W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2024 – 03:33 PM EDT

PDB ID	:	1UA2
Title	:	Crystal Structure of Human CDK7
Authors	:	Lolli, G.; Lowe, E.D.; Brown, N.R.; Johnson, L.N.
Deposited on	:	2004-08-11
Resolution	:	3.02 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

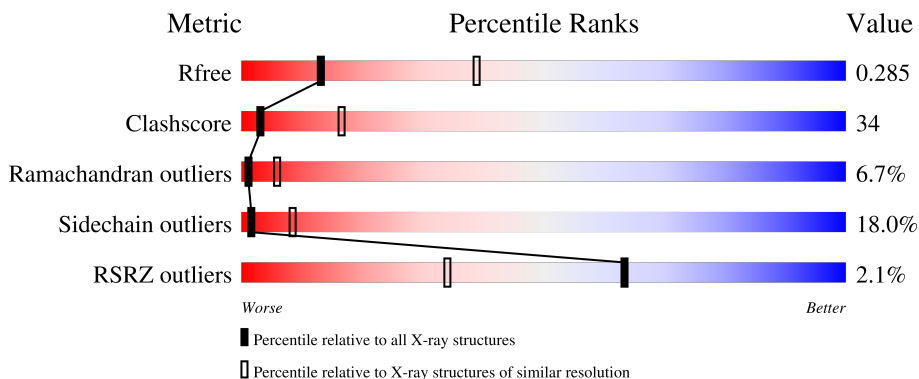|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 3.02 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	Percentile Ranks	Value
Rfree		0.285
Clashscore		34
Ramachandran outliers		6.7%
Sidechain outliers		18.0%
RSRZ outliers		2.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	346	34% 38% 9% · 17%
1	B	346	.% 29% 36% 15% · 17%
1	C	346	4% 36% 35% 11% · 17%
1	D	346	2% 35% 34% 12% · 17%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9336 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 Cell division protein kinase 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	P	S	0	0	0
			2291	1480	387	412	1	11			
1	B	287	Total	C	N	O	P	S	0	0	0
			2291	1480	387	412	1	11			
1	C	287	Total	C	N	O	P	S	0	0	0
			2291	1480	387	412	1	11			
1	D	287	Total	C	N	O	P	S	0	0	0
			2291	1480	387	412	1	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	TPO	THR	modified residue	UNP P50613
B	170	TPO	THR	modified residue	UNP P50613
C	170	TPO	THR	modified residue	UNP P50613
D	170	TPO	THR	modified residue	UNP P50613

- Molecule 2 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
2	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	D	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 3 is water.

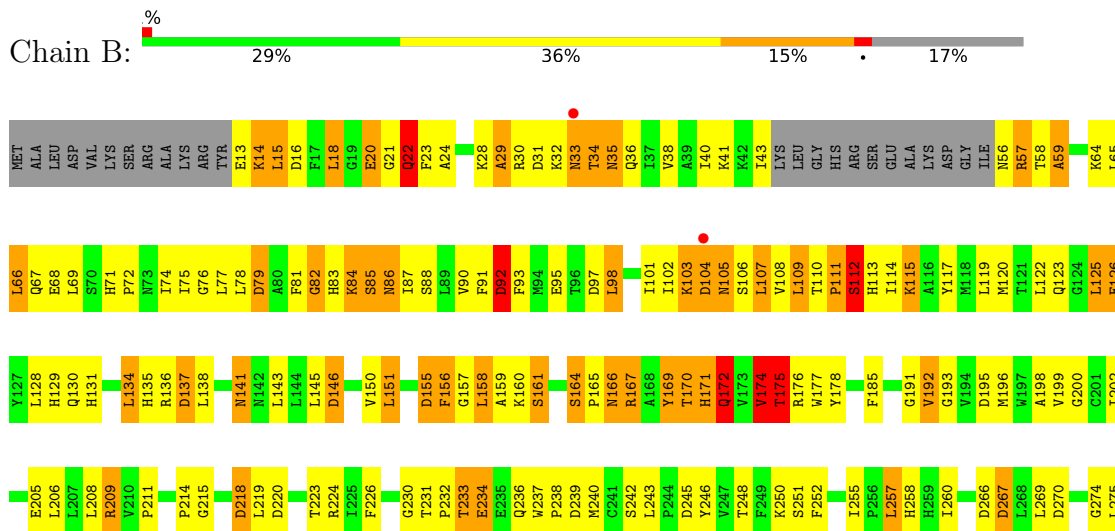| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total 16	O 16	0	0
3	B	13	Total 13	O 13	0	0
3	C	12	Total 12	O 12	0	0
3	D	7	Total 7	O 7	0	0

3 Residue-property plots ⓘ

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: Cell division protein kinase 7

Chain A:

• Molecule 1: Cell division protein kinase 7

Chain B:

F276 L277 F278 C281 A282 R283 I284 T285 A286 T287 Q288 A289 L290 K291 M292 K293 Y294 F295 S296 N297 R298 P299 G304 L307 P308 R309 P310 N311 CYS PRO VAL GLU THR LEU LYS GLU GLN SER ASN PRO ALA LEU ALA ILE LYS ARG LYS ARG THR GLU ALA LEU GLU GLN GLY GLY LEU

PRO LYS LYS LEU ILE PHE

• Molecule 1: Cell division protein kinase 7

Chain C:

4%

36% 35% 11% • 17%

MET ALA LEU ASP VAL LYS SER ARG ALA LYS ARG TYR E13 K14 L15 D16 F17 L18 G21 Q22 F23 V26 Y27 K28 D31 K32 N33 T34 N35 Q36 I40 K41 K42 I43 LYS LEU GLY HIS SER GLU ALA LYS ASP GLY ILE N56 R57 T58 A59 L60 I63 K64 L65 L66

H71 P72 N73 I74 L77 L78 D79 H83 K84 S85 N86 L89 V90 F91 D92 F93 M94 E95 L98 E99 V100 I101 I102 K103 D104 N105 S106 L107 V108 L109 T110 P111 S112 H113 I114 K115 A116 Y117 M118 L119 M120 Q123 G124 L125 H129 Q130 H131 W132 I133 L134 H135 R136 D137

L138 K139 P140 N141 N142 L143 L144 L145 D146 E147 N148 L151 K152 L153 A154 D155 F156 G157 L158 A159 K160 S161 F162 P165 N166 R167 A168 Y169 T170 H171 Q172 V173 V174 T175 R176 W177 Y178 R179 A180 P181 E182 L183 L184 F185 M189 Y190 G191 V192 G193 V194 D195 M196 V199 L203 A204

E205 L206 L207 L208 R209 F212 L213 P214 G215 D216 S217 D218 L219 D220 Q221 L222 T223 R224 I225 P232 T233 E234 E235 Q236 W237 P238 D239 S242 L243 P244 D245 Y246 H259 A264 G265 D266 D267 L268 L269 I272 Q273 L275 N279 P280 C281 A282 R283 I284 T285 Q288 A289

M292 K293 Y294 N297 R298 P301 G304 L307 P308 N311 CYS PRO VAL GLU THR LEU LYS GLU GLN SER ASN PRO ALA LEU ALA ILE LYS ARG LYS ARG THR GLU ALA LEU GLU GLU GLY GLY LEU PRO LYS LYS LEU ILE PHE

• Molecule 1: Cell division protein kinase 7

Chain D:

2%

35% 34% 12% • 17%

MET ALA LEU ASP VAL LYS SER ARG ALA LYS ARG TYR E13 K14 L15 D16 E20 G21 Q22 F23 K28 A29 R30 N33 T34 N35 Q36 I37 I40 K41 K42 I43 LYS LEU GLY HIS ARG SER GLU ALA LYS ASP GLY ILE N56 R57 T58 A59 L60 L65 L78 D79 A80 F81

G82 H83 K84 S88 L89 V90 F91 D92 F93 M94 E95 T96 D97 L98 E99 V100 I101 I102 K103 D104 N105 S106 T110 P111 S112 H113 I114 Y117 T121 L122 L125 L128 H129 Q130 I133 L134 R135 R136 D137 L138 K139 P140 N141 N142 L143 L144 L145 D146 E147 V150 L151

A154 D155 F156 G157 L158 A159 K160 S161 F162 G163 S164 P165 N166 R167 A168 Y169 T170 H171 Q172 V173 V174 T175 R176 W177 Y178 R179 A180 P181 E182 L183 L184 F185 G186 A187 R188 M189 V192 D195 V199 L202 L203 A204 E205 L206 L207 L208 R209 P214 G215 D216 S217 D218 L219 D220 Q221

L222 T223 R224 I225 F226 G230 T231 P232 T233 E234 E235 Q236 W237 P238 D239 M240 C241 S242 L243 P244 D245 V246 V247 T248 F249 K250 I255 P256 L267 H258 H259 I260 F261 S262 D266 D267 L268 L269 D270 L271 I272 Q273 L277 F278 C281 A282 R283 I284 T285 A286 T287 Q288 A289 L290 K291

M292 K293 Y294 R298 T302 P303 G304 L307 P308 R309 P310 N311 CYS PRO VAL GLU THR LEU LYS GLU GLN SER ASN PRO ALA LEU ALA ILE LYS ARG LYS ARG THR GLU ALA LEU GLU GLN GLY GLY LEU PRO LYS LYS LEU ILE PHE

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.50Å 191.63Å 75.79Å 90.00° 94.40° 90.00°	Depositor
Resolution (Å)	49.45 – 3.02 29.42 – 2.96	Depositor EDS
% Data completeness (in resolution range)	95.5 (49.45-3.02) 91.2 (29.42-2.96)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.213 , 0.288 0.210 , 0.285	Depositor DCC
R_{free} test set	1767 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9336	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: TPO, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.79	0/2336	1.04	8/3169 (0.3%)
1	B	0.76	0/2336	1.05	16/3169 (0.5%)
1	C	0.76	0/2336	1.00	11/3169 (0.3%)
1	D	0.68	0/2336	0.99	11/3169 (0.3%)
All	All	0.75	0/9344	1.02	46/12676 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
1	C	0	2
All	All	0	9

There are no bond length outliers.

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	195	ASP	CB-CG-OD2	9.33	126.70	118.30
1	A	92	ASP	CB-CG-OD2	7.60	125.14	118.30
1	A	216	ASP	CB-CG-OD2	7.57	125.11	118.30
1	B	270	ASP	CB-CG-OD2	7.17	124.75	118.30
1	D	195	ASP	CB-CG-OD2	7.12	124.70	118.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

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Mol	Chain	Res	Type	Group
1	A	112	SER	Peptide
1	A	164	SER	Peptide
1	A	297	ASN	Peptide
1	A	304	GLY	Peptide
1	B	34	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2291	0	2300	182	0
1	B	2291	0	2300	169	0
1	C	2291	0	2300	134	0
1	D	2291	0	2300	138	0
2	A	31	0	12	2	0
2	B	31	0	12	3	0
2	C	31	0	12	1	0
2	D	31	0	12	0	0
3	A	16	0	0	9	0
3	B	13	0	0	5	0
3	C	12	0	0	1	0
3	D	7	0	0	2	0
All	All	9336	0	9248	625	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 34.

The worst 5 of 625 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:234:GLU:OE2	1:A:238:PRO:HA	1.21	1.34
1:A:43:ILE:CD1	1:A:160:LYS:HE2	1.70	1.21
1:A:32:LYS:HB2	1:A:32:LYS:NZ	1.49	1.20
1:A:24:ALA:CB	1:A:160:LYS:NZ	2.06	1.18
1:A:103:LYS:O	1:A:105:ASN:N	1.75	1.17

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	282/346 (82%)	242 (86%)	22 (8%)	18 (6%)	1	7
1	B	282/346 (82%)	231 (82%)	26 (9%)	25 (9%)	1	3
1	C	282/346 (82%)	237 (84%)	30 (11%)	15 (5%)	2	11
1	D	282/346 (82%)	227 (80%)	37 (13%)	18 (6%)	1	7
All	All	1128/1384 (82%)	937 (83%)	115 (10%)	76 (7%)	1	6

5 of 76 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	22	GLN
1	A	84	LYS
1	A	104	ASP
1	A	112	SER

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	249/298 (84%)	213 (86%)	36 (14%)	3	14
1	B	249/298 (84%)	200 (80%)	49 (20%)	1	7
1	C	249/298 (84%)	207 (83%)	42 (17%)	2	10
1	D	249/298 (84%)	197 (79%)	52 (21%)	1	5
All	All	996/1192 (84%)	817 (82%)	179 (18%)	1	8

5 of 179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	206	LEU
1	D	104	ASP
1	C	233	THR
1	D	20	GLU
1	D	139	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	35	ASN
1	C	141	ASN
1	C	86	ASN
1	C	236	GLN
1	B	33	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	#$|Z| > 2$
1	TPO	B	170	1	8,10,11	3.30	4 (50%)	10,14,16	0.88	0
1	TPO	D	170	1	8,10,11	3.40	4 (50%)	10,14,16	1.06	0
1	TPO	C	170	1	8,10,11	3.25	4 (50%)	10,14,16	0.78	0
1	TPO	A	170	1	8,10,11	3.23	4 (50%)	10,14,16	1.36	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
1	TPO	B	170	1	-	2/9/11/13	-
1	TPO	D	170	1	-	6/9/11/13	-
1	TPO	C	170	1	-	5/9/11/13	-
1	TPO	A	170	1	-	4/9/11/13	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	170	TPO	P-O1P	6.71	1.72	1.50
1	B	170	TPO	P-O1P	6.66	1.72	1.50
1	C	170	TPO	P-O1P	6.43	1.71	1.50
1	A	170	TPO	P-O1P	6.24	1.70	1.50
1	D	170	TPO	P-O2P	4.41	1.71	1.54

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	170	TPO	N-CA-CB-CG2
1	A	170	TPO	N-CA-CB-OG1
1	A	170	TPO	C-CA-CB-CG2
1	A	170	TPO	O-C-CA-CB
1	B	170	TPO	N-CA-CB-OG1

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	170	TPO	1	0
1	D	170	TPO	3	0
1	C	170	TPO	1	0
1	A	170	TPO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6   Ligand geometry   ⓘ

4 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	#$|Z| > 2$
2	ATP	C	383	-	26,33,33	1.03	2 (7%)	31,52,52	1.63	6 (19%)
2	ATP	A	381	-	26,33,33	0.98	2 (7%)	31,52,52	1.44	5 (16%)
2	ATP	B	382	-	26,33,33	1.02	2 (7%)	31,52,52	1.74	7 (22%)
2	ATP	D	384	-	26,33,33	0.91	1 (3%)	31,52,52	1.64	8 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	C	383	-	-	4/18/38/38	0/3/3/3
2	ATP	A	381	-	-	6/18/38/38	0/3/3/3
2	ATP	B	382	-	-	5/18/38/38	0/3/3/3
2	ATP	D	384	-	-	3/18/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	383	ATP	C5-C4	2.56	1.47	1.40
2	D	384	ATP	C5-C4	2.39	1.47	1.40
2	A	381	ATP	C5-C4	2.38	1.47	1.40
2	B	382	ATP	O4'-C1'	2.33	1.44	1.41
2	C	383	ATP	O4'-C1'	2.19	1.44	1.41

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	381	ATP	PA-O3A-PB	-4.17	118.52	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	382	ATP	PB-O3B-PG	-4.14	118.62	132.83
2	B	382	ATP	C4-C5-N7	-3.84	105.39	109.40
2	C	383	ATP	C3'-C2'-C1'	3.84	106.76	100.98
2	D	384	ATP	N3-C2-N1	-3.84	122.67	128.68

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	381	ATP	PB-O3B-PG-O2G
2	A	381	ATP	PB-O3B-PG-O3G
2	C	383	ATP	O4'-C4'-C5'-O5'
2	C	383	ATP	C3'-C4'-C5'-O5'
2	D	384	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	383	ATP	1	0
2	A	381	ATP	2	0
2	B	382	ATP	3	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 C 383

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 381

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 382

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP D 384

Bond lengths

Bond angles

Torsions

Rings
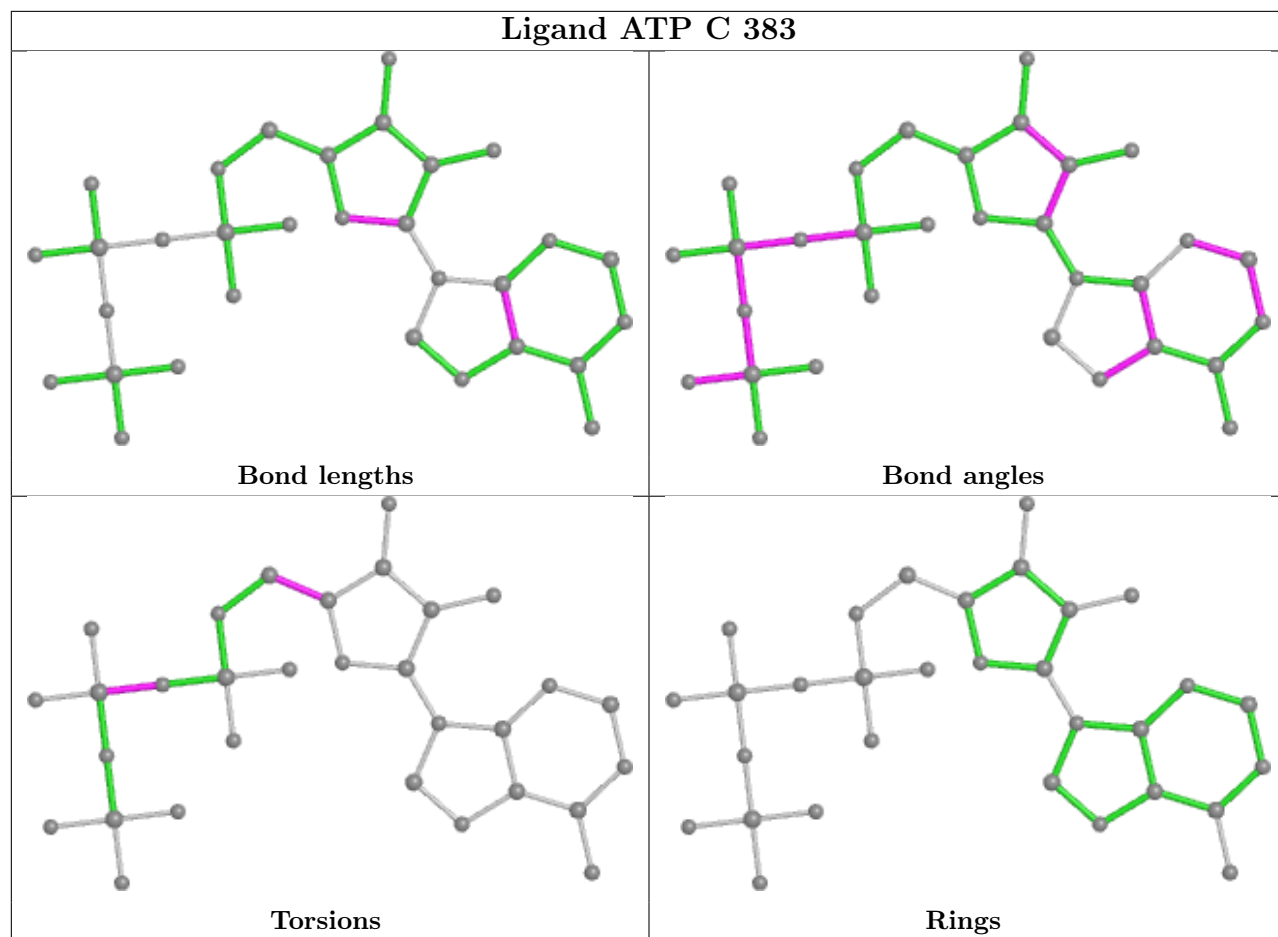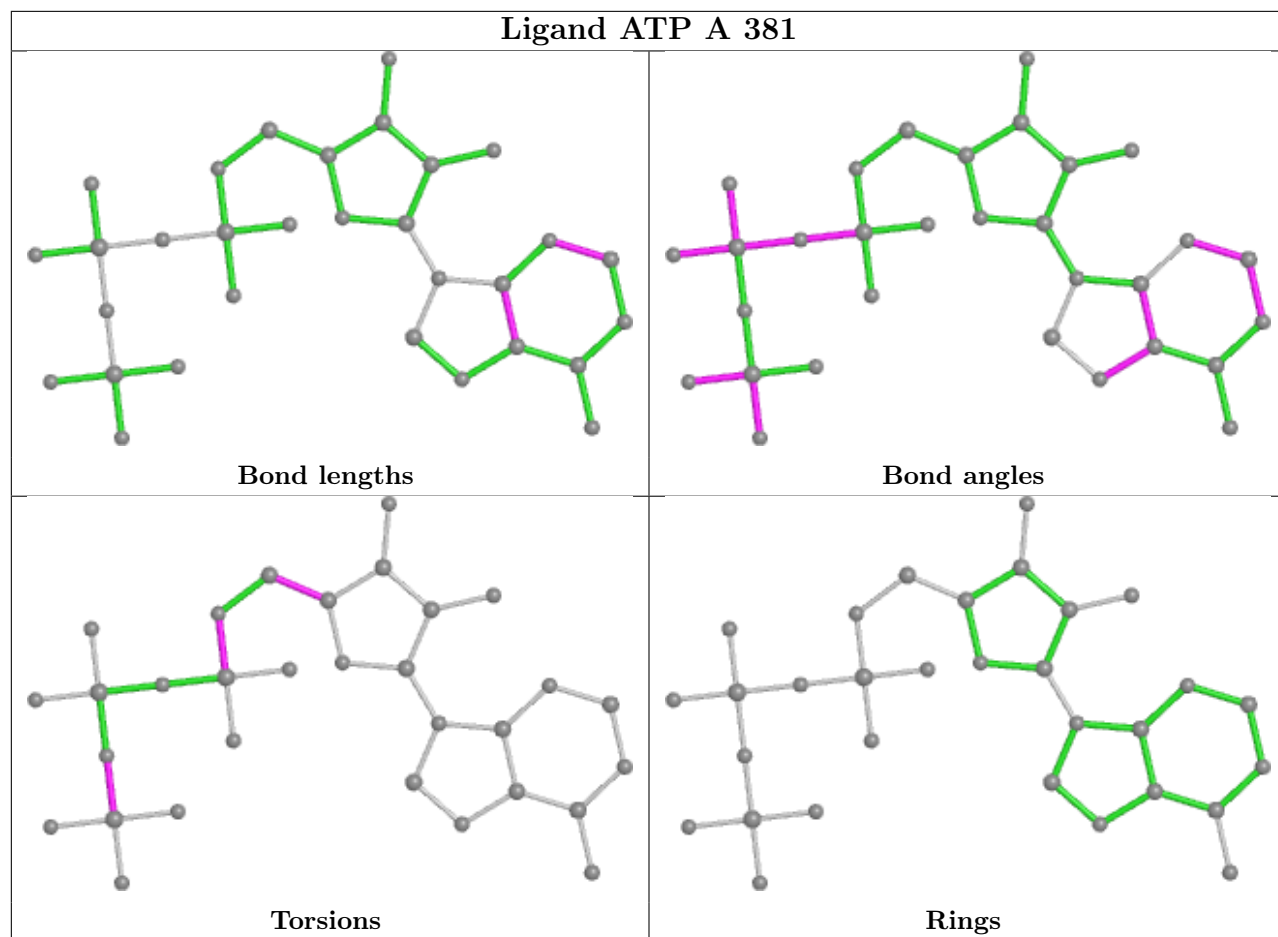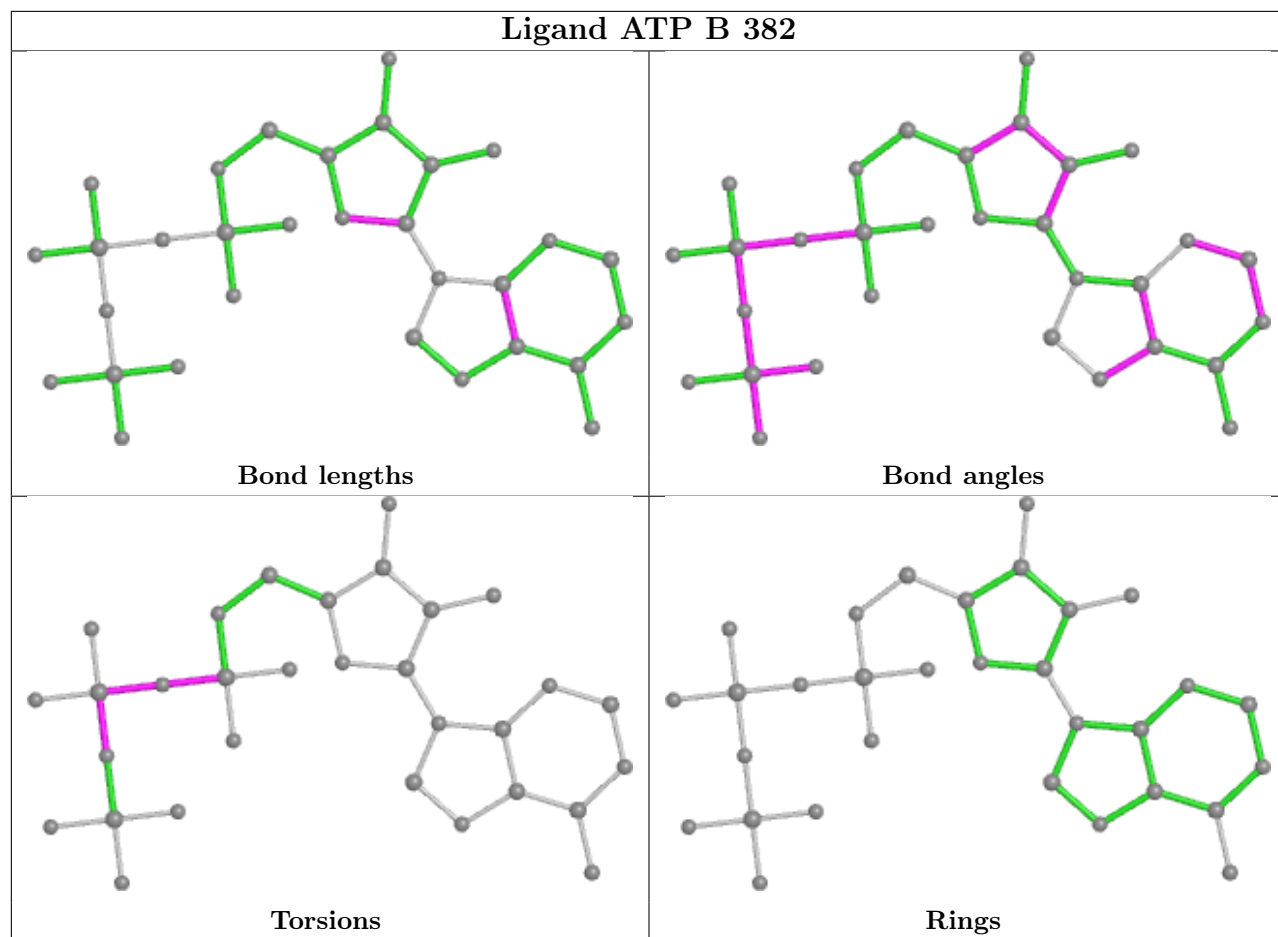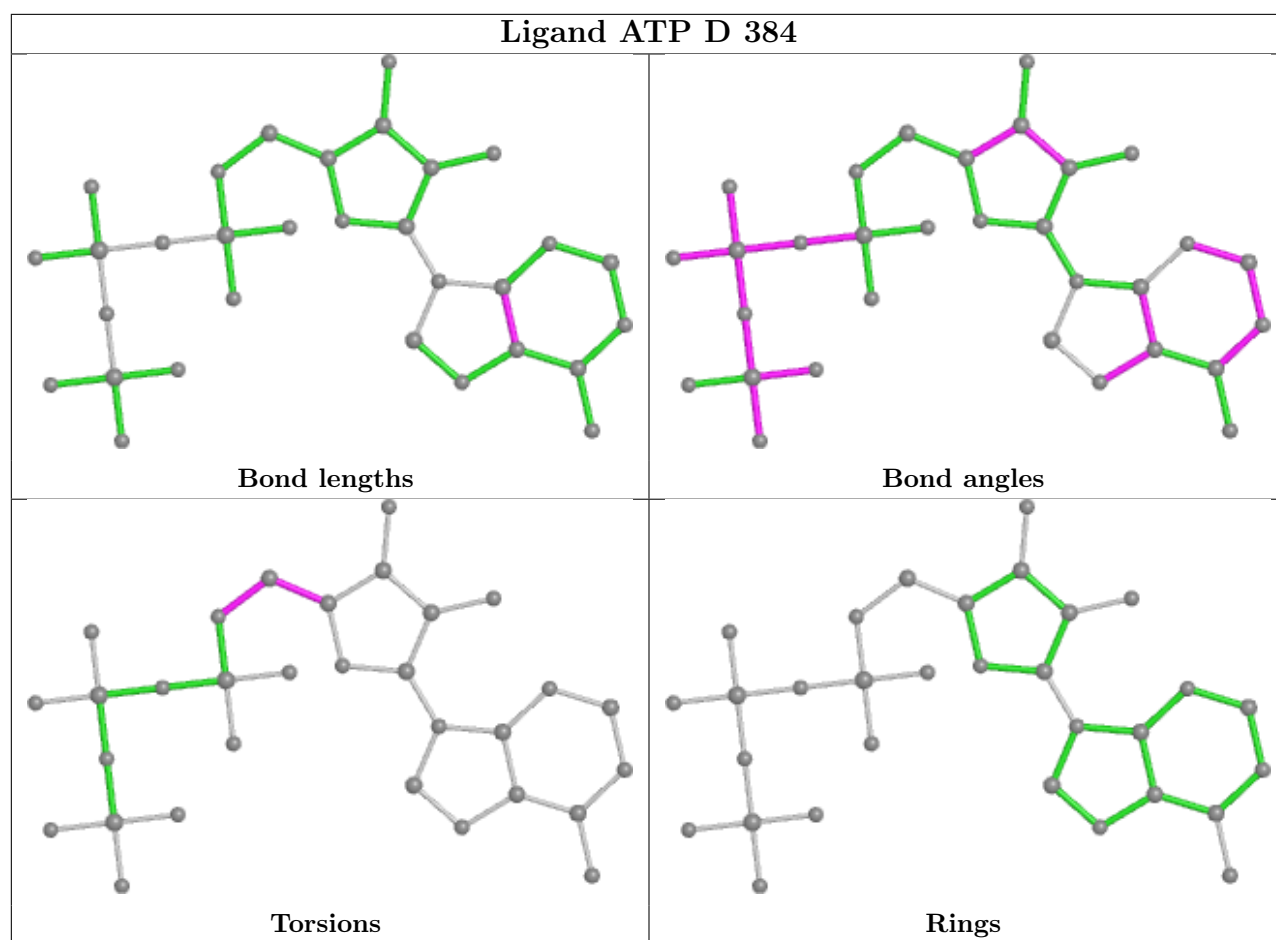
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	286/346 (82%)	-0.39	1 (0%)	94	83	18, 36, 68, 79	0
1	B	286/346 (82%)	-0.35	2 (0%)	87	68	16, 40, 74, 82	0
1	C	286/346 (82%)	-0.17	13 (4%)	33	12	20, 37, 78, 86	0
1	D	286/346 (82%)	-0.22	8 (2%)	53	24	23, 46, 79, 87	0
All	All	1144/1384 (82%)	-0.28	24 (2%)	63	34	16, 40, 74, 87	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	ASP	4.1
1	C	33	ASN	3.3
1	A	165	PRO	3.2
1	C	171	HIS	3.2
1	C	84	LYS	2.9

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

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.

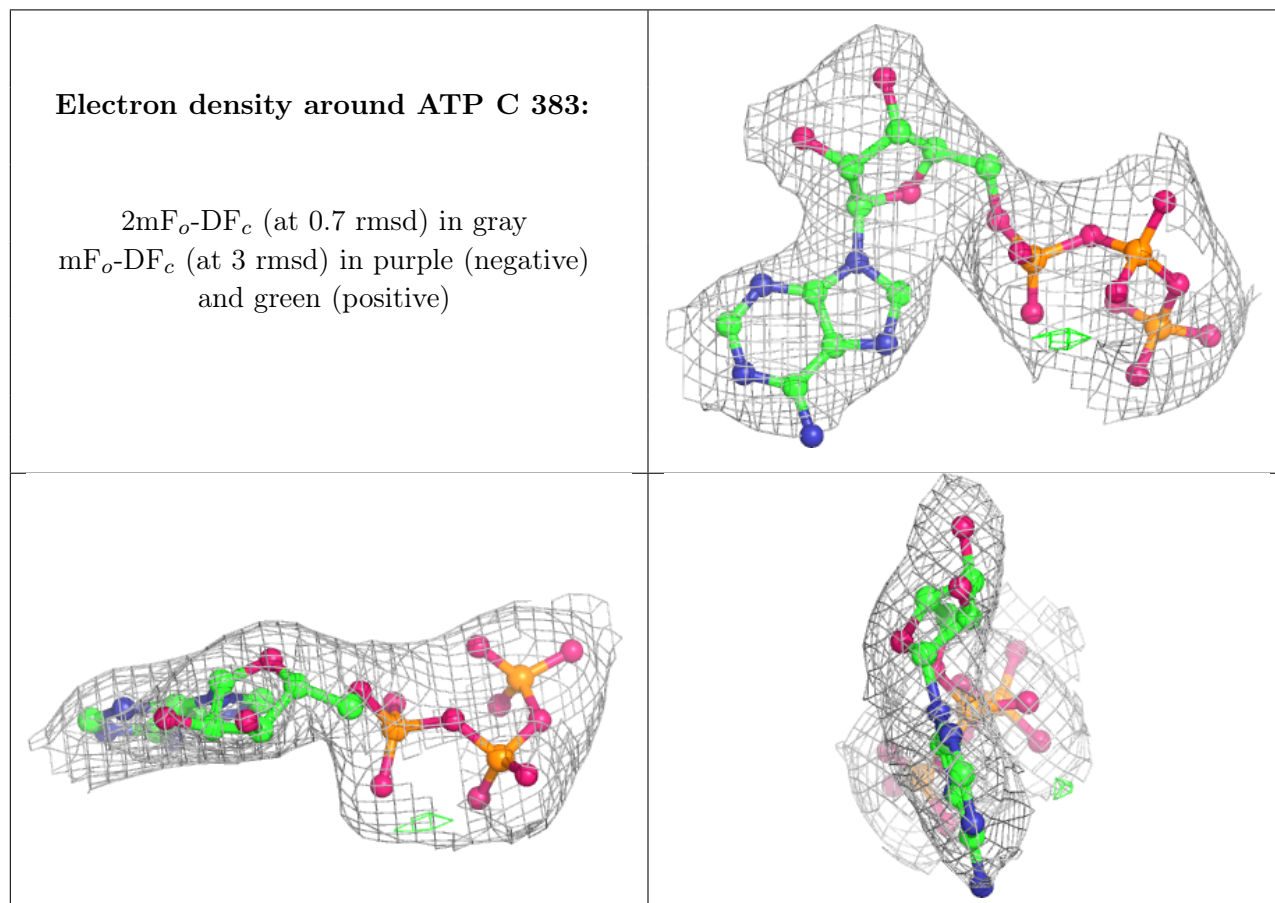| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPO	D	170	11/12	0.73	0.36	74,76,84,84	0
1	TPO	C	170	11/12	0.82	0.38	76,78,83,84	0
1	TPO	B	170	11/12	0.83	0.26	71,72,77,77	0
1	TPO	A	170	11/12	0.87	0.26	64,65,66,68	0

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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	ATP	C	383	31/31	0.94	0.15	54,59,66,66	0
2	ATP	D	384	31/31	0.95	0.21	59,65,70,70	0
2	ATP	A	381	31/31	0.96	0.12	32,35,46,47	0
2	ATP	B	382	31/31	0.96	0.17	50,57,67,68	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 383:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
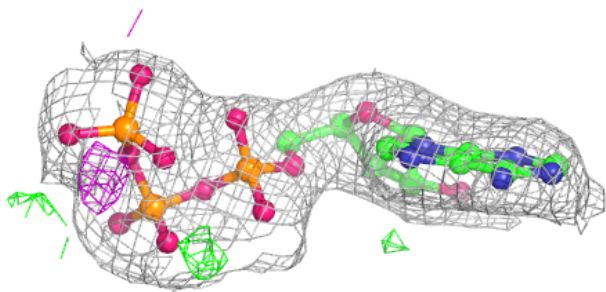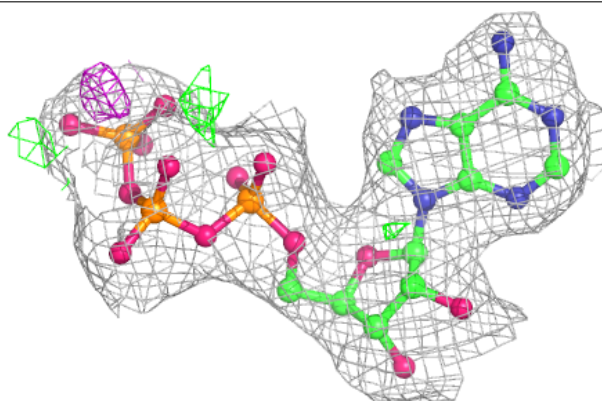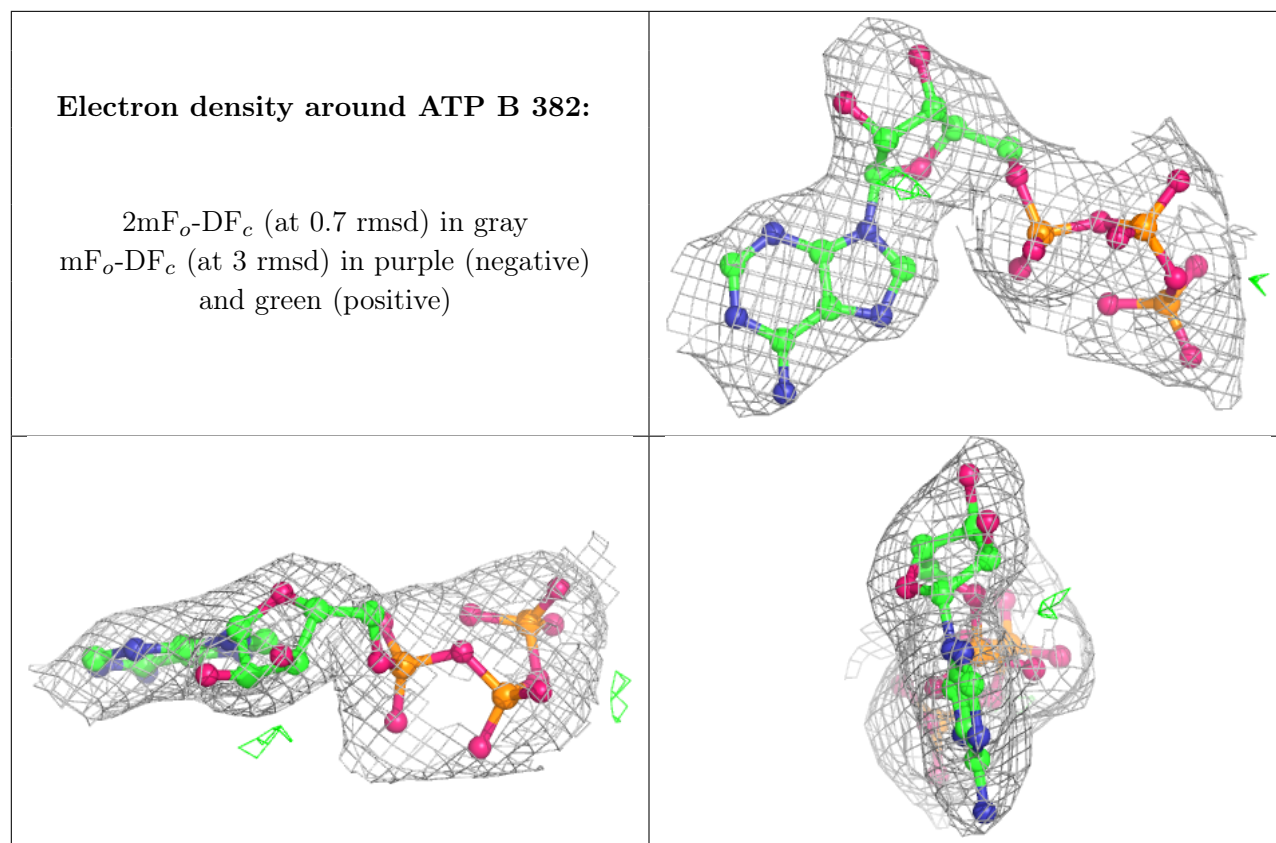
Electron density around ATP D 384:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
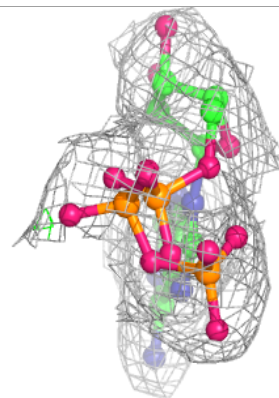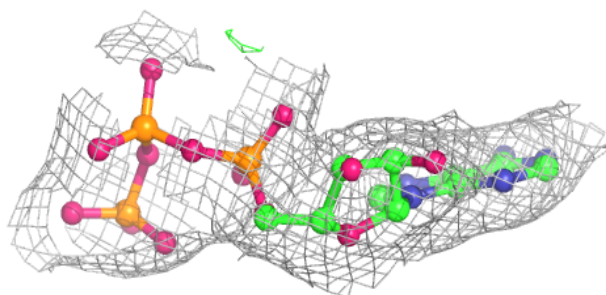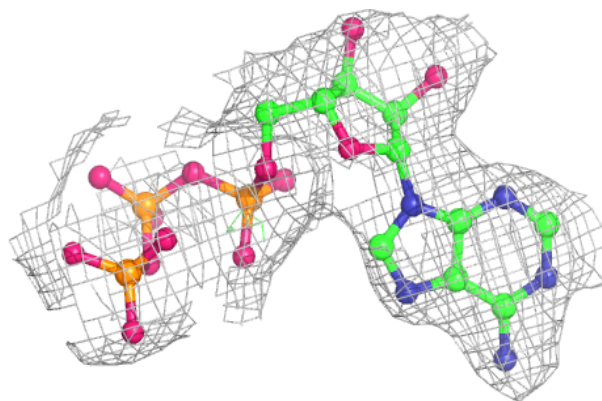
Electron density around ATP A 381:

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

Electron density around ATP B 382:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
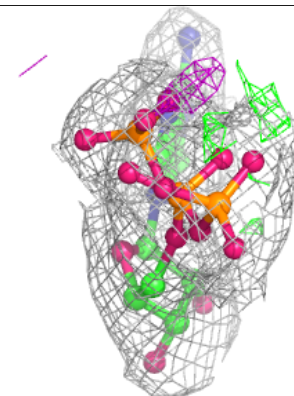
6.5   Other polymers (i)

There are no such residues in this entry.