wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 05:15 PM EDT

PDB ID	:	2AFI
Title	:	Crystal Structure of MgADP bound Av2-Av1 Complex
Authors	:	Tezcan, F.A.; Kaiser, J.T.; Mustafi, D.; Walton, M.Y.; Howard, J.B.; Rees, D.C.
Deposited on	:	2005-07-25
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:

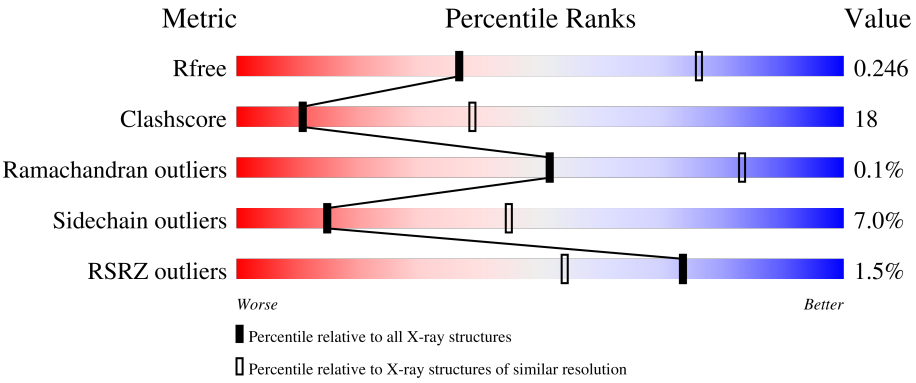
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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	491	60% 34%
1	C	491	59% 36%
1	I	491	57% 37%
1	K	491	60% 34%
2	B	522	68% 29%

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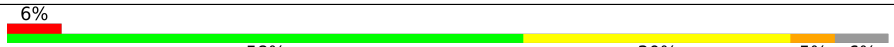
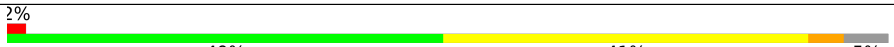
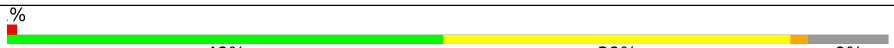
Mol	Chain	Length	Quality of chain
2	D	522	
2	J	522	
2	L	522	
3	E	289	
3	F	289	
3	G	289	
3	H	289	
3	M	289	
3	N	289	
3	O	289	
3	P	289	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 48501 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 Nitrogenase molybdenum-iron protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	31	0	0
			3782	2405	645	708	24			
1	C	476	Total	C	N	O	S	28	0	0
			3782	2405	645	708	24			
1	I	476	Total	C	N	O	S	0	0	0
			3782	2405	645	708	24			
1	K	476	Total	C	N	O	S	17	0	0
			3782	2405	645	708	24			

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	39	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	10	0	0
			4174	2666	705	775	28			
2	J	522	Total	C	N	O	S	5	0	0
			4174	2666	705	775	28			
2	L	522	Total	C	N	O	S	5	0	0
			4174	2666	705	775	28			

- Molecule 3 is a protein called Nitrogenase iron protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	271	Total	C	N	O	S	453	0	0
			2053	1283	350	400	20			
3	F	275	Total	C	N	O	S	242	0	0
			2082	1301	354	406	21			
3	G	263	Total	C	N	O	S	280	0	0
			1983	1236	342	386	19			
3	H	269	Total	C	N	O	S	1031	0	0
			2037	1271	348	398	20			

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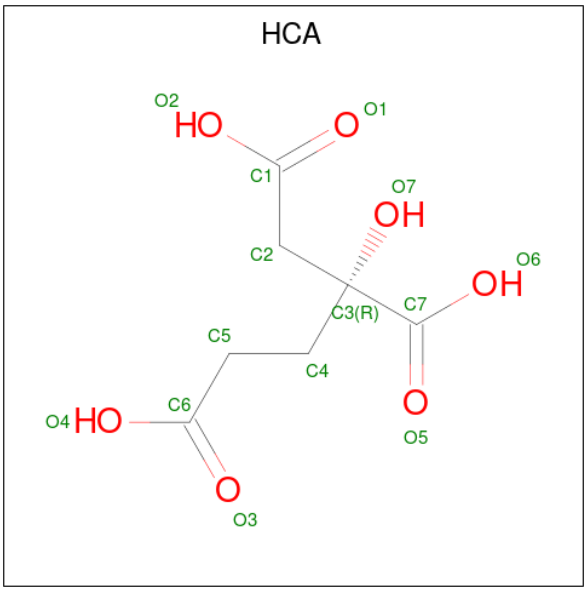
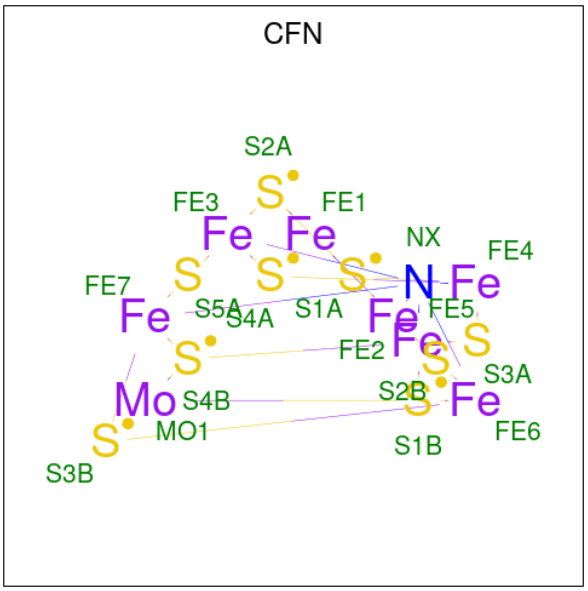
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	268	Total	C	N	O	S	458	0	0
			2029	1269	344	397	19			
3	N	270	Total	C	N	O	S	1220	0	0
			2041	1277	346	399	19			
3	O	262	Total	C	N	O	S	302	0	0
			1978	1233	341	385	19			
3	P	267	Total	C	N	O	S	868	0	0
			2018	1263	342	395	18			

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: $C_7H_{10}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	7	7		
4	C	1	Total	C	O	0	0
			14	7	7		
4	I	1	Total	C	O	0	0
			14	7	7		
4	K	1	Total	C	O	0	0
			14	7	7		

- Molecule 5 is FE(7)-MO-S(9)-N CLUSTER (three-letter code: CFN) (formula: Fe_7MoNS_9).

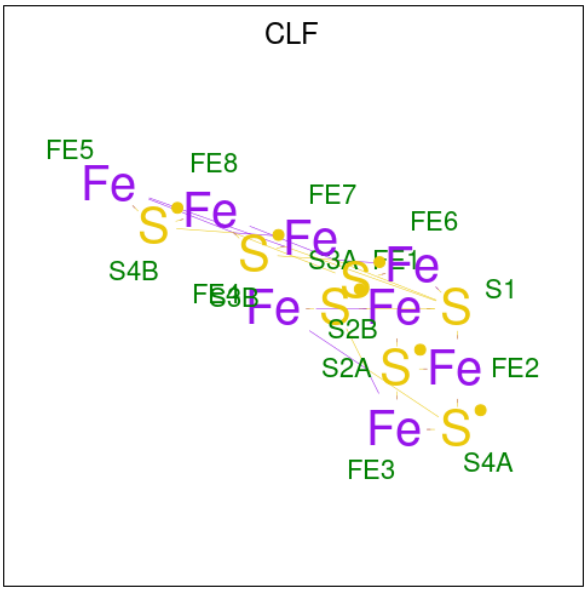


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	Fe	Mo	N	S	0	0
			18	7	1	1	9		
5	C	1	Total	Fe	Mo	N	S	0	0
			18	7	1	1	9		
5	I	1	Total	Fe	Mo	N	S	0	0
			18	7	1	1	9		
5	K	1	Total	Fe	Mo	N	S	0	0
			18	7	1	1	9		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Ca	0	0
			2	2		
6	J	1	Total	Ca	0	0
			1	1		
6	L	1	Total	Ca	0	0
			1	1		

- Molecule 7 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe_8S_7).

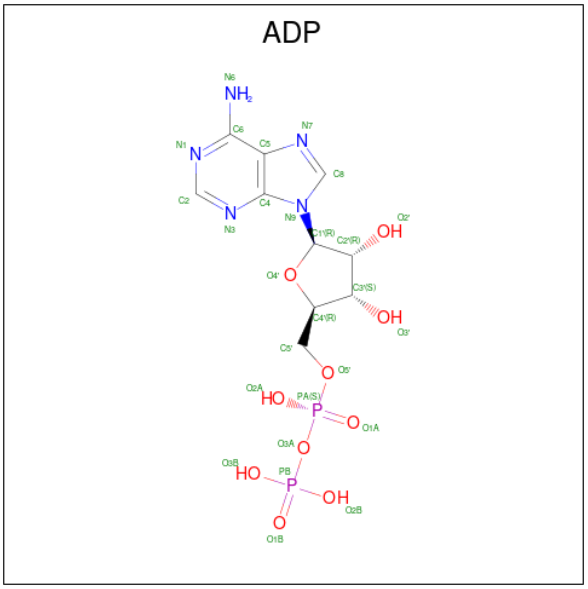


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Fe S 15 8 7	0	0
7	D	1	Total Fe S 15 8 7	0	0
7	J	1	Total Fe S 15 8 7	0	0
7	L	1	Total Fe S 15 8 7	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

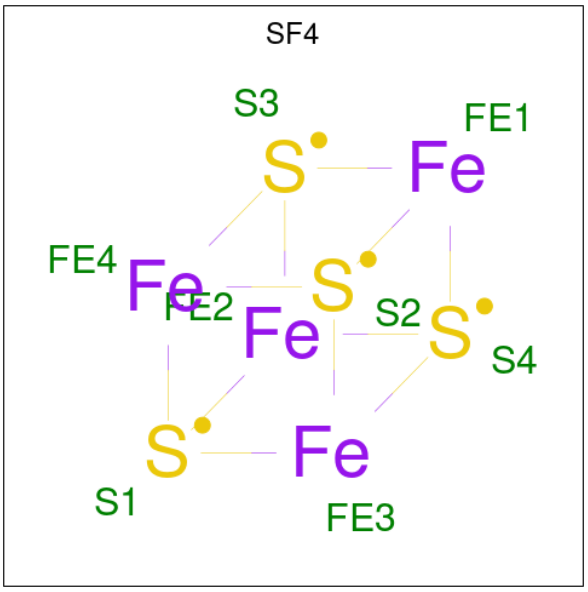
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total Mg 1 1	0	0
8	F	1	Total Mg 1 1	0	0
8	G	1	Total Mg 1 1	0	0
8	H	1	Total Mg 1 1	0	0
8	M	1	Total Mg 1 1	0	0
8	N	1	Total Mg 1 1	0	0
8	O	1	Total Mg 1 1	0	0
8	P	1	Total Mg 1 1	0	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	F	1	Total Fe S 8 4 4	0	0
10	G	1	Total Fe S 8 4 4	0	0
10	N	1	Total Fe S 8 4 4	0	0
10	P	1	Total Fe S 8 4 4	0	0

- Molecule 11 is water.

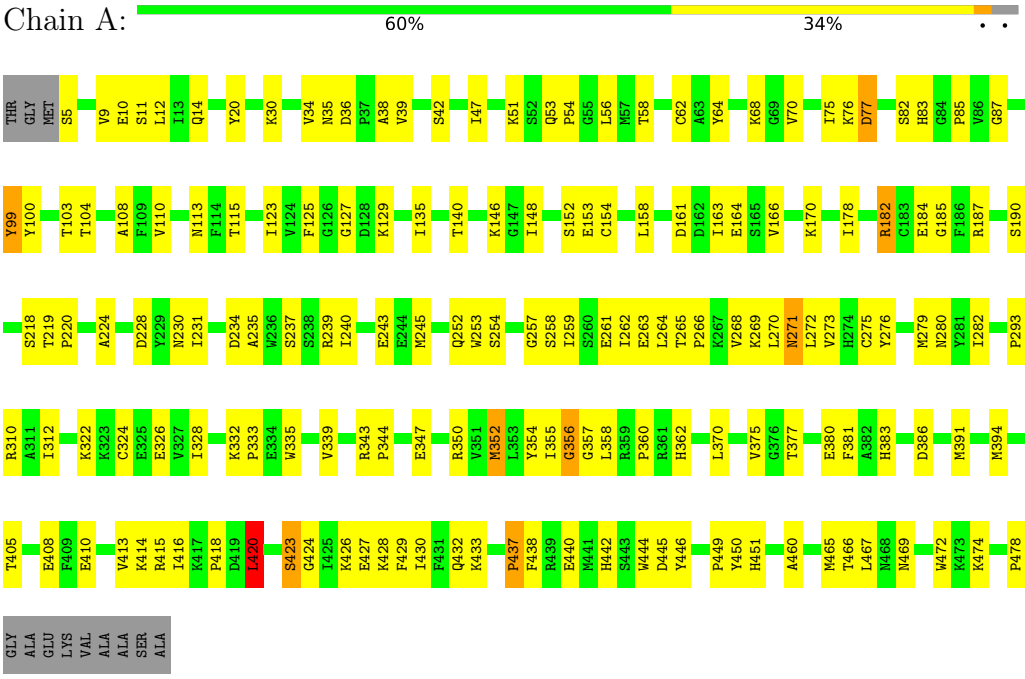
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	2	Total O 2 2	0	0
11	D	2	Total O 2 2	0	0
11	J	2	Total O 2 2	0	0
11	L	2	Total O 2 2	0	0

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.

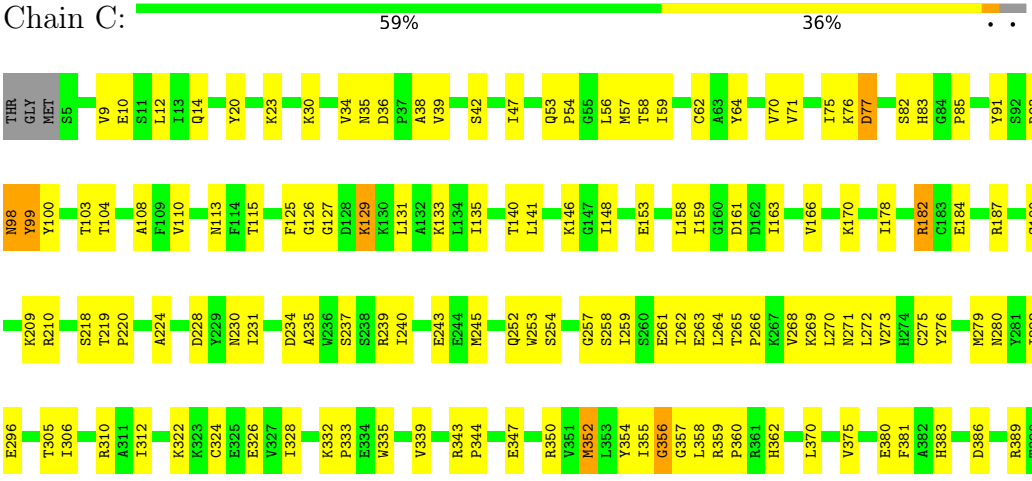
• Molecule 1: Nitrogenase molybdenum-iron protein

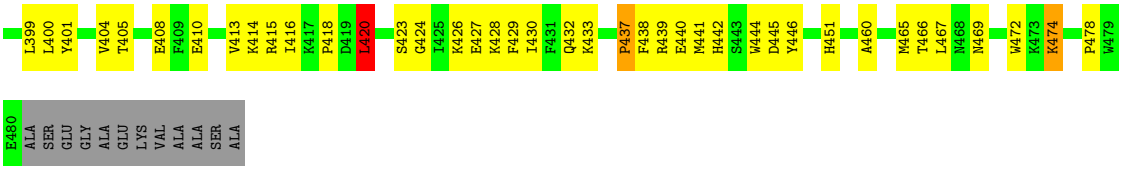
Chain A:



• Molecule 1: Nitrogenase molybdenum-iron protein

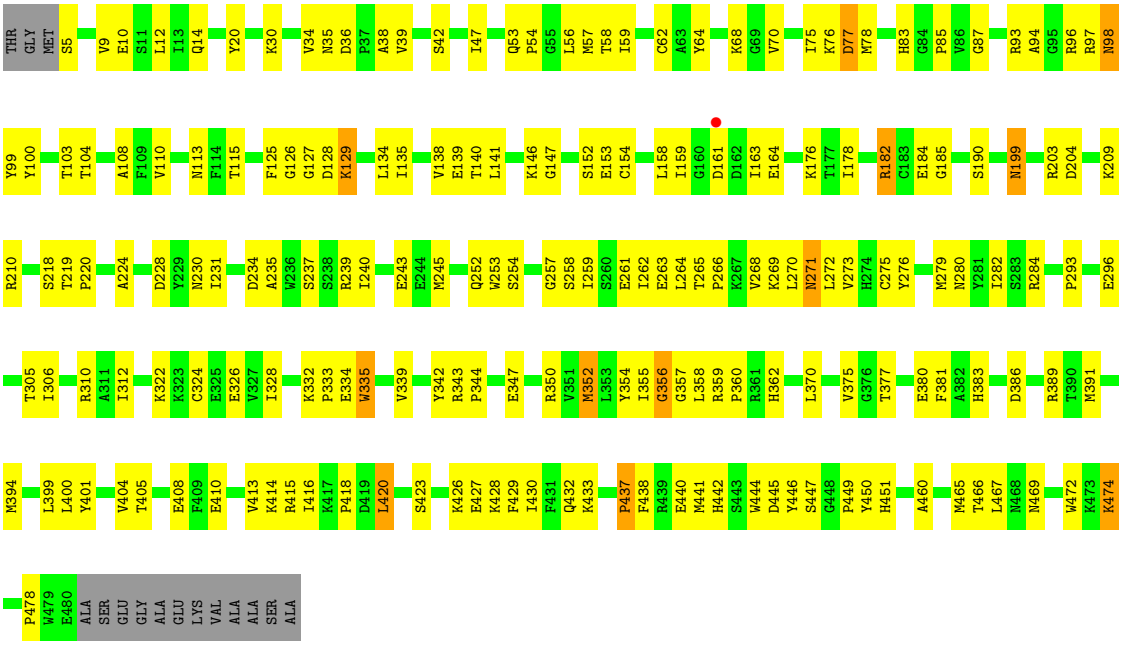
Chain C:





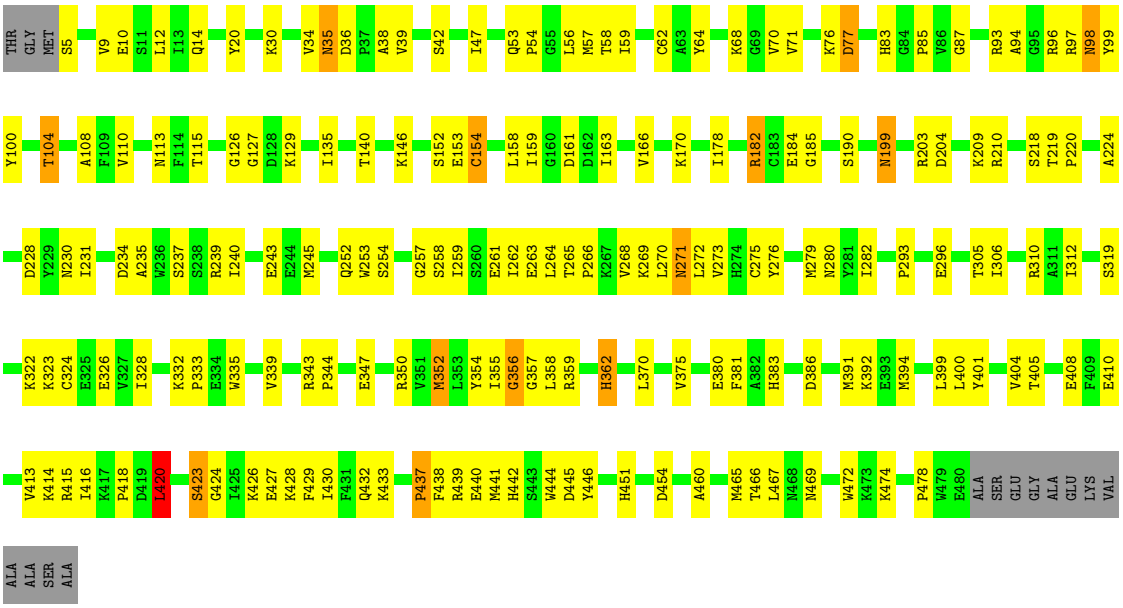
• Molecule 1: Nitrogenase molybdenum-iron protein

Chain I:



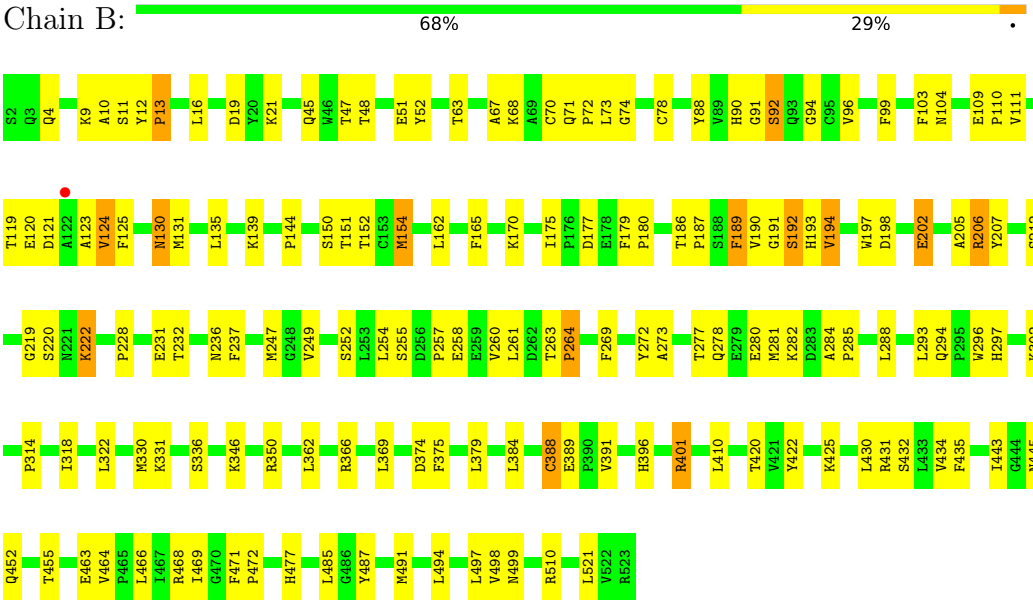
• Molecule 1: Nitrogenase molybdenum-iron protein

Chain K:



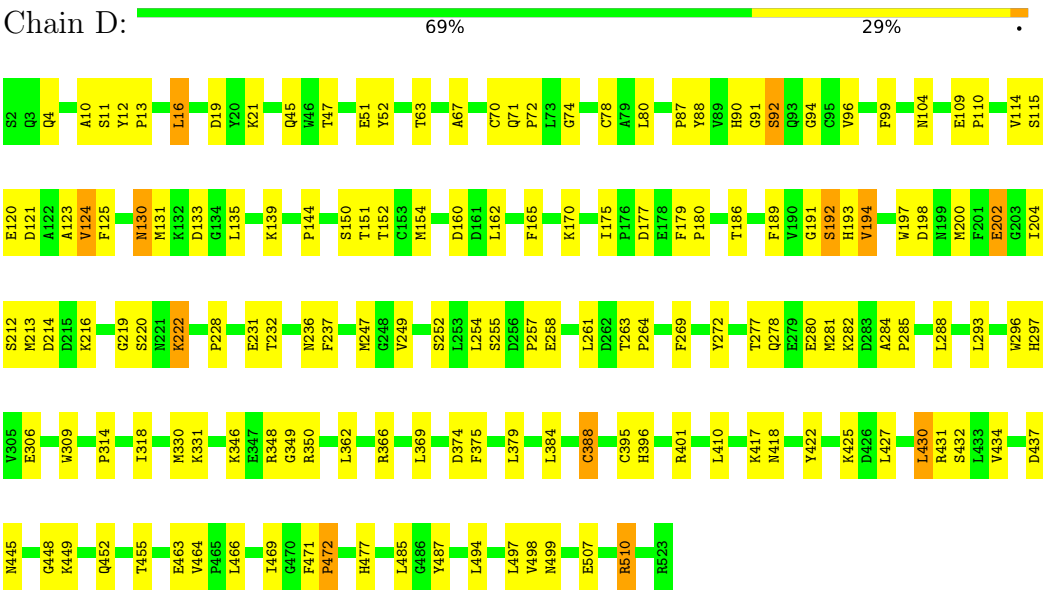
• Molecule 2: Nitrogenase molybdenum-iron protein

Chain B:



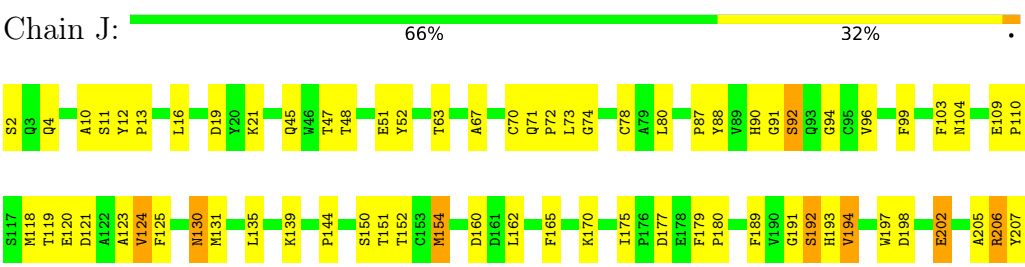
• Molecule 2: Nitrogenase molybdenum-iron protein

Chain D:



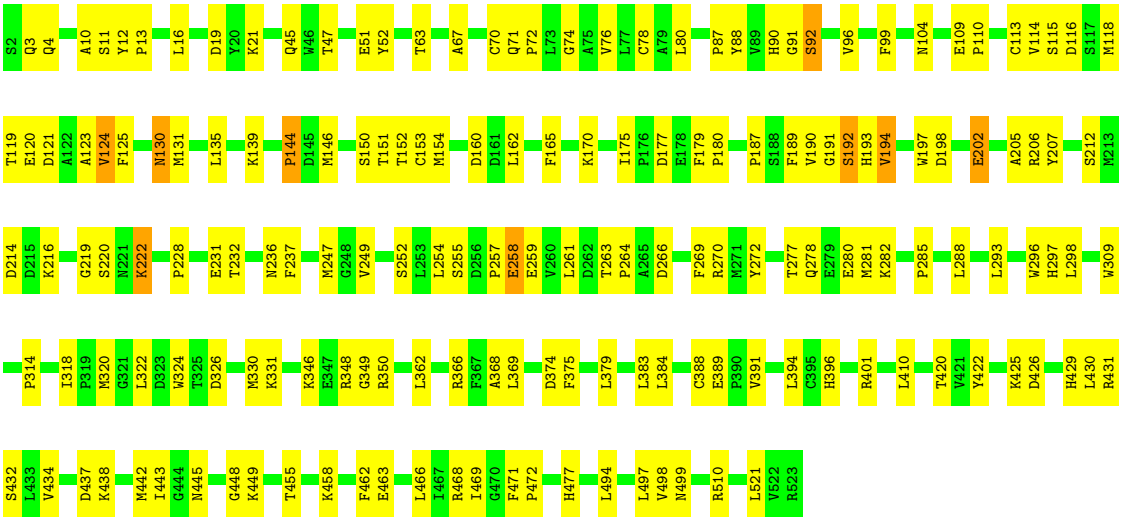
• Molecule 2: Nitrogenase molybdenum-iron protein

Chain J:



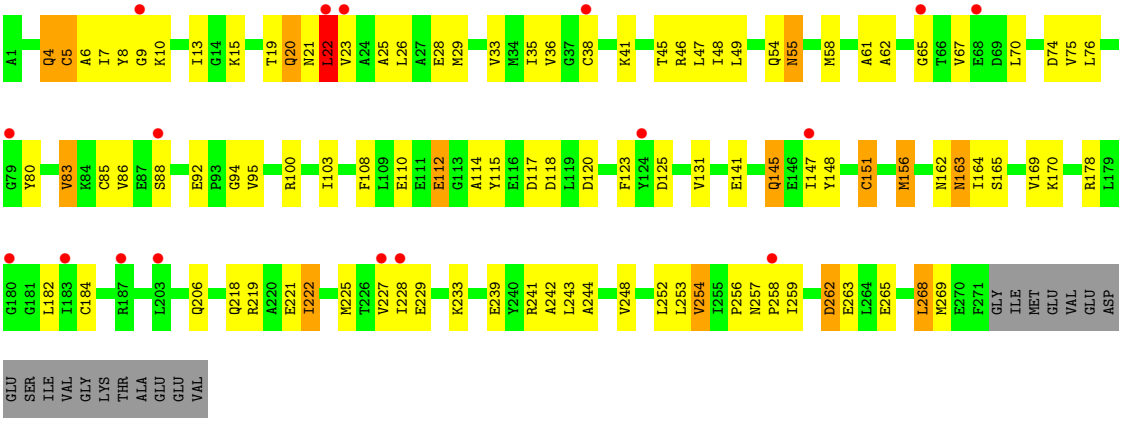
• Molecule 2: Nitrogenase molybdenum-iron protein

Chain L:



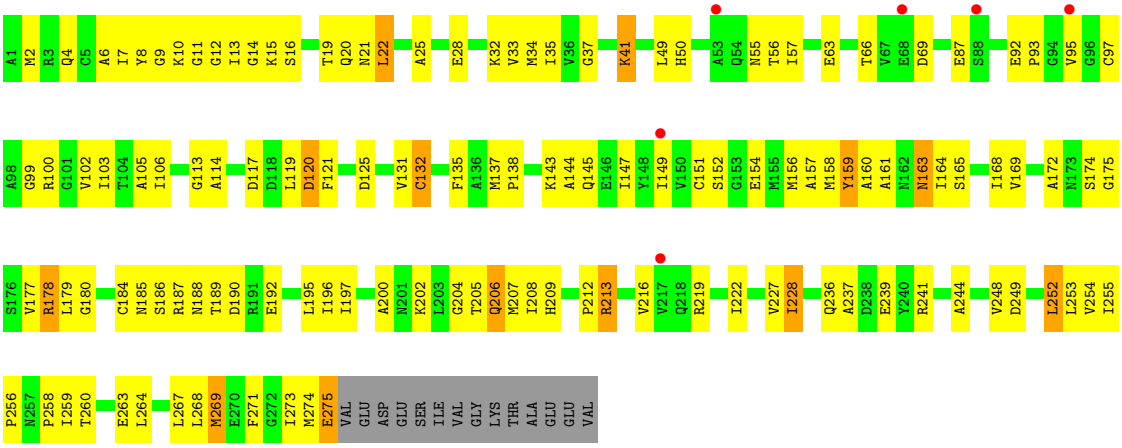
• Molecule 3: Nitrogenase iron protein 1

Chain E:



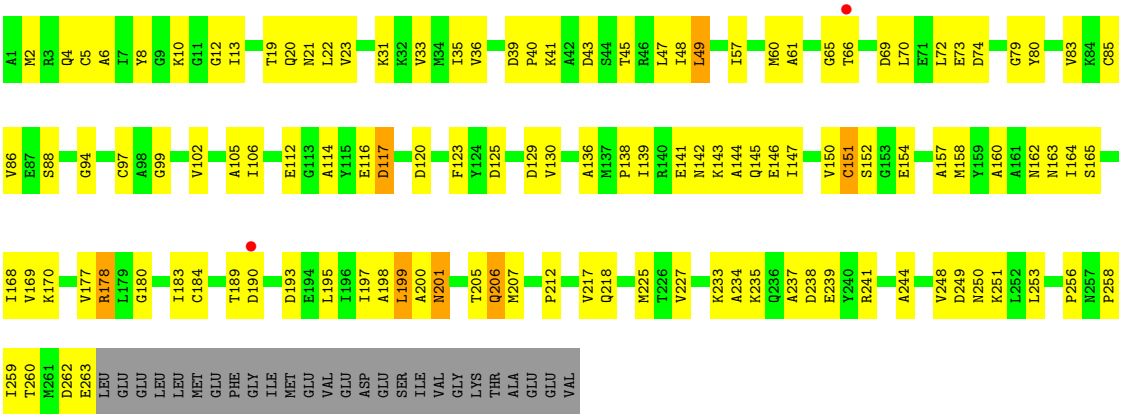
• Molecule 3: Nitrogenase iron protein 1

Chain F:



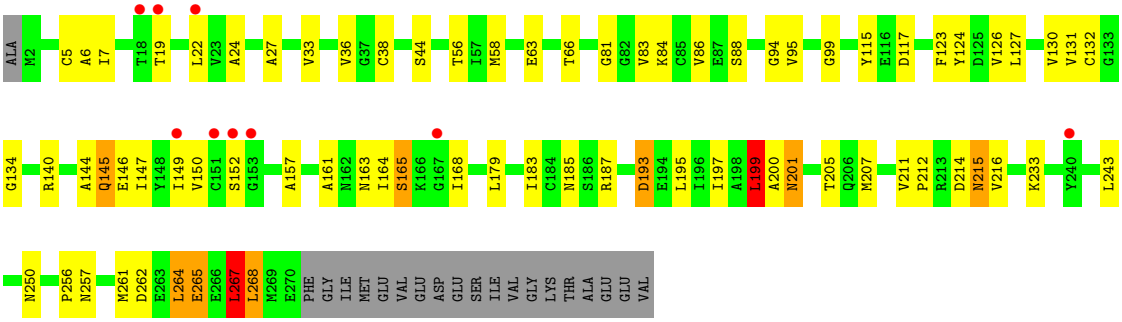
• Molecule 3: Nitrogenase iron protein 1

Chain G:



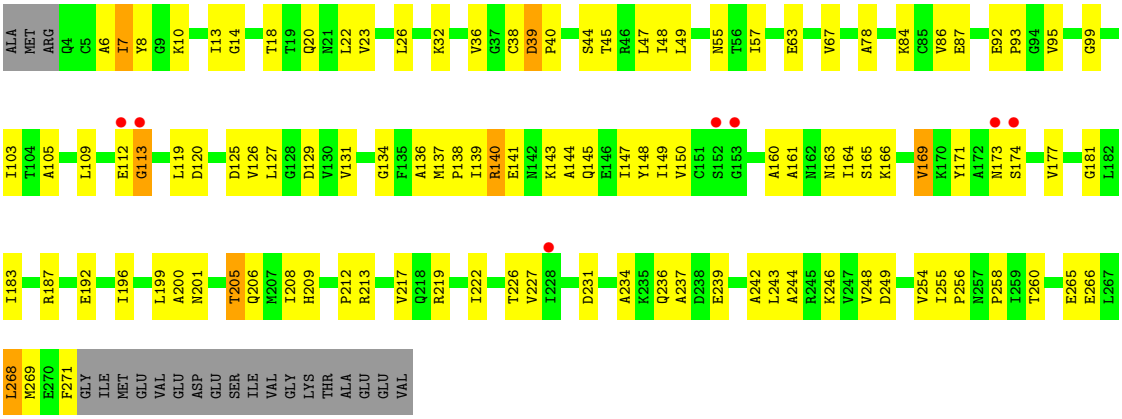
• Molecule 3: Nitrogenase iron protein 1

Chain H:



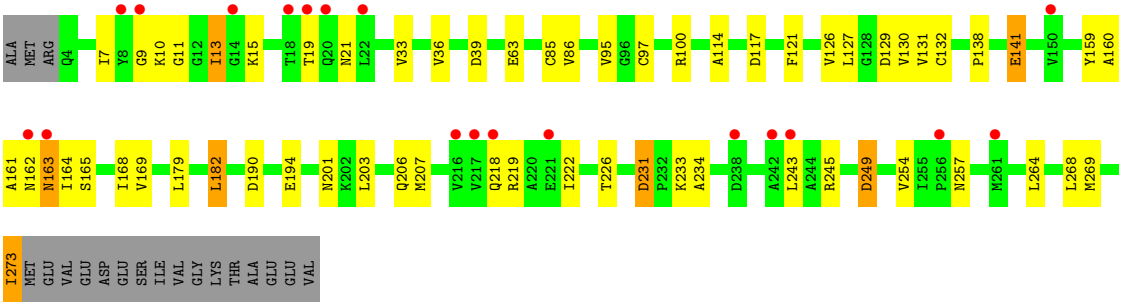
• Molecule 3: Nitrogenase iron protein 1

Chain M:



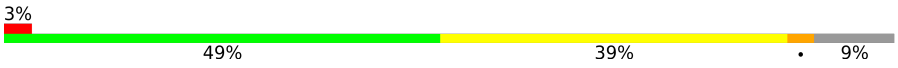
• Molecule 3: Nitrogenase iron protein 1

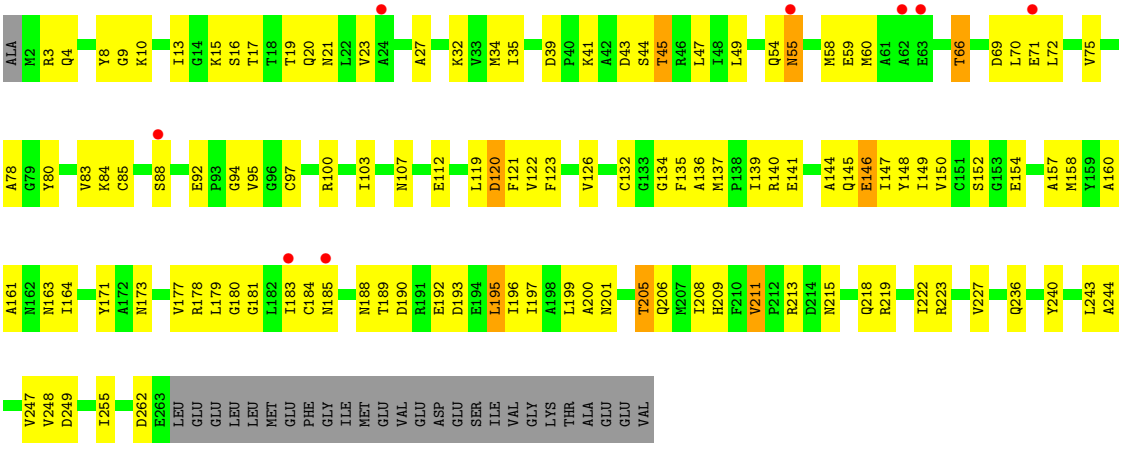
Chain N:



• Molecule 3: Nitrogenase iron protein 1

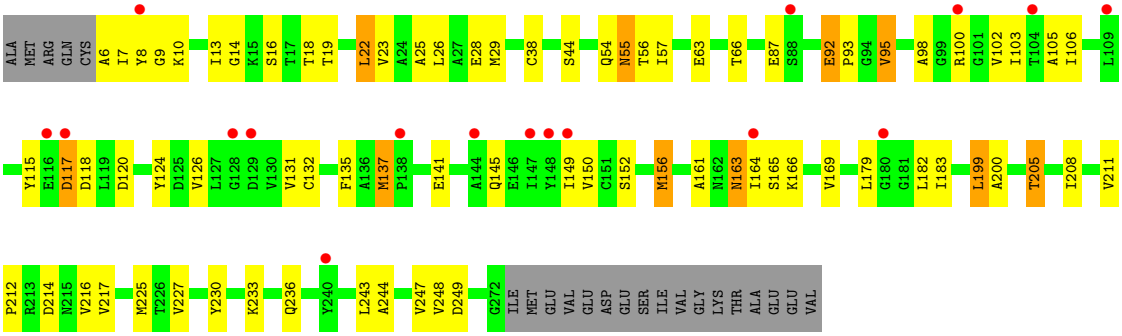
Chain O:





• Molecule 3: Nitrogenase iron protein 1

Chain P:


ALA MET ARG GLN CYS A6 I7 Y8 G9 K10 I13 G14 K15 S16 T17 T18 T19 L22 V23 A24 A25 L26 A27 E28 M29 C38 S44 Q54 N55 T56 I57 E63 T66 E87 S88 E92 P93 G94 V95 A98 G99 R100 G101 V102 I103 T104 A105 I106 L109
Y115 E116 D117 D118 L119 D120 Y124 D125 V126 L127 G128 D129 V130 V131 C132 F135 A136 M137 P138 E141 A144 Q145 E146 I147 Y148 I149 V150 G151 S152 M156 A161 N162 N163 I164 S165 K166 V169 L179 G180 G181 L182 I183 L199 A200 T206 I208 V211
P212 R213 D214 N215 V216 V217 M225 T226 V227 Y230 K233 Q236 Y240 L243 A244 V247 V248 D249 G272 ILE MET GLU VAL GLU ASP GLU SER ILE VAL GLY LYS THR ALA GLU GLU VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.92Å 141.43Å 165.55Å 73.69° 79.37° 76.58°	Depositor
Resolution (Å)	49.43 – 3.10 49.43 – 3.10	Depositor EDS
% Data completeness (in resolution range)	87.5 (49.43-3.10) 87.5 (49.43-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.270 0.207 , 0.246	Depositor DCC
R_{free} test set	10115 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 26.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.048 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	48501	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, CFN, HCA, MG, CLF, SF4, 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	0.67	0/3870	0.97	12/5219 (0.2%)
1	C	0.71	0/3870	0.97	11/5219 (0.2%)
1	I	0.67	1/3870 (0.0%)	0.98	12/5219 (0.2%)
1	K	0.68	1/3870 (0.0%)	1.11	10/5219 (0.2%)
2	B	0.78	1/4280 (0.0%)	0.97	6/5786 (0.1%)
2	D	0.76	2/4280 (0.0%)	0.96	7/5786 (0.1%)
2	J	0.77	0/4280	0.96	7/5786 (0.1%)
2	L	0.74	2/4280 (0.0%)	0.98	7/5786 (0.1%)
3	E	0.60	0/2077	1.00	5/2798 (0.2%)
3	F	0.62	0/2106	1.00	3/2836 (0.1%)
3	G	0.66	1/2006 (0.0%)	1.02	4/2703 (0.1%)
3	H	0.55	0/2060	0.98	5/2775 (0.2%)
3	M	0.59	0/2053	0.98	3/2767 (0.1%)
3	N	0.54	0/2065	0.99	8/2783 (0.3%)
3	O	0.62	0/2001	1.01	4/2696 (0.1%)
3	P	0.56	0/2042	0.98	3/2752 (0.1%)
All	All	0.68	8/49010 (0.0%)	0.99	107/66130 (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	2
1	C	0	3
1	I	0	1
1	K	0	1
2	B	0	1
2	D	0	1
2	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
3	F	0	1
All	All	0	12

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	388	CYS	CB-SG	-7.12	1.70	1.82
2	L	113	CYS	CB-SG	-6.13	1.71	1.82
3	G	151	CYS	CB-SG	-5.63	1.72	1.81
2	L	153	CYS	CB-SG	-5.61	1.72	1.81
2	D	388	CYS	CB-SG	-5.35	1.73	1.81

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	182	ARG	NE-CZ-NH1	-27.96	106.32	120.30
1	K	182	ARG	NE-CZ-NH2	26.72	133.66	120.30
2	B	510	ARG	NE-CZ-NH1	-15.74	112.43	120.30
2	L	510	ARG	NE-CZ-NH2	-14.60	113.00	120.30
1	K	182	ARG	CD-NE-CZ	14.03	143.24	123.60

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	446	TYR	Sidechain
1	A	99	TYR	Sidechain
2	B	12	TYR	Sidechain
1	C	91	TYR	Sidechain
1	C	99	TYR	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	3782	0	3720	133	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3782	0	3720	150	0
1	I	3782	0	3720	159	0
1	K	3782	0	3720	148	0
2	B	4174	0	4088	125	0
2	D	4174	0	4088	113	0
2	J	4174	0	4088	129	0
2	L	4174	0	4088	127	0
3	E	2053	0	2069	83	0
3	F	2082	0	2097	117	0
3	G	1983	0	2000	79	0
3	H	2037	0	2052	45	0
3	M	2029	0	2039	86	0
3	N	2041	0	2053	27	0
3	O	1978	0	1991	98	0
3	P	2018	0	2029	48	0
4	A	14	0	6	1	0
4	C	14	0	6	1	0
4	I	14	0	6	1	0
4	K	14	0	6	1	0
5	A	18	0	0	2	0
5	C	18	0	0	3	0
5	I	18	0	0	2	0
5	K	18	0	0	3	0
6	B	2	0	0	0	0
6	J	1	0	0	0	0
6	L	1	0	0	0	0
7	B	15	0	0	2	0
7	D	15	0	0	2	0
7	J	15	0	0	2	0
7	L	15	0	0	2	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
8	O	1	0	0	0	0
8	P	1	0	0	0	0
9	E	27	0	12	0	0
9	F	27	0	12	4	0
9	G	27	0	12	1	0
9	H	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	M	27	0	12	2	0
9	N	27	0	12	0	0
9	O	27	0	12	0	0
9	P	27	0	12	1	0
10	F	8	0	0	1	0
10	G	8	0	0	0	0
10	N	8	0	0	0	0
10	P	8	0	0	0	0
11	B	2	0	0	0	0
11	D	2	0	0	0	0
11	J	2	0	0	0	0
11	L	2	0	0	0	0
All	All	48501	0	47682	1542	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 18.

The worst 5 of 1542 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:I:356:GLY:HA2	1:I:380:GLU:HB2	1.42	1.02
1:C:356:GLY:HA2	1:C:380:GLU:HB2	1.36	1.00
1:K:356:GLY:HA2	1:K:380:GLU:HB2	1.40	1.00
1:I:129:LYS:H	1:I:129:LYS:HD2	1.27	0.97
2:B:499:ASN:HD21	2:D:477:HIS:H	1.09	0.95

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	474/491 (96%)	467 (98%)	6 (1%)	1 (0%)	47 79
1	C	474/491 (96%)	467 (98%)	6 (1%)	1 (0%)	47 79
1	I	474/491 (96%)	467 (98%)	6 (1%)	1 (0%)	47 79
1	K	474/491 (96%)	467 (98%)	6 (1%)	1 (0%)	47 79
2	B	520/522 (100%)	514 (99%)	6 (1%)	0	100 100
2	D	520/522 (100%)	514 (99%)	6 (1%)	0	100 100
2	J	520/522 (100%)	514 (99%)	6 (1%)	0	100 100
2	L	520/522 (100%)	513 (99%)	7 (1%)	0	100 100
3	E	269/289 (93%)	268 (100%)	1 (0%)	0	100 100
3	F	273/289 (94%)	270 (99%)	3 (1%)	0	100 100
3	G	261/289 (90%)	259 (99%)	2 (1%)	0	100 100
3	H	267/289 (92%)	265 (99%)	2 (1%)	0	100 100
3	M	266/289 (92%)	264 (99%)	2 (1%)	0	100 100
3	N	268/289 (93%)	267 (100%)	1 (0%)	0	100 100
3	O	260/289 (90%)	259 (100%)	1 (0%)	0	100 100
3	P	265/289 (92%)	264 (100%)	1 (0%)	0	100 100
All	All	6105/6364 (96%)	6039 (99%)	62 (1%)	4 (0%)	51 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	357	GLY
1	A	357	GLY
1	K	357	GLY
1	I	357	GLY

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	406/414 (98%)	386 (95%)	20 (5%)	25 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	406/414 (98%)	389 (96%)	17 (4%)	30 62
1	I	406/414 (98%)	389 (96%)	17 (4%)	30 62
1	K	406/414 (98%)	386 (95%)	20 (5%)	25 57
2	B	454/454 (100%)	428 (94%)	26 (6%)	20 52
2	D	454/454 (100%)	429 (94%)	25 (6%)	21 53
2	J	454/454 (100%)	429 (94%)	25 (6%)	21 53
2	L	454/454 (100%)	430 (95%)	24 (5%)	22 54
3	E	218/233 (94%)	192 (88%)	26 (12%)	5 20
3	F	221/233 (95%)	202 (91%)	19 (9%)	10 37
3	G	210/233 (90%)	187 (89%)	23 (11%)	6 25
3	H	217/233 (93%)	192 (88%)	25 (12%)	5 22
3	M	216/233 (93%)	194 (90%)	22 (10%)	7 27
3	N	217/233 (93%)	193 (89%)	24 (11%)	6 24
3	O	210/233 (90%)	188 (90%)	22 (10%)	7 26
3	P	214/233 (92%)	189 (88%)	25 (12%)	5 22
All	All	5163/5336 (97%)	4803 (93%)	360 (7%)	15 45

5 of 360 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	218	SER
3	M	266	GLU
1	K	401	TYR
2	L	252	SER
3	N	194	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	14	GLN
3	P	215	ASN
2	J	499	ASN
3	P	201	ASN
3	O	21	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)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
9	ADP	G	3292	8	24,29,29	1.41	4 (16%)	29,45,45	1.70	6 (20%)
7	CLF	J	5498	1,2	0,24,24	-	-	-		
10	SF4	P	7290	3	0,12,12	-	-	-		
7	CLF	D	3498	1,2	0,24,24	-	-	-		
9	ADP	F	2292	8	24,29,29	1.05	1 (4%)	29,45,45	1.61	5 (17%)
7	CLF	L	7498	1,2	0,24,24	-	-	-		
9	ADP	N	6292	8	24,29,29	1.18	1 (4%)	29,45,45	1.79	7 (24%)
5	CFN	C	496	1	18,30,30	3.26	12 (66%)	-		
5	CFN	I	496	1	18,30,30	2.77	12 (66%)	-		
10	SF4	G	3290	3	0,12,12	-	-	-		
4	HCA	K	494	-	13,13,13	4.19	5 (38%)	14,18,18	1.53	4 (28%)
4	HCA	C	494	-	13,13,13	3.18	5 (38%)	14,18,18	1.58	4 (28%)
9	ADP	M	5292	8	24,29,29	1.10	1 (4%)	29,45,45	1.68	6 (20%)
9	ADP	P	8292	8	24,29,29	1.17	2 (8%)	29,45,45	1.73	6 (20%)
9	ADP	E	1292	-	24,29,29	1.03	1 (4%)	29,45,45	1.72	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	ADP	O	7292	8	24,29,29	1.23	2 (8%)	29,45,45	1.71	5 (17%)
9	ADP	H	4292	-	24,29,29	1.22	1 (4%)	29,45,45	1.82	6 (20%)
10	SF4	N	5290	3	0,12,12	-	-	-		
7	CLF	B	1498	1,2	0,24,24	-	-	-		
4	HCA	A	494	-	13,13,13	4.00	4 (30%)	14,18,18	1.40	2 (14%)
10	SF4	F	1290	3	0,12,12	-	-	-		
5	CFN	K	496	1	18,30,30	3.01	9 (50%)	-		
5	CFN	A	496	1	18,30,30	2.46	9 (50%)	-		
4	HCA	I	494	-	13,13,13	4.27	4 (30%)	14,18,18	1.32	3 (21%)

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
9	ADP	G	3292	8	-	0/12/32/32	0/3/3/3
7	CLF	J	5498	1,2	-	-	0/12/10/10
10	SF4	P	7290	3	-	-	0/6/5/5
7	CLF	D	3498	1,2	-	-	0/12/10/10
9	ADP	F	2292	8	-	7/12/32/32	0/3/3/3
9	ADP	N	6292	8	-	4/12/32/32	0/3/3/3
7	CLF	L	7498	1,2	-	-	0/12/10/10
10	SF4	G	3290	3	-	-	0/6/5/5
4	HCA	K	494	-	-	9/17/17/17	-
4	HCA	C	494	-	-	9/17/17/17	-
9	ADP	M	5292	8	-	3/12/32/32	0/3/3/3
9	ADP	P	8292	8	-	6/12/32/32	0/3/3/3
9	ADP	E	1292	-	-	2/12/32/32	0/3/3/3
9	ADP	O	7292	8	-	2/12/32/32	0/3/3/3
10	SF4	N	5290	3	-	-	0/6/5/5
9	ADP	H	4292	-	-	3/12/32/32	0/3/3/3
7	CLF	B	1498	1,2	-	-	0/12/10/10
4	HCA	A	494	-	-	8/17/17/17	-
10	SF4	F	1290	3	-	-	0/6/5/5
4	HCA	I	494	-	-	8/17/17/17	-

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	494	HCA	C3-C7	-12.97	1.39	1.53
4	A	494	HCA	C3-C7	-11.44	1.41	1.53
4	K	494	HCA	C3-C7	-10.78	1.42	1.53
4	K	494	HCA	C4-C3	-6.93	1.42	1.54
4	C	494	HCA	C3-C7	-6.37	1.46	1.53

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	6292	ADP	C5-C6-N6	4.76	127.59	120.35
9	M	5292	ADP	C5-C6-N6	4.72	127.52	120.35
9	O	7292	ADP	C5-C6-N6	4.71	127.52	120.35
9	H	4292	ADP	C5-C6-N6	4.67	127.44	120.35
9	G	3292	ADP	C5-C6-N6	4.65	127.41	120.35

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	494	HCA	C2-C3-C4-C5
4	A	494	HCA	C7-C3-C4-C5
4	A	494	HCA	O7-C3-C4-C5
4	C	494	HCA	C2-C3-C4-C5
4	C	494	HCA	C7-C3-C4-C5

There are no ring outliers.

17 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	G	3292	ADP	1	0
7	J	5498	CLF	2	0
7	D	3498	CLF	2	0
9	F	2292	ADP	4	0
7	L	7498	CLF	2	0
5	C	496	CFN	3	0
5	I	496	CFN	2	0
4	K	494	HCA	1	0
4	C	494	HCA	1	0
9	M	5292	ADP	2	0
9	P	8292	ADP	1	0
7	B	1498	CLF	2	0
4	A	494	HCA	1	0

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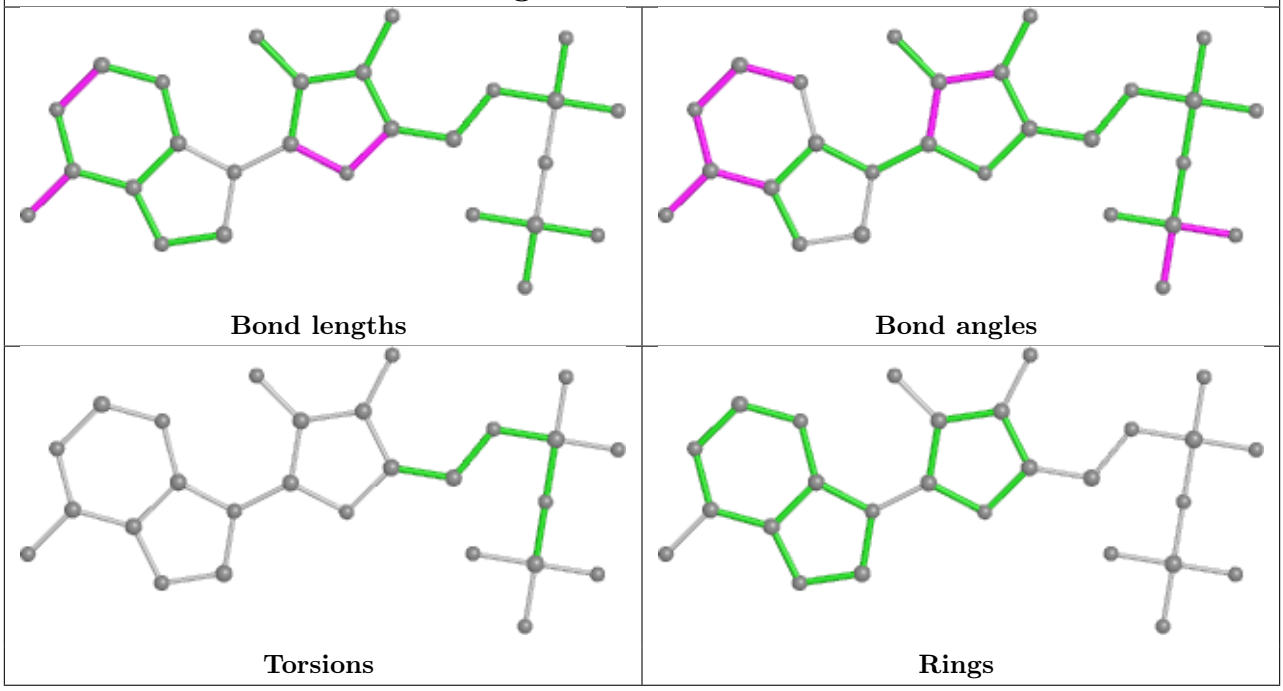
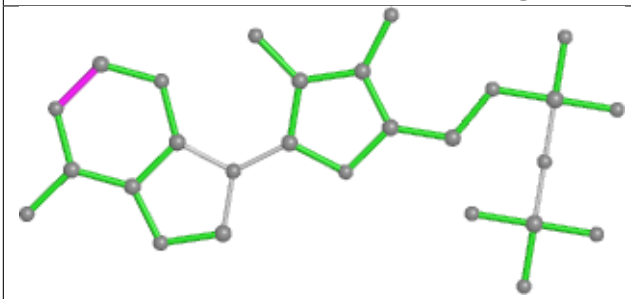
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	1290	SF4	1	0
5	K	496	CFN	3	0
5	A	496	CFN	2	0
4	I	494	HCA	1	0

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.

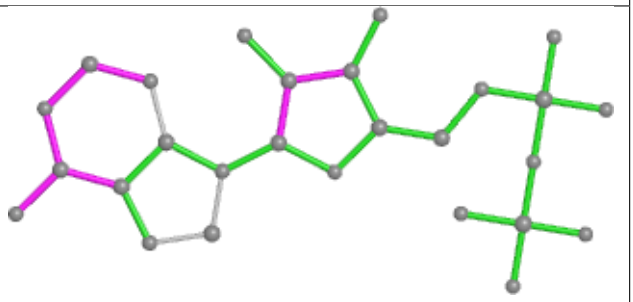
Ligand ADP G 3292



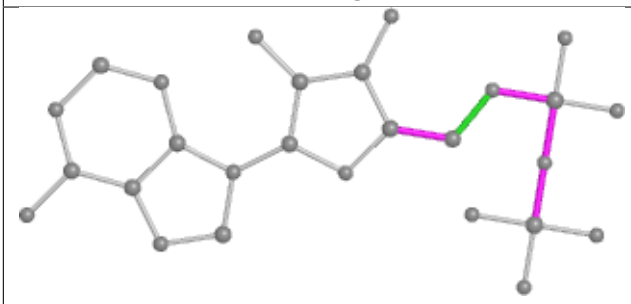
Ligand ADP F 2292



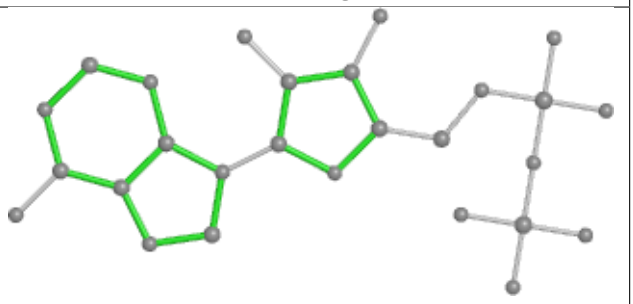
Bond lengths



Bond angles

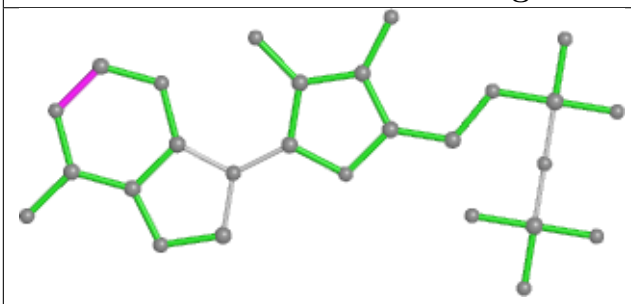


Torsions

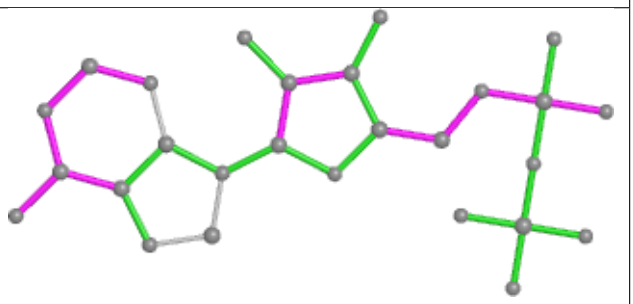


Rings

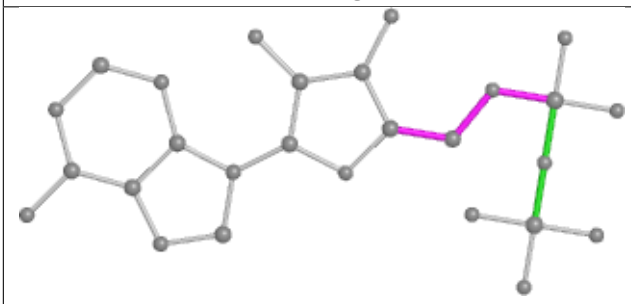
Ligand ADP N 6292



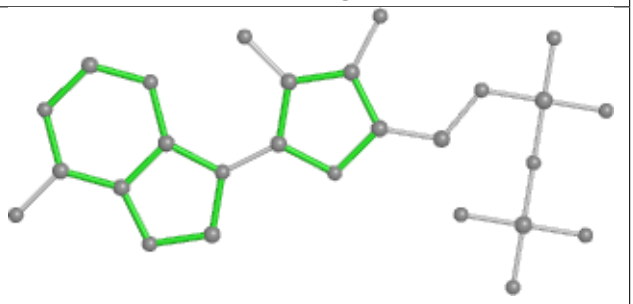
Bond lengths



Bond angles

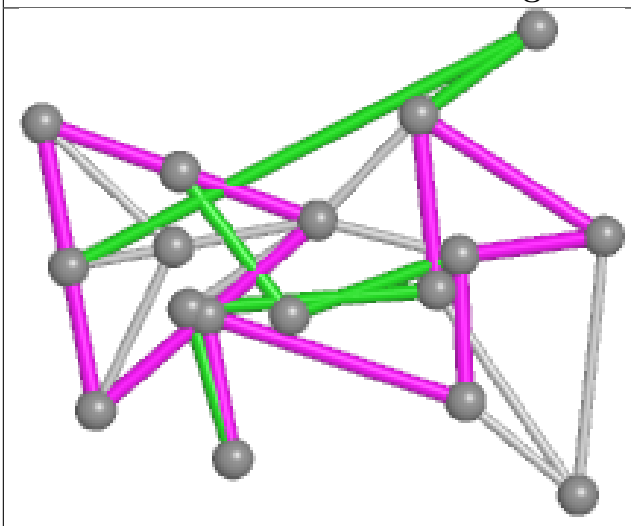


Torsions

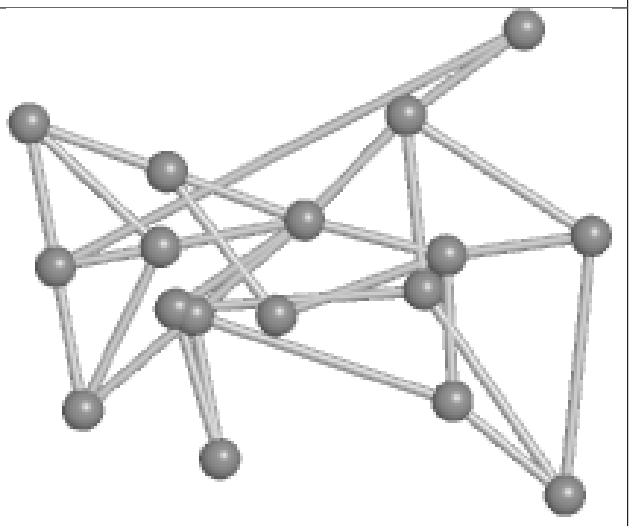


Rings

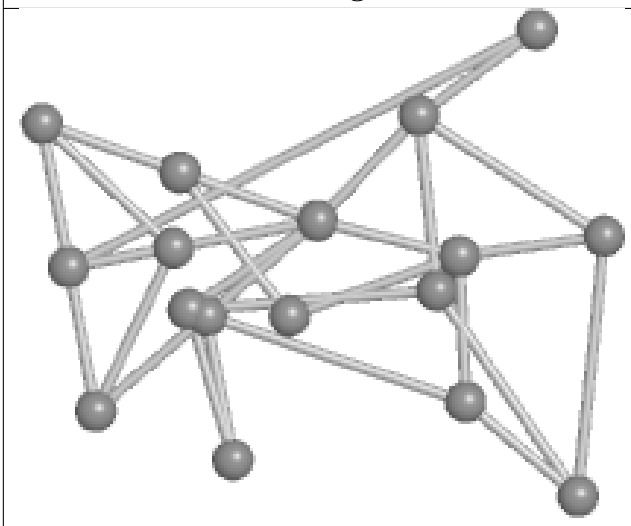
Ligand CFN C 496



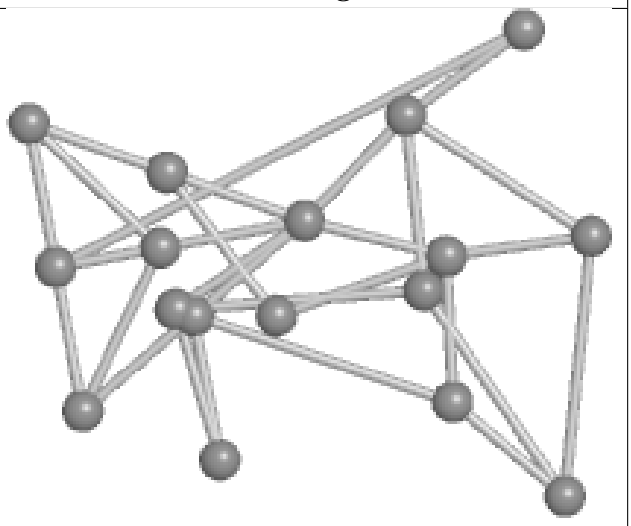
Bond lengths



Bond angles

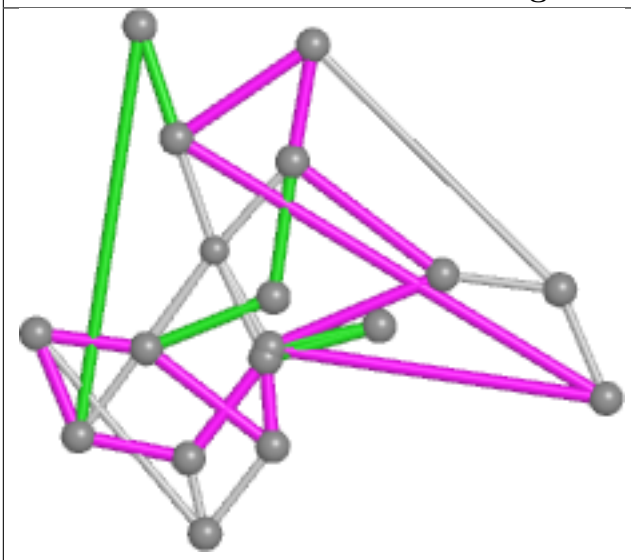


Torsions



Rings

Ligand CFN I 496



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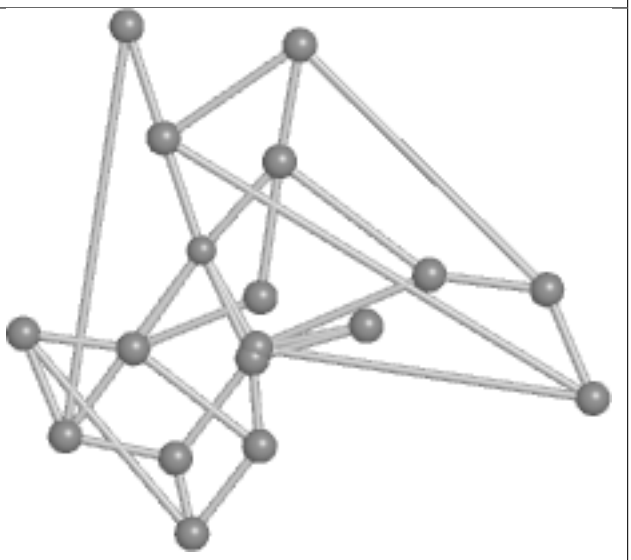
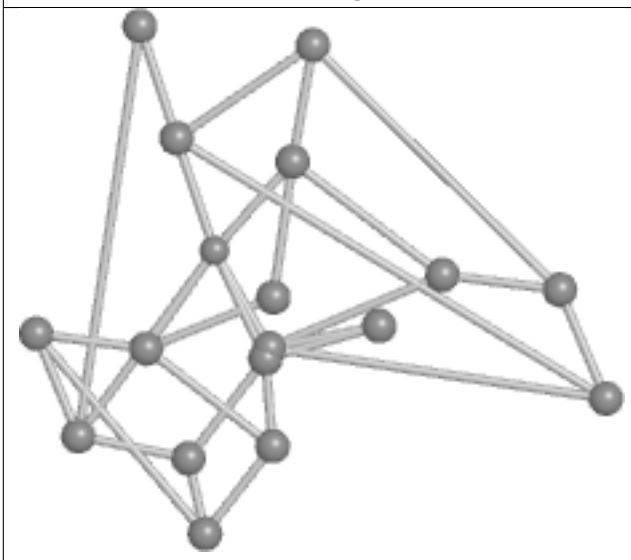
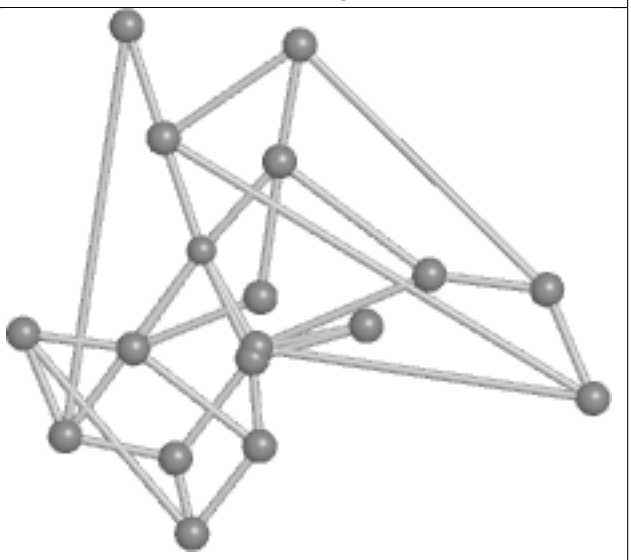


Bond angles

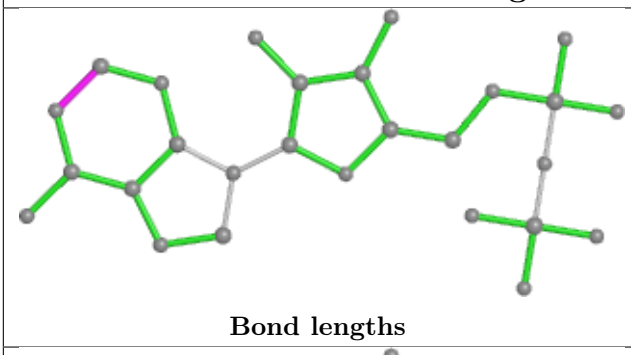


Torsions



Rings

Ligand ADP M 5292



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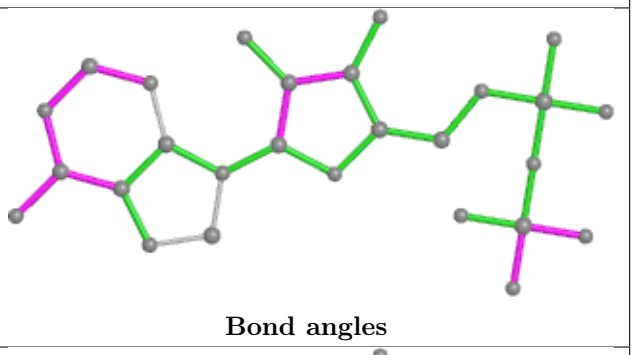
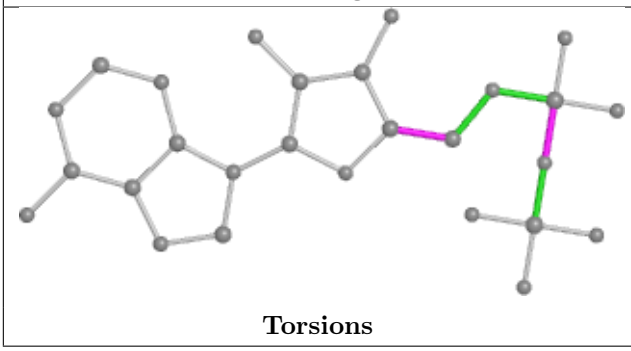
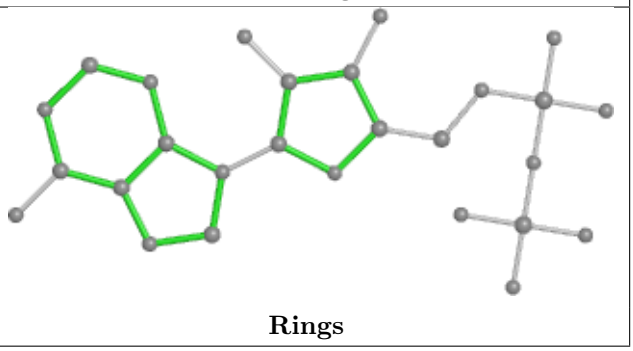


Bond angles

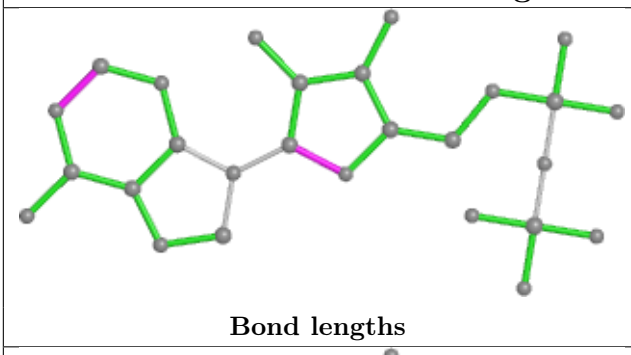


Torsions

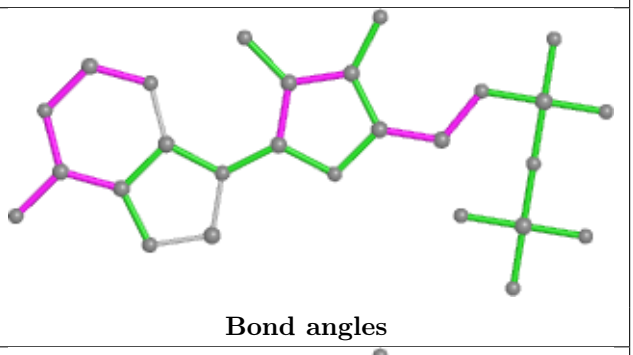


Rings

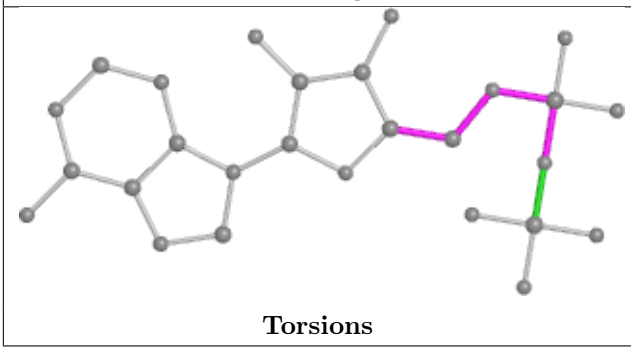
Ligand ADP P 8292



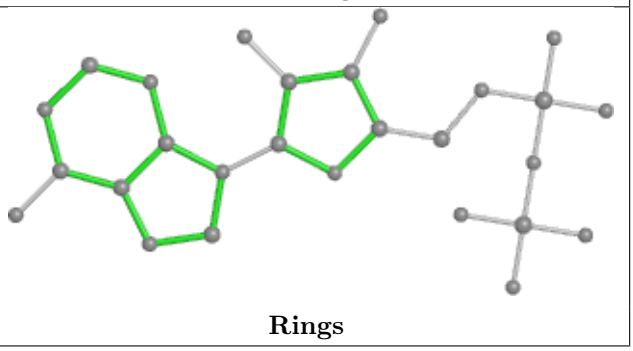
Bond lengths



Bond angles

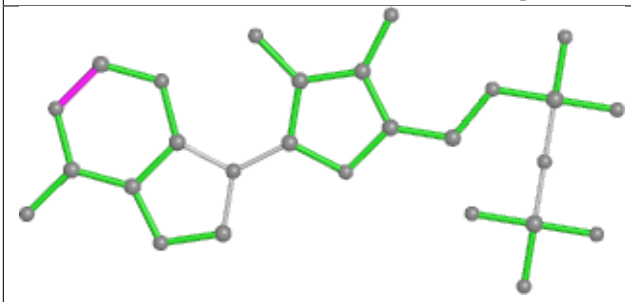


Torsions

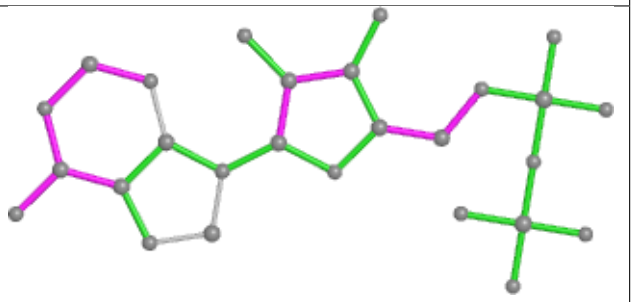


Rings

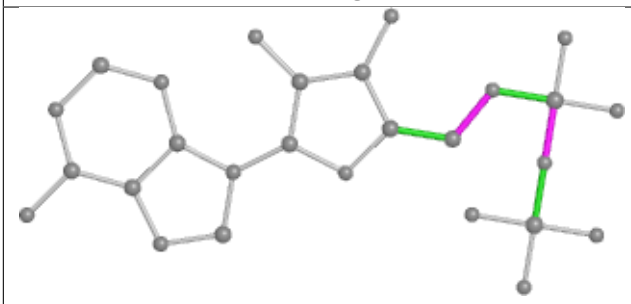
Ligand ADP E 1292



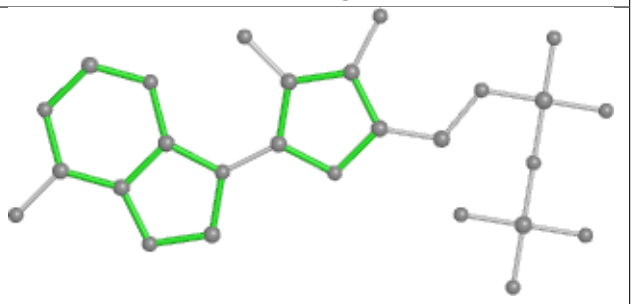
Bond lengths



Bond angles

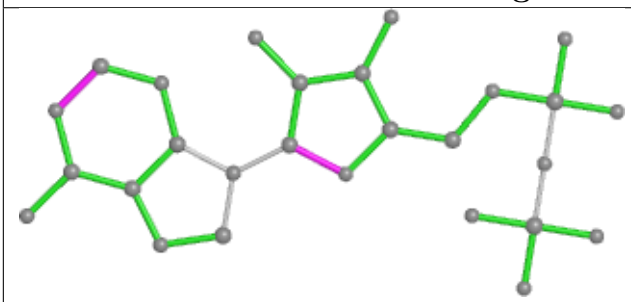


Torsions



Rings

Ligand ADP O 7292



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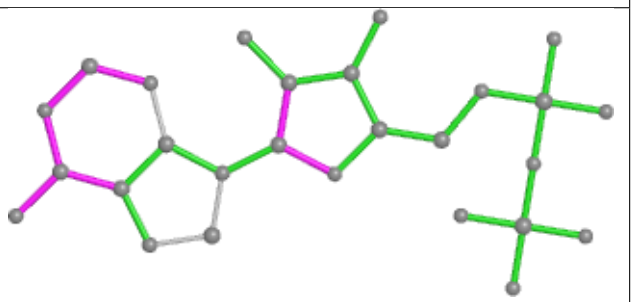
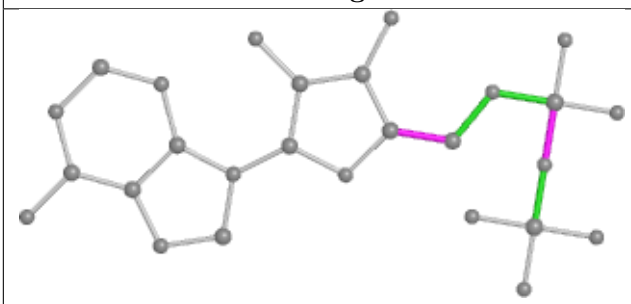


Bond angles



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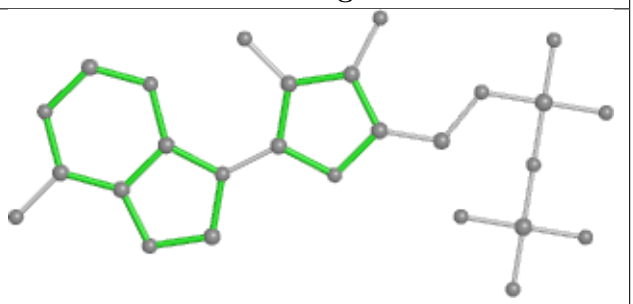
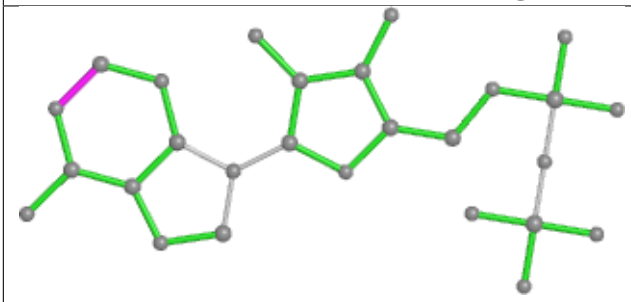


Rings

Ligand ADP H 4292



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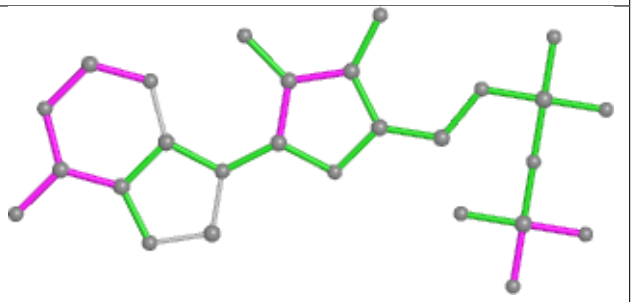
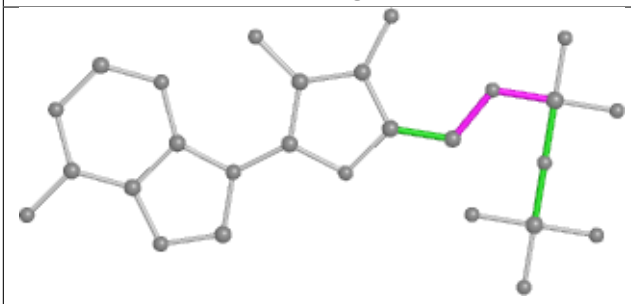
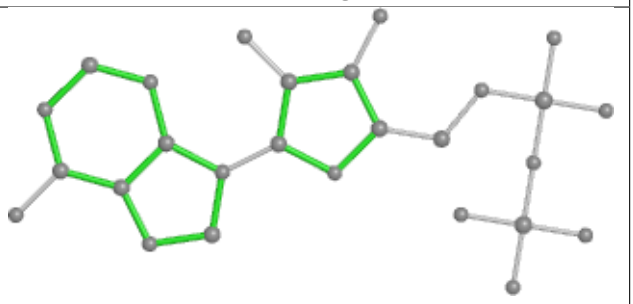


Bond angles

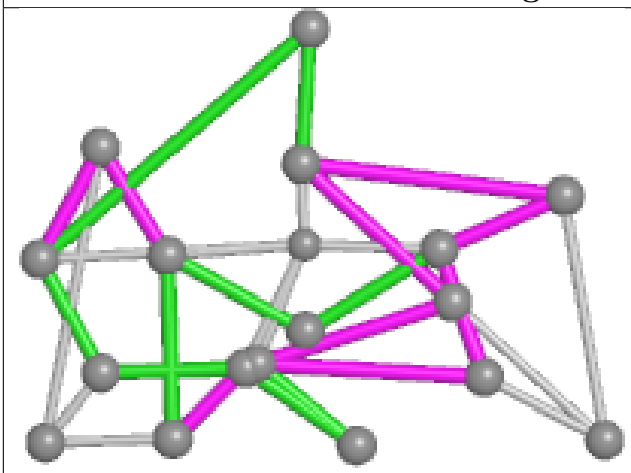


Torsions

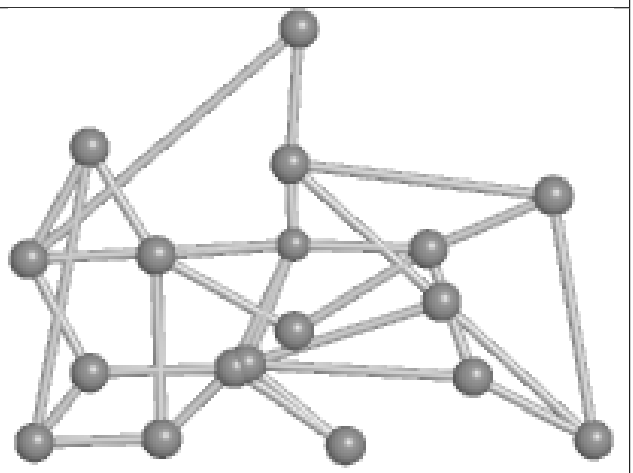


Rings

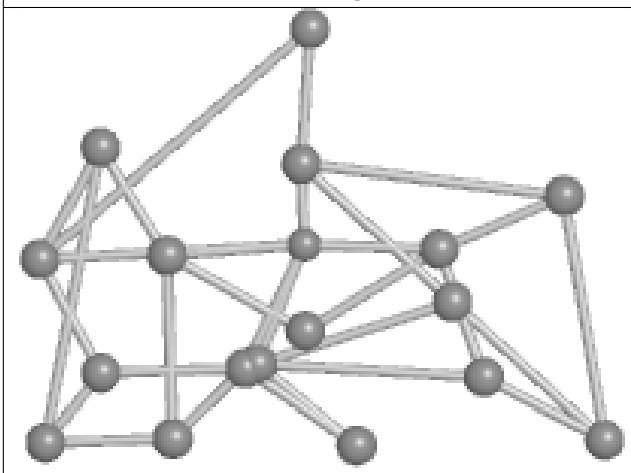
Ligand CFN K 496



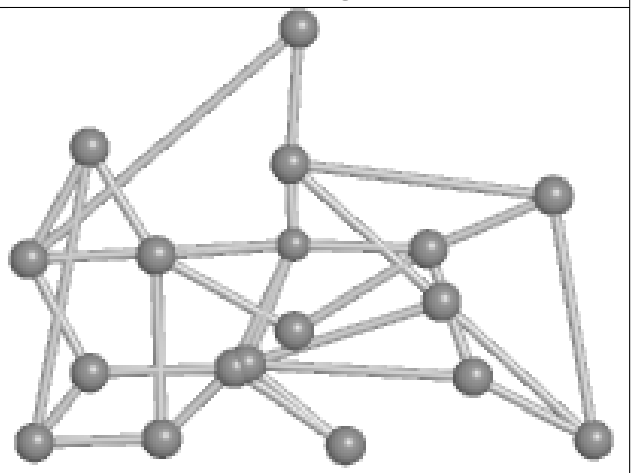
Bond lengths



Bond angles

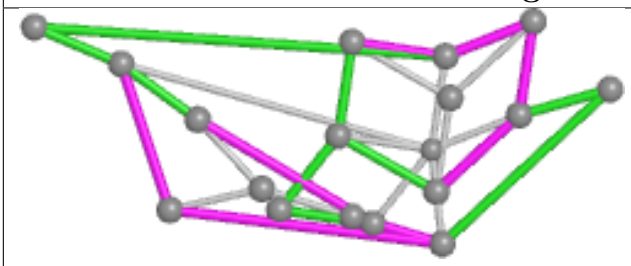


Torsions

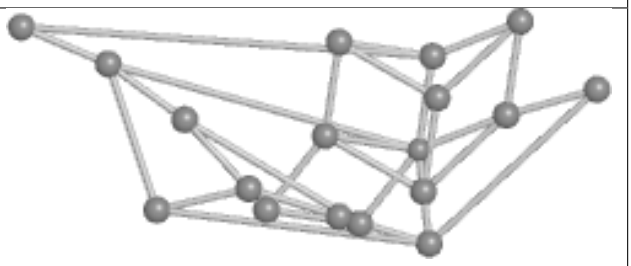


Rings

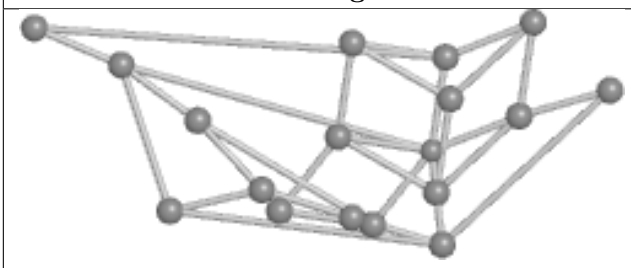
Ligand CFN A 496



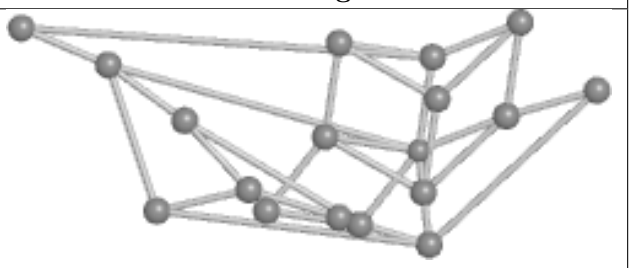
Bond lengths



Bond angles



Torsions



Rings

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	476/491 (96%)	-0.68	0 100 100	16, 34, 57, 86	7 (1%)
1	C	476/491 (96%)	-0.65	0 100 100	15, 33, 58, 85	6 (1%)
1	I	476/491 (96%)	-0.64	1 (0%) 95 90	18, 35, 59, 86	0
1	K	476/491 (96%)	-0.66	0 100 100	15, 34, 58, 85	3 (0%)
2	B	522/522 (100%)	-0.75	1 (0%) 95 90	9, 28, 49, 69	8 (1%)
2	D	522/522 (100%)	-0.73	0 100 100	9, 28, 49, 69	2 (0%)
2	J	522/522 (100%)	-0.78	0 100 100	10, 29, 50, 69	1 (0%)
2	L	522/522 (100%)	-0.79	0 100 100	9, 29, 51, 70	1 (0%)
3	E	252/289 (87%)	-0.02	17 (6%) 17 7	52, 87, 114, 127	65 (25%)
3	F	270/289 (93%)	-0.21	6 (2%) 62 41	45, 81, 116, 131	43 (15%)
3	G	257/289 (88%)	-0.31	2 (0%) 86 72	34, 73, 111, 128	49 (19%)
3	H	170/289 (58%)	0.03	9 (5%) 26 12	56, 86, 114, 121	55 (32%)
3	M	253/289 (87%)	-0.17	7 (2%) 53 30	55, 93, 126, 134	72 (28%)
3	N	157/289 (54%)	0.56	19 (12%) 4 1	74, 103, 129, 138	77 (49%)
3	O	260/289 (89%)	-0.22	8 (3%) 49 26	54, 82, 115, 131	61 (23%)
3	P	190/289 (65%)	0.22	17 (8%) 9 3	70, 100, 124, 131	54 (28%)
All	All	5801/6364 (91%)	-0.51	87 (1%) 73 54	9, 38, 106, 138	504 (8%)

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	19	THR	7.9
3	N	18	THR	6.8
3	N	8	TYR	5.2
3	N	22	LEU	5.2
3	N	9	GLY	4.6

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
9	ADP	N	6292	27/27	0.75	0.22	139,148,148,149	10
8	MG	M	5291	1/1	0.87	0.29	47,47,47,47	0
9	ADP	P	8292	27/27	0.87	0.17	114,122,127,128	0
8	MG	H	4291	1/1	0.90	0.28	68,68,68,68	0
9	ADP	M	5292	27/27	0.91	0.14	78,82,85,87	0
9	ADP	H	4292	27/27	0.92	0.20	124,133,136,136	10
9	ADP	F	2292	27/27	0.92	0.14	68,75,91,93	0
9	ADP	E	1292	27/27	0.93	0.14	61,68,71,73	0
8	MG	G	3291	1/1	0.93	0.19	41,41,41,41	0
8	MG	N	6291	1/1	0.93	0.17	46,46,46,46	0
8	MG	P	8291	1/1	0.94	0.15	66,66,66,66	0
8	MG	F	2291	1/1	0.94	0.20	23,23,23,23	0
8	MG	O	7291	1/1	0.94	0.23	39,39,39,39	0
9	ADP	G	3292	27/27	0.94	0.15	50,56,59,60	0
6	CA	B	2492	1/1	0.95	0.10	34,34,34,34	0
9	ADP	O	7292	27/27	0.95	0.15	66,81,93,96	0
6	CA	J	8492	1/1	0.95	0.10	42,42,42,42	0
4	HCA	C	494	14/14	0.96	0.17	18,22,30,32	0
4	HCA	A	494	14/14	0.96	0.12	21,25,29,30	0
4	HCA	K	494	14/14	0.98	0.15	17,23,31,33	0
6	CA	L	6492	1/1	0.98	0.09	37,37,37,37	0
8	MG	E	1291	1/1	0.98	0.17	44,44,44,44	0
10	SF4	F	1290	8/8	0.98	0.13	55,59,61,62	0
10	SF4	P	7290	8/8	0.98	0.11	74,76,80,82	0
7	CLF	J	5498	15/15	0.99	0.19	21,27,34,35	0
7	CLF	L	7498	15/15	0.99	0.16	24,28,34,35	0
5	CFN	I	496	18/18	0.99	0.16	17,22,25,27	0

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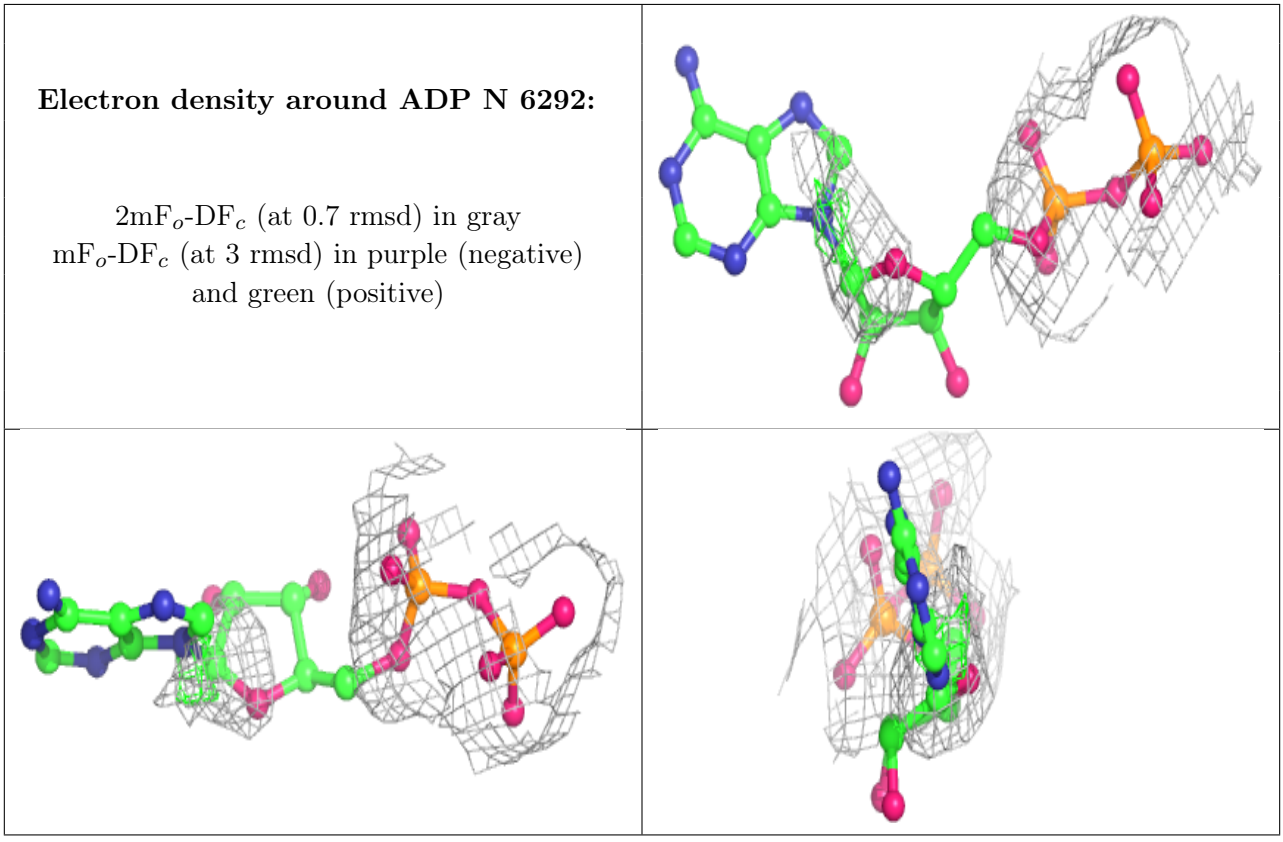
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CFN	K	496	18/18	0.99	0.17	12,21,25,26	0
4	HCA	I	494	14/14	0.99	0.14	19,27,32,37	0
6	CA	B	4492	1/1	0.99	0.10	32,32,32,32	0
5	CFN	A	496	18/18	0.99	0.17	14,19,23,28	0
5	CFN	C	496	18/18	0.99	0.20	9,15,18,18	0
7	CLF	B	1498	15/15	0.99	0.17	17,21,30,33	0
10	SF4	G	3290	8/8	0.99	0.09	42,46,48,49	0
10	SF4	N	5290	8/8	0.99	0.11	53,57,60,63	0
7	CLF	D	3498	15/15	0.99	0.18	15,20,28,29	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.

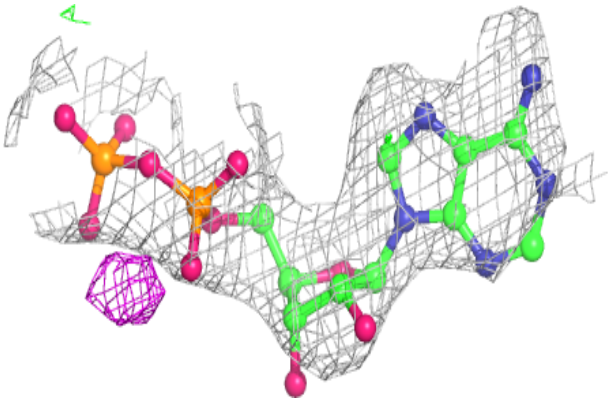
Electron density around ADP N 6292:

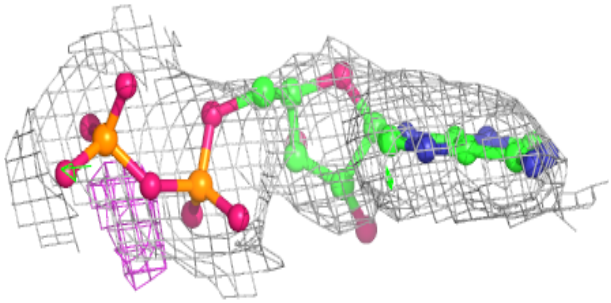
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

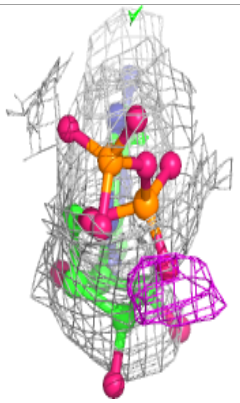


Electron density around ADP P 8292:

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

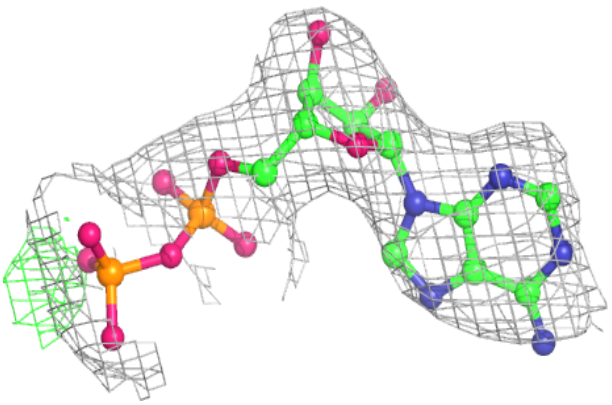


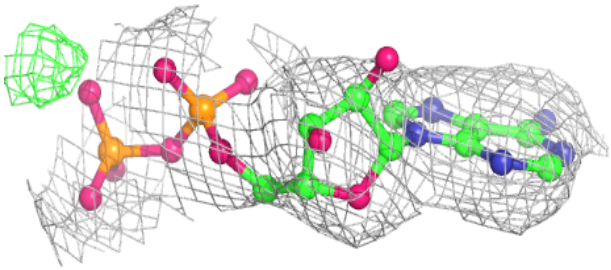


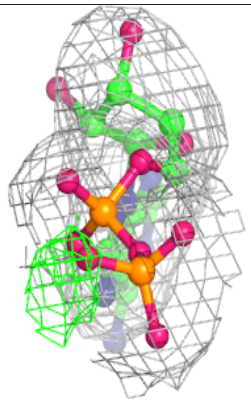


Electron density around ADP M 5292:

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

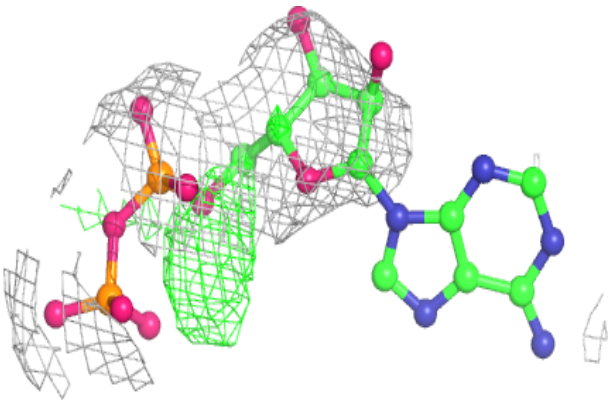


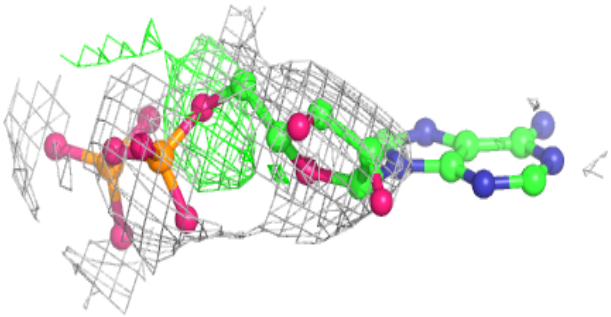


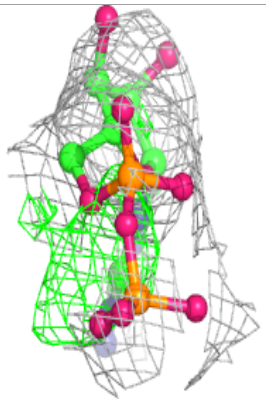


Electron density around ADP H 4292:

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

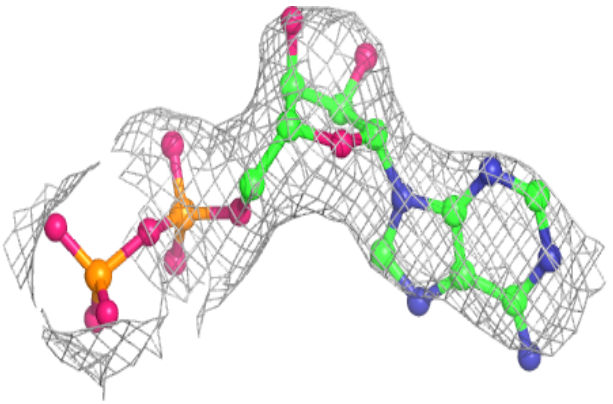


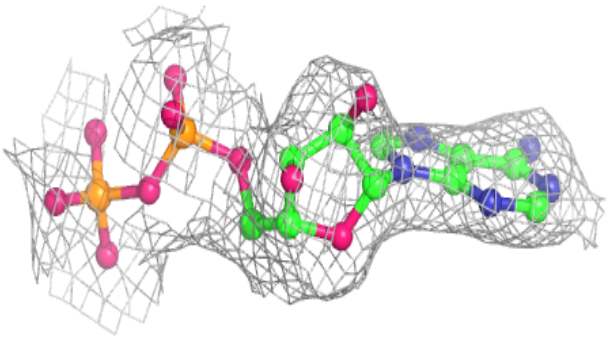


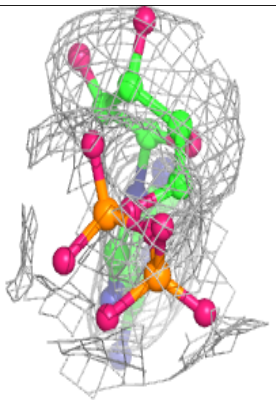


Electron density around ADP F 2292:

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

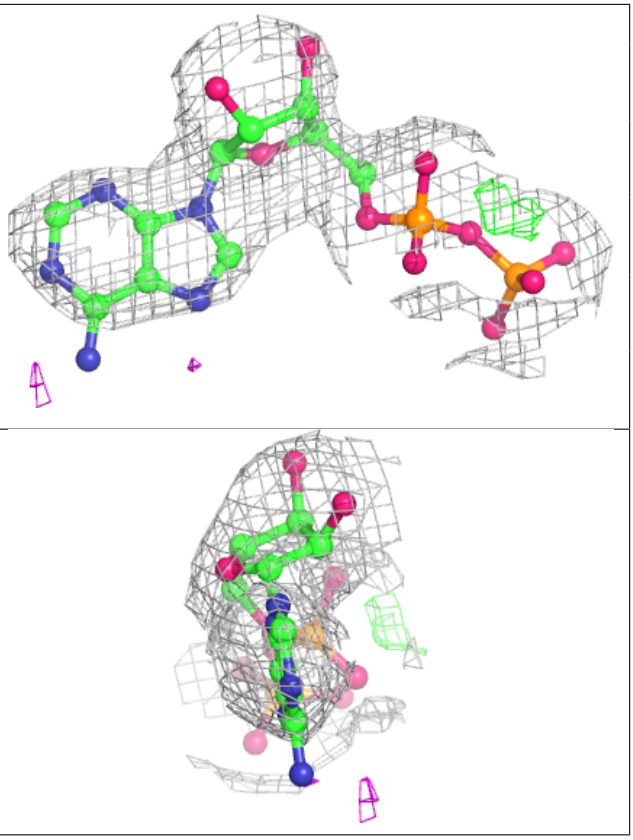






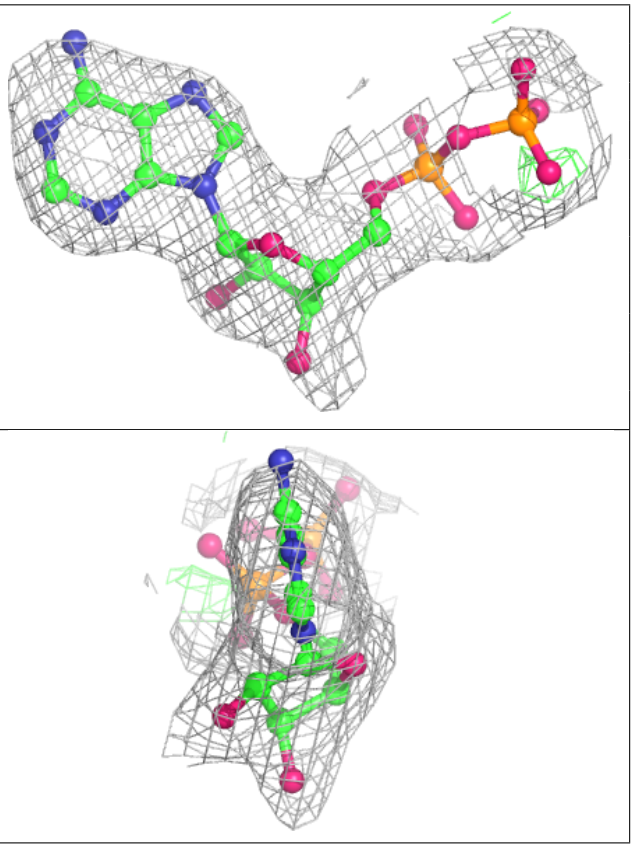
Electron density around ADP E 1292:

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



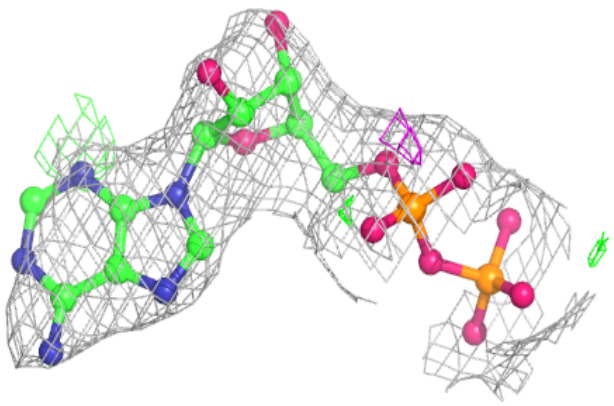
Electron density around ADP G 3292:

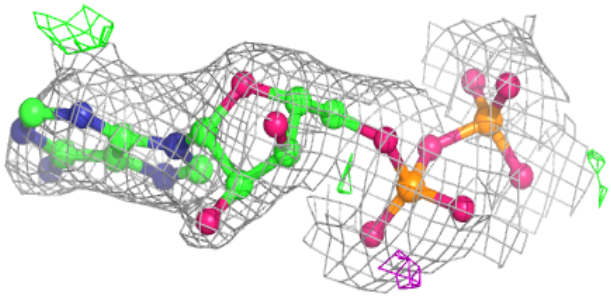
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

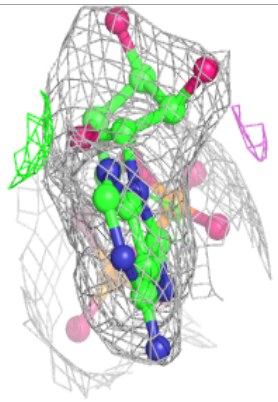


Electron density around ADP O 7292:

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

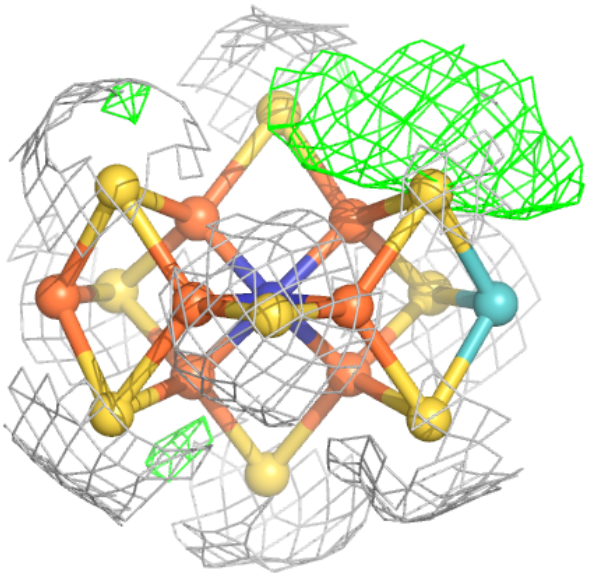


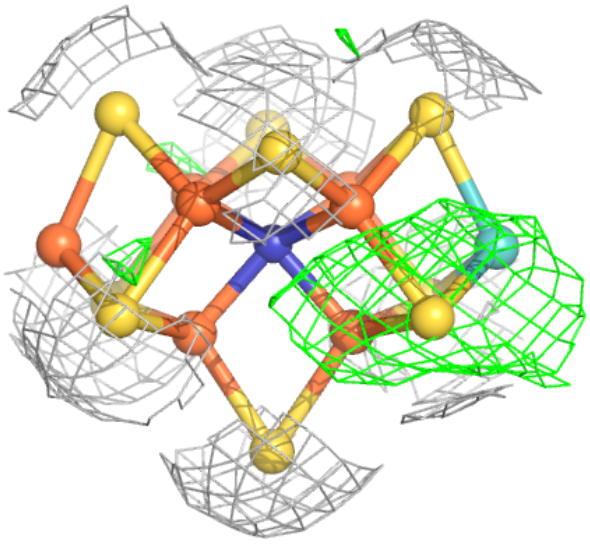


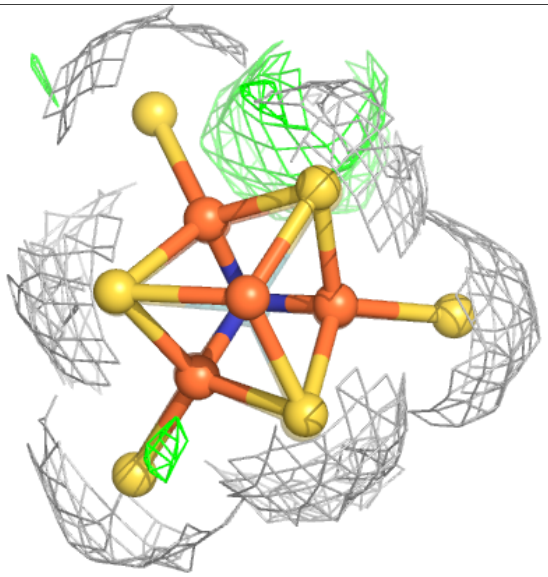


Electron density around CFN I 496:

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

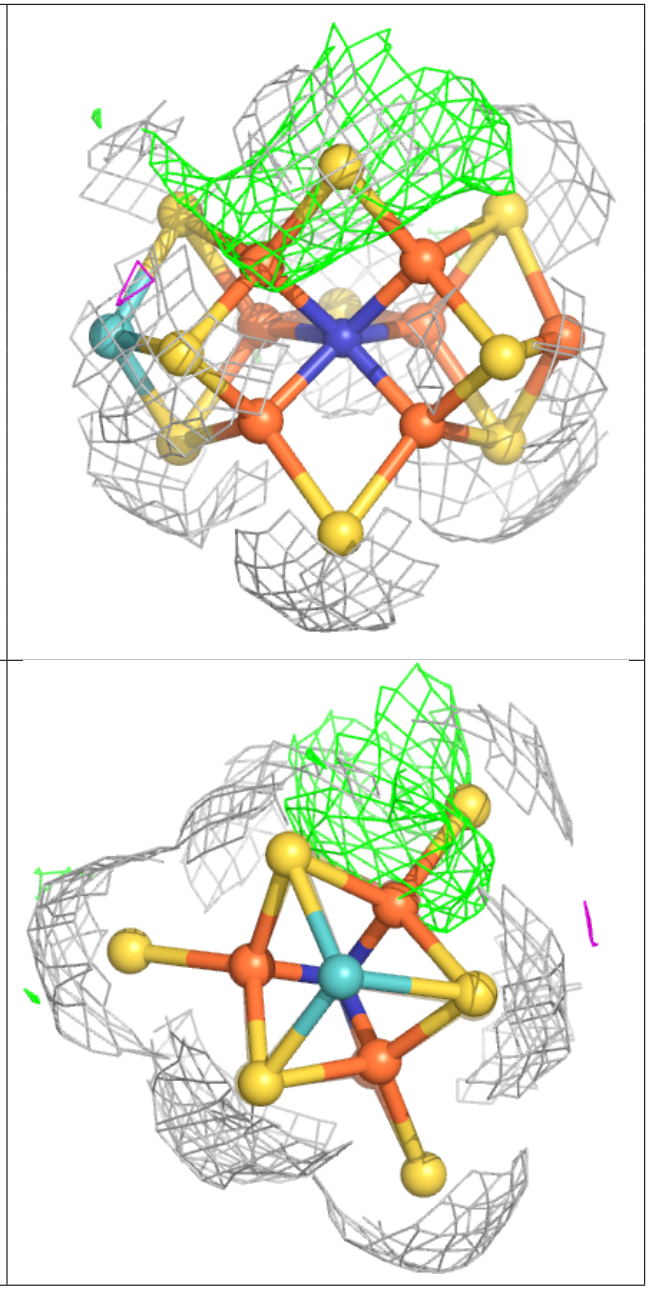






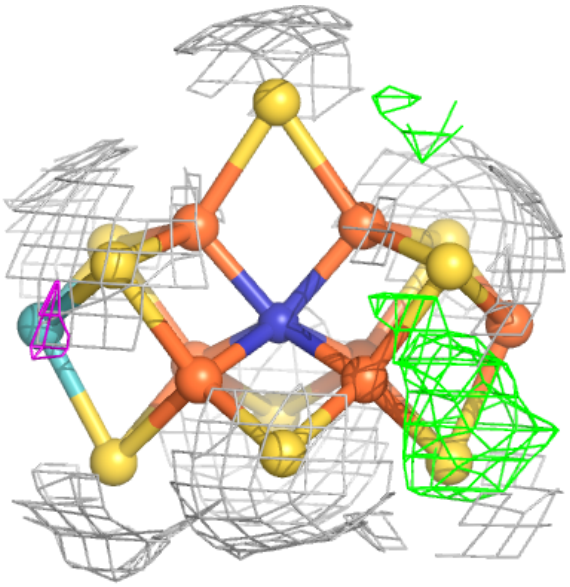
Electron density around CFN K 496:

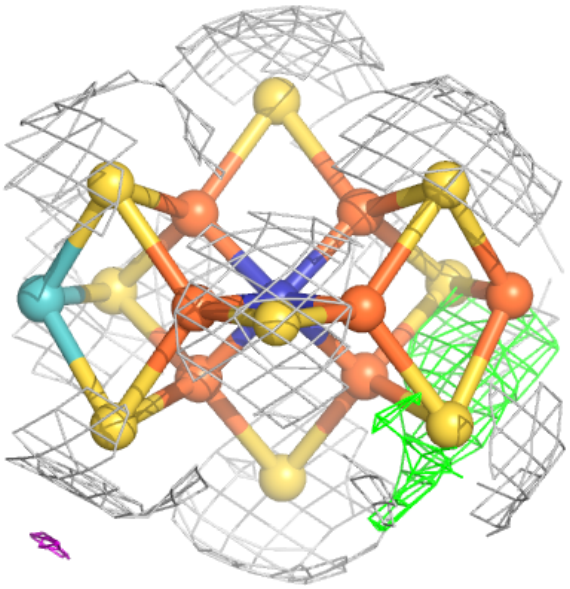
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

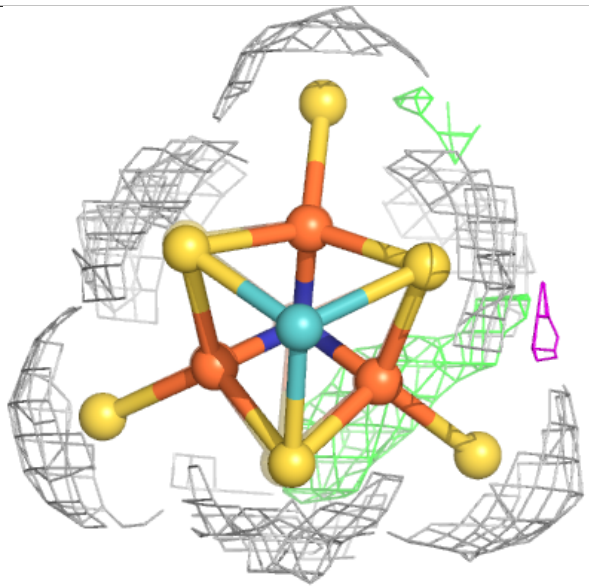


Electron density around CFN A 496:

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

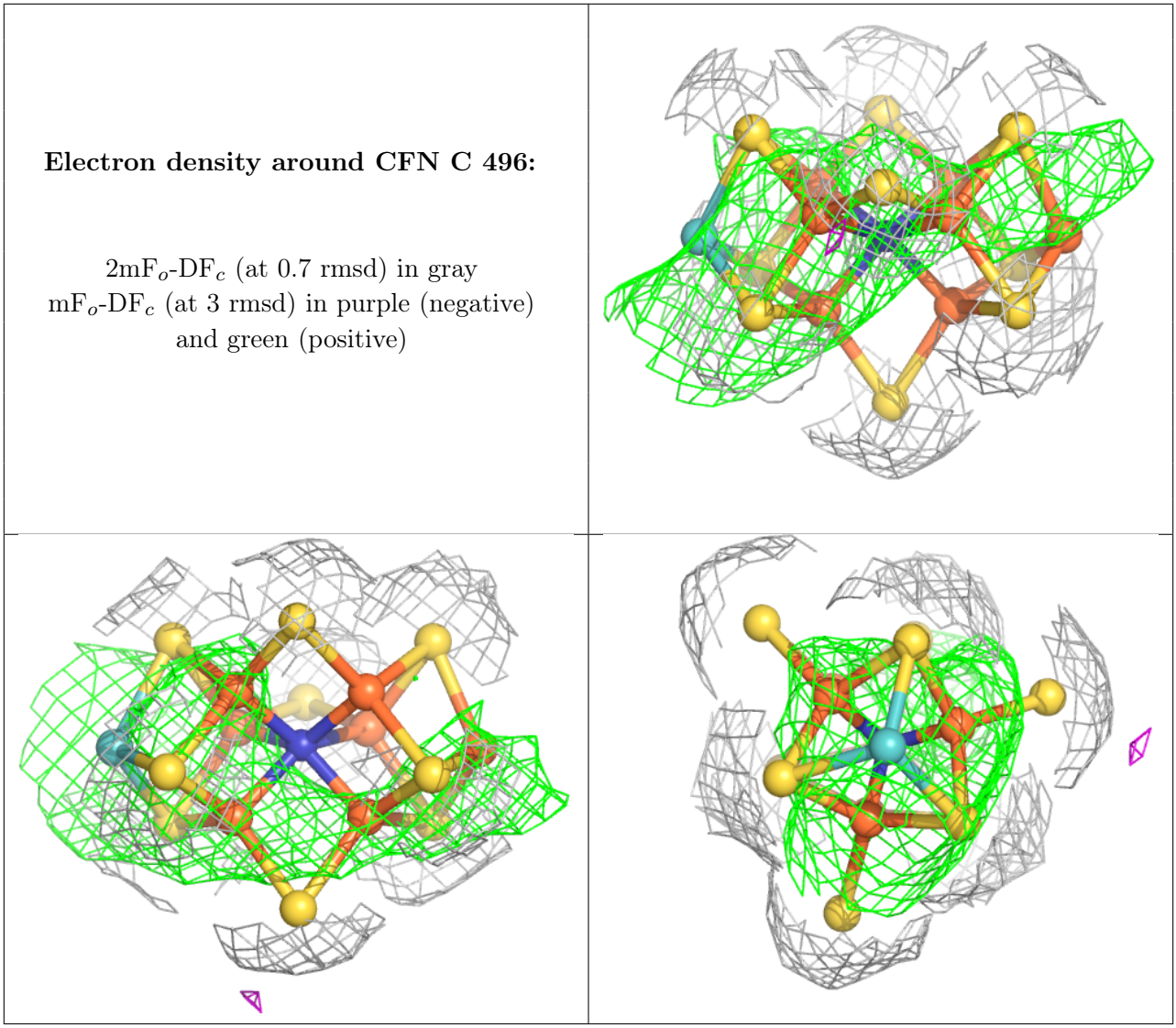






Electron density around CFN C 496:

$2mF_o$-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.