WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 19, 2023 – 06:10 PM JST

PDB ID : 6LUF
Title : Trans-acting mutant Y290A of the central AAA+ domain of the flagellar regulatory protein FlrC
Authors : Dasgupta, J.; Chakraborty, S.
Deposited on : 2020-01-27
Resolution : 3.45 Å(reported)

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 3.45 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.
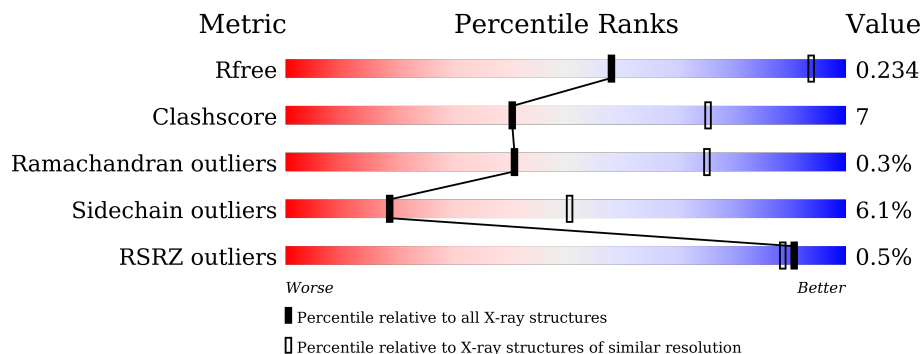
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	271	71% 17% · 9%
1	B	271	71% 16% · 9%
1	C	271	% 77% 13% · 9%
1	D	271	73% 15% · 9%
1	E	271	70% 19% · 9%
1	F	271	% 70% 20% · 9%

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Mol	Chain	Length	Quality of chain
1	G	271	69% 20% 9%

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	ADP	D	401	-	-	-	X
2	ADP	F	401	-	-	-	X

2　Entry composition　ⓘ

There are 2 unique types of molecules in this entry. The entry contains 13613 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 Flagellar regulatory protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total 1923	C 1217	N 343	O 354	S 9	0	0	0
1	B	247	Total 1923	C 1217	N 343	O 354	S 9	0	0	0
1	C	246	Total 1921	C 1216	N 343	O 353	S 9	0	1	0
1	D	246	Total 1913	C 1211	N 340	O 353	S 9	0	0	0
1	E	246	Total 1913	C 1211	N 340	O 353	S 9	0	0	0
1	F	247	Total 1918	C 1214	N 341	O 354	S 9	0	0	0
1	G	246	Total 1913	C 1211	N 340	O 353	S 9	0	0	0

There are 154 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	MET	-	initiating methionine	UNP A0A0H3AHP1
A	112	GLY	-	expression tag	UNP A0A0H3AHP1
A	113	SER	-	expression tag	UNP A0A0H3AHP1
A	114	SER	-	expression tag	UNP A0A0H3AHP1
A	115	HIS	-	expression tag	UNP A0A0H3AHP1
A	116	HIS	-	expression tag	UNP A0A0H3AHP1
A	117	HIS	-	expression tag	UNP A0A0H3AHP1
A	118	HIS	-	expression tag	UNP A0A0H3AHP1
A	119	HIS	-	expression tag	UNP A0A0H3AHP1
A	120	HIS	-	expression tag	UNP A0A0H3AHP1
A	121	SER	-	expression tag	UNP A0A0H3AHP1
A	122	SER	-	expression tag	UNP A0A0H3AHP1
A	123	GLY	-	expression tag	UNP A0A0H3AHP1
A	124	LEU	-	expression tag	UNP A0A0H3AHP1
A	125	VAL	-	expression tag	UNP A0A0H3AHP1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	126	PRO	-	expression tag	UNP A0A0H3AHP1
A	127	ARG	-	expression tag	UNP A0A0H3AHP1
A	128	GLY	-	expression tag	UNP A0A0H3AHP1
A	129	SER	-	expression tag	UNP A0A0H3AHP1
A	130	HIS	-	expression tag	UNP A0A0H3AHP1
A	131	MET	-	expression tag	UNP A0A0H3AHP1
A	290	ALA	TYR	engineered mutation	UNP A0A0H3AHP1
B	111	MET	-	initiating methionine	UNP A0A0H3AHP1
B	112	GLY	-	expression tag	UNP A0A0H3AHP1
B	113	SER	-	expression tag	UNP A0A0H3AHP1
B	114	SER	-	expression tag	UNP A0A0H3AHP1
B	115	HIS	-	expression tag	UNP A0A0H3AHP1
B	116	HIS	-	expression tag	UNP A0A0H3AHP1
B	117	HIS	-	expression tag	UNP A0A0H3AHP1
B	118	HIS	-	expression tag	UNP A0A0H3AHP1
B	119	HIS	-	expression tag	UNP A0A0H3AHP1
B	120	HIS	-	expression tag	UNP A0A0H3AHP1
B	121	SER	-	expression tag	UNP A0A0H3AHP1
B	122	SER	-	expression tag	UNP A0A0H3AHP1
B	123	GLY	-	expression tag	UNP A0A0H3AHP1
B	124	LEU	-	expression tag	UNP A0A0H3AHP1
B	125	VAL	-	expression tag	UNP A0A0H3AHP1
B	126	PRO	-	expression tag	UNP A0A0H3AHP1
B	127	ARG	-	expression tag	UNP A0A0H3AHP1
B	128	GLY	-	expression tag	UNP A0A0H3AHP1
B	129	SER	-	expression tag	UNP A0A0H3AHP1
B	130	HIS	-	expression tag	UNP A0A0H3AHP1
B	131	MET	-	expression tag	UNP A0A0H3AHP1
B	290	ALA	TYR	engineered mutation	UNP A0A0H3AHP1
C	111	MET	-	initiating methionine	UNP A0A0H3AHP1
C	112	GLY	-	expression tag	UNP A0A0H3AHP1
C	113	SER	-	expression tag	UNP A0A0H3AHP1
C	114	SER	-	expression tag	UNP A0A0H3AHP1
C	115	HIS	-	expression tag	UNP A0A0H3AHP1
C	116	HIS	-	expression tag	UNP A0A0H3AHP1
C	117	HIS	-	expression tag	UNP A0A0H3AHP1
C	118	HIS	-	expression tag	UNP A0A0H3AHP1
C	119	HIS	-	expression tag	UNP A0A0H3AHP1
C	120	HIS	-	expression tag	UNP A0A0H3AHP1
C	121	SER	-	expression tag	UNP A0A0H3AHP1
C	122	SER	-	expression tag	UNP A0A0H3AHP1
C	123	GLY	-	expression tag	UNP A0A0H3AHP1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	124	LEU	-	expression tag	UNP A0A0H3AHP1
C	125	VAL	-	expression tag	UNP A0A0H3AHP1
C	126	PRO	-	expression tag	UNP A0A0H3AHP1
C	127	ARG	-	expression tag	UNP A0A0H3AHP1
C	128	GLY	-	expression tag	UNP A0A0H3AHP1
C	129	SER	-	expression tag	UNP A0A0H3AHP1
C	130	HIS	-	expression tag	UNP A0A0H3AHP1
C	131	MET	-	expression tag	UNP A0A0H3AHP1
C	290	ALA	TYR	engineered mutation	UNP A0A0H3AHP1
D	111	MET	-	initiating methionine	UNP A0A0H3AHP1
D	112	GLY	-	expression tag	UNP A0A0H3AHP1
D	113	SER	-	expression tag	UNP A0A0H3AHP1
D	114	SER	-	expression tag	UNP A0A0H3AHP1
D	115	HIS	-	expression tag	UNP A0A0H3AHP1
D	116	HIS	-	expression tag	UNP A0A0H3AHP1
D	117	HIS	-	expression tag	UNP A0A0H3AHP1
D	118	HIS	-	expression tag	UNP A0A0H3AHP1
D	119	HIS	-	expression tag	UNP A0A0H3AHP1
D	120	HIS	-	expression tag	UNP A0A0H3AHP1
D	121	SER	-	expression tag	UNP A0A0H3AHP1
D	122	SER	-	expression tag	UNP A0A0H3AHP1
D	123	GLY	-	expression tag	UNP A0A0H3AHP1
D	124	LEU	-	expression tag	UNP A0A0H3AHP1
D	125	VAL	-	expression tag	UNP A0A0H3AHP1
D	126	PRO	-	expression tag	UNP A0A0H3AHP1
D	127	ARG	-	expression tag	UNP A0A0H3AHP1
D	128	GLY	-	expression tag	UNP A0A0H3AHP1
D	129	SER	-	expression tag	UNP A0A0H3AHP1
D	130	HIS	-	expression tag	UNP A0A0H3AHP1
D	131	MET	-	expression tag	UNP A0A0H3AHP1
D	290	ALA	TYR	engineered mutation	UNP A0A0H3AHP1
E	111	MET	-	initiating methionine	UNP A0A0H3AHP1
E	112	GLY	-	expression tag	UNP A0A0H3AHP1
E	113	SER	-	expression tag	UNP A0A0H3AHP1
E	114	SER	-	expression tag	UNP A0A0H3AHP1
E	115	HIS	-	expression tag	UNP A0A0H3AHP1
E	116	HIS	-	expression tag	UNP A0A0H3AHP1
E	117	HIS	-	expression tag	UNP A0A0H3AHP1
E	118	HIS	-	expression tag	UNP A0A0H3AHP1
E	119	HIS	-	expression tag	UNP A0A0H3AHP1
E	120	HIS	-	expression tag	UNP A0A0H3AHP1
E	121	SER	-	expression tag	UNP A0A0H3AHP1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	122	SER	-	expression tag	UNP A0A0H3AHP1
E	123	GLY	-	expression tag	UNP A0A0H3AHP1
E	124	LEU	-	expression tag	UNP A0A0H3AHP1
E	125	VAL	-	expression tag	UNP A0A0H3AHP1
E	126	PRO	-	expression tag	UNP A0A0H3AHP1
E	127	ARG	-	expression tag	UNP A0A0H3AHP1
E	128	GLY	-	expression tag	UNP A0A0H3AHP1
E	129	SER	-	expression tag	UNP A0A0H3AHP1
E	130	HIS	-	expression tag	UNP A0A0H3AHP1
E	131	MET	-	expression tag	UNP A0A0H3AHP1
E	290	ALA	TYR	engineered mutation	UNP A0A0H3AHP1
F	111	MET	-	initiating methionine	UNP A0A0H3AHP1
F	112	GLY	-	expression tag	UNP A0A0H3AHP1
F	113	SER	-	expression tag	UNP A0A0H3AHP1
F	114	SER	-	expression tag	UNP A0A0H3AHP1
F	115	HIS	-	expression tag	UNP A0A0H3AHP1
F	116	HIS	-	expression tag	UNP A0A0H3AHP1
F	117	HIS	-	expression tag	UNP A0A0H3AHP1
F	118	HIS	-	expression tag	UNP A0A0H3AHP1
F	119	HIS	-	expression tag	UNP A0A0H3AHP1
F	120	HIS	-	expression tag	UNP A0A0H3AHP1
F	121	SER	-	expression tag	UNP A0A0H3AHP1
F	122	SER	-	expression tag	UNP A0A0H3AHP1
F	123	GLY	-	expression tag	UNP A0A0H3AHP1
F	124	LEU	-	expression tag	UNP A0A0H3AHP1
F	125	VAL	-	expression tag	UNP A0A0H3AHP1
F	126	PRO	-	expression tag	UNP A0A0H3AHP1
F	127	ARG	-	expression tag	UNP A0A0H3AHP1
F	128	GLY	-	expression tag	UNP A0A0H3AHP1
F	129	SER	-	expression tag	UNP A0A0H3AHP1
F	130	HIS	-	expression tag	UNP A0A0H3AHP1
F	131	MET	-	expression tag	UNP A0A0H3AHP1
F	290	ALA	TYR	engineered mutation	UNP A0A0H3AHP1
G	111	MET	-	initiating methionine	UNP A0A0H3AHP1
G	112	GLY	-	expression tag	UNP A0A0H3AHP1
G	113	SER	-	expression tag	UNP A0A0H3AHP1
G	114	SER	-	expression tag	UNP A0A0H3AHP1
G	115	HIS	-	expression tag	UNP A0A0H3AHP1
G	116	HIS	-	expression tag	UNP A0A0H3AHP1
G	117	HIS	-	expression tag	UNP A0A0H3AHP1
G	118	HIS	-	expression tag	UNP A0A0H3AHP1
G	119	HIS	-	expression tag	UNP A0A0H3AHP1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	120	HIS	-	expression tag	UNP A0A0H3AHP1
G	121	SER	-	expression tag	UNP A0A0H3AHP1
G	122	SER	-	expression tag	UNP A0A0H3AHP1
G	123	GLY	-	expression tag	UNP A0A0H3AHP1
G	124	LEU	-	expression tag	UNP A0A0H3AHP1
G	125	VAL	-	expression tag	UNP A0A0H3AHP1
G	126	PRO	-	expression tag	UNP A0A0H3AHP1
G	127	ARG	-	expression tag	UNP A0A0H3AHP1
G	128	GLY	-	expression tag	UNP A0A0H3AHP1
G	129	SER	-	expression tag	UNP A0A0H3AHP1
G	130	HIS	-	expression tag	UNP A0A0H3AHP1
G	131	MET	-	expression tag	UNP A0A0H3AHP1
G	290	ALA	TYR	engineered mutation	UNP A0A0H3AHP1

- Molecule 2 is A D E N O S I N E - 5 ' - D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).
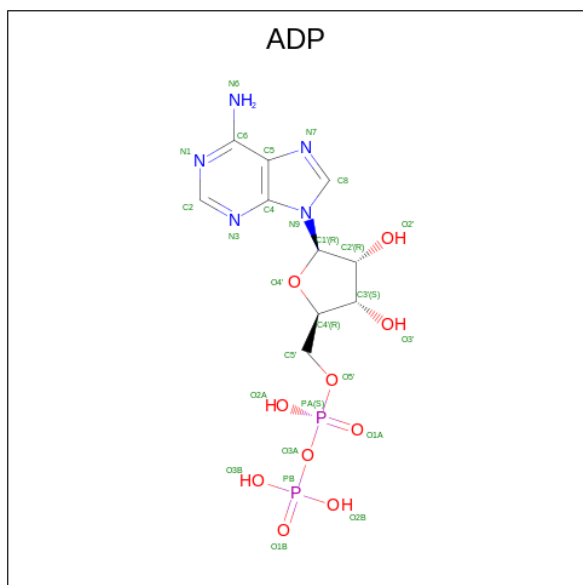
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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.

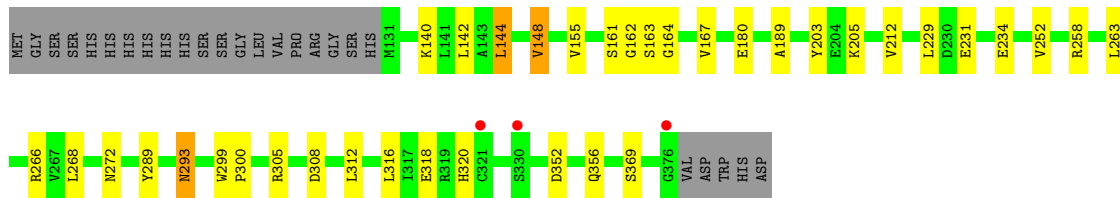• Molecule 1: Flagellar regulatory protein C

Chain A:

• Molecule 1: Flagellar regulatory protein C

Chain B:

• Molecule 1: Flagellar regulatory protein C
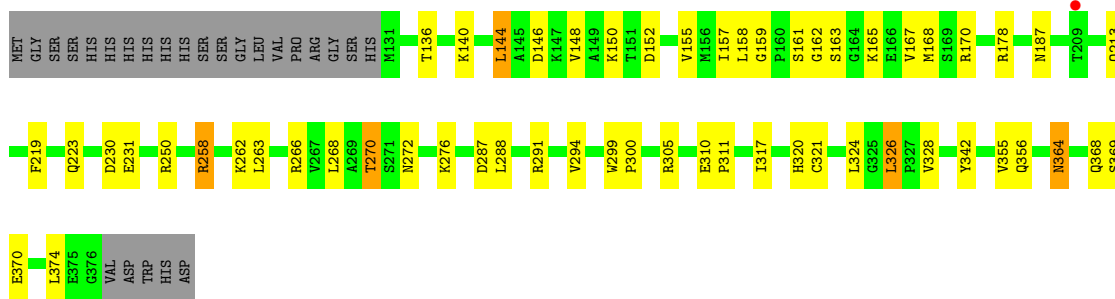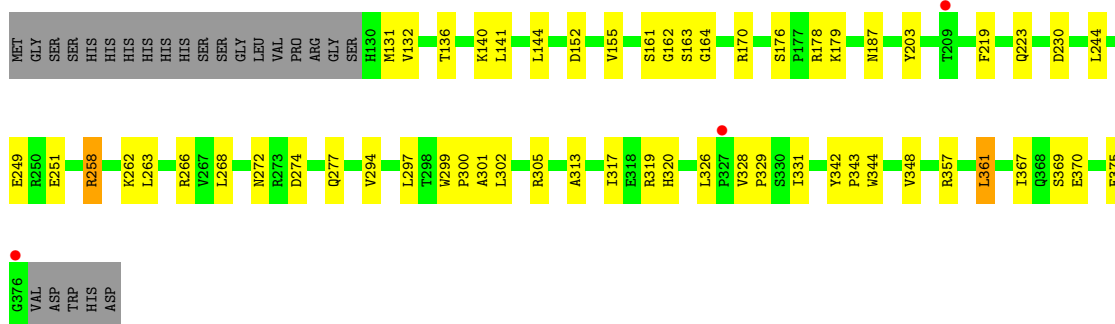
Chain C:

• Molecule 1: Flagellar regulatory protein C

Chain D:

G256 S257 R258 L263 R266 V267 L268 R273 D287 L288 R291 W299 P300 R305 D308 L312 A313 I317 H320 C321 L324 G325 L326 P327 V328 Y342 P343 Q356 R357 L361 Q368 S369 E370 G376 VAL ASP TRP HIS ASP

• Molecule 1: Flagellar regulatory protein C

Chain E:
70%					19%		•	9%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS M131 T136 K140 L144 A145 D146 K147 V148 A149 K150 T151 D152 V155 M156 I157 L158 G159 P160 S161 G162 S163 G164 K165 E166 V167 M168 S169 R170 R178 N187 T209 Q213

F219 Q223 D230 E231 R250 R258 K262 L263 R266 V267 L268 A269 T270 S271 N272 K276 D287 L288 R291 V294 W299 P300 R305 E310 P311 I317 H320 C321 L324 G325 L326 P327 V328 Y342 V355 Q356 N364 Q368 S369

E370 L374 E375 G376 VAL ASP TRP HIS ASP

• Molecule 1: Flagellar regulatory protein C

Chain F:
%
70%					20%		•	9%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER H130 M131 V132 T136 K140 L141 L144 D152 V155 S161 G162 S163 G164 R170 R178 S176 P177 K179 N187 Y203 T209 F219 Q223 D230 L244

E249 R250 E251 R258 K262 L263 R266 V267 L268 N272 R273 D274 Q277 V294 L297 T298 W299 P300 A301 L302 R305 A313 I317 E318 R319 H320 L326 P327 V328 P329 S330 I331 Y342 P343 W344 V348 R357 L361 I367 Q368 S369 E370 E375

G376 VAL ASP TRP HIS ASP

• Molecule 1: Flagellar regulatory protein C

Chain G:
69%					20%		•	9%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS M131 K140 L141 L144 D152 V155 M156 P160 S161 G162 S163 G164 K165 R170 S176 P177 R178 K179 I186 N187 L200 Y203 E204 K205 T209 V212 Q223

D230 E231 R254 R258 L263 R266 V267 L268 A269 T270 S271 N272 K276 D287 L288 F295 T298 W299 P300 R305 D308 L312 A313 I317 H320 C321 K322 K323 L324 G325 L326 P327 V328 P329 L339 V348 R349 Q356 I360 N364

Q368 S369 E370 H371 I372 G376 VAL ASP TRP HIS ASP

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.93Å 154.13Å 194.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.28 – 3.45 48.01 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.28-3.45) 93.2 (48.01-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.188 , 0.234 0.192 , 0.234	Depositor DCC
R_{free} test set	1633 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	57.9	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 26.2	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13613	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.41% 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 $< \lvert L \rvert >$, $< L^2 >$ 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: 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	0.23	0/1957	0.45	0/2648
1	B	0.23	0/1957	0.45	0/2648
1	C	0.23	0/1957	0.43	0/2647
1	D	0.23	0/1946	0.46	0/2633
1	E	0.23	0/1946	0.43	0/2633
1	F	0.23	0/1951	0.43	0/2640
1	G	0.24	0/1946	0.46	0/2633
All	All	0.23	0/13660	0.45	0/18482

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 ⓘ

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	1923	0	1970	31	0
1	B	1923	0	1970	30	0
1	C	1921	0	1976	20	0
1	D	1913	0	1963	32	0
1	E	1913	0	1963	29	0
1	F	1918	0	1965	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1913	0	1963	34	0
2	A	27	0	12	4	0
2	B	27	0	12	2	0
2	C	27	0	12	4	0
2	D	27	0	12	2	0
2	E	27	0	12	2	0
2	F	27	0	12	3	0
2	G	27	0	12	1	0
All	All	13613	0	13854	198	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 7.

The worst 5 of 198 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:F:164:GLY:N	2:F:401:ADP:O2A	2.10	0.81
1:B:178:ARG:NH1	1:B:225:GLY:O	2.18	0.76
1:A:258:ARG:NH2	1:G:203:TYR:OH	2.19	0.76
1:A:163:SER:O	1:A:299:TRP:NE1	2.21	0.73
1:F:163:SER:O	1:F:299:TRP:NE1	2.19	0.72

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	245/271 (90%)	233 (95%)	11 (4%)	1 (0%)	34	70
1	B	245/271 (90%)	236 (96%)	9 (4%)	0	100	100
1	C	245/271 (90%)	235 (96%)	9 (4%)	1 (0%)	34	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	244/271 (90%)	233 (96%)	11 (4%)	0	100	100
1	E	244/271 (90%)	233 (96%)	10 (4%)	1 (0%)	34	70
1	F	245/271 (90%)	235 (96%)	8 (3%)	2 (1%)	19	57
1	G	244/271 (90%)	233 (96%)	11 (4%)	0	100	100
All	All	1712/1897 (90%)	1638 (96%)	69 (4%)	5 (0%)	41	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	369	SER
1	F	369	SER
1	A	369	SER
1	E	369	SER
1	F	132	VAL

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	208/229 (91%)	194 (93%)	14 (7%)	16	48
1	B	208/229 (91%)	190 (91%)	18 (9%)	10	37
1	C	208/229 (91%)	200 (96%)	8 (4%)	33	64
1	D	207/229 (90%)	196 (95%)	11 (5%)	22	54
1	E	207/229 (90%)	194 (94%)	13 (6%)	18	50
1	F	207/229 (90%)	195 (94%)	12 (6%)	20	52
1	G	207/229 (90%)	195 (94%)	12 (6%)	20	52
All	All	1452/1603 (91%)	1364 (94%)	88 (6%)	18	51

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	258	ARG

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Mol	Chain	Res	Type
1	F	320	HIS
1	E	270	THR
1	F	170	ARG
1	F	370	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	174	ASN
1	G	320	HIS
1	G	356	GLN
1	C	320	HIS
1	D	356	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	ADP	G	401	-	24,29,29	1.00	2 (8%)	29,45,45	1.35	4 (13%)
2	ADP	C	401	-	24,29,29	1.00	1 (4%)	29,45,45	1.32	3 (10%)
2	ADP	E	401	-	24,29,29	1.00	2 (8%)	29,45,45	1.29	4 (13%)
2	ADP	A	401	-	24,29,29	1.02	3 (12%)	29,45,45	1.30	3 (10%)
2	ADP	F	401	-	24,29,29	1.03	2 (8%)	29,45,45	1.38	3 (10%)
2	ADP	B	401	-	24,29,29	1.02	2 (8%)	29,45,45	1.24	2 (6%)
2	ADP	D	401	-	24,29,29	1.01	2 (8%)	29,45,45	1.25	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	G	401	-	-	3/12/32/32	0/3/3/3
2	ADP	C	401	-	-	5/12/32/32	0/3/3/3
2	ADP	E	401	-	-	1/12/32/32	0/3/3/3
2	ADP	A	401	-	-	1/12/32/32	0/3/3/3
2	ADP	F	401	-	-	5/12/32/32	0/3/3/3
2	ADP	B	401	-	-	2/12/32/32	0/3/3/3
2	ADP	D	401	-	-	5/12/32/32	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	ADP	C5-C4	2.53	1.47	1.40
2	D	401	ADP	C5-C4	2.52	1.47	1.40
2	A	401	ADP	C5-C4	2.52	1.47	1.40
2	F	401	ADP	C5-C4	2.50	1.47	1.40
2	G	401	ADP	C5-C4	2.50	1.47	1.40

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	401	ADP	PA-O3A-PB	-4.11	118.73	132.83
2	D	401	ADP	PA-O3A-PB	-3.33	121.39	132.83
2	G	401	ADP	PA-O3A-PB	-3.29	121.53	132.83
2	C	401	ADP	PA-O3A-PB	-3.24	121.70	132.83
2	A	401	ADP	N3-C2-N1	-3.14	123.78	128.68

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

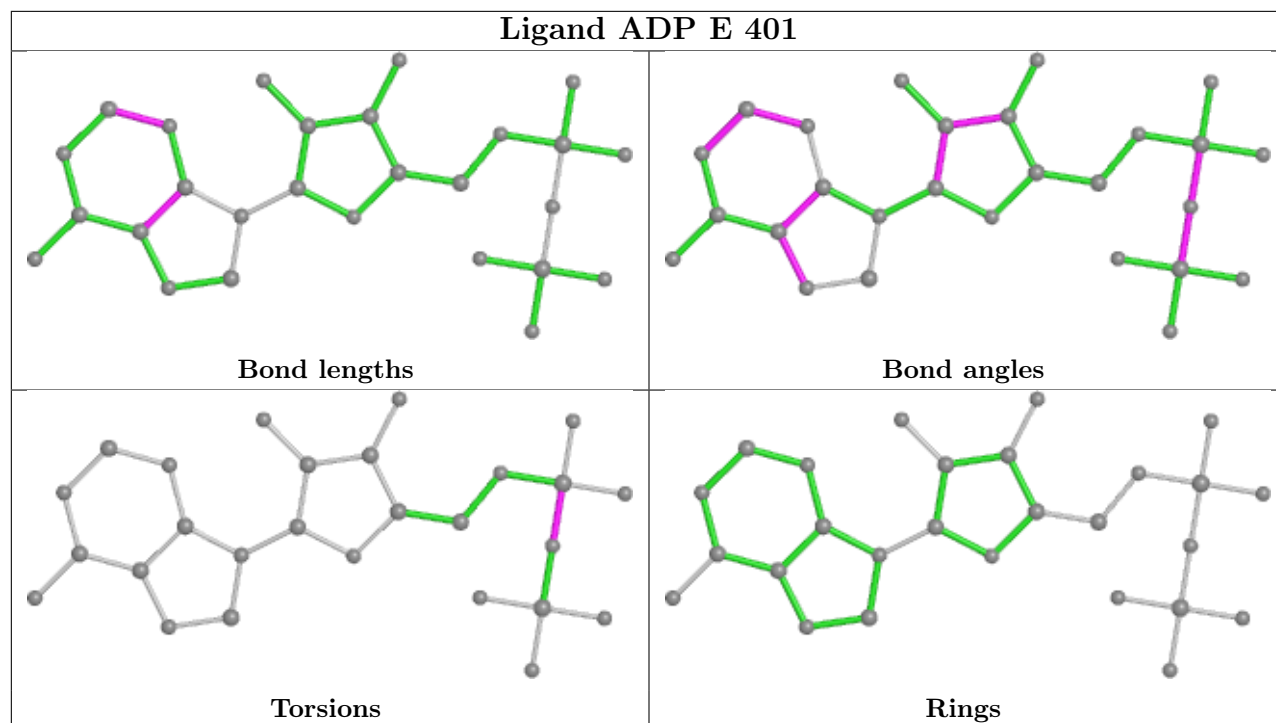| Mol	Chain	Res	Type	Atoms
2	C	401	ADP	PA-O3A-PB-O2B
2	C	401	ADP	C5'-O5'-PA-O1A
2	C	401	ADP	C5'-O5'-PA-O2A
2	D	401	ADP	C5'-O5'-PA-O2A
2	D	401	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

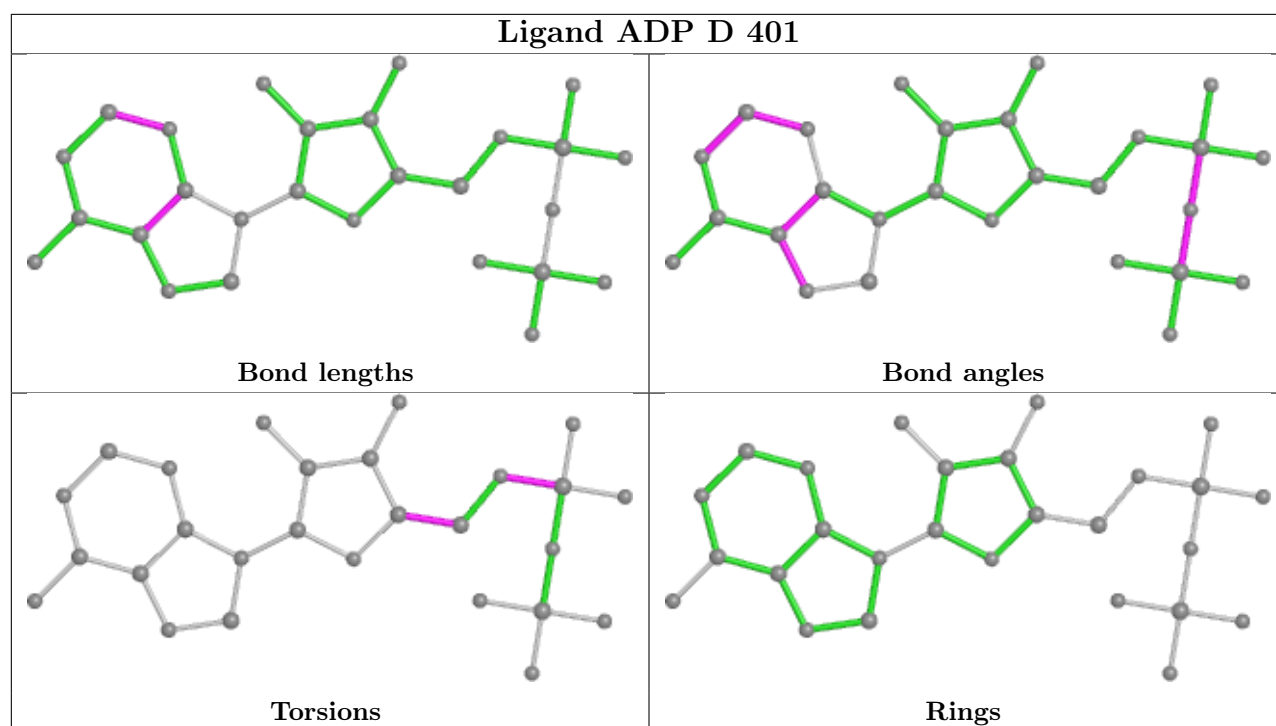7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	401	ADP	1	0
2	C	401	ADP	4	0
2	E	401	ADP	2	0
2	A	401	ADP	4	0
2	F	401	ADP	3	0
2	B	401	ADP	2	0
2	D	401	ADP	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 ADP G 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP F 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 401

Bond lengths

Bond angles

Torsions

Rings
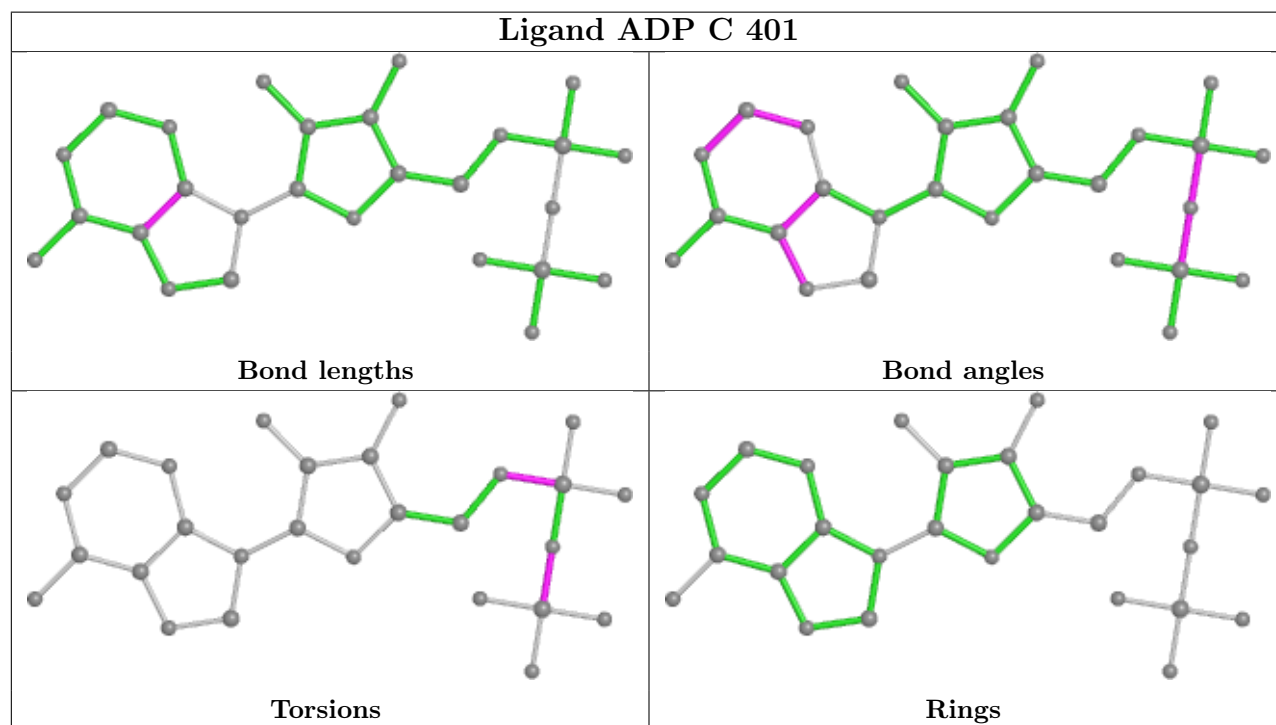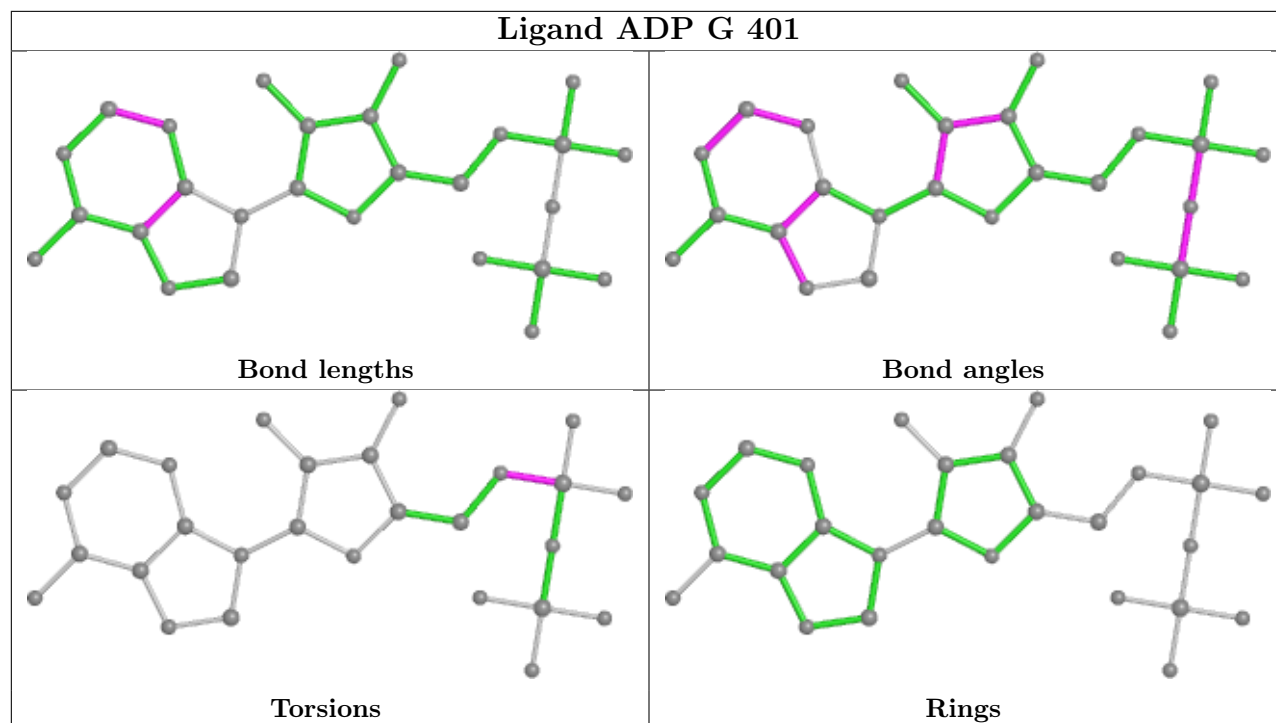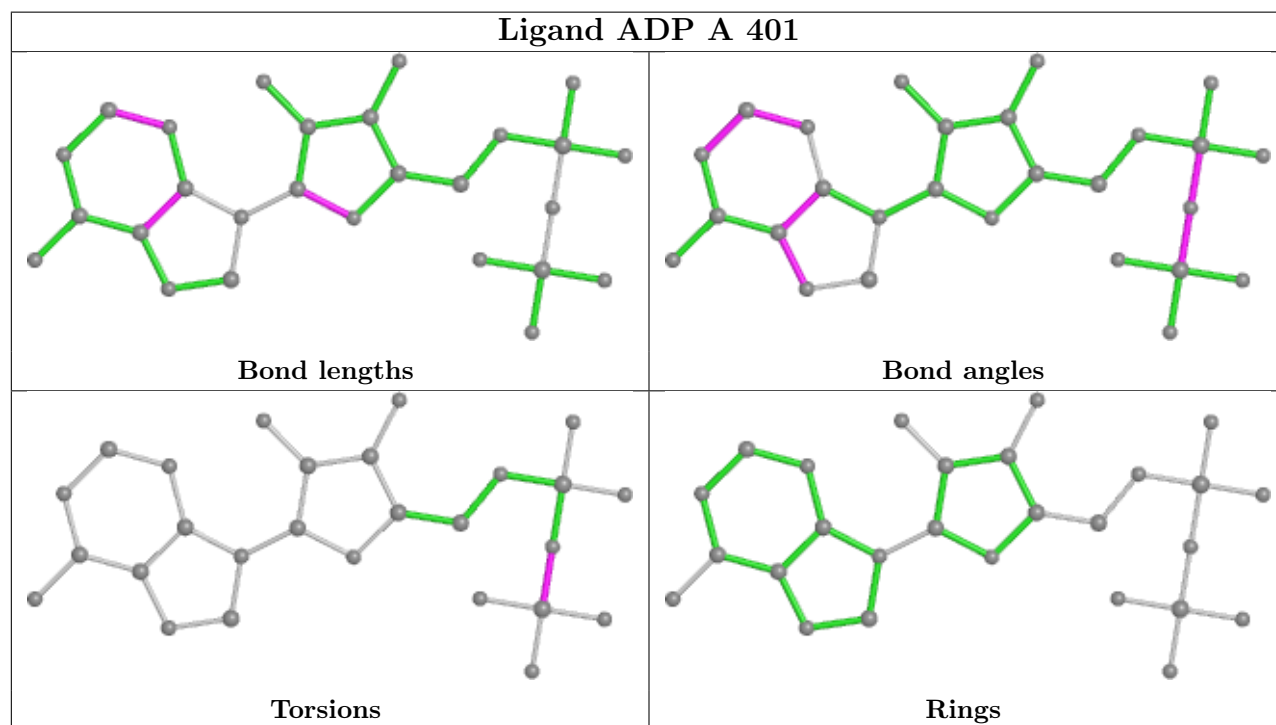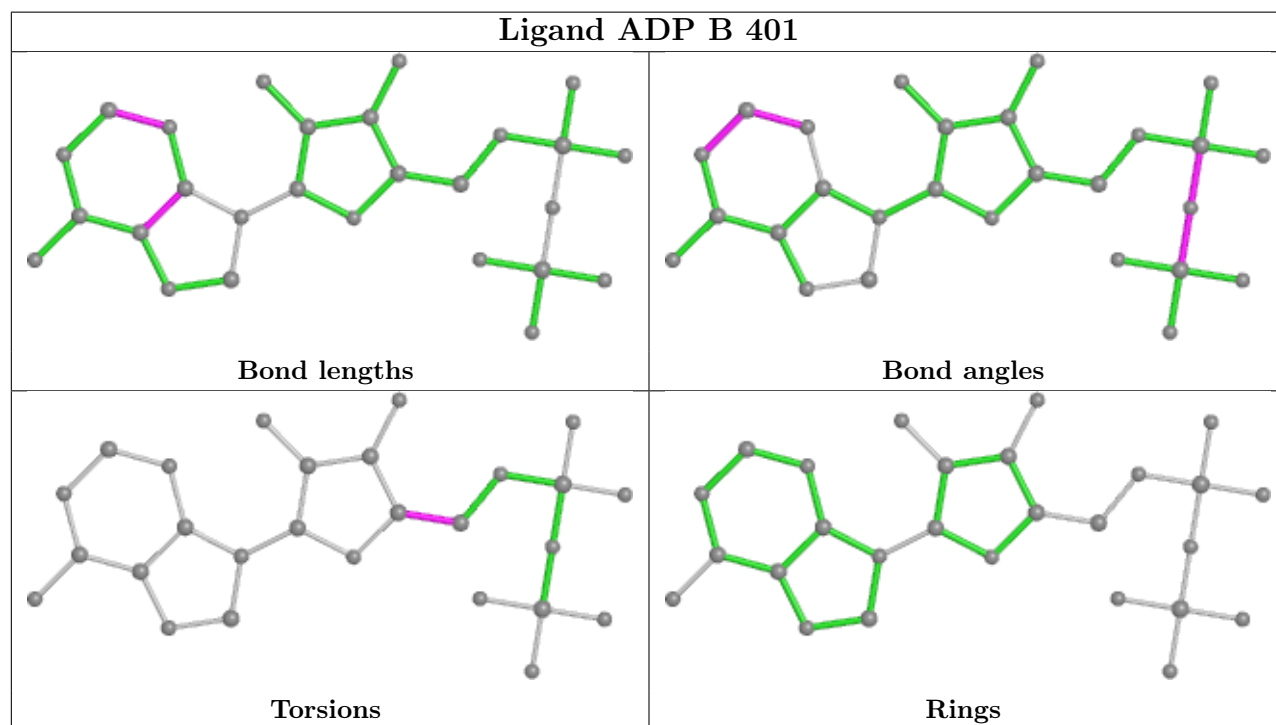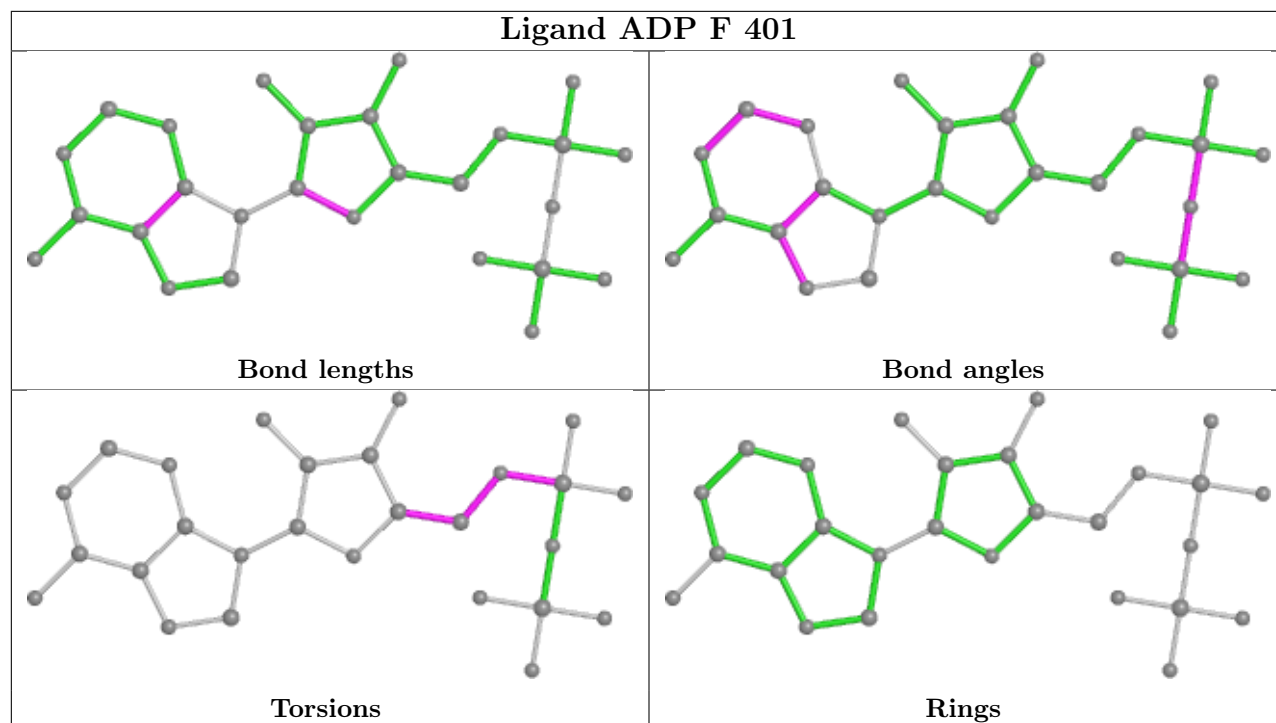
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	247/271 (91%)	-0.03	0	100	100	28, 54, 88, 100	0
1	B	247/271 (91%)	-0.09	0	100	100	33, 52, 81, 103	0
1	C	246/271 (90%)	-0.04	3 (1%)	79	75	31, 54, 84, 93	0
1	D	246/271 (90%)	-0.07	1 (0%)	92	90	33, 53, 80, 105	0
1	E	246/271 (90%)	-0.13	1 (0%)	92	90	30, 50, 79, 109	0
1	F	247/271 (91%)	0.01	3 (1%)	79	75	34, 55, 88, 122	0
1	G	246/271 (90%)	-0.16	0	100	100	32, 51, 77, 105	0
All	All	1725/1897 (90%)	-0.07	8 (0%)	91	89	28, 53, 84, 122	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	376	GLY	2.9
1	D	256	GLY	2.6
1	E	209	THR	2.4
1	F	327	PRO	2.3
1	C	376	GLY	2.2

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 ⓘ

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	ADP	F	401	27/27	0.72	0.45	126,142,172,175	0
2	ADP	B	401	27/27	0.77	0.38	103,110,152,210	0
2	ADP	D	401	27/27	0.78	0.44	100,106,193,219	0
2	ADP	A	401	27/27	0.79	0.38	98,109,137,139	0
2	ADP	C	401	27/27	0.79	0.37	99,112,143,149	0
2	ADP	G	401	27/27	0.85	0.35	91,98,134,139	0
2	ADP	E	401	27/27	0.86	0.33	104,113,132,193	0

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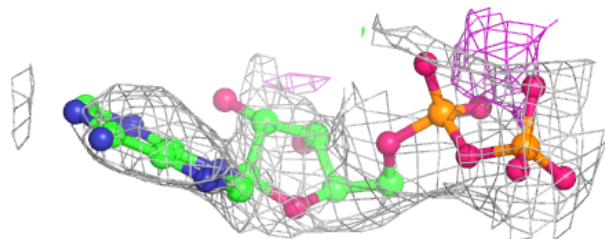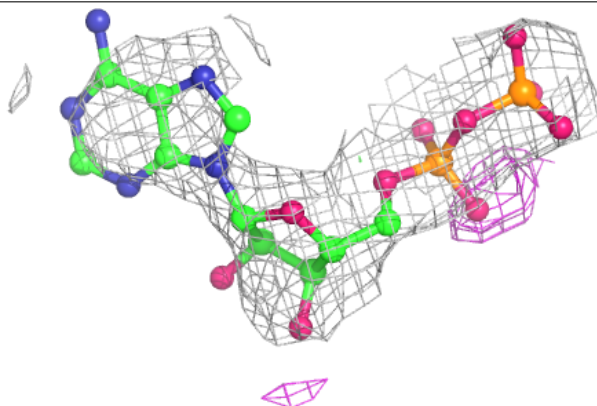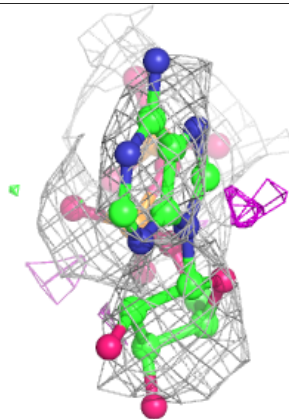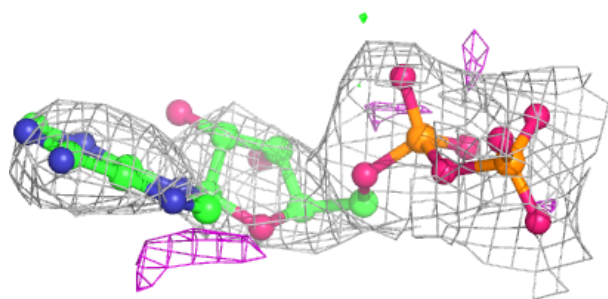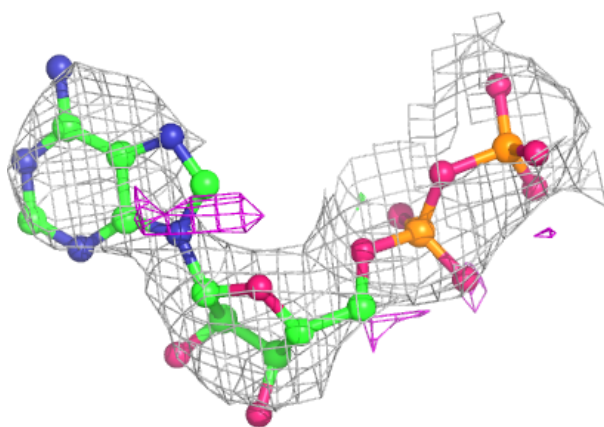

Electron density around ADP F 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
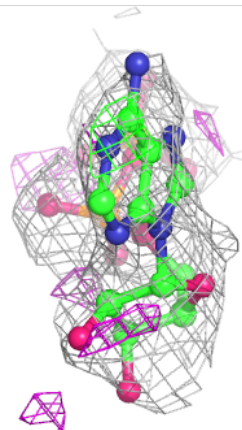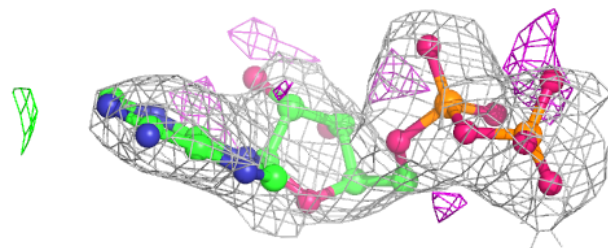mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
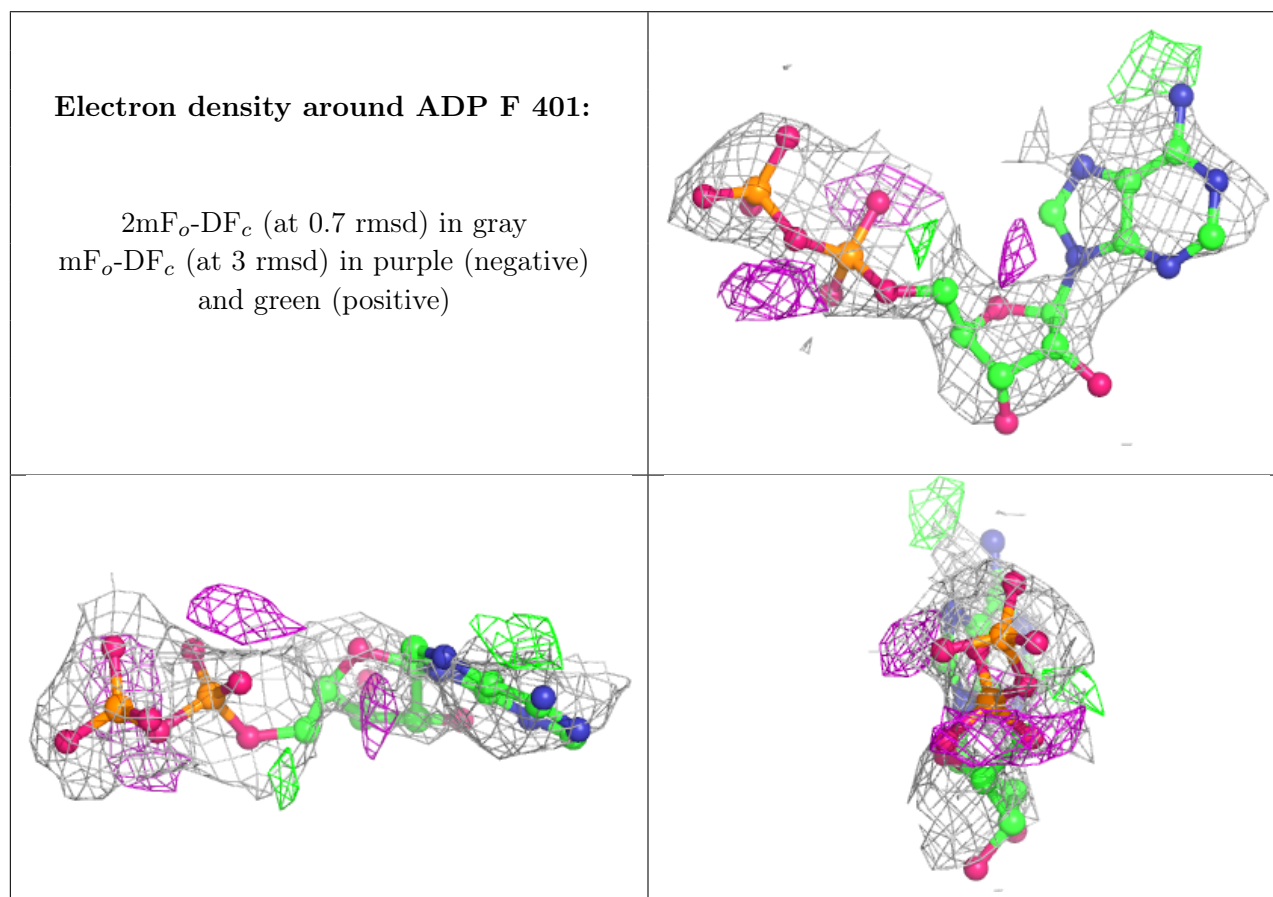
Electron density around ADP B 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
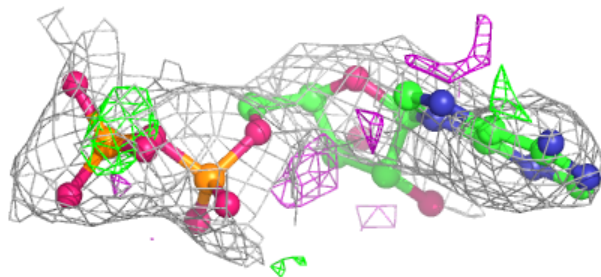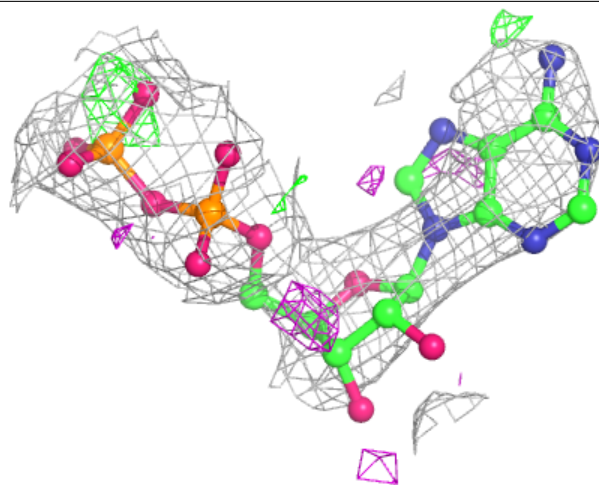
Electron density around ADP D 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
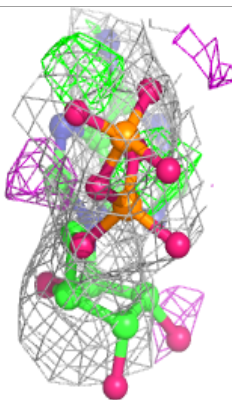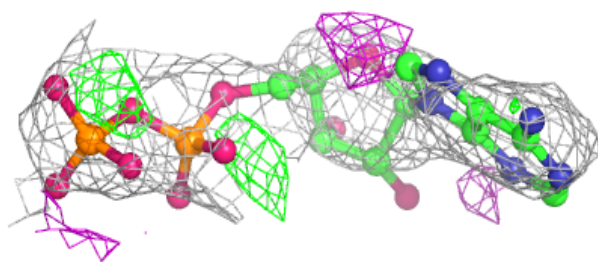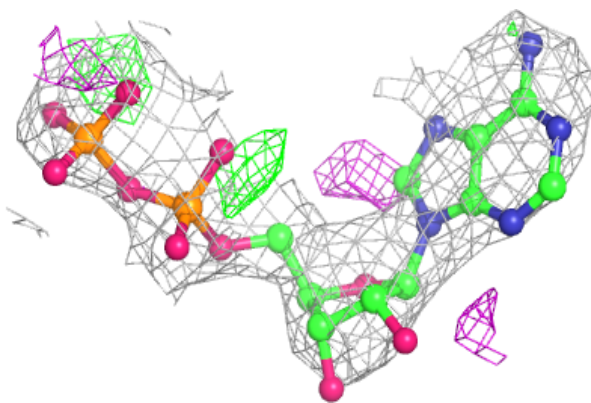
Electron density around ADP A 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
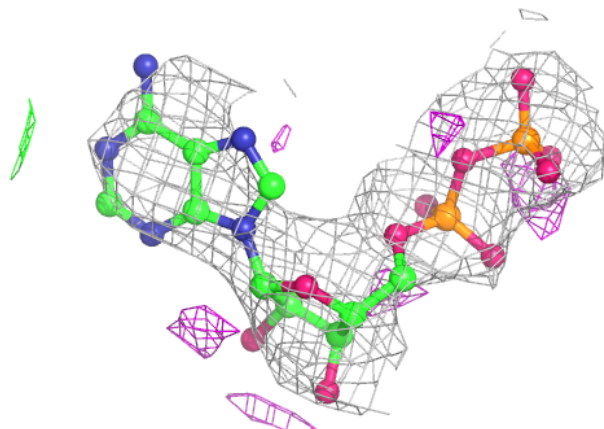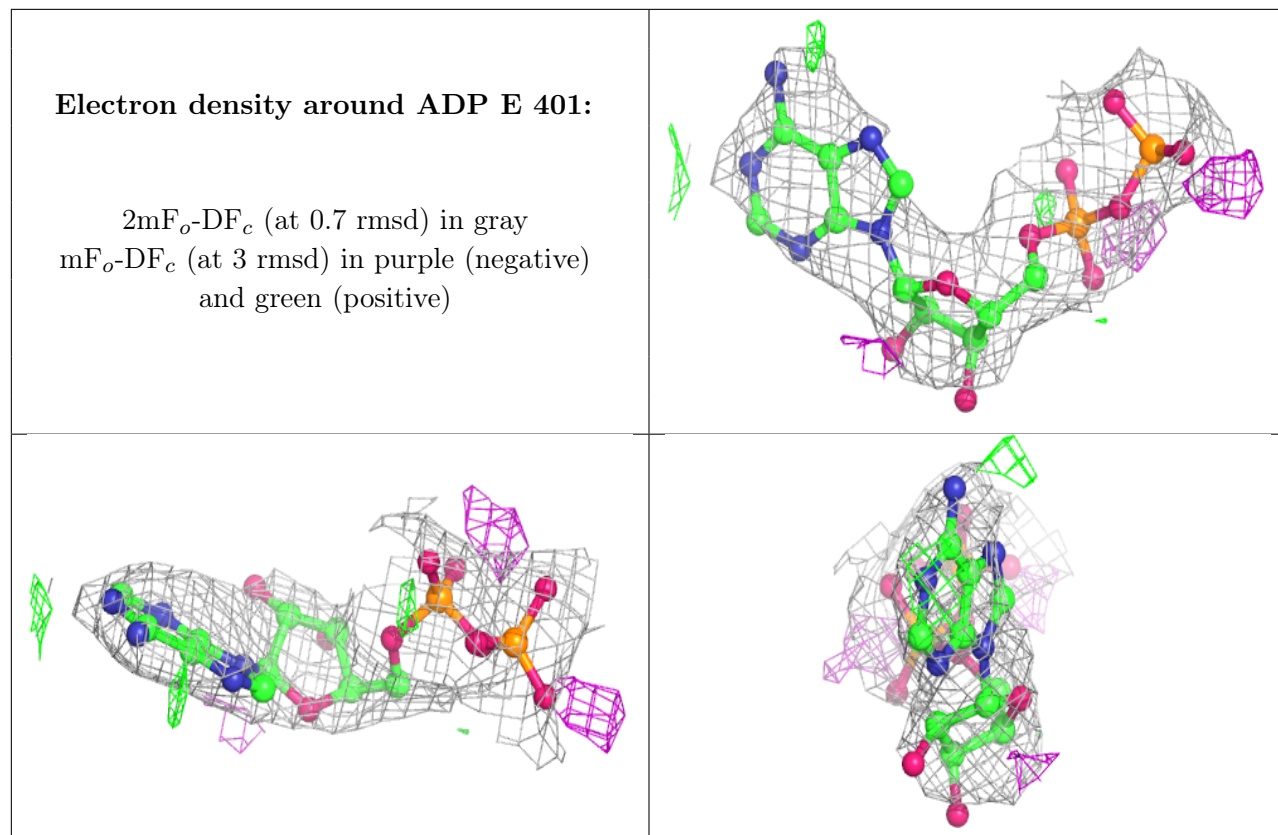$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
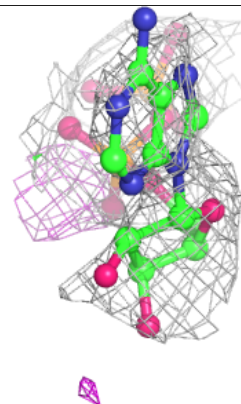
Electron density around ADP C 401:

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

Electron density around ADP G 401:

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

Electron density around ADP E 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 ⓘ

There are no such residues in this entry.