Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 – 01:49 am GMT

PDB ID	:	6EP2
Title	:	Enterococcus faecalis FIC protein in complex with ADP and calcium ion.
Authors	:	Veyron, S.; Cherfils, J.
Deposited on	:	2017-10-10
Resolution	:	2.15 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

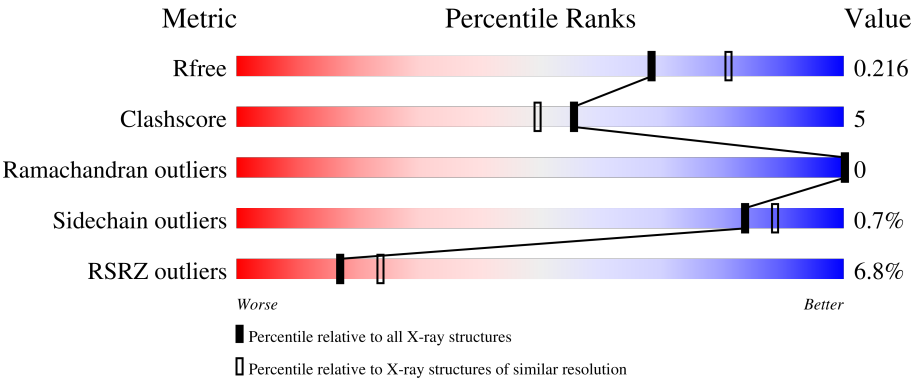
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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.



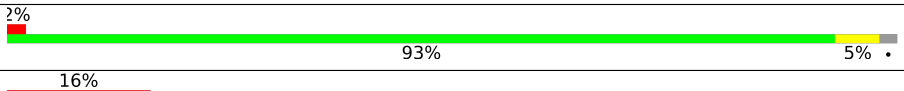
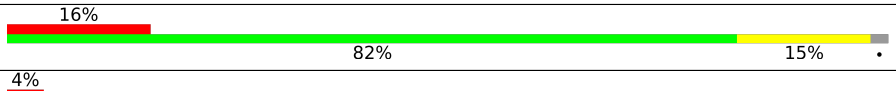
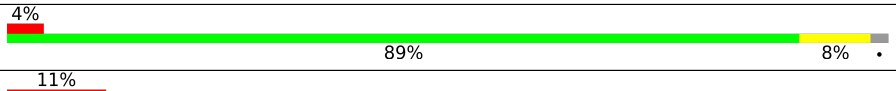
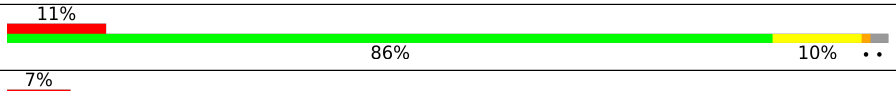
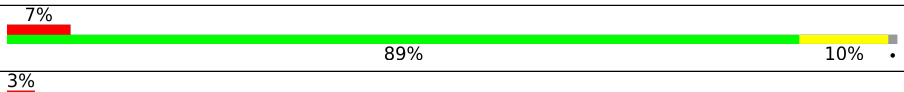
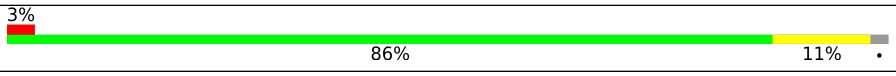
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	207	6% 90% 7%
1	B	207	4% 86% 11%
1	C	207	3% 89% 8%
1	D	207	2% 91% 7%
1	E	207	4% 92% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	207	
1	G	207	
1	H	207	
1	I	207	
1	J	207	
1	K	207	
1	L	207	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22137 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 Fic family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1686	1077	287	316	6			
1	B	202	Total	C	N	O	S	0	0	0
			1686	1077	287	316	6			
1	C	202	Total	C	N	O	S	0	0	0
			1686	1077	287	316	6			
1	D	203	Total	C	N	O	S	0	0	0
			1696	1083	290	317	6			
1	E	203	Total	C	N	O	S	0	0	0
			1696	1083	290	317	6			
1	F	202	Total	C	N	O	S	0	1	0
			1693	1082	289	316	6			
1	G	203	Total	C	N	O	S	0	0	0
			1696	1083	290	317	6			
1	H	202	Total	C	N	O	S	0	0	0
			1686	1077	287	316	6			
1	I	202	Total	C	N	O	S	0	0	0
			1686	1077	287	316	6			
1	J	202	Total	C	N	O	S	0	0	0
			1686	1077	287	316	6			
1	K	204	Total	C	N	O	S	0	0	0
			1706	1089	293	318	6			
1	L	203	Total	C	N	O	S	0	0	0
			1696	1083	290	317	6			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP U6S0Y1
A	2	HIS	-	expression tag	UNP U6S0Y1
A	3	HIS	-	expression tag	UNP U6S0Y1
A	4	HIS	-	expression tag	UNP U6S0Y1
A	5	HIS	-	expression tag	UNP U6S0Y1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	HIS	-	expression tag	UNP U6S0Y1
A	7	HIS	-	expression tag	UNP U6S0Y1
A	32	ASN	LYS	conflict	UNP U6S0Y1
A	35	ARG	GLN	conflict	UNP U6S0Y1
A	45	ILE	VAL	conflict	UNP U6S0Y1
A	47	VAL	ILE	conflict	UNP U6S0Y1
A	142	ARG	GLN	conflict	UNP U6S0Y1
A	150	ASN	ASP	conflict	UNP U6S0Y1
A	205	ASP	GLU	conflict	UNP U6S0Y1
A	206	GLU	ASP	conflict	UNP U6S0Y1
B	1	MET	-	initiating methionine	UNP U6S0Y1
B	2	HIS	-	expression tag	UNP U6S0Y1
B	3	HIS	-	expression tag	UNP U6S0Y1
B	4	HIS	-	expression tag	UNP U6S0Y1
B	5	HIS	-	expression tag	UNP U6S0Y1
B	6	HIS	-	expression tag	UNP U6S0Y1
B	7	HIS	-	expression tag	UNP U6S0Y1
B	32	ASN	LYS	conflict	UNP U6S0Y1
B	35	ARG	GLN	conflict	UNP U6S0Y1
B	45	ILE	VAL	conflict	UNP U6S0Y1
B	47	VAL	ILE	conflict	UNP U6S0Y1
B	142	ARG	GLN	conflict	UNP U6S0Y1
B	150	ASN	ASP	conflict	UNP U6S0Y1
B	205	ASP	GLU	conflict	UNP U6S0Y1
B	206	GLU	ASP	conflict	UNP U6S0Y1
C	1	MET	-	initiating methionine	UNP U6S0Y1
C	2	HIS	-	expression tag	UNP U6S0Y1
C	3	HIS	-	expression tag	UNP U6S0Y1
C	4	HIS	-	expression tag	UNP U6S0Y1
C	5	HIS	-	expression tag	UNP U6S0Y1
C	6	HIS	-	expression tag	UNP U6S0Y1
C	7	HIS	-	expression tag	UNP U6S0Y1
C	32	ASN	LYS	conflict	UNP U6S0Y1
C	35	ARG	GLN	conflict	UNP U6S0Y1
C	45	ILE	VAL	conflict	UNP U6S0Y1
C	47	VAL	ILE	conflict	UNP U6S0Y1
C	142	ARG	GLN	conflict	UNP U6S0Y1
C	150	ASN	ASP	conflict	UNP U6S0Y1
C	205	ASP	GLU	conflict	UNP U6S0Y1
C	206	GLU	ASP	conflict	UNP U6S0Y1
D	1	MET	-	initiating methionine	UNP U6S0Y1
D	2	HIS	-	expression tag	UNP U6S0Y1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	3	HIS	-	expression tag	UNP U6S0Y1
D	4	HIS	-	expression tag	UNP U6S0Y1
D	5	HIS	-	expression tag	UNP U6S0Y1
D	6	HIS	-	expression tag	UNP U6S0Y1
D	7	HIS	-	expression tag	UNP U6S0Y1
D	32	ASN	LYS	conflict	UNP U6S0Y1
D	35	ARG	GLN	conflict	UNP U6S0Y1
D	45	ILE	VAL	conflict	UNP U6S0Y1
D	47	VAL	ILE	conflict	UNP U6S0Y1
D	142	ARG	GLN	conflict	UNP U6S0Y1
D	150	ASN	ASP	conflict	UNP U6S0Y1
D	205	ASP	GLU	conflict	UNP U6S0Y1
D	206	GLU	ASP	conflict	UNP U6S0Y1
E	1	MET	-	initiating methionine	UNP U6S0Y1
E	2	HIS	-	expression tag	UNP U6S0Y1
E	3	HIS	-	expression tag	UNP U6S0Y1
E	4	HIS	-	expression tag	UNP U6S0Y1
E	5	HIS	-	expression tag	UNP U6S0Y1
E	6	HIS	-	expression tag	UNP U6S0Y1
E	7	HIS	-	expression tag	UNP U6S0Y1
E	32	ASN	LYS	conflict	UNP U6S0Y1
E	35	ARG	GLN	conflict	UNP U6S0Y1
E	45	ILE	VAL	conflict	UNP U6S0Y1
E	47	VAL	ILE	conflict	UNP U6S0Y1
E	142	ARG	GLN	conflict	UNP U6S0Y1
E	150	ASN	ASP	conflict	UNP U6S0Y1
E	205	ASP	GLU	conflict	UNP U6S0Y1
E	206	GLU	ASP	conflict	UNP U6S0Y1
F	1	MET	-	initiating methionine	UNP U6S0Y1
F	2	HIS	-	expression tag	UNP U6S0Y1
F	3	HIS	-	expression tag	UNP U6S0Y1
F	4	HIS	-	expression tag	UNP U6S0Y1
F	5	HIS	-	expression tag	UNP U6S0Y1
F	6	HIS	-	expression tag	UNP U6S0Y1
F	7	HIS	-	expression tag	UNP U6S0Y1
F	32	ASN	LYS	conflict	UNP U6S0Y1
F	35	ARG	GLN	conflict	UNP U6S0Y1
F	45	ILE	VAL	conflict	UNP U6S0Y1
F	47	VAL	ILE	conflict	UNP U6S0Y1
F	142	ARG	GLN	conflict	UNP U6S0Y1
F	150	ASN	ASP	conflict	UNP U6S0Y1
F	205	ASP	GLU	conflict	UNP U6S0Y1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	206	GLU	ASP	conflict	UNP U6S0Y1
G	1	MET	-	initiating methionine	UNP U6S0Y1
G	2	HIS	-	expression tag	UNP U6S0Y1
G	3	HIS	-	expression tag	UNP U6S0Y1
G	4	HIS	-	expression tag	UNP U6S0Y1
G	5	HIS	-	expression tag	UNP U6S0Y1
G	6	HIS	-	expression tag	UNP U6S0Y1
G	7	HIS	-	expression tag	UNP U6S0Y1
G	32	ASN	LYS	conflict	UNP U6S0Y1
G	35	ARG	GLN	conflict	UNP U6S0Y1
G	45	ILE	VAL	conflict	UNP U6S0Y1
G	47	VAL	ILE	conflict	UNP U6S0Y1
G	142	ARG	GLN	conflict	UNP U6S0Y1
G	150	ASN	ASP	conflict	UNP U6S0Y1
G	205	ASP	GLU	conflict	UNP U6S0Y1
G	206	GLU	ASP	conflict	UNP U6S0Y1
H	1	MET	-	initiating methionine	UNP U6S0Y1
H	2	HIS	-	expression tag	UNP U6S0Y1
H	3	HIS	-	expression tag	UNP U6S0Y1
H	4	HIS	-	expression tag	UNP U6S0Y1
H	5	HIS	-	expression tag	UNP U6S0Y1
H	6	HIS	-	expression tag	UNP U6S0Y1
H	7	HIS	-	expression tag	UNP U6S0Y1
H	32	ASN	LYS	conflict	UNP U6S0Y1
H	35	ARG	GLN	conflict	UNP U6S0Y1
H	45	ILE	VAL	conflict	UNP U6S0Y1
H	47	VAL	ILE	conflict	UNP U6S0Y1
H	142	ARG	GLN	conflict	UNP U6S0Y1
H	150	ASN	ASP	conflict	UNP U6S0Y1
H	205	ASP	GLU	conflict	UNP U6S0Y1
H	206	GLU	ASP	conflict	UNP U6S0Y1
I	1	MET	-	initiating methionine	UNP U6S0Y1
I	2	HIS	-	expression tag	UNP U6S0Y1
I	3	HIS	-	expression tag	UNP U6S0Y1
I	4	HIS	-	expression tag	UNP U6S0Y1
I	5	HIS	-	expression tag	UNP U6S0Y1
I	6	HIS	-	expression tag	UNP U6S0Y1
I	7	HIS	-	expression tag	UNP U6S0Y1
I	32	ASN	LYS	conflict	UNP U6S0Y1
I	35	ARG	GLN	conflict	UNP U6S0Y1
I	45	ILE	VAL	conflict	UNP U6S0Y1
I	47	VAL	ILE	conflict	UNP U6S0Y1

Continued on next page...

Continued from previous page...

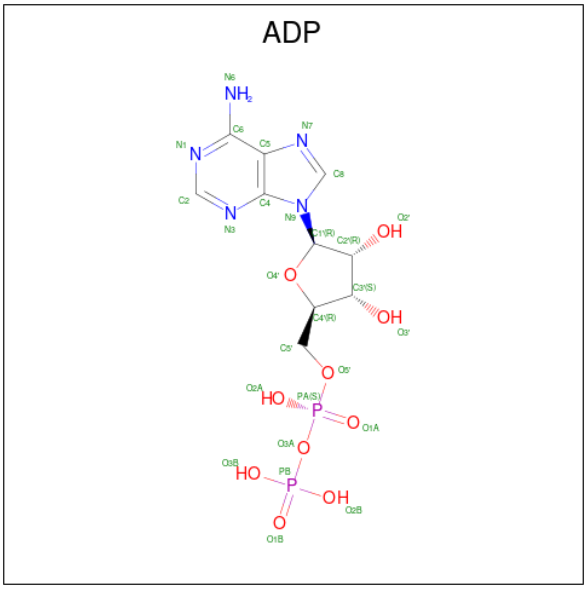
Chain	Residue	Modelled	Actual	Comment	Reference
I	142	ARG	GLN	conflict	UNP U6S0Y1
I	150	ASN	ASP	conflict	UNP U6S0Y1
I	205	ASP	GLU	conflict	UNP U6S0Y1
I	206	GLU	ASP	conflict	UNP U6S0Y1
J	1	MET	-	initiating methionine	UNP U6S0Y1
J	2	HIS	-	expression tag	UNP U6S0Y1
J	3	HIS	-	expression tag	UNP U6S0Y1
J	4	HIS	-	expression tag	UNP U6S0Y1
J	5	HIS	-	expression tag	UNP U6S0Y1
J	6	HIS	-	expression tag	UNP U6S0Y1
J	7	HIS	-	expression tag	UNP U6S0Y1
J	32	ASN	LYS	conflict	UNP U6S0Y1
J	35	ARG	GLN	conflict	UNP U6S0Y1
J	45	ILE	VAL	conflict	UNP U6S0Y1
J	47	VAL	ILE	conflict	UNP U6S0Y1
J	142	ARG	GLN	conflict	UNP U6S0Y1
J	150	ASN	ASP	conflict	UNP U6S0Y1
J	205	ASP	GLU	conflict	UNP U6S0Y1
J	206	GLU	ASP	conflict	UNP U6S0Y1
K	1	MET	-	initiating methionine	UNP U6S0Y1
K	2	HIS	-	expression tag	UNP U6S0Y1
K	3	HIS	-	expression tag	UNP U6S0Y1
K	4	HIS	-	expression tag	UNP U6S0Y1
K	5	HIS	-	expression tag	UNP U6S0Y1
K	6	HIS	-	expression tag	UNP U6S0Y1
K	7	HIS	-	expression tag	UNP U6S0Y1
K	32	ASN	LYS	conflict	UNP U6S0Y1
K	35	ARG	GLN	conflict	UNP U6S0Y1
K	45	ILE	VAL	conflict	UNP U6S0Y1
K	47	VAL	ILE	conflict	UNP U6S0Y1
K	142	ARG	GLN	conflict	UNP U6S0Y1
K	150	ASN	ASP	conflict	UNP U6S0Y1
K	205	ASP	GLU	conflict	UNP U6S0Y1
K	206	GLU	ASP	conflict	UNP U6S0Y1
L	1	MET	-	initiating methionine	UNP U6S0Y1
L	2	HIS	-	expression tag	UNP U6S0Y1
L	3	HIS	-	expression tag	UNP U6S0Y1
L	4	HIS	-	expression tag	UNP U6S0Y1
L	5	HIS	-	expression tag	UNP U6S0Y1
L	6	HIS	-	expression tag	UNP U6S0Y1
L	7	HIS	-	expression tag	UNP U6S0Y1
L	32	ASN	LYS	conflict	UNP U6S0Y1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	35	ARG	GLN	conflict	UNP U6S0Y1
L	45	ILE	VAL	conflict	UNP U6S0Y1
L	47	VAL	ILE	conflict	UNP U6S0Y1
L	142	ARG	GLN	conflict	UNP U6S0Y1
L	150	ASN	ASP	conflict	UNP U6S0Y1
L	205	ASP	GLU	conflict	UNP U6S0Y1
L	206	GLU	ASP	conflict	UNP U6S0Y1

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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		
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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		
3	C	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		
3	E	2	Total	Ca	0	0
			2	2		
3	F	2	Total	Ca	0	0
			2	2		
3	G	3	Total	Ca	0	0
			3	3		
3	H	3	Total	Ca	0	0
			3	3		
3	I	1	Total	Ca	0	0
			1	1		
3	J	2	Total	Ca	0	0
			2	2		
3	K	1	Total	Ca	0	0
			1	1		
3	L	2	Total	Ca	0	0
			2	2		

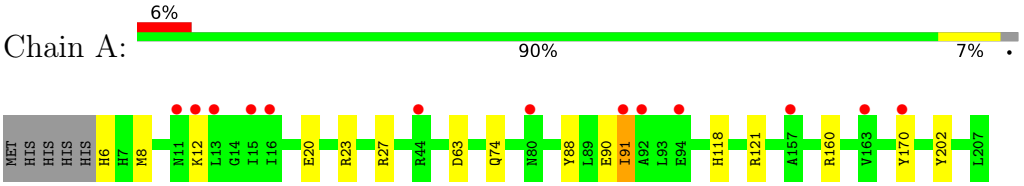
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	179	Total O 179 179	0	0
4	B	175	Total O 175 175	0	0
4	C	166	Total O 166 166	0	0
4	D	176	Total O 176 176	0	0
4	E	148	Total O 148 148	0	0
4	F	41	Total O 41 41	0	0
4	G	119	Total O 119 119	0	0
4	H	37	Total O 37 37	0	0
4	I	165	Total O 165 165	0	0
4	J	61	Total O 61 61	0	0
4	K	68	Total O 68 68	0	0
4	L	155	Total O 155 155	0	0

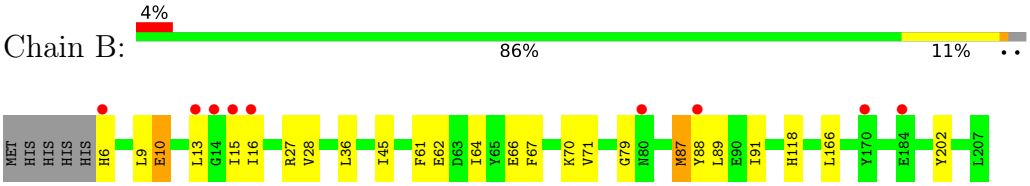
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

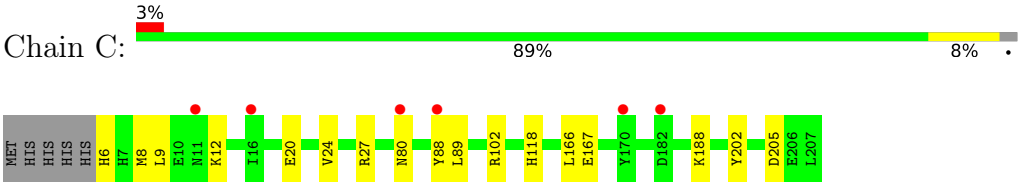
• Molecule 1: Fic family protein



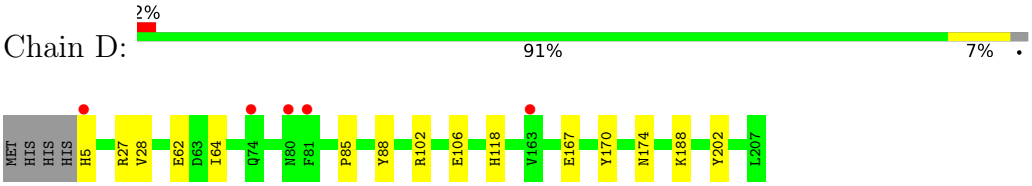
• Molecule 1: Fic family protein



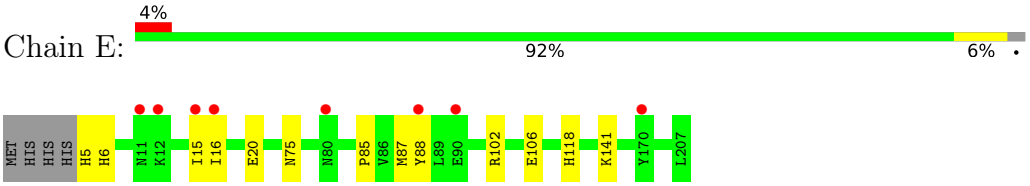
• Molecule 1: Fic family protein



• Molecule 1: Fic family protein

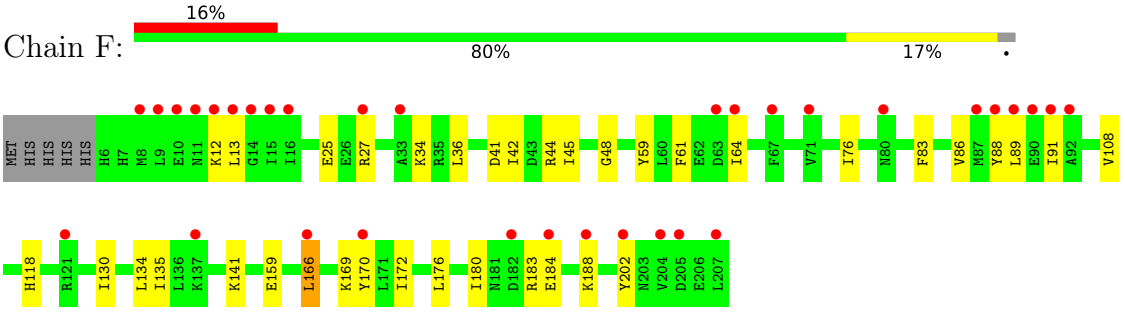


• Molecule 1: Fic family protein



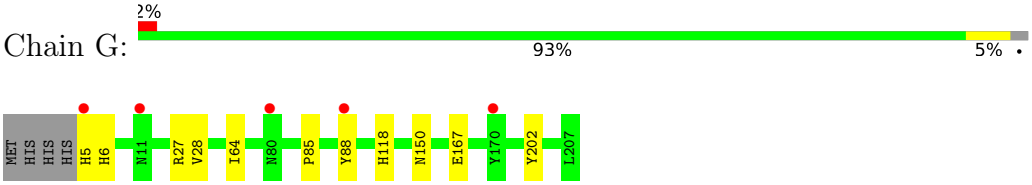
• Molecule 1: Fic family protein

Chain F:



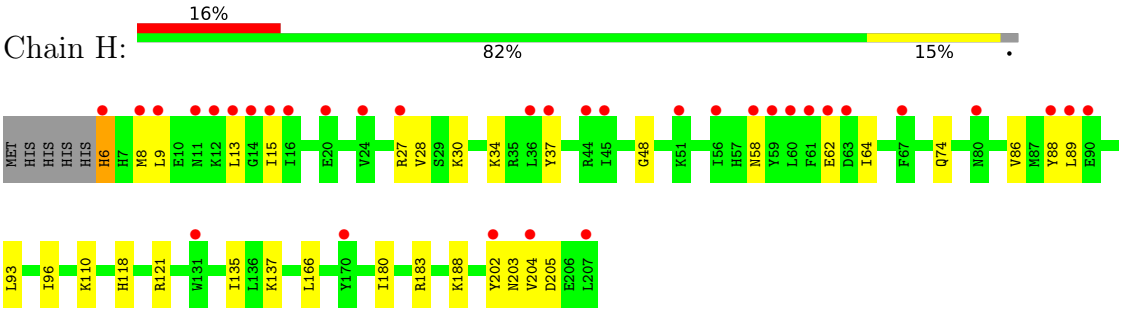
• Molecule 1: Fic family protein

Chain G:



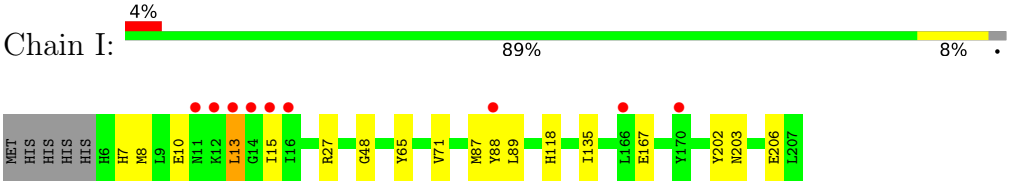
• Molecule 1: Fic family protein

Chain H:



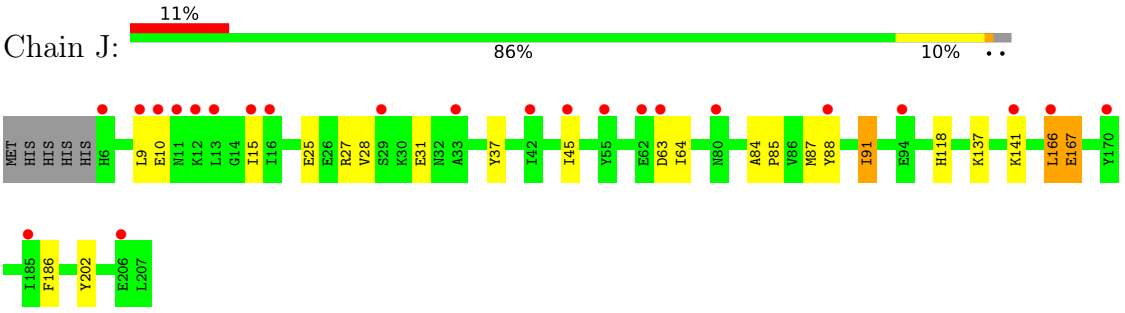
• Molecule 1: Fic family protein

Chain I:



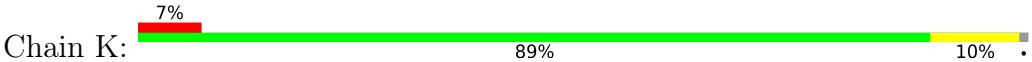
• Molecule 1: Fic family protein

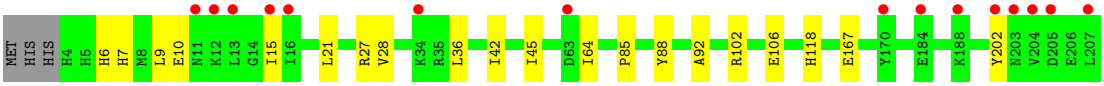
Chain J:



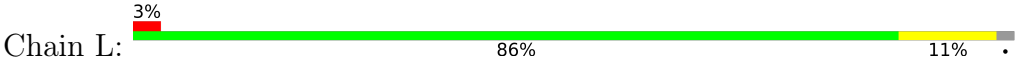
• Molecule 1: Fic family protein

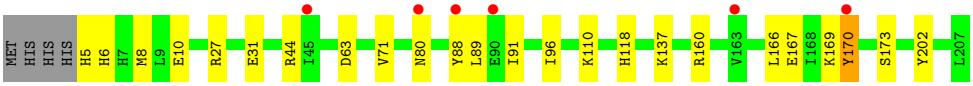
Chain K:





• Molecule 1: Fic family protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	125.31Å 125.31Å 362.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.04 – 2.15 56.04 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (56.04-2.15) 99.9 (56.04-2.15)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.14Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.187 , 0.218 0.187 , 0.216	Depositor DCC
R_{free} test set	7890 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22137	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, CA

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	0.42	0/1718	0.53	0/2312
1	B	0.48	0/1718	0.68	4/2312 (0.2%)
1	C	0.47	0/1718	0.55	0/2312
1	D	0.42	0/1729	0.53	0/2327
1	E	0.42	0/1729	0.53	0/2327
1	F	0.55	0/1729	0.58	1/2327 (0.0%)
1	G	0.50	0/1729	0.54	0/2327
1	H	0.55	1/1718 (0.1%)	0.64	1/2312 (0.0%)
1	I	0.42	0/1718	0.57	1/2312 (0.0%)
1	J	0.58	2/1718 (0.1%)	0.59	1/2312 (0.0%)
1	K	0.34	0/1740	0.52	0/2342
1	L	0.66	6/1729 (0.3%)	0.58	0/2327
All	All	0.49	9/20693 (0.0%)	0.57	8/27849 (0.0%)

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	H	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	6	HIS	C-N	-10.38	1.10	1.34
1	J	167	GLU	CD-OE2	-6.94	1.18	1.25
1	L	167	GLU	CD-OE2	-6.43	1.18	1.25
1	L	170	TYR	CB-CG	-6.16	1.42	1.51
1	J	167	GLU	CD-OE1	-6.09	1.19	1.25
1	L	80	ASN	C-O	-6.01	1.11	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	167	GLU	CD-OE1	-5.93	1.19	1.25
1	L	173	SER	CB-OG	-5.38	1.35	1.42
1	L	169	LYS	C-O	-5.05	1.13	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	13	LEU	CA-CB-CG	9.74	137.70	115.30
1	H	6	HIS	O-C-N	-7.54	110.64	122.70
1	F	166	LEU	CB-CG-CD2	-6.44	100.05	111.00
1	B	13	LEU	CB-CG-CD2	-6.29	100.31	111.00
1	B	166	LEU	CB-CG-CD1	-6.03	100.75	111.00
1	B	9	LEU	CB-CG-CD1	5.83	120.91	111.00
1	I	13	LEU	CA-CB-CG	5.66	128.32	115.30
1	J	166	LEU	CA-CB-CG	5.56	128.09	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	6	HIS	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1686	0	1676	24	0
1	B	1686	0	1676	20	0
1	C	1686	0	1676	15	0
1	D	1696	0	1683	17	0
1	E	1696	0	1683	14	0
1	F	1693	0	1683	30	0
1	G	1696	0	1683	8	0
1	H	1686	0	1675	23	0
1	I	1686	0	1675	14	0
1	J	1686	0	1676	30	0
1	K	1706	0	1690	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1696	0	1683	17	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	1	0
2	G	27	0	12	0	0
2	H	27	0	12	0	0
2	I	27	0	12	0	0
2	J	27	0	12	0	0
2	K	27	0	12	0	0
2	L	27	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	1	0	0	0	0
3	J	2	0	0	0	0
3	K	1	0	0	0	0
3	L	2	0	0	0	0
4	A	179	0	0	4	0
4	B	175	0	0	2	0
4	C	166	0	0	8	0
4	D	176	0	0	2	0
4	E	148	0	0	0	0
4	F	41	0	0	0	0
4	G	119	0	0	3	0
4	H	37	0	0	1	0
4	I	165	0	0	1	0
4	J	61	0	0	5	0
4	K	68	0	0	1	0
4	L	155	0	0	3	0
All	All	22137	0	20303	207	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 5.

All (207) 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:88:TYR:HB2	1:A:91:ILE:CD1	1.33	1.53
1:A:88:TYR:CB	1:A:91:ILE:HD11	1.39	1.49
1:J:45:ILE:CD1	4:J:459:HOH:O	1.74	1.30
4:G:435:HOH:O	1:J:166:LEU:HD11	1.28	1.29
1:A:88:TYR:O	1:A:91:ILE:HG13	1.22	1.28
1:J:166:LEU:HG	4:J:454:HOH:O	1.18	1.26
1:C:20:GLU:OE2	4:C:401:HOH:O	1.53	1.22
1:F:12:LYS:HG2	1:F:13:LEU:HD12	1.20	1.14
1:F:12:LYS:HG2	1:F:13:LEU:CD1	1.86	1.06
1:A:88:TYR:CG	1:A:91:ILE:HD11	1.96	0.99
1:A:88:TYR:O	1:A:91:ILE:CG1	2.11	0.97
1:J:45:ILE:HD12	4:J:459:HOH:O	1.47	0.97
1:D:170:TYR:CE1	1:D:174:ASN:ND2	2.33	0.95
1:A:88:TYR:HB2	1:A:91:ILE:CG1	1.99	0.93
1:H:9:LEU:HD12	1:H:9:LEU:N	1.84	0.90
1:J:9:LEU:CD1	1:J:64:ILE:HA	2.02	0.88
1:H:203:ASN:O	1:H:205:ASP:O	1.91	0.88
1:J:45:ILE:HD11	4:J:459:HOH:O	1.52	0.83
1:A:63:ASP:O	4:A:401:HOH:O	1.98	0.81
1:J:9:LEU:HD11	1:J:63:ASP:O	1.80	0.81
1:J:88:TYR:OH	1:K:88:TYR:HB2	1.82	0.80
1:B:6:HIS:CD2	1:B:66:GLU:OE1	2.35	0.79
1:J:9:LEU:HD11	1:J:64:ILE:HA	1.66	0.78
1:H:9:LEU:N	1:H:9:LEU:CD1	2.49	0.75
1:L:27:ARG:NH1	1:L:31:GLU:OE2	2.20	0.74
1:J:27:ARG:NH1	1:J:31:GLU:OE2	2.19	0.74
1:E:16:ILE:O	1:E:16:ILE:HG22	1.87	0.74
1:F:12:LYS:CG	1:F:13:LEU:HD12	2.11	0.73
1:K:10:GLU:HA	1:K:15:ILE:HG22	1.72	0.71
1:C:6:HIS:N	4:C:402:HOH:O	2.21	0.71
1:K:28:VAL:HB	1:K:64:ILE:HD11	1.73	0.71
1:J:9:LEU:HD13	1:J:64:ILE:HA	1.71	0.70
1:A:74:GLN:HE21	1:A:121:ARG:HD3	1.56	0.70
1:B:87:MET:HE1	1:D:88:TYR:CE1	2.27	0.69
1:C:102:ARG:NH1	4:C:404:HOH:O	2.24	0.68
1:L:71:VAL:CG1	1:L:89:LEU:HD13	2.23	0.68
1:H:74:GLN:OE1	1:H:121:ARG:NH1	2.27	0.68
1:F:88:TYR:HD1	1:F:91:ILE:HD13	1.59	0.68
1:D:102:ARG:NH2	1:D:106:GLU:OE2	2.28	0.67
1:A:20:GLU:OE1	4:A:402:HOH:O	2.13	0.67
1:J:137:LYS:O	1:J:141:LYS:HD3	1.95	0.67
1:H:203:ASN:C	1:H:205:ASP:O	2.33	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:LYS:HE2	1:F:183:ARG:HH22	1.58	0.66
1:J:88:TYR:HH	1:K:88:TYR:HB2	1.61	0.66
1:B:6:HIS:HD2	1:B:66:GLU:OE1	1.78	0.66
1:E:85:PRO:HG2	1:E:88:TYR:CE2	2.31	0.66
1:F:27:ARG:HB2	1:F:202:TYR:CE2	2.31	0.66
1:J:9:LEU:N	1:J:9:LEU:HD12	2.11	0.65
1:E:102:ARG:HG2	1:E:106:GLU:OE1	1.95	0.65
1:B:87:MET:CE	1:D:88:TYR:CE1	2.79	0.65
4:G:435:HOH:O	1:J:166:LEU:CD1	2.08	0.65
1:B:88:TYR:HB2	1:B:91:ILE:HD12	1.79	0.64
1:E:15:ILE:HD11	1:E:20:GLU:HB2	1.80	0.64
1:E:85:PRO:HD2	1:E:88:TYR:OH	1.99	0.63
1:L:71:VAL:HG13	1:L:89:LEU:HD13	1.80	0.63
1:E:5:HIS:CG	1:E:6:HIS:H	2.17	0.63
1:I:8:MET:HE2	1:I:65:TYR:C	2.19	0.63
1:G:150:ASN:ND2	4:G:401:HOH:O	2.27	0.62
1:C:6:HIS:N	4:C:405:HOH:O	2.31	0.62
1:H:166:LEU:HD22	1:I:167:GLU:HG3	1.80	0.62
1:F:13:LEU:HD12	1:F:13:LEU:N	2.14	0.61
1:G:5:HIS:CG	1:G:6:HIS:H	2.19	0.61
1:C:80:ASN:ND2	4:C:407:HOH:O	2.34	0.60
1:A:91:ILE:HD12	1:E:87:MET:CE	2.31	0.60
1:B:87:MET:HE3	1:D:88:TYR:CD1	2.36	0.60
1:A:90:GLU:HG2	4:A:406:HOH:O	2.02	0.59
1:A:88:TYR:CB	1:A:91:ILE:CD1	2.28	0.59
1:H:34:LYS:HE2	1:H:183:ARG:HH22	1.67	0.59
1:F:88:TYR:CD1	1:F:91:ILE:HD13	2.37	0.59
1:F:13:LEU:CD1	1:F:13:LEU:N	2.66	0.58
1:A:88:TYR:HB2	1:A:91:ILE:HD11	0.61	0.58
1:F:25:GLU:HB3	1:F:64:ILE:HD11	1.85	0.58
1:F:86:VAL:HA	1:F:89:LEU:HG	1.86	0.58
1:E:16:ILE:O	1:E:16:ILE:CG2	2.52	0.57
1:A:6:HIS:N	4:A:408:HOH:O	2.38	0.57
1:F:41:ASP:OD1	1:F:44:ARG:NH2	2.38	0.57
1:A:74:GLN:HE22	1:A:121:ARG:CZ	2.18	0.56
1:J:9:LEU:CD1	1:J:9:LEU:N	2.68	0.56
1:K:7:HIS:O	1:K:10:GLU:HG2	2.06	0.55
1:H:27:ARG:HB2	1:H:202:TYR:CE2	2.42	0.55
1:L:166:LEU:HD21	1:L:170:TYR:HE2	1.70	0.55
1:D:170:TYR:CD1	1:D:174:ASN:ND2	2.75	0.54
1:J:166:LEU:CG	4:J:454:HOH:O	2.02	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:9:LEU:CD1	1:J:63:ASP:O	2.52	0.54
1:B:61:PHE:HA	1:B:64:ILE:HD13	1.88	0.54
1:H:8:MET:C	1:H:9:LEU:HD12	2.28	0.54
1:I:87:MET:HG3	1:I:88:TYR:CE1	2.43	0.54
1:F:76:ILE:HD12	1:F:83:PHE:CD2	2.44	0.53
1:I:71:VAL:HG13	1:I:89:LEU:HD23	1.90	0.53
1:K:102:ARG:HG2	1:K:106:GLU:OE1	2.09	0.53
1:B:62:GLU:O	1:B:64:ILE:HD12	2.09	0.53
1:J:10:GLU:HG3	1:J:15:ILE:O	2.08	0.53
1:K:27:ARG:HB2	1:K:202:TYR:CE2	2.44	0.52
1:B:88:TYR:HB2	1:B:91:ILE:CD1	2.39	0.52
1:C:27:ARG:HB2	1:C:202:TYR:CE2	2.44	0.52
1:I:27:ARG:HB2	1:I:202:TYR:CE2	2.44	0.52
1:L:44:ARG:NH2	4:L:408:HOH:O	2.42	0.52
1:C:12:LYS:NZ	4:C:410:HOH:O	2.40	0.51
1:F:184:GLU:O	1:F:188:LYS:HG2	2.11	0.51
1:J:9:LEU:HD21	1:J:64:ILE:HG12	1.93	0.51
1:E:85:PRO:HD2	1:E:88:TYR:CZ	2.45	0.51
1:H:30:LYS:NZ	1:H:202:TYR:O	2.43	0.51
1:C:166:LEU:HD22	1:D:167:GLU:HG2	1.93	0.51
1:E:5:HIS:CG	1:E:6:HIS:N	2.79	0.51
1:H:188:LYS:NZ	4:H:406:HOH:O	2.44	0.51
1:A:91:ILE:HD12	1:E:87:MET:HE2	1.91	0.50
1:J:27:ARG:HB2	1:J:202:TYR:CE2	2.46	0.50
1:F:12:LYS:CG	1:F:13:LEU:CD1	2.76	0.50
1:F:12:LYS:C	1:F:13:LEU:HD12	2.32	0.50
1:J:88:TYR:HH	1:K:88:TYR:CB	2.24	0.50
1:A:27:ARG:HB2	1:A:202:TYR:CE2	2.47	0.50
1:F:34:LYS:HE2	1:F:183:ARG:NH2	2.26	0.49
1:D:170:TYR:CZ	1:D:174:ASN:ND2	2.80	0.49
1:A:20:GLU:OE2	1:A:23:ARG:NH1	2.45	0.49
1:E:75:ASN:OD1	1:E:85:PRO:HA	2.11	0.49
1:D:28:VAL:HG12	1:D:64:ILE:HD11	1.94	0.49
1:L:27:ARG:HB2	1:L:202:TYR:CE2	2.48	0.48
1:C:88:TYR:OH	1:E:88:TYR:CD2	2.66	0.48
1:G:27:ARG:HB2	1:G:202:TYR:CE2	2.48	0.48
1:H:13:LEU:O	1:H:15:ILE:HG13	2.12	0.48
1:B:27:ARG:HB2	1:B:202:TYR:CE2	2.48	0.48
1:H:28:VAL:HG12	1:H:64:ILE:HD11	1.96	0.48
1:L:166:LEU:HD21	1:L:170:TYR:CE2	2.48	0.48
1:L:88:TYR:HD1	1:L:91:ILE:HG12	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ILE:HD13	1:L:88:TYR:OH	2.13	0.48
1:D:5:HIS:HB3	4:D:491:HOH:O	2.14	0.48
1:H:166:LEU:HD22	1:I:167:GLU:CG	2.43	0.48
1:J:84:ALA:HA	1:J:85:PRO:HD3	1.64	0.47
1:A:88:TYR:CB	1:A:91:ILE:CG1	2.83	0.47
1:B:87:MET:HE3	1:D:88:TYR:CE1	2.48	0.47
1:A:74:GLN:NE2	1:A:121:ARG:HD3	2.27	0.47
1:I:48:GLY:HA2	1:I:135:ILE:HD11	1.97	0.47
1:F:61:PHE:O	1:F:64:ILE:HG22	2.15	0.47
1:K:85:PRO:HD2	1:K:88:TYR:CZ	2.50	0.47
1:E:141:LYS:HA	1:E:141:LYS:HD3	1.61	0.47
1:F:42:ILE:HA	1:F:45:ILE:HD12	1.96	0.47
1:F:141:LYS:HE3	1:F:180:ILE:CD1	2.45	0.47
1:I:7:HIS:O	1:I:10:GLU:HG2	2.15	0.46
1:B:71:VAL:HG13	1:B:89:LEU:HD23	1.97	0.46
1:J:37:TYR:HB2	1:J:186:PHE:CE2	2.49	0.46
1:I:87:MET:HG3	1:I:88:TYR:CD1	2.51	0.46
1:D:28:VAL:CG1	1:D:64:ILE:HD11	2.44	0.46
1:B:6:HIS:HD2	1:B:66:GLU:CD	2.18	0.46
1:F:130:ILE:O	1:F:134:LEU:HD13	2.16	0.46
1:F:159:GLU:HG2	2:F:301:ADP:N6	2.31	0.46
1:H:93:LEU:HD23	1:H:93:LEU:HA	1.73	0.46
1:F:36:LEU:HB2	1:F:59:TYR:CE1	2.51	0.45
1:G:85:PRO:HD2	1:G:88:TYR:CZ	2.52	0.45
1:H:48:GLY:HA2	1:H:135:ILE:HD11	1.98	0.45
1:D:62:GLU:O	1:D:64:ILE:HD12	2.17	0.45
1:C:9:LEU:HD13	1:C:24:VAL:HG12	1.98	0.45
1:F:166:LEU:HG	1:F:170:TYR:CZ	2.52	0.45
1:J:9:LEU:HD22	1:J:25:GLU:HG2	1.98	0.45
1:H:96:ILE:O	1:H:110:LYS:HE3	2.16	0.45
1:J:88:TYR:OH	1:K:88:TYR:CB	2.61	0.45
1:F:88:TYR:CG	1:H:88:TYR:OH	2.70	0.45
1:G:5:HIS:CG	1:G:6:HIS:N	2.81	0.44
1:I:13:LEU:HD12	1:I:15:ILE:HD11	1.98	0.44
1:H:58:ASN:O	1:H:62:GLU:HB2	2.16	0.44
1:B:28:VAL:HG12	1:B:64:ILE:HD11	1.99	0.44
1:B:15:ILE:HD12	1:B:16:ILE:H	1.82	0.44
1:I:10:GLU:OE2	4:I:401:HOH:O	2.21	0.44
1:H:86:VAL:HA	1:H:89:LEU:HG	1.99	0.44
1:I:203:ASN:O	1:I:206:GLU:HG2	2.18	0.44
1:J:28:VAL:HB	1:J:64:ILE:HD11	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:204:VAL:C	1:H:205:ASP:O	2.53	0.44
1:L:137:LYS:NZ	4:L:411:HOH:O	2.50	0.44
1:B:10:GLU:HB2	4:B:434:HOH:O	2.18	0.44
1:I:89:LEU:HD12	1:I:89:LEU:HA	1.84	0.44
1:G:167:GLU:HG3	1:J:167:GLU:HG3	2.00	0.43
1:C:167:GLU:HG3	1:D:167:GLU:HG3	2.00	0.43
1:B:36:LEU:HD11	1:B:45:ILE:HD11	2.00	0.43
1:B:79:GLY:O	4:B:401:HOH:O	2.21	0.43
1:F:141:LYS:HE3	1:F:180:ILE:HD11	2.00	0.43
1:K:36:LEU:HG	1:K:42:ILE:HB	2.00	0.43
1:L:6:HIS:ND1	4:L:404:HOH:O	2.36	0.43
1:F:166:LEU:CD2	1:K:167:GLU:HG2	2.49	0.43
1:L:8:MET:CE	1:L:63:ASP:HA	2.49	0.43
1:A:74:GLN:HE21	1:A:121:ARG:CD	2.27	0.42
1:K:42:ILE:HA	1:K:45:ILE:HD12	2.02	0.42
1:C:89:LEU:HD23	1:C:89:LEU:HA	1.83	0.42
1:F:48:GLY:HA2	1:F:135:ILE:HD11	2.02	0.42
1:D:27:ARG:HB2	1:D:202:TYR:CE2	2.54	0.42
1:H:37:TYR:CE2	1:H:183:ARG:HG3	2.55	0.42
1:K:102:ARG:HG2	1:K:102:ARG:H	1.64	0.42
1:G:85:PRO:HD2	1:G:88:TYR:CE1	2.54	0.42
1:D:188:LYS:NZ	4:D:421:HOH:O	2.53	0.41
1:L:89:LEU:HD23	1:L:89:LEU:HA	1.80	0.41
1:C:188:LYS:NZ	4:C:418:HOH:O	2.53	0.41
1:L:96:ILE:O	1:L:110:LYS:HE3	2.21	0.41
1:F:172:ILE:O	1:F:176:LEU:HG	2.19	0.41
1:G:28:VAL:HB	1:G:64:ILE:HD11	2.03	0.41
1:C:205:ASP:OD1	4:C:403:HOH:O	2.22	0.41
1:H:137:LYS:HG3	1:H:180:ILE:HB	2.02	0.41
1:L:5:HIS:CE1	1:L:10:GLU:HB3	2.56	0.41
1:A:8:MET:O	1:A:12:LYS:HG3	2.21	0.41
1:A:170:TYR:HB3	1:L:170:TYR:CZ	2.56	0.41
1:J:87:MET:SD	1:K:92:ALA:HA	2.61	0.41
1:F:108:VAL:HG11	1:F:169:LYS:HB2	2.02	0.41
1:K:15:ILE:HG21	1:K:21:LEU:HD13	2.03	0.41
1:K:6:HIS:HE1	4:K:435:HOH:O	2.04	0.41
1:K:9:LEU:HD23	1:K:9:LEU:HA	1.83	0.41
1:A:160:ARG:HD3	1:L:160:ARG:HD3	2.04	0.40
1:I:88:TYR:HE1	1:J:91:ILE:HD11	1.87	0.40
1:B:67:PHE:HB3	1:B:70:LYS:HB2	2.03	0.40
1:C:8:MET:O	1:C:12:LYS:HG3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:PRO:HD2	1:D:88:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	200/207 (97%)	198 (99%)	2 (1%)	0	100	100
1	B	200/207 (97%)	197 (98%)	3 (2%)	0	100	100
1	C	200/207 (97%)	198 (99%)	2 (1%)	0	100	100
1	D	201/207 (97%)	200 (100%)	1 (0%)	0	100	100
1	E	201/207 (97%)	199 (99%)	2 (1%)	0	100	100
1	F	201/207 (97%)	199 (99%)	2 (1%)	0	100	100
1	G	201/207 (97%)	199 (99%)	2 (1%)	0	100	100
1	H	200/207 (97%)	197 (98%)	3 (2%)	0	100	100
1	I	200/207 (97%)	198 (99%)	2 (1%)	0	100	100
1	J	200/207 (97%)	198 (99%)	2 (1%)	0	100	100
1	K	202/207 (98%)	200 (99%)	2 (1%)	0	100	100
1	L	201/207 (97%)	199 (99%)	2 (1%)	0	100	100
All	All	2407/2484 (97%)	2382 (99%)	25 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/188 (97%)	181 (99%)	2 (1%)	73	78
1	B	183/188 (97%)	180 (98%)	3 (2%)	62	67
1	C	183/188 (97%)	182 (100%)	1 (0%)	88	92
1	D	184/188 (98%)	183 (100%)	1 (0%)	88	92
1	E	184/188 (98%)	183 (100%)	1 (0%)	88	92
1	F	184/188 (98%)	183 (100%)	1 (0%)	88	92
1	G	184/188 (98%)	183 (100%)	1 (0%)	88	92
1	H	183/188 (97%)	182 (100%)	1 (0%)	88	92
1	I	183/188 (97%)	182 (100%)	1 (0%)	88	92
1	J	183/188 (97%)	181 (99%)	2 (1%)	73	78
1	K	185/188 (98%)	184 (100%)	1 (0%)	88	92
1	L	184/188 (98%)	183 (100%)	1 (0%)	88	92
All	All	2203/2256 (98%)	2187 (99%)	16 (1%)	84	89

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ILE
1	A	118	HIS
1	B	10	GLU
1	B	87	MET
1	B	118	HIS
1	C	118	HIS
1	D	118	HIS
1	E	118	HIS
1	F	118	HIS
1	G	118	HIS
1	H	118	HIS
1	I	118	HIS
1	J	91	ILE
1	J	118	HIS
1	K	118	HIS
1	L	118	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	B	6	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	C	301	3	24,29,29	0.91	1 (4%)	29,45,45	1.25	4 (13%)
2	ADP	D	301	3	24,29,29	0.98	2 (8%)	29,45,45	1.22	2 (6%)
2	ADP	F	301	3	24,29,29	0.99	2 (8%)	29,45,45	1.25	4 (13%)
2	ADP	B	301	3	24,29,29	0.98	2 (8%)	29,45,45	1.18	3 (10%)
2	ADP	H	301	3	24,29,29	0.97	1 (4%)	29,45,45	1.27	4 (13%)
2	ADP	J	301	3	24,29,29	1.02	1 (4%)	29,45,45	1.25	4 (13%)
2	ADP	K	301	3	24,29,29	0.95	1 (4%)	29,45,45	1.22	3 (10%)
2	ADP	A	301	3	24,29,29	0.95	1 (4%)	29,45,45	1.25	2 (6%)
2	ADP	L	301	3	24,29,29	0.98	1 (4%)	29,45,45	1.24	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ADP	G	301	3	24,29,29	0.95	1 (4%)	29,45,45	1.22	3 (10%)
2	ADP	I	301	3	24,29,29	1.00	1 (4%)	29,45,45	1.20	3 (10%)
2	ADP	E	301	3	24,29,29	1.02	2 (8%)	29,45,45	1.19	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	C	301	3	-	1/12/32/32	0/3/3/3
2	ADP	D	301	3	-	0/12/32/32	0/3/3/3
2	ADP	F	301	3	-	0/12/32/32	0/3/3/3
2	ADP	B	301	3	-	0/12/32/32	0/3/3/3
2	ADP	H	301	3	-	2/12/32/32	0/3/3/3
2	ADP	J	301	3	-	2/12/32/32	0/3/3/3
2	ADP	K	301	3	-	1/12/32/32	0/3/3/3
2	ADP	A	301	3	-	1/12/32/32	0/3/3/3
2	ADP	L	301	3	-	0/12/32/32	0/3/3/3
2	ADP	G	301	3	-	1/12/32/32	0/3/3/3
2	ADP	I	301	3	-	1/12/32/32	0/3/3/3
2	ADP	E	301	3	-	0/12/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	ADP	C5-C4	2.63	1.47	1.40
2	G	301	ADP	C5-C4	2.56	1.47	1.40
2	J	301	ADP	C5-C4	2.52	1.47	1.40
2	F	301	ADP	C5-C4	2.51	1.47	1.40
2	K	301	ADP	C5-C4	2.48	1.47	1.40
2	A	301	ADP	C5-C4	2.47	1.47	1.40
2	H	301	ADP	C5-C4	2.43	1.47	1.40
2	E	301	ADP	C5-C4	2.43	1.47	1.40
2	B	301	ADP	C5-C4	2.41	1.47	1.40
2	L	301	ADP	C5-C4	2.40	1.47	1.40
2	D	301	ADP	C5-C4	2.33	1.47	1.40
2	C	301	ADP	C5-C4	2.17	1.46	1.40
2	B	301	ADP	C2-N3	2.15	1.35	1.32
2	E	301	ADP	O4'-C1'	2.12	1.44	1.41
2	F	301	ADP	C2-N3	2.03	1.35	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	ADP	C2-N3	2.02	1.35	1.32

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	ADP	N3-C2-N1	-3.54	123.15	128.68
2	C	301	ADP	N3-C2-N1	-3.51	123.19	128.68
2	L	301	ADP	N3-C2-N1	-3.50	123.20	128.68
2	A	301	ADP	N3-C2-N1	-3.36	123.42	128.68
2	G	301	ADP	N3-C2-N1	-3.34	123.46	128.68
2	D	301	ADP	N3-C2-N1	-3.33	123.47	128.68
2	J	301	ADP	N3-C2-N1	-3.26	123.58	128.68
2	F	301	ADP	N3-C2-N1	-3.18	123.71	128.68
2	H	301	ADP	N3-C2-N1	-3.17	123.72	128.68
2	B	301	ADP	N3-C2-N1	-3.13	123.79	128.68
2	K	301	ADP	N3-C2-N1	-3.12	123.81	128.68
2	I	301	ADP	N3-C2-N1	-3.09	123.86	128.68
2	G	301	ADP	C4-C5-N7	-2.79	106.50	109.40
2	I	301	ADP	C4-C5-N7	-2.69	106.60	109.40
2	H	301	ADP	C4-C5-N7	-2.62	106.67	109.40
2	A	301	ADP	C4-C5-N7	-2.57	106.72	109.40
2	D	301	ADP	C4-C5-N7	-2.56	106.73	109.40
2	H	301	ADP	C3'-C2'-C1'	2.49	104.72	100.98
2	F	301	ADP	C4-C5-N7	-2.46	106.83	109.40
2	F	301	ADP	C3'-C2'-C1'	2.43	104.64	100.98
2	K	301	ADP	C4-C5-N7	-2.43	106.87	109.40
2	L	301	ADP	C3'-C2'-C1'	2.38	104.56	100.98
2	E	301	ADP	C4-C5-N7	-2.38	106.92	109.40
2	G	301	ADP	C3'-C2'-C1'	2.33	104.48	100.98
2	L	301	ADP	C4-C5-N7	-2.32	106.98	109.40
2	C	301	ADP	C4-C5-N7	-2.31	106.99	109.40
2	K	301	ADP	C3'-C2'-C1'	2.31	104.45	100.98
2	I	301	ADP	C3'-C2'-C1'	2.25	104.36	100.98
2	B	301	ADP	C4-C5-N7	-2.23	107.08	109.40
2	J	301	ADP	C4-C5-N7	-2.20	107.11	109.40
2	H	301	ADP	PA-O3A-PB	-2.20	125.28	132.83
2	J	301	ADP	C3'-C2'-C1'	2.19	104.28	100.98
2	J	301	ADP	PA-O3A-PB	-2.19	125.31	132.83
2	F	301	ADP	PA-O3A-PB	-2.08	125.69	132.83
2	B	301	ADP	C3'-C2'-C1'	2.07	104.09	100.98
2	C	301	ADP	O2A-PA-O1A	2.05	122.37	112.24
2	C	301	ADP	C2-N1-C6	2.01	122.20	118.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	ADP	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	301	ADP	C5'-O5'-PA-O1A
2	J	301	ADP	PB-O3A-PA-O2A
2	A	301	ADP	PB-O3A-PA-O2A
2	K	301	ADP	PB-O3A-PA-O2A
2	H	301	ADP	C5'-O5'-PA-O3A
2	C	301	ADP	PB-O3A-PA-O1A
2	G	301	ADP	PB-O3A-PA-O2A
2	I	301	ADP	PB-O3A-PA-O2A
2	J	301	ADP	PB-O3A-PA-O1A

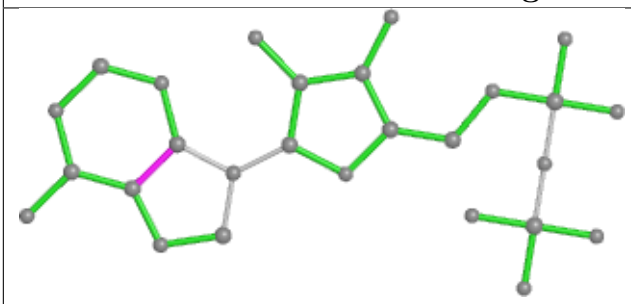
There are no ring outliers.

1 monomer is involved in 1 short contact:

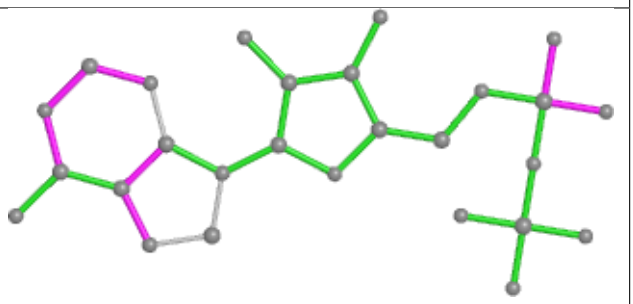
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	ADP	1	0

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

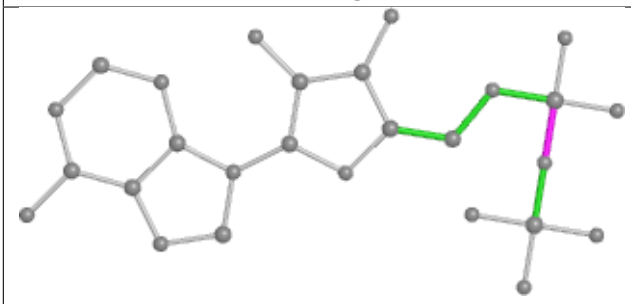
Ligand ADP C 301



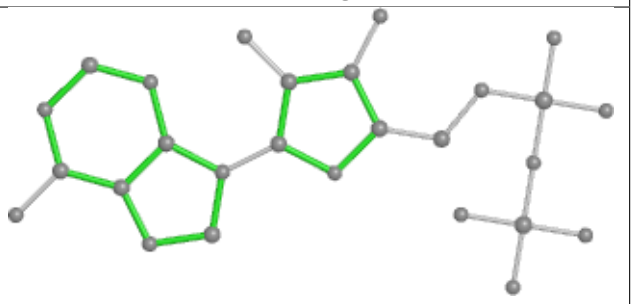
Bond lengths



Bond angles

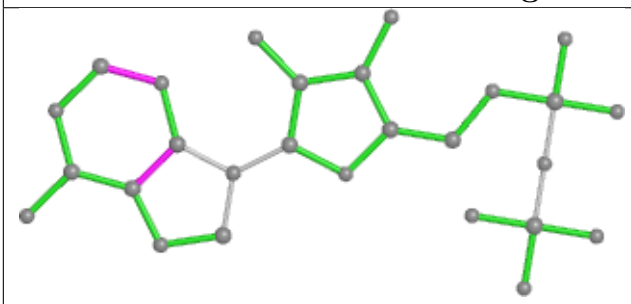


Torsions

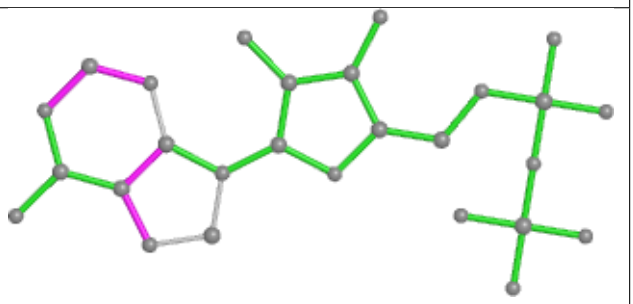


Rings

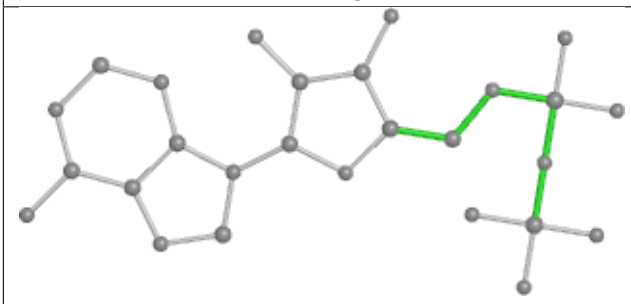
Ligand ADP D 301



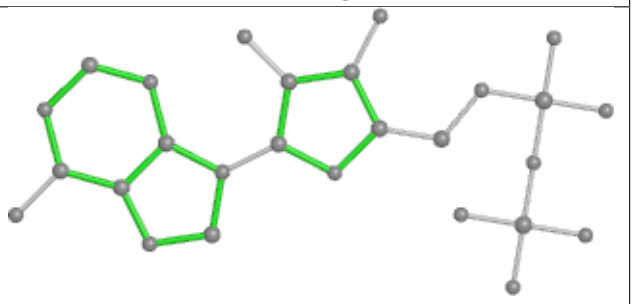
Bond lengths



Bond angles

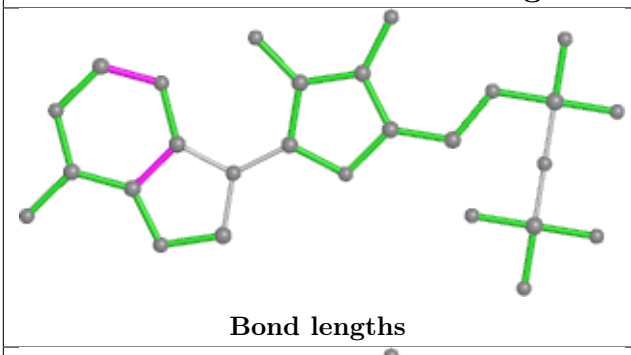


Torsions

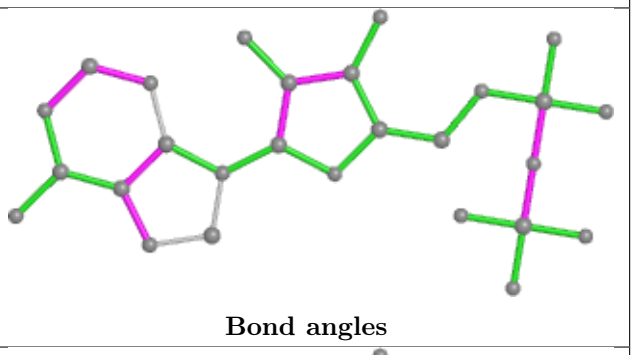


Rings

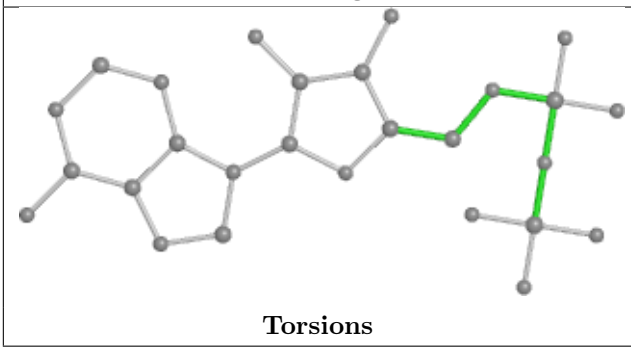
Ligand ADP F 301



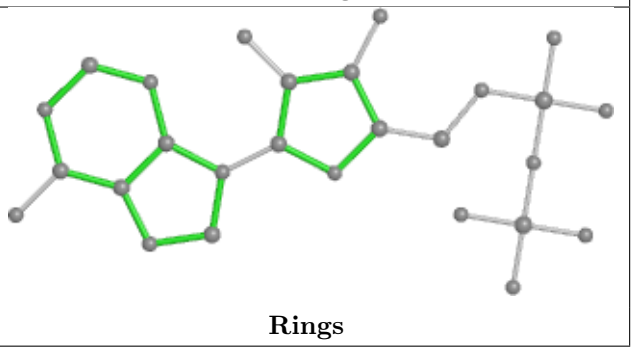
Bond lengths



Bond angles

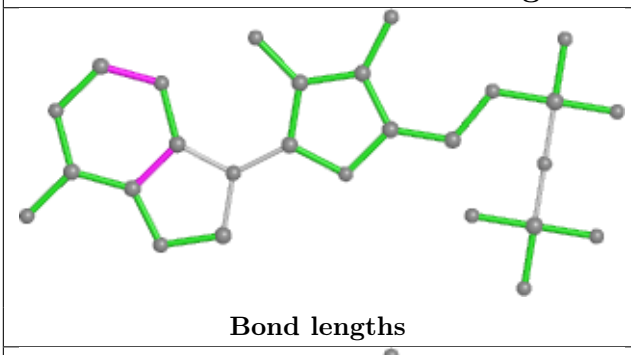


Torsions

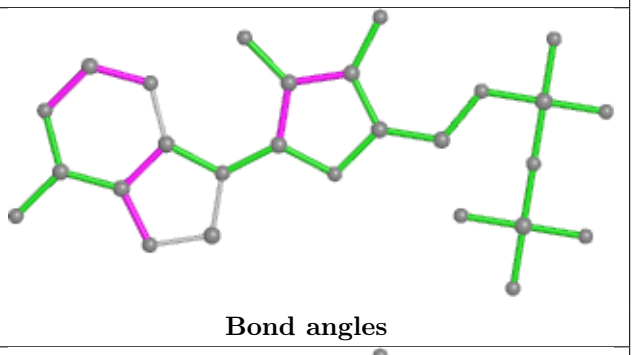


Rings

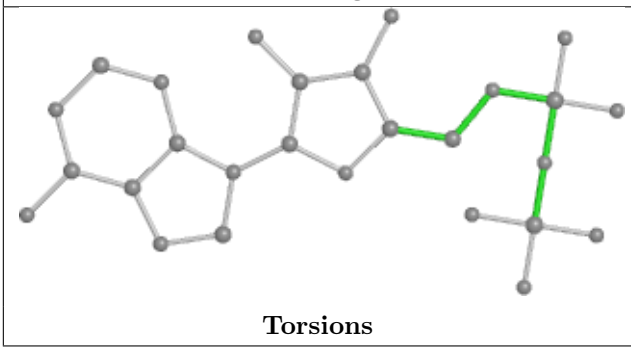
Ligand ADP B 301



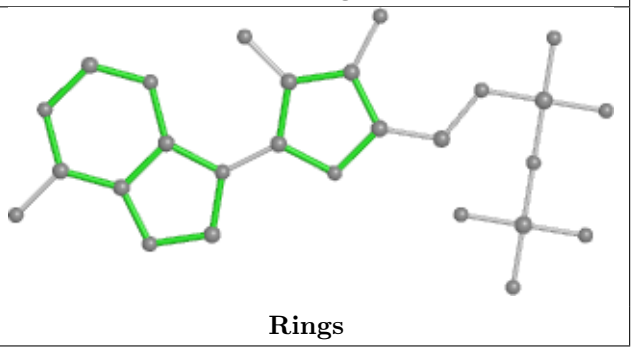
Bond lengths



Bond angles

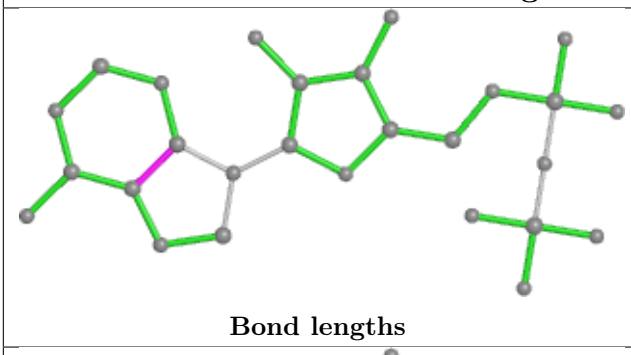


Torsions

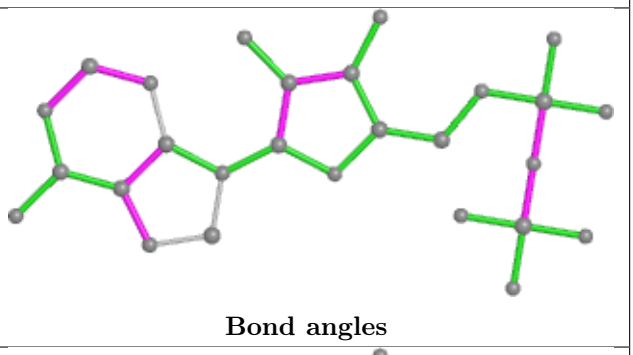


Rings

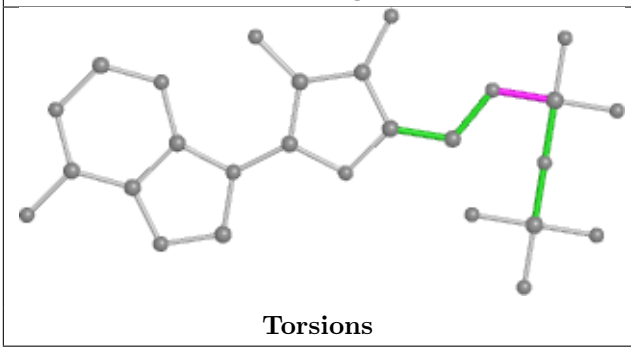
Ligand ADP H 301



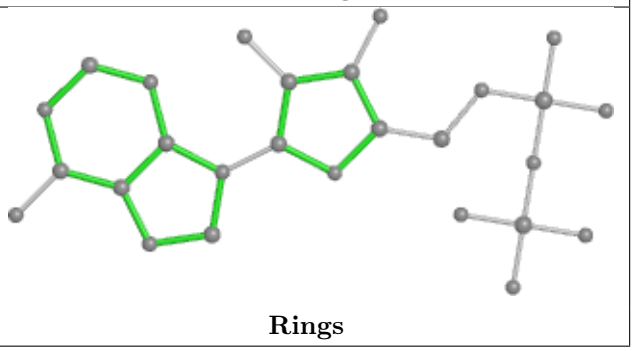
Bond lengths



Bond angles

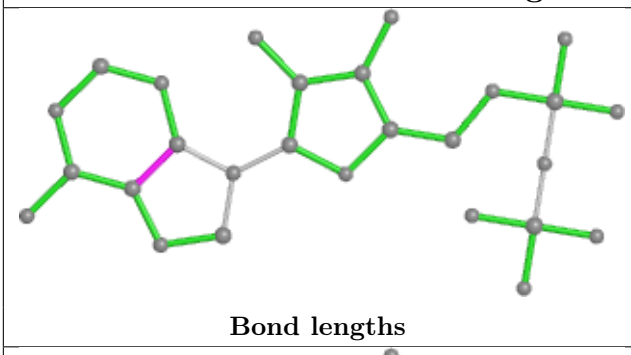


Torsions

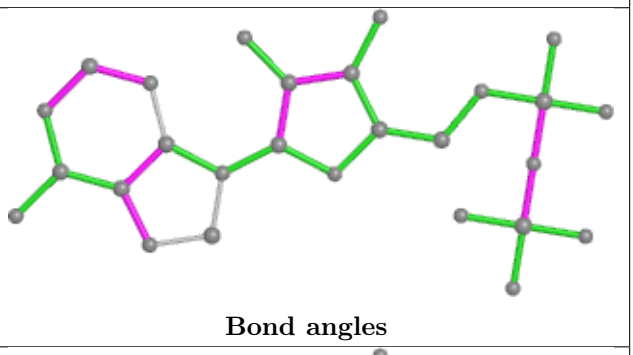


Rings

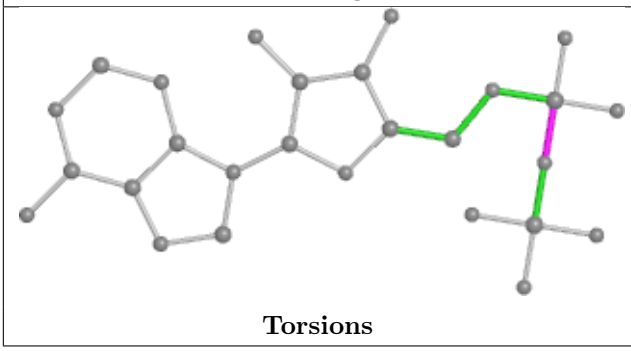
Ligand ADP J 301



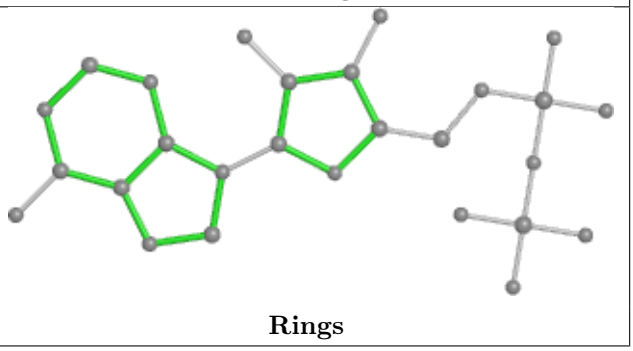
Bond lengths



Bond angles

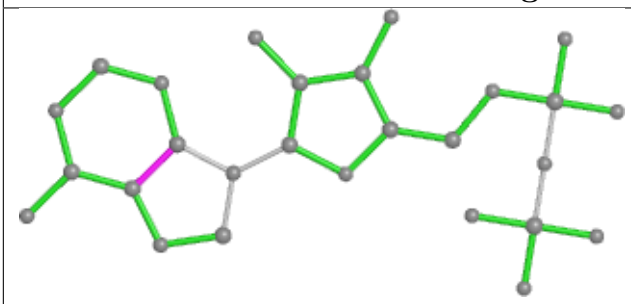


Torsions

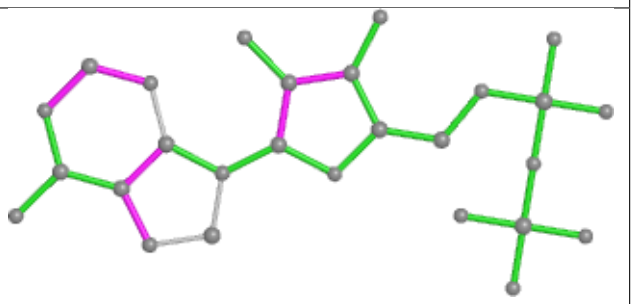


Rings

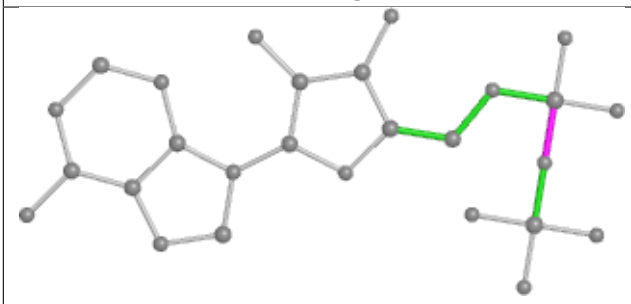
Ligand ADP K 301



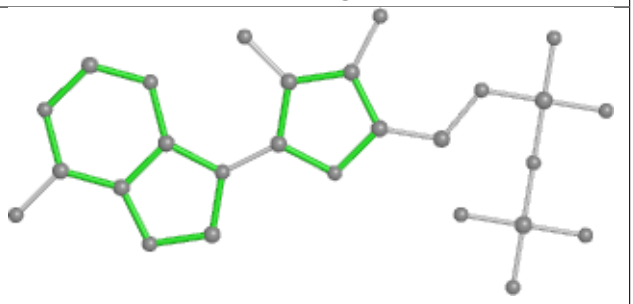
Bond lengths



Bond angles

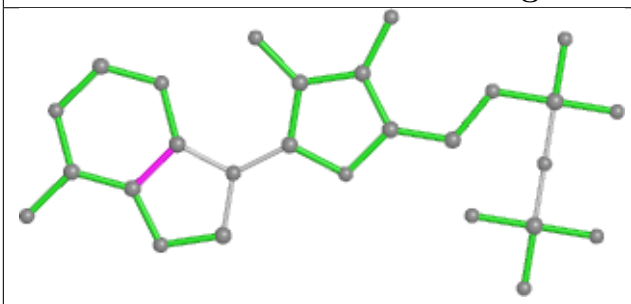


Torsions

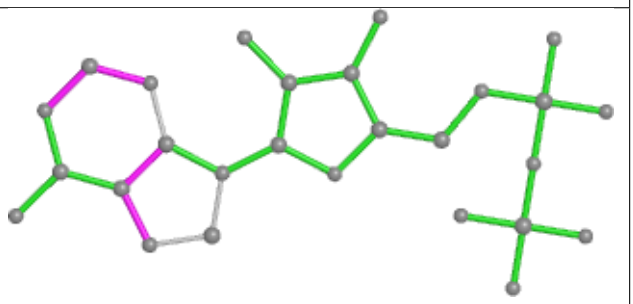


Rings

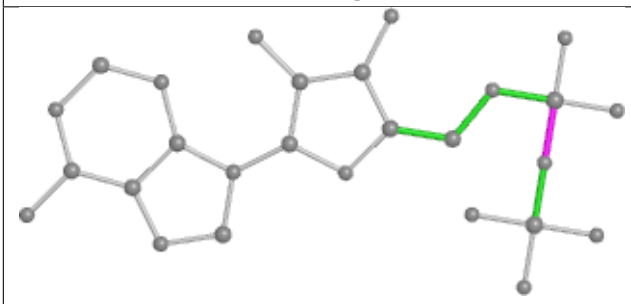
Ligand ADP A 301



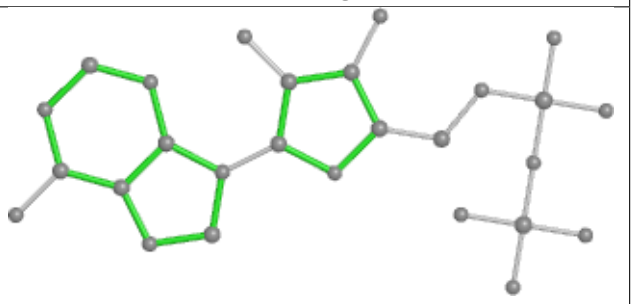
Bond lengths



Bond angles

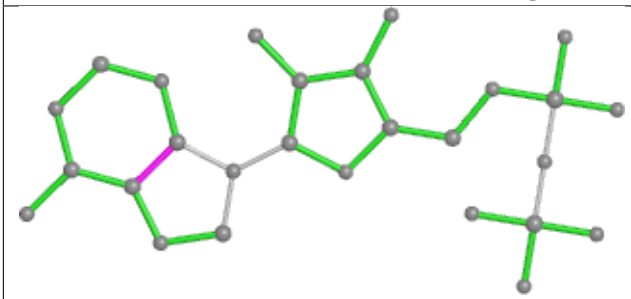


Torsions

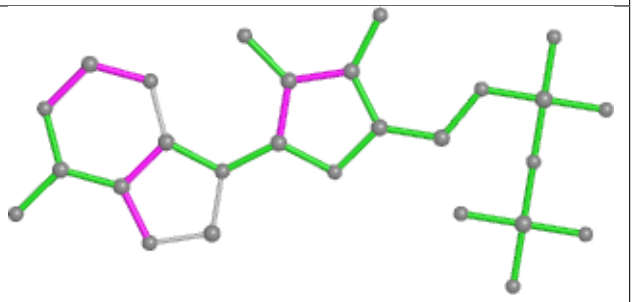


Rings

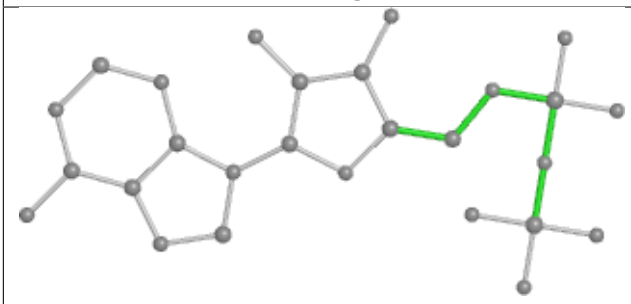
Ligand ADP L 301



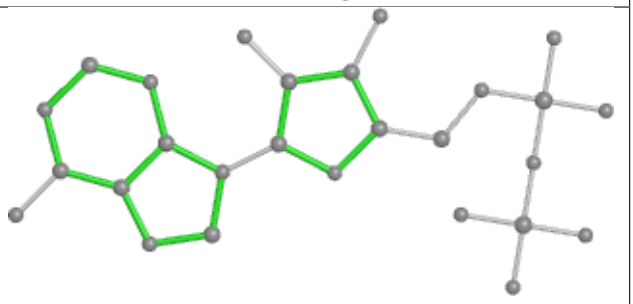
Bond lengths



Bond angles

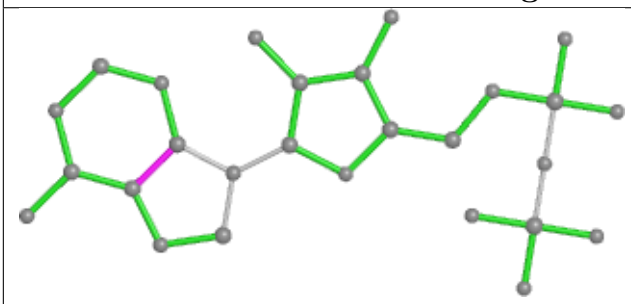


Torsions

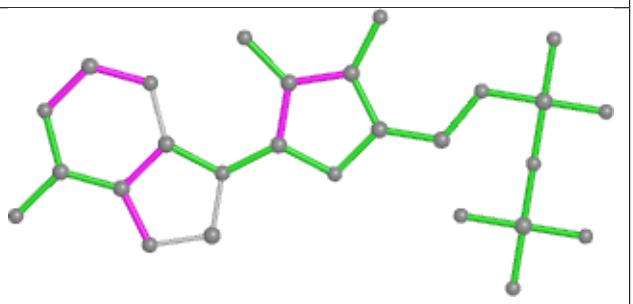


Rings

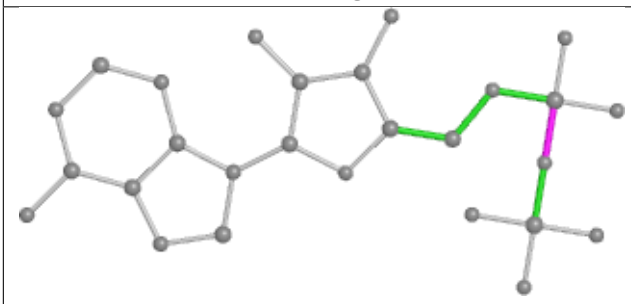
Ligand ADP G 301



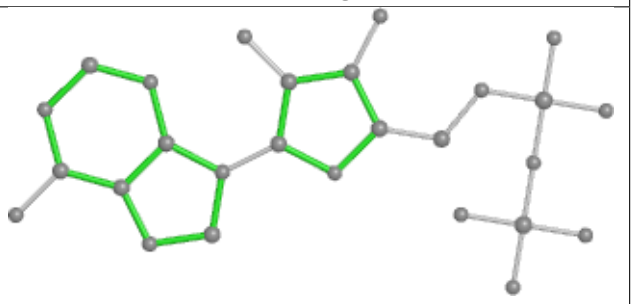
Bond lengths



Bond angles

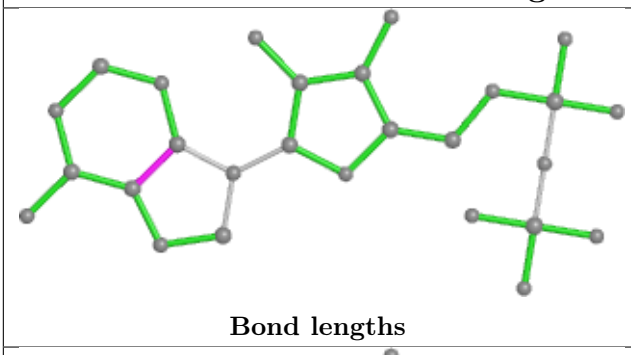


Torsions

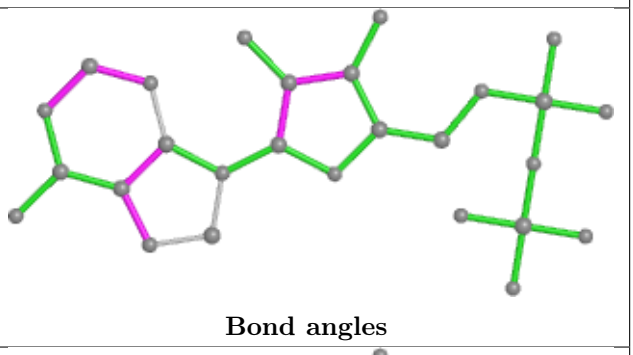


Rings

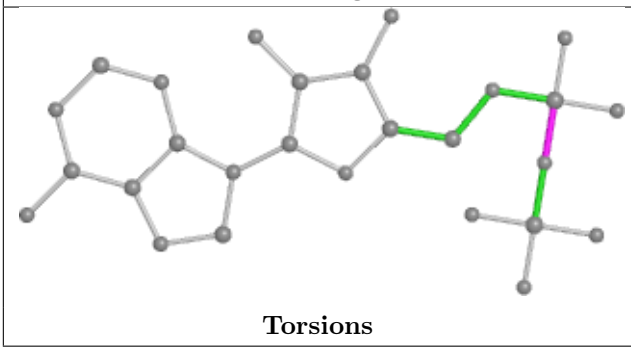
Ligand ADP I 301



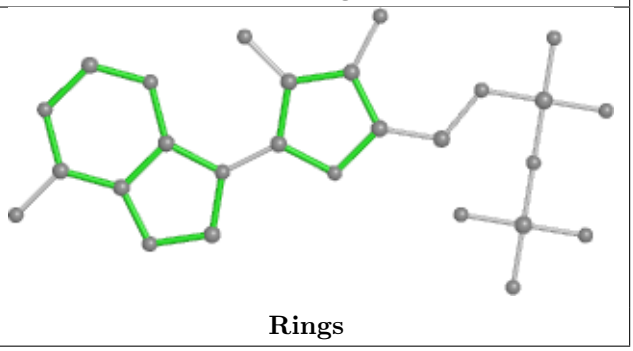
Bond lengths



Bond angles

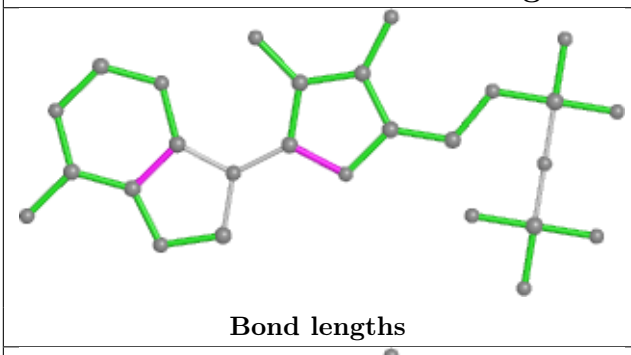


Torsions

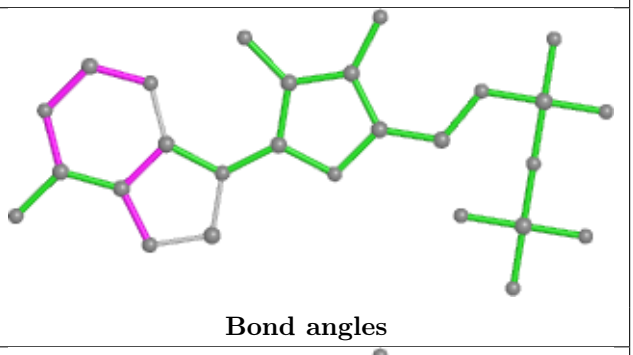


Rings

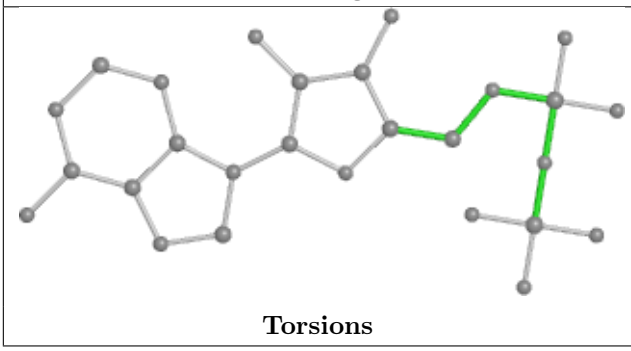
Ligand ADP E 301



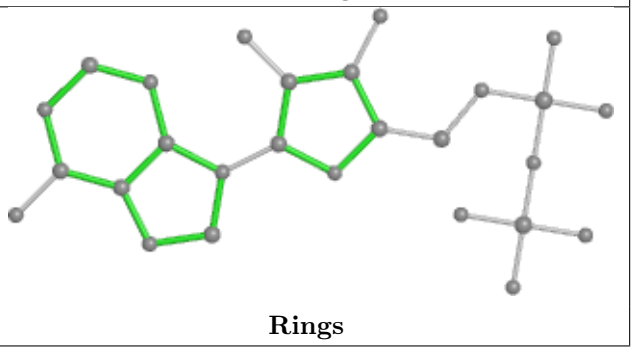
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	6:HIS	C	7:HIS	N	1.10

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, 95^{th} 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	202/207 (97%)	0.27	13 (6%) 19 26	18, 30, 52, 89	0
1	B	202/207 (97%)	0.09	9 (4%) 33 42	20, 28, 50, 90	0
1	C	202/207 (97%)	0.07	6 (2%) 50 59	22, 34, 50, 66	0
1	D	203/207 (98%)	0.11	5 (2%) 57 65	22, 32, 47, 73	0
1	E	203/207 (98%)	0.09	8 (3%) 39 48	21, 32, 58, 95	0
1	F	202/207 (97%)	0.85	33 (16%) 1 2	33, 56, 85, 117	0
1	G	203/207 (98%)	-0.03	5 (2%) 57 65	26, 37, 57, 87	0
1	H	202/207 (97%)	0.88	34 (16%) 1 2	32, 58, 91, 109	0
1	I	202/207 (97%)	0.06	9 (4%) 33 42	23, 33, 52, 98	0
1	J	202/207 (97%)	0.68	23 (11%) 5 7	30, 49, 79, 102	0
1	K	204/207 (98%)	0.44	15 (7%) 14 20	33, 51, 71, 117	0
1	L	203/207 (98%)	0.07	6 (2%) 50 59	20, 34, 53, 80	0
All	All	2430/2484 (97%)	0.30	166 (6%) 17 24	18, 38, 73, 117	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	16	ILE	7.5
1	I	88	TYR	7.4
1	J	9	LEU	7.4
1	J	88	TYR	7.2
1	F	15	ILE	7.1
1	I	15	ILE	6.8
1	J	16	ILE	6.6
1	H	88	TYR	6.6
1	F	11	ASN	6.3
1	F	13	LEU	6.3
1	F	88	TYR	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	16	ILE	5.9
1	E	88	TYR	5.8
1	B	16	ILE	5.7
1	K	15	ILE	5.7
1	L	88	TYR	5.2
1	F	16	ILE	5.1
1	B	15	ILE	5.0
1	H	14	GLY	5.0
1	H	44	ARG	4.9
1	I	14	GLY	4.8
1	F	12	LYS	4.7
1	H	90	GLU	4.7
1	I	170	TYR	4.7
1	I	13	LEU	4.6
1	K	205	ASP	4.6
1	H	204	VAL	4.6
1	E	15	ILE	4.5
1	F	91	ILE	4.3
1	A	170	TYR	4.3
1	H	59	TYR	4.2
1	J	13	LEU	4.2
1	A	15	ILE	4.2
1	J	45	ILE	4.2
1	H	15	ILE	4.1
1	F	170	TYR	4.0
1	B	14	GLY	3.9
1	K	170	TYR	3.9
1	H	13	LEU	3.9
1	K	16	ILE	3.9
1	C	88	TYR	3.8
1	H	170	TYR	3.7
1	B	13	LEU	3.7
1	L	170	TYR	3.7
1	F	89	LEU	3.7
1	J	170	TYR	3.6
1	H	58	ASN	3.6
1	F	121	ARG	3.6
1	F	63	ASP	3.6
1	J	166	LEU	3.6
1	E	16	ILE	3.6
1	G	170	TYR	3.5
1	K	11	ASN	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	207	LEU	3.5
1	H	45	ILE	3.4
1	F	14	GLY	3.4
1	F	205	ASP	3.4
1	J	141	LYS	3.3
1	H	11	ASN	3.3
1	A	44	ARG	3.3
1	B	170	TYR	3.3
1	K	204	VAL	3.3
1	I	16	ILE	3.3
1	L	163	VAL	3.2
1	K	202	TYR	3.2
1	D	74	GLN	3.1
1	F	9	LEU	3.1
1	J	12	LYS	3.1
1	J	55	TYR	3.1
1	G	88	TYR	3.1
1	D	80	ASN	3.0
1	A	13	LEU	3.0
1	J	6	HIS	3.0
1	K	207	LEU	3.0
1	E	12	LYS	3.0
1	G	5	HIS	2.9
1	H	37	TYR	2.9
1	I	12	LYS	2.9
1	J	63	ASP	2.9
1	A	11	ASN	2.9
1	K	34	LYS	2.8
1	H	131	TRP	2.8
1	H	63	ASP	2.8
1	F	10	GLU	2.8
1	J	11	ASN	2.7
1	E	80	ASN	2.7
1	F	184	GLU	2.7
1	F	67	PHE	2.7
1	D	5	HIS	2.6
1	K	63	ASP	2.6
1	F	27	ARG	2.6
1	H	24	VAL	2.6
1	A	16	ILE	2.6
1	H	36	LEU	2.6
1	F	202	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	8	MET	2.6
1	F	188	LYS	2.5
1	K	203	ASN	2.5
1	A	80	ASN	2.5
1	E	170	TYR	2.5
1	H	27	ARG	2.5
1	C	182	ASP	2.5
1	I	11	ASN	2.4
1	F	166	LEU	2.4
1	H	60	LEU	2.4
1	F	33	ALA	2.4
1	H	9	LEU	2.4
1	K	188	LYS	2.4
1	L	90	GLU	2.4
1	J	42	ILE	2.4
1	H	67	PHE	2.4
1	J	15	ILE	2.3
1	B	88	TYR	2.3
1	F	204	VAL	2.3
1	A	157	ALA	2.3
1	F	8	MET	2.3
1	J	29	SER	2.3
1	H	89	LEU	2.3
1	A	94	GLU	2.3
1	A	163	VAL	2.3
1	G	80	ASN	2.3
1	J	80	ASN	2.3
1	J	206	GLU	2.3
1	A	12	LYS	2.2
1	F	92	ALA	2.2
1	I	166	LEU	2.2
1	K	184	GLU	2.2
1	J	185	ILE	2.2
1	F	182	ASP	2.2
1	H	61	PHE	2.2
1	J	10	GLU	2.2
1	D	163	VAL	2.2
1	A	92	ALA	2.2
1	C	80	ASN	2.2
1	E	11	ASN	2.2
1	K	12	LYS	2.2
1	J	62	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	11	ASN	2.2
1	F	87	MET	2.2
1	G	11	ASN	2.2
1	H	20	GLU	2.2
1	H	202	TYR	2.2
1	J	94	GLU	2.2
1	L	45	ILE	2.1
1	J	33	ALA	2.1
1	F	71	VAL	2.1
1	H	6	HIS	2.1
1	B	6	HIS	2.1
1	B	184	GLU	2.1
1	A	91	ILE	2.1
1	F	137	LYS	2.1
1	D	81	PHE	2.1
1	L	80	ASN	2.1
1	H	207	LEU	2.1
1	E	90	GLU	2.0
1	F	90	GLU	2.0
1	B	80	ASN	2.0
1	F	64	ILE	2.0
1	C	170	TYR	2.0
1	H	51	LYS	2.0
1	K	13	LEU	2.0
1	F	80	ASN	2.0
1	H	80	ASN	2.0
1	H	62	GLU	2.0
1	H	56	ILE	2.0
1	H	12	LYS	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

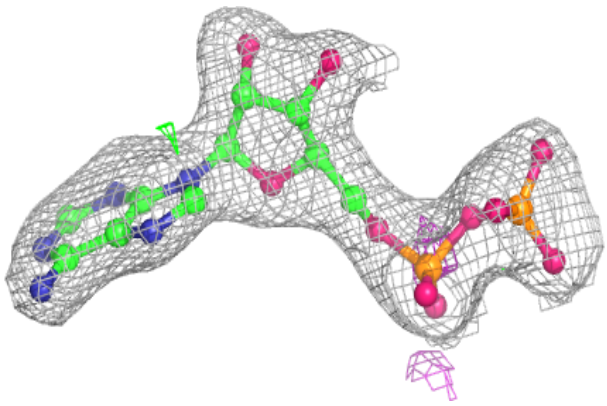
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

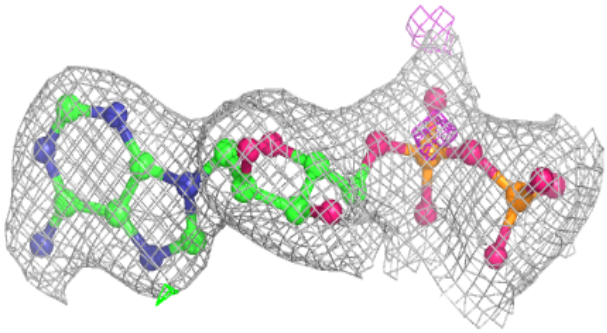
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	J	302	1/1	0.69	0.06	77,77,77,77	0
3	CA	H	303	1/1	0.81	0.06	93,93,93,93	0
3	CA	H	304	1/1	0.86	0.08	61,61,61,61	0
3	CA	H	302	1/1	0.86	0.08	74,74,74,74	0
2	ADP	F	301	27/27	0.94	0.09	39,44,46,48	0
2	ADP	J	301	27/27	0.95	0.11	35,41,44,47	0
3	CA	G	302	1/1	0.95	0.07	39,39,39,39	0
2	ADP	H	301	27/27	0.95	0.11	36,42,47,49	0
3	CA	C	303	1/1	0.96	0.05	45,45,45,45	0
2	ADP	C	301	27/27	0.96	0.14	23,25,27,28	0
2	ADP	K	301	27/27	0.96	0.10	35,41,44,47	0
3	CA	A	302	1/1	0.96	0.11	37,37,37,37	0
3	CA	B	302	1/1	0.96	0.07	36,36,36,36	0
3	CA	B	303	1/1	0.96	0.04	44,44,44,44	0
3	CA	K	302	1/1	0.96	0.04	53,53,53,53	0
3	CA	C	302	1/1	0.97	0.09	40,40,40,40	0
2	ADP	E	301	27/27	0.97	0.13	23,26,28,30	0
3	CA	D	302	1/1	0.97	0.11	34,34,34,34	0
3	CA	F	303	1/1	0.97	0.06	53,53,53,53	0
2	ADP	G	301	27/27	0.97	0.12	29,30,33,34	0
3	CA	L	302	1/1	0.97	0.09	39,39,39,39	0
3	CA	F	302	1/1	0.98	0.05	75,75,75,75	0
3	CA	A	303	1/1	0.98	0.06	43,43,43,43	0
2	ADP	I	301	27/27	0.98	0.11	26,29,31,33	0
2	ADP	A	301	27/27	0.98	0.15	22,25,28,29	0
2	ADP	D	301	27/27	0.98	0.16	21,24,27,27	0
2	ADP	L	301	27/27	0.98	0.12	22,25,26,29	0
3	CA	I	302	1/1	0.98	0.07	38,38,38,38	0
2	ADP	B	301	27/27	0.98	0.13	20,25,26,28	0
3	CA	J	303	1/1	0.98	0.10	61,61,61,61	0
3	CA	D	303	1/1	0.98	0.05	40,40,40,40	0
3	CA	E	303	1/1	0.98	0.06	43,43,43,43	0
3	CA	G	304	1/1	0.99	0.13	30,30,30,30	0
3	CA	E	302	1/1	0.99	0.10	37,37,37,37	0
3	CA	G	303	1/1	0.99	0.10	26,26,26,26	0
3	CA	L	303	1/1	0.99	0.05	49,49,49,49	0

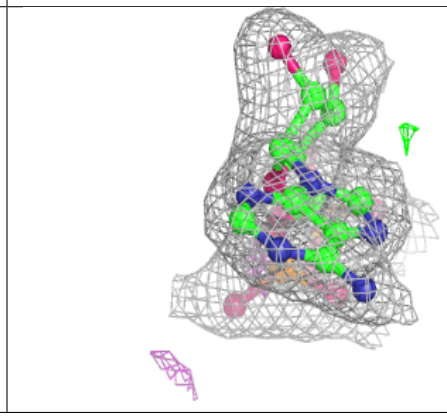
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP F 301:

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

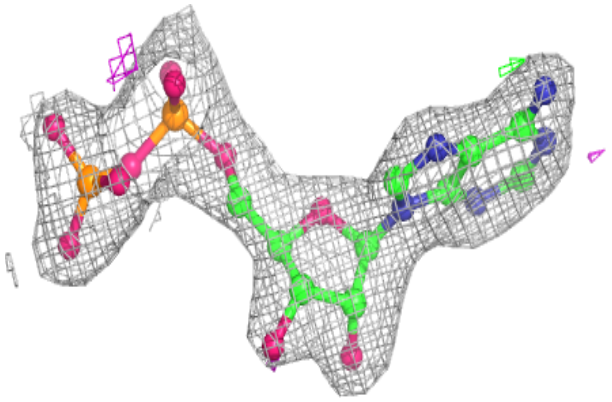


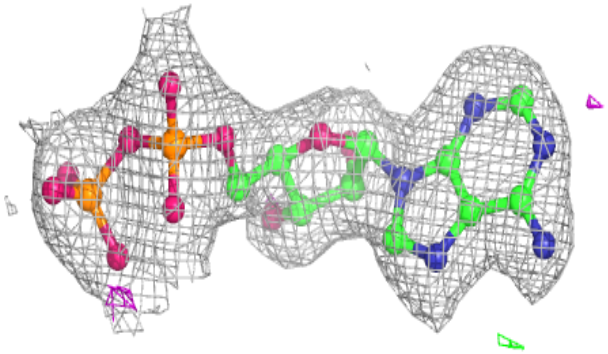


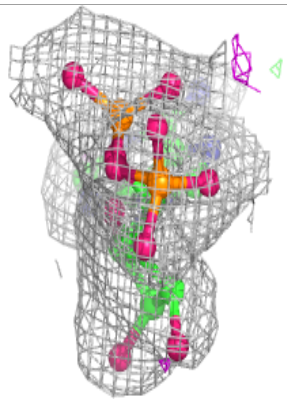


Electron density around ADP J 301:

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

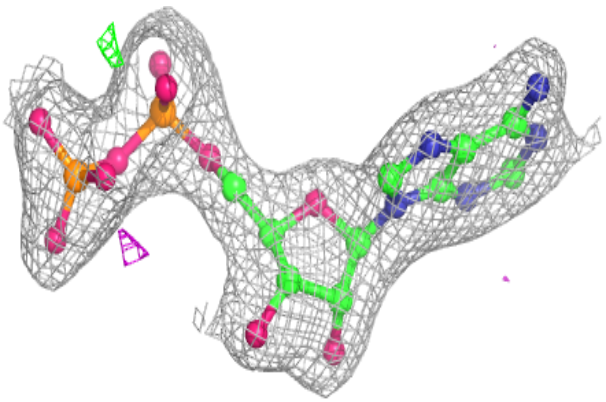


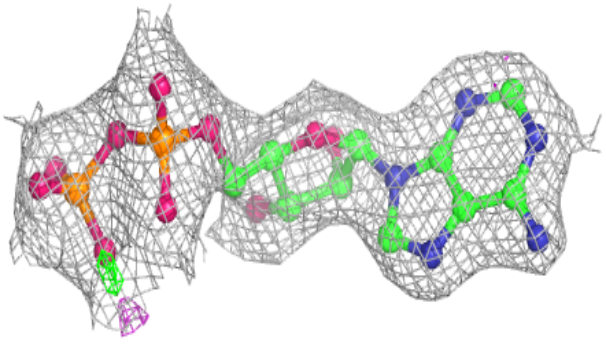


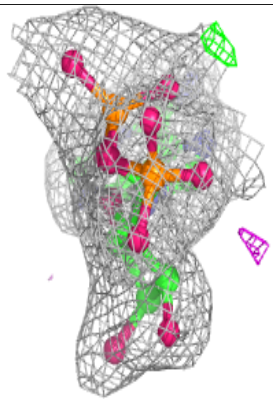


Electron density around ADP H 301:

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

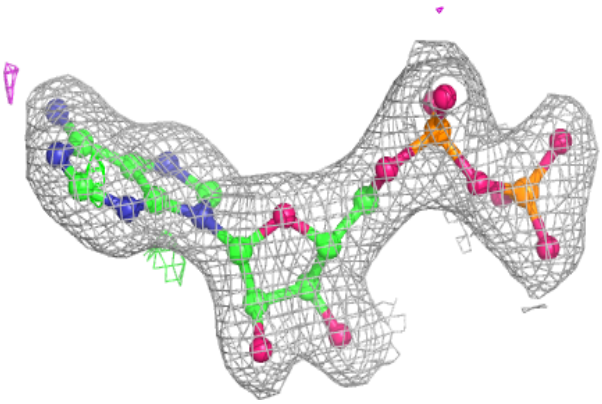


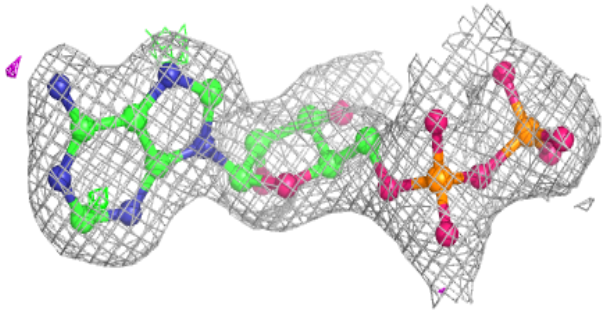


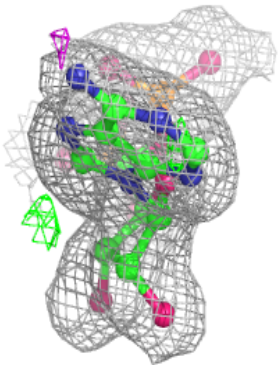


Electron density around ADP C 301:

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

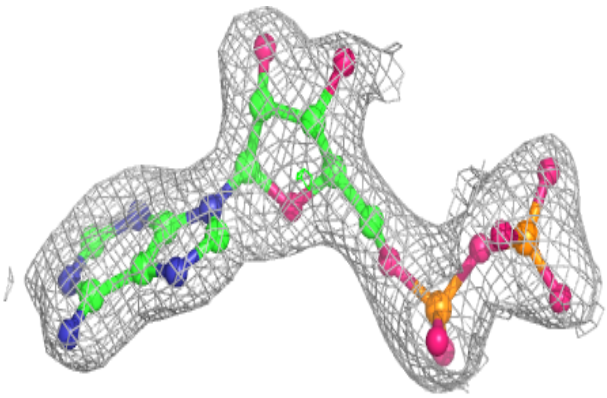


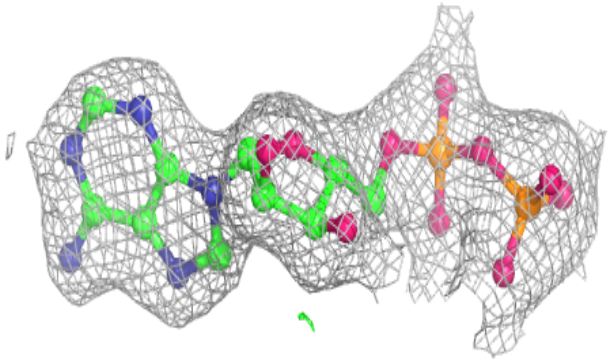


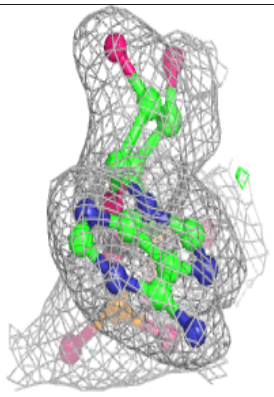


Electron density around ADP K 301:

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

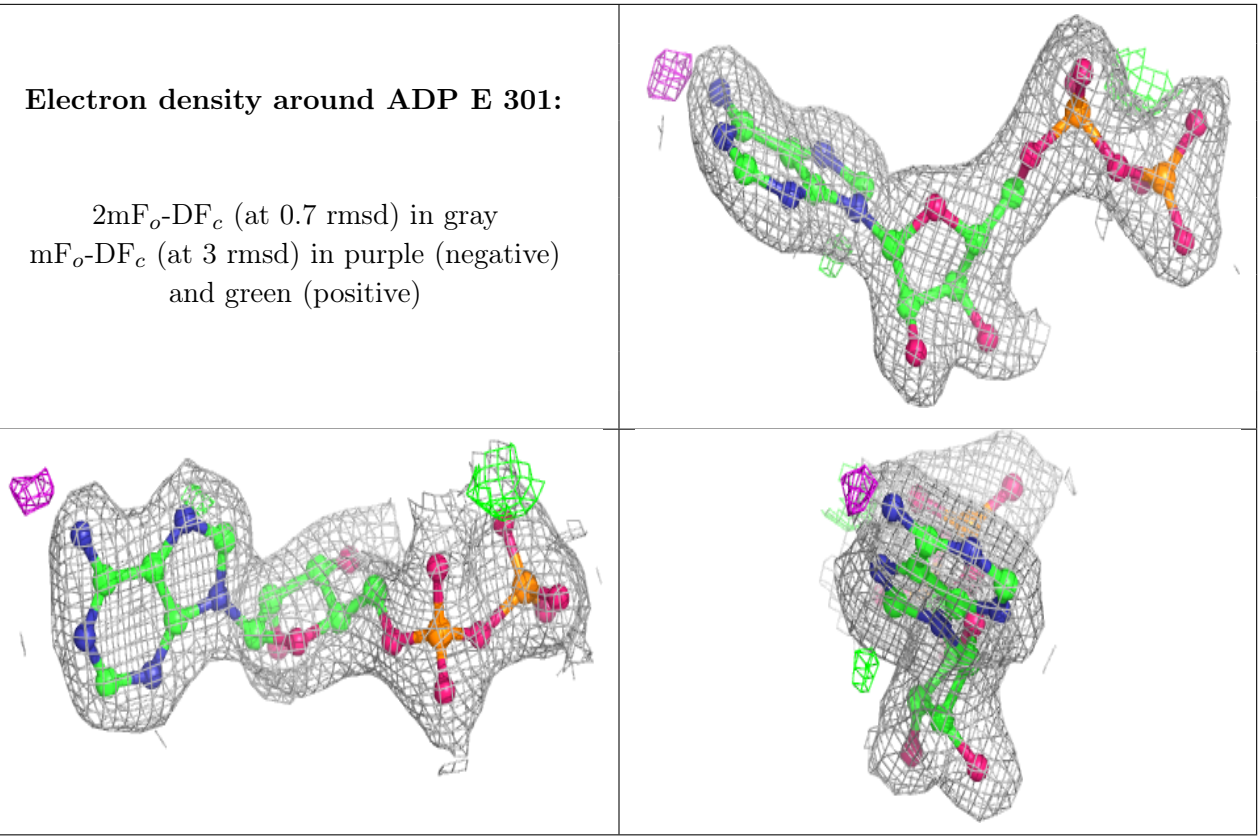






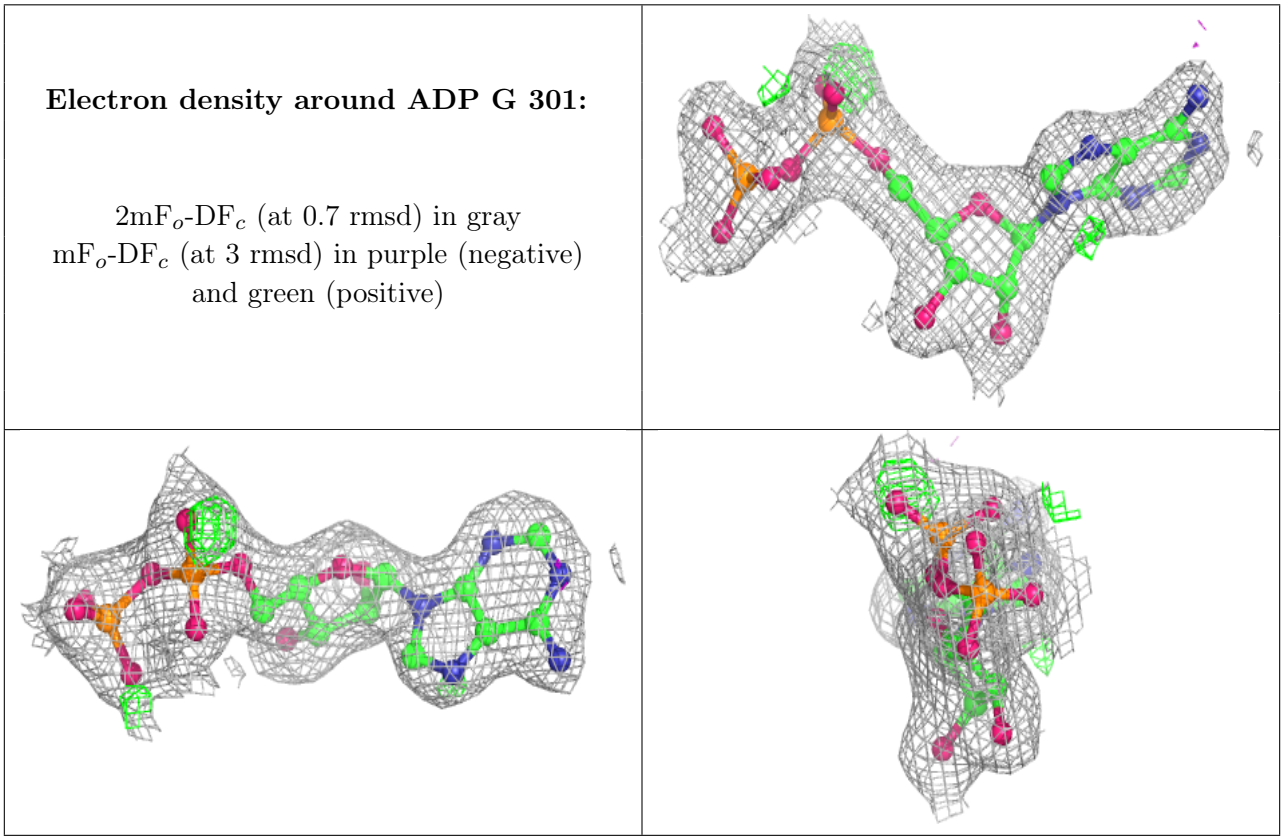
Electron density around ADP E 301:

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



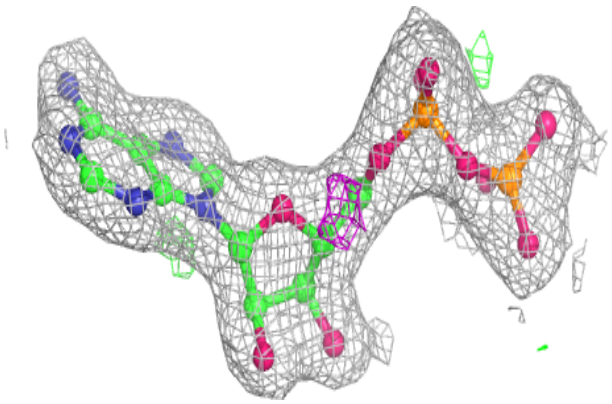
Electron density around ADP G 301:

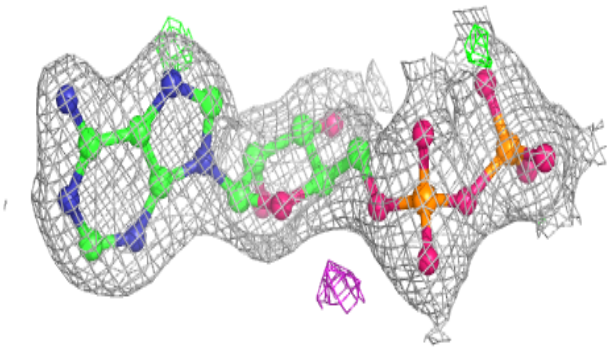
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

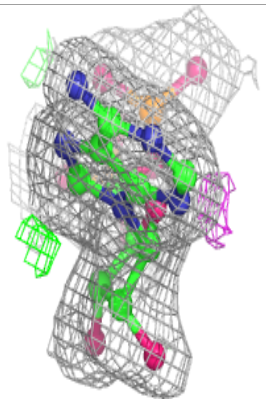


Electron density around ADP I 301:

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

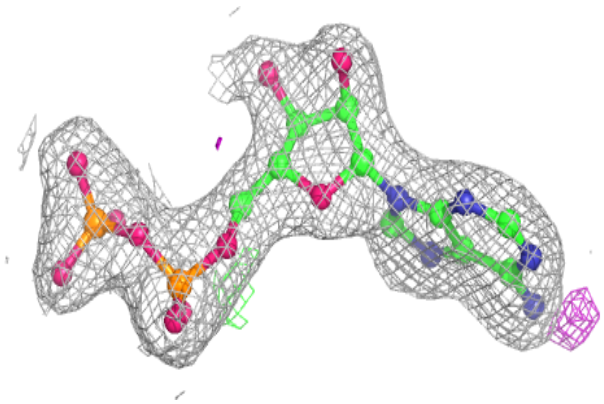


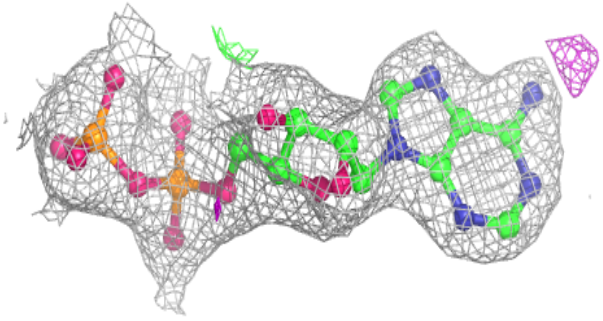


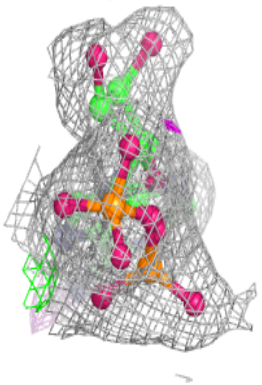


Electron density around ADP A 301:

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

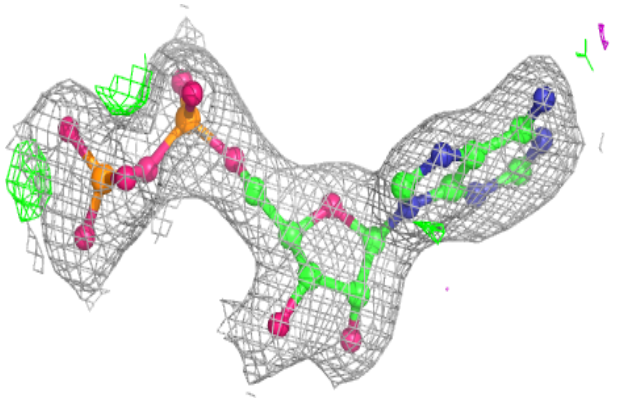


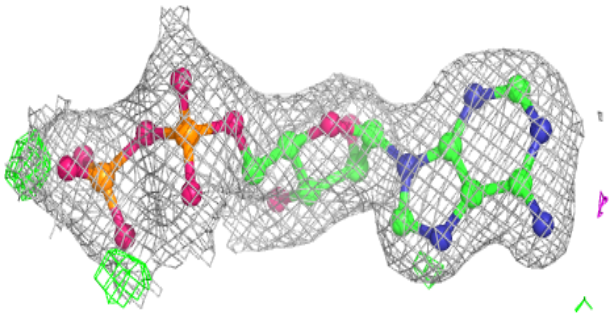


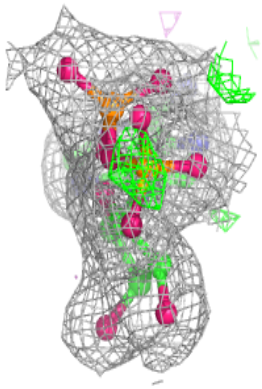


Electron density around ADP D 301:

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

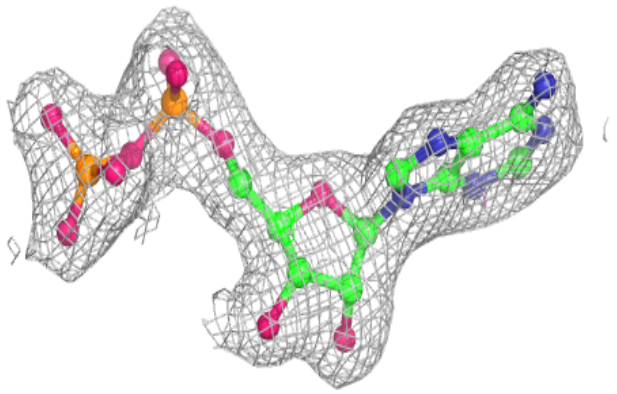


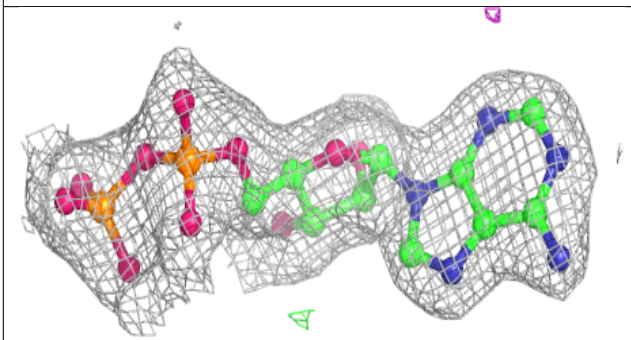


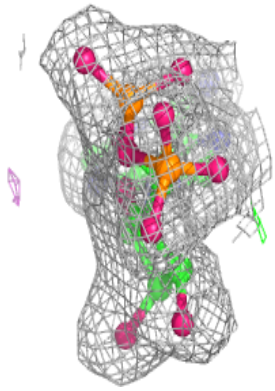


Electron density around ADP L 301:

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

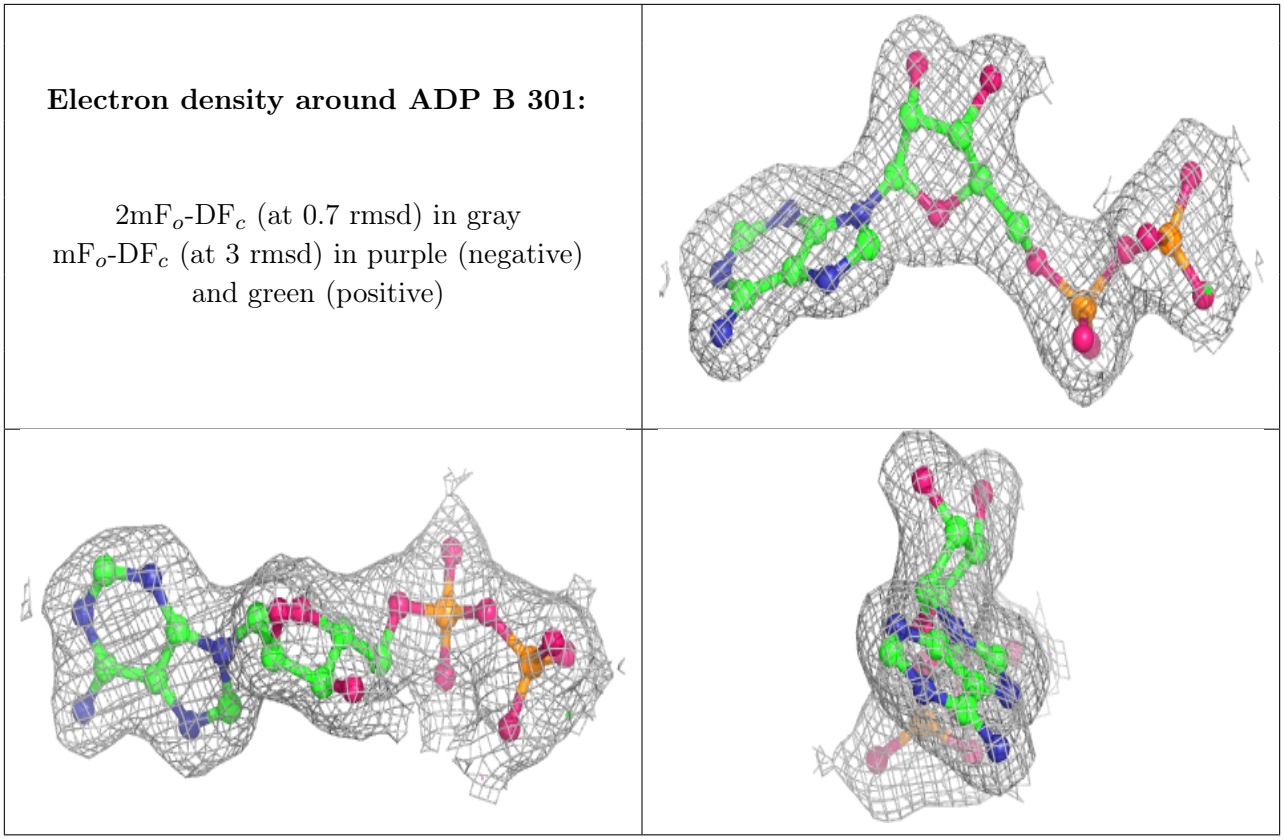






Electron density around ADP B 301:

$2mF_o$-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.