Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 07:51 pm GMT

PDB ID	:	4D79
Title	:	Crystal structure of E. coli tRNA N6-threonylcarbamoyladenosine dehydratase, TcdA, in complex with ATP at 1.768 Angstroem resolution
Authors	:	Lopez-Estepa, M.; Arda, A.; Savko, M.; Round, A.; Shepard, W.; Bruix, M.; Coll, M.; Fernandez, F.J.; Jimenez-Barbero, J.; Vega, M.C.
Deposited on	:	2014-11-21
Resolution	:	1.77 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:

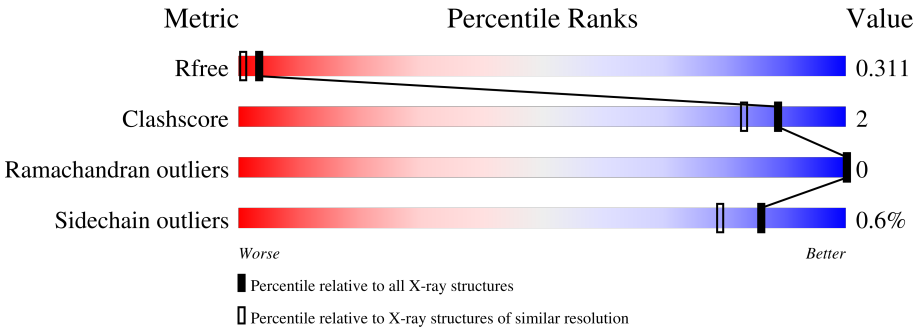
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.77 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	276	86% · 12%
1	B	276	82% 7% 11%
1	C	276	88% · 9%
1	D	276	86% · 12%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8167 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 TRNA THREONYLCARBAMOYLADENOSINE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	3	0
			1846	1161	332	341	12			
1	B	247	Total	C	N	O	S	0	3	0
			1872	1176	334	350	12			
1	C	252	Total	C	N	O	S	0	4	1
			1923	1210	348	353	12			
1	D	244	Total	C	N	O	S	0	1	0
			1843	1160	329	343	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	269	LEU	-	expression tag	UNP Q46927
A	270	GLU	-	expression tag	UNP Q46927
A	271	HIS	-	expression tag	UNP Q46927
A	272	HIS	-	expression tag	UNP Q46927
A	273	HIS	-	expression tag	UNP Q46927
A	274	HIS	-	expression tag	UNP Q46927
A	275	HIS	-	expression tag	UNP Q46927
A	276	HIS	-	expression tag	UNP Q46927
B	269	LEU	-	expression tag	UNP Q46927
B	270	GLU	-	expression tag	UNP Q46927
B	271	HIS	-	expression tag	UNP Q46927
B	272	HIS	-	expression tag	UNP Q46927
B	273	HIS	-	expression tag	UNP Q46927
B	274	HIS	-	expression tag	UNP Q46927
B	275	HIS	-	expression tag	UNP Q46927
B	276	HIS	-	expression tag	UNP Q46927
C	269	LEU	-	expression tag	UNP Q46927
C	270	GLU	-	expression tag	UNP Q46927
C	271	HIS	-	expression tag	UNP Q46927
C	272	HIS	-	expression tag	UNP Q46927

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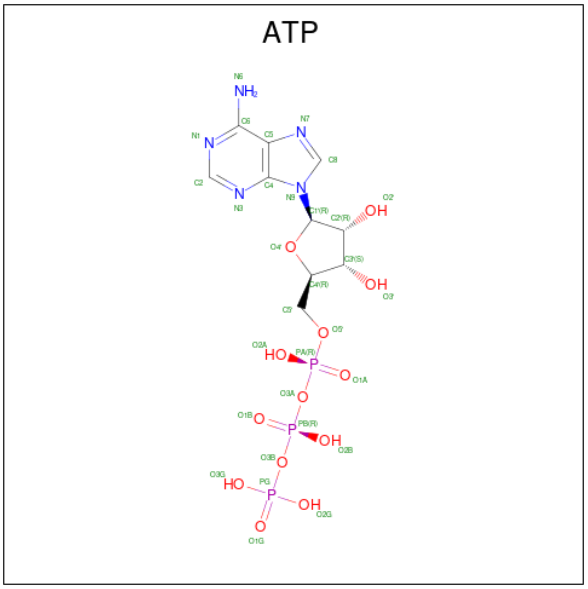
Chain	Residue	Modelled	Actual	Comment	Reference
C	273	HIS	-	expression tag	UNP Q46927
C	274	HIS	-	expression tag	UNP Q46927
C	275	HIS	-	expression tag	UNP Q46927
C	276	HIS	-	expression tag	UNP Q46927
D	269	LEU	-	expression tag	UNP Q46927
D	270	GLU	-	expression tag	UNP Q46927
D	271	HIS	-	expression tag	UNP Q46927
D	272	HIS	-	expression tag	UNP Q46927
D	273	HIS	-	expression tag	UNP Q46927
D	274	HIS	-	expression tag	UNP Q46927
D	275	HIS	-	expression tag	UNP Q46927
D	276	HIS	-	expression tag	UNP Q46927

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

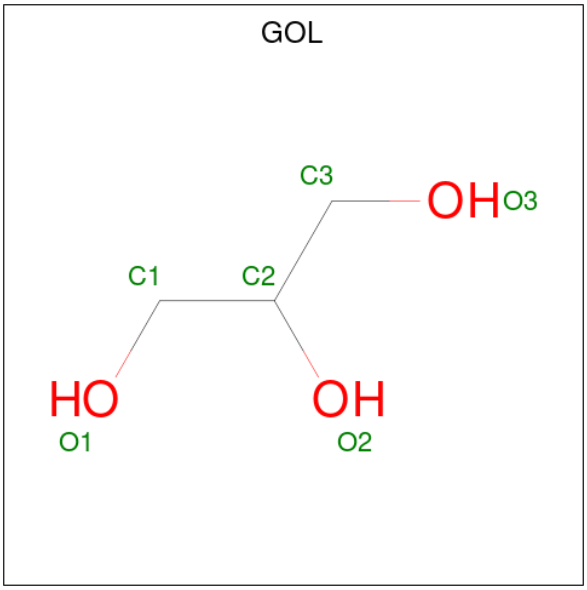
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0

- Molecule 6 is water.

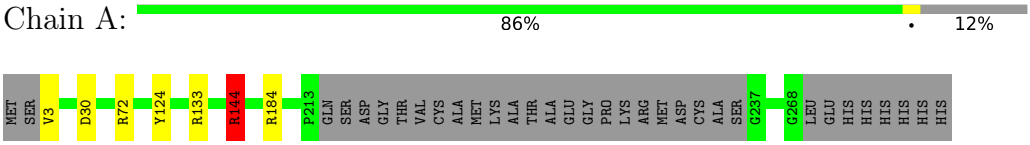
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	123	Total O 123 123	0	0
6	B	140	Total O 140 140	0	0
6	C	144	Total O 144 144	0	0
6	D	104	Total O 104 104	0	0

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. 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. 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.

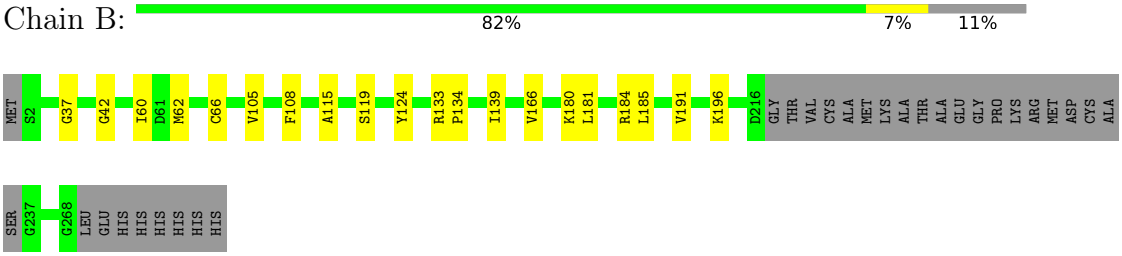
• Molecule 1: TRNA THREONYLCARBAMOYLADENOSINE DEHYDRATASE

Chain A:



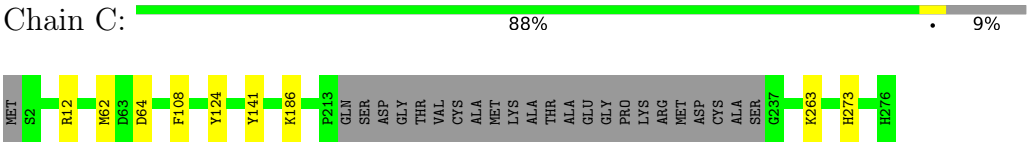
• Molecule 1: TRNA THREONYLCARBAMOYLADENOSINE DEHYDRATASE

Chain B:



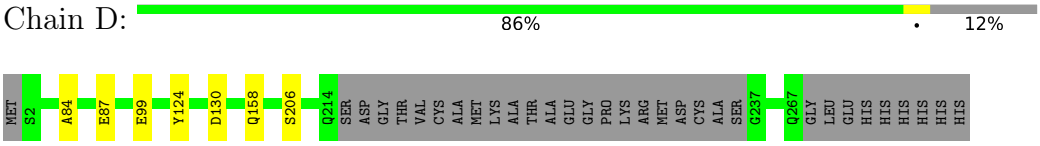
• Molecule 1: TRNA THREONYLCARBAMOYLADENOSINE DEHYDRATASE

Chain C:



• Molecule 1: TRNA THREONYLCARBAMOYLADENOSINE DEHYDRATASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.69Å 97.16Å 83.19Å 90.00° 111.61° 90.00°	Depositor
Resolution (Å)	41.13 – 1.77 77.34 – 1.77	Depositor EDS
% Data completeness (in resolution range)	96.0 (41.13-1.77) 95.0 (77.34-1.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.89 (at 1.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.142 , 0.183 0.297 , 0.311	Depositor DCC
R_{free} test set	4502 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8167	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, K, ATP, NA

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	0.52	0/1872	0.73	4/2533 (0.2%)
1	B	0.49	0/1898	0.65	0/2570
1	C	0.48	0/1957	0.63	0/2651
1	D	0.46	0/1869	0.64	0/2530
All	All	0.49	0/7596	0.66	4/10284 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	144[A]	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	144[B]	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	144[A]	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	A	144[B]	ARG	NE-CZ-NH1	6.81	123.70	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1846	0	1883	6	0
1	B	1872	0	1903	14	0
1	C	1923	0	1947	6	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1843	0	1878	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	1	0
3	B	31	0	12	0	0
3	C	31	0	12	2	0
3	D	31	0	12	0	0
4	A	12	0	16	0	0
4	B	12	0	16	0	0
4	C	12	0	16	0	0
4	D	6	0	8	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	123	0	0	0	0
6	B	140	0	0	3	0
6	C	144	0	0	3	1
6	D	104	0	0	1	2
All	All	8167	0	7715	29	3

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 (29) 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:66[A]:CYS:SG	6:B:2046:HOH:O	2.31	0.87
1:A:133:ARG:CG	1:A:184:ARG:HH12	2.18	0.57
1:C:108:PHE:HB2	3:C:401:ATP:C6	2.42	0.55
1:A:133:ARG:HG3	1:A:184:ARG:HH12	1.72	0.54
1:B:180:LYS:HG3	6:B:2106:HOH:O	2.11	0.51
1:B:133:ARG:HG2	1:B:184:ARG:HH12	1.77	0.50
1:C:186:LYS:NZ	6:C:2120:HOH:O	2.44	0.50
1:B:133:ARG:HB2	1:B:134:PRO:CD	2.42	0.50
1:C:108:PHE:HB2	3:C:401:ATP:N6	2.27	0.49
1:B:133:ARG:HB2	1:B:134:PRO:HD3	1.95	0.48
1:B:196:LYS:NZ	1:D:130:ASP:OD2	2.46	0.48
1:C:12:ARG:NH2	6:C:2019:HOH:O	2.46	0.48
1:B:139:ILE:CD1	1:B:181:LEU:HD21	2.45	0.47
1:A:72:ARG:NH2	3:A:401:ATP:O3B	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ARG:HG2	1:A:184:ARG:NH1	2.31	0.46
1:A:144[A]:ARG:CG	1:A:144[A]:ARG:HH11	2.29	0.46
1:B:37:GLY:O	1:B:42:GLY:HA3	2.17	0.45
1:D:99:GLU:OE2	6:D:2048:HOH:O	2.21	0.45
1:C:62:MET:SD	1:C:108:PHE:HD1	2.40	0.45
1:B:166[B]:VAL:HG21	6:B:2126:HOH:O	2.18	0.44
1:A:3:VAL:N	1:A:30:ASP:OD1	2.52	0.43
1:B:62:MET:HG2	1:B:108:PHE:CZ	2.54	0.42
1:B:115:ALA:O	1:B:119:SER:OG	2.27	0.42
1:C:263:LYS:NZ	6:C:2138:HOH:O	2.53	0.41
1:B:185:LEU:HB3	1:B:191:VAL:HB	2.03	0.41
1:B:62:MET:CG	1:B:108:PHE:CE2	3.04	0.41
1:D:158:GLN:OE1	1:D:206:SER:HB3	2.22	0.40
1:B:60:ILE:HG12	1:B:105:VAL:HB	2.03	0.40
1:D:84:ALA:HB3	1:D:87[B]:GLU:HG3	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:2100:HOH:O	6:D:2003:HOH:O[2_657]	1.82	0.38
1:C:64:ASP:OD1	1:C:273:HIS:ND1[2_647]	2.00	0.20
1:C:141:TYR:OH	6:D:2048:HOH:O[2_657]	2.19	0.01

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	242/276 (88%)	237 (98%)	5 (2%)	0	100	100
1	B	246/276 (89%)	241 (98%)	5 (2%)	0	100	100
1	C	252/276 (91%)	248 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	241/276 (87%)	237 (98%)	4 (2%)	0	100	100
All	All	981/1104 (89%)	963 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	192/216 (89%)	189 (98%)	3 (2%)	62	45
1	B	196/216 (91%)	195 (100%)	1 (0%)	88	83
1	C	201/216 (93%)	200 (100%)	1 (0%)	88	83
1	D	192/216 (89%)	191 (100%)	1 (0%)	88	83
All	All	781/864 (90%)	775 (99%)	6 (1%)	86	72

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	TYR
1	A	144[A]	ARG
1	A	144[B]	ARG
1	B	124	TYR
1	C	124	TYR
1	D	124	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
4	GOL	B	501	-	5,5,5	0.49	0	5,5,5	0.43	0
4	GOL	A	501	-	5,5,5	0.41	0	5,5,5	0.42	0
4	GOL	C	502	-	5,5,5	0.34	0	5,5,5	0.42	0
3	ATP	B	401	-	26,33,33	1.19	3 (11%)	31,52,52	1.58	6 (19%)
4	GOL	C	501	-	5,5,5	0.67	0	5,5,5	0.67	0
3	ATP	A	401	-	26,33,33	1.12	3 (11%)	31,52,52	1.47	4 (12%)
3	ATP	C	401	-	26,33,33	1.05	2 (7%)	31,52,52	1.51	5 (16%)
4	GOL	D	501	-	5,5,5	0.47	0	5,5,5	0.31	0
3	ATP	D	401	-	26,33,33	1.06	3 (11%)	31,52,52	1.54	5 (16%)
4	GOL	B	502	-	5,5,5	0.34	0	5,5,5	0.63	0
4	GOL	A	502	-	5,5,5	0.49	0	5,5,5	0.39	0

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
4	GOL	B	501	-	-	0/4/4/4	-
4	GOL	A	501	-	-	0/4/4/4	-
4	GOL	C	502	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	401	-	-	5/18/38/38	0/3/3/3
4	GOL	C	501	-	-	0/4/4/4	-
3	ATP	A	401	-	-	6/18/38/38	0/3/3/3
3	ATP	C	401	-	-	6/18/38/38	0/3/3/3
4	GOL	D	501	-	-	0/4/4/4	-
3	ATP	D	401	-	-	4/18/38/38	0/3/3/3
4	GOL	B	502	-	-	2/4/4/4	-
4	GOL	A	502	-	-	2/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ATP	O4'-C1'	3.32	1.45	1.41
3	C	401	ATP	O4'-C1'	2.74	1.44	1.41
3	A	401	ATP	C5-C4	2.57	1.47	1.40
3	B	401	ATP	C5-C4	2.54	1.47	1.40
3	A	401	ATP	C2-N3	2.47	1.36	1.32
3	A	401	ATP	O4'-C1'	2.41	1.44	1.41
3	D	401	ATP	C5-C4	2.36	1.47	1.40
3	C	401	ATP	C5-C4	2.24	1.46	1.40
3	B	401	ATP	C2-N3	2.19	1.35	1.32
3	D	401	ATP	C2-N1	2.09	1.37	1.33
3	D	401	ATP	C2'-C1'	-2.06	1.50	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	401	ATP	N3-C2-N1	-4.51	121.63	128.68
3	A	401	ATP	N3-C2-N1	-4.05	122.35	128.68
3	B	401	ATP	N3-C2-N1	-3.75	122.81	128.68
3	B	401	ATP	O4'-C1'-C2'	-3.69	101.53	106.93
3	C	401	ATP	N3-C2-N1	-3.63	123.00	128.68
3	D	401	ATP	C1'-N9-C4	-3.52	120.46	126.64
3	C	401	ATP	PB-O3B-PG	-3.17	121.96	132.83
3	C	401	ATP	O4'-C1'-C2'	-2.99	102.56	106.93
3	A	401	ATP	PB-O3B-PG	-2.95	122.70	132.83
3	B	401	ATP	PA-O3A-PB	-2.82	123.14	132.83
3	A	401	ATP	N6-C6-N1	2.69	124.17	118.57
3	B	401	ATP	PB-O3B-PG	-2.64	123.78	132.83
3	D	401	ATP	C2-N1-C6	2.61	123.21	118.75
3	D	401	ATP	PB-O3B-PG	-2.55	124.06	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	ATP	N6-C6-N1	2.54	123.84	118.57
3	D	401	ATP	N6-C6-N1	2.46	123.67	118.57
3	A	401	ATP	C5-C6-N6	-2.31	116.84	120.35
3	B	401	ATP	C3'-C2'-C1'	2.20	104.29	100.98
3	C	401	ATP	PA-O3A-PB	-2.12	125.55	132.83
3	B	401	ATP	O3G-PG-O2G	2.07	115.53	107.64

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	ATP	C5'-O5'-PA-O1A
3	B	401	ATP	C5'-O5'-PA-O1A
3	C	401	ATP	C5'-O5'-PA-O1A
4	A	502	GOL	C1-C2-C3-O3
4	A	502	GOL	O2-C2-C3-O3
4	B	502	GOL	O2-C2-C3-O3
4	C	502	GOL	O2-C2-C3-O3
4	B	502	GOL	C1-C2-C3-O3
4	C	502	GOL	C1-C2-C3-O3
3	A	401	ATP	PB-O3A-PA-O5'
3	B	401	ATP	PB-O3A-PA-O5'
3	C	401	ATP	PB-O3A-PA-O5'
3	D	401	ATP	PB-O3A-PA-O5'
3	C	401	ATP	C5'-O5'-PA-O3A
3	A	401	ATP	C5'-O5'-PA-O2A
3	B	401	ATP	C5'-O5'-PA-O2A
3	C	401	ATP	C5'-O5'-PA-O2A
3	D	401	ATP	PA-O3A-PB-O2B
3	C	401	ATP	O4'-C4'-C5'-O5'
3	A	401	ATP	O4'-C4'-C5'-O5'
3	A	401	ATP	C5'-O5'-PA-O3A
3	B	401	ATP	C5'-O5'-PA-O3A
3	D	401	ATP	O4'-C4'-C5'-O5'
3	A	401	ATP	PB-O3A-PA-O2A
3	C	401	ATP	PB-O3A-PA-O2A
3	D	401	ATP	PA-O3A-PB-O1B
3	B	401	ATP	O4'-C4'-C5'-O5'

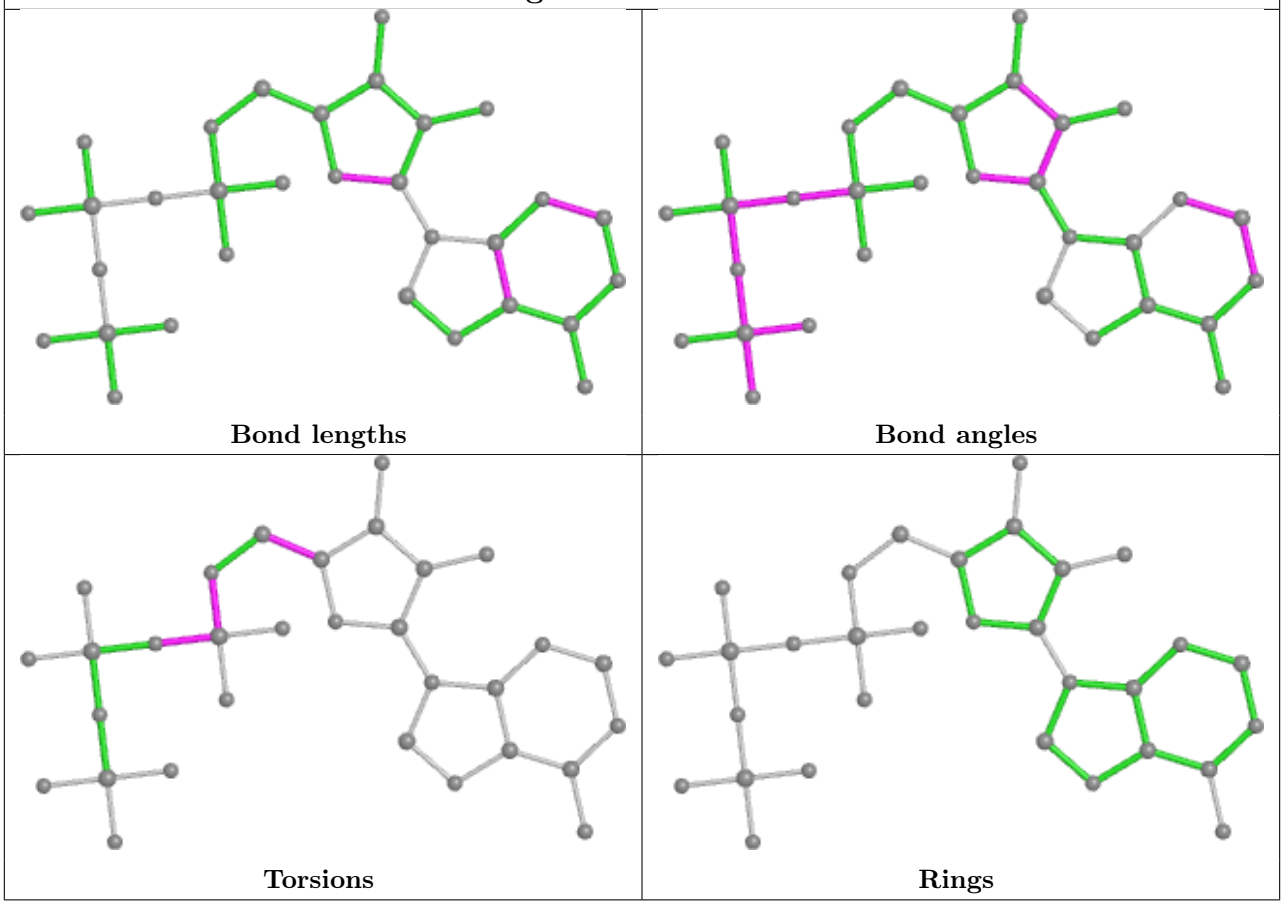
There are no ring outliers.

2 monomers are involved in 3 short contacts:

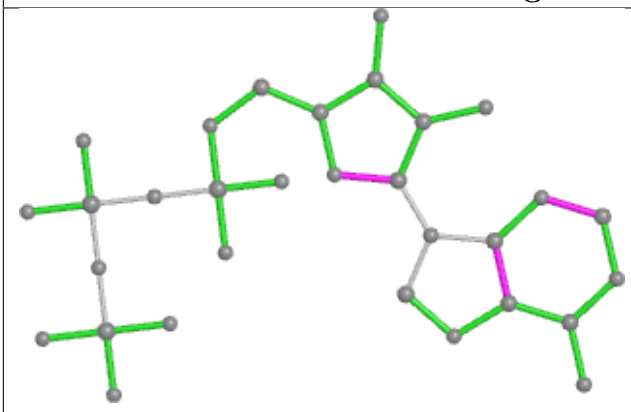
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ATP	1	0
3	C	401	ATP	2	0

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 then 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.

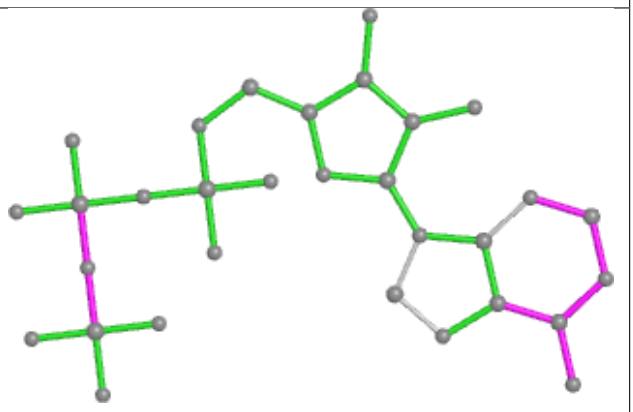
Ligand ATP B 401



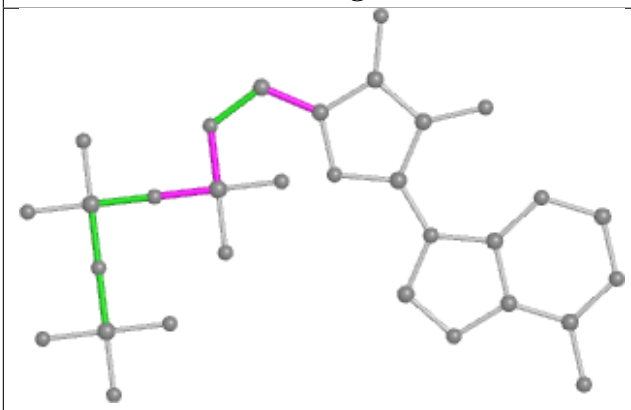
Ligand ATP A 401



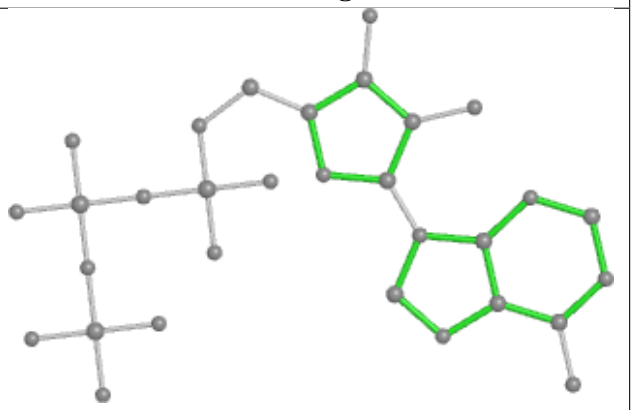
Bond lengths



Bond angles

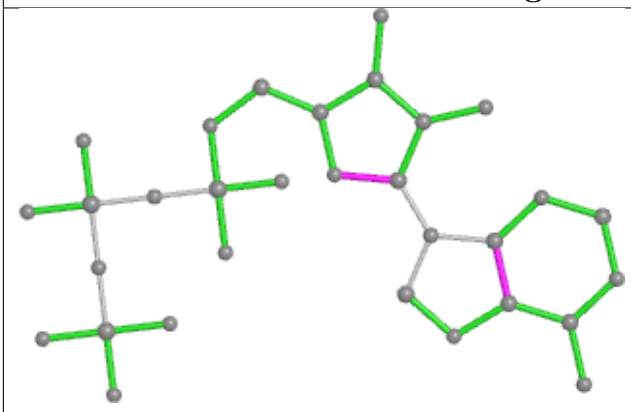


Torsions

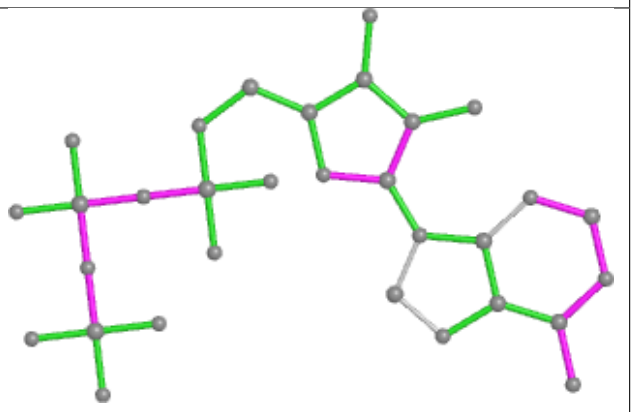


Rings

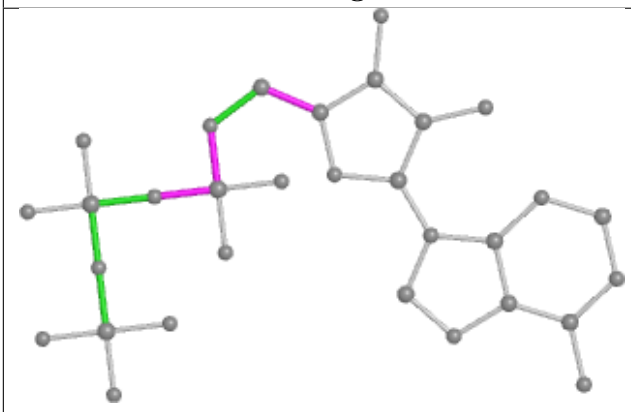
Ligand ATP C 401



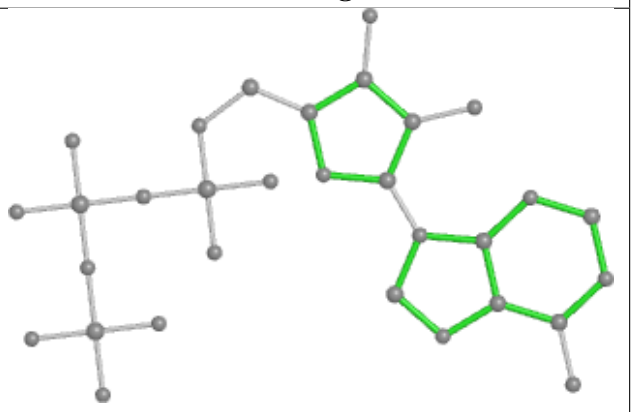
Bond lengths



Bond angles

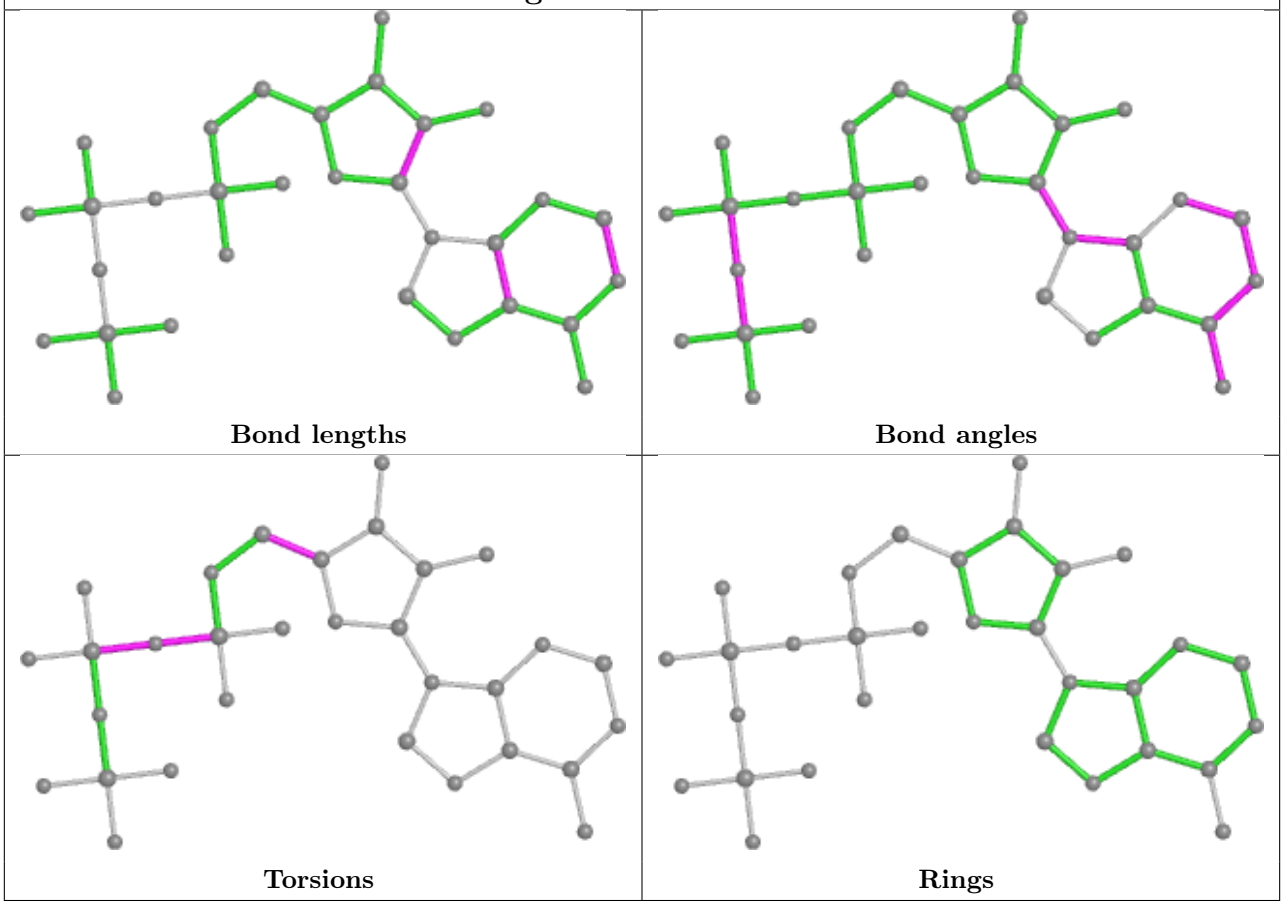


Torsions



Rings

Ligand ATP D 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

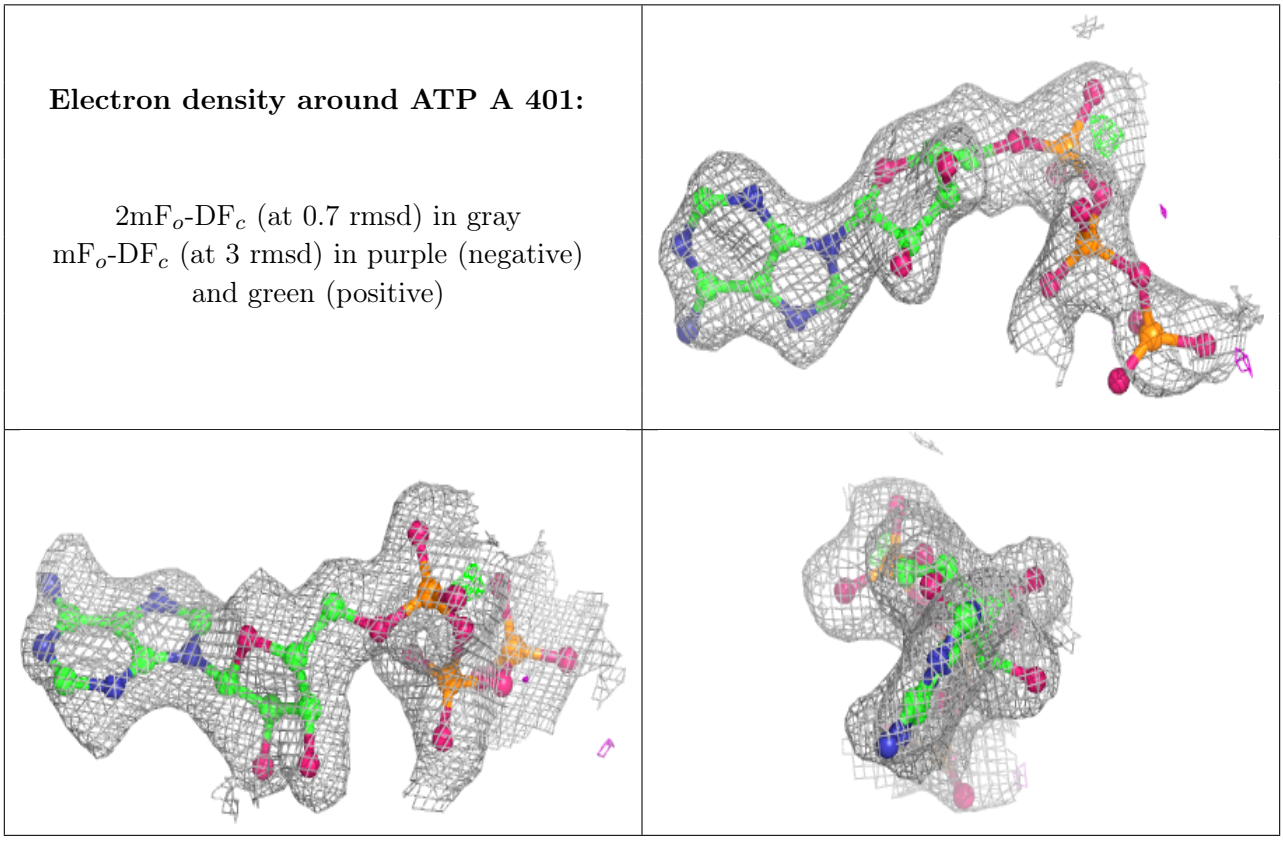
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

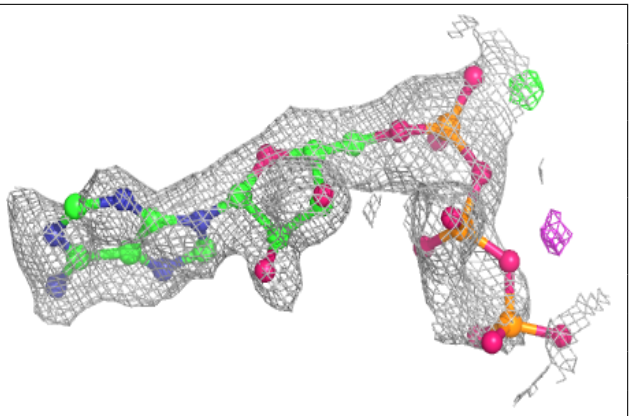
Electron density around ATP A 401:

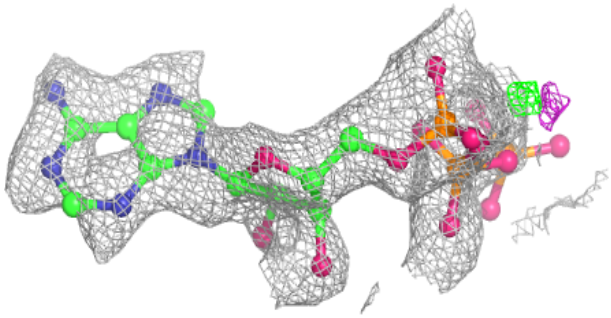
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

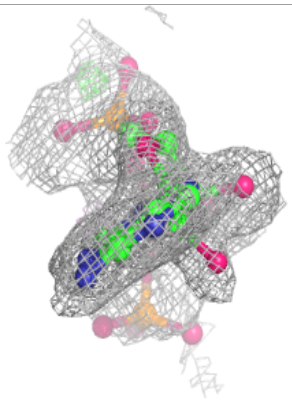


Electron density around ATP B 401:

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

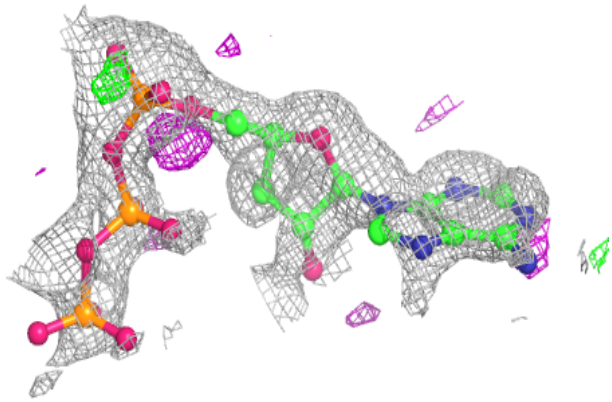


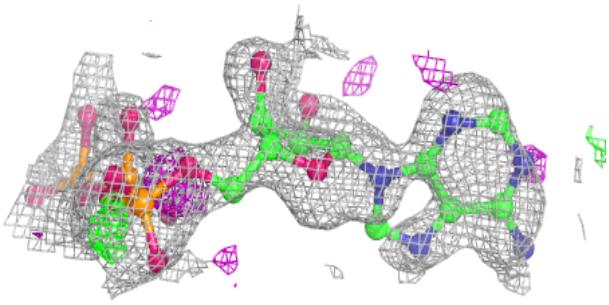


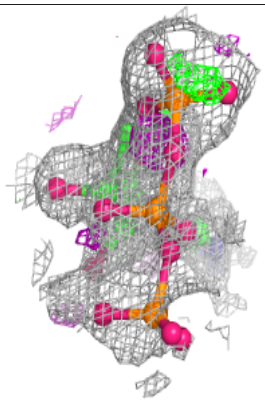


Electron density around ATP C 401:

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

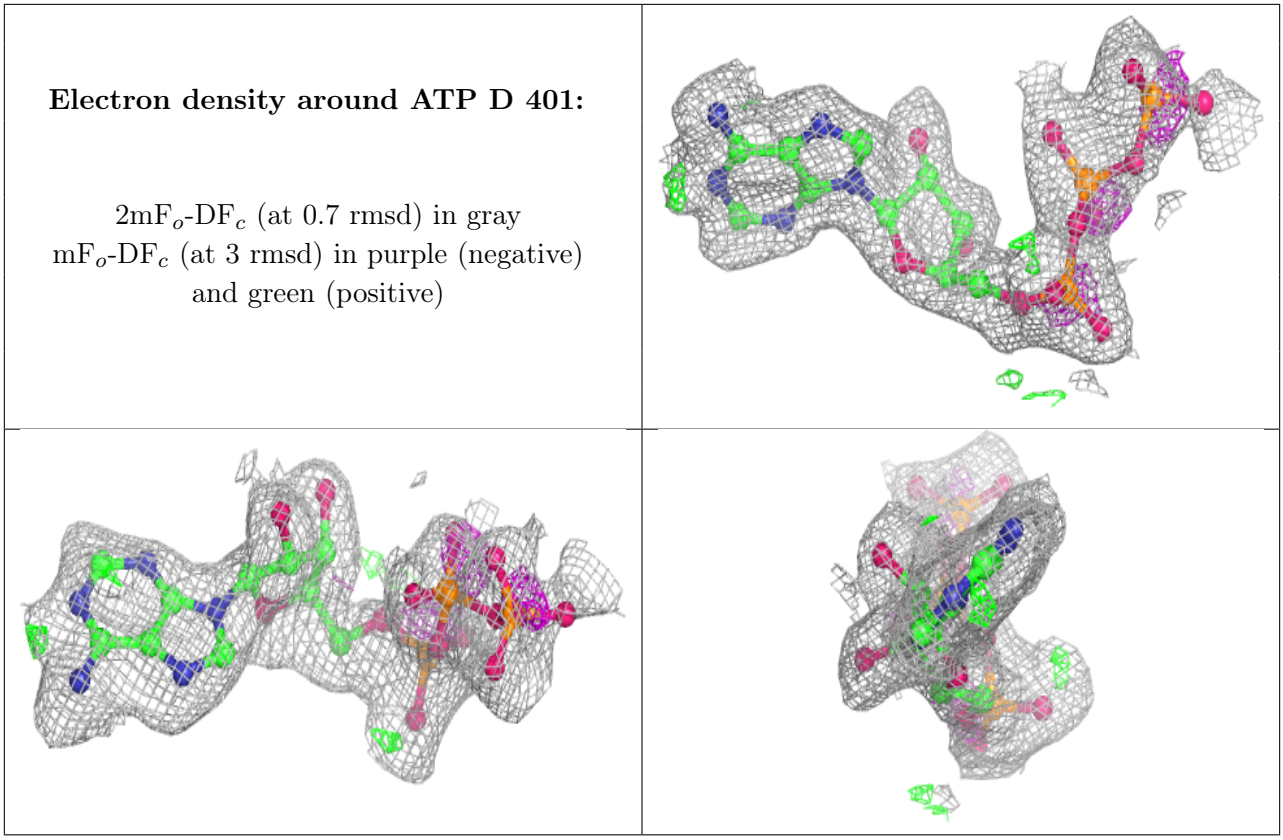






Electron density around ATP D 401:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.