wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2024 – 10:18 AM JST

PDB ID	:	8KG2
Title	:	Crystal structure of p97-N/D1 hexamer in complex with FAF1-UBX domain
Authors	:	Kang, W.
Deposited on	:	2023-08-17
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

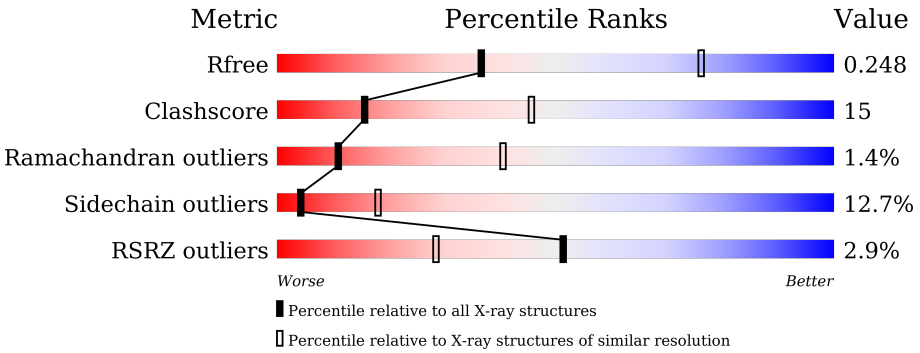
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	438	70% 25%
1	B	438	69% 25% 5%
1	C	438	70% 26%
1	D	438	71% 24%
1	E	438	71% 22% 6%
1	F	438	67% 26% 5%

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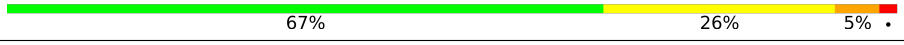
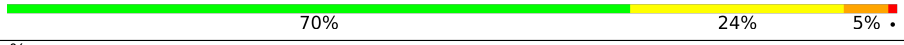
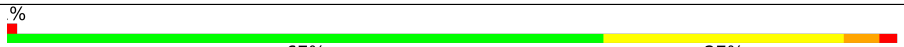
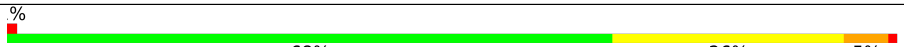
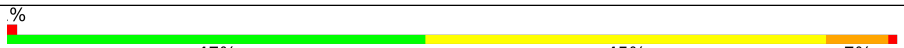
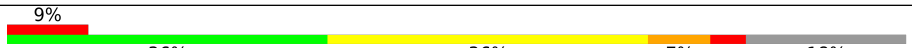
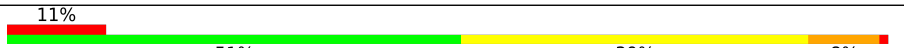
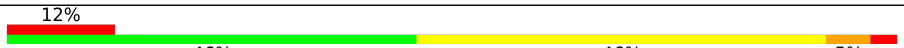
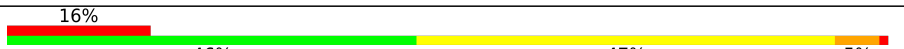
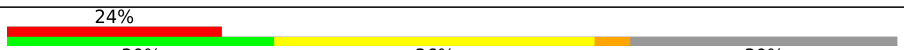
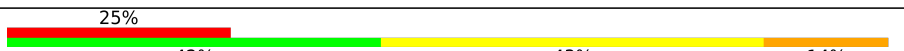
Mol	Chain	Length	Quality of chain
1	G	438	
1	H	438	
1	I	438	
1	J	438	
1	K	438	
1	L	438	
2	M	76	
2	N	76	
2	O	76	
2	P	76	
2	Q	76	
2	R	76	
2	S	76	
2	T	76	
2	U	76	
2	V	76	
2	W	76	
2	X	76	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 48735 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	B	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	C	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	D	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	E	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	F	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	G	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	H	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	I	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	J	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	K	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	L	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	ALA	GLU	engineered mutation	UNP P55072
A	193	ALA	ASP	engineered mutation	UNP P55072
A	194	ALA	GLU	engineered mutation	UNP P55072
B	192	ALA	GLU	engineered mutation	UNP P55072
B	193	ALA	ASP	engineered mutation	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
B	194	ALA	GLU	engineered mutation	UNP P55072
C	192	ALA	GLU	engineered mutation	UNP P55072
C	193	ALA	ASP	engineered mutation	UNP P55072
C	194	ALA	GLU	engineered mutation	UNP P55072
D	192	ALA	GLU	engineered mutation	UNP P55072
D	193	ALA	ASP	engineered mutation	UNP P55072
D	194	ALA	GLU	engineered mutation	UNP P55072
E	192	ALA	GLU	engineered mutation	UNP P55072
E	193	ALA	ASP	engineered mutation	UNP P55072
E	194	ALA	GLU	engineered mutation	UNP P55072
F	192	ALA	GLU	engineered mutation	UNP P55072
F	193	ALA	ASP	engineered mutation	UNP P55072
F	194	ALA	GLU	engineered mutation	UNP P55072
G	192	ALA	GLU	engineered mutation	UNP P55072
G	193	ALA	ASP	engineered mutation	UNP P55072
G	194	ALA	GLU	engineered mutation	UNP P55072
H	192	ALA	GLU	engineered mutation	UNP P55072
H	193	ALA	ASP	engineered mutation	UNP P55072
H	194	ALA	GLU	engineered mutation	UNP P55072
I	192	ALA	GLU	engineered mutation	UNP P55072
I	193	ALA	ASP	engineered mutation	UNP P55072
I	194	ALA	GLU	engineered mutation	UNP P55072
J	192	ALA	GLU	engineered mutation	UNP P55072
J	193	ALA	ASP	engineered mutation	UNP P55072
J	194	ALA	GLU	engineered mutation	UNP P55072
K	192	ALA	GLU	engineered mutation	UNP P55072
K	193	ALA	ASP	engineered mutation	UNP P55072
K	194	ALA	GLU	engineered mutation	UNP P55072
L	192	ALA	GLU	engineered mutation	UNP P55072
L	193	ALA	ASP	engineered mutation	UNP P55072
L	194	ALA	GLU	engineered mutation	UNP P55072

- Molecule 2 is a protein called FAS-associated factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	76	Total	C	N	O	0	0	0
			637	417	107	113			
2	N	62	Total	C	N	O	0	0	0
			524	340	89	95			
2	O	76	Total	C	N	O	0	0	0
			637	417	107	113			
2	P	76	Total	C	N	O	0	0	0
			637	417	107	113			

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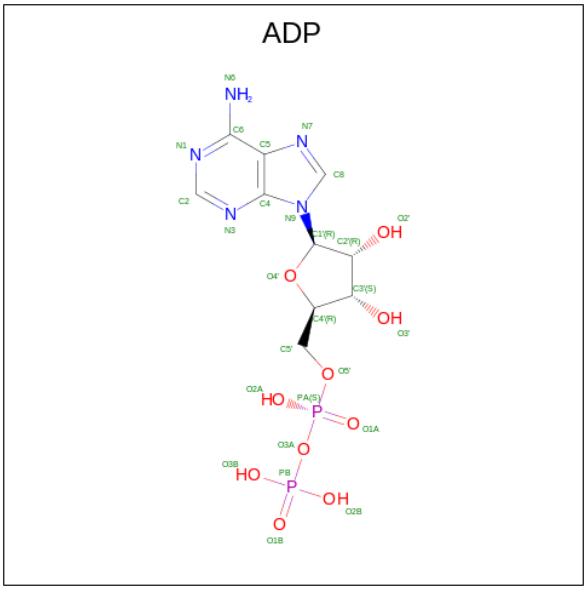
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	76	Total 637	C 417	N 107	O 113	0	0	0
2	R	76	Total 637	C 417	N 107	O 113	0	0	0
2	S	76	Total 637	C 417	N 107	O 113	0	0	0
2	T	76	Total 637	C 417	N 107	O 113	0	0	0
2	U	76	Total 637	C 417	N 107	O 113	0	0	0
2	V	76	Total 637	C 417	N 107	O 113	0	0	0
2	W	53	Total 453	C 299	N 79	O 75	0	0	0
2	X	76	Total 637	C 417	N 107	O 113	0	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0

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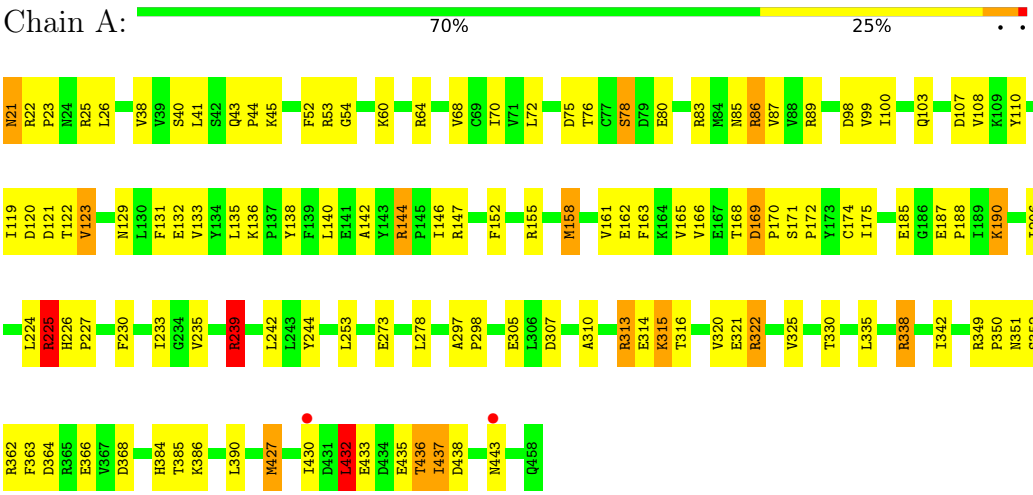
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J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

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.

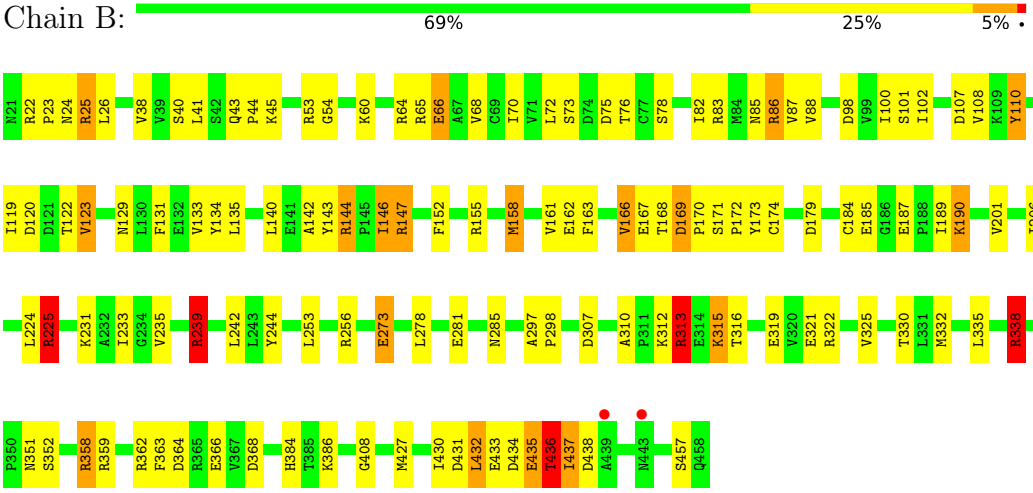
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain A:



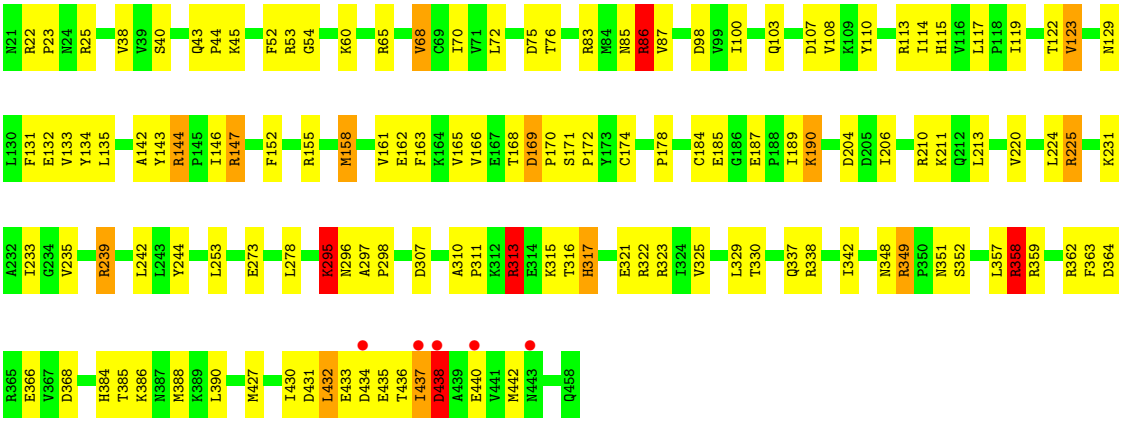
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain B:



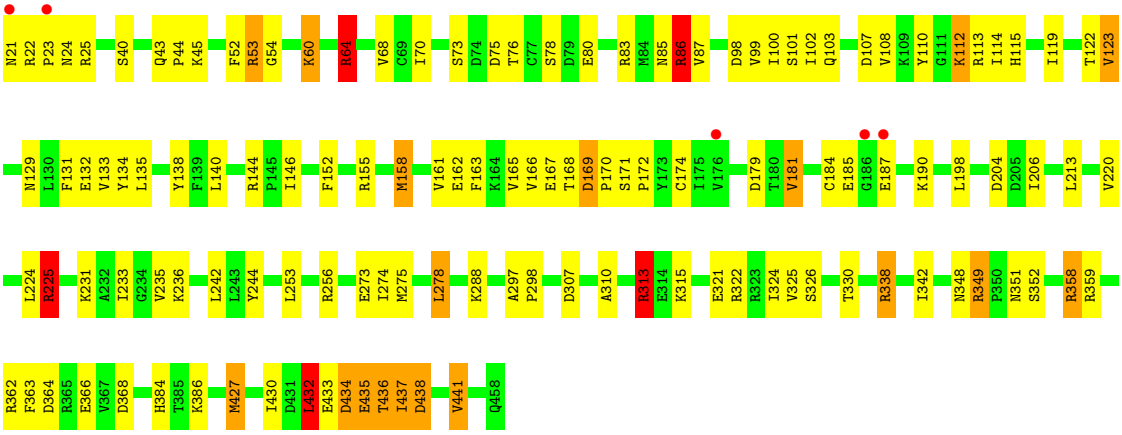
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C:



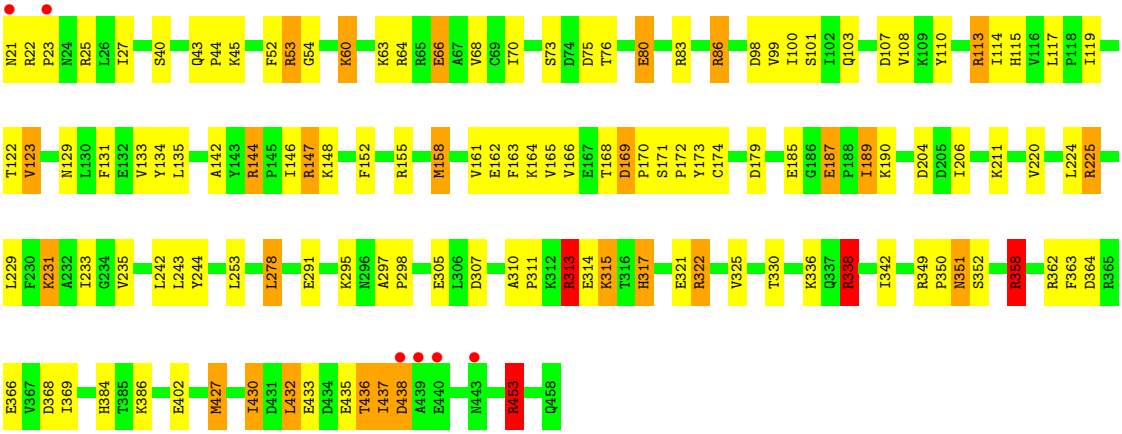
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain D:



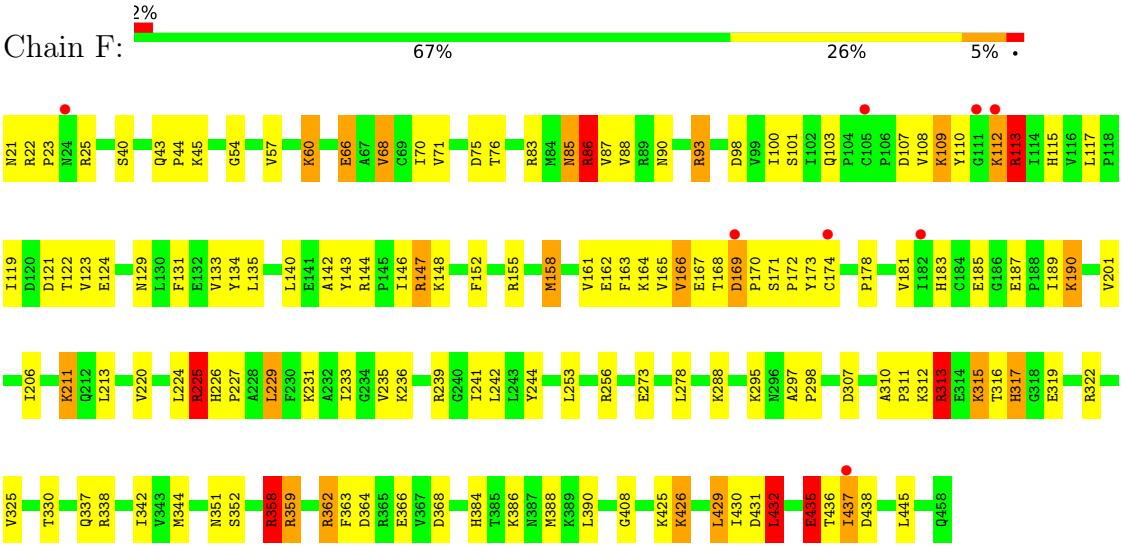
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain E:



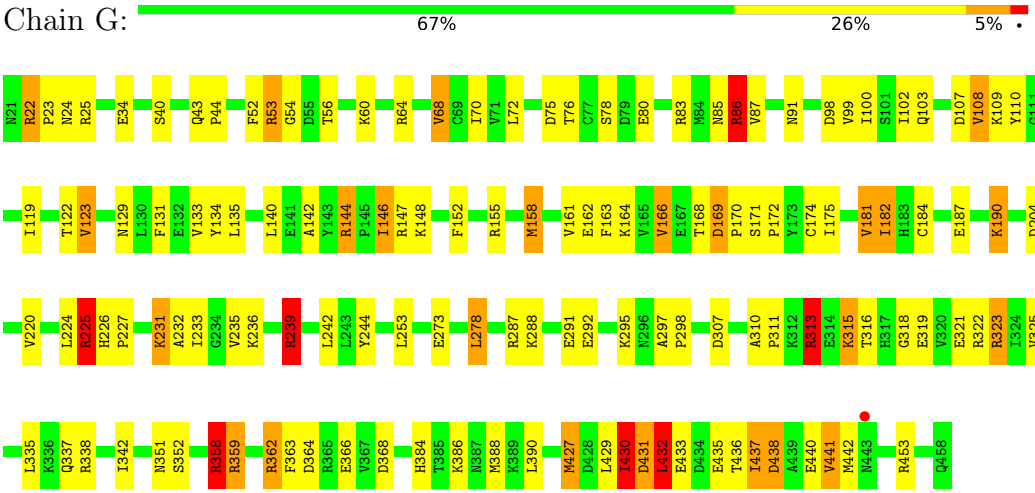
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F:



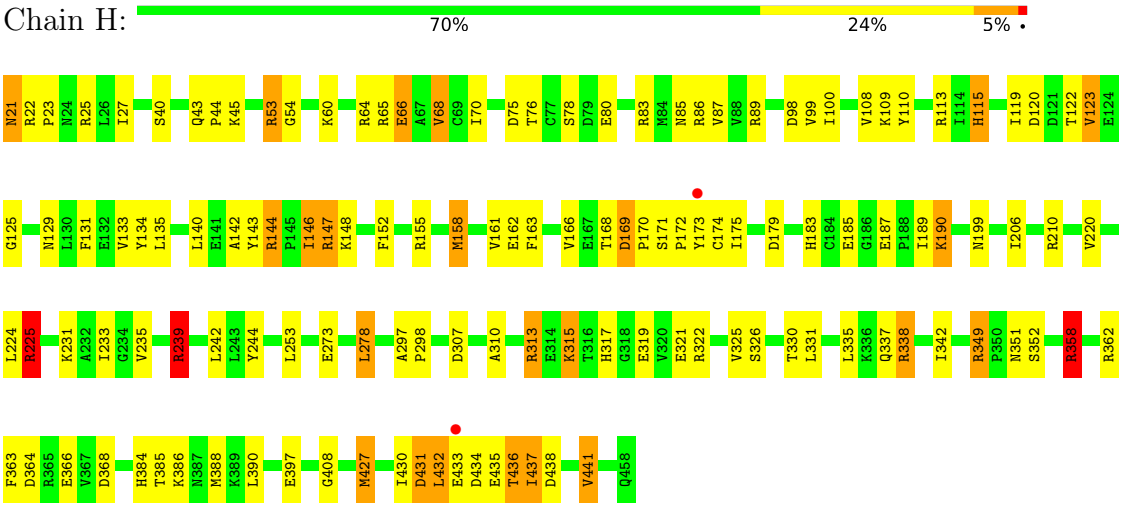
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain G:



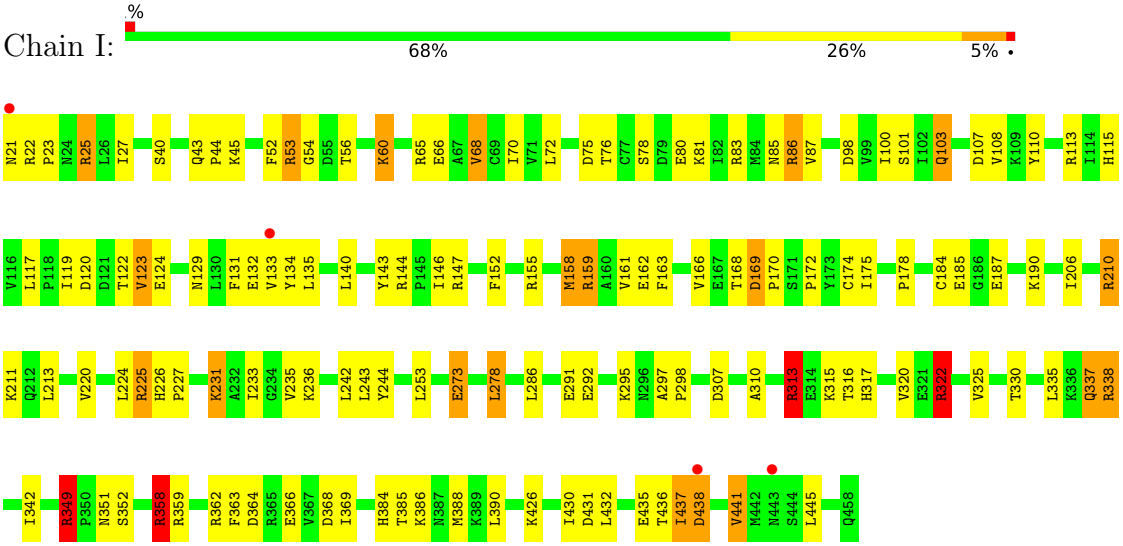
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain H:



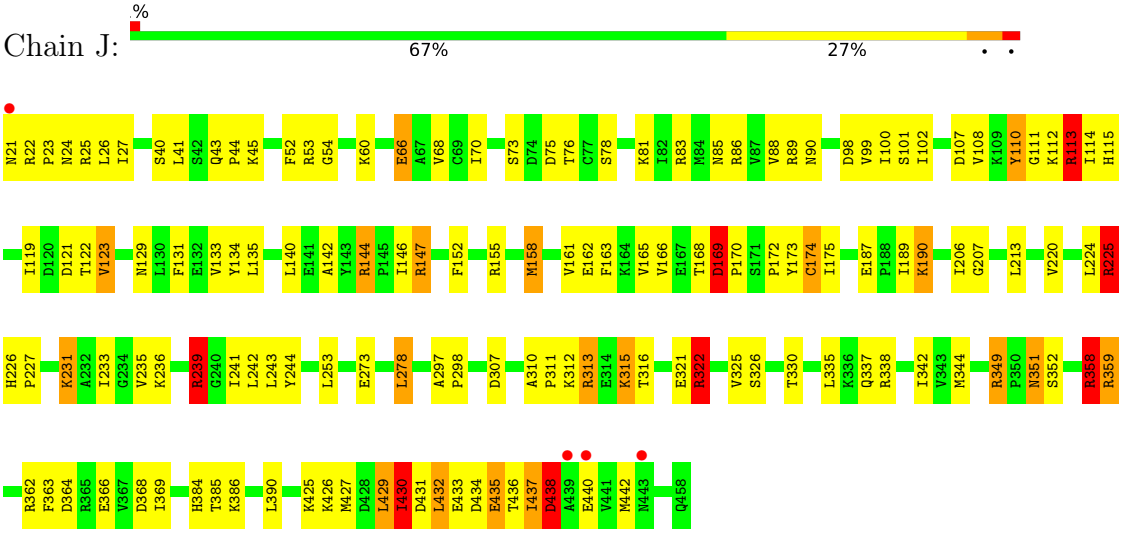
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain I:



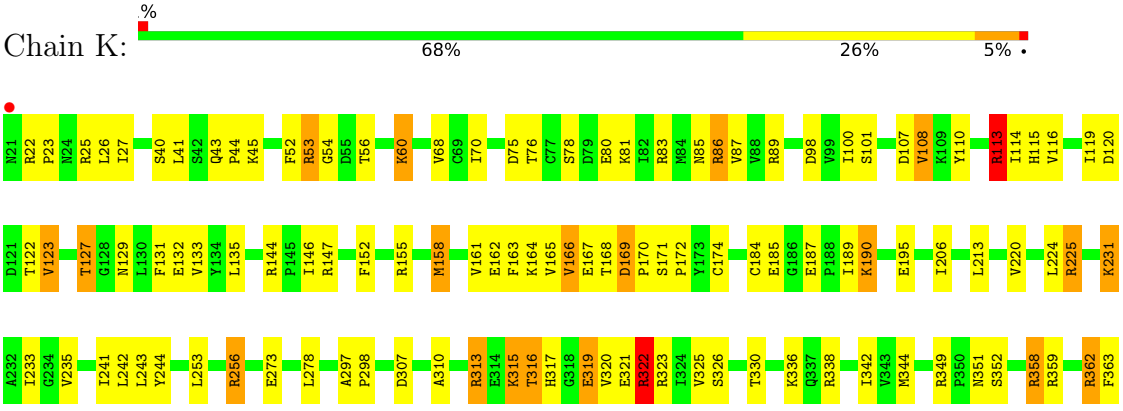
• Molecule 1: Transitional endoplasmic reticulum ATPase

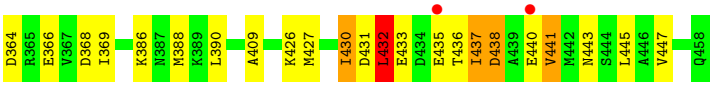
Chain J:



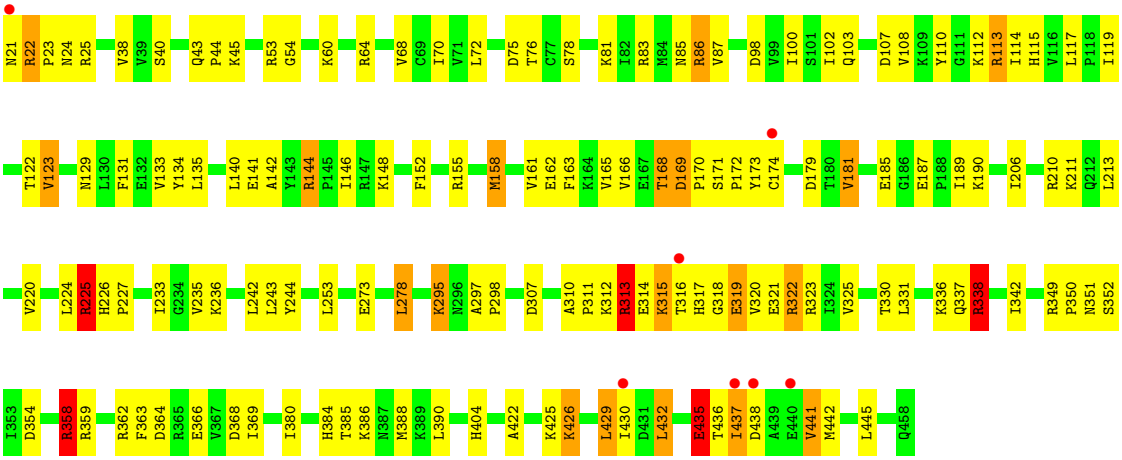
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain K:

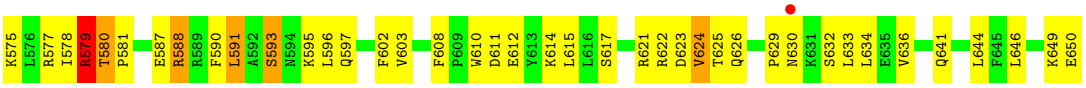




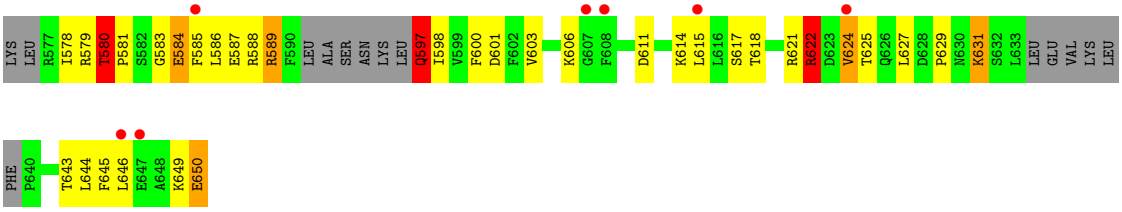
• Molecule 1: Transitional endoplasmic reticulum ATPase



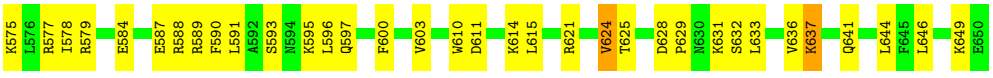
• Molecule 2: FAS-associated factor 1



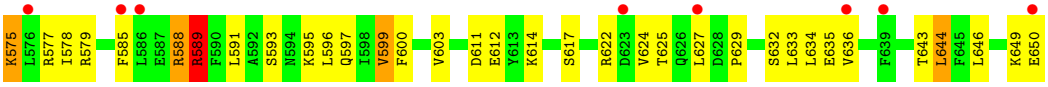
• Molecule 2: FAS-associated factor 1



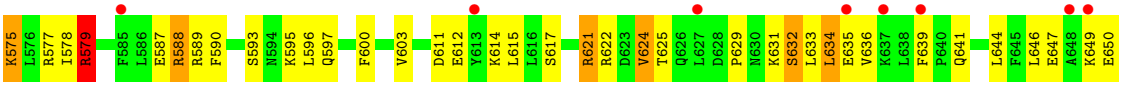
• Molecule 2: FAS-associated factor 1



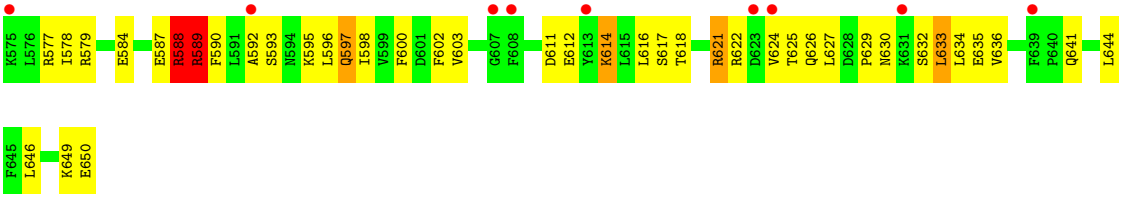
• Molecule 2: FAS-associated factor 1



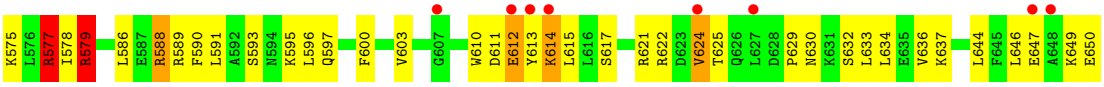
• Molecule 2: FAS-associated factor 1



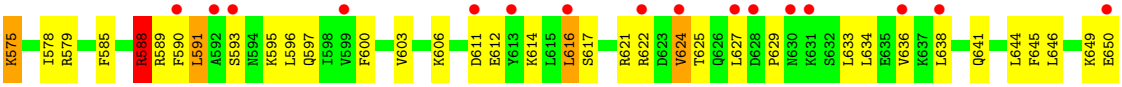
• Molecule 2: FAS-associated factor 1



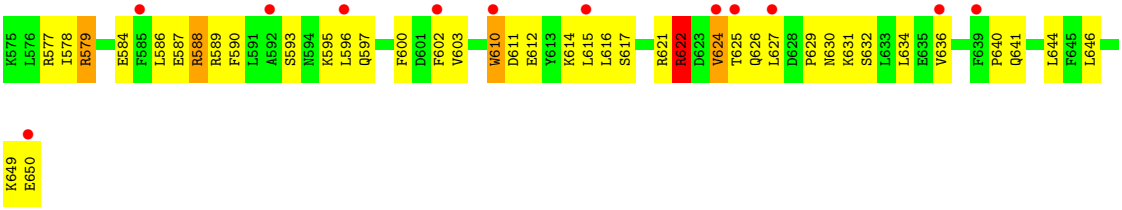
• Molecule 2: FAS-associated factor 1



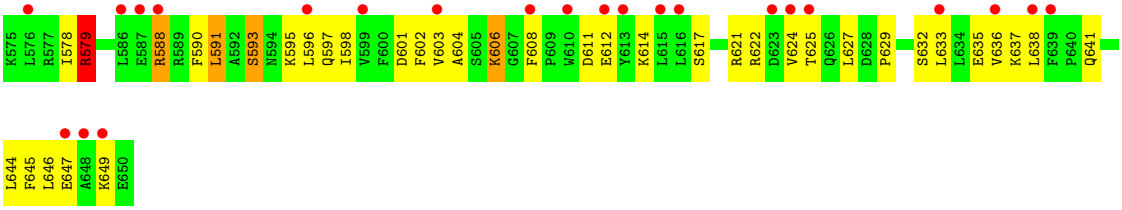
• Molecule 2: FAS-associated factor 1



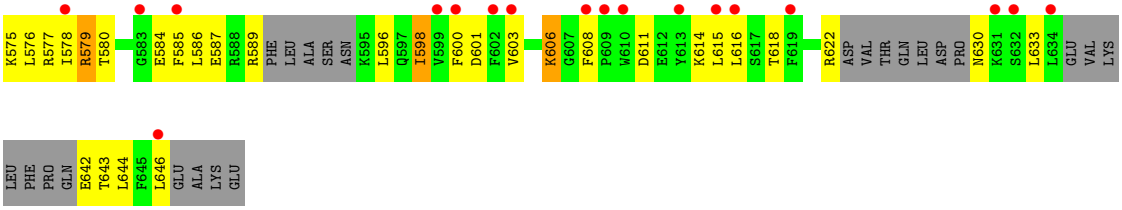
• Molecule 2: FAS-associated factor 1



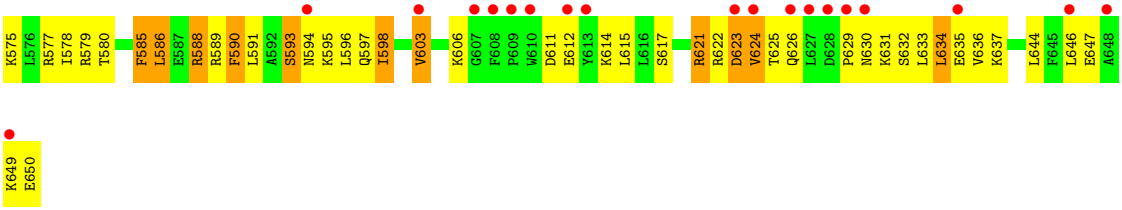
• Molecule 2: FAS-associated factor 1



• Molecule 2: FAS-associated factor 1



• Molecule 2: FAS-associated factor 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	106.67Å 134.48Å 148.22Å 71.52° 80.87° 87.53°	Depositor
Resolution (Å)	48.80 – 3.10 48.80 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.80-3.10) 97.4 (48.80-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.198 , 0.246 0.200 , 0.248	Depositor DCC
R_{free} test set	6798 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	78.3	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 65.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	48735	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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

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	0.39	0/3475	0.83	5/4696 (0.1%)
1	B	0.39	0/3475	0.82	3/4696 (0.1%)
1	C	0.39	0/3475	0.83	6/4696 (0.1%)
1	D	0.40	0/3475	0.89	9/4696 (0.2%)
1	E	0.40	0/3475	0.85	6/4696 (0.1%)
1	F	0.41	1/3475 (0.0%)	0.95	13/4696 (0.3%)
1	G	0.39	0/3475	0.86	10/4696 (0.2%)
1	H	0.39	0/3475	0.90	8/4696 (0.2%)
1	I	0.39	0/3475	0.83	7/4696 (0.1%)
1	J	0.40	0/3475	0.87	10/4696 (0.2%)
1	K	0.40	0/3475	0.87	9/4696 (0.2%)
1	L	0.37	0/3475	0.82	5/4696 (0.1%)
2	M	0.34	0/652	0.82	1/878 (0.1%)
2	N	0.53	0/536	1.26	6/719 (0.8%)
2	O	0.39	0/652	0.92	3/878 (0.3%)
2	P	0.39	0/652	0.88	3/878 (0.3%)
2	Q	0.33	0/652	0.91	3/878 (0.3%)
2	R	0.40	0/652	0.95	5/878 (0.6%)
2	S	0.36	0/652	0.89	3/878 (0.3%)
2	T	0.37	0/652	0.88	1/878 (0.1%)
2	U	0.35	0/652	0.95	3/878 (0.3%)
2	V	0.35	0/652	0.81	0/878
2	W	0.39	0/461	0.97	1/613 (0.2%)
2	X	0.36	0/652	0.87	3/878 (0.3%)
All	All	0.39	1/49217 (0.0%)	0.87	123/66464 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
1	B	0	8
1	C	0	6
1	D	0	7
1	E	0	8
1	F	0	11
1	G	0	11
1	H	0	8
1	I	0	11
1	J	0	9
1	K	0	7
1	L	0	7
2	M	0	2
2	N	0	1
2	Q	0	2
2	R	0	2
2	S	0	3
2	T	0	2
2	U	0	1
2	V	0	1
2	X	0	2
All	All	0	121

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	167	GLU	CD-OE2	-6.63	1.18	1.25

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	93	ARG	NE-CZ-NH1	-19.83	110.38	120.30
1	H	358	ARG	NE-CZ-NH1	-19.37	110.62	120.30
1	D	86	ARG	NE-CZ-NH1	17.71	129.16	120.30
1	D	86	ARG	NE-CZ-NH2	-16.14	112.23	120.30
1	H	358	ARG	NE-CZ-NH2	13.29	126.94	120.30

There are no chirality outliers.

5 of 121 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	22	ARG	Sidechain
1	A	64	ARG	Sidechain
1	A	86	ARG	Sidechain
1	A	89	ARG	Sidechain

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	3422	0	3486	96	3
1	B	3422	0	3486	106	0
1	C	3422	0	3486	96	4
1	D	3422	0	3486	92	0
1	E	3422	0	3486	96	0
1	F	3422	0	3486	115	0
1	G	3422	0	3486	109	3
1	H	3422	0	3486	115	4
1	I	3422	0	3486	96	0
1	J	3422	0	3486	116	0
1	K	3422	0	3486	106	0
1	L	3422	0	3486	116	0
2	M	637	0	652	31	0
2	N	524	0	517	31	0
2	O	637	0	652	18	0
2	P	637	0	652	27	0
2	Q	637	0	652	26	0
2	R	637	0	652	25	0
2	S	637	0	652	25	0
2	T	637	0	652	32	0
2	U	637	0	652	35	0
2	V	637	0	652	35	0
2	W	453	0	470	20	0
2	X	637	0	652	35	0
3	A	27	0	12	1	0
3	B	27	0	12	2	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
3	E	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	27	0	12	2	0
3	G	27	0	12	1	0
3	H	27	0	12	3	0
3	I	27	0	12	1	0
3	J	27	0	12	4	0
3	K	27	0	12	1	0
3	L	27	0	12	2	0
All	All	48735	0	49483	1442	7

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 15.

The worst 5 of 1442 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:E:147:ARG:NH2	1:E:173:TYR:HD2	1.14	1.44
1:G:430:ILE:CD1	1:G:431:ASP:H	1.31	1.43
1:B:147:ARG:NH2	1:B:173:TYR:HD2	1.13	1.43
1:H:147:ARG:NH2	1:H:173:TYR:HD2	1.14	1.43
1:G:430:ILE:HD12	1:G:431:ASP:N	1.28	1.43

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ASN:OD1	1:H:185:GLU:OE2[1_565]	1.41	0.79
1:A:120:ASP:OD2	1:G:64:ARG:NH2[1_655]	1.79	0.41
1:A:188:PRO:O	1:G:64:ARG:NH1[1_655]	1.81	0.39
1:C:296:ASN:OD1	1:H:185:GLU:CD[1_565]	1.81	0.39
1:A:190:LYS:CA	1:G:64:ARG:NH2[1_655]	2.13	0.07

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	436/438 (100%)	415 (95%)	14 (3%)	7 (2%)	9 37
1	B	436/438 (100%)	417 (96%)	13 (3%)	6 (1%)	11 40
1	C	436/438 (100%)	413 (95%)	16 (4%)	7 (2%)	9 37
1	D	436/438 (100%)	416 (95%)	13 (3%)	7 (2%)	9 37
1	E	436/438 (100%)	417 (96%)	12 (3%)	7 (2%)	9 37
1	F	436/438 (100%)	415 (95%)	14 (3%)	7 (2%)	9 37
1	G	436/438 (100%)	415 (95%)	11 (2%)	10 (2%)	6 28
1	H	436/438 (100%)	415 (95%)	15 (3%)	6 (1%)	11 40
1	I	436/438 (100%)	418 (96%)	11 (2%)	7 (2%)	9 37
1	J	436/438 (100%)	415 (95%)	14 (3%)	7 (2%)	9 37
1	K	436/438 (100%)	416 (95%)	12 (3%)	8 (2%)	8 34
1	L	436/438 (100%)	416 (95%)	14 (3%)	6 (1%)	11 40
2	M	74/76 (97%)	71 (96%)	3 (4%)	0	100 100
2	N	56/76 (74%)	50 (89%)	4 (7%)	2 (4%)	3 20
2	O	74/76 (97%)	70 (95%)	4 (5%)	0	100 100
2	P	74/76 (97%)	71 (96%)	3 (4%)	0	100 100
2	Q	74/76 (97%)	71 (96%)	3 (4%)	0	100 100
2	R	74/76 (97%)	71 (96%)	3 (4%)	0	100 100
2	S	74/76 (97%)	71 (96%)	3 (4%)	0	100 100
2	T	74/76 (97%)	71 (96%)	3 (4%)	0	100 100
2	U	74/76 (97%)	71 (96%)	3 (4%)	0	100 100
2	V	74/76 (97%)	71 (96%)	3 (4%)	0	100 100
2	W	45/76 (59%)	43 (96%)	2 (4%)	0	100 100
2	X	74/76 (97%)	71 (96%)	3 (4%)	0	100 100
All	All	6073/6168 (98%)	5790 (95%)	196 (3%)	87 (1%)	11 40

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	THR
1	C	438	ASP
1	D	436	THR
1	E	363	PHE

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Mol	Chain	Res	Type
1	F	363	PHE

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	372/372 (100%)	333 (90%)	39 (10%)	7 26
1	B	372/372 (100%)	328 (88%)	44 (12%)	5 21
1	C	372/372 (100%)	330 (89%)	42 (11%)	6 23
1	D	372/372 (100%)	327 (88%)	45 (12%)	5 20
1	E	372/372 (100%)	327 (88%)	45 (12%)	5 20
1	F	372/372 (100%)	328 (88%)	44 (12%)	5 21
1	G	372/372 (100%)	321 (86%)	51 (14%)	3 16
1	H	372/372 (100%)	332 (89%)	40 (11%)	6 25
1	I	372/372 (100%)	335 (90%)	37 (10%)	8 29
1	J	372/372 (100%)	331 (89%)	41 (11%)	6 25
1	K	372/372 (100%)	330 (89%)	42 (11%)	6 23
1	L	372/372 (100%)	323 (87%)	49 (13%)	4 17
2	M	71/71 (100%)	59 (83%)	12 (17%)	2 9
2	N	58/71 (82%)	48 (83%)	10 (17%)	2 9
2	O	71/71 (100%)	62 (87%)	9 (13%)	4 18
2	P	71/71 (100%)	60 (84%)	11 (16%)	2 11
2	Q	71/71 (100%)	58 (82%)	13 (18%)	1 7
2	R	71/71 (100%)	56 (79%)	15 (21%)	1 5
2	S	71/71 (100%)	56 (79%)	15 (21%)	1 5
2	T	71/71 (100%)	58 (82%)	13 (18%)	1 7
2	U	71/71 (100%)	56 (79%)	15 (21%)	1 5
2	V	71/71 (100%)	60 (84%)	11 (16%)	2 11
2	W	50/71 (70%)	41 (82%)	9 (18%)	1 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	X	71/71 (100%)	54 (76%)	17 (24%)	0 2
All	All	5282/5316 (99%)	4613 (87%)	669 (13%)	4 18

5 of 669 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	107	ASP
1	L	315	LYS
1	J	225	ARG
1	J	78	SER
1	K	256	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	327	GLN
1	K	129	ASN
1	I	129	ASN
1	J	351	ASN
1	K	348	ASN

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)

12 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	$\#\|Z\| > 2$
3	ADP	B	501	-	24,29,29	0.72	0	29,45,45	1.10	1 (3%)
3	ADP	D	501	-	24,29,29	0.66	0	29,45,45	0.87	0
3	ADP	L	501	-	24,29,29	0.68	0	29,45,45	0.97	1 (3%)
3	ADP	J	501	-	24,29,29	0.72	0	29,45,45	1.07	2 (6%)
3	ADP	C	501	-	24,29,29	0.64	0	29,45,45	0.91	2 (6%)
3	ADP	A	501	-	24,29,29	0.69	0	29,45,45	1.01	1 (3%)
3	ADP	E	501	-	24,29,29	0.66	0	29,45,45	0.93	2 (6%)
3	ADP	G	501	-	24,29,29	0.66	0	29,45,45	0.97	2 (6%)
3	ADP	H	501	-	24,29,29	0.67	0	29,45,45	0.99	1 (3%)
3	ADP	F	501	-	24,29,29	0.66	0	29,45,45	1.07	1 (3%)
3	ADP	K	501	-	24,29,29	0.68	0	29,45,45	0.90	1 (3%)
3	ADP	I	501	-	24,29,29	0.76	0	29,45,45	0.84	1 (3%)

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
3	ADP	B	501	-	-	2/12/32/32	0/3/3/3
3	ADP	D	501	-	-	3/12/32/32	0/3/3/3
3	ADP	L	501	-	-	3/12/32/32	0/3/3/3
3	ADP	J	501	-	-	5/12/32/32	0/3/3/3
3	ADP	C	501	-	-	2/12/32/32	0/3/3/3
3	ADP	A	501	-	-	4/12/32/32	0/3/3/3
3	ADP	E	501	-	-	3/12/32/32	0/3/3/3
3	ADP	G	501	-	-	4/12/32/32	0/3/3/3
3	ADP	H	501	-	-	3/12/32/32	0/3/3/3
3	ADP	F	501	-	-	4/12/32/32	0/3/3/3
3	ADP	K	501	-	-	5/12/32/32	0/3/3/3
3	ADP	I	501	-	-	4/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	501	ADP	C5-C6-N6	2.85	124.69	120.35
3	J	501	ADP	C5-C6-N6	2.80	124.60	120.35
3	A	501	ADP	C3'-C2'-C1'	2.63	104.93	100.98
3	B	501	ADP	C3'-C2'-C1'	2.50	104.75	100.98
3	J	501	ADP	O3'-C3'-C2'	-2.49	103.78	111.82

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ADP	C5'-O5'-PA-O3A
3	C	501	ADP	C5'-O5'-PA-O2A
3	C	501	ADP	C5'-O5'-PA-O3A
3	D	501	ADP	C5'-O5'-PA-O1A
3	D	501	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

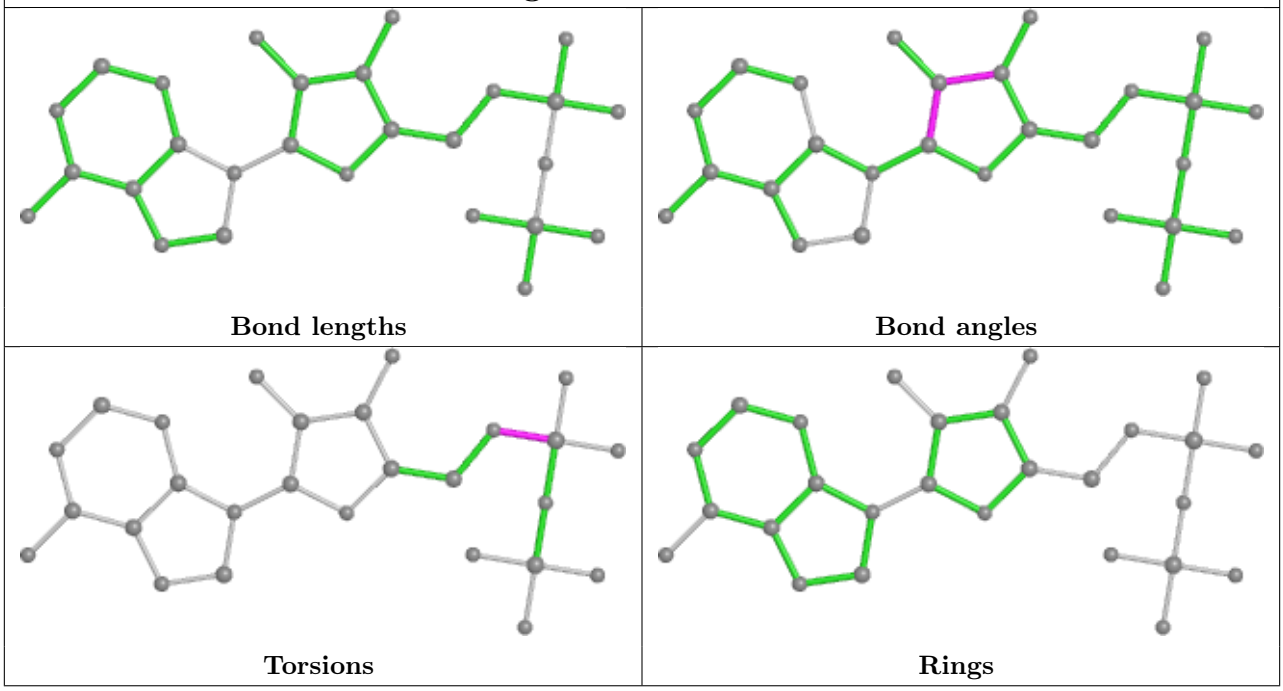
12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	ADP	2	0
3	D	501	ADP	1	0
3	L	501	ADP	2	0
3	J	501	ADP	4	0
3	C	501	ADP	1	0
3	A	501	ADP	1	0
3	E	501	ADP	1	0
3	G	501	ADP	1	0
3	H	501	ADP	3	0
3	F	501	ADP	2	0
3	K	501	ADP	1	0
3	I	501	ADP	1	0

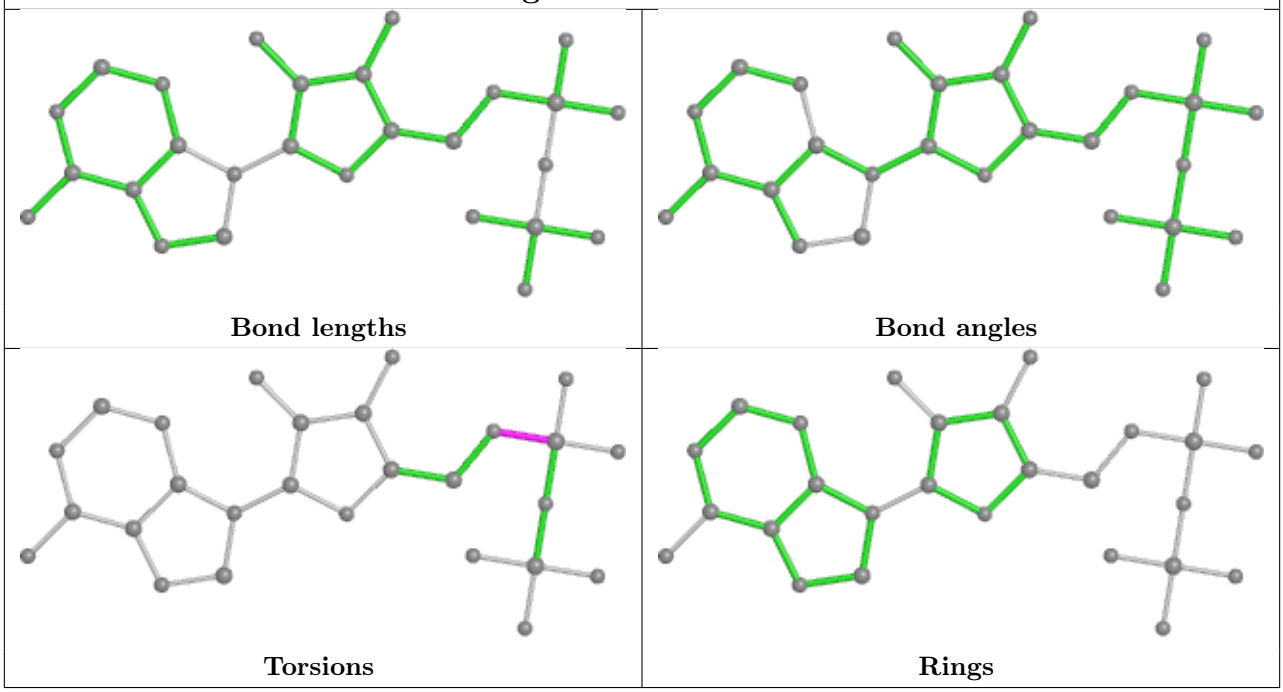
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

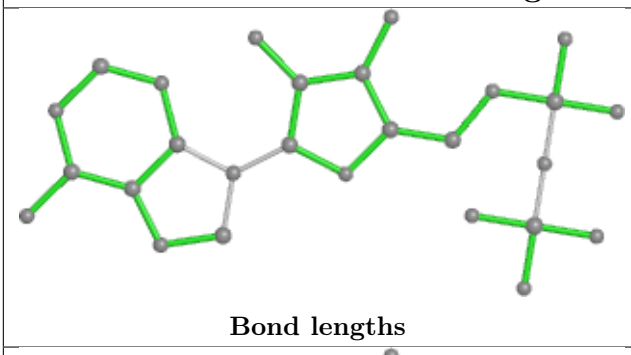
Ligand ADP B 501



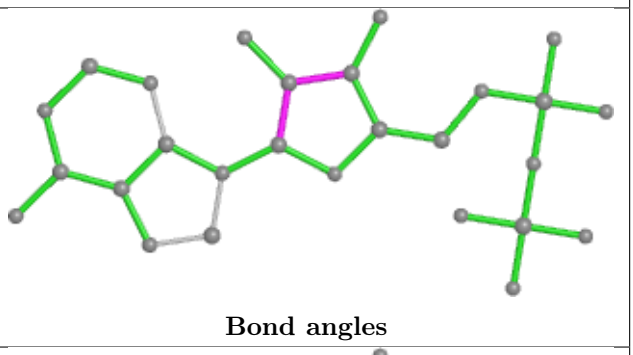
Ligand ADP D 501



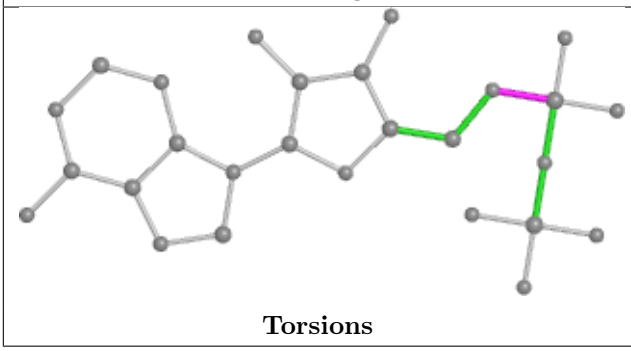
Ligand ADP L 501



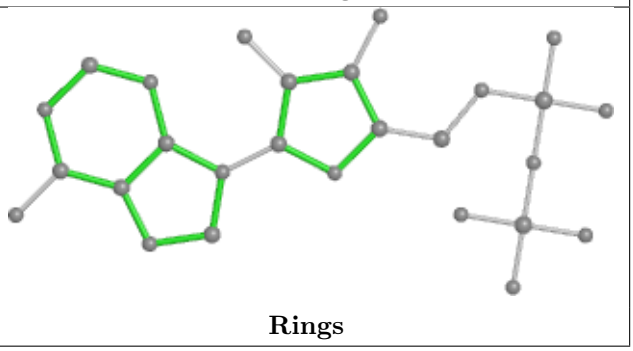
Bond lengths



Bond angles

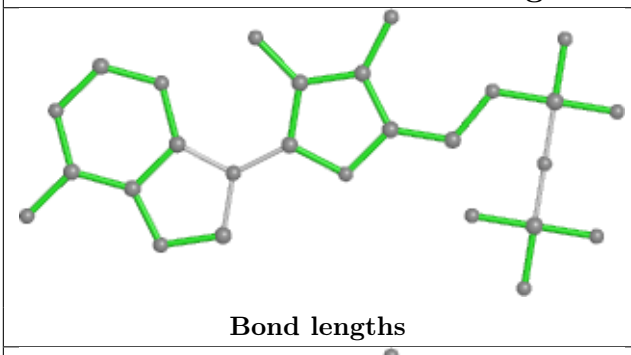


Torsions

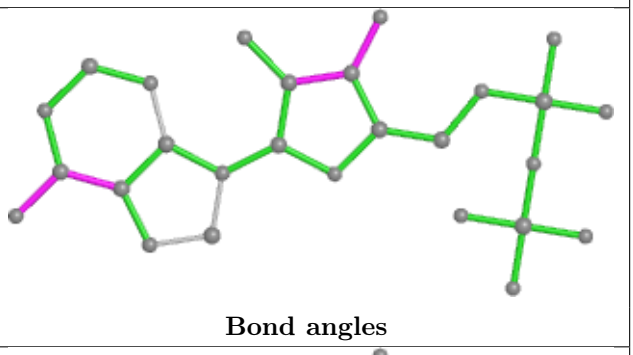


Rings

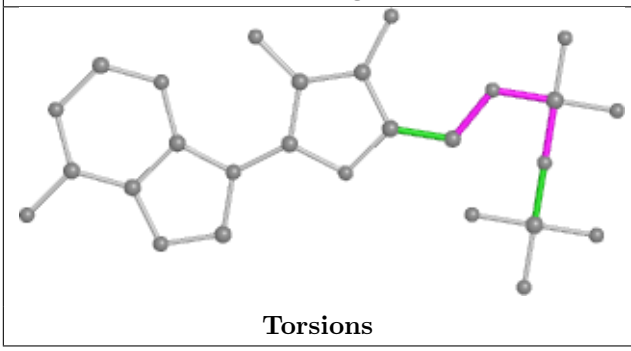
Ligand ADP J 501



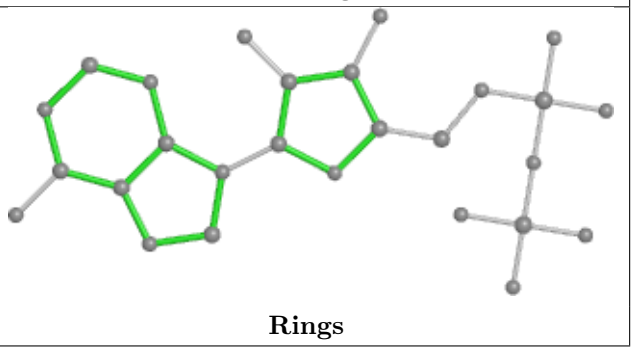
Bond lengths



Bond angles

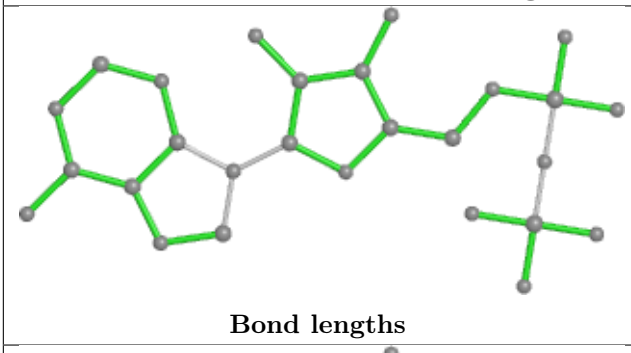


Torsions

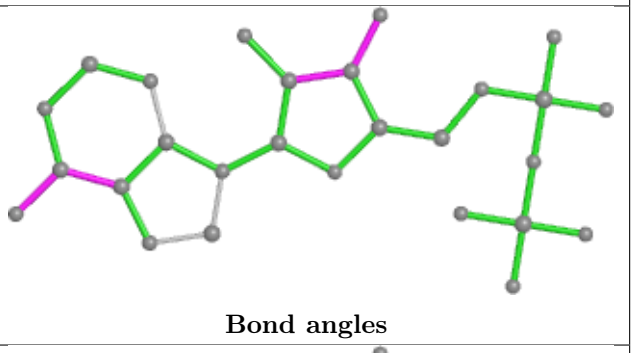


Rings

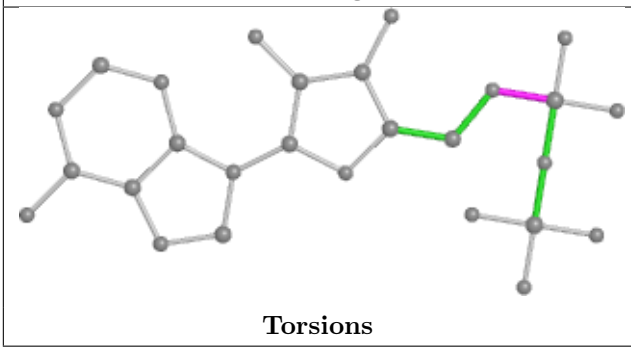
Ligand ADP C 501



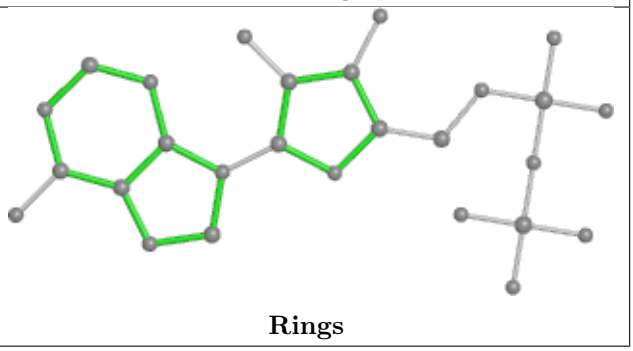
Bond lengths



Bond angles

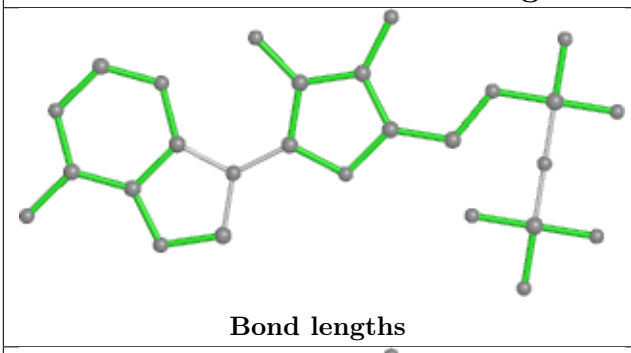


Torsions

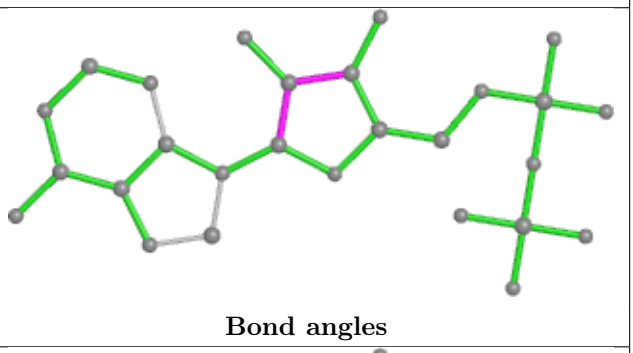


Rings

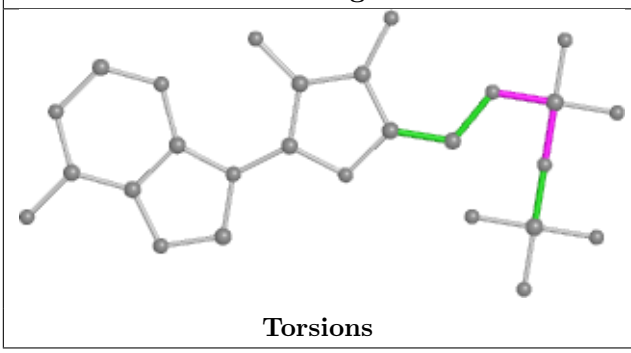
Ligand ADP A 501



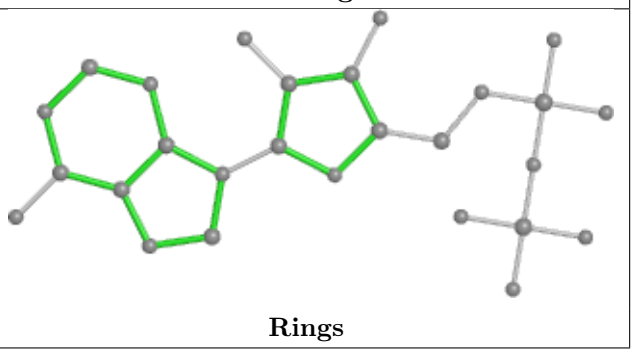
Bond lengths



Bond angles

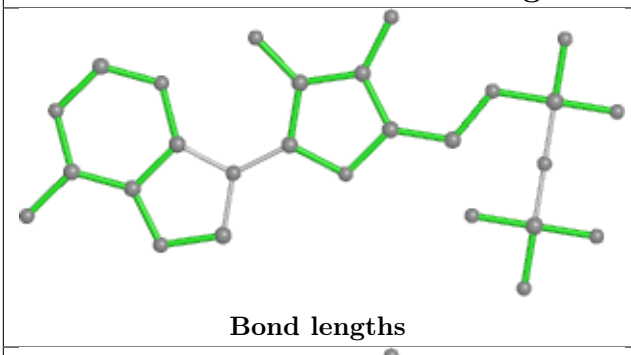


Torsions

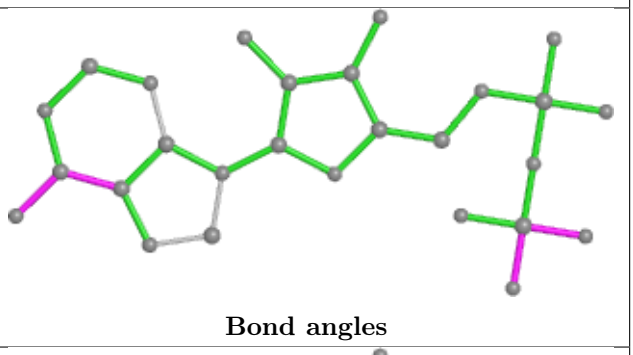


Rings

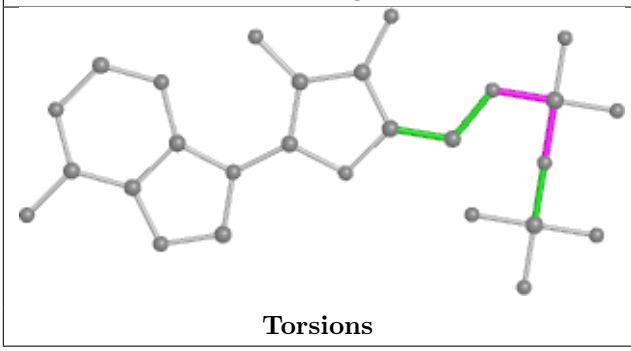
Ligand ADP E 501



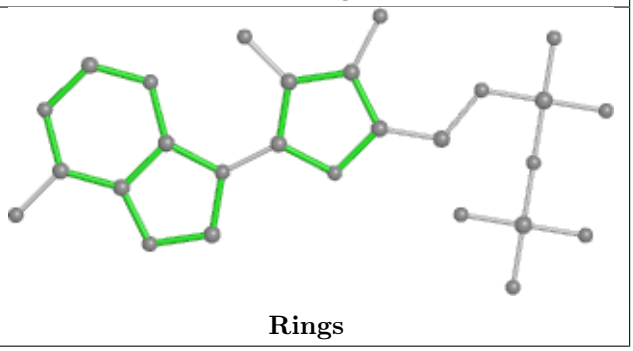
Bond lengths



Bond angles

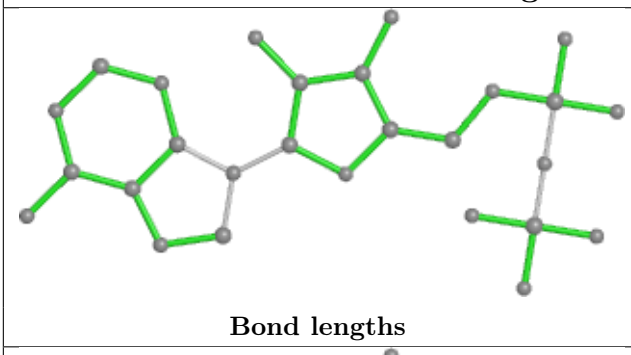


Torsions

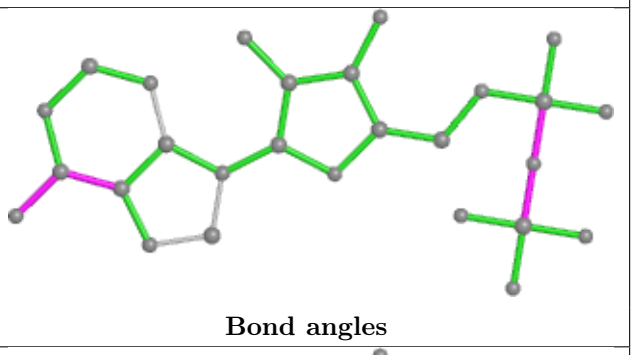


Rings

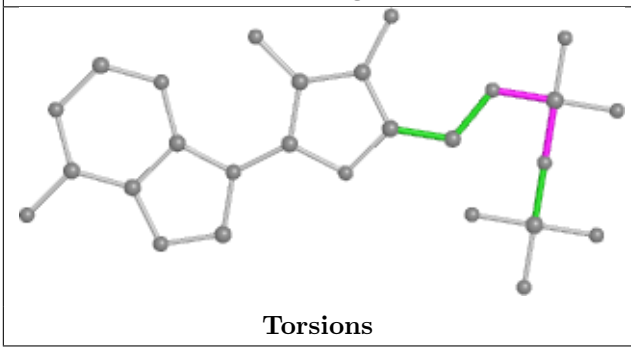
Ligand ADP G 501



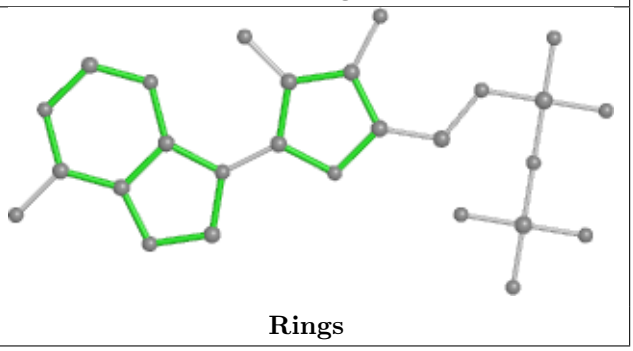
Bond lengths



Bond angles

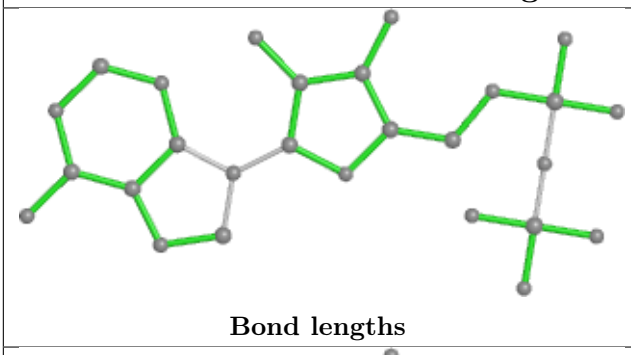


Torsions

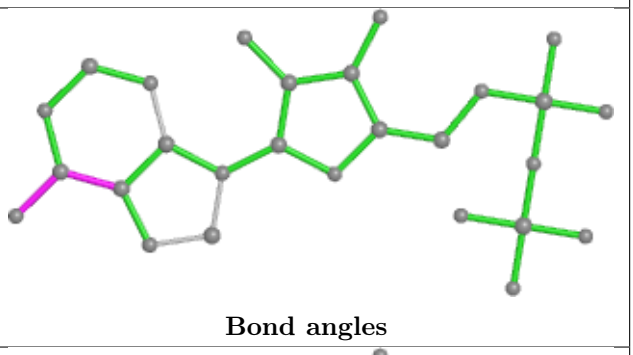


Rings

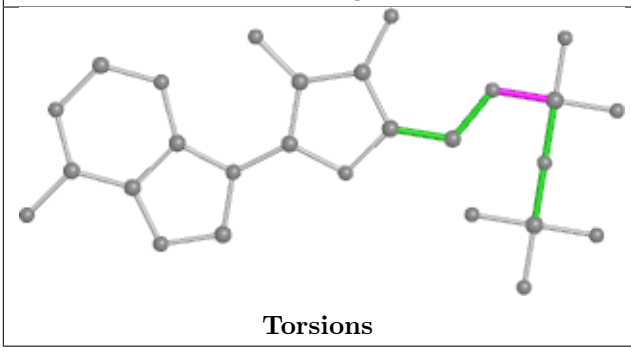
Ligand ADP H 501



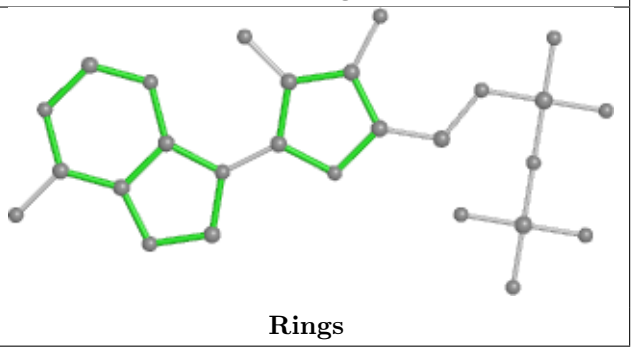
Bond lengths



Bond angles

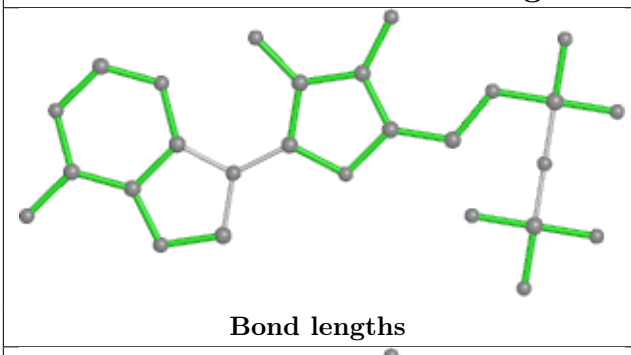


Torsions

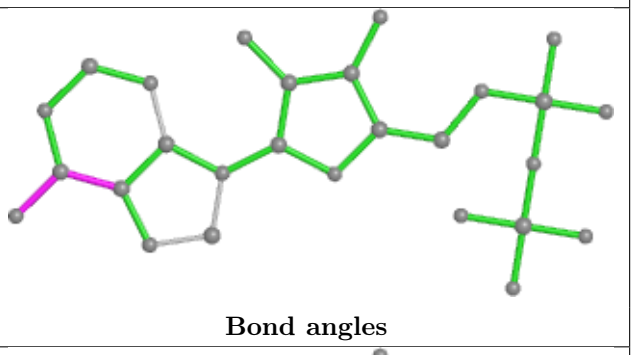


Rings

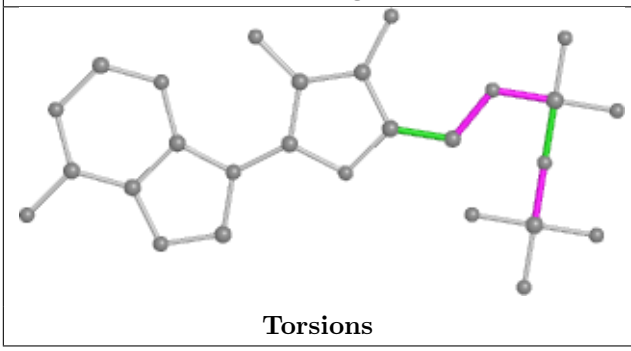
Ligand ADP F 501



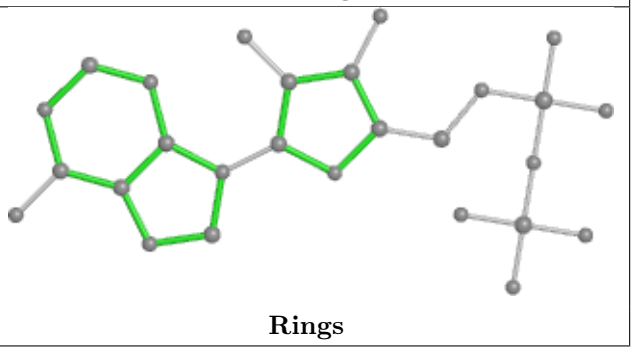
Bond lengths



Bond angles

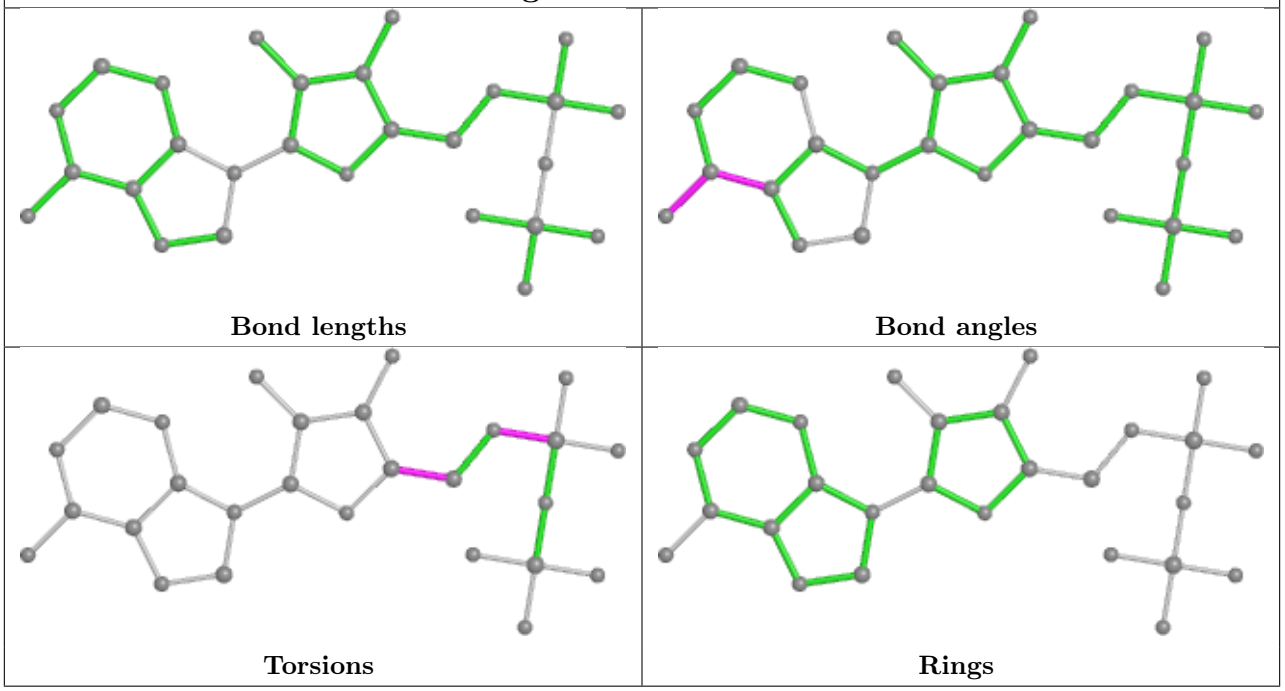


Torsions

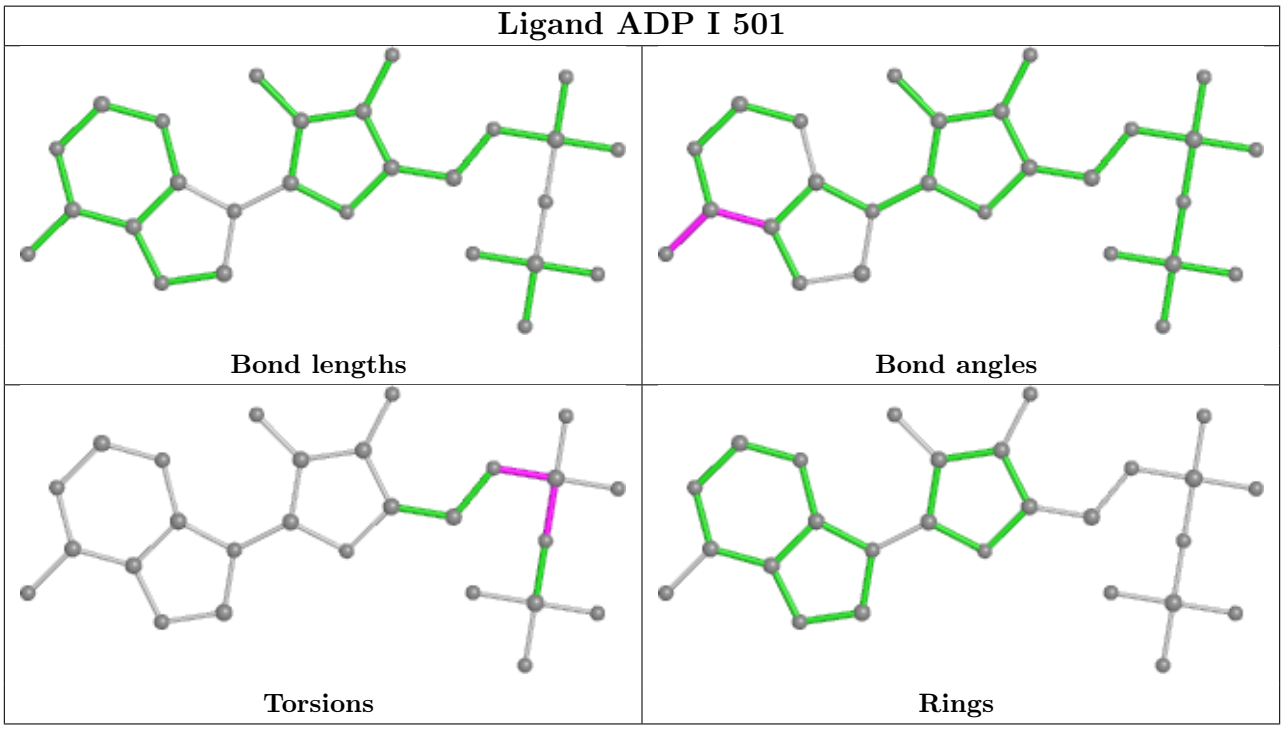


Rings

Ligand ADP K 501



Ligand ADP I 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	438/438 (100%)	-0.25	2 (0%) 91 81	30, 64, 127, 190	0
1	B	438/438 (100%)	-0.29	2 (0%) 91 81	38, 73, 138, 207	0
1	C	438/438 (100%)	-0.26	5 (1%) 80 64	34, 66, 129, 214	0
1	D	438/438 (100%)	-0.24	5 (1%) 80 64	37, 73, 136, 214	0
1	E	438/438 (100%)	-0.23	6 (1%) 75 56	38, 76, 143, 252	0
1	F	438/438 (100%)	-0.09	8 (1%) 68 47	36, 81, 157, 205	0
1	G	438/438 (100%)	-0.24	1 (0%) 95 90	38, 75, 133, 194	0
1	H	438/438 (100%)	-0.24	2 (0%) 91 81	37, 73, 134, 200	0
1	I	438/438 (100%)	-0.26	4 (0%) 84 69	36, 75, 145, 240	0
1	J	438/438 (100%)	-0.23	4 (0%) 84 69	36, 78, 153, 252	0
1	K	438/438 (100%)	-0.25	3 (0%) 87 75	39, 77, 138, 203	0
1	L	438/438 (100%)	-0.14	7 (1%) 72 51	44, 85, 150, 209	0
2	M	76/76 (100%)	-0.21	1 (1%) 77 59	71, 110, 143, 168	0
2	N	62/76 (81%)	0.79	7 (11%) 5 2	91, 133, 172, 194	0
2	O	76/76 (100%)	-0.17	0 100 100	65, 96, 137, 160	0
2	P	76/76 (100%)	0.55	8 (10%) 6 2	97, 148, 188, 229	0
2	Q	76/76 (100%)	0.58	8 (10%) 6 2	109, 159, 192, 233	0
2	R	76/76 (100%)	0.73	9 (11%) 4 2	111, 161, 203, 219	0
2	S	76/76 (100%)	0.43	8 (10%) 6 2	84, 120, 158, 182	0
2	T	76/76 (100%)	1.00	16 (21%) 1 0	114, 157, 197, 216	0
2	U	76/76 (100%)	0.99	12 (15%) 2 1	101, 137, 178, 232	0
2	V	76/76 (100%)	1.17	23 (30%) 0 0	108, 164, 199, 210	0
2	W	53/76 (69%)	1.27	18 (33%) 0 0	80, 133, 195, 219	0
2	X	76/76 (100%)	1.19	19 (25%) 0 0	111, 159, 185, 208	0

Continued on next page...

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	6131/6168 (99%)	-0.10	178 (2%)	51	28	30, 80, 165, 252	0

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	443	ASN	5.4
2	U	627	LEU	5.1
2	T	592	ALA	5.0
1	D	21	ASN	5.0
2	W	609	PRO	5.0

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)

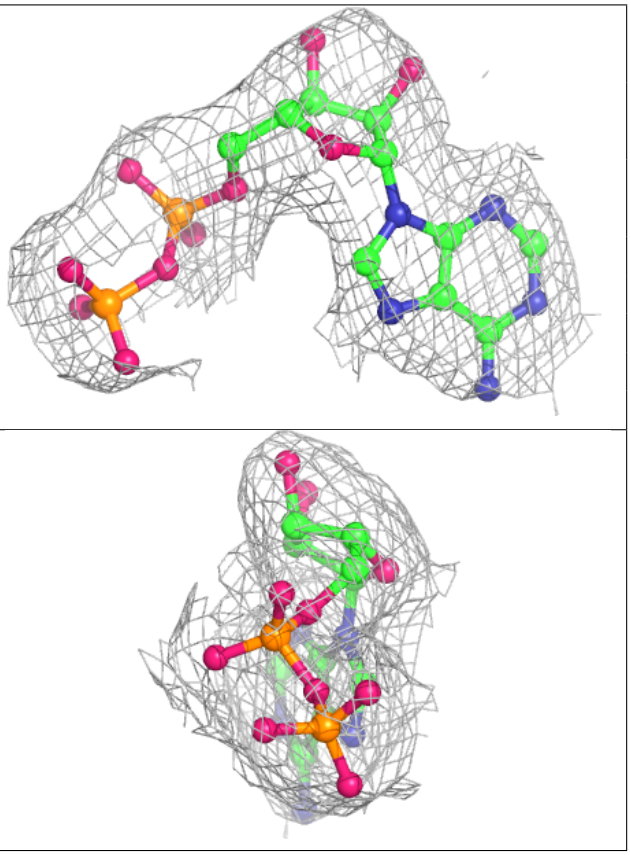
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

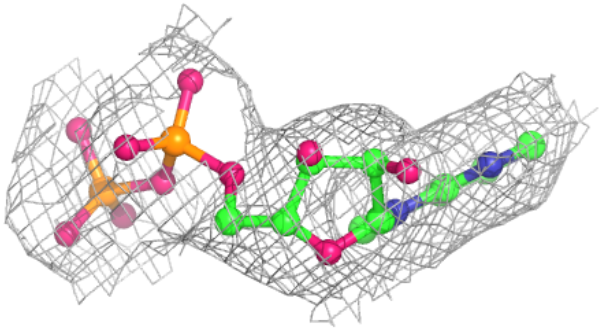
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	B	501	27/27	0.96	0.16	52,62,84,94	0
3	ADP	C	501	27/27	0.97	0.18	45,60,77,94	0
3	ADP	D	501	27/27	0.97	0.16	51,60,76,99	0
3	ADP	E	501	27/27	0.97	0.18	55,63,87,91	0
3	ADP	H	501	27/27	0.97	0.17	55,65,93,109	0
3	ADP	J	501	27/27	0.97	0.19	53,60,79,94	0
3	ADP	L	501	27/27	0.97	0.15	59,75,90,98	0
3	ADP	I	501	27/27	0.98	0.17	45,57,81,83	0
3	ADP	G	501	27/27	0.98	0.15	56,69,102,122	0
3	ADP	K	501	27/27	0.98	0.17	55,63,86,108	0
3	ADP	A	501	27/27	0.98	0.17	50,59,74,95	0
3	ADP	F	501	27/27	0.99	0.16	48,54,74,89	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 B 501:

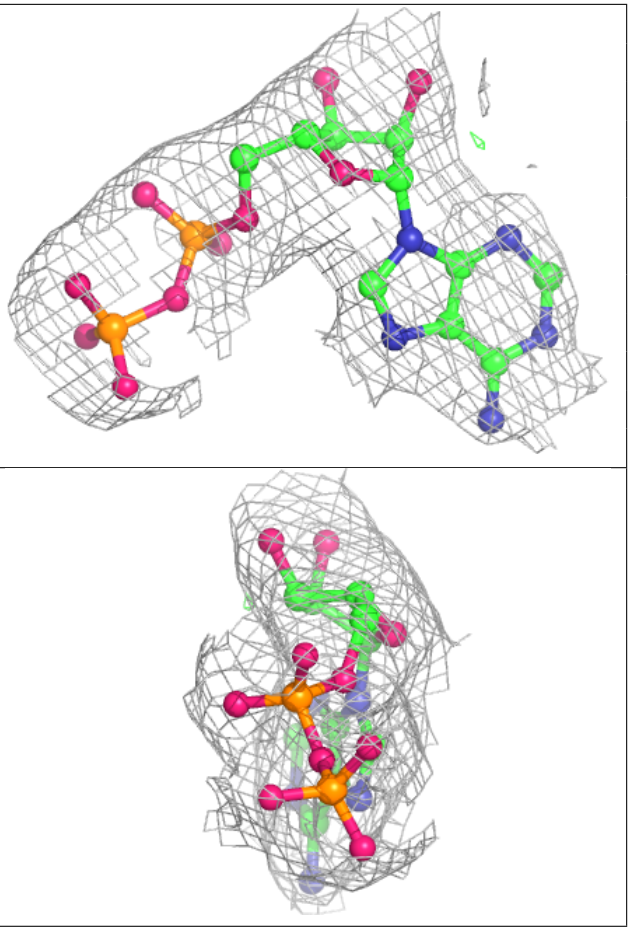
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

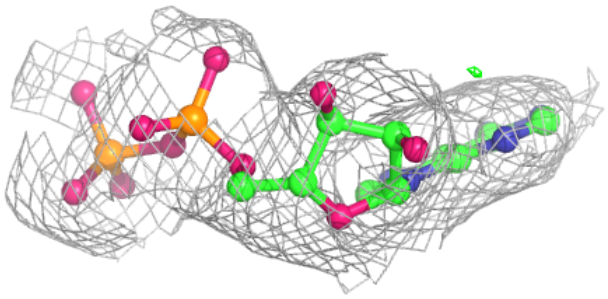




Electron density around ADP C 501:

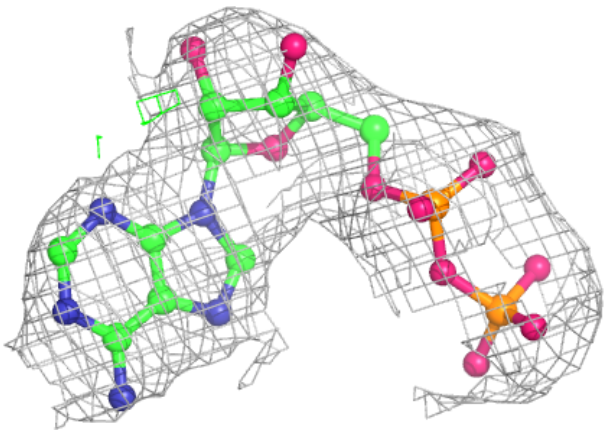
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

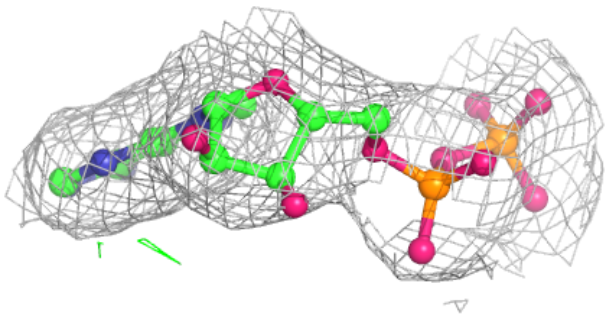


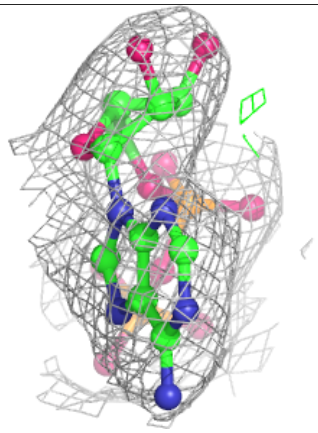


Electron density around ADP D 501:

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

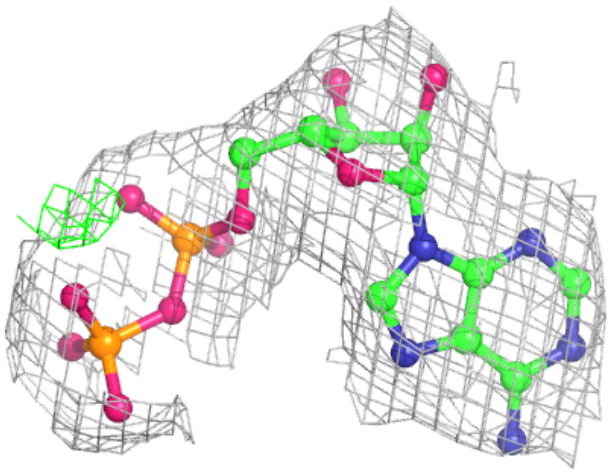


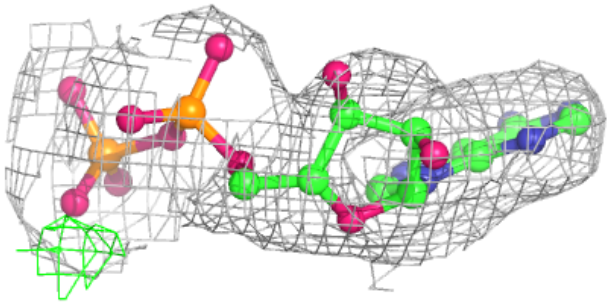


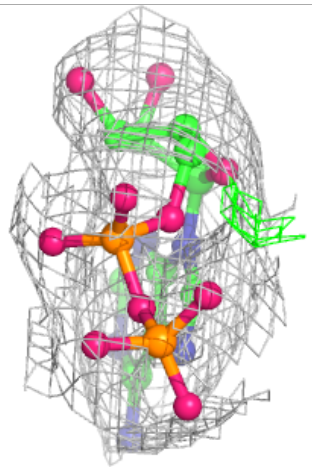


Electron density around ADP E 501:

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

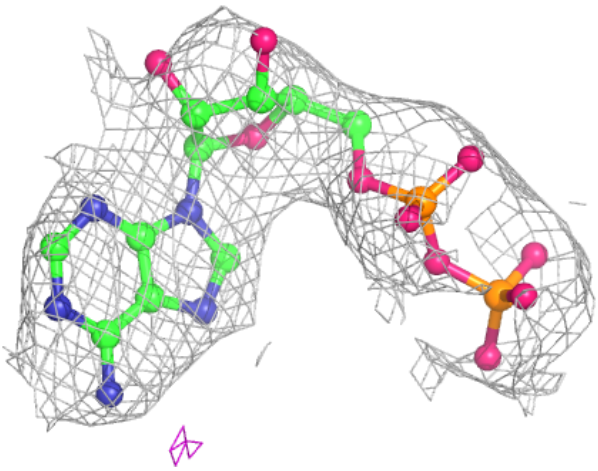


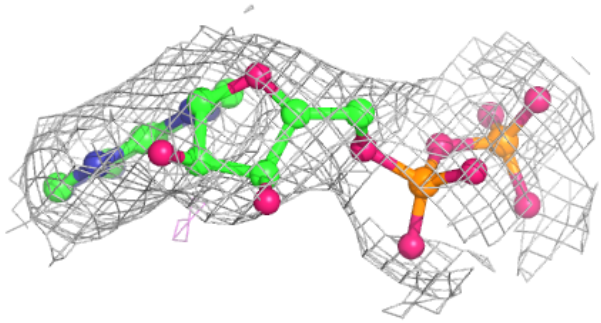


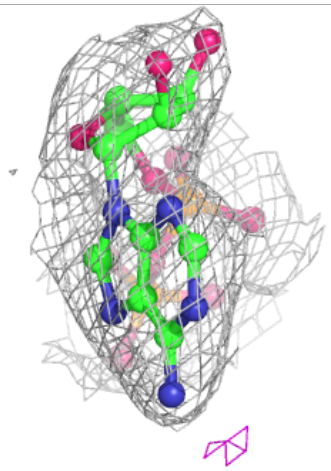


Electron density around ADP H 501:

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

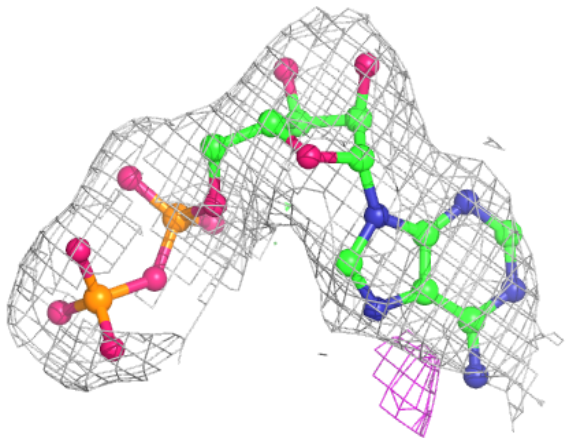


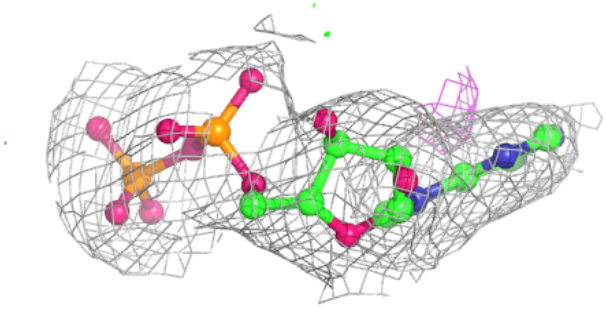


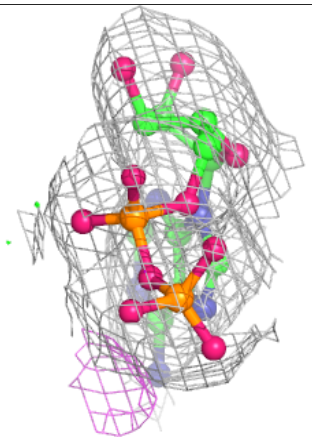


Electron density around ADP J 501:

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

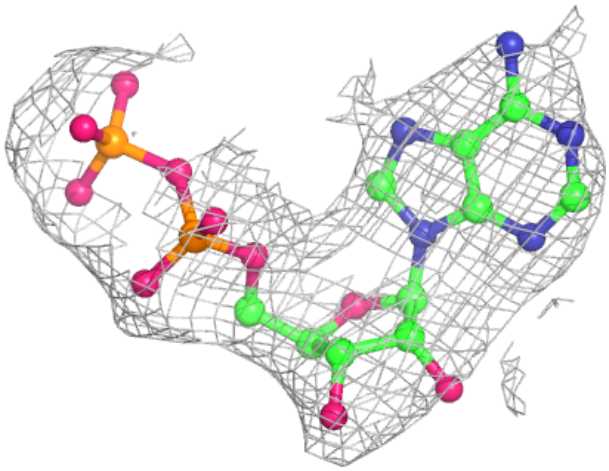


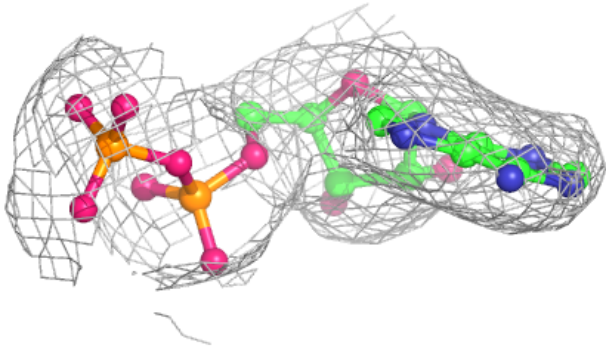


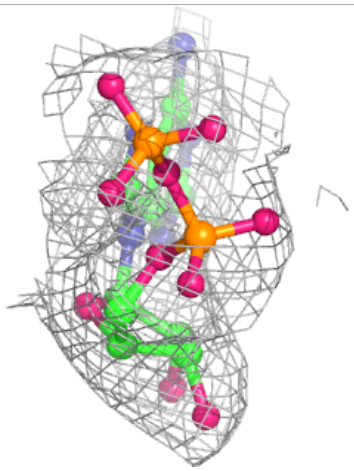


Electron density around ADP L 501:

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

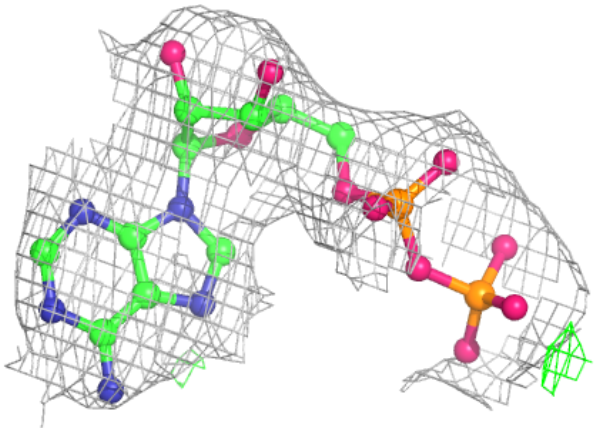


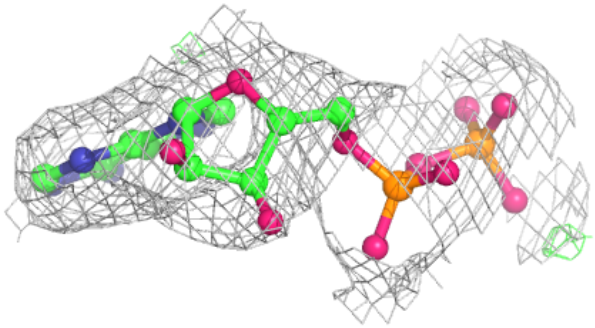


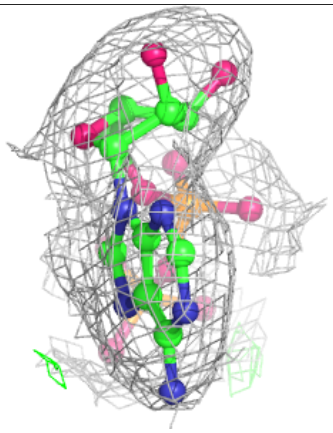


Electron density around ADP I 501:

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

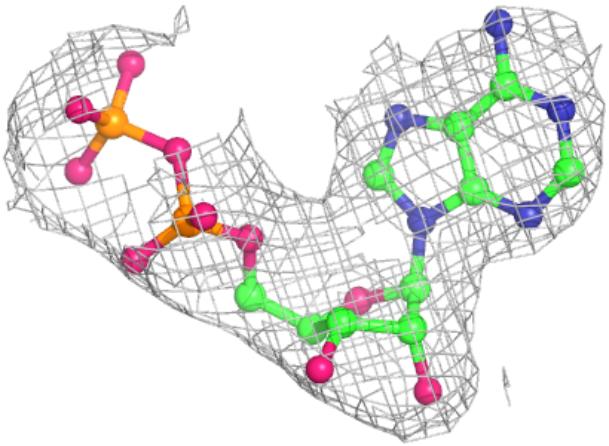


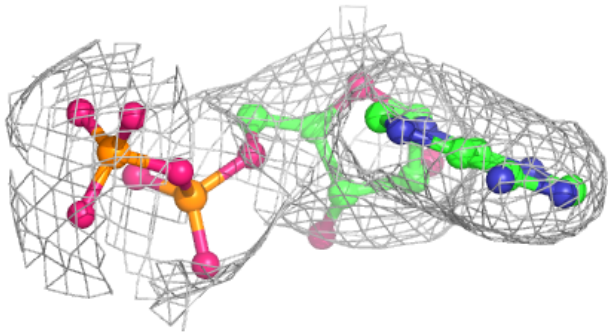


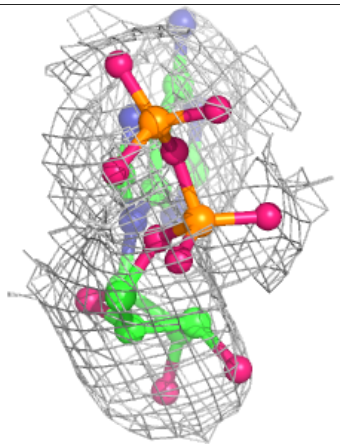


Electron density around ADP G 501:

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

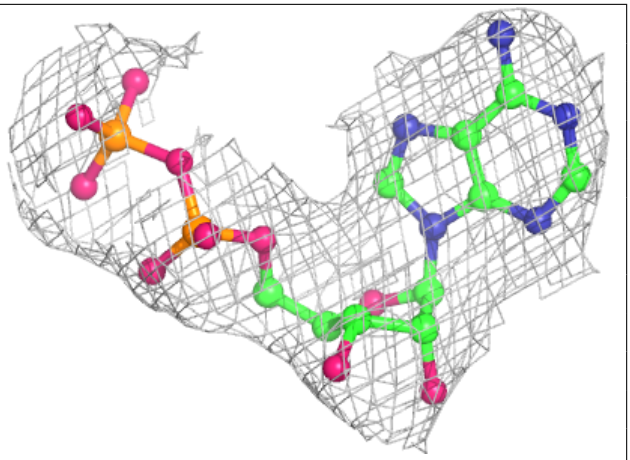


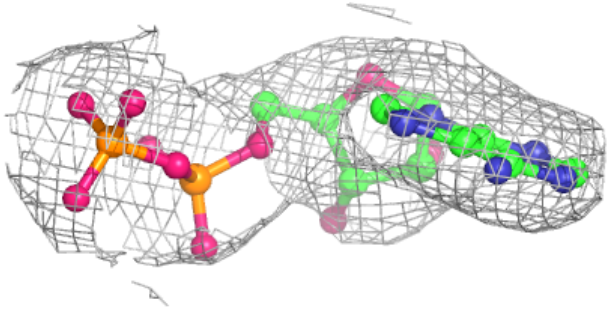


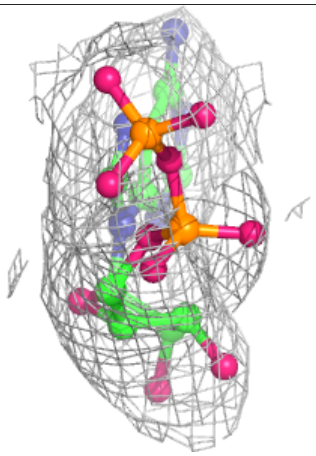


Electron density around ADP K 501:

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

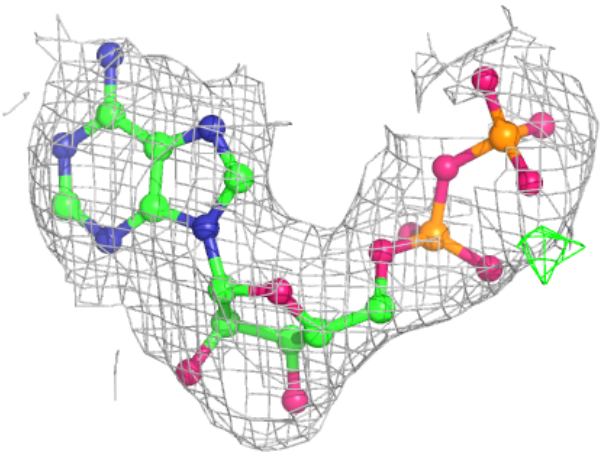


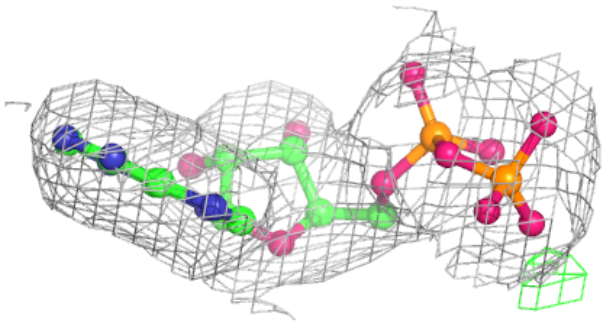


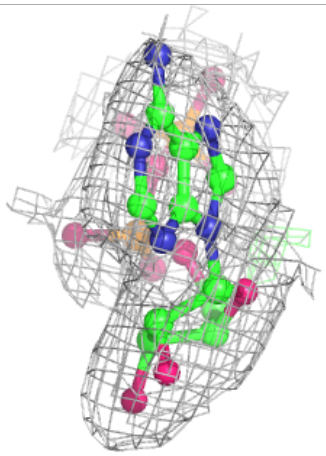


Electron density around ADP A 501:

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

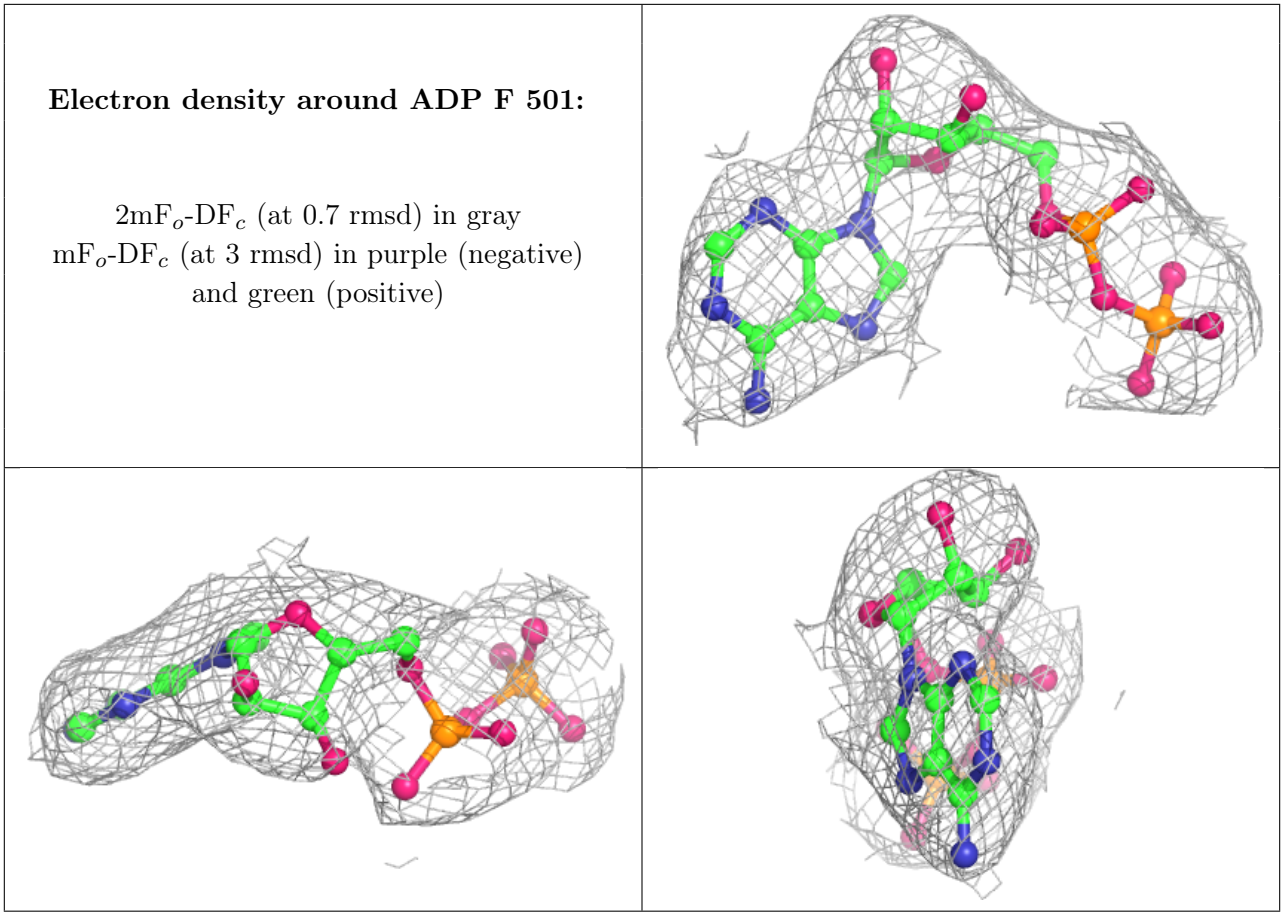






Electron density around ADP F 501:

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



6.5 Other polymers

There are no such residues in this entry.