wwPDB X-ray Structure Validation Summary Report (i)

Nov 7, 2023 – 02:43 AM EST

PDB ID	:	1PJ4
Title	:	Crystal structure of human mitochondrial NAD(P)+-dependent malic enzyme in a pentary complex with natural substrate malate, ATP, Mn++, and allosteric activator fumarate.
Authors	:	Tao, X.; Yang, Z.; Tong, L.
Deposited on	:	2003-05-31
Resolution	:	2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

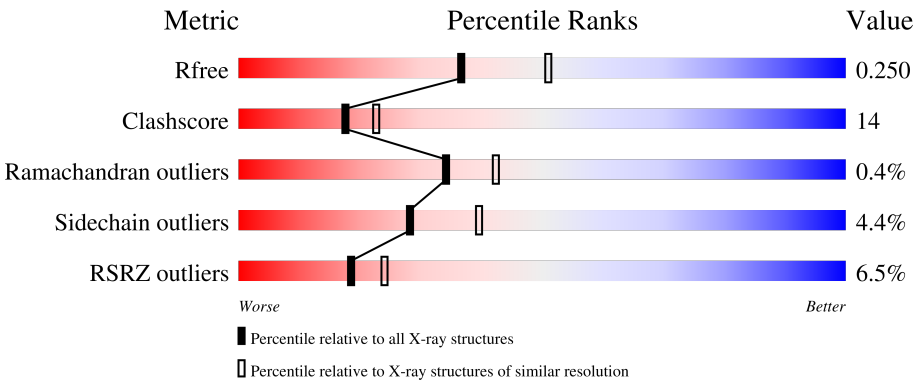
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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% 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	564	6% 73% 23% • •
1	B	564	7% 69% 26% • •
1	C	564	7% 71% 26% • •
1	D	564	5% 74% 21% • •

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
2	MLT	A	701	X	-	-	-
2	MLT	B	1701	X	-	-	-
2	MLT	C	2701	X	-	-	-
2	MLT	D	3701	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18442 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 NAD-dependent malic enzyme, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	552	4359	2790	743	803	9	14	0	0	0
1	B	552	4359	2790	743	803	9	14	0	0	0
1	C	552	4359	2790	743	803	9	14	0	0	0
1	D	552	4359	2790	743	803	9	14	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	MET	modified residue	UNP P23368
A	38	MSE	MET	modified residue	UNP P23368
A	47	MSE	MET	modified residue	UNP P23368
A	75	MSE	MET	modified residue	UNP P23368
A	86	MSE	MET	modified residue	UNP P23368
A	108	MSE	MET	modified residue	UNP P23368
A	177	MSE	MET	modified residue	UNP P23368
A	219	MSE	MET	modified residue	UNP P23368
A	239	MSE	MET	modified residue	UNP P23368
A	325	MSE	MET	modified residue	UNP P23368
A	327	MSE	MET	modified residue	UNP P23368
A	343	MSE	MET	modified residue	UNP P23368
A	407	MSE	MET	modified residue	UNP P23368
A	539	MSE	MET	modified residue	UNP P23368
B	1029	MSE	MET	modified residue	UNP P23368
B	1038	MSE	MET	modified residue	UNP P23368
B	1047	MSE	MET	modified residue	UNP P23368
B	1075	MSE	MET	modified residue	UNP P23368
B	1086	MSE	MET	modified residue	UNP P23368
B	1108	MSE	MET	modified residue	UNP P23368
B	1177	MSE	MET	modified residue	UNP P23368

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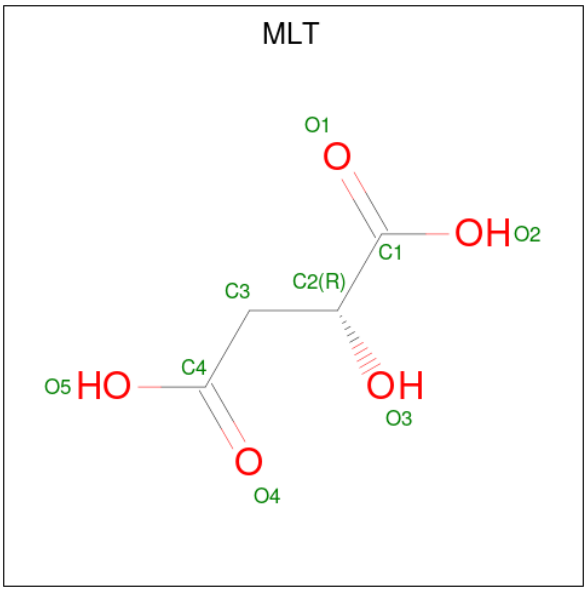
Chain	Residue	Modelled	Actual	Comment	Reference
B	1219	MSE	MET	modified residue	UNP P23368
B	1239	MSE	MET	modified residue	UNP P23368
B	1325	MSE	MET	modified residue	UNP P23368
B	1327	MSE	MET	modified residue	UNP P23368
B	1343	MSE	MET	modified residue	UNP P23368
B	1407	MSE	MET	modified residue	UNP P23368
B	1539	MSE	MET	modified residue	UNP P23368
C	2029	MSE	MET	modified residue	UNP P23368
C	2038	MSE	MET	modified residue	UNP P23368
C	2047	MSE	MET	modified residue	UNP P23368
C	2075	MSE	MET	modified residue	UNP P23368
C	2086	MSE	MET	modified residue	UNP P23368
C	2108	MSE	MET	modified residue	UNP P23368
C	2177	MSE	MET	modified residue	UNP P23368
C	2219	MSE	MET	modified residue	UNP P23368
C	2239	MSE	MET	modified residue	UNP P23368
C	2325	MSE	MET	modified residue	UNP P23368
C	2327	MSE	MET	modified residue	UNP P23368
C	2343	MSE	MET	modified residue	UNP P23368
C	2407	MSE	MET	modified residue	UNP P23368
C	2539	MSE	MET	modified residue	UNP P23368
D	3029	MSE	MET	modified residue	UNP P23368
D	3038	MSE	MET	modified residue	UNP P23368
D	3047	MSE	MET	modified residue	UNP P23368
D	3075	MSE	MET	modified residue	UNP P23368
D	3086	MSE	MET	modified residue	UNP P23368
D	3108	MSE	MET	modified residue	UNP P23368
D	3177	MSE	MET	modified residue	UNP P23368
D	3219	MSE	MET	modified residue	UNP P23368
D	3239	MSE	MET	modified residue	UNP P23368
D	3325	MSE	MET	modified residue	UNP P23368
D	3327	MSE	MET	modified residue	UNP P23368
D	3343	MSE	MET	modified residue	UNP P23368
D	3407	MSE	MET	modified residue	UNP P23368
D	3539	MSE	MET	modified residue	UNP P23368

- Molecule 2 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).



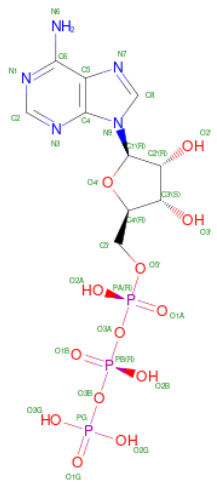
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 4 5	0	0
2	B	1	Total C O 9 4 5	0	0
2	C	1	Total C O 9 4 5	0	0
2	D	1	Total C O 9 4 5	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0

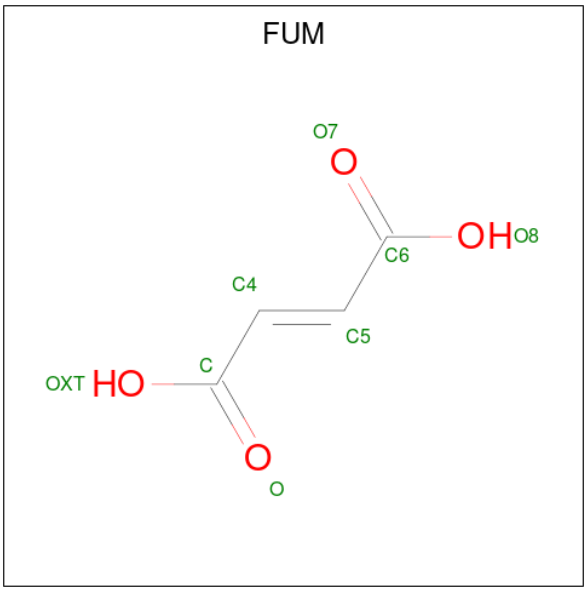
- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

ATP



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

- Molecule 5 is FUMARIC ACID (three-letter code: FUM) (formula: $C_4H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	8	4	4	0	0
5	B	1	8	4	4	0	0
5	C	1	8	4	4	0	0
5	D	1	8	4	4	0	0

- Molecule 6 is water.

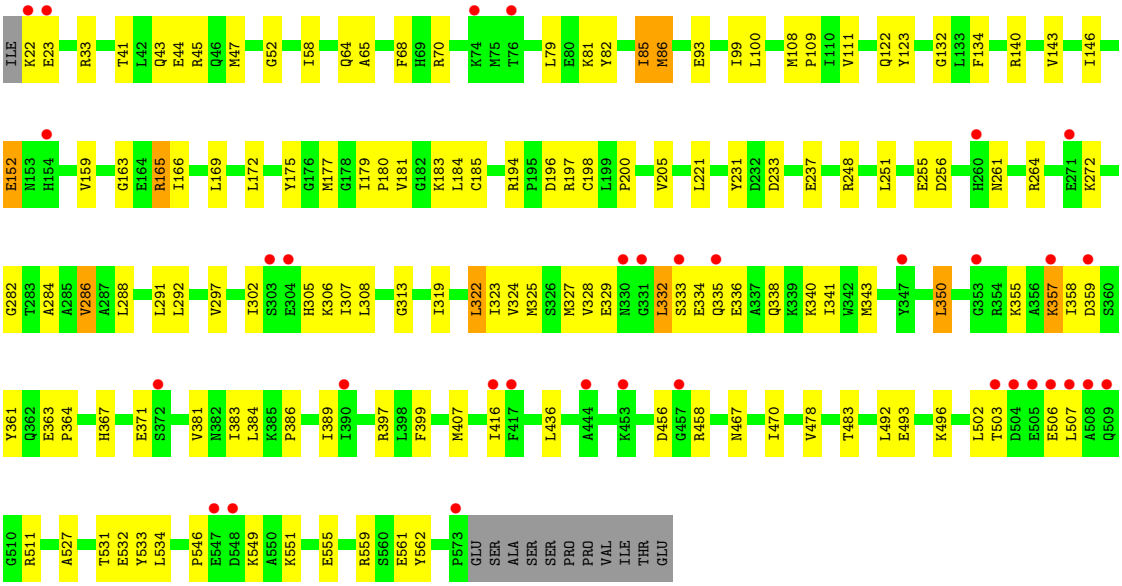
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	165	165	165	0	0
6	B	176	176	176	0	0
6	C	169	169	169	0	0
6	D	176	176	176	0	0

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 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.

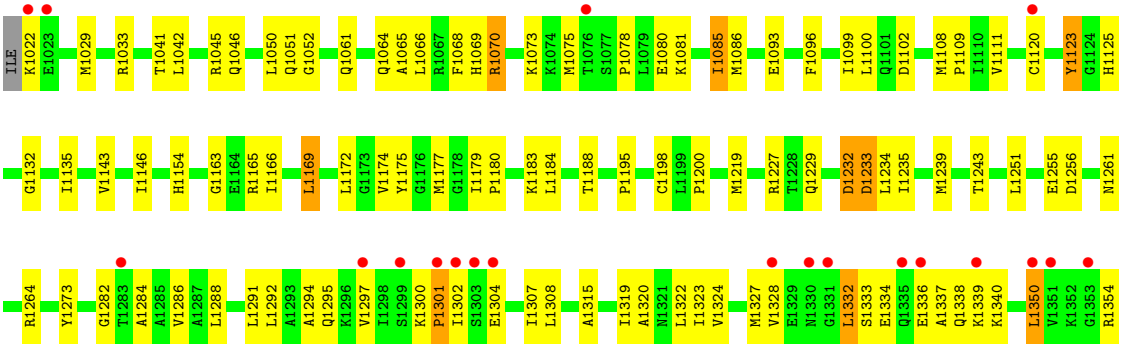
• Molecule 1: NAD-dependent malic enzyme, mitochondrial

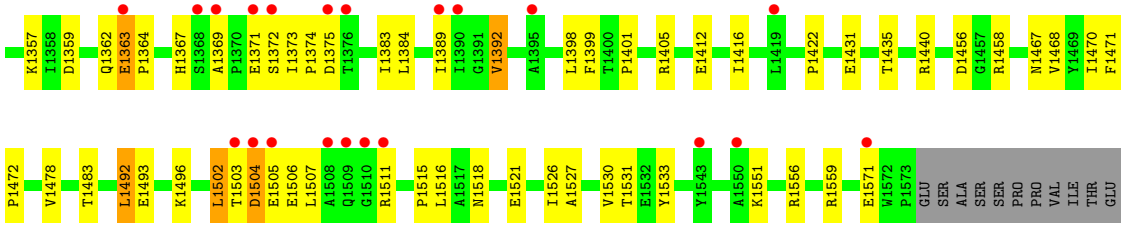
Chain A:



• Molecule 1: NAD-dependent malic enzyme, mitochondrial

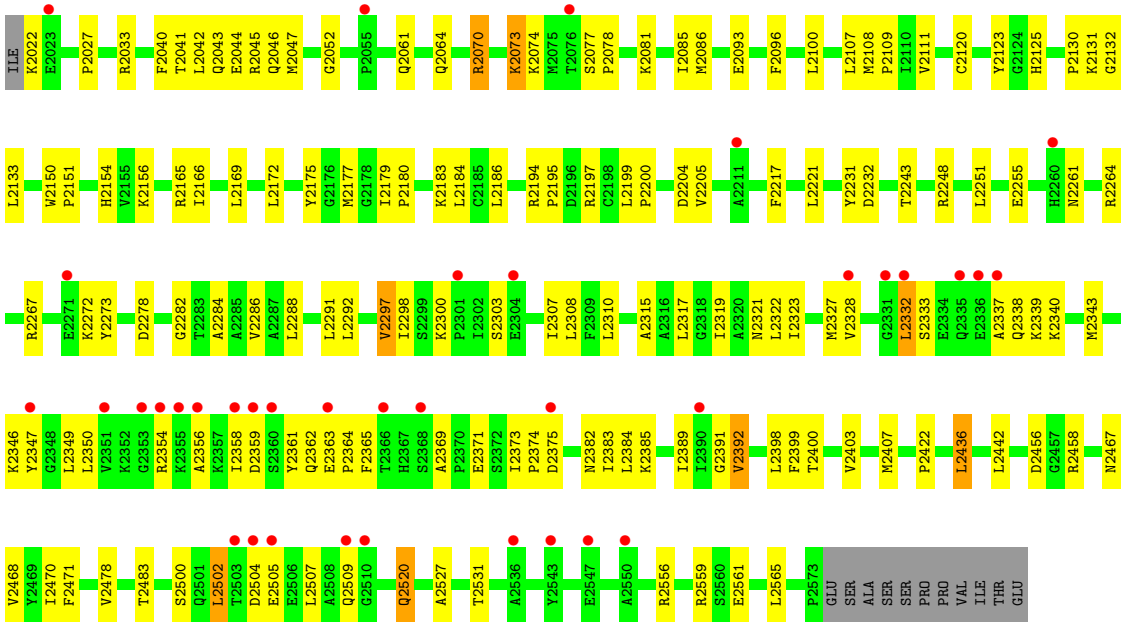
Chain B:





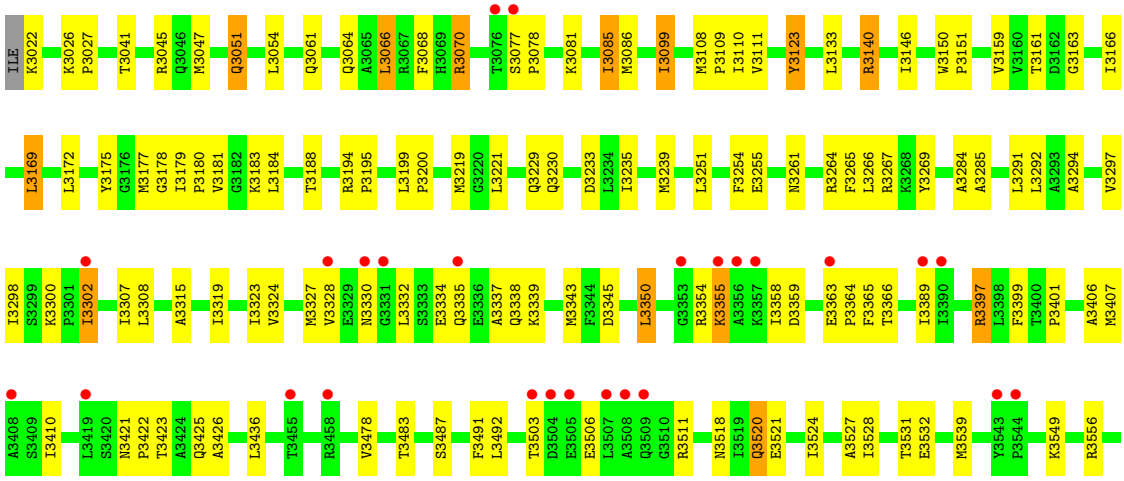
• Molecule 1: NAD-dependent malic enzyme, mitochondrial

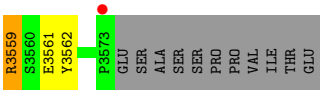
Chain C:



• Molecule 1: NAD-dependent malic enzyme, mitochondrial

Chain D:




R3559
S3560
E3561
Y3562
P3573
GLU
SER
ALA
SER
SER
PRO
PRO
VAL
ILE
THR
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	226.05Å 117.34Å 111.31Å 90.00° 109.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.30 29.55 – 2.29	Depositor EDS
% Data completeness (in resolution range)	92.7 (19.94-2.30) 96.7 (29.55-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.93 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.252 0.211 , 0.250	Depositor DCC
R_{free} test set	8990 reflections (7.52%)	wwPDB-VP
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18442	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.37% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FUM, MN, ATP, MLT

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	0.36	0/4439	0.60	0/5987
1	B	0.36	0/4439	0.60	0/5987
1	C	0.36	0/4439	0.60	0/5987
1	D	0.36	0/4439	0.60	0/5987
All	All	0.36	0/17756	0.60	0/23948

There are no bond length outliers.

There are no bond angle outliers.

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	4359	0	4396	112	0
1	B	4359	0	4396	138	0
1	C	4359	0	4396	131	0
1	D	4359	0	4396	111	0
2	A	9	0	3	0	0
2	B	9	0	3	0	0
2	C	9	0	3	0	0
2	D	9	0	3	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	1	0
4	B	62	0	24	1	0
4	C	62	0	24	1	0
4	D	62	0	24	1	0
5	A	8	0	1	0	0
5	B	8	0	1	0	0
5	C	8	0	1	0	0
5	D	8	0	1	0	0
6	A	165	0	0	2	0
6	B	176	0	0	7	0
6	C	169	0	0	8	0
6	D	176	0	0	4	0
All	All	18442	0	17696	485	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 14.

The worst 5 of 485 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:1315:ALA:HB3	1:B:1392:VAL:HG21	1.25	1.14
1:D:3177:MSE:HE1	1:D:3200:PRO:HB2	1.14	1.07
1:C:2286:VAL:HG21	1:C:2467:ASN:HA	1.38	1.05
1:B:1323:ILE:HG22	1:B:1327:MSE:HE2	1.40	1.03
1:C:2132:GLY:HA3	1:C:2177:MSE:CE	1.89	1.01

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	550/564 (98%)	531 (96%)	16 (3%)	3 (0%)	29	35
1	B	550/564 (98%)	534 (97%)	14 (2%)	2 (0%)	34	42
1	C	550/564 (98%)	532 (97%)	16 (3%)	2 (0%)	34	42
1	D	550/564 (98%)	531 (96%)	17 (3%)	2 (0%)	34	42
All	All	2200/2256 (98%)	2128 (97%)	63 (3%)	9 (0%)	34	42

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	LYS
1	C	2332	LEU
1	A	397	ARG
1	B	1332	LEU
1	A	332	LEU

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	468/465 (101%)	447 (96%)	21 (4%)	27	39
1	B	468/465 (101%)	449 (96%)	19 (4%)	30	43
1	C	468/465 (101%)	450 (96%)	18 (4%)	33	47
1	D	468/465 (101%)	443 (95%)	25 (5%)	22	31
All	All	1872/1860 (101%)	1789 (96%)	83 (4%)	28	39

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2561	GLU
1	D	3251	LEU
1	D	3047	MSE
1	D	3123	TYR
1	D	3330	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2520	GLN
1	D	3261	ASN
1	D	3051	GLN
1	D	3089	GLN
1	D	3338	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)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
5	FUM	D	3700	-	7,7,7	2.41	4 (57%)	8,8,8	1.69	2 (25%)
4	ATP	D	3601	-	26,33,33	1.59	6 (23%)	31,52,52	1.49	3 (9%)
4	ATP	A	4602	-	26,33,33	1.59	6 (23%)	31,52,52	1.57	3 (9%)
2	MLT	C	2701	3	8,8,8	1.28	0	10,10,10	1.60	3 (30%)
5	FUM	C	2700	-	7,7,7	2.36	4 (57%)	8,8,8	1.28	0
4	ATP	A	4601	-	26,33,33	1.61	6 (23%)	31,52,52	1.49	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ATP	B	1601	-	26,33,33	1.67	6 (23%)	31,52,52	1.52	3 (9%)
5	FUM	A	700	-	7,7,7	2.31	5 (71%)	8,8,8	1.54	2 (25%)
4	ATP	C	2601	-	26,33,33	1.52	6 (23%)	31,52,52	1.53	2 (6%)
2	MLT	A	701	3	8,8,8	1.26	2 (25%)	10,10,10	1.60	3 (30%)
2	MLT	D	3701	3	8,8,8	1.26	2 (25%)	10,10,10	1.59	2 (20%)
4	ATP	C	2602	-	26,33,33	1.54	4 (15%)	31,52,52	1.57	3 (9%)
5	FUM	B	1700	-	7,7,7	2.28	6 (85%)	8,8,8	1.43	1 (12%)
4	ATP	D	3602	-	26,33,33	1.62	5 (19%)	31,52,52	1.57	3 (9%)
4	ATP	B	1602	-	26,33,33	1.57	5 (19%)	31,52,52	1.60	3 (9%)
2	MLT	B	1701	3	8,8,8	1.34	2 (25%)	10,10,10	1.60	2 (20%)

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
5	FUM	D	3700	-	-	0/5/5/5	-
4	ATP	D	3601	-	-	7/18/38/38	0/3/3/3
4	ATP	A	4602	-	-	1/18/38/38	0/3/3/3
2	MLT	C	2701	3	1/1/3/3	1/8/8/8	-
5	FUM	C	2700	-	-	0/5/5/5	-
4	ATP	A	4601	-	-	8/18/38/38	0/3/3/3
4	ATP	B	1601	-	-	6/18/38/38	0/3/3/3
5	FUM	A	700	-	-	0/5/5/5	-
4	ATP	C	2601	-	-	5/18/38/38	0/3/3/3
2	MLT	A	701	3	1/1/3/3	0/8/8/8	-
2	MLT	D	3701	3	1/1/3/3	0/8/8/8	-
4	ATP	C	2602	-	-	1/18/38/38	0/3/3/3
5	FUM	B	1700	-	-	0/5/5/5	-
4	ATP	D	3602	-	-	1/18/38/38	0/3/3/3
4	ATP	B	1602	-	-	1/18/38/38	0/3/3/3
2	MLT	B	1701	3	1/1/3/3	2/8/8/8	-

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3602	ATP	O4'-C1'	4.45	1.47	1.41
4	B	1601	ATP	O4'-C1'	3.87	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3601	ATP	C2-N3	3.70	1.38	1.32
4	A	4601	ATP	O4'-C1'	3.68	1.46	1.41
4	A	4602	ATP	O4'-C1'	3.60	1.46	1.41

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1602	ATP	N3-C2-N1	-5.27	120.44	128.68
4	C	2601	ATP	N3-C2-N1	-5.21	120.53	128.68
4	D	3602	ATP	N3-C2-N1	-5.18	120.58	128.68
4	C	2602	ATP	N3-C2-N1	-5.13	120.66	128.68
4	A	4602	ATP	N3-C2-N1	-5.10	120.71	128.68

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	701	MLT	C2
2	B	1701	MLT	C2
2	C	2701	MLT	C2
2	D	3701	MLT	C2

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1601	ATP	PB-O3B-PG-O1G
4	D	3601	ATP	PB-O3B-PG-O1G
4	A	4601	ATP	PG-O3B-PB-O2B
4	B	1601	ATP	PG-O3B-PB-O2B
4	C	2601	ATP	PG-O3B-PB-O2B

There are no ring outliers.

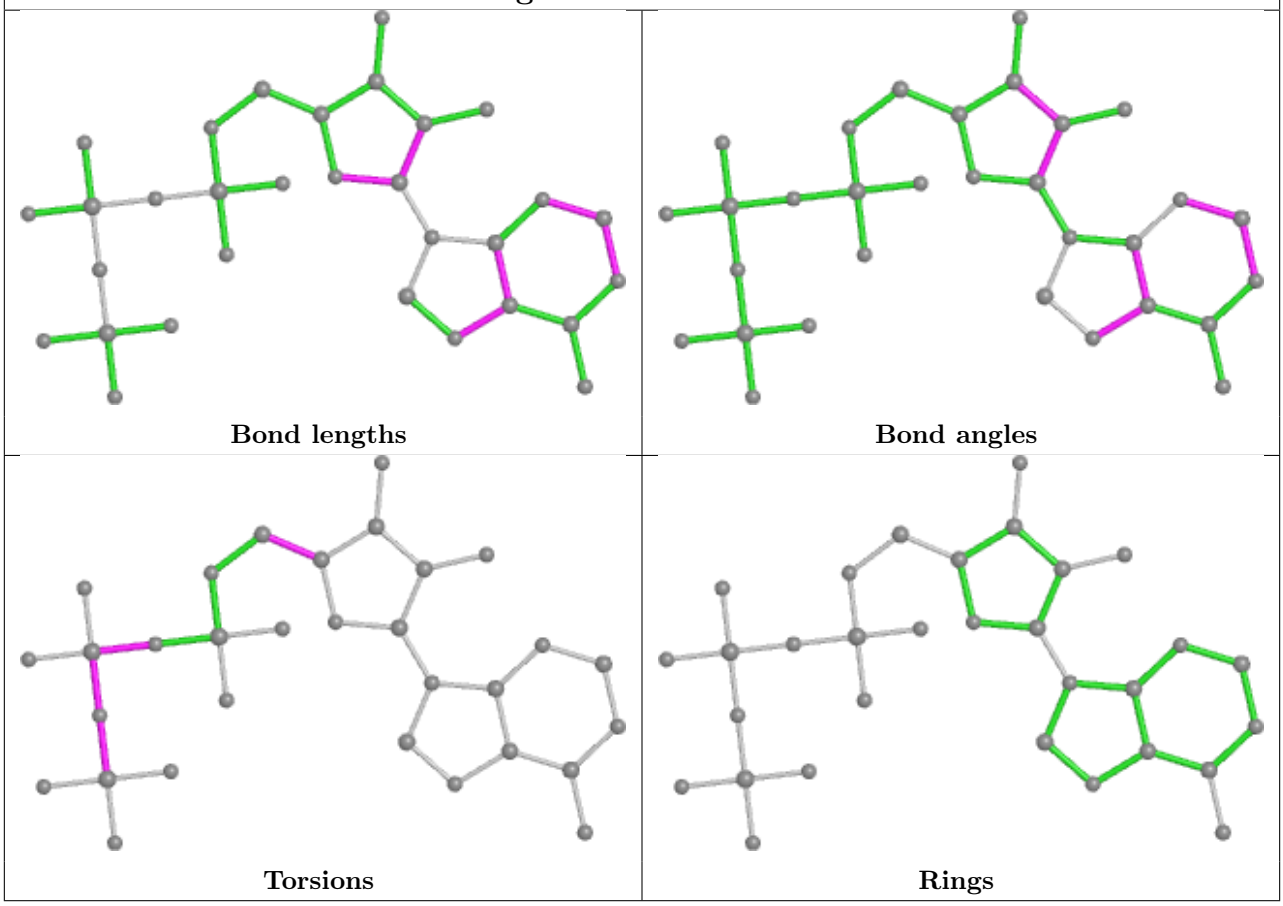
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3601	ATP	1	0
4	A	4601	ATP	1	0
4	B	1601	ATP	1	0
2	D	3701	MLT	1	0
4	C	2602	ATP	1	0

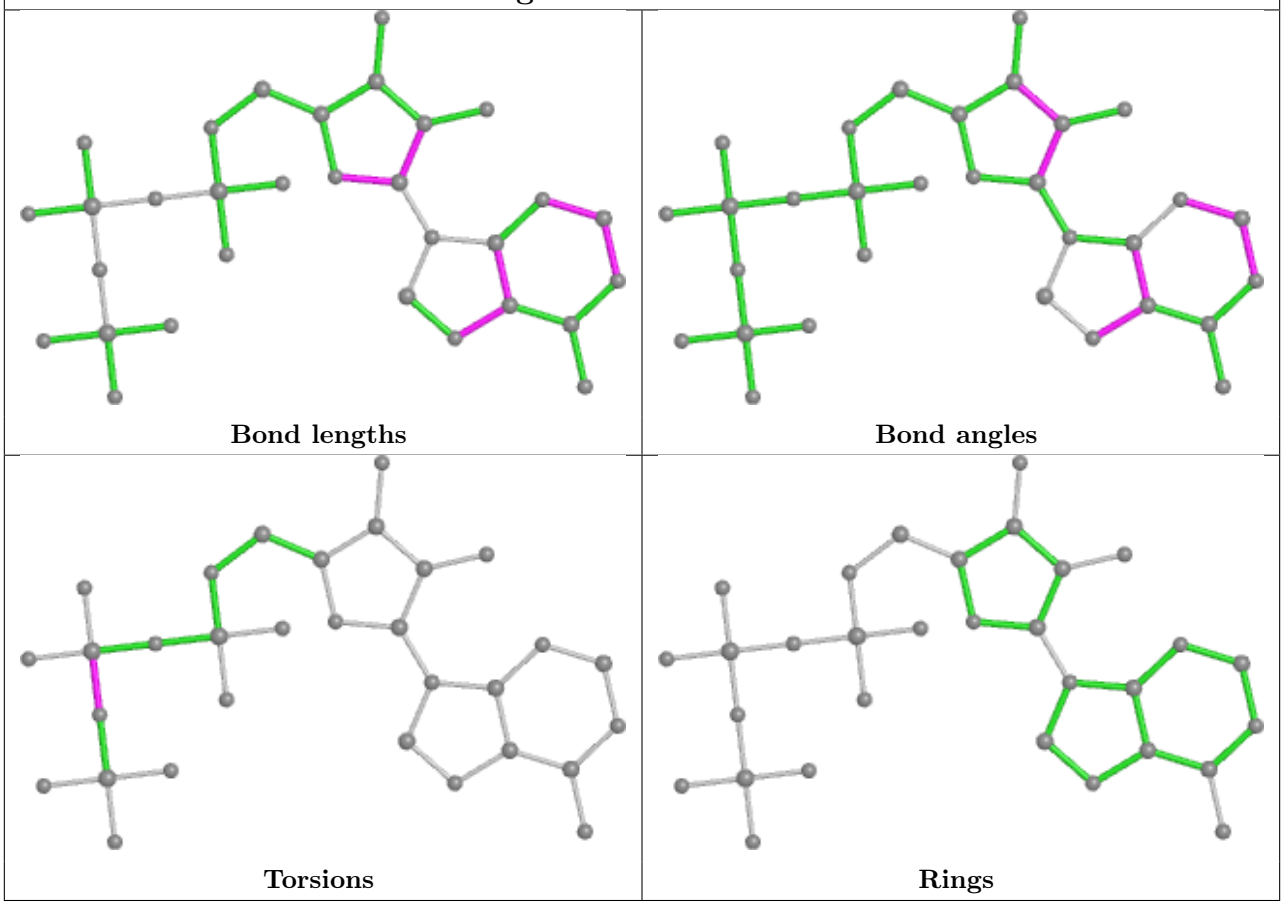
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 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.

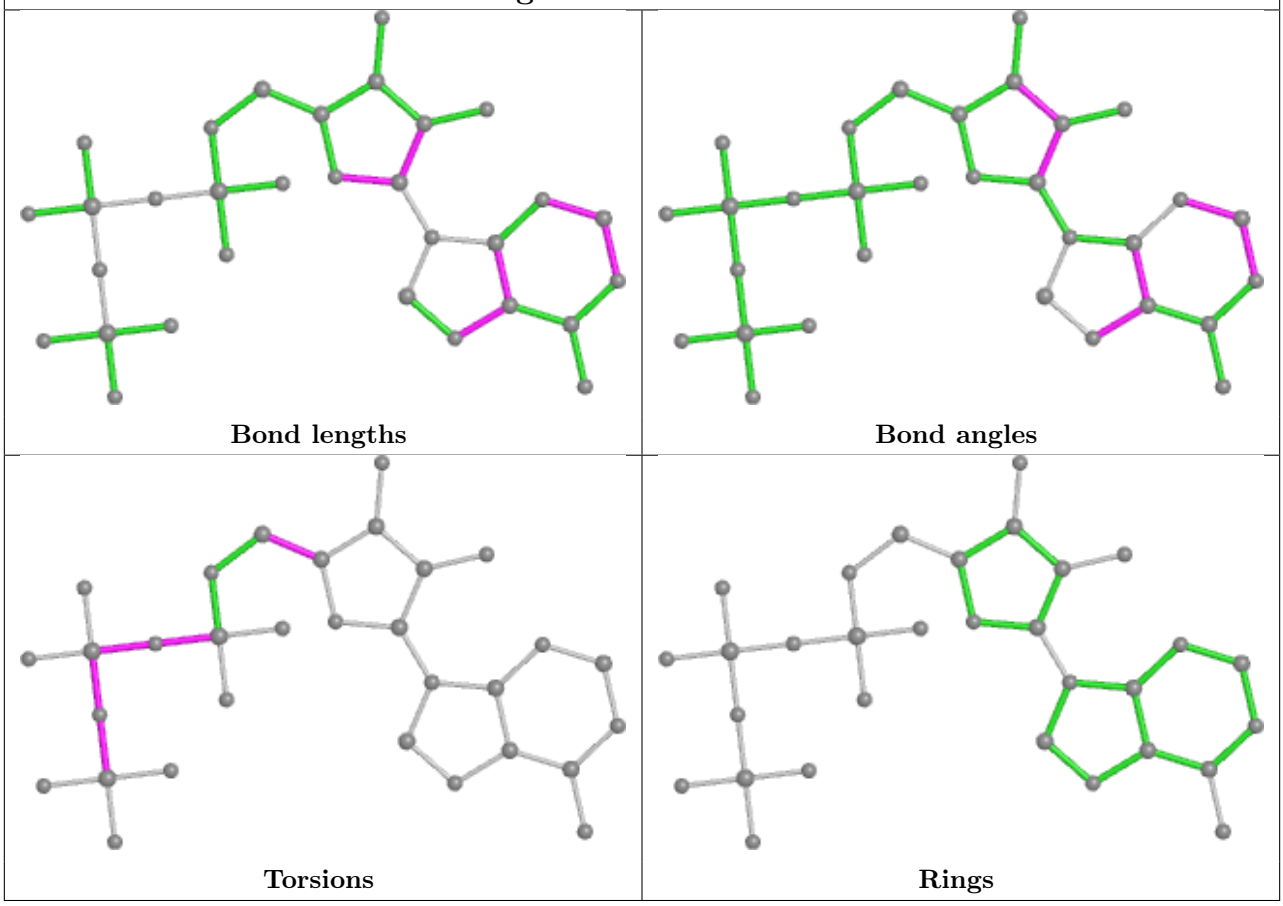
Ligand ATP D 3601



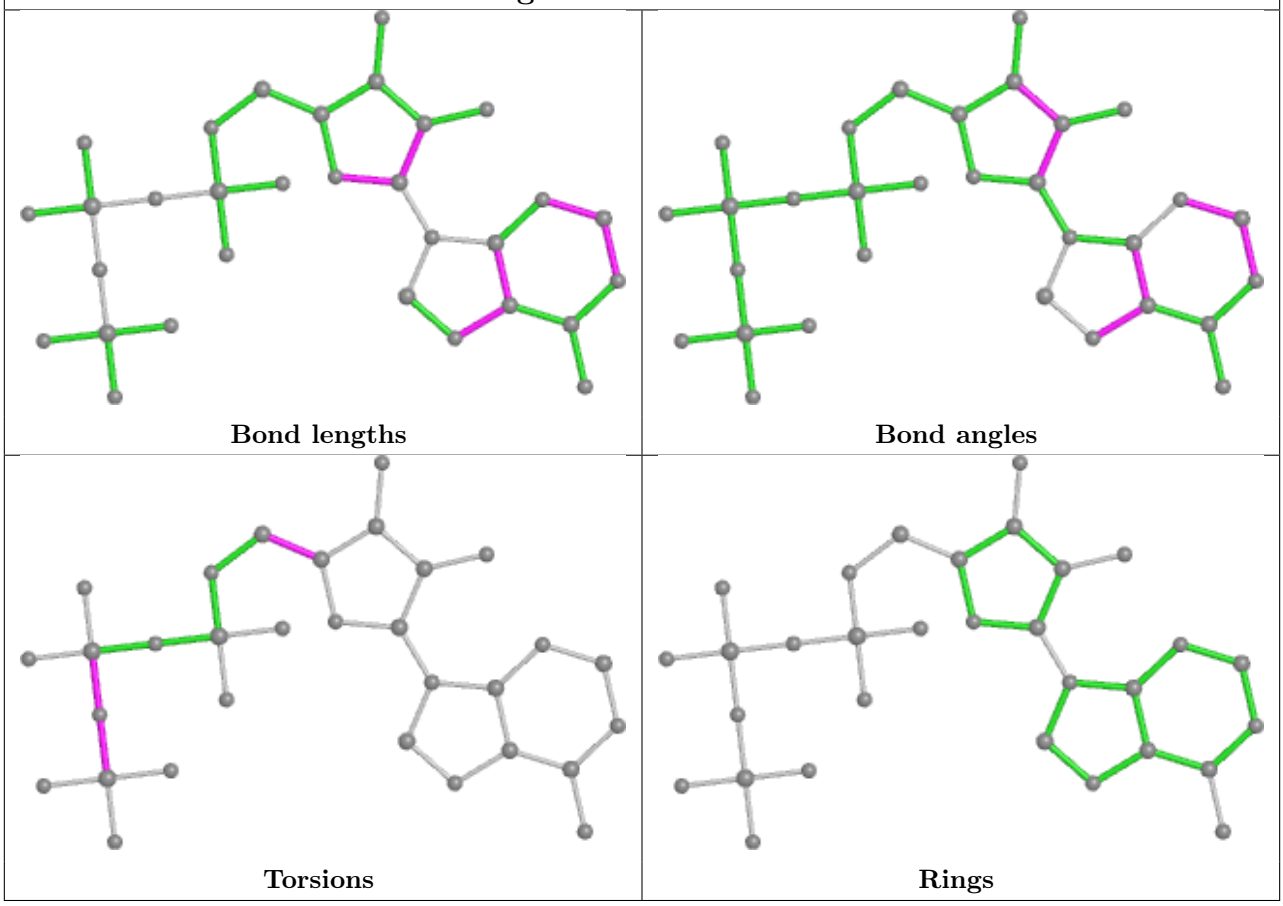
Ligand ATP A 4602



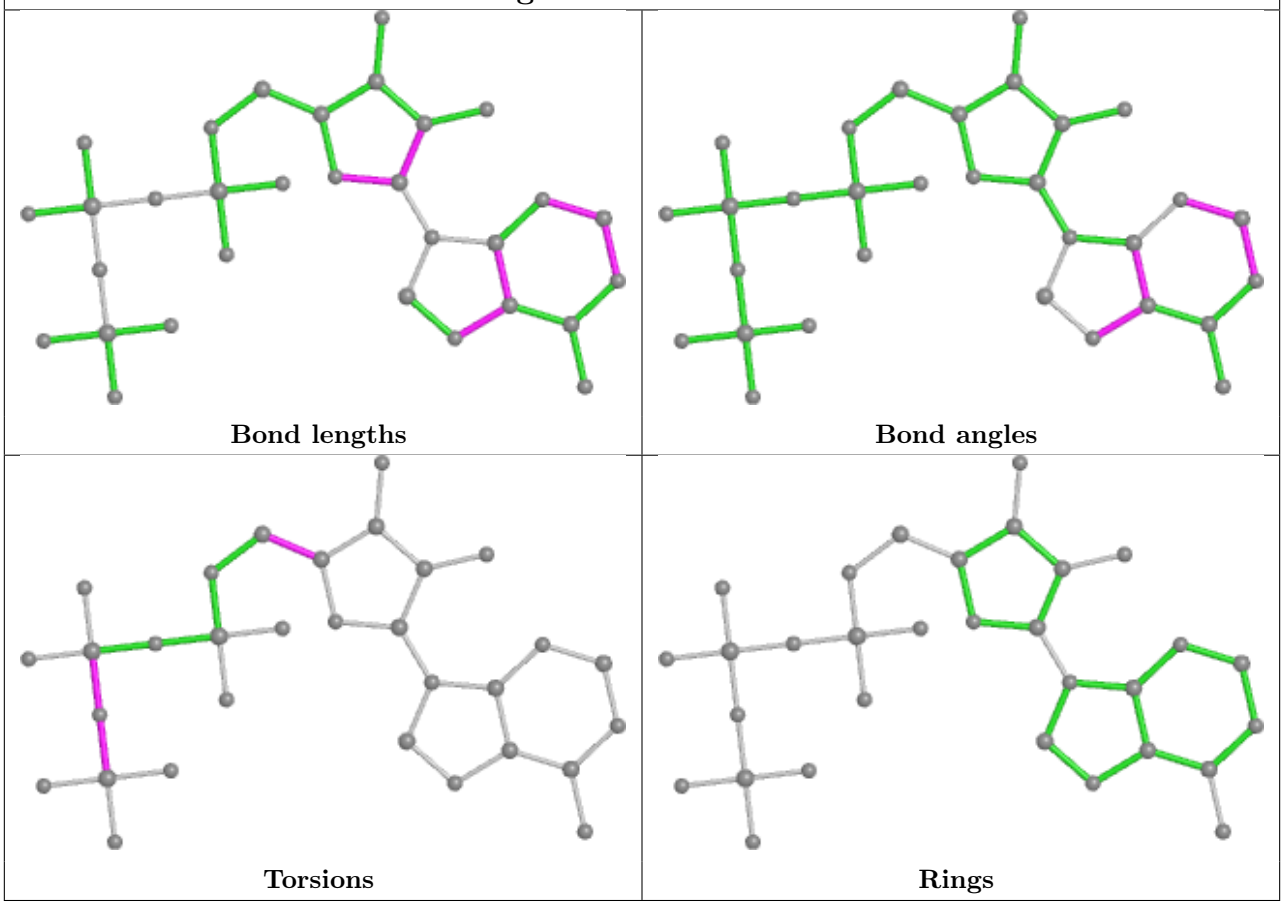
Ligand ATP A 4601



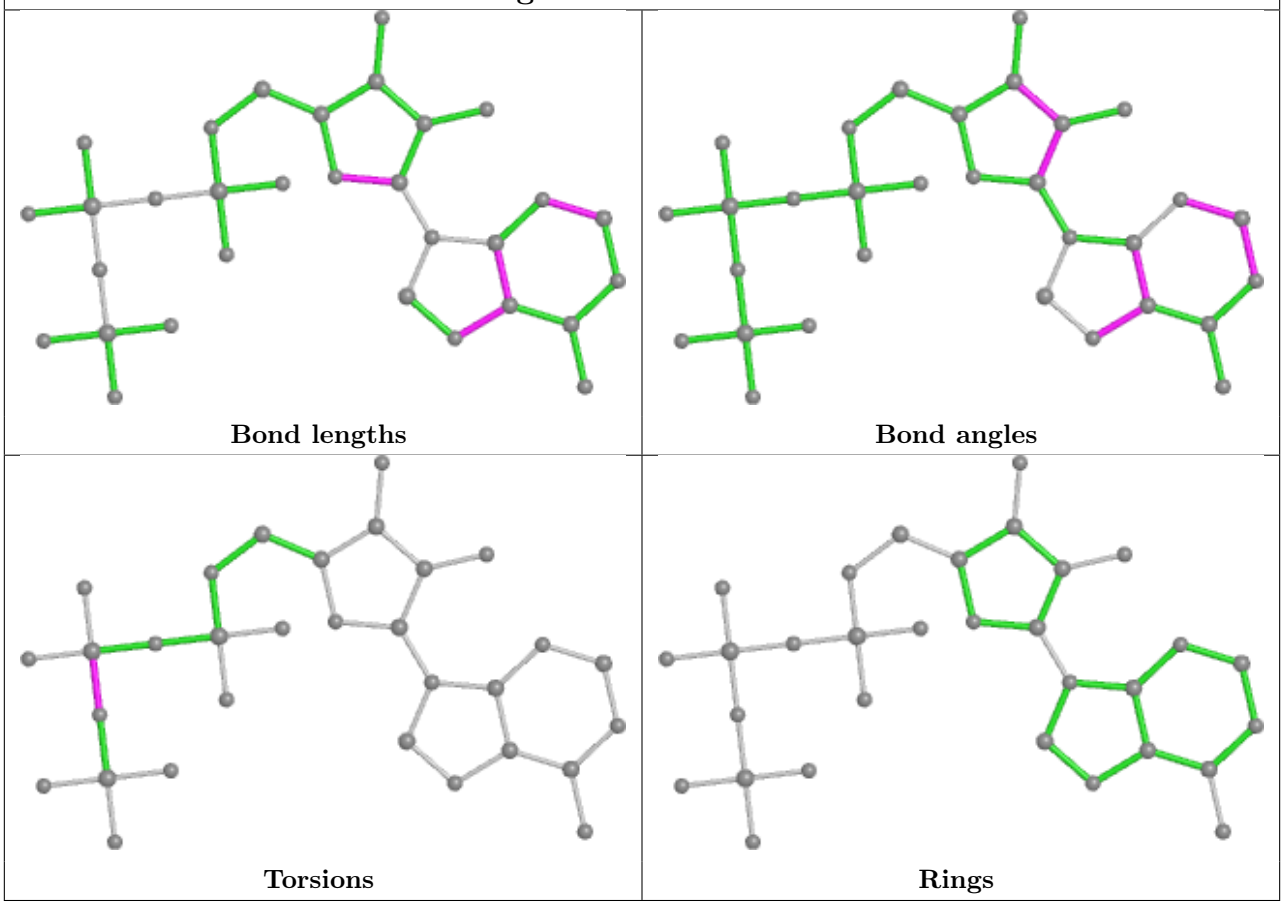
Ligand ATP B 1601



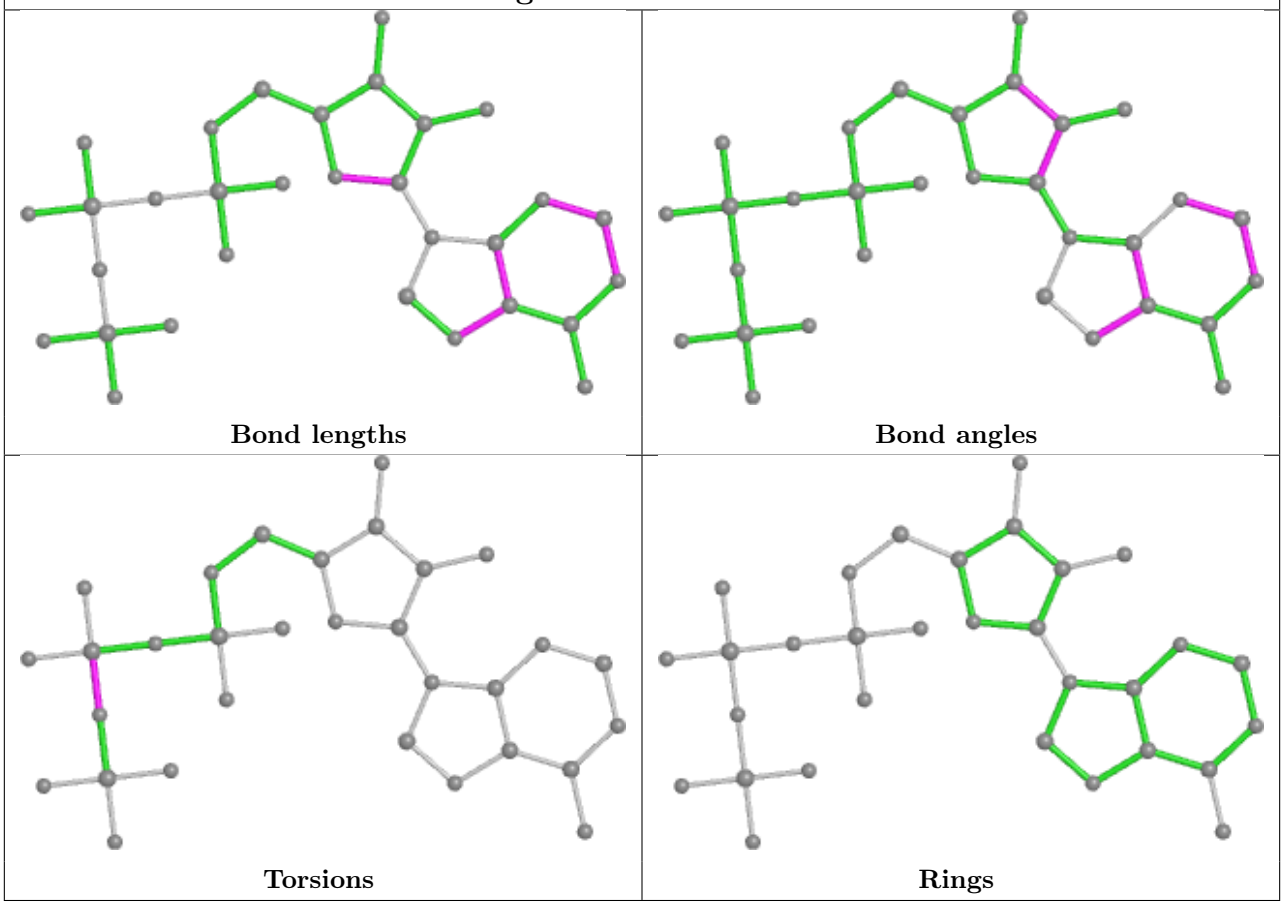
Ligand ATP C 2601



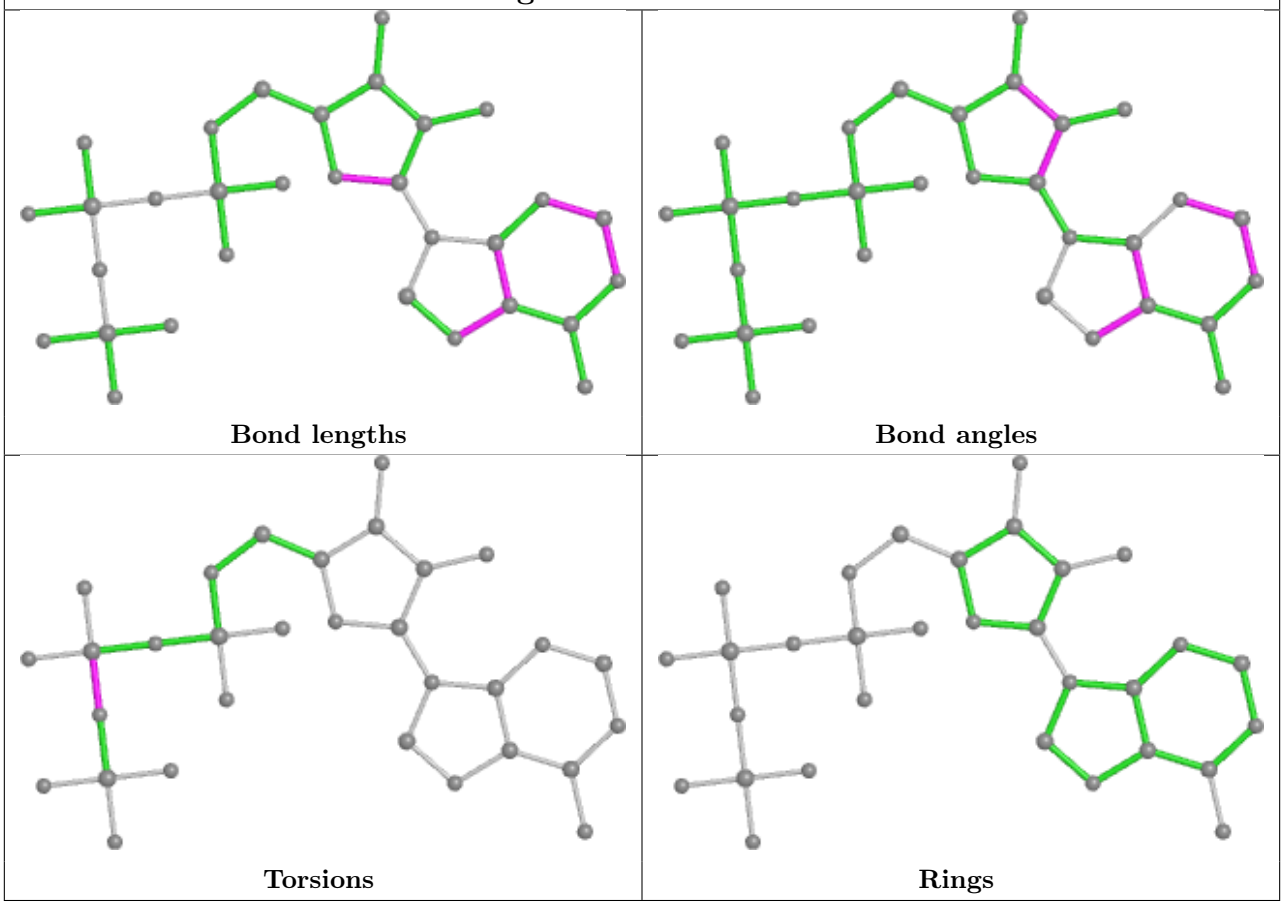
Ligand ATP C 2602



Ligand ATP D 3602



Ligand ATP B 1602



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	538/564 (95%)	0.34	34 (6%)	20	25	16, 27, 52, 66	0
1	B	538/564 (95%)	0.46	41 (7%)	13	18	16, 27, 53, 68	0
1	C	538/564 (95%)	0.37	37 (6%)	16	22	16, 28, 52, 60	0
1	D	538/564 (95%)	0.34	27 (5%)	28	35	15, 28, 52, 67	0
All	All	2152/2256 (95%)	0.38	139 (6%)	18	24	15, 27, 52, 68	0

The worst 5 of 139 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3353	GLY	6.0
1	B	1510	GLY	5.8
1	C	2358	ILE	5.3
1	A	507	LEU	4.6
1	B	1301	PRO	4.4

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)

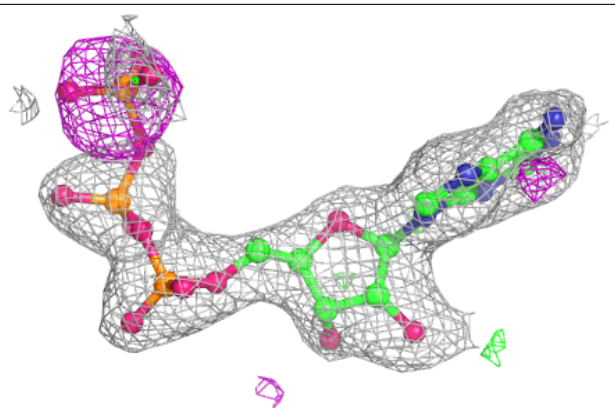
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

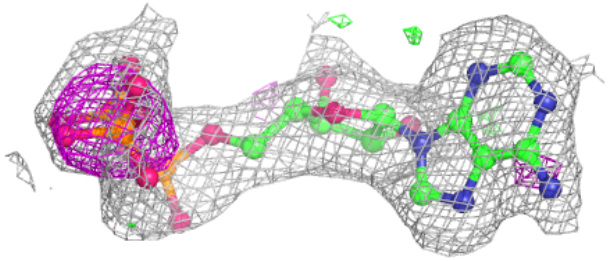
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ATP	C	2601	31/31	0.86	0.19	30,32,60,61	0
4	ATP	A	4602	31/31	0.87	0.17	21,35,73,74	0
4	ATP	D	3602	31/31	0.87	0.17	23,37,73,75	0
4	ATP	A	4601	31/31	0.88	0.18	25,28,60,62	0
4	ATP	C	2602	31/31	0.88	0.17	24,35,73,75	0
4	ATP	B	1602	31/31	0.88	0.15	24,34,71,73	0
2	MLT	C	2701	9/9	0.89	0.17	26,30,32,32	0
4	ATP	D	3601	31/31	0.90	0.16	27,30,59,60	0
4	ATP	B	1601	31/31	0.90	0.18	28,30,59,60	0
2	MLT	D	3701	9/9	0.92	0.17	27,29,31,33	0
5	FUM	B	1700	8/8	0.94	0.14	35,39,39,40	0
5	FUM	C	2700	8/8	0.94	0.17	35,37,39,39	0
2	MLT	A	701	9/9	0.95	0.14	25,28,31,33	0
5	FUM	A	700	8/8	0.95	0.23	35,37,38,38	0
2	MLT	B	1701	9/9	0.96	0.15	27,30,34,34	0
5	FUM	D	3700	8/8	0.96	0.21	35,38,38,39	0
3	MN	B	1604	1/1	0.99	0.13	28,28,28,28	0
3	MN	C	2604	1/1	0.99	0.12	29,29,29,29	0
3	MN	D	3604	1/1	0.99	0.08	28,28,28,28	0
3	MN	A	4604	1/1	1.00	0.09	23,23,23,23	0

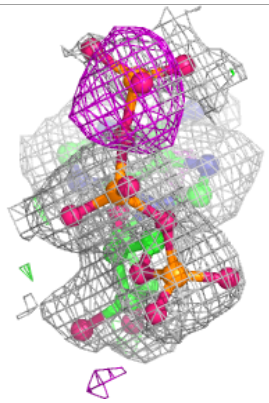
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP C 2601:

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

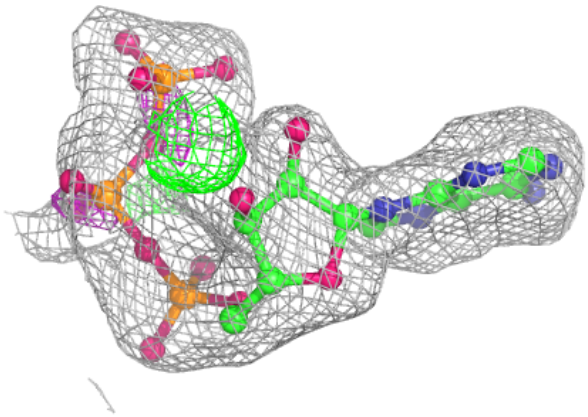


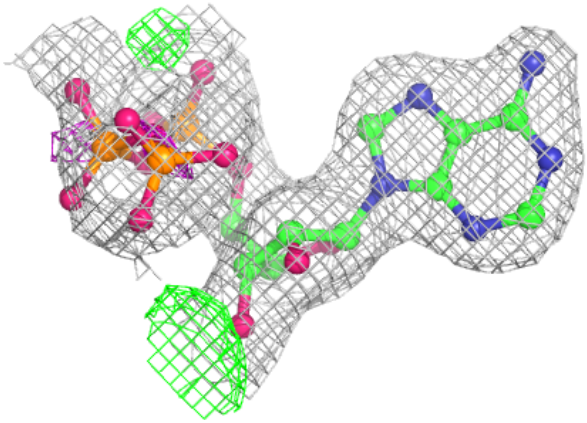


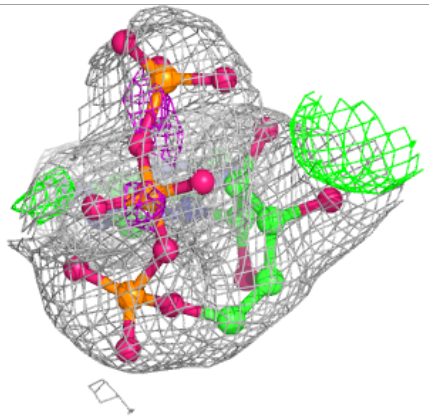


Electron density around ATP A 4602:

$2mF_o$-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 3602:

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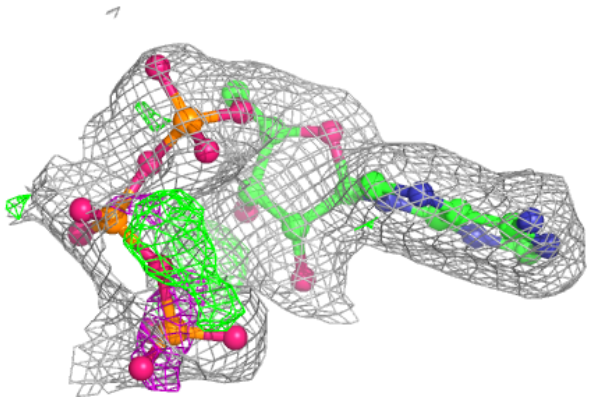
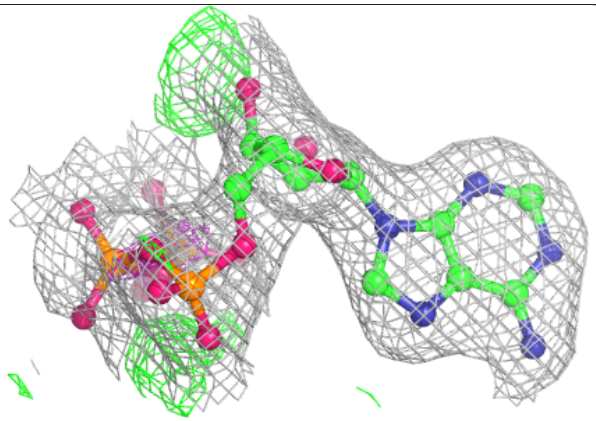
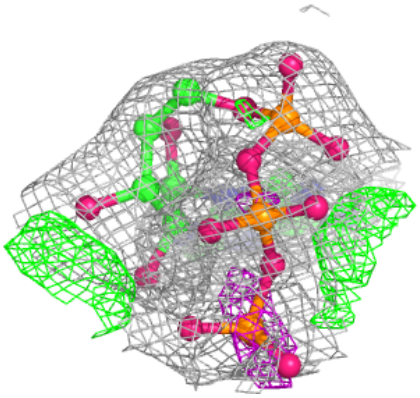
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

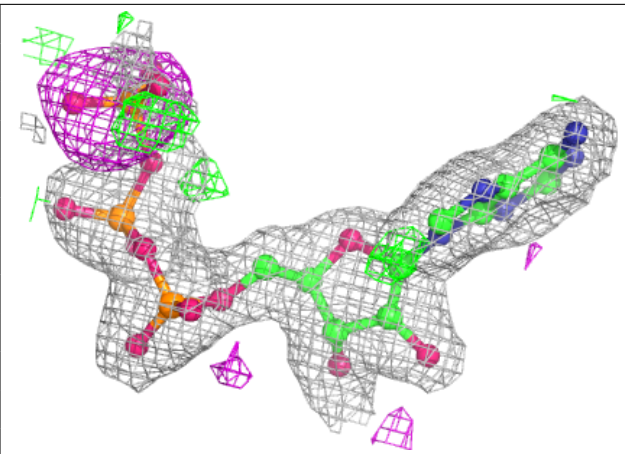


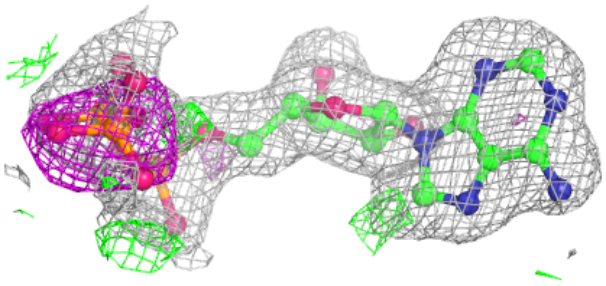


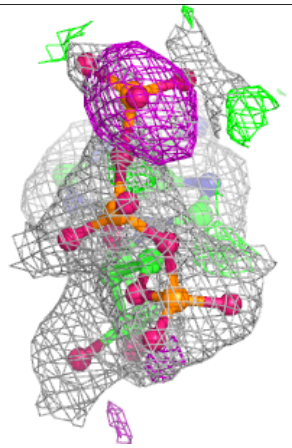


Electron density around ATP A 4601:

$2mF_o$-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 2602:

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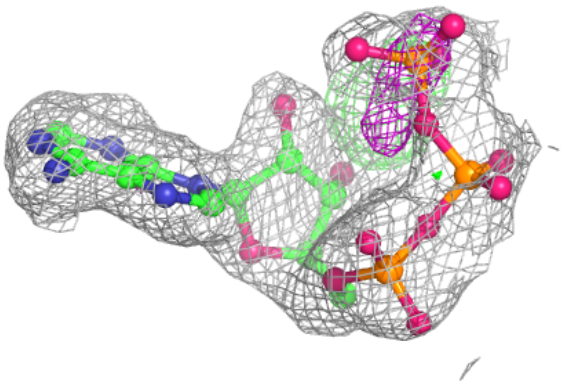
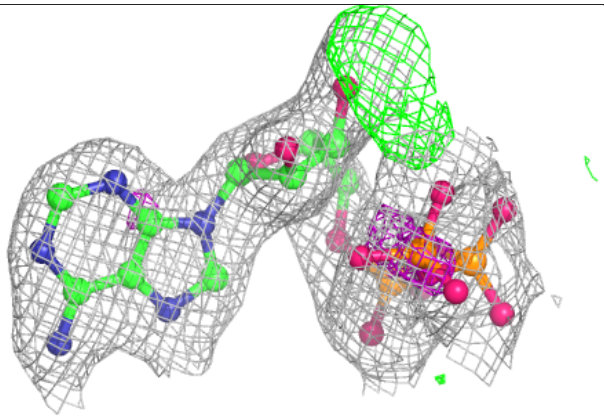
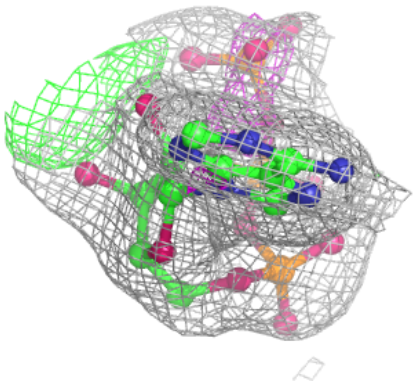
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around ATP B 1602:

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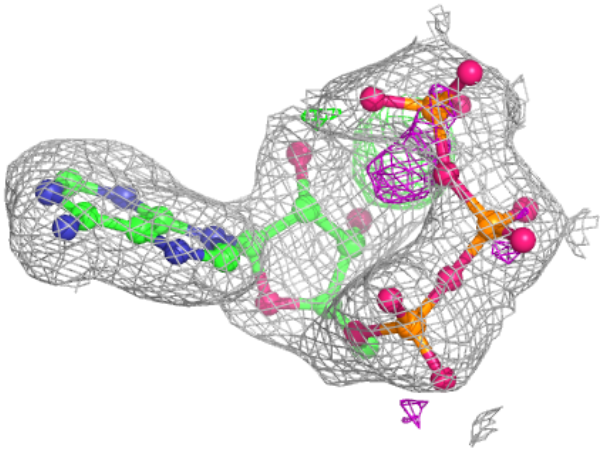
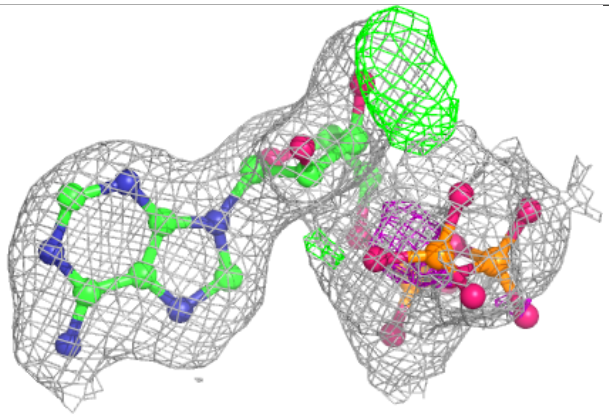
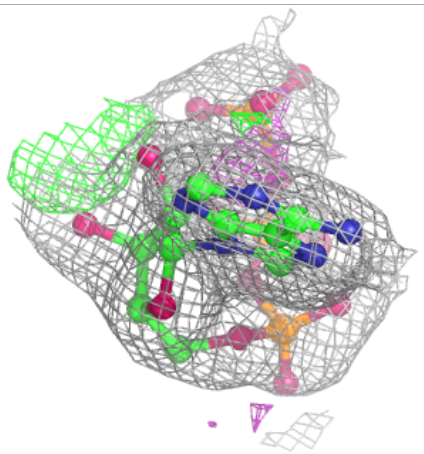
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around ATP D 3601:

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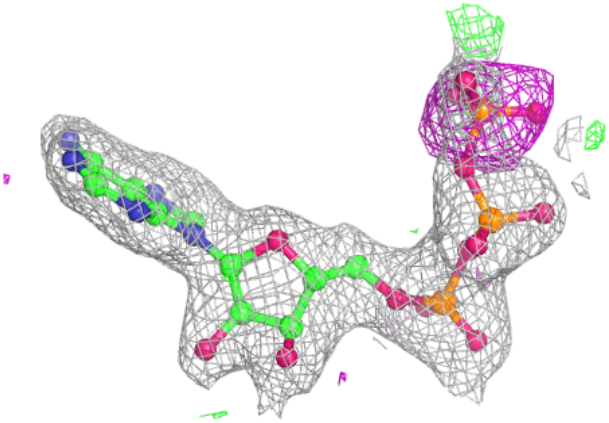
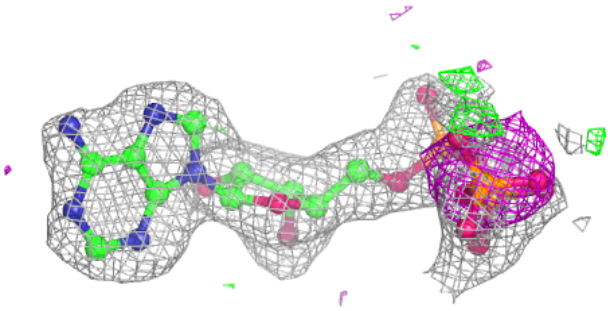
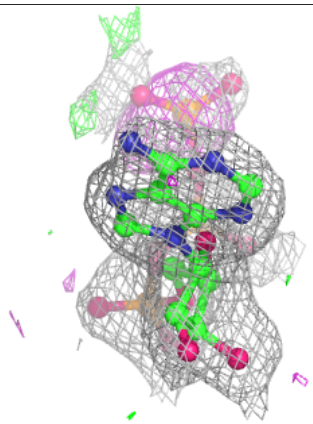
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

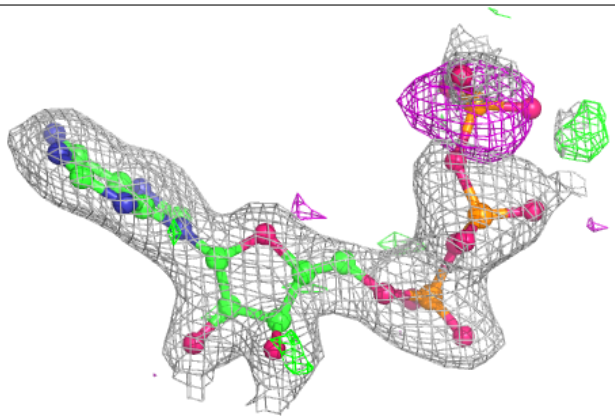


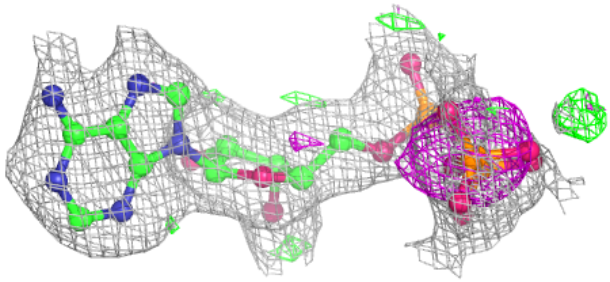


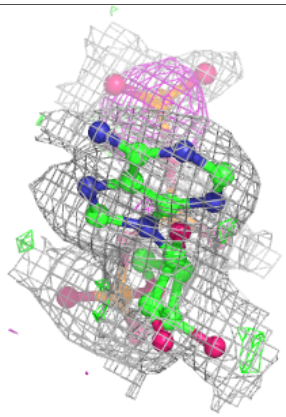


Electron density around ATP B 1601:

$2mF_o$-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.