



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2020 – 12:10 PM JST

PDB ID : 7C1Y
Title : Pseudouridine and ADP bound structure of Pseudouridine kinase (PUKI) from Arabidopsis thaliana
Authors : Kim, S.H.; Rhee, S.
Deposited on : 2020-05-06
Resolution : 2.08 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 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 : 2.14.6
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) : 2.14.6

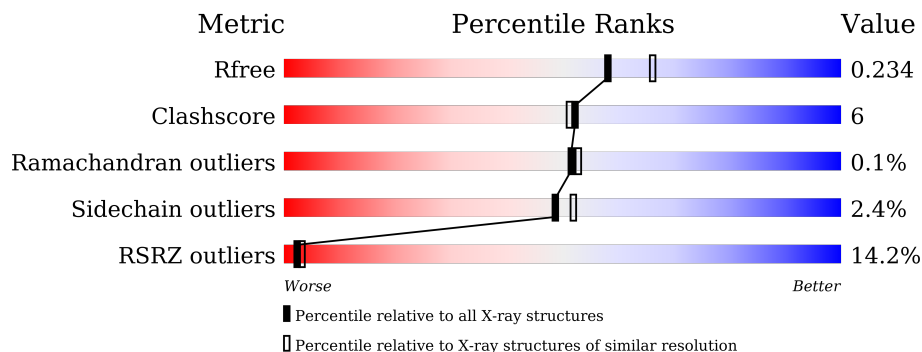
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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 on 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	378	
1	B	378	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5380 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.

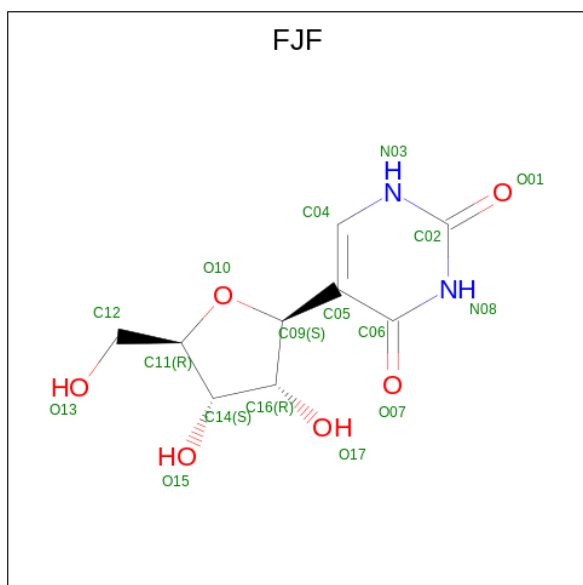
- Molecule 1 is a protein called PfkB-like carbohydrate kinase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	356	Total 2638	C 1695	N 435	O 493	S 15	0	0	0
1	B	347	Total 2569	C 1648	N 424	O 482	S 15	0	0	0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

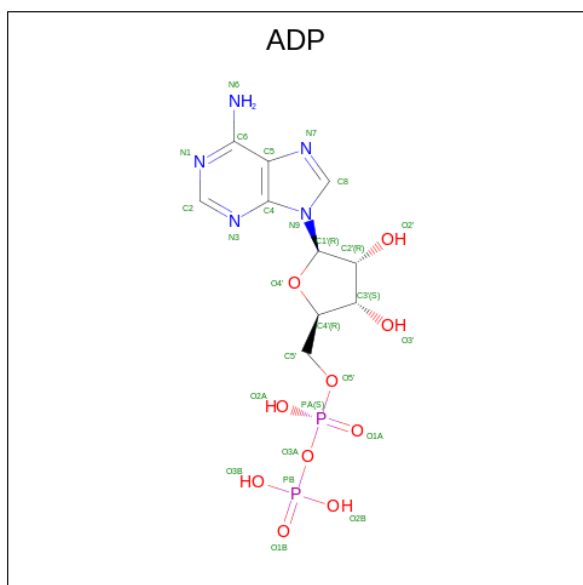
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Na 1	0	0
2	A	1	Total 1	Na 1	0	0

- Molecule 3 is 5-[(2 {S},3 {R},4 {S},5 {R})-5-(hydroxymethyl)-3,4-bis(oxidanyl)oxolan-2-yl]-1 {H}-pyrimidine-2,4-dione (three-letter code: FJF) (formula: C₉H₁₂N₂O₆) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	2	6		
3	B	1	Total	C	N	O	0	0
			17	9	2	6		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

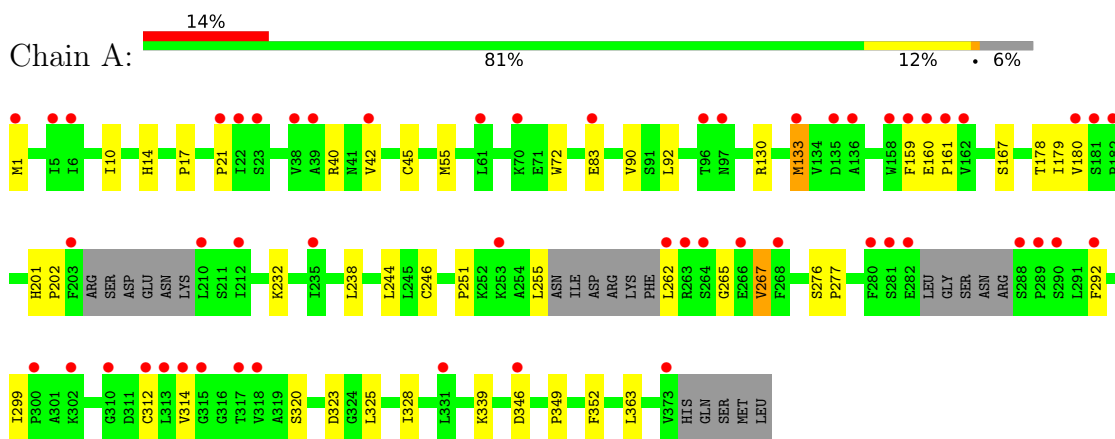
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total	O	0	0
			53	53		
5	B	30	Total	O	0	0
			30	30		

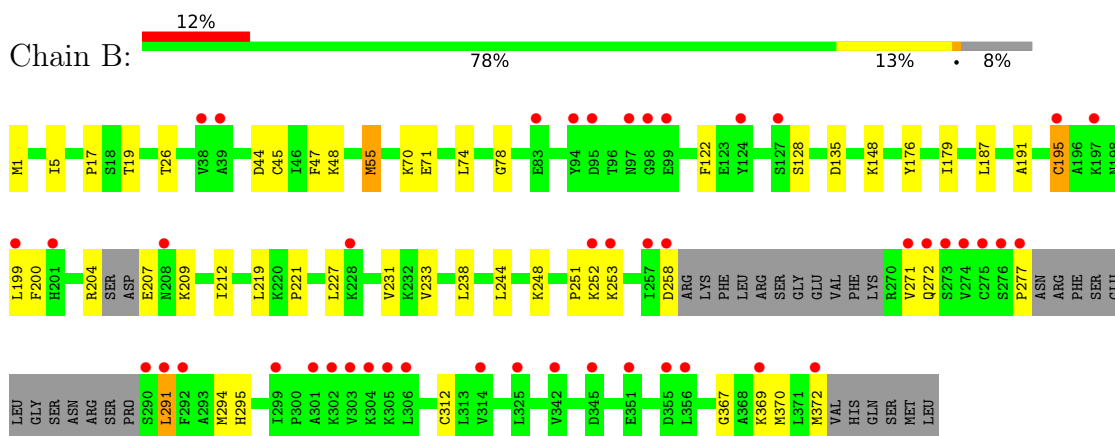
3 Residue-property plots [i](#)

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: PfkB-like carbohydrate kinase family protein



- Molecule 1: PfkB-like carbohydrate kinase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.33Å 48.86Å 91.79Å 90.00° 107.52° 90.00°	Depositor
Resolution (Å)	30.62 – 2.08 30.62 – 2.08	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.62-2.08) 98.5 (30.62-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.08Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.190 , 0.235 0.193 , 0.234	Depositor DCC
R_{free} test set	2000 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtrriage
Anisotropy	0.382	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5380	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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: NA, FJF, ADP

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	0.43	0/2682	0.59	0/3642
1	B	0.38	0/2610	0.57	2/3545 (0.1%)
All	All	0.40	0/5292	0.58	2/7187 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	199	LEU	CA-CB-CG	5.11	127.05	115.30

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	2638	0	2739	31	0
1	B	2569	0	2669	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	17	0	0	1	0
3	B	17	0	0	0	0
4	A	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	12	1	0
5	A	53	0	0	2	0
5	B	30	0	0	1	0
All	All	5380	0	5432	59	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 6.

All (59) 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:40:ARG:HA	1:A:55:MET:HE1	1.59	0.85
1:A:42:VAL:HG21	1:A:133:MET:HE3	1.68	0.76
4:A:403:ADP:O1B	5:A:501:HOH:O	2.08	0.70
1:B:1:MET:HB2	1:B:128:SER:O	1.94	0.67
1:A:10:ILE:HG21	1:A:90:VAL:HG23	1.76	0.67
1:B:187:LEU:HD23	1:B:219:LEU:HD22	1.79	0.64
1:A:1:MET:N	5:A:504:HOH:O	2.29	0.64
1:B:148:LYS:NZ	1:B:176:TYR:OH	2.29	0.63
1:B:70:LYS:HG3	1:B:71:GLU:HG2	1.82	0.61
1:A:17:PRO:HG3	1:A:21:PRO:HG3	1.81	0.61
1:A:14:HIS:CD2	1:A:92:LEU:HD12	2.36	0.61
1:A:178:THR:HG23	1:A:232:LYS:HD2	1.82	0.60
4:B:403:ADP:O3B	5:B:501:HOH:O	2.16	0.60
1:B:238:LEU:HD11	1:B:244:LEU:HG	1.86	0.57
1:A:55:MET:HE2	1:A:72:TRP:HH2	1.69	0.57
1:B:200:PHE:HE1	1:B:221:PRO:HB2	1.70	0.56
1:A:251:PRO:HG2	1:A:328:ILE:HD11	1.88	0.56
1:A:320:SER:HB3	1:A:325:LEU:HD12	1.89	0.55
1:A:251:PRO:HG3	1:A:292:PHE:CE2	2.41	0.54
1:A:299:ILE:HB	1:A:339:LYS:HD2	1.88	0.53
1:A:133:MET:HE3	1:A:314:VAL:HG11	1.91	0.52
1:B:5:ILE:HB	1:B:55:MET:HE2	1.89	0.52
1:B:212:ILE:HD13	1:B:295:HIS:CE1	2.46	0.51
1:B:179:ILE:HG12	1:B:233:VAL:HB	1.94	0.50
1:B:5:ILE:HB	1:B:55:MET:CE	2.42	0.49
1:A:42:VAL:HG21	1:A:133:MET:CE	2.38	0.49
1:B:251:PRO:O	1:B:253:LYS:N	2.45	0.48
1:B:78:GLY:HA2	1:B:122:PHE:CZ	2.48	0.48
1:A:238:LEU:HD11	1:A:244:LEU:HG	1.95	0.47
1:B:294:MET:HG2	1:B:370:MET:SD	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:HG13	1:A:323:ASP:OD2	2.15	0.47
1:A:160:GLU:HA	1:A:161:PRO:HD3	1.65	0.47
1:B:44:ASP:OD1	1:B:48:LYS:NZ	2.38	0.46
1:A:1:MET:HG3	1:A:130:ARG:NE	2.31	0.45
1:A:201:HIS:HA	1:A:202:PRO:HD3	1.79	0.44
1:A:55:MET:CE	1:A:72:TRP:HH2	2.28	0.44
1:B:227:LEU:HD23	1:B:231:VAL:O	2.18	0.44
1:A:40:ARG:HA	1:A:55:MET:CE	2.37	0.44
1:A:349:PRO:HG2	1:A:352:PHE:CE1	2.53	0.44
1:B:191:ALA:O	1:B:195:CYS:HB2	2.18	0.43
1:B:272:GLN:OE1	1:B:277:PRO:HD3	2.18	0.43
1:A:299:ILE:HD11	1:A:363:LEU:HB3	2.00	0.43
1:B:291:LEU:HD23	1:B:372:MET:SD	2.59	0.43
3:A:402:FJF:N03	1:B:26:THR:OG1	2.51	0.43
1:A:133:MET:CE	1:A:314:VAL:HG11	2.49	0.43
1:A:179:ILE:HD11	1:A:255:LEU:HD11	2.01	0.42
1:B:367:GLY:O	1:B:369:LYS:HE2	2.20	0.42
1:A:328:ILE:N	1:A:328:ILE:HD12	2.34	0.42
1:A:276:SER:HA	1:A:277:PRO:HD3	1.93	0.42
1:B:209:LYS:HA	1:B:209:LYS:HD3	1.69	0.42
1:B:47:PHE:CD1	1:B:74:LEU:HD21	2.55	0.42
1:A:265:GLY:H	1:A:323:ASP:CG	2.24	0.41
1:B:204:ARG:C	1:B:207:GLU:HA	2.40	0.41
1:B:248:LYS:HB2	1:B:248:LYS:HE3	1.65	0.41
1:B:55:MET:HB2	1:B:55:MET:HE3	1.95	0.41
1:A:159:PHE:HB3	1:A:180:VAL:HG12	2.02	0.41
1:A:246:CYS:HA	1:A:292:PHE:O	2.20	0.41
1:A:161:PRO:HB3	1:A:167:SER:HB2	2.03	0.41
1:B:17:PRO:HB2	1:B:19:THR:O	2.21	0.41

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	348/378 (92%)	339 (97%)	9 (3%)	0	100	100
1	B	339/378 (90%)	334 (98%)	4 (1%)	1 (0%)	41	39
All	All	687/756 (91%)	673 (98%)	13 (2%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	252	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	292/314 (93%)	285 (98%)	7 (2%)	49	52
1	B	284/314 (90%)	277 (98%)	7 (2%)	47	50
All	All	576/628 (92%)	562 (98%)	14 (2%)	49	52

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	CYS
1	A	83	GLU
1	A	133	MET
1	A	262	LEU
1	A	267	VAL
1	A	312	CYS
1	A	346	ASP
1	B	45	CYS
1	B	55	MET
1	B	195	CYS
1	B	258	ASP
1	B	271	VAL
1	B	291	LEU
1	B	312	CYS

Some 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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
3	FJF	A	402	-	17,18,18	4.84	12 (70%)	20,26,26	4.04	7 (35%)
4	ADP	B	403	-	24,29,29	1.02	2 (8%)	29,45,45	1.22	3 (10%)
4	ADP	A	403	-	24,29,29	0.92	1 (4%)	29,45,45	1.38	3 (10%)
3	FJF	B	402	-	17,18,18	4.94	11 (64%)	20,26,26	3.69	7 (35%)

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	FJF	A	402	-	-	0/6/22/22	0/2/2/2
4	ADP	B	403	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	403	-	-	4/12/32/32	0/3/3/3
3	FJF	B	402	-	-	3/6/22/22	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	FJF	O10-C09	-11.69	1.27	1.44
3	A	402	FJF	O10-C09	-11.12	1.28	1.44
3	B	402	FJF	C14-C11	-9.49	1.28	1.53
3	A	402	FJF	C14-C11	-9.34	1.29	1.53
3	A	402	FJF	O10-C11	7.29	1.61	1.45
3	B	402	FJF	O10-C11	7.20	1.61	1.45
3	B	402	FJF	C04-C05	5.89	1.47	1.38
3	A	402	FJF	C04-C05	5.20	1.46	1.38
3	A	402	FJF	C06-N08	5.12	1.41	1.33
3	B	402	FJF	C06-N08	4.97	1.41	1.33
3	A	402	FJF	O15-C14	4.18	1.52	1.43
3	A	402	FJF	C02-N03	4.09	1.46	1.38
3	B	402	FJF	O15-C14	4.06	1.52	1.43
3	B	402	FJF	C02-N03	4.06	1.46	1.38
3	A	402	FJF	C04-N03	3.92	1.42	1.34
3	B	402	FJF	C02-N08	3.88	1.45	1.38
3	B	402	FJF	C04-N03	3.62	1.42	1.34
3	A	402	FJF	C02-N08	3.21	1.44	1.38
3	A	402	FJF	C16-C09	2.77	1.57	1.54
3	A	402	FJF	C06-C05	2.68	1.47	1.41
3	B	402	FJF	O17-C16	-2.55	1.37	1.43
3	B	402	FJF	C06-C05	2.55	1.46	1.41
4	B	403	ADP	C5-C4	2.52	1.47	1.40
4	A	403	ADP	C5-C4	2.39	1.47	1.40
4	B	403	ADP	O4'-C1'	2.27	1.44	1.41
3	A	402	FJF	O17-C16	-2.26	1.37	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	FJF	N03-C02-N08	-12.54	118.46	128.43
3	B	402	FJF	N03-C02-N08	-10.59	120.01	128.43
3	A	402	FJF	C11-O10-C09	-8.43	99.02	109.42
3	B	402	FJF	C11-O10-C09	-7.54	100.12	109.42
3	A	402	FJF	C06-N08-C02	7.11	121.14	115.14
3	B	402	FJF	C06-N08-C02	6.10	120.30	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	FJF	C05-C06-N08	-4.38	119.72	125.36
3	B	402	FJF	C05-C04-N03	-4.37	119.06	124.44
4	A	403	ADP	N3-C2-N1	-3.53	123.15	128.68
3	A	402	FJF	C04-N03-C02	3.50	121.13	115.36
3	A	402	FJF	C05-C06-N08	-3.49	120.87	125.36
3	A	402	FJF	C05-C04-N03	-3.35	120.33	124.44
4	B	403	ADP	N3-C2-N1	-3.20	123.67	128.68
3	B	402	FJF	C04-N03-C02	3.18	120.61	115.36
4	A	403	ADP	O2'-C2'-C3'	-2.79	102.80	111.82
4	B	403	ADP	C3'-C2'-C1'	2.61	104.90	100.98
3	B	402	FJF	C06-C05-C09	-2.49	116.42	121.12
3	A	402	FJF	O10-C09-C16	-2.46	100.67	104.66
4	A	403	ADP	C2-N1-C6	2.22	122.56	118.75
4	B	403	ADP	C4-C5-N7	-2.09	107.23	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	ADP	C5'-O5'-PA-O1A
4	A	403	ADP	C5'-O5'-PA-O3A
3	B	402	FJF	C04-C05-C09-O10
3	B	402	FJF	C04-C05-C09-C16
3	B	402	FJF	C06-C05-C09-O10
4	A	403	ADP	PB-O3A-PA-O2A
4	A	403	ADP	C5'-O5'-PA-O2A

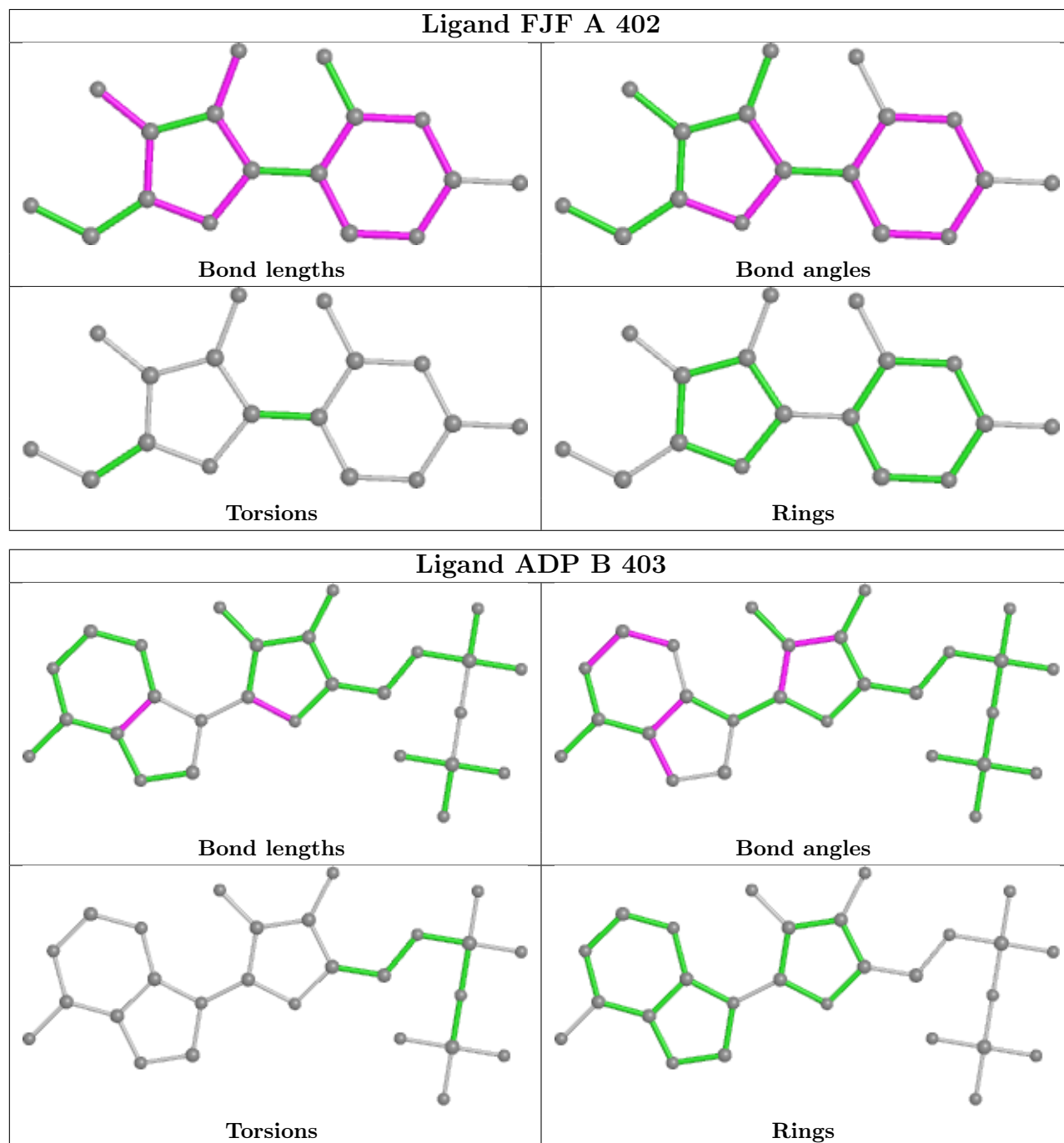
There are no ring outliers.

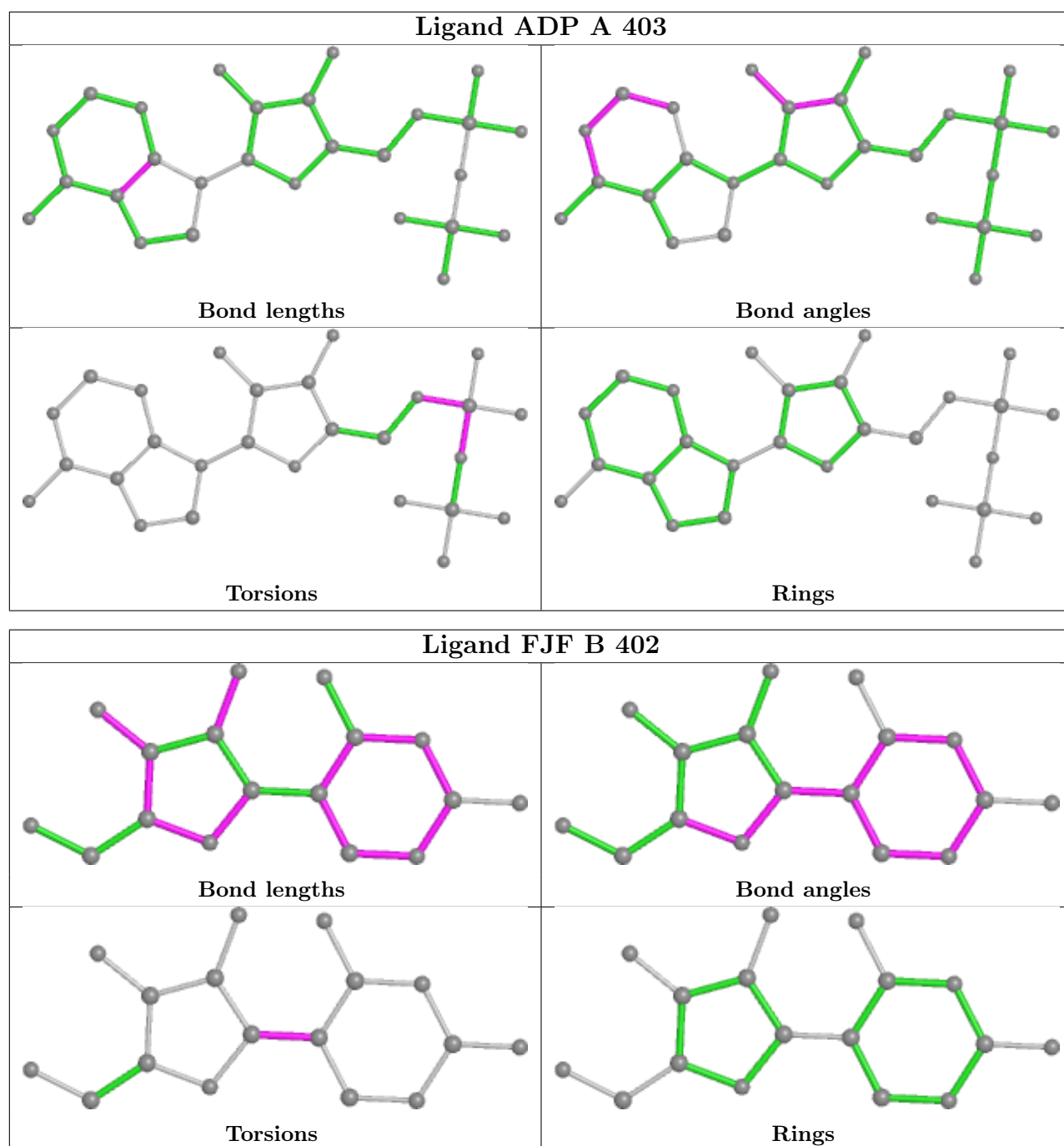
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	FJF	1	0
4	B	403	ADP	1	0
4	A	403	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	356/378 (94%)	0.64	54 (15%) 2 2	30, 45, 76, 101	0
1	B	347/378 (91%)	0.67	46 (13%) 3 4	35, 56, 88, 102	0
All	All	703/756 (92%)	0.66	100 (14%) 2 3	30, 51, 84, 102	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	LEU	6.9
1	A	253	LYS	5.9
1	B	273	SER	5.8
1	B	302	LYS	5.2
1	A	268	PHE	5.1
1	B	97	ASN	5.0
1	A	21	PRO	5.0
1	B	306	LEU	4.9
1	B	301	ALA	4.8
1	A	22	ILE	4.4
1	A	314	VAL	4.4
1	B	199	LEU	4.3
1	A	96	THR	4.3
1	A	302	LYS	4.2
1	B	252	LYS	4.2
1	B	292	PHE	4.2
1	A	1	MET	4.2
1	A	203	PHE	4.1
1	A	38	VAL	4.1
1	B	257	ILE	4.0
1	A	23	SER	4.0
1	B	342	VAL	3.8
1	B	291	LEU	3.7
1	B	372	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	282	GLU	3.7
1	B	304	LYS	3.5
1	B	39	ALA	3.5
1	B	303	VAL	3.5
1	A	162	VAL	3.3
1	B	274	VAL	3.3
1	A	161	PRO	3.3
1	A	300	PRO	3.3
1	B	124	TYR	3.2
1	A	42	VAL	3.2
1	A	346	ASP	3.1
1	A	136	ALA	3.1
1	A	313	LEU	3.1
1	B	276	SER	3.1
1	B	208	ASN	3.1
1	B	345	ASP	3.0
1	A	263	ARG	3.0
1	A	210	LEU	3.0
1	A	5	ILE	3.0
1	B	201	HIS	3.0
1	B	299	ILE	3.0
1	A	159	PHE	2.9
1	A	373	VAL	2.9
1	A	292	PHE	2.8
1	A	39	ALA	2.8
1	A	212	ILE	2.8
1	B	195	CYS	2.7
1	A	83	GLU	2.7
1	B	351	GLU	2.7
1	B	355	ASP	2.7
1	B	98	GLY	2.7
1	A	158	TRP	2.7
1	B	272	GLN	2.7
1	B	253	LYS	2.6
1	B	277	PRO	2.6
1	B	275	CYS	2.6
1	B	369	LYS	2.6
1	B	290	SER	2.6
1	A	317	THR	2.5
1	A	6	ILE	2.5
1	A	70	LYS	2.5
1	A	318	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	271	VAL	2.4
1	B	197	LYS	2.4
1	A	312	CYS	2.4
1	A	310	GLY	2.4
1	A	235	ILE	2.4
1	A	331	LEU	2.3
1	B	305	LYS	2.3
1	B	127	SER	2.3
1	A	281	SER	2.3
1	B	228	LYS	2.3
1	B	83	GLU	2.3
1	B	356	LEU	2.3
1	B	258	ASP	2.3
1	A	290	SER	2.3
1	B	95	ASP	2.3
1	B	314	VAL	2.2
1	A	315	GLY	2.2
1	A	61	LEU	2.2
1	A	97	ASN	2.2
1	A	288	SER	2.2
1	A	289	PRO	2.2
1	A	133	MET	2.2
1	A	182	PRO	2.2
1	A	180	VAL	2.1
1	B	38	VAL	2.1
1	A	280	PHE	2.1
1	A	181	SER	2.1
1	A	160	GLU	2.0
1	A	264	SER	2.0
1	A	135	ASP	2.0
1	B	99	GLU	2.0
1	B	325	LEU	2.0
1	B	94	TYR	2.0
1	A	266	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

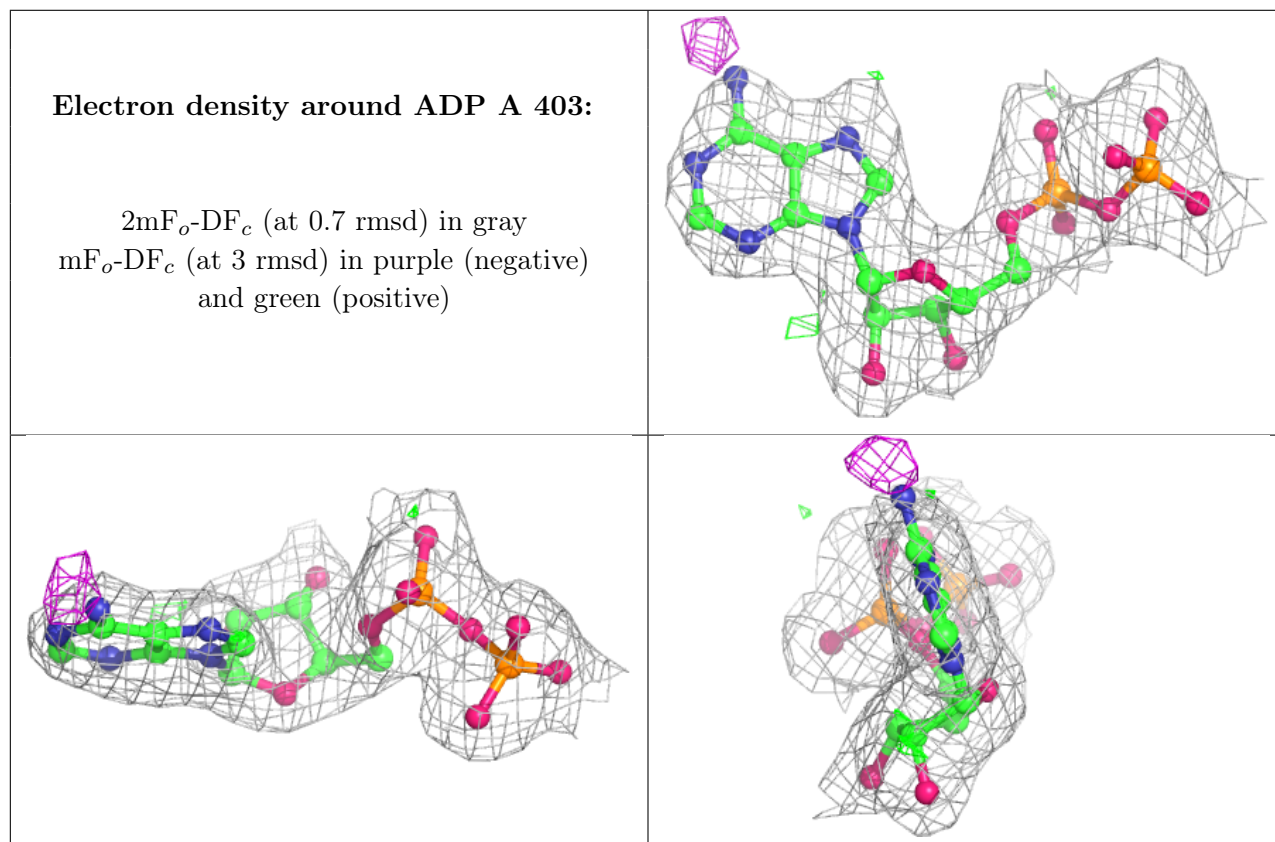
There are no monosaccharides in this entry.

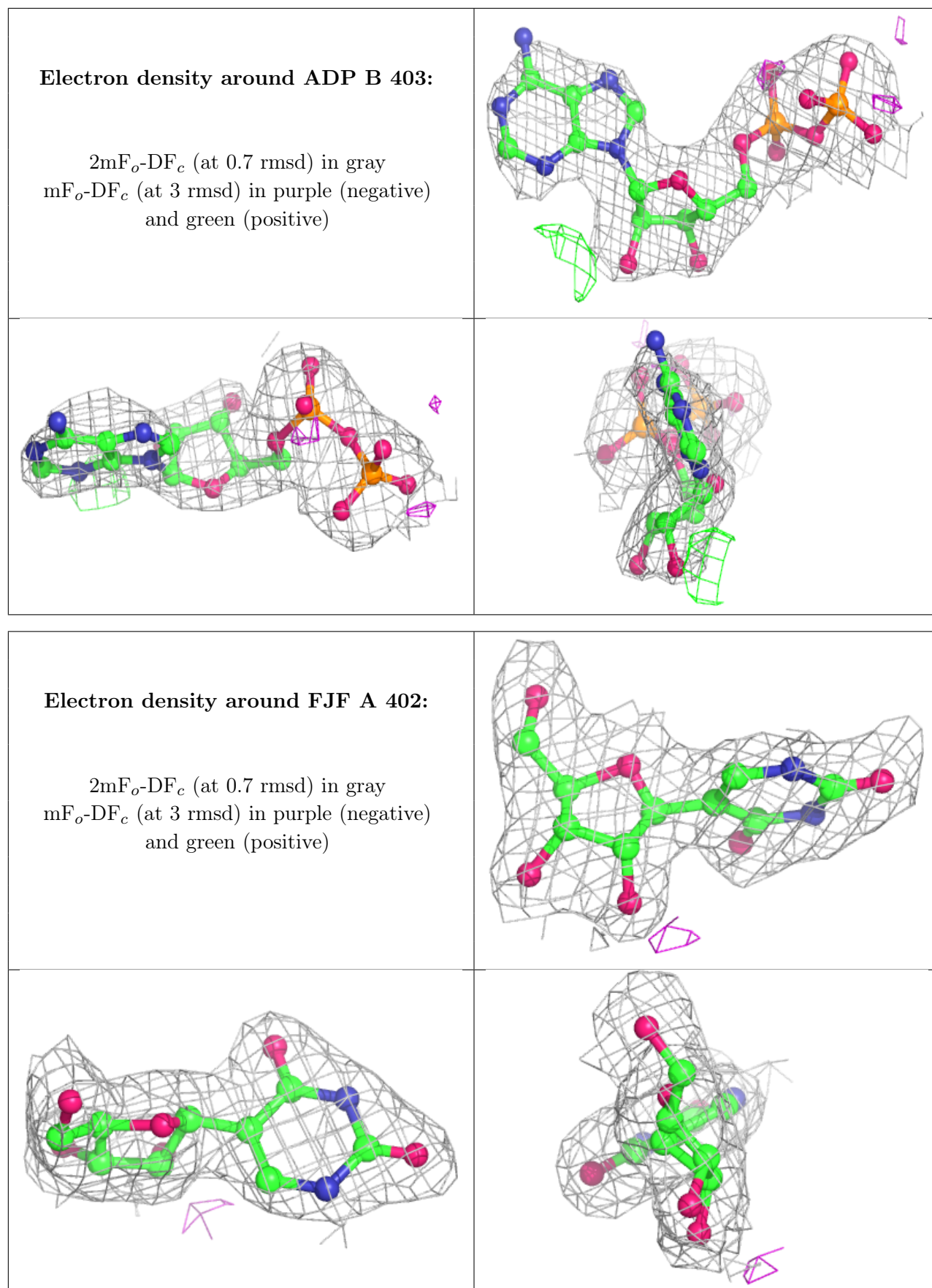
6.4 Ligands [i](#)

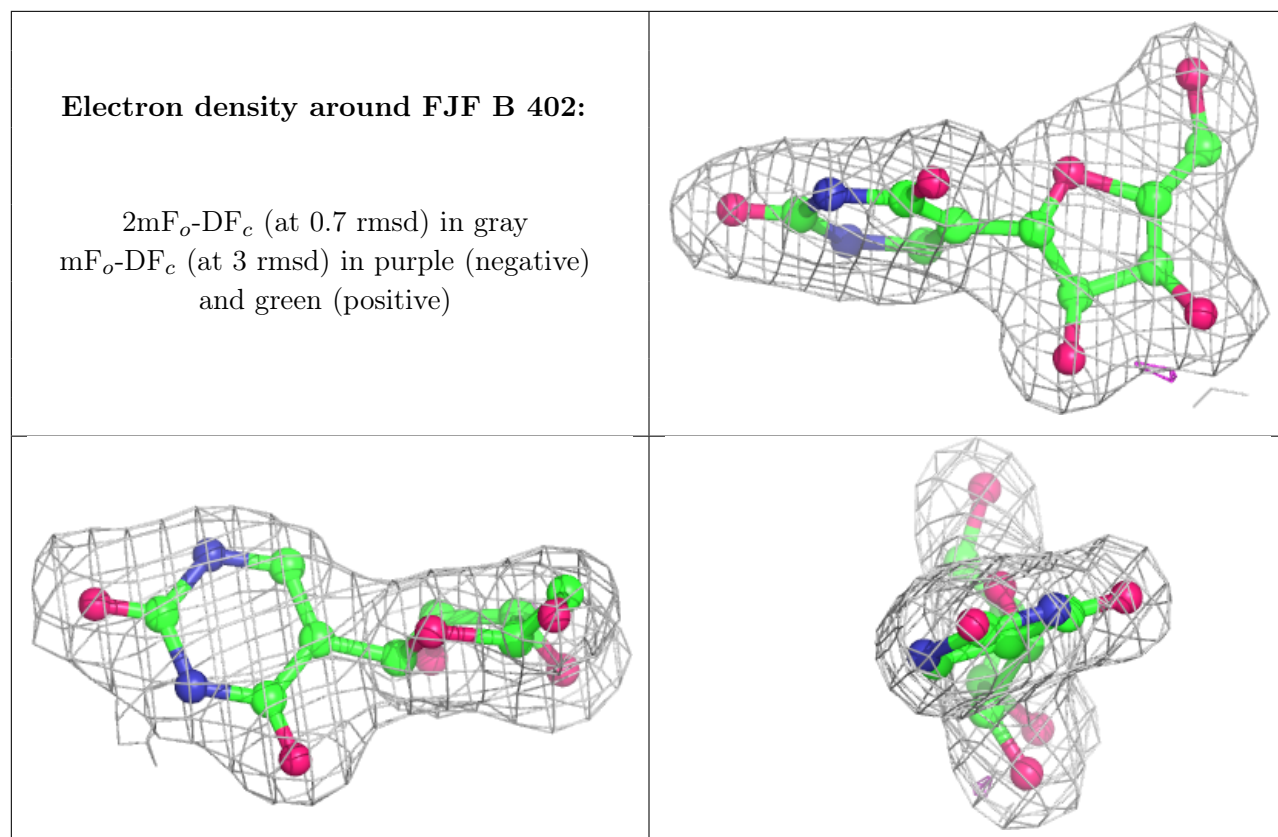
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	A	401	1/1	0.63	0.21	56,56,56,56	0
2	NA	B	401	1/1	0.89	0.36	73,73,73,73	0
4	ADP	A	403	27/27	0.92	0.15	31,47,59,65	0
4	ADP	B	403	27/27	0.92	0.15	47,68,85,86	0
3	FJF	A	402	17/17	0.96	0.23	25,31,38,41	0
3	FJF	B	402	17/17	0.96	0.18	33,40,44,45	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.