0.61
1:B:254:ASP:HB3	1:B:261:PRO:HD3	1.81	0.61
1:A:263:ASN:CG	1:A:264:GLY:N	2.59	0.60
1:B:212:ALA:HB2	4:B:404:OOC:H8	1.84	0.60
1:B:260:MET:SD	1:B:261:PRO:HD2	2.42	0.60
1:B:160:LYS:CE	5:B:405:GOL:H31	2.20	0.60
1:A:69:ASN:HD22	1:A:72:GLN:H	1.52	0.57
1:A:41:GLY:O	7:A:678:HOH:O	2.17	0.56
1:A:151:ARG:NH2	1:B:151:ARG:HG3	2.22	0.55
1:B:160:LYS:NZ	5:B:405:GOL:H11	2.22	0.54
1:A:151:ARG:NH2	1:B:151:ARG:CG	2.71	0.54
1:A:260:MET:HE1	7:A:660:HOH:O	2.08	0.53
1:B:212:ALA:HB2	4:B:404:OOC:CAE	2.39	0.52
1:B:260:MET:CE	1:B:287:ILE:HG12	2.40	0.52
1:A:25:ARG:NH1	7:A:614:HOH:O	2.38	0.51
1:B:56[A]:ARG:NH1	7:B:637:HOH:O	2.42	0.51
1:A:69:ASN:ND2	1:A:72:GLN:N	2.59	0.51
1:B:160:LYS:CE	5:B:405:GOL:C3	2.86	0.50
1:B:208:ALA:HB1	4:B:404:OOC:CAA	2.36	0.50
1:B:160:LYS:HZ2	5:B:405:GOL:C1	2.24	0.50
1:B:25:ARG:NH2	1:B:151:ARG:HH22	2.11	0.49
1:A:160:LYS:HE2	1:A:195:MET:O	2.13	0.49
1:B:263:ASN:N	1:B:263:ASN:OD1	2.45	0.48
5:B:405:GOL:C1	7:B:691:HOH:O	2.62	0.47
1:A:84:ARG:O	1:A:86:PRO:HD3	2.14	0.47
1:B:22:ASP:OD1	1:B:25:ARG:NH1	2.47	0.47
1:B:160:LYS:NZ	5:B:405:GOL:C1	2.78	0.47
1:A:198:ARG:HD3	1:A:278:ARG:O	2.15	0.46
1:A:69:ASN:HB3	1:A:70[B]:PRO:C	2.40	0.46
1:A:69:ASN:ND2	1:A:72:GLN:H	2.14	0.45
1:B:287:ILE:HA	1:B:287:ILE:HD13	1.60	0.45
1:B:160:LYS:HZ2	1:B:196:SER:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:PRO:HD3	1:A:201:TYR:OH	2.16	0.45
1:B:160:LYS:HE2	1:B:160:LYS:HB3	1.79	0.44
1:B:25:ARG:NH2	1:B:151:ARG:NH2	2.66	0.44
1:A:157:PHE:CZ	1:A:168:ILE:HD13	2.52	0.44
1:B:208:ALA:O	1:B:211:VAL:HG12	2.17	0.44
7:A:613:HOH:O	6:B:407:EOH:H21	2.16	0.43
5:B:405:GOL:H11	7:B:691:HOH:O	2.18	0.42
1:A:71:MET:SD	1:A:138:GLY:HA2	2.59	0.42
1:B:260:MET:HE2	1:B:287:ILE:HG12	2.01	0.41
1:A:120:PRO:HB2	1:A:124:ALA:HB2	2.04	0.40
2:B:401:ATP:O3G	5:B:405:GOL:H12	2.21	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	288/301 (96%)	273 (95%)	9 (3%)	6 (2%)	5	1
1	B	272/301 (90%)	267 (98%)	5 (2%)	0	100	100
All	All	560/602 (93%)	540 (96%)	14 (2%)	6 (1%)	14	3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ALA
1	A	76	GLY
1	A	87	ASP
1	A	69	ASN
1	A	70[A]	PRO
1	A	70[B]	PRO

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	217/223 (97%)	210 (97%)	7 (3%)	34	22
1	B	207/223 (93%)	201 (97%)	6 (3%)	37	25
All	All	424/446 (95%)	411 (97%)	13 (3%)	35	23

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	87	ASP
1	A	94	ARG
1	A	151	ARG
1	A	160	LYS
1	A	229	GLN
1	A	263	ASN
1	B	17	PRO
1	B	28	ARG
1	B	55	LYS
1	B	151	ARG
1	B	196	SER
1	B	263	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	148	GLN
1	A	164	GLN
1	A	170	GLN
1	A	222	HIS
1	B	119	GLN
1	B	164	GLN
1	B	170	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	401	3	32,33,33	2.17	6 (18%)	48,52,52	2.11	14 (29%)
6	EOH	A	406	-	2,2,2	0.59	0	1,1,1	0.64	0
5	GOL	A	404	-	5,5,5	1.01	0	5,5,5	1.01	0
5	GOL	B	405	-	5,5,5	0.40	0	5,5,5	1.21	0
4	0OC	B	404	-	10,11,11	4.23	4 (40%)	11,16,16	4.30	6 (54%)
6	EOH	B	406	-	2,2,2	0.70	0	1,1,1	0.17	0
4	0OC	A	403	-	10,11,11	3.47	4 (40%)	11,16,16	2.30	3 (27%)
2	ATP	B	401	3	32,33,33	2.28	7 (21%)	48,52,52	2.43	19 (39%)
6	EOH	B	407	-	2,2,2	0.47	0	1,1,1	0.46	0
6	EOH	A	405	-	2,2,2	0.32	0	1,1,1	0.79	0
4	0OC	B	403	-	10,11,11	4.45	4 (40%)	11,16,16	4.26	5 (45%)

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	401	3	-	3/22/38/38	0/3/3/3
5	GOL	A	404	-	-	1/4/4/4	-
5	GOL	B	405	-	-	4/4/4/4	-
4	0OC	B	404	-	-	7/10/12/12	0/1/1/1
4	0OC	A	403	-	-	6/10/12/12	0/1/1/1
2	ATP	B	401	3	-	4/22/38/38	0/3/3/3
4	0OC	B	403	-	-	8/10/12/12	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	0OC	OAD-SAK	9.74	1.53	1.43
4	B	403	0OC	SAK-NAJ	7.89	1.75	1.63
2	A	401	ATP	PB-O3A	7.64	1.67	1.59
4	B	404	0OC	OAC-SAK	7.46	1.50	1.43
4	B	404	0OC	OAD-SAK	7.06	1.50	1.43
2	B	401	ATP	PB-O3A	6.97	1.67	1.59
4	B	404	0OC	SAK-NAJ	-6.67	1.53	1.63
4	A	403	0OC	CAF-CAI	-6.59	1.34	1.42
4	A	403	0OC	OAC-SAK	6.43	1.49	1.43
2	A	401	ATP	PA-O3A	6.14	1.66	1.59
2	B	401	ATP	C5-C4	5.96	1.49	1.39
4	B	403	0OC	OAC-SAK	5.92	1.49	1.43
4	B	404	0OC	CAF-CAI	-5.13	1.35	1.42
2	B	401	ATP	PA-O3A	5.04	1.64	1.59
2	A	401	ATP	C5-C4	4.79	1.47	1.39
4	A	403	0OC	SAK-NAJ	4.16	1.69	1.63
4	A	403	0OC	OAD-SAK	3.95	1.47	1.43
2	B	401	ATP	C8-N7	3.70	1.38	1.31
2	A	401	ATP	C8-N7	2.76	1.37	1.31
2	B	401	ATP	C2-N1	2.60	1.38	1.33
2	B	401	ATP	C5'-C4'	2.33	1.58	1.51
4	B	403	0OC	CAF-CAI	-2.28	1.39	1.42
2	B	401	ATP	PB-O1B	2.18	1.58	1.50
2	A	401	ATP	C4-N9	-2.09	1.33	1.37
2	A	401	ATP	C5-C6	2.08	1.46	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	0OC	OAD-SAK-OAC	-9.78	105.65	119.69
4	B	404	0OC	CAA-NAJ-SAK	-7.71	99.93	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	0OC	CAB-NAJ-SAK	-7.36	100.68	116.53
4	B	404	0OC	OAD-SAK-OAC	-7.12	109.47	119.69
4	B	403	0OC	OAC-SAK-NAJ	5.95	118.68	106.87
2	B	401	ATP	O2A-PA-O3A	-5.92	91.28	107.27
4	B	403	0OC	CAE-CAF-CAI	5.19	116.03	110.84
4	B	403	0OC	OAD-SAK-NAJ	5.16	117.11	106.87
2	B	401	ATP	N3-C2-N1	-5.07	120.90	128.58
2	B	401	ATP	C5-C4-N3	-4.93	119.94	126.72
2	A	401	ATP	C5-C4-N3	-4.86	120.03	126.72
2	A	401	ATP	N3-C2-N1	-4.67	121.52	128.58
4	A	403	0OC	OAC-SAK-NAJ	4.65	116.11	106.87
2	A	401	ATP	O2A-PA-O1A	4.53	133.51	112.44
2	B	401	ATP	N3-C4-N9	4.28	134.44	127.17
2	B	401	ATP	O2B-PB-O3B	-4.27	95.73	107.27
2	A	401	ATP	N3-C4-N9	4.23	134.37	127.17
2	A	401	ATP	C2-N3-C4	4.10	121.86	111.83
2	B	401	ATP	C4-N9-C8	4.02	109.95	105.74
2	B	401	ATP	O2A-PA-O1A	3.99	131.03	112.44
4	B	404	0OC	CAE-CAF-CAI	3.99	114.83	110.84
2	B	401	ATP	C2-N3-C4	3.97	121.53	111.83
4	A	403	0OC	CAB-NAJ-CAA	3.69	122.08	114.75
2	A	401	ATP	C4-N9-C8	3.68	109.61	105.74
4	B	404	0OC	CAB-NAJ-CAA	-3.58	107.65	114.75
4	A	403	0OC	OAD-SAK-OAC	-3.54	114.60	119.69
2	A	401	ATP	O3A-PA-O1A	-3.45	100.33	110.70
2	B	401	ATP	O3B-PB-O1B	3.37	120.85	110.70
2	B	401	ATP	O2A-PA-O5'	3.17	121.95	107.57
2	B	401	ATP	N9-C8-N7	-3.10	109.54	113.94
2	B	401	ATP	C4-N9-C1'	-2.84	119.99	126.63
2	B	401	ATP	O3G-PG-O3B	2.74	113.83	104.64
2	B	401	ATP	C4-C5-N7	-2.70	107.49	110.58
2	B	401	ATP	O5'-PA-O1A	-2.68	98.31	108.94
2	A	401	ATP	C5-C6-N6	-2.68	116.65	123.29
2	A	401	ATP	N6-C6-N1	2.58	124.12	118.38
2	B	401	ATP	C5-N7-C8	2.57	107.49	103.45
2	B	401	ATP	C2-N1-C6	2.56	122.93	118.73
2	A	401	ATP	O3'-C3'-C4'	-2.53	103.83	111.08
4	B	403	0OC	OAD-SAK-CAI	2.48	112.37	107.88
2	A	401	ATP	C4-C5-N7	-2.48	107.75	110.58
2	A	401	ATP	N9-C8-N7	-2.42	110.51	113.94
2	A	401	ATP	O2B-PB-O3B	2.32	113.55	107.27
4	B	404	0OC	OAC-SAK-NAJ	-2.27	102.37	106.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ATP	C6-C5-N7	2.23	136.39	132.09
2	B	401	ATP	O2B-PB-O3A	2.21	113.25	107.27
2	B	401	ATP	C6-C5-N7	2.20	136.33	132.09

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ATP	C5'-O5'-PA-O2A
2	A	401	ATP	C5'-O5'-PA-O3A
2	B	401	ATP	C5'-O5'-PA-O1A
2	B	401	ATP	C5'-O5'-PA-O3A
4	A	403	0OC	CAB-NAJ-SAK-OAC
4	A	403	0OC	CAB-NAJ-SAK-OAD
4	B	403	0OC	CAA-NAJ-SAK-OAC
4	B	403	0OC	CAA-NAJ-SAK-OAD
4	B	403	0OC	CAB-NAJ-SAK-OAC
4	B	403	0OC	CAB-NAJ-SAK-OAD
4	B	403	0OC	CAB-NAJ-SAK-CAI
4	B	403	0OC	CAF-CAI-SAK-OAD
4	B	404	0OC	CAA-NAJ-SAK-OAD
4	B	404	0OC	CAF-CAI-SAK-OAC
5	B	405	GOL	O1-C1-C2-O2
5	B	405	GOL	O1-C1-C2-C3
5	B	405	GOL	C1-C2-C3-O3
5	B	405	GOL	O2-C2-C3-O3
4	A	403	0OC	CAA-NAJ-SAK-OAC
4	B	404	0OC	CAB-NAJ-SAK-OAC
5	A	404	GOL	O1-C1-C2-C3
4	A	403	0OC	CAA-NAJ-SAK-OAD
4	A	403	0OC	CAB-NAJ-SAK-CAI
4	B	403	0OC	CAA-NAJ-SAK-CAI
4	A	403	0OC	CAA-NAJ-SAK-CAI
4	B	404	0OC	CAB-NAJ-SAK-CAI
2	A	401	ATP	C5'-O5'-PA-O1A
2	B	401	ATP	C5'-O5'-PA-O2A
4	B	403	0OC	CAF-CAI-SAK-OAC
4	B	404	0OC	CAA-NAJ-SAK-OAC
4	B	404	0OC	CAB-NAJ-SAK-OAD
4	B	404	0OC	CAA-NAJ-SAK-CAI
2	B	401	ATP	PG-O3B-PB-O2B

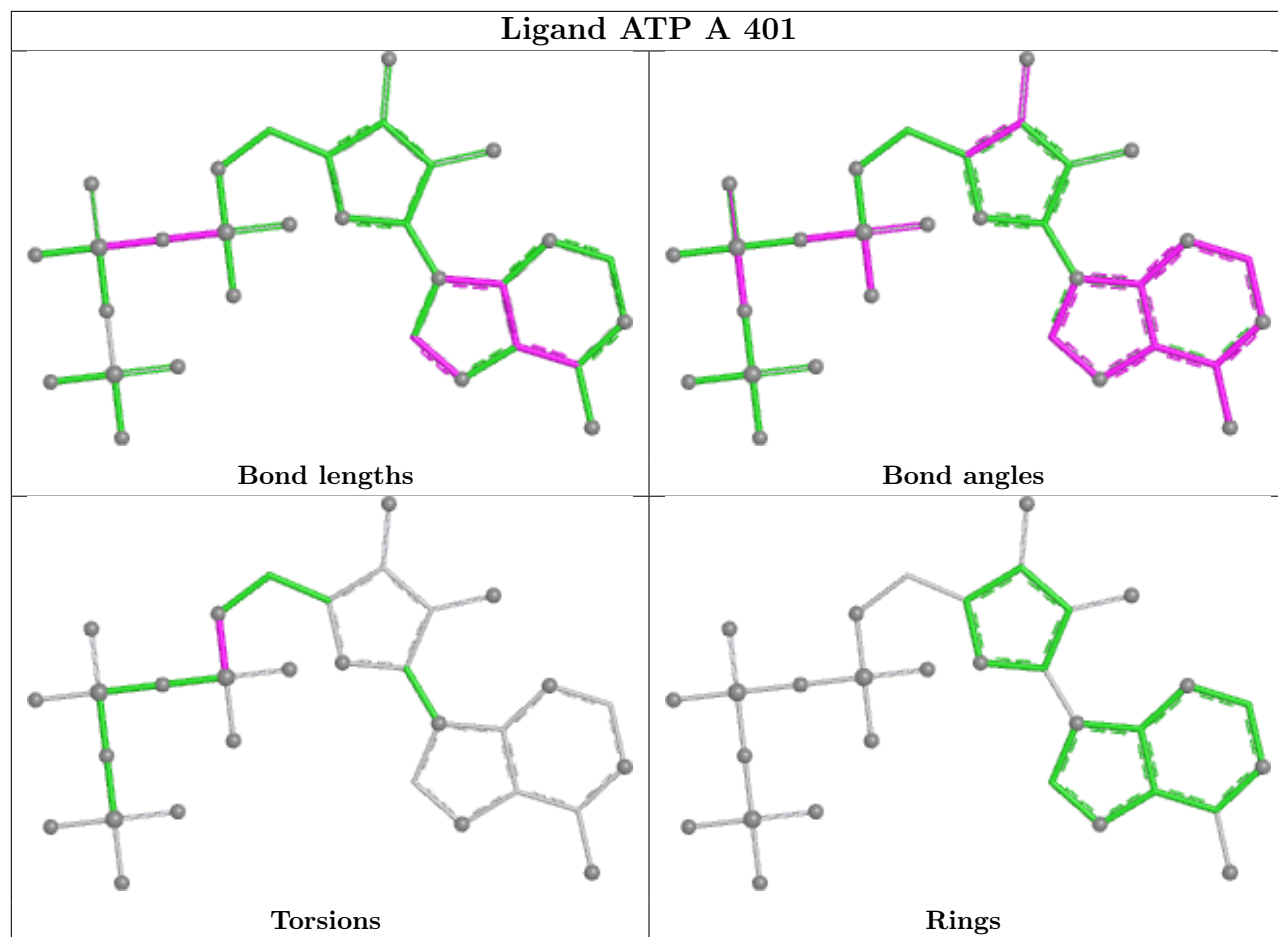
There are no ring outliers.

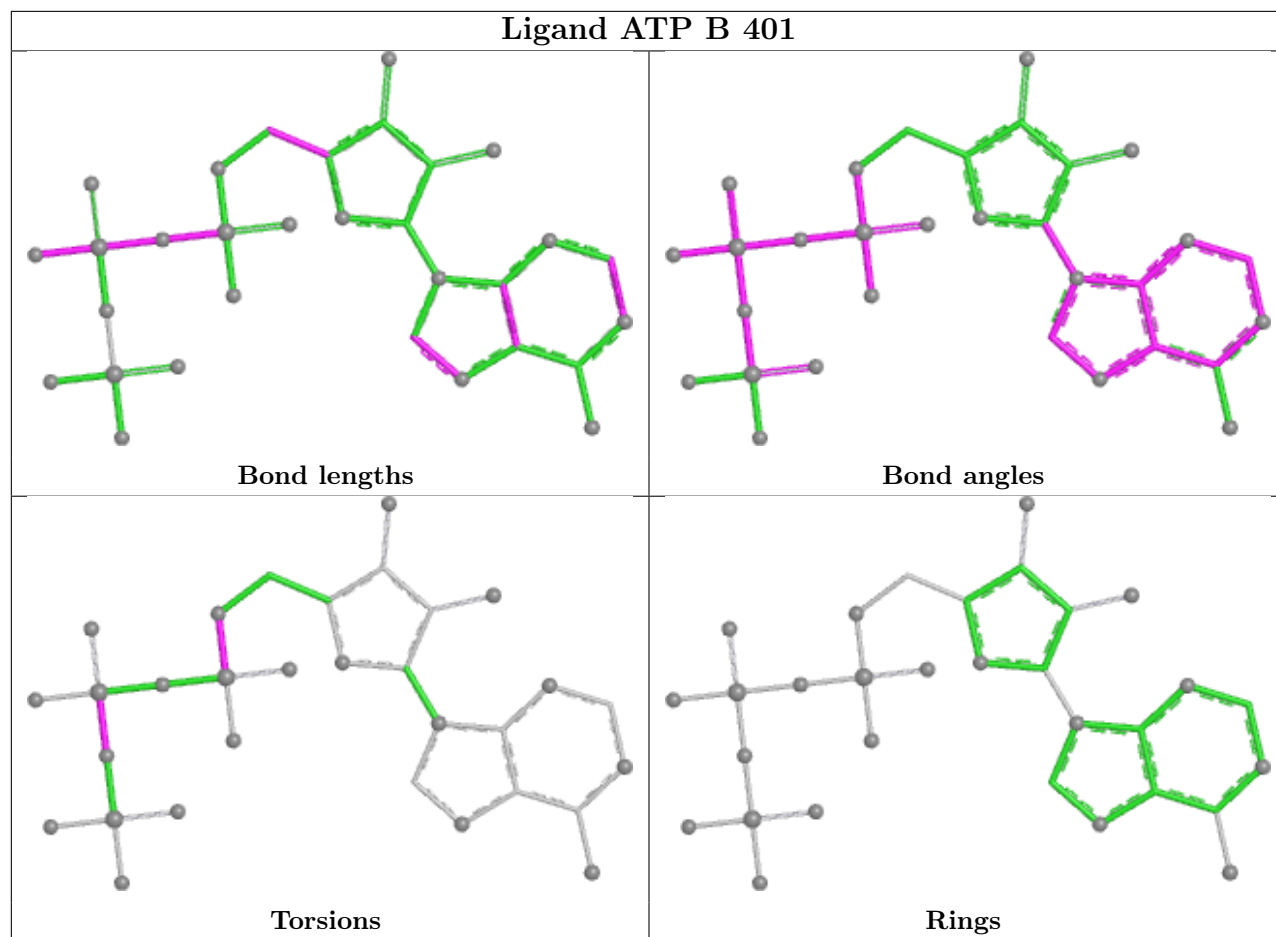
6 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	405	GOL	18	0
4	B	404	OOC	7	0
2	B	401	ATP	1	0
6	B	407	EOH	3	0
6	A	405	EOH	2	0
4	B	403	OOC	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.

Ligand ATP A 401





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	286/301 (95%)	-0.02	18 (6%) 26 24	11, 26, 56, 85	14 (4%)
1	B	272/301 (90%)	-0.32	6 (2%) 62 62	9, 25, 53, 86	4 (1%)
All	All	558/602 (92%)	-0.17	24 (4%) 40 39	9, 25, 57, 86	18 (3%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	GLY	5.8
1	A	76	GLY	5.3
1	A	75	ALA	5.2
1	A	70[A]	PRO	4.9
1	A	74	GLY	4.3
1	A	289	THR	4.1
1	A	81	ALA	4.0
1	A	258	GLY	3.5
1	B	288	GLY	3.2
1	A	87	ASP	3.1
1	A	259	PRO	2.8
1	A	85	THR	2.5
1	A	82	TYR	2.5
1	B	86	PRO	2.5
1	B	2	ALA	2.4
1	B	69	ASN	2.4
1	A	73	PHE	2.3
1	A	261	PRO	2.2
1	A	28[A]	ARG	2.2
1	A	88	ASP	2.1
1	A	243	PRO	2.1
1	A	262	LEU	2.0
1	B	262	LEU	2.0
1	B	88	ASP	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](#)

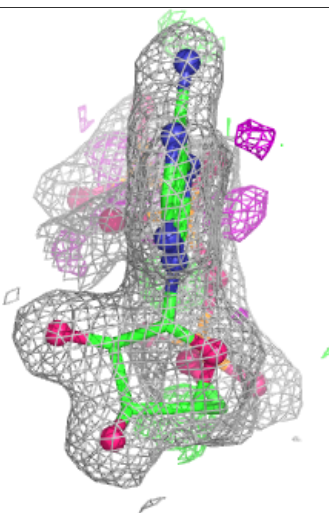
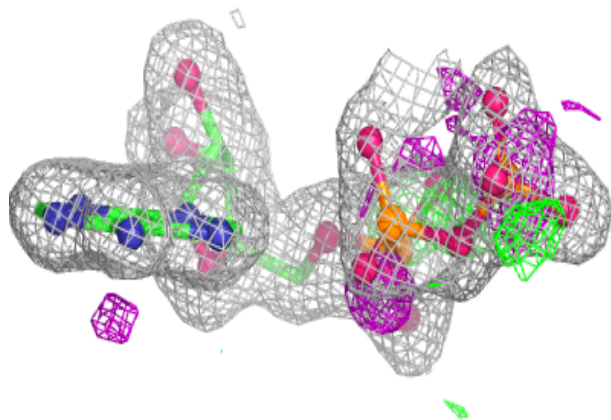
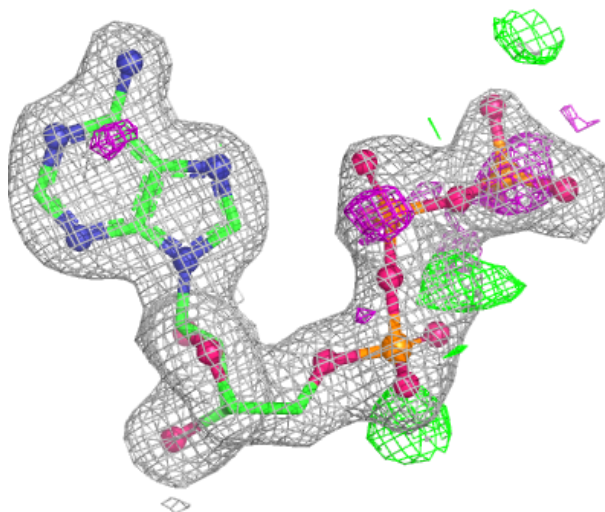
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

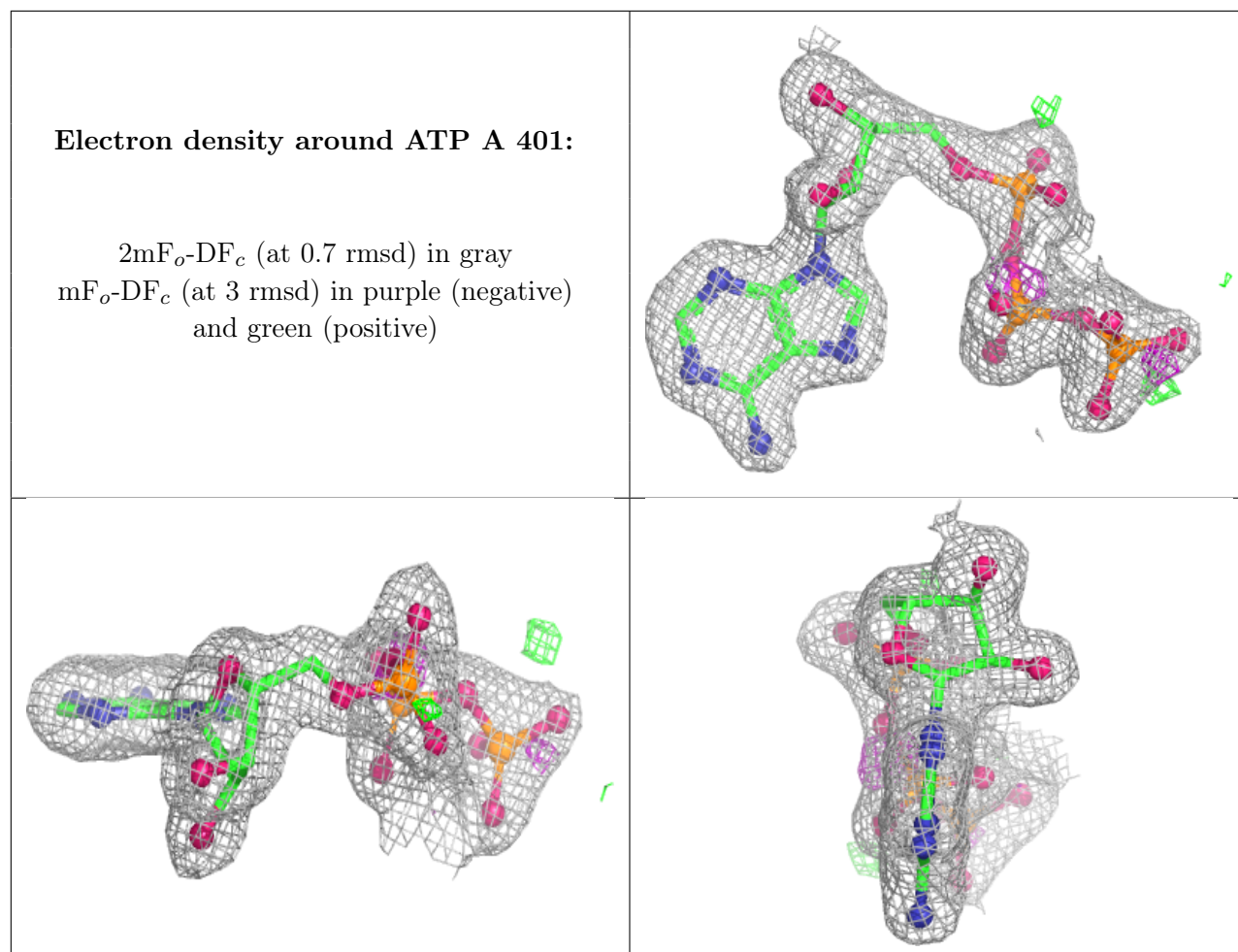
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EOH	A	406	3/3	0.78	0.19	41,41,42,42	0
6	EOH	B	406	3/3	0.81	0.17	33,33,33,34	0
5	GOL	B	405	6/6	0.82	0.21	18,39,46,62	6
4	OOC	B	404	11/11	0.83	0.17	21,33,61,64	11
6	EOH	B	407	3/3	0.84	0.16	39,39,40,45	0
6	EOH	A	405	3/3	0.90	0.12	22,22,38,63	0
4	OOC	B	403	11/11	0.92	0.10	28,42,48,52	0
4	OOC	A	403	11/11	0.93	0.10	14,23,28,30	11
2	ATP	B	401	31/31	0.95	0.07	20,24,46,50	0
3	MG	B	402	1/1	0.95	0.18	44,44,44,44	0
5	GOL	A	404	6/6	0.96	0.07	18,23,24,24	0
3	MG	A	402	1/1	0.96	0.07	43,43,43,43	0
2	ATP	A	401	31/31	0.97	0.06	21,30,44,46	0

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

Electron density around ATP B 401:

$2mF_o-DF_c$ (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.