



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:38 PM UTC

PDB ID : 6LUF / pdb_00006luf
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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

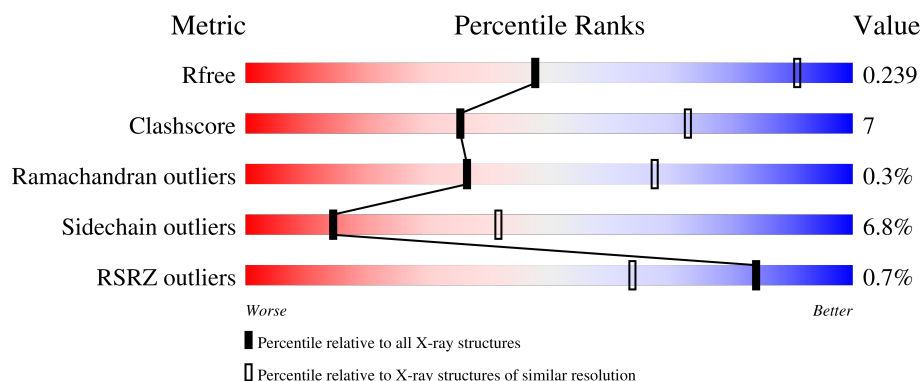
1 Overall quality at a glance

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}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	271	70%17%•9%
1	B	271	% 71%17%•9%
1	C	271	77%13%•9%
1	D	271	% 72%16%•9%
1	E	271	% 70%18%•9%

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Mol	Chain	Length	Quality of chain
1	F	271	% 69% 20% • 9%
1	G	271	% 67% 21% • 9%

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	C	N	O	S	0	0	0
			1923	1217	343	354	9			
1	B	247	Total	C	N	O	S	0	0	0
			1923	1217	343	354	9			
1	C	246	Total	C	N	O	S	0	1	0
			1921	1216	343	353	9			
1	D	246	Total	C	N	O	S	0	0	0
			1913	1211	340	353	9			
1	E	246	Total	C	N	O	S	0	0	0
			1913	1211	340	353	9			
1	F	247	Total	C	N	O	S	0	0	0
			1918	1214	341	354	9			
1	G	246	Total	C	N	O	S	0	0	0
			1913	1211	340	353	9			

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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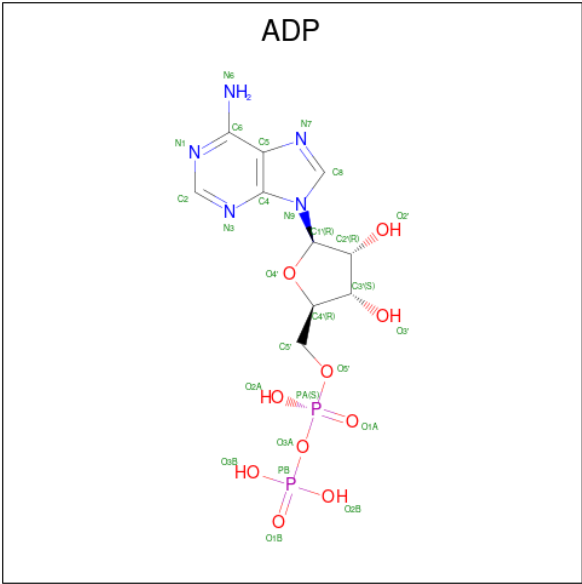
Chain	Residue	Modelled	Actual	Comment	Reference
E	122	SER	-	expression tag	UNP A0A0H3AHP1
E	123	GLY	-	expression tag	UNP A0A0H3AHP1
E	124	LEU	-	expression tag	UNP A0A0H3AHP1
E	125	VAL	-	expression tag	UNP A0A0H3AHP1
E	126	PRO	-	expression tag	UNP A0A0H3AHP1
E	127	ARG	-	expression tag	UNP A0A0H3AHP1
E	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 ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (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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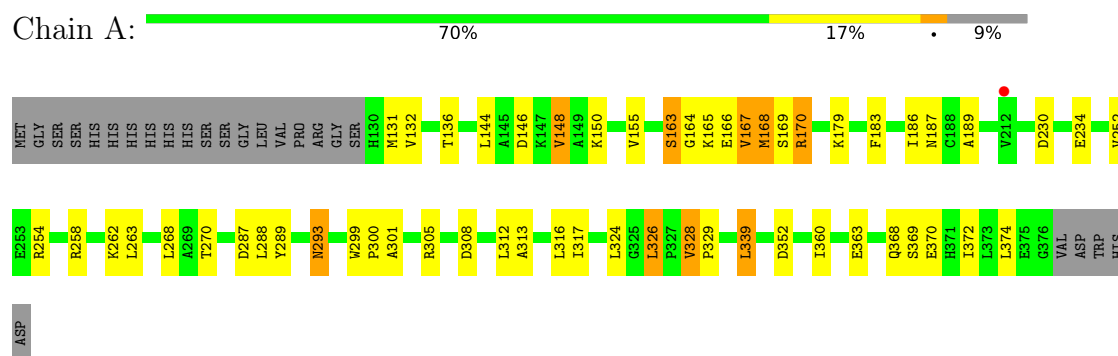
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

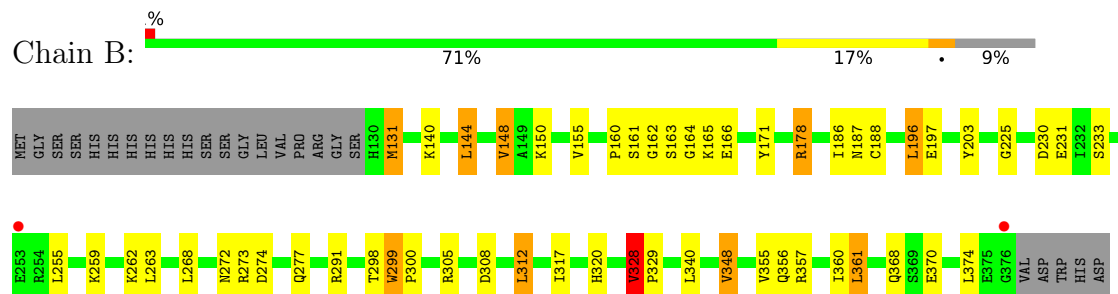
3 Residue-property plots

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.

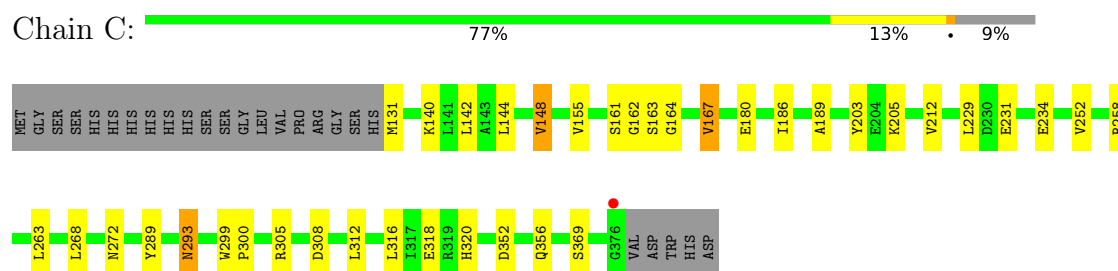
- Molecule 1: Flagellar regulatory protein C



- Molecule 1: Flagellar regulatory protein C

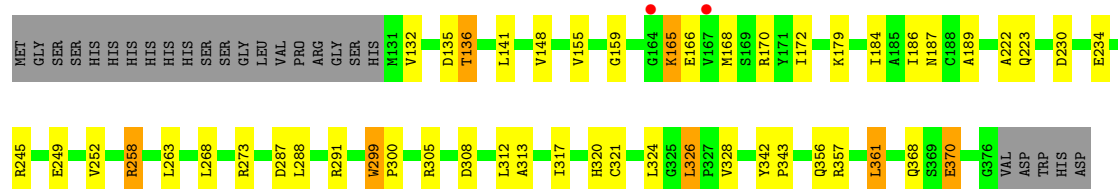


- Molecule 1: Flagellar regulatory protein C

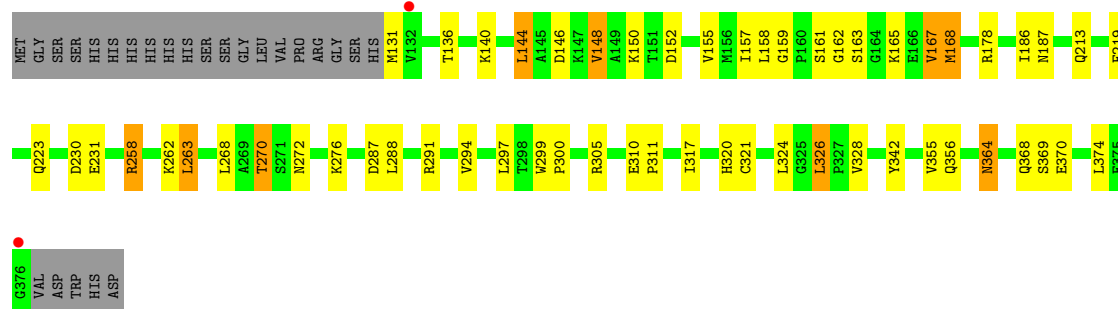


- Molecule 1: Flagellar regulatory protein C

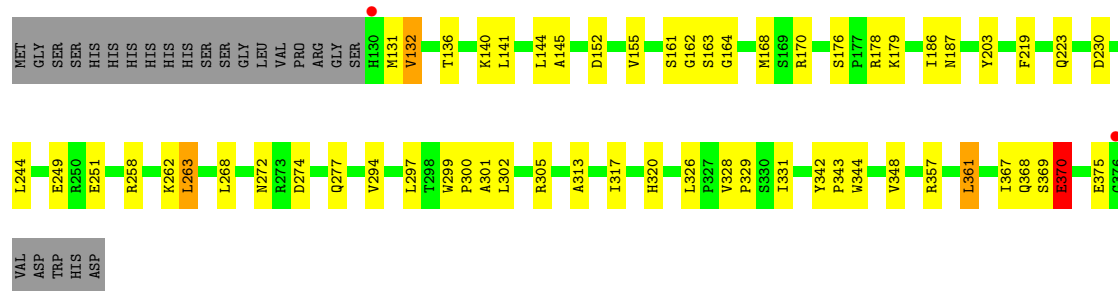




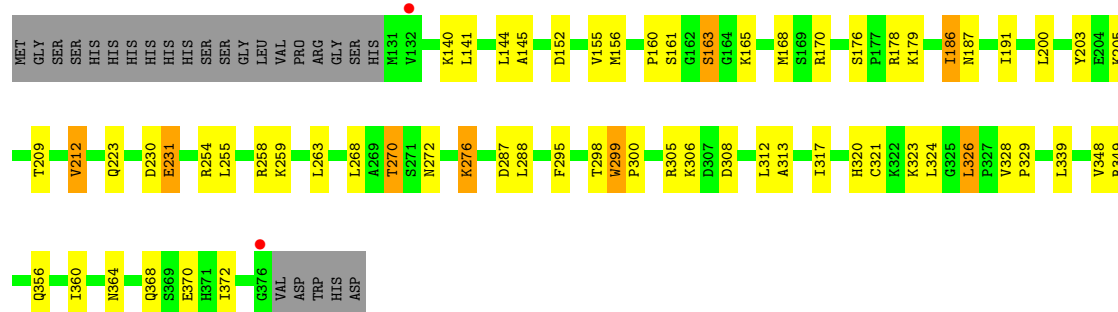
• Molecule 1: Flagellar regulatory protein C



• Molecule 1: Flagellar regulatory protein C



• Molecule 1: Flagellar regulatory protein C



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 46.28 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.28-3.45) 93.2 (46.28-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.188 , 0.234 0.195 , 0.239	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 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.30	0/1957	0.78	0/2648
1	B	0.31	0/1957	0.81	4/2648 (0.2%)
1	C	0.29	0/1957	0.76	0/2647
1	D	0.30	0/1946	0.80	0/2633
1	E	0.31	0/1946	0.77	0/2633
1	F	0.30	0/1951	0.75	1/2640 (0.0%)
1	G	0.31	0/1946	0.78	1/2633 (0.0%)
All	All	0.30	0/13660	0.78	6/18482 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	VAL	CA-C-N	5.49	126.78	120.85
1	B	328	VAL	C-N-CA	5.49	126.78	120.85
1	B	328	VAL	N-CA-C	5.41	113.28	108.63
1	B	291	ARG	N-CA-C	-5.19	106.79	113.23
1	G	191	ILE	N-CA-C	5.14	112.23	107.56
1	F	370	GLU	N-CA-C	-5.11	107.07	113.72

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	32	0
1	B	1923	0	1970	30	0
1	C	1921	0	1976	21	0
1	D	1913	0	1963	32	0
1	E	1913	0	1963	30	0
1	F	1918	0	1965	35	0
1	G	1913	0	1963	35	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	204	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.

All (204) 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
1:A:339:LEU:HD13	1:A:372:ILE:HD13	1.72	0.71
1:C:167:VAL:HG11	2:C:401:ADP:H2'	1.71	0.71
1:E:300:PRO:HG2	1:E:305:ARG:HD3	1.73	0.71
1:E:231:GLU:H	1:E:270:THR:HG22	1.56	0.70
1:F:141:LEU:HD23	1:F:299:TRP:HE3	1.57	0.69
1:F:219:PHE:HB3	1:F:263:LEU:HD21	1.74	0.69
1:D:321:CYS:HB2	1:D:328:VAL:HG12	1.75	0.68
1:A:300:PRO:HG2	1:A:305:ARG:HD3	1.77	0.67
1:B:162:GLY:N	2:B:401:ADP:O3B	2.26	0.67
1:C:300:PRO:HG2	1:C:305:ARG:HD3	1.76	0.67
1:G:320:HIS:HD2	1:G:323:LYS:HE3	1.62	0.65
1:B:299:TRP:HE3	1:B:300:PRO:HD2	1.60	0.65
1:E:219:PHE:HB3	1:E:263:LEU:HD21	1.78	0.64
1:B:203:TYR:OH	1:C:258:ARG:NH1	2.31	0.63
1:E:320:HIS:CD2	1:E:356:GLN:HE21	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:ASN:HA	1:E:230:ASP:HB3	1.80	0.63
1:A:131:MET:HE1	1:A:168:MET:HB2	1.82	0.62
1:B:320:HIS:CD2	1:B:356:GLN:HE21	2.17	0.62
1:G:152:ASP:OD1	1:G:178:ARG:NH1	2.33	0.62
1:G:205:LYS:HG3	1:G:212:VAL:O	2.00	0.62
1:A:324:LEU:HB2	1:A:326:LEU:HD22	1.81	0.61
1:D:187:ASN:HA	1:D:230:ASP:HB3	1.83	0.61
1:F:375:GLU:OE1	1:G:276:LYS:NZ	2.35	0.60
1:E:163:SER:O	1:E:299:TRP:NE1	2.35	0.60
1:G:187:ASN:HA	1:G:230:ASP:HB3	1.83	0.60
1:B:308:ASP:O	1:B:312:LEU:HB2	2.01	0.60
1:F:163:SER:HB3	1:F:299:TRP:CD1	2.37	0.59
1:B:155:VAL:HB	1:B:268:LEU:HD22	1.85	0.59
1:F:145:ALA:HB2	1:F:168:MET:HE1	1.84	0.59
1:E:223:GLN:HE22	1:E:263:LEU:HD12	1.68	0.58
1:E:324:LEU:HB2	1:E:326:LEU:HD22	1.84	0.58
1:F:300:PRO:HG2	1:F:305:ARG:HD3	1.83	0.58
1:A:155:VAL:HB	1:A:268:LEU:HD22	1.85	0.58
1:F:249:GLU:HB3	1:F:251:GLU:HG2	1.84	0.58
1:C:162:GLY:N	2:C:401:ADP:O3B	2.33	0.58
1:E:162:GLY:N	2:E:401:ADP:O1B	2.33	0.57
1:G:320:HIS:CD2	1:G:323:LYS:HE3	2.40	0.57
1:C:164:GLY:HA3	2:C:401:ADP:C8	2.39	0.57
1:G:320:HIS:CD2	1:G:356:GLN:HE21	2.23	0.57
1:E:155:VAL:HB	1:E:268:LEU:HD22	1.86	0.57
1:G:160:PRO:O	1:G:165:LYS:NZ	2.38	0.57
1:G:300:PRO:HG2	1:G:305:ARG:HD3	1.87	0.57
1:F:164:GLY:HA2	2:F:401:ADP:H5'2	1.86	0.56
1:B:188:CYS:HB3	1:B:196:LEU:HD11	1.87	0.56
1:C:308:ASP:O	1:C:312:LEU:HB2	2.05	0.56
1:D:308:ASP:O	1:D:312:LEU:HB2	2.04	0.56
1:A:252:VAL:HB	1:A:263:LEU:HD11	1.88	0.56
1:D:300:PRO:HG2	1:D:305:ARG:HD3	1.88	0.55
1:D:357:ARG:O	1:D:361:LEU:HD22	2.06	0.55
1:C:252:VAL:HB	1:C:263:LEU:HD11	1.88	0.55
1:B:300:PRO:HG2	1:B:305:ARG:HD3	1.89	0.55
1:G:163:SER:O	1:G:299:TRP:NE1	2.41	0.54
1:C:140:LYS:O	1:C:144:LEU:HD12	2.08	0.54
1:E:152:ASP:OD1	1:E:178:ARG:NH1	2.40	0.54
1:F:203:TYR:OH	1:G:258:ARG:NH1	2.41	0.54
1:D:155:VAL:HB	1:D:268:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ASP:O	1:B:277:GLN:HG3	2.08	0.54
1:B:187:ASN:HA	1:B:230:ASP:HB3	1.90	0.53
1:F:331:ILE:HD12	1:F:367:ILE:HD11	1.89	0.53
1:G:321:CYS:HB2	1:G:328:VAL:HG12	1.89	0.53
1:G:161:SER:OG	1:G:272:ASN:ND2	2.23	0.53
1:E:161:SER:OG	1:E:272:ASN:ND2	2.32	0.53
1:G:308:ASP:O	1:G:312:LEU:HB2	2.09	0.53
1:A:167:VAL:HG11	2:A:401:ADP:H2'	1.91	0.52
1:A:368:GLN:HB2	1:A:370:GLU:HG2	1.91	0.52
1:D:320:HIS:CE1	1:D:356:GLN:HE21	2.27	0.52
1:G:155:VAL:HB	1:G:268:LEU:HD22	1.91	0.52
1:A:164:GLY:HA2	2:A:401:ADP:PA	2.50	0.52
1:D:234:GLU:OE2	1:D:273:ARG:NH1	2.43	0.52
1:E:131:MET:HE1	1:E:168:MET:HG2	1.91	0.52
1:F:152:ASP:OD1	1:F:178:ARG:NH1	2.43	0.52
1:C:316:LEU:HD13	1:C:352:ASP:HA	1.93	0.51
1:F:162:GLY:N	2:F:401:ADP:O1B	2.41	0.51
1:D:299:TRP:HE3	1:D:300:PRO:HD2	1.74	0.51
1:G:176:SER:O	1:G:179:LYS:HG3	2.11	0.51
1:B:162:GLY:O	1:B:348:VAL:HG13	2.11	0.51
1:B:164:GLY:O	1:B:299:TRP:NE1	2.41	0.51
1:B:357:ARG:O	1:B:361:LEU:HD22	2.11	0.51
1:B:317:ILE:HG12	1:B:355:VAL:HG13	1.93	0.51
1:A:163:SER:HB2	1:A:299:TRP:CD1	2.45	0.51
1:A:289:TYR:O	1:A:293:ASN:HB2	2.10	0.51
1:B:360:ILE:HG21	1:C:148:VAL:HG13	1.92	0.51
1:D:184:ILE:HD13	1:D:222:ALA:HA	1.92	0.50
1:E:364:ASN:O	1:E:364:ASN:ND2	2.35	0.50
1:C:131:MET:HE2	1:C:142:LEU:HD21	1.92	0.50
1:C:155:VAL:HB	1:C:268:LEU:HD22	1.92	0.50
1:A:308:ASP:O	1:A:312:LEU:HB2	2.11	0.50
1:A:363:GLU:OE1	1:B:150:LYS:NZ	2.44	0.50
1:F:140:LYS:O	1:F:144:LEU:HD12	2.10	0.50
1:B:368:GLN:HB2	1:B:370:GLU:HG2	1.94	0.50
1:D:313:ALA:O	1:D:317:ILE:HG13	2.12	0.50
1:A:165:LYS:HD2	1:A:270:THR:HB	1.93	0.50
1:A:368:GLN:C	1:A:370:GLU:H	2.20	0.50
1:G:231:GLU:H	1:G:270:THR:HG22	1.76	0.49
1:C:189:ALA:HB2	1:C:234:GLU:HG3	1.94	0.49
1:A:287:ASP:OD1	1:A:288:LEU:N	2.45	0.49
1:G:324:LEU:HB2	1:G:326:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:LEU:O	1:E:148:VAL:HG23	2.13	0.49
1:G:145:ALA:HB2	1:G:168:MET:HE1	1.92	0.49
1:B:299:TRP:CE3	1:B:300:PRO:HD2	2.43	0.49
1:B:161:SER:OG	1:B:272:ASN:ND2	2.28	0.48
1:G:339:LEU:HD21	1:G:372:ILE:HD12	1.95	0.48
1:F:223:GLN:NE2	1:F:262:LYS:O	2.46	0.48
1:B:131:MET:HG3	1:B:171:TYR:HB2	1.97	0.47
1:B:368:GLN:C	1:B:370:GLU:H	2.22	0.47
1:D:165:LYS:HG3	2:D:401:ADP:O3B	2.14	0.47
1:A:316:LEU:HD13	1:A:352:ASP:HA	1.95	0.47
1:F:136:THR:O	1:F:140:LYS:HG3	2.15	0.47
1:B:197:GLU:HG2	1:B:255:LEU:HD11	1.96	0.47
1:F:163:SER:HB3	1:F:299:TRP:HD1	1.76	0.46
1:D:368:GLN:C	1:D:370:GLU:H	2.23	0.46
1:E:368:GLN:C	1:E:370:GLU:H	2.23	0.46
1:E:321:CYS:HB2	1:E:328:VAL:HG12	1.97	0.46
1:C:163:SER:O	1:C:299:TRP:NE1	2.48	0.46
1:G:368:GLN:HB2	1:G:370:GLU:HG2	1.97	0.46
1:A:189:ALA:HB2	1:A:234:GLU:HG3	1.98	0.46
1:F:176:SER:O	1:F:179:LYS:HG3	2.15	0.46
1:B:160:PRO:O	1:B:165:LYS:HE2	2.16	0.45
1:D:324:LEU:HB2	1:D:326:LEU:HD22	1.98	0.45
1:G:368:GLN:C	1:G:370:GLU:H	2.24	0.45
1:C:161:SER:OG	1:C:272:ASN:ND2	2.37	0.45
1:A:166:GLU:HB3	2:A:401:ADP:O1A	2.16	0.45
1:A:131:MET:HE1	1:A:168:MET:HE3	1.99	0.45
1:F:302:LEU:HD21	1:F:348:VAL:CG2	2.47	0.45
1:F:302:LEU:HD21	1:F:348:VAL:HG23	1.99	0.45
1:D:223:GLN:HE22	1:D:263:LEU:HD23	1.82	0.45
1:F:155:VAL:HB	1:F:268:LEU:HD22	1.99	0.45
1:D:342:TYR:CD1	1:D:343:PRO:HD2	2.52	0.45
1:C:320:HIS:CE1	1:C:356:GLN:HE21	2.35	0.44
1:G:313:ALA:O	1:G:317:ILE:HG13	2.17	0.44
1:E:146:ASP:O	1:E:150:LYS:HG3	2.17	0.44
1:C:289:TYR:O	1:C:293:ASN:HB2	2.17	0.44
1:D:299:TRP:CE3	1:D:300:PRO:HD2	2.52	0.44
1:D:299:TRP:CE3	1:D:299:TRP:HA	2.53	0.44
1:E:342:TYR:HB2	1:E:374:LEU:HD13	1.99	0.44
1:F:328:VAL:HA	1:F:329:PRO:HD3	1.86	0.44
1:E:310:GLU:HB3	1:E:311:PRO:HD3	2.00	0.44
1:B:233:SER:HB2	1:B:273:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:LEU:HA	1:F:141:LEU:HD12	1.78	0.44
1:F:161:SER:OG	1:F:272:ASN:ND2	2.29	0.44
1:F:297:LEU:HD23	1:F:297:LEU:HA	1.85	0.44
1:D:168:MET:O	1:D:168:MET:HG3	2.14	0.44
1:E:317:ILE:HG12	1:E:355:VAL:HG13	1.98	0.44
1:B:328:VAL:HA	1:B:329:PRO:HD3	1.69	0.44
1:C:299:TRP:HZ2	2:C:401:ADP:HN61	1.65	0.44
1:A:301:ALA:O	1:A:305:ARG:HG2	2.18	0.43
1:A:148:VAL:HG13	1:G:360:ILE:HG21	2.00	0.43
1:A:164:GLY:HA3	2:A:401:ADP:C8	2.53	0.43
1:A:170:ARG:HG3	1:A:183:PHE:CE2	2.53	0.43
1:A:328:VAL:HA	1:A:329:PRO:HD3	1.85	0.43
1:E:258:ARG:HE	1:E:258:ARG:HB2	1.30	0.43
1:F:368:GLN:C	1:F:370:GLU:H	2.26	0.43
1:D:189:ALA:HB2	1:D:234:GLU:HG3	2.00	0.43
1:G:141:LEU:HD11	1:G:298:THR:O	2.18	0.43
1:D:245:ARG:NH2	1:D:249:GLU:HG3	2.34	0.43
1:A:166:GLU:OE1	1:A:170:ARG:NH1	2.52	0.43
1:F:361:LEU:HD11	1:G:295:PHE:HE1	1.83	0.43
1:G:287:ASP:OD1	1:G:288:LEU:N	2.52	0.43
1:G:328:VAL:HA	1:G:329:PRO:HD3	1.85	0.42
1:A:146:ASP:O	1:A:150:LYS:HG3	2.19	0.42
1:A:187:ASN:HA	1:A:230:ASP:HB3	2.01	0.42
1:A:360:ILE:HG21	1:B:148:VAL:HG13	2.01	0.42
1:B:140:LYS:O	1:B:144:LEU:HD22	2.19	0.42
1:B:348:VAL:HG21	2:B:401:ADP:C8	2.54	0.42
1:D:141:LEU:HD12	1:D:141:LEU:HA	1.86	0.42
1:D:287:ASP:OD1	1:D:288:LEU:N	2.53	0.42
1:E:136:THR:O	1:E:140:LYS:HG3	2.19	0.42
1:E:159:GLY:O	1:E:165:LYS:NZ	2.51	0.42
1:G:349:ARG:O	1:G:349:ARG:HG2	2.18	0.42
1:B:262:LYS:HD3	1:B:263:LEU:N	2.34	0.42
1:G:223:GLN:HE22	1:G:263:LEU:HD23	1.83	0.42
1:E:213:GLN:OE1	1:F:258:ARG:HG3	2.20	0.42
1:G:186:ILE:HD13	1:G:200:LEU:HD13	2.01	0.42
1:D:159:GLY:O	1:D:165:LYS:NZ	2.52	0.42
1:F:187:ASN:HA	1:F:230:ASP:HB3	2.02	0.42
1:D:252:VAL:HB	1:D:263:LEU:HD11	2.02	0.42
1:E:163:SER:O	1:E:299:TRP:CD1	2.73	0.41
1:E:262:LYS:HD3	1:E:262:LYS:HA	1.78	0.41
1:F:342:TYR:CD1	1:F:343:PRO:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:GLU:O	1:D:170:ARG:HG3	2.19	0.41
1:E:167:VAL:HG11	2:E:401:ADP:H2'	2.02	0.41
1:G:348:VAL:HG11	2:G:401:ADP:C8	2.55	0.41
1:C:205:LYS:HE3	1:C:212:VAL:O	2.21	0.41
1:E:276:LYS:HA	1:E:276:LYS:HD2	1.87	0.41
1:G:140:LYS:O	1:G:144:LEU:HD13	2.20	0.41
1:D:312:LEU:HD12	1:D:312:LEU:HA	1.94	0.41
1:D:312:LEU:HD11	2:D:401:ADP:C6	2.56	0.41
1:A:313:ALA:O	1:A:317:ILE:HG13	2.20	0.41
1:F:342:TYR:HD2	1:F:344:TRP:CD2	2.38	0.41
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.87	0.41
1:D:135:ASP:OD1	1:D:136:THR:N	2.53	0.41
1:D:320:HIS:CE1	1:D:324:LEU:HD11	2.56	0.41
1:D:168:MET:O	1:D:172:ILE:HG13	2.20	0.41
1:E:287:ASP:OD1	1:E:288:LEU:N	2.54	0.41
1:F:301:ALA:O	1:F:305:ARG:HG2	2.21	0.40
1:F:313:ALA:O	1:F:317:ILE:HG13	2.21	0.40
1:C:203:TYR:OH	1:D:258:ARG:NH1	2.54	0.40
1:G:312:LEU:HD12	1:G:312:LEU:HA	1.99	0.40
1:F:274:ASP:O	1:F:277:GLN:HG3	2.22	0.40

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%)	30 62
1	B	245/271 (90%)	236 (96%)	9 (4%)	0	100 100
1	C	245/271 (90%)	235 (96%)	9 (4%)	1 (0%)	30 62
1	D	244/271 (90%)	233 (96%)	11 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	244/271 (90%)	233 (96%)	10 (4%)	1 (0%)	30	62
1	F	245/271 (90%)	235 (96%)	8 (3%)	2 (1%)	16	49
1	G	244/271 (90%)	233 (96%)	11 (4%)	0	100	100
All	All	1712/1897 (90%)	1638 (96%)	69 (4%)	5 (0%)	36	67

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%)	190 (91%)	18 (9%)	9	34
1	B	208/229 (91%)	190 (91%)	18 (9%)	9	34
1	C	208/229 (91%)	200 (96%)	8 (4%)	29	57
1	D	207/229 (90%)	195 (94%)	12 (6%)	18	45
1	E	207/229 (90%)	192 (93%)	15 (7%)	13	39
1	F	207/229 (90%)	195 (94%)	12 (6%)	18	45
1	G	207/229 (90%)	191 (92%)	16 (8%)	12	38
All	All	1452/1603 (91%)	1353 (93%)	99 (7%)	14	41

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	VAL
1	A	136	THR

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Mol	Chain	Res	Type
1	A	144	LEU
1	A	148	VAL
1	A	163	SER
1	A	167	VAL
1	A	168	MET
1	A	169	SER
1	A	170	ARG
1	A	179	LYS
1	A	186	ILE
1	A	254	ARG
1	A	262	LYS
1	A	293	ASN
1	A	326	LEU
1	A	328	VAL
1	A	339	LEU
1	A	374	LEU
1	B	131	MET
1	B	144	LEU
1	B	148	VAL
1	B	163	SER
1	B	166	GLU
1	B	178	ARG
1	B	186	ILE
1	B	196	LEU
1	B	231	GLU
1	B	259	LYS
1	B	298	THR
1	B	299	TRP
1	B	312	LEU
1	B	328	VAL
1	B	340	LEU
1	B	348	VAL
1	B	361	LEU
1	B	374	LEU
1	C	148	VAL
1	C	167	VAL
1	C	180	GLU
1	C	186	ILE
1	C	229	LEU
1	C	231	GLU
1	C	293	ASN
1	C	318	GLU

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Mol	Chain	Res	Type
1	D	132	VAL
1	D	136	THR
1	D	148	VAL
1	D	165	LYS
1	D	179	LYS
1	D	186	ILE
1	D	258	ARG
1	D	291	ARG
1	D	299	TRP
1	D	326	LEU
1	D	361	LEU
1	D	370	GLU
1	E	144	LEU
1	E	148	VAL
1	E	157	ILE
1	E	158	LEU
1	E	167	VAL
1	E	168	MET
1	E	186	ILE
1	E	258	ARG
1	E	263	LEU
1	E	270	THR
1	E	291	ARG
1	E	294	VAL
1	E	297	LEU
1	E	326	LEU
1	E	364	ASN
1	F	131	MET
1	F	132	VAL
1	F	170	ARG
1	F	186	ILE
1	F	244	LEU
1	F	263	LEU
1	F	294	VAL
1	F	320	HIS
1	F	326	LEU
1	F	357	ARG
1	F	361	LEU
1	F	370	GLU
1	G	156	MET
1	G	163	SER
1	G	170	ARG

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Mol	Chain	Res	Type
1	G	186	ILE
1	G	209	THR
1	G	212	VAL
1	G	231	GLU
1	G	254	ARG
1	G	255	LEU
1	G	259	LYS
1	G	270	THR
1	G	276	LYS
1	G	299	TRP
1	G	306	LYS
1	G	326	LEU
1	G	364	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	HIS
1	A	221	GLN
1	A	277	GLN
1	A	293	ASN
1	A	314	ASN
1	A	356	GLN
1	B	221	GLN
1	B	356	GLN
1	C	221	GLN
1	C	320	HIS
1	C	356	GLN
1	D	356	GLN
1	D	364	ASN
1	E	320	HIS
1	E	356	GLN
1	F	174	ASN
1	F	368	GLN
1	G	221	GLN
1	G	320	HIS
1	G	356	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	28,29,29	1.43	4 (14%)	43,45,45	1.86	7 (16%)
2	ADP	E	401	-	28,29,29	1.44	5 (17%)	43,45,45	1.82	7 (16%)
2	ADP	C	401	-	28,29,29	1.45	5 (17%)	43,45,45	1.80	7 (16%)
2	ADP	F	401	-	28,29,29	1.42	4 (14%)	43,45,45	1.86	8 (18%)
2	ADP	D	401	-	28,29,29	1.48	5 (17%)	43,45,45	1.83	8 (18%)
2	ADP	B	401	-	28,29,29	1.45	5 (17%)	43,45,45	1.83	8 (18%)
2	ADP	A	401	-	28,29,29	1.43	4 (14%)	43,45,45	1.83	7 (16%)

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	-	-	3/16/32/32	0/3/3/3
2	ADP	E	401	-	-	1/16/32/32	0/3/3/3
2	ADP	C	401	-	-	5/16/32/32	0/3/3/3
2	ADP	F	401	-	-	5/16/32/32	0/3/3/3
2	ADP	D	401	-	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	401	-	-	2/16/32/32	0/3/3/3
2	ADP	A	401	-	-	1/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	ADP	C5-C4	4.78	1.47	1.39
2	D	401	ADP	C5-C4	4.77	1.47	1.39
2	A	401	ADP	C5-C4	4.77	1.47	1.39
2	F	401	ADP	C5-C4	4.74	1.47	1.39
2	G	401	ADP	C5-C4	4.74	1.47	1.39
2	E	401	ADP	C5-C4	4.73	1.47	1.39
2	B	401	ADP	C5-C4	4.73	1.47	1.39
2	F	401	ADP	C5-N7	-2.74	1.34	1.39
2	D	401	ADP	PA-O3A	2.67	1.62	1.59
2	B	401	ADP	C5-N7	-2.64	1.34	1.39
2	A	401	ADP	C5-C6	2.63	1.48	1.41
2	D	401	ADP	C5-C6	2.59	1.48	1.41
2	G	401	ADP	C5-C6	2.58	1.48	1.41
2	E	401	ADP	C5-C6	2.57	1.48	1.41
2	C	401	ADP	C5-C6	2.54	1.48	1.41
2	F	401	ADP	C5-C6	2.52	1.48	1.41
2	E	401	ADP	C5-N7	-2.51	1.34	1.39
2	C	401	ADP	C5-N7	-2.51	1.34	1.39
2	G	401	ADP	C5-N7	-2.49	1.34	1.39
2	B	401	ADP	C5-C6	2.49	1.47	1.41
2	D	401	ADP	C5-N7	-2.48	1.34	1.39
2	A	401	ADP	C5-N7	-2.39	1.34	1.39
2	C	401	ADP	PA-O3A	2.27	1.61	1.59
2	D	401	ADP	C8-N7	2.25	1.36	1.31
2	G	401	ADP	C8-N7	2.25	1.36	1.31
2	A	401	ADP	C8-N7	2.22	1.35	1.31
2	B	401	ADP	PA-O3A	2.18	1.61	1.59
2	C	401	ADP	C8-N7	2.18	1.35	1.31
2	E	401	ADP	C8-N7	2.16	1.35	1.31
2	B	401	ADP	C8-N7	2.14	1.35	1.31
2	F	401	ADP	C8-N7	2.12	1.35	1.31
2	E	401	ADP	PA-O3A	2.06	1.61	1.59

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	ADP	C5-C4-N3	-6.34	117.98	126.72
2	D	401	ADP	C5-C4-N3	-6.22	118.15	126.72
2	G	401	ADP	C5-C4-N3	-6.19	118.20	126.72
2	E	401	ADP	C5-C4-N3	-6.13	118.27	126.72
2	A	401	ADP	C5-C4-N3	-6.13	118.28	126.72
2	C	401	ADP	C5-C4-N3	-6.12	118.30	126.72
2	B	401	ADP	C5-C4-N3	-6.11	118.31	126.72
2	F	401	ADP	N3-C4-N9	5.35	136.27	127.17
2	B	401	ADP	N3-C4-N9	5.29	136.16	127.17
2	D	401	ADP	N3-C4-N9	5.29	136.16	127.17
2	C	401	ADP	N3-C4-N9	5.16	135.94	127.17
2	A	401	ADP	N3-C4-N9	5.15	135.93	127.17
2	G	401	ADP	N3-C4-N9	5.14	135.91	127.17
2	E	401	ADP	N3-C4-N9	5.11	135.85	127.17
2	D	401	ADP	C2-N3-C4	3.74	120.97	111.83
2	A	401	ADP	C2-N3-C4	3.74	120.95	111.83
2	G	401	ADP	C2-N3-C4	3.68	120.82	111.83
2	C	401	ADP	C2-N3-C4	3.68	120.81	111.83
2	F	401	ADP	C2-N3-C4	3.67	120.80	111.83
2	E	401	ADP	C2-N3-C4	3.63	120.69	111.83
2	B	401	ADP	C2-N3-C4	3.61	120.64	111.83
2	A	401	ADP	N3-C2-N1	-3.17	123.78	128.58
2	G	401	ADP	C4-C5-N7	-3.17	106.96	110.58
2	F	401	ADP	C4-C5-N7	-3.14	107.00	110.58
2	E	401	ADP	C4-C5-N7	-3.12	107.01	110.58
2	C	401	ADP	N3-C2-N1	-3.09	123.90	128.58
2	A	401	ADP	C4-C5-N7	-3.08	107.06	110.58
2	D	401	ADP	N3-C2-N1	-3.07	123.93	128.58
2	B	401	ADP	N3-C2-N1	-3.07	123.94	128.58
2	G	401	ADP	N3-C2-N1	-3.01	124.02	128.58
2	C	401	ADP	C4-C5-N7	-3.00	107.15	110.58
2	E	401	ADP	N3-C2-N1	-2.99	124.05	128.58
2	F	401	ADP	N3-C2-N1	-2.92	124.17	128.58
2	D	401	ADP	C4-C5-N7	-2.91	107.25	110.58
2	B	401	ADP	C4-C5-N7	-2.83	107.35	110.58
2	B	401	ADP	C4-N9-C8	2.65	108.52	105.74
2	D	401	ADP	C4-N9-C8	2.65	108.52	105.74
2	G	401	ADP	C4-N9-C8	2.64	108.50	105.74
2	A	401	ADP	C4-N9-C8	2.60	108.47	105.74
2	F	401	ADP	C5-N7-C8	2.56	107.47	103.45
2	F	401	ADP	C4-N9-C8	2.56	108.42	105.74
2	E	401	ADP	C4-N9-C8	2.54	108.40	105.74
2	C	401	ADP	C4-N9-C8	2.51	108.38	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	ADP	C5-N7-C8	2.48	107.36	103.45
2	A	401	ADP	C5-N7-C8	2.44	107.29	103.45
2	E	401	ADP	C5-N7-C8	2.35	107.15	103.45
2	C	401	ADP	C5-N7-C8	2.30	107.06	103.45
2	B	401	ADP	C5-N7-C8	2.28	107.03	103.45
2	D	401	ADP	C5-N7-C8	2.27	107.01	103.45
2	F	401	ADP	C1'-N9-C8	-2.24	122.12	127.09
2	B	401	ADP	C1'-N9-C8	-2.12	122.39	127.09
2	D	401	ADP	C1'-N9-C8	-2.03	122.59	127.09

There are no chirality outliers.

All (21) 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	C	401	ADP	C5'-O5'-PA-O3A
2	D	401	ADP	C5'-O5'-PA-O2A
2	D	401	ADP	C5'-O5'-PA-O3A
2	F	401	ADP	C5'-O5'-PA-O3A
2	G	401	ADP	C5'-O5'-PA-O1A
2	G	401	ADP	C5'-O5'-PA-O3A
2	F	401	ADP	O4'-C4'-C5'-O5'
2	F	401	ADP	C3'-C4'-C5'-O5'
2	A	401	ADP	PA-O3A-PB-O1B
2	F	401	ADP	C4'-C5'-O5'-PA
2	B	401	ADP	O4'-C4'-C5'-O5'
2	D	401	ADP	C5'-O5'-PA-O1A
2	F	401	ADP	C5'-O5'-PA-O1A
2	G	401	ADP	C5'-O5'-PA-O2A
2	E	401	ADP	PB-O3A-PA-O2A
2	C	401	ADP	PA-O3A-PB-O3B
2	B	401	ADP	C3'-C4'-C5'-O5'
2	D	401	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 18 short contacts:

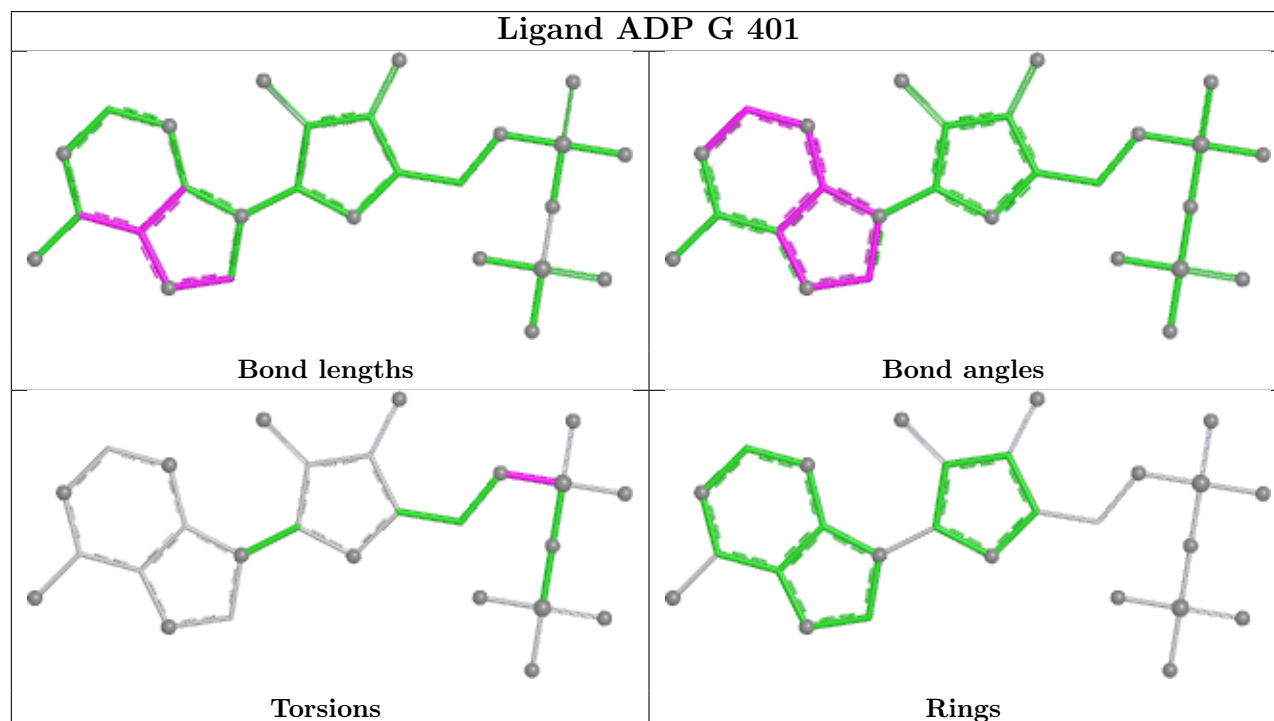
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	401	ADP	1	0

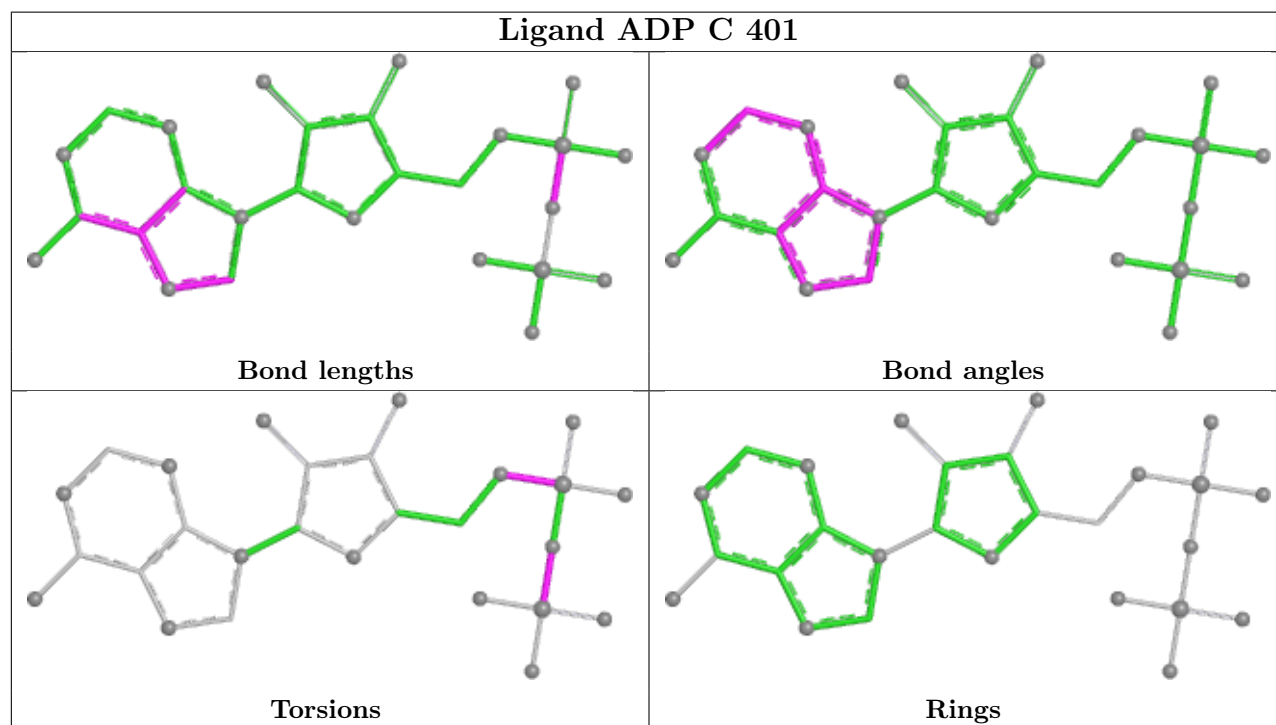
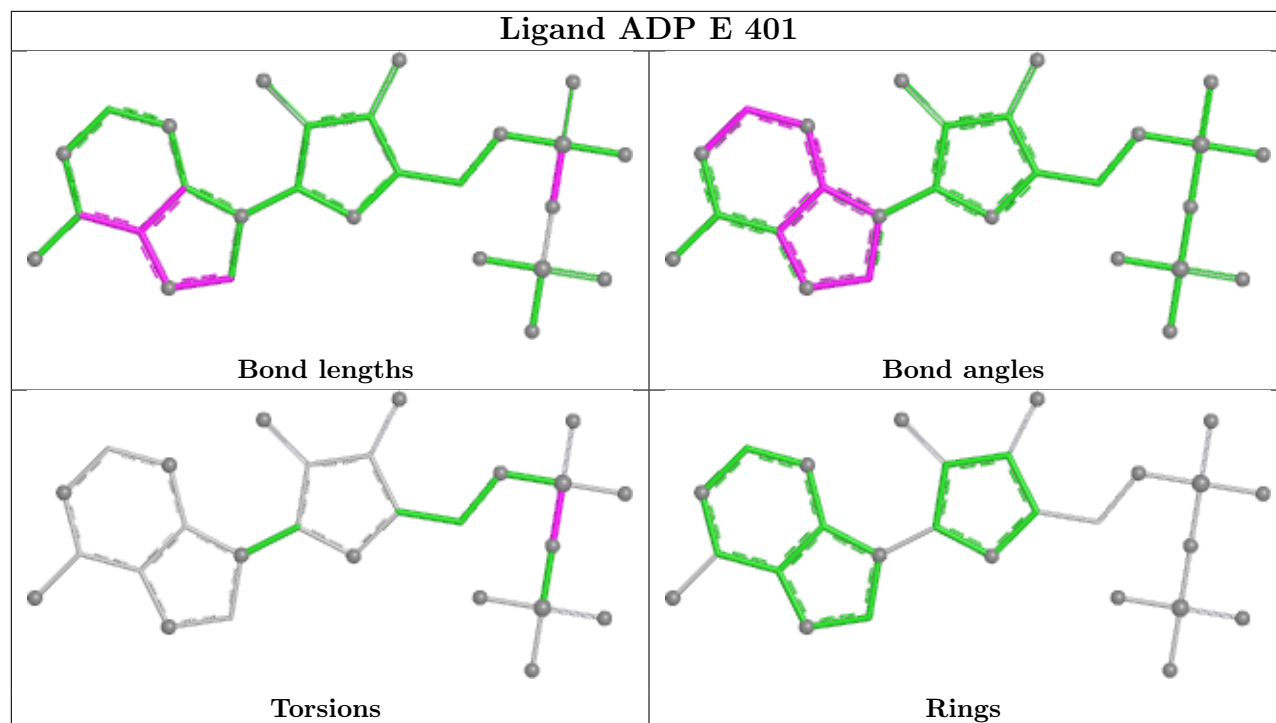
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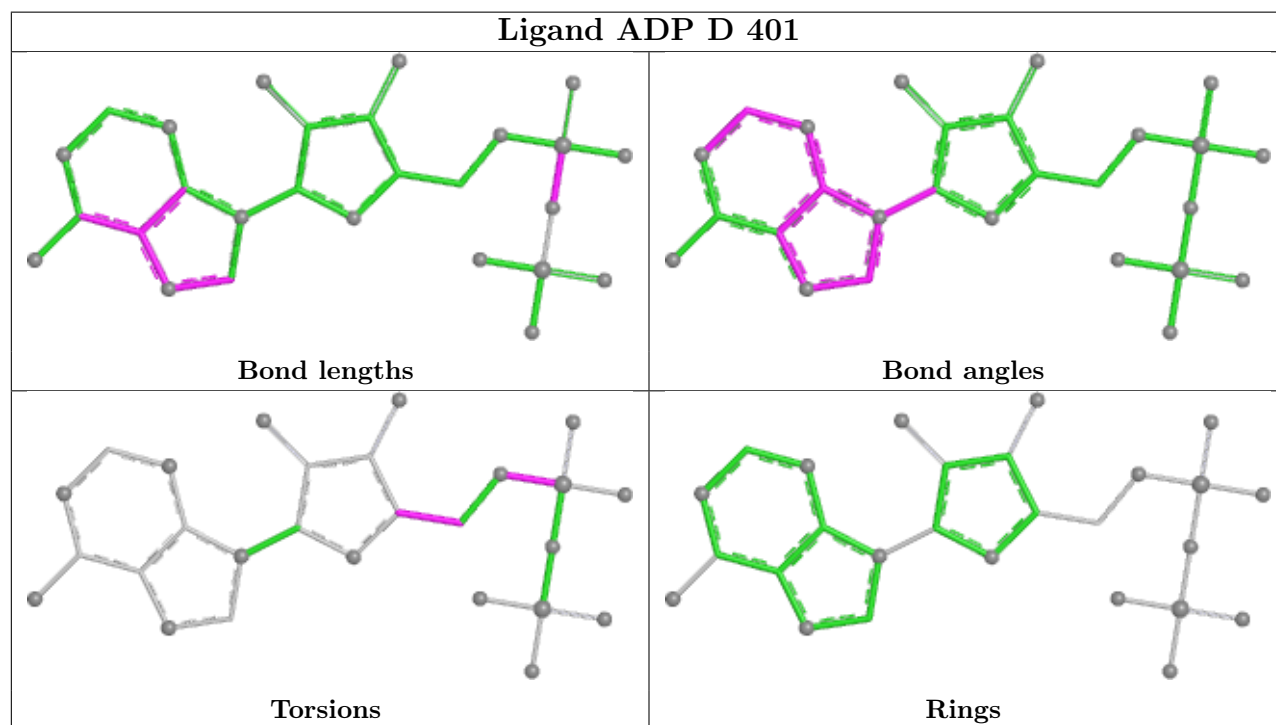
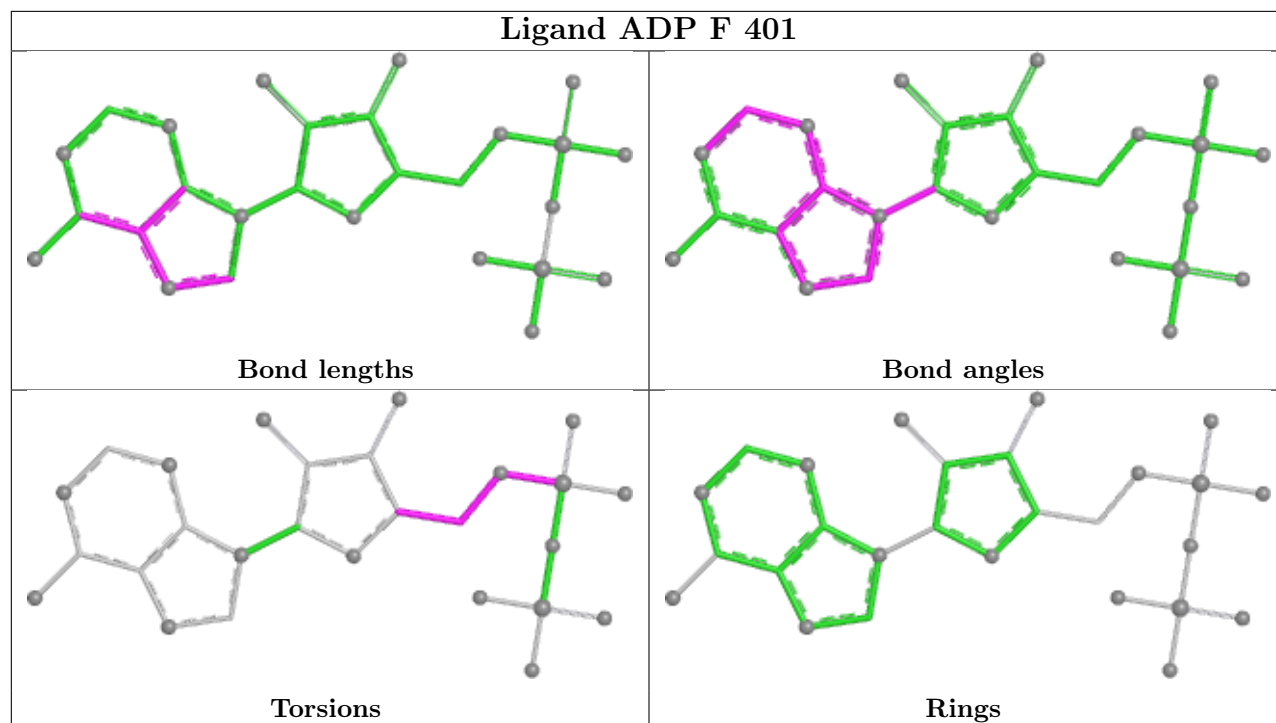
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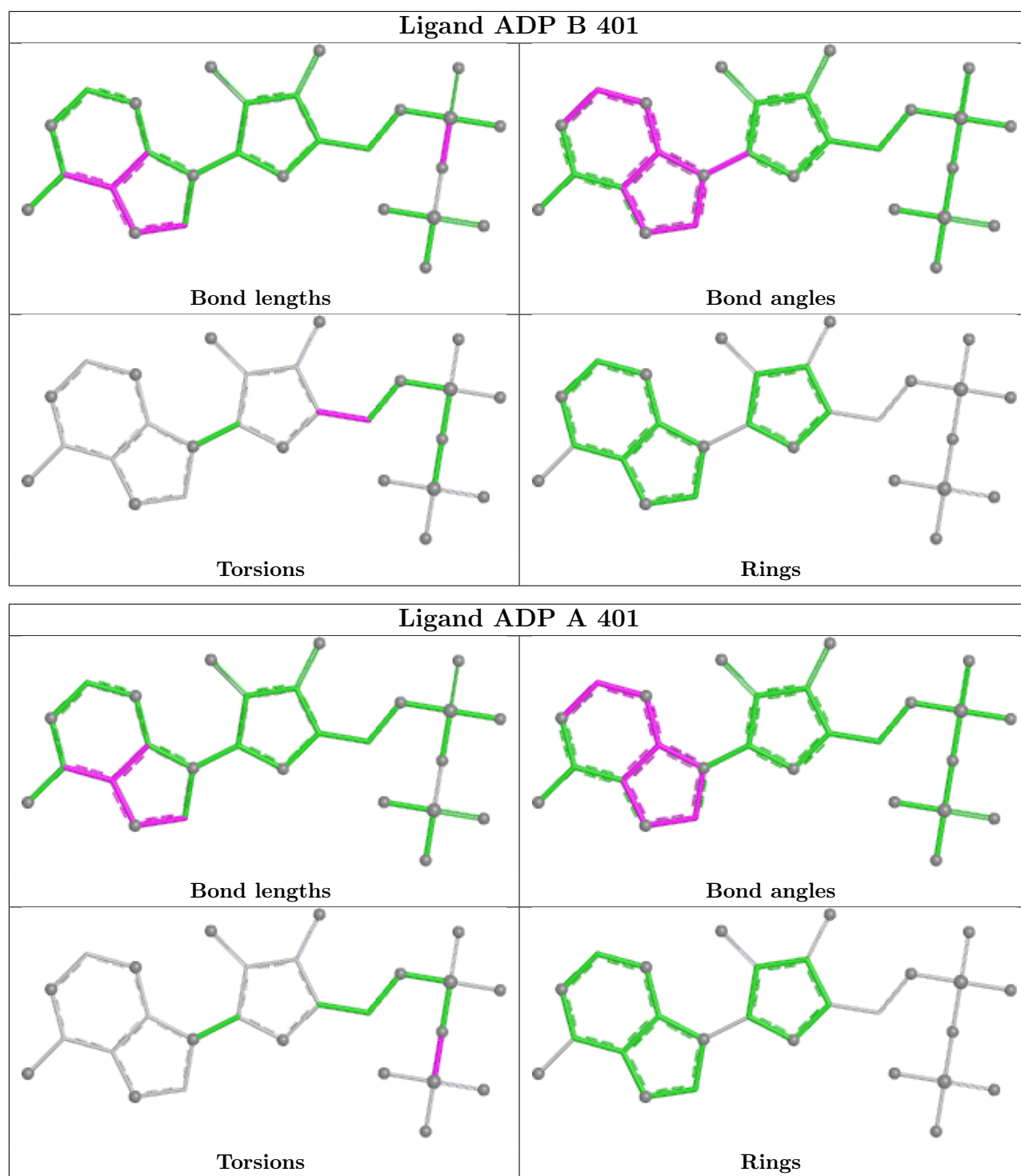
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	ADP	2	0
2	C	401	ADP	4	0
2	F	401	ADP	3	0
2	D	401	ADP	2	0
2	B	401	ADP	2	0
2	A	401	ADP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

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 [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	247/271 (91%)	-0.11	1 (0%) 88 73	28, 54, 88, 100	0
1	B	247/271 (91%)	-0.14	2 (0%) 82 61	33, 52, 81, 103	0
1	C	246/271 (90%)	-0.17	1 (0%) 88 73	31, 54, 84, 93	1 (0%)
1	D	246/271 (90%)	-0.15	2 (0%) 82 61	33, 53, 80, 105	0
1	E	246/271 (90%)	-0.18	2 (0%) 82 61	30, 50, 79, 109	0
1	F	247/271 (91%)	-0.10	2 (0%) 82 61	34, 55, 88, 122	0
1	G	246/271 (90%)	-0.20	2 (0%) 82 61	32, 51, 77, 105	0
All	All	1725/1897 (90%)	-0.15	12 (0%) 84 64	28, 53, 84, 122	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	132	VAL	4.0
1	G	376	GLY	3.9
1	E	132	VAL	3.6
1	D	164	GLY	3.0
1	E	376	GLY	2.5
1	C	376	GLY	2.4
1	F	376	GLY	2.2
1	B	253	GLU	2.2
1	B	376	GLY	2.1
1	F	130	HIS	2.1
1	A	212	VAL	2.0
1	D	167	VAL	2.0

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

There are no oligosaccharides in this entry.

6.4 Ligands

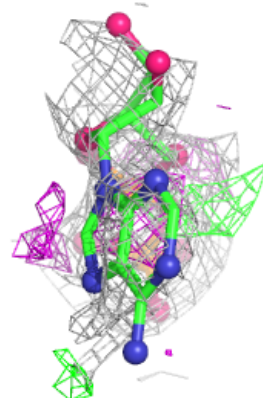
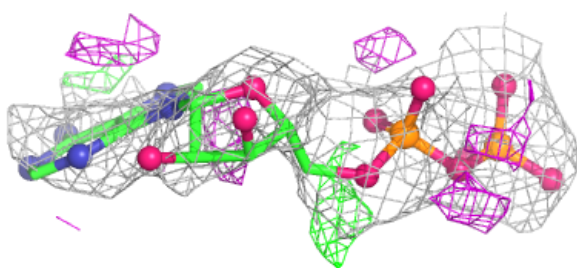
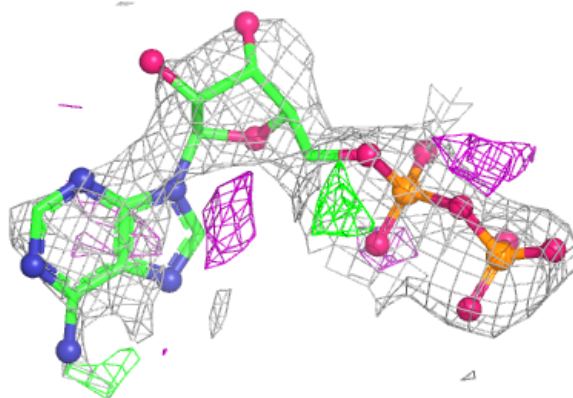
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.74	0.20	126,142,172,175	0
2	ADP	D	401	27/27	0.75	0.19	100,106,193,219	0
2	ADP	C	401	27/27	0.78	0.17	99,112,143,149	0
2	ADP	B	401	27/27	0.79	0.18	103,110,152,210	0
2	ADP	A	401	27/27	0.80	0.16	98,109,137,139	0
2	ADP	G	401	27/27	0.80	0.17	91,98,134,139	0
2	ADP	E	401	27/27	0.81	0.20	104,113,132,193	0

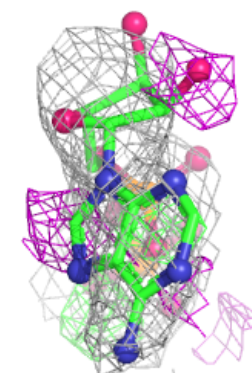
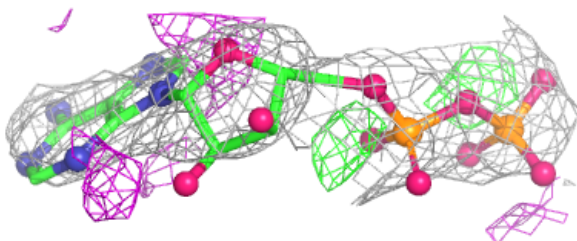
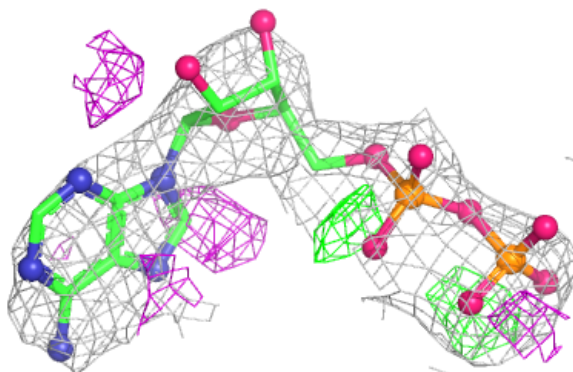
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

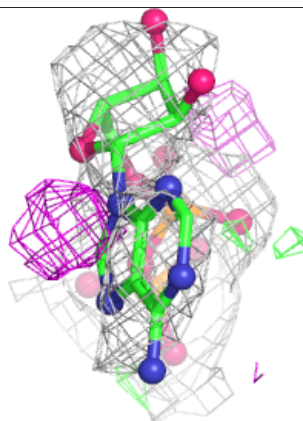
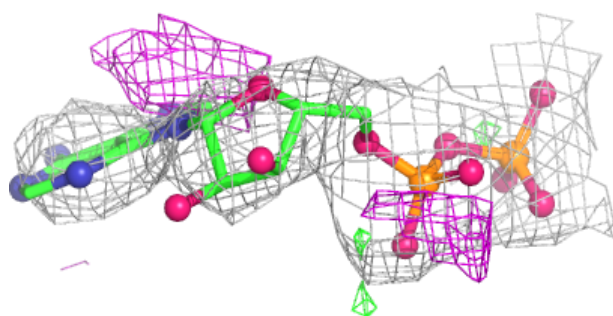
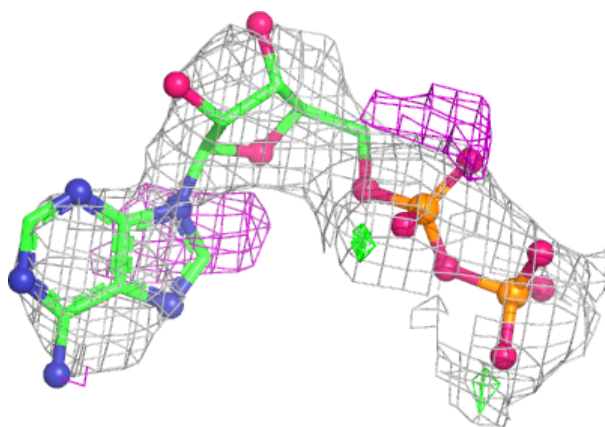
**Electron density around ADP D 401:**

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



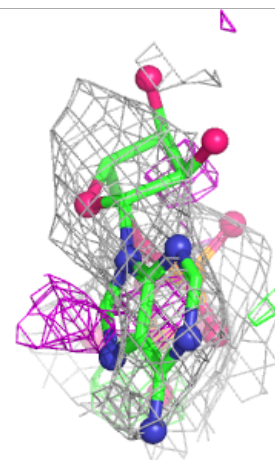
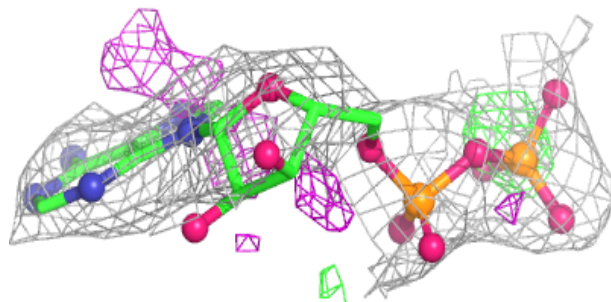
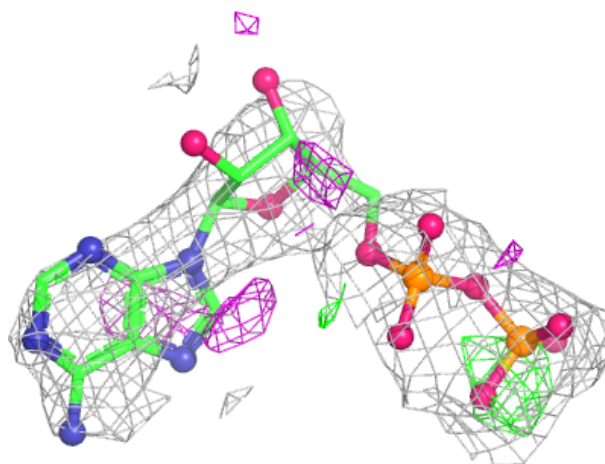
Electron density around ADP C 401:

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



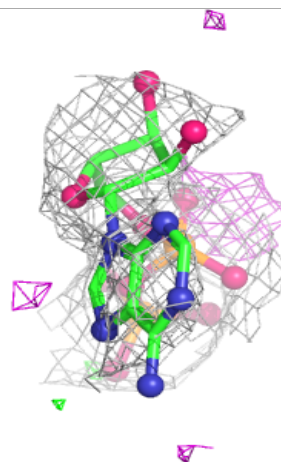
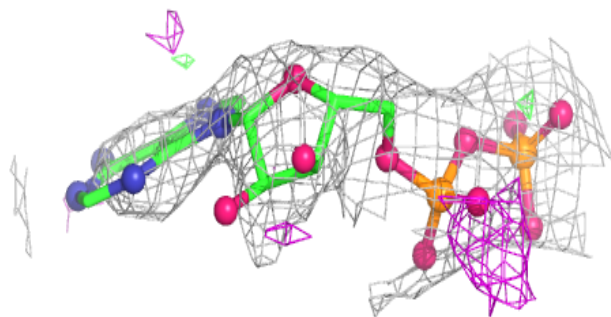
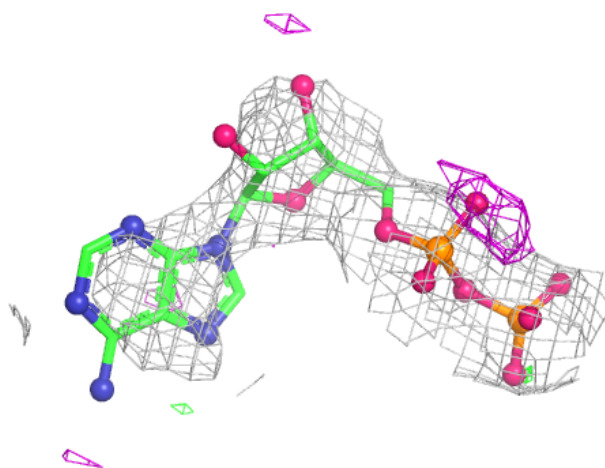
Electron density around ADP B 401:

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



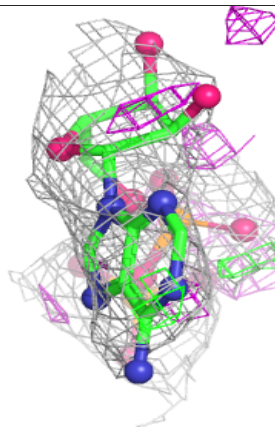
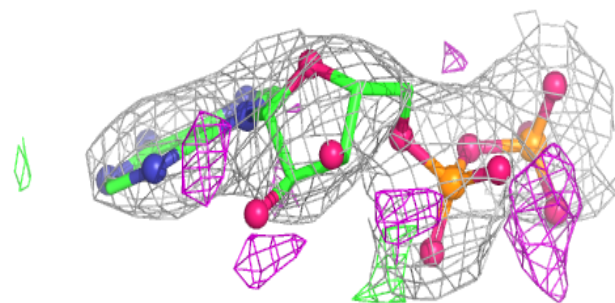
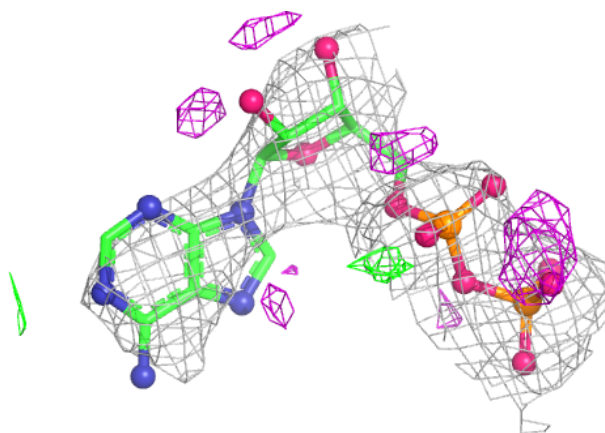
Electron density around ADP A 401:

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

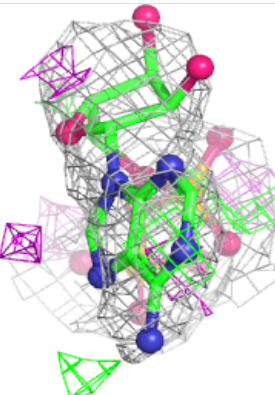
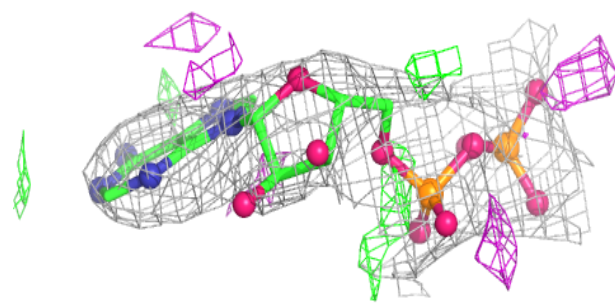
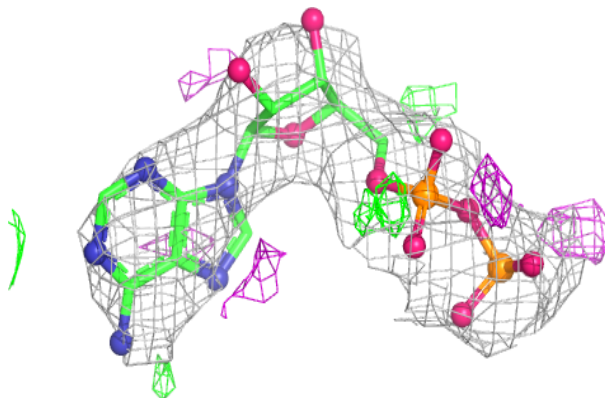


Electron density around ADP G 401:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.