



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 07:57 PM EDT

PDB ID : 5T3O
Title : Crystal structure of the Phosphorybosylpyrophosphate synthetase II from *Thermus thermophilus*
Authors : Timofeev, V.I.; Sinitsyna, E.V.; Abramchik, Y.A.; Kostromina, M.A.; Esipov, R.S.; Kuranova, I.P.
Deposited on : 2016-08-26
Resolution : 2.20 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

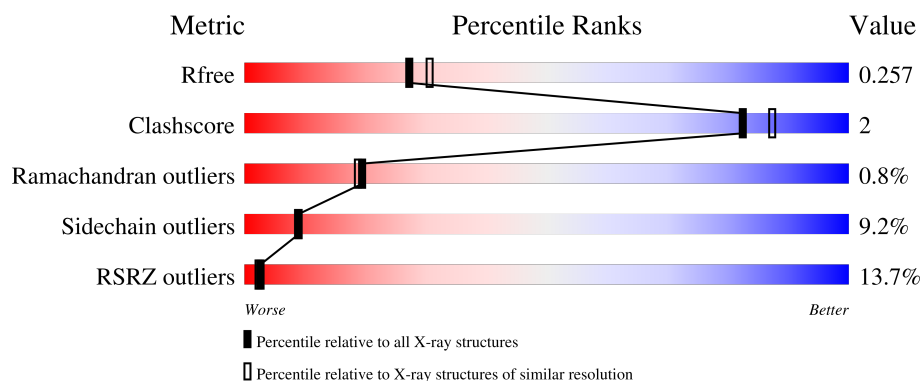
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 ≥ 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	307	<div> <div>28%</div> <div>86%</div> <div>13%</div> </div>
1	B	307	<div> <div>4%</div> <div>89%</div> <div>10%</div> </div>
1	C	307	<div> <div>9%</div> <div>87%</div> <div>10%</div> </div>

2 Entry composition [i](#)

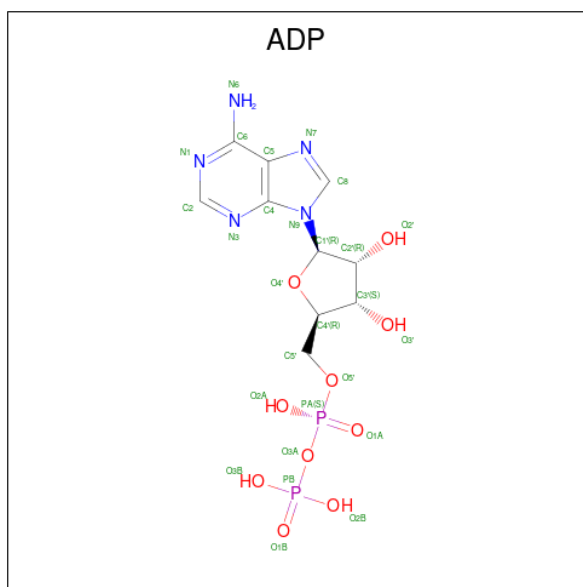
There are 4 unique types of molecules in this entry. The entry contains 7294 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribose-phosphate pyrophosphokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2331	1483	405	436	7			
1	B	307	Total	C	N	O	S	0	0	0
			2331	1483	405	436	7			
1	C	307	Total	C	N	O	S	0	0	0
			2331	1483	405	436	7			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	102	Total	O	0	0
			102	102		
4	C	59	Total	O	0	0
			59	59		

- Molecule 1: Ribose-phosphate pyrophosphokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	115.97Å 115.97Å 207.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.39 – 2.20 64.39 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.39-2.20) 100.0 (64.39-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.16 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.227 , 0.254 0.231 , 0.257	Depositor DCC
R_{free} test set	3548 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.9	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	0.93	EDS
Total number of atoms	7294	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: ADP, SO4

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	0.44	0/2374	0.75	3/3227 (0.1%)
1	B	0.44	0/2374	0.74	0/3227
1	C	0.44	0/2374	0.75	4/3227 (0.1%)
All	All	0.44	0/7122	0.74	7/9681 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	ARG	NE-CZ-NH2	9.10	124.85	120.30
1	C	111	ARG	NE-CZ-NH1	-8.53	116.04	120.30
1	A	111	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	C	124	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	C	124	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	111	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	A	124	ARG	NE-CZ-NH1	5.67	123.13	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2331	0	2387	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2331	0	2387	12	0
1	C	2331	0	2387	11	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
4	A	29	0	0	0	0
4	B	102	0	0	0	0
4	C	59	0	0	0	0
All	All	7294	0	7197	35	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 2.

All (35) 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:167:VAL:HG11	1:A:182:ALA:HB2	1.76	0.67
1:B:181:LEU:HD22	1:B:219:VAL:HG11	1.79	0.63
1:A:65:GLN:NE2	1:A:95:TYR:OH	2.33	0.60
1:A:181:LEU:HB3	1:A:182:ALA:HB3	1.87	0.57
1:B:192:ILE:HG23	1:B:204:VAL:HG23	1.88	0.56
1:C:33:THR:HG22	1:C:43:VAL:HG22	1.86	0.56
1:B:181:LEU:CD2	1:B:219:VAL:HG11	2.37	0.54
1:B:277:PRO:HB3	1:B:285:THR:HG21	1.90	0.53
1:B:53:ASP:OD1	1:B:85:ARG:HD2	2.11	0.51
1:A:33:THR:HG21	1:A:70:GLU:OE2	2.11	0.49
1:A:246:ALA:HB3	1:A:269:VAL:HG12	1.93	0.48
1:C:111:ARG:HD2	1:C:115:ASP:OD2	2.14	0.48
1:A:160:VAL:HG12	1:A:162:LEU:HD13	1.96	0.48
1:C:160:VAL:O	1:C:161:ASP:HB3	2.15	0.47
1:B:115:ASP:O	1:B:119:THR:HG23	2.13	0.47
1:A:33:THR:HG22	1:A:43:VAL:HG22	1.97	0.47
1:C:118:GLN:HE22	1:C:140:LYS:H	1.63	0.47
1:C:61:VAL:O	1:C:67:HIS:HD2	1.99	0.46
1:B:118:GLN:HE22	1:B:140:LYS:H	1.64	0.45
1:A:79:LYS:HE3	1:A:86:VAL:HG13	1.99	0.44
1:C:11:GLN:NE2	1:C:33:THR:OG1	2.49	0.44
1:A:178:ALA:O	1:A:182:ALA:HB1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:VAL:HG13	1:B:182:ALA:HB2	2.00	0.43
1:A:61:VAL:O	1:A:67:HIS:HD2	2.02	0.43
1:C:277:PRO:CB	1:C:285:THR:HG21	2.49	0.42
1:B:277:PRO:CB	1:B:285:THR:HG21	2.49	0.42
1:C:193:ASP:O	1:C:205:ARG:NE	2.53	0.42
1:A:179:SER:C	1:A:182:ALA:O	2.59	0.42
1:B:271:ALA:O	1:B:285:THR:HA	2.21	0.41
1:B:167:VAL:CG1	1:B:182:ALA:HB2	2.51	0.41
1:B:248:ALA:O	1:B:271:ALA:HA	2.20	0.41
1:C:248:ALA:O	1:C:271:ALA:HA	2.21	0.41
1:C:196:ARG:O	1:C:197:VAL:C	2.59	0.41
1:C:160:VAL:O	1:C:161:ASP:CB	2.68	0.40
1:A:45:TYR:CG	1:A:49:LEU:HD11	2.56	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	305/307 (99%)	277 (91%)	26 (8%)	2 (1%)	22	22
1	B	305/307 (99%)	293 (96%)	11 (4%)	1 (0%)	41	46
1	C	305/307 (99%)	289 (95%)	12 (4%)	4 (1%)	12	9
All	All	915/921 (99%)	859 (94%)	49 (5%)	7 (1%)	19	19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	VAL
1	C	197	VAL
1	B	212	GLU
1	C	199	ASP

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Mol	Chain	Res	Type
1	C	161	ASP
1	A	281	PRO
1	C	170	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	247/247 (100%)	225 (91%)	22 (9%)	9	9
1	B	247/247 (100%)	225 (91%)	22 (9%)	9	9
1	C	247/247 (100%)	223 (90%)	24 (10%)	8	7
All	All	741/741 (100%)	673 (91%)	68 (9%)	9	9

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	49	LEU
1	A	68	LEU
1	A	86	VAL
1	A	111	ARG
1	A	116	LEU
1	A	117	LEU
1	A	126	LEU
1	A	146	LEU
1	A	183	ARG
1	A	189	LEU
1	A	192	ILE
1	A	194	LYS
1	A	196	ARG
1	A	202	VAL
1	A	205	ARG
1	A	215	THR
1	A	229	LEU
1	A	242	LYS

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Mol	Chain	Res	Type
1	A	258	LEU
1	A	284	ARG
1	A	286	LEU
1	B	5	LEU
1	B	6	LEU
1	B	28	LEU
1	B	49	LEU
1	B	68	LEU
1	B	79	LYS
1	B	86	VAL
1	B	117	LEU
1	B	119	THR
1	B	140	LYS
1	B	143	VAL
1	B	159	ARG
1	B	163	GLU
1	B	167	VAL
1	B	217	LEU
1	B	229	LEU
1	B	238	GLN
1	B	282	LYS
1	B	284	ARG
1	B	285	THR
1	B	286	LEU
1	B	308	LEU
1	C	4	PRO
1	C	6	LEU
1	C	43	VAL
1	C	54	VAL
1	C	68	LEU
1	C	111	ARG
1	C	116	LEU
1	C	117	LEU
1	C	119	THR
1	C	126	LEU
1	C	167	VAL
1	C	176	LYS
1	C	192	ILE
1	C	195	GLU
1	C	196	ARG
1	C	199	ASP
1	C	205	ARG

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Mol	Chain	Res	Type
1	C	219	VAL
1	C	229	LEU
1	C	258	LEU
1	C	284	ARG
1	C	285	THR
1	C	286	LEU
1	C	308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	67	HIS
1	A	118	GLN
1	B	67	HIS
1	B	118	GLN
1	B	136	HIS
1	B	238	GLN
1	B	300	HIS
1	C	11	GLN
1	C	67	HIS
1	C	118	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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	$\# Z > 2$
3	SO4	C	402	-	4,4,4	0.25	0	6,6,6	0.53	0
3	SO4	A	402	-	4,4,4	0.30	0	6,6,6	0.61	0
2	ADP	B	401	-	24,29,29	1.07	3 (12%)	29,45,45	1.32	2 (6%)
3	SO4	B	403	-	4,4,4	0.34	0	6,6,6	0.29	0
2	ADP	A	401	-	24,29,29	0.97	2 (8%)	29,45,45	1.31	3 (10%)
3	SO4	A	403	-	4,4,4	0.33	0	6,6,6	0.30	0
3	SO4	B	402	-	4,4,4	0.29	0	6,6,6	0.28	0
3	SO4	C	403	-	4,4,4	0.34	0	6,6,6	0.30	0
2	ADP	C	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.33	4 (13%)

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	ADP	A	401	-	-	5/12/32/32	0/3/3/3
2	ADP	B	401	-	-	6/12/32/32	0/3/3/3
2	ADP	C	401	-	-	3/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ADP	C2-N3	2.68	1.36	1.32
2	A	401	ADP	C5-C4	2.42	1.47	1.40
2	C	401	ADP	C5-C4	2.33	1.47	1.40
2	A	401	ADP	C2-N3	2.26	1.35	1.32
2	B	401	ADP	C5-C4	2.25	1.46	1.40
2	B	401	ADP	O4'-C1'	2.17	1.44	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ADP	N3-C2-N1	-3.80	122.75	128.68
2	C	401	ADP	N3-C2-N1	-3.66	122.95	128.68
2	B	401	ADP	N3-C2-N1	-3.65	122.97	128.68
2	B	401	ADP	PA-O3A-PB	-3.32	121.42	132.83
2	A	401	ADP	PA-O3A-PB	-2.90	122.89	132.83
2	C	401	ADP	C3'-C2'-C1'	2.38	104.56	100.98
2	C	401	ADP	C4-C5-N7	-2.19	107.11	109.40
2	C	401	ADP	PA-O3A-PB	-2.16	125.43	132.83
2	A	401	ADP	C4-C5-N7	-2.12	107.19	109.40

There are no chirality outliers.

All (14) torsion outliers are listed below:

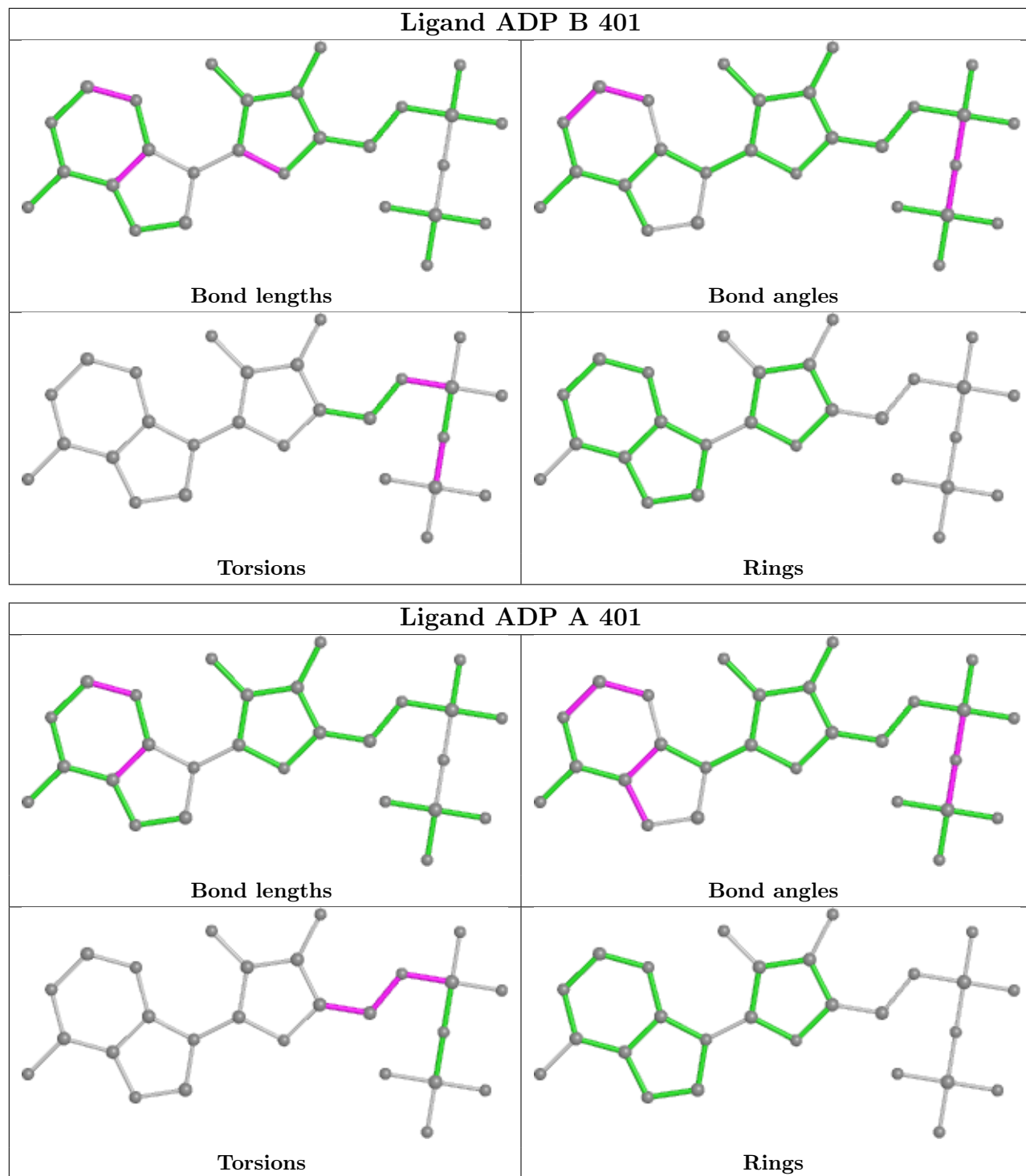
Mol	Chain	Res	Type	Atoms
2	A	401	ADP	C5'-O5'-PA-O2A
2	B	401	ADP	PA-O3A-PB-O2B
2	B	401	ADP	C5'-O5'-PA-O2A
2	B	401	ADP	PA-O3A-PB-O3B
2	B	401	ADP	C5'-O5'-PA-O3A
2	C	401	ADP	C4'-C5'-O5'-PA
2	A	401	ADP	C3'-C4'-C5'-O5'
2	A	401	ADP	C4'-C5'-O5'-PA
2	C	401	ADP	C3'-C4'-C5'-O5'
2	B	401	ADP	PA-O3A-PB-O1B
2	A	401	ADP	C5'-O5'-PA-O3A
2	A	401	ADP	C5'-O5'-PA-O1A
2	B	401	ADP	C5'-O5'-PA-O1A
2	C	401	ADP	C5'-O5'-PA-O1A

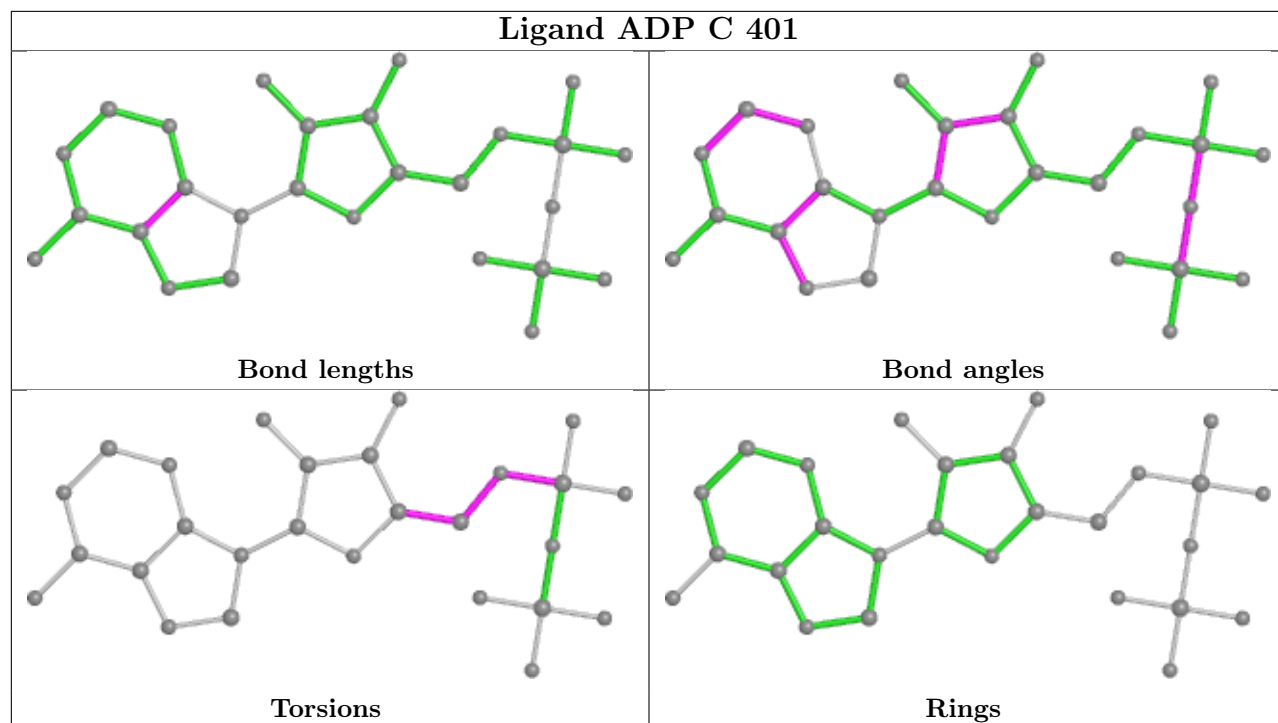
There are no ring outliers.

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

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	307/307 (100%)	1.58	86 (28%) 0 0	22, 52, 139, 170	0
1	B	307/307 (100%)	0.01	13 (4%) 36 34	12, 29, 65, 93	0
1	C	307/307 (100%)	0.50	27 (8%) 10 8	15, 33, 97, 167	0
All	All	921/921 (100%)	0.70	126 (13%) 3 2	12, 37, 113, 170	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	198	SER	14.8
1	C	199	ASP	13.7
1	A	202	VAL	12.7
1	A	197	VAL	12.3
1	A	204	VAL	11.5
1	A	198	SER	11.1
1	A	213	GLY	11.1
1	C	202	VAL	10.5
1	A	200	THR	10.0
1	C	197	VAL	9.9
1	A	201	GLU	9.7
1	C	200	THR	9.2
1	A	310	THR	9.2
1	A	191	PHE	8.9
1	A	193	ASP	8.6
1	C	195	GLU	8.4
1	A	199	ASP	8.1
1	A	208	VAL	7.9
1	A	211	VAL	7.7
1	C	203	ARG	7.5
1	A	206	MET	7.3
1	C	204	VAL	6.7
1	C	201	GLU	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	183	ARG	6.4
1	C	194	LYS	6.2
1	A	309	PHE	6.1
1	A	238	GLN	6.0
1	A	205	ARG	5.9
1	A	195	GLU	5.8
1	A	192	ILE	5.8
1	A	161	ASP	5.8
1	A	236	LEU	5.8
1	A	203	ARG	5.7
1	C	206	MET	5.6
1	A	207	LEU	5.5
1	A	169	ALA	5.3
1	A	194	LYS	5.3
1	A	245	TYR	5.1
1	A	182	ALA	5.0
1	A	234	GLU	4.9
1	A	190	ALA	4.8
1	A	163	GLU	4.8
1	C	196	ARG	4.8
1	B	201	GLU	4.7
1	A	166	VAL	4.6
1	A	189	LEU	4.6
1	A	162	LEU	4.4
1	A	210	GLU	4.4
1	A	215	THR	4.4
1	A	216	ALA	4.3
1	A	212	GLU	4.2
1	A	214	LYS	4.1
1	C	310	THR	4.1
1	A	171	ASP	4.1
1	C	210	GLU	4.1
1	A	240	GLY	4.1
1	C	171	ASP	3.9
1	A	172	ALA	3.9
1	A	174	ASP	3.9
1	B	212	GLU	3.9
1	A	164	ASN	3.9
1	A	157	ALA	3.9
1	B	210	GLU	3.9
1	A	158	THR	3.8
1	B	310	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	167	VAL	3.7
1	A	155	TYR	3.7
1	C	207	LEU	3.7
1	C	205	ARG	3.6
1	A	209	GLY	3.6
1	A	168	VAL	3.5
1	A	307	SER	3.4
1	A	165	ALA	3.3
1	A	218	ILE	3.2
1	A	265	PRO	3.2
1	A	160	VAL	3.2
1	A	283	LEU	3.2
1	A	196	ARG	3.1
1	A	267	LYS	3.1
1	C	213	GLY	3.1
1	A	284	ARG	3.1
1	A	244	VAL	3.0
1	A	282	LYS	3.0
1	A	186	GLY	3.0
1	A	308	LEU	3.0
1	A	156	PHE	2.9
1	A	239	ALA	2.9
1	A	173	GLY	2.8
1	A	266	VAL	2.8
1	C	193	ASP	2.8
1	A	263	LYS	2.7
1	B	238	GLN	2.7
1	A	179	SER	2.7
1	A	185	LEU	2.7
1	A	242	LYS	2.6
1	A	241	ALA	2.6
1	A	175	LEU	2.5
1	B	200	THR	2.5
1	A	187	LEU	2.5
1	C	212	GLU	2.5
1	B	205	ARG	2.5
1	B	308	LEU	2.5
1	C	238	GLN	2.5
1	A	188	PRO	2.4
1	A	176	LYS	2.4
1	A	217	LEU	2.4
1	A	4	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	211	VAL	2.3
1	C	159	ARG	2.3
1	C	163	GLU	2.3
1	C	170	PRO	2.3
1	A	269	VAL	2.3
1	B	202	VAL	2.3
1	A	159	ARG	2.2
1	A	231	GLU	2.2
1	B	233	VAL	2.2
1	B	279	GLU	2.2
1	A	152	ILE	2.2
1	A	259	ASP	2.1
1	C	231	GLU	2.1
1	C	174	ASP	2.1
1	B	173	GLY	2.1
1	A	229	LEU	2.1
1	A	280	GLY	2.0
1	B	204	VAL	2.0
1	A	261	ILE	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, 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(\AA^2)	Q<0.9
2	ADP	A	401	27/27	0.87	0.14	40,54,88,89	0
2	ADP	C	401	27/27	0.90	0.13	36,53,79,81	0
3	SO4	A	403	5/5	0.92	0.16	58,58,60,65	0
2	ADP	B	401	27/27	0.93	0.11	24,35,72,75	0

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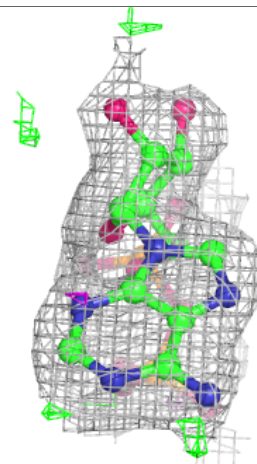
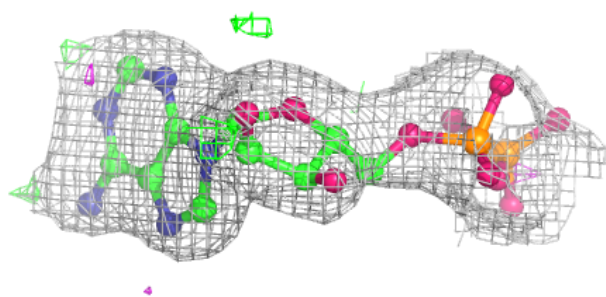
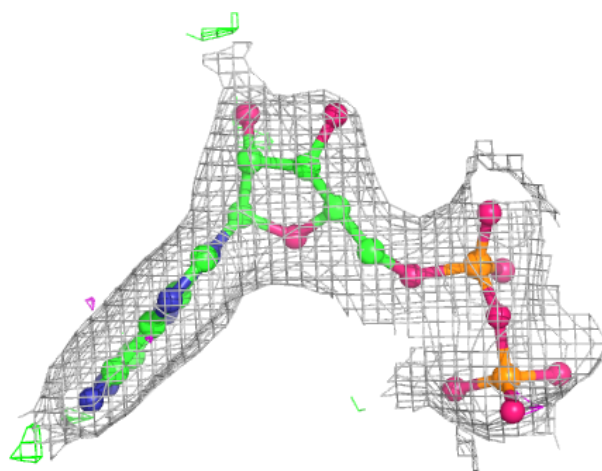
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	402	5/5	0.96	0.13	32,33,36,40	0
3	SO4	C	403	5/5	0.97	0.09	39,39,41,41	0
3	SO4	B	403	5/5	0.98	0.11	31,31,34,35	0
3	SO4	B	402	5/5	0.98	0.13	37,38,39,39	0
3	SO4	C	402	5/5	0.99	0.10	21,21,22,22	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.

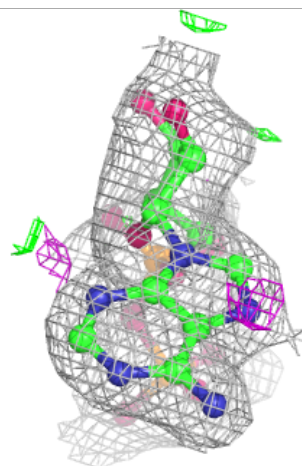
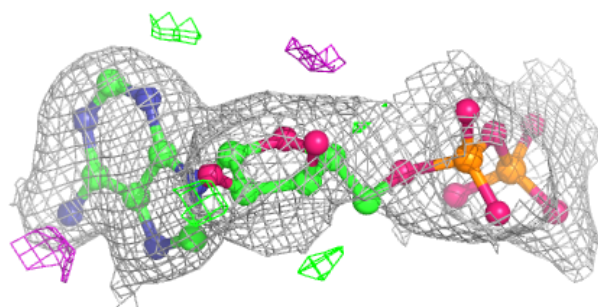
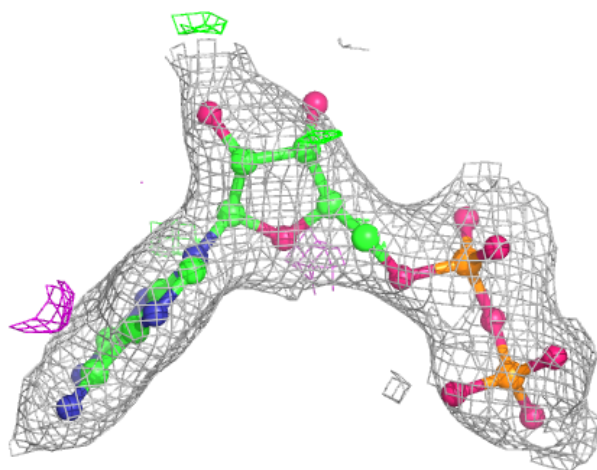
Electron density around ADP A 401:

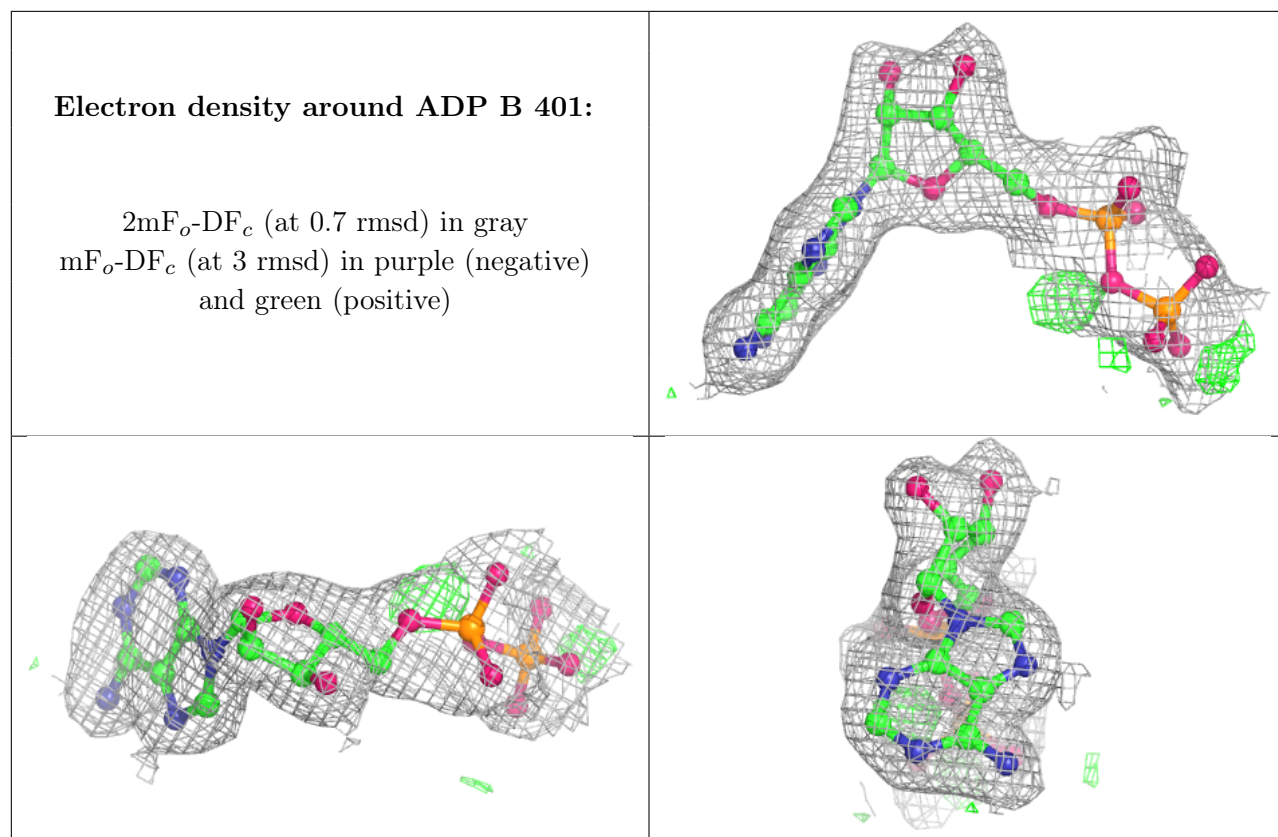
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP C 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.