wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 09:35 PM EDT

PDB ID	:	8F6M
Title	:	Complex of Rabbit muscle pyruvate kinase with ADP and the phosphonate analogue of PEP mimicking the Michaelis complex.
Authors	:	Holyoak, T.; Fenton, A.W.
Deposited on	:	2022-11-16
Resolution	:	2.15 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:

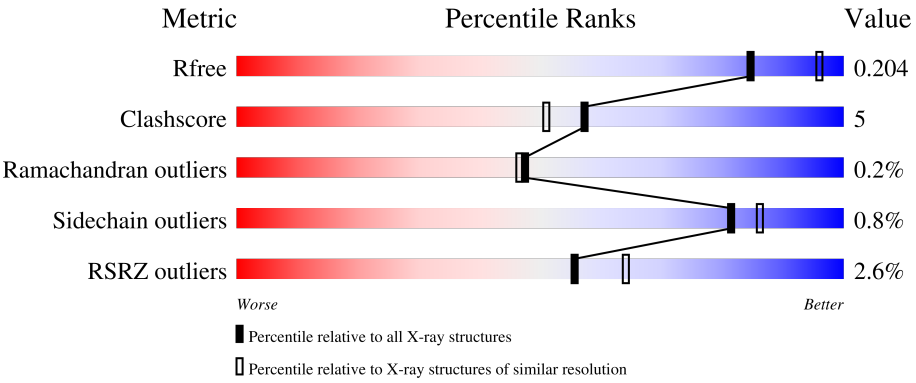
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	531	% 88% 9%
1	B	531	89% 9%
1	C	531	5% 86% 11%
1	D	531	% 89% 9%
1	E	531	90% 8%

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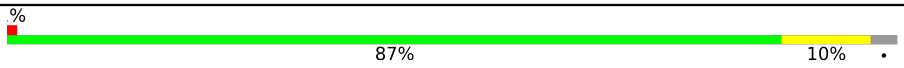
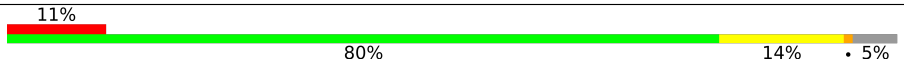
Mol	Chain	Length	Quality of chain
1	F	531	
1	G	531	
1	H	531	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	GZ3	G	601	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 35355 atoms, of which 64 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.

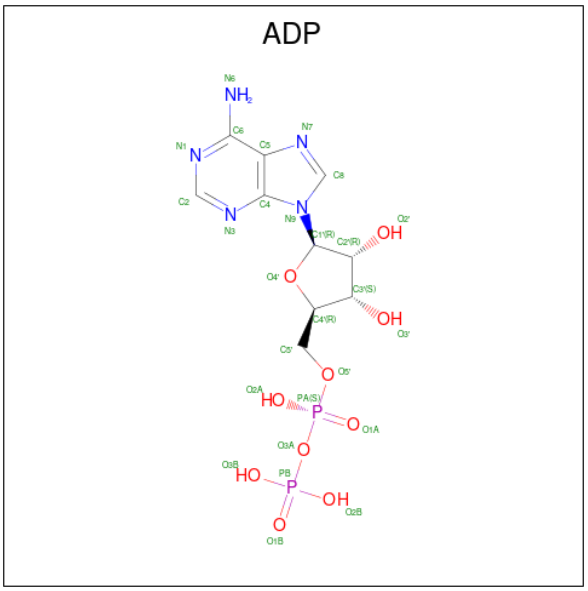
- Molecule 1 is a protein called Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	3	0
			3999	2512	714	745	28			
1	B	519	Total	C	N	O	S	0	4	0
			4004	2516	715	745	28			
1	C	519	Total	C	N	O	S	0	2	0
			3989	2506	708	746	29			
1	D	522	Total	C	N	O	S	0	5	0
			4031	2534	716	752	29			
1	E	519	Total	C	N	O	S	0	5	0
			4011	2521	715	746	29			
1	F	515	Total	C	N	O	S	0	3	0
			3978	2501	709	740	28			
1	G	506	Total	C	N	O	S	0	1	0
			3889	2442	692	726	29			
1	H	522	Total	C	N	O	S	0	2	0
			4010	2520	712	749	29			

There are 8 discrepancies between the modelled and reference sequences:

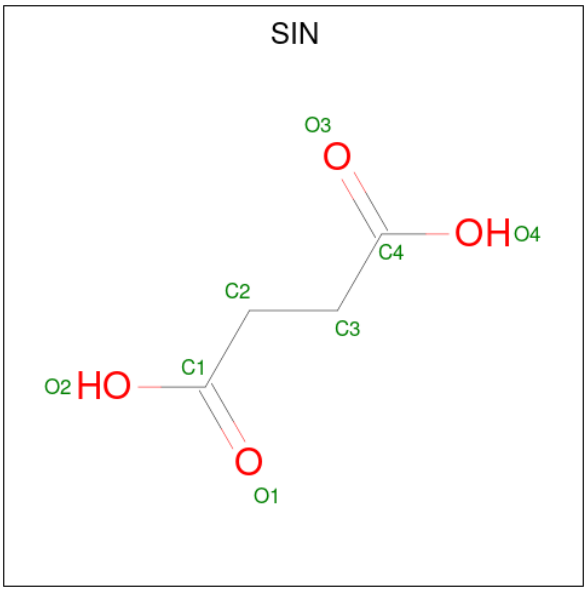
Chain	Residue	Modelled	Actual	Comment	Reference
A	400	ALA	SER	variant	UNP P11974
B	400	ALA	SER	variant	UNP P11974
C	400	ALA	SER	variant	UNP P11974
D	400	ALA	SER	variant	UNP P11974
E	400	ALA	SER	variant	UNP P11974
F	400	ALA	SER	variant	UNP P11974
G	400	ALA	SER	variant	UNP P11974
H	400	ALA	SER	variant	UNP P11974

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 4 4	0	0
3	A	1	Total C H O 12 4 4 4	0	0
3	B	1	Total C O 8 4 4	0	0
3	B	1	Total C H O 12 4 4 4	0	0
3	C	1	Total C O 8 4 4	0	0
3	C	1	Total C H O 12 4 4 4	0	0
3	D	1	Total C O 8 4 4	0	0
3	D	1	Total C H O 12 4 4 4	0	0
3	E	1	Total C H O 12 4 4 4	0	0
3	F	1	Total C H O 12 4 4 4	0	0
3	G	1	Total C H O 12 4 4 4	0	0
3	H	1	Total C H O 12 4 4 4	0	0

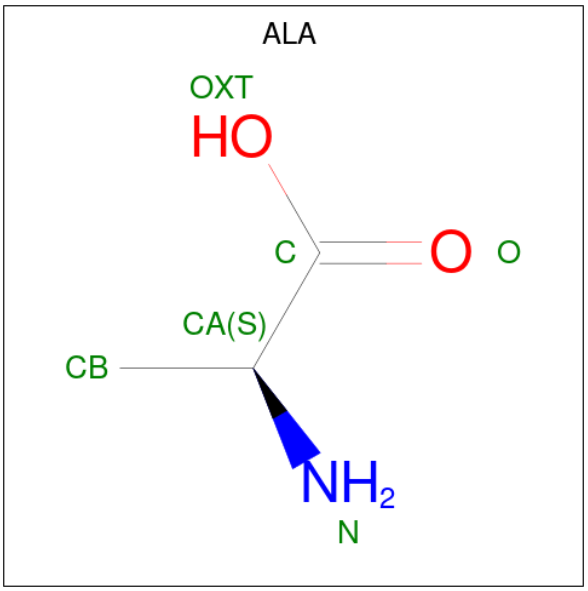
- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mn 2 2	0	0
4	B	2	Total Mn 2 2	0	0
4	C	2	Total Mn 2 2	0	0
4	D	2	Total Mn 2 2	0	0
4	E	2	Total Mn 2 2	0	0
4	F	2	Total Mn 2 2	0	0
4	G	1	Total Mn 1 1	0	0
4	H	2	Total Mn 2 2	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

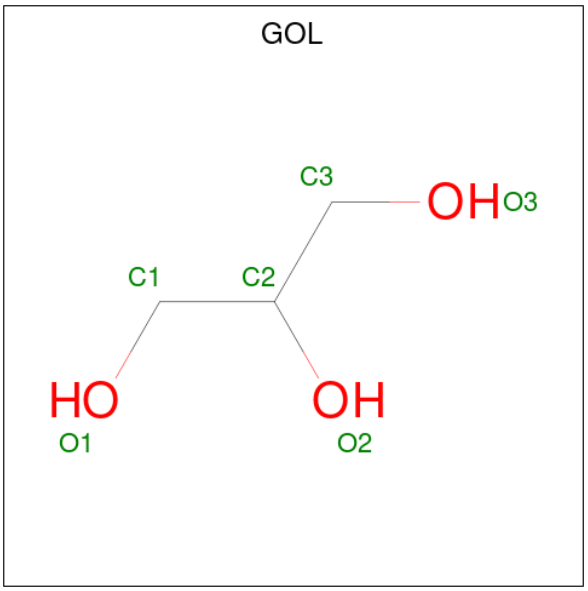
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0
5	E	1	Total K 1 1	0	0
5	F	1	Total K 1 1	0	0
5	G	1	Total K 1 1	0	0
5	H	1	Total K 1 1	0	0

- Molecule 6 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 6 3 1 2	0	0
6	B	1	Total C N O 6 3 1 2	0	0
6	C	1	Total C N O 6 3 1 2	0	0
6	D	1	Total C N O 6 3 1 2	0	0
6	E	1	Total C N O 6 3 1 2	0	0
6	F	1	Total C N O 6 3 1 2	0	0
6	G	1	Total C N O 6 3 1 2	0	0
6	H	1	Total C N O 6 3 1 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C H O 14 3 8 3	0	0
7	C	1	Total C O 6 3 3	0	0
7	C	1	Total C O 6 3 3	0	0
7	C	1	Total C O 6 3 3	0	0
7	C	1	Total C H O 14 3 8 3	0	0
7	C	1	Total C H O 14 3 8 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0

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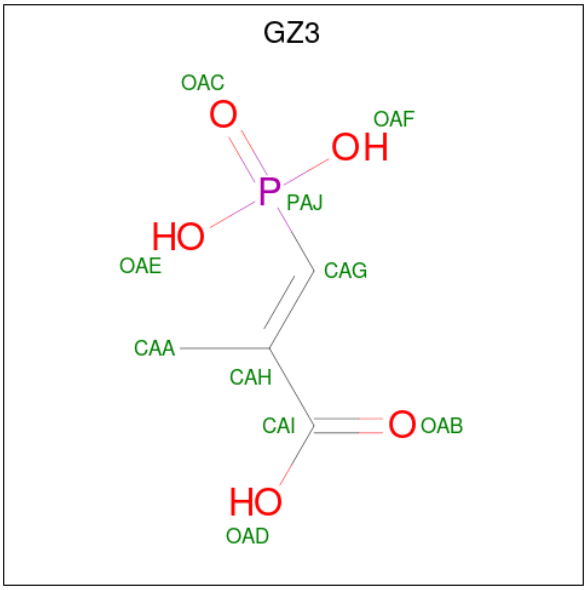
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0
7	F	1	Total C O 6 3 3	0	0
7	F	1	Total C O 6 3 3	0	0
7	F	1	Total C O 6 3 3	0	0
7	F	1	Total C O 6 3 3	0	0
7	F	1	Total C H O 14 3 8 3	0	0
7	G	1	Total C O 6 3 3	0	0
7	G	1	Total C O 6 3 3	0	0
7	H	1	Total C O 6 3 3	0	0
7	H	1	Total C O 6 3 3	0	0

- Molecule 8 is (E)-2-METHYL-3-PHOSPHONOACRYLATE (three-letter code: GZ3) (formula: $C_4H_7O_5P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	1	Total	C	O	P	0	0
			10	4	5	1		
8	F	1	Total	C	O	P	0	0
			10	4	5	1		
8	G	1	Total	C	O	P	0	0
			10	4	5	1		
8	H	1	Total	C	O	P	0	0
			10	4	5	1		

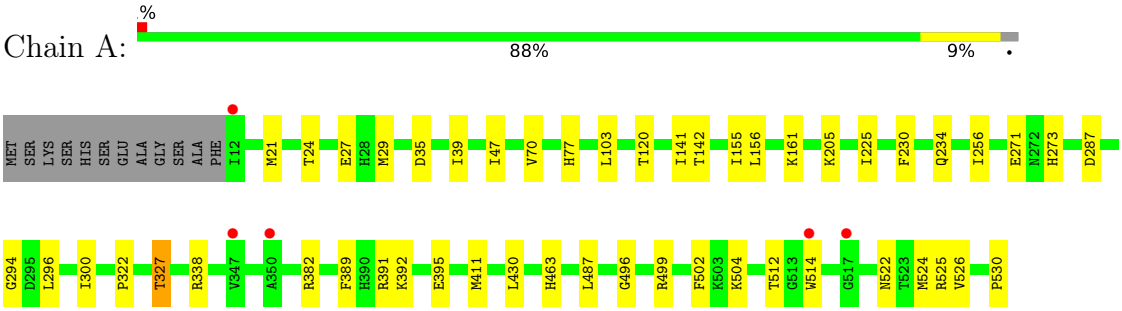
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	414	Total	O	0	0
			414	414		
9	B	402	Total	O	0	0
			402	402		
9	C	256	Total	O	0	0
			256	256		
9	D	344	Total	O	0	0
			344	344		
9	E	412	Total	O	0	0
			412	412		
9	F	358	Total	O	0	0
			358	358		
9	G	332	Total	O	0	0
			332	332		
9	H	364	Total	O	0	0
			364	364		

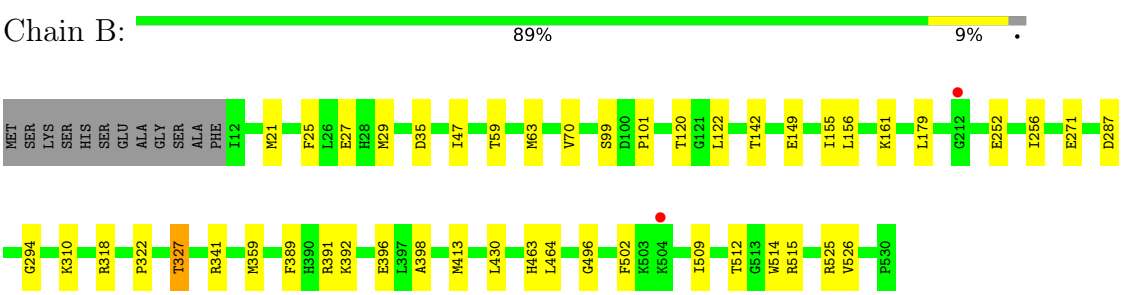
3 Residue-property plots (i)

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.

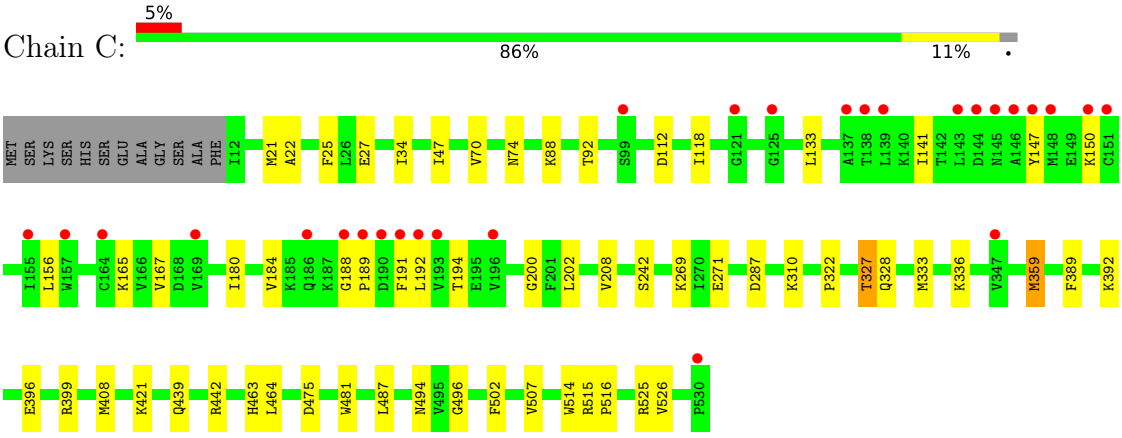
• Molecule 1: Pyruvate kinase PKM



• Molecule 1: Pyruvate kinase PKM

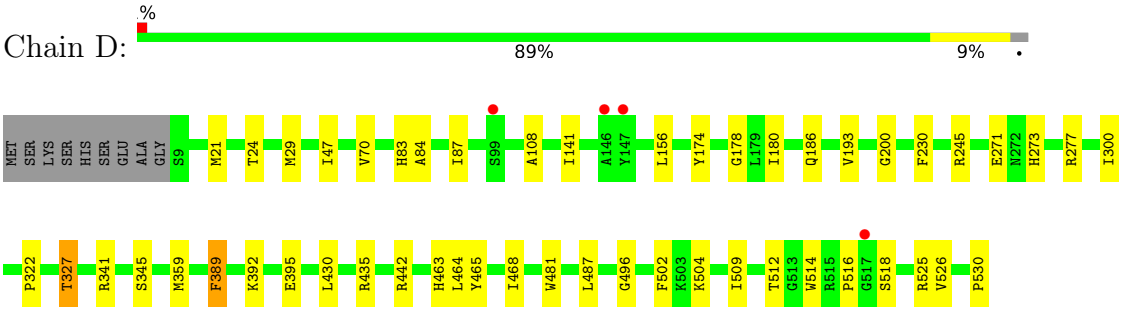


• Molecule 1: Pyruvate kinase PKM



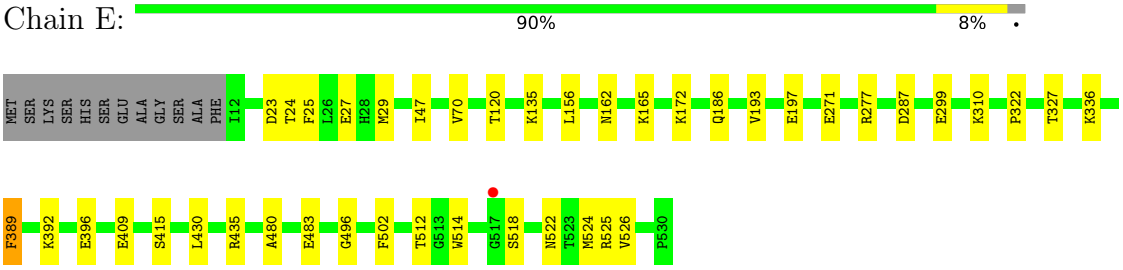
• Molecule 1: Pyruvate kinase PKM

Chain D:



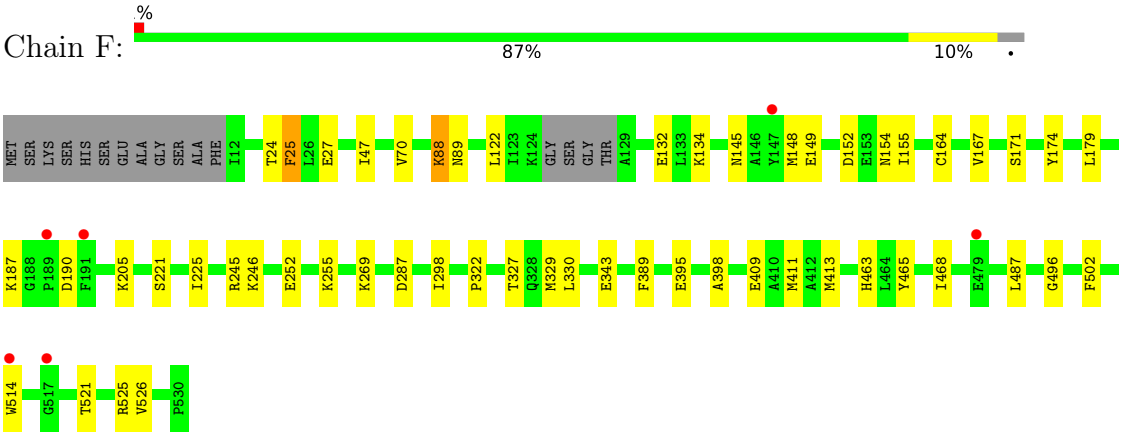
• Molecule 1: Pyruvate kinase PKM

Chain E:



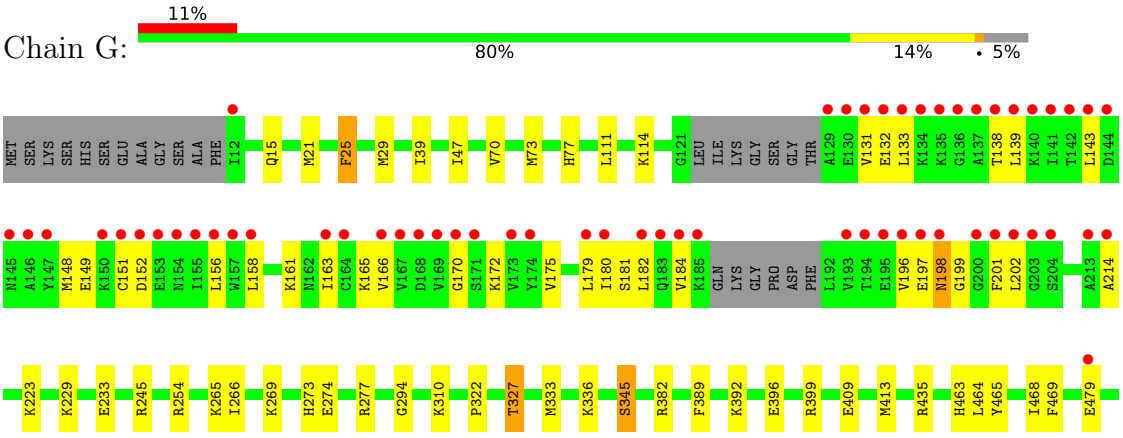
• Molecule 1: Pyruvate kinase PKM

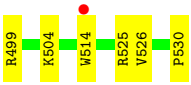
Chain F:



• Molecule 1: Pyruvate kinase PKM

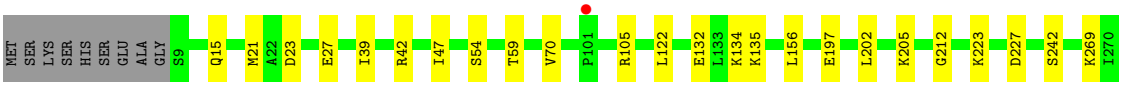
Chain G:





• Molecule 1: Pyruvate kinase PKM

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.03Å 216.40Å 258.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.02 – 2.15 46.02 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.02-2.15) 99.8 (46.02-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.156 , 0.205 0.156 , 0.204	Depositor DCC
R_{free} test set	14172 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	22.7	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	35355	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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: MN, ADP, GZ3, SIN, GOL, K

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	0.62	0/4072	0.70	1/5492 (0.0%)
1	B	0.60	0/4080	0.68	0/5503
1	C	0.55	0/4058	0.67	2/5473 (0.0%)
1	D	0.58	0/4111	0.67	0/5544
1	E	0.64	0/4091	0.71	0/5517
1	F	0.61	1/4050 (0.0%)	0.71	1/5461 (0.0%)
1	G	0.58	0/3951	0.67	1/5327 (0.0%)
1	H	0.64	0/4080	0.71	0/5503
All	All	0.60	1/32493 (0.0%)	0.69	5/43820 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	27	GLU	CG-CD	5.39	1.60	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	329	MET	CG-SD-CE	-5.91	90.75	100.20
1	G	21	MET	CG-SD-CE	5.56	109.10	100.20
1	A	524	MET	CG-SD-CE	-5.23	91.84	100.20
1	C	359	MET	CG-SD-CE	5.11	108.38	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	408	MET	CG-SD-CE	5.01	108.22	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	341	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	3999	0	4083	44	0
1	B	4004	0	4094	35	0
1	C	3989	0	4070	47	0
1	D	4031	0	4113	38	0
1	E	4011	0	4097	35	0
1	F	3978	0	4062	45	0
1	G	3889	0	3965	68	0
1	H	4010	0	4089	36	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	F	27	0	12	0	0
3	A	16	4	8	1	0
3	B	16	4	8	2	0
3	C	16	4	8	1	0
3	D	16	4	8	2	0
3	E	8	4	4	0	0
3	F	8	4	4	0	0
3	G	8	4	4	1	0
3	H	8	4	4	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	1	0	0	0	0
4	H	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	6	0	4	1	0
6	B	6	0	4	1	0
6	C	6	0	4	1	0
6	D	6	0	4	1	0
6	E	6	0	4	0	0
6	F	6	0	4	1	0
6	G	6	0	4	1	0
6	H	6	0	4	1	0
7	A	24	0	32	3	0
7	B	18	8	24	1	0
7	C	30	16	40	6	0
7	D	6	0	8	0	0
7	E	24	0	32	2	0
7	F	30	8	40	4	0
7	G	12	0	16	1	0
7	H	12	0	15	1	0
8	E	10	0	4	0	0
8	F	10	0	4	1	0
8	G	10	0	4	4	0
8	H	10	0	4	1	0
9	A	414	0	0	8	0
9	B	402	0	0	5	0
9	C	256	0	0	3	0
9	D	344	0	0	2	0
9	E	412	0	0	1	0
9	F	358	0	0	7	0
9	G	332	0	0	7	0
9	H	364	0	0	6	0
All	All	35291	64	32936	318	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 318 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:MET:HG3	9:A:1377:HOH:O	1.53	1.06
1:G:175:VAL:HG22	1:G:180:ILE:HB	1.43	0.97
1:F:122:LEU:CD1	1:F:205:LYS:HE3	2.06	0.85
1:F:152:ASP:HB2	1:F:155:ILE:HG22	1.58	0.85
1:A:21:MET:HE1	9:A:1113:HOH:O	1.78	0.83

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	520/531 (98%)	508 (98%)	11 (2%)	1 (0%)	47	46
1	B	521/531 (98%)	509 (98%)	11 (2%)	1 (0%)	47	46
1	C	519/531 (98%)	505 (97%)	13 (2%)	1 (0%)	47	46
1	D	525/531 (99%)	514 (98%)	10 (2%)	1 (0%)	47	46
1	E	522/531 (98%)	513 (98%)	8 (2%)	1 (0%)	47	46
1	F	514/531 (97%)	503 (98%)	10 (2%)	1 (0%)	47	46
1	G	501/531 (94%)	493 (98%)	7 (1%)	1 (0%)	47	46
1	H	522/531 (98%)	513 (98%)	8 (2%)	1 (0%)	47	46
All	All	4144/4248 (98%)	4058 (98%)	78 (2%)	8 (0%)	47	46

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	THR
1	B	327	THR

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Mol	Chain	Res	Type
1	D	327	THR
1	E	327	THR
1	G	327	THR

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	428/434 (99%)	426 (100%)	2 (0%)	88	92
1	B	429/434 (99%)	427 (100%)	2 (0%)	88	92
1	C	427/434 (98%)	422 (99%)	5 (1%)	71	76
1	D	432/434 (100%)	427 (99%)	5 (1%)	71	76
1	E	430/434 (99%)	428 (100%)	2 (0%)	88	92
1	F	426/434 (98%)	423 (99%)	3 (1%)	84	89
1	G	416/434 (96%)	409 (98%)	7 (2%)	60	65
1	H	429/434 (99%)	427 (100%)	2 (0%)	88	92
All	All	3417/3472 (98%)	3389 (99%)	28 (1%)	81	86

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	389	PHE
1	H	515	ARG
1	F	88	LYS
1	G	389	PHE
1	F	25	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	403	HIS
1	G	273	HIS

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Mol	Chain	Res	Type
1	H	273	HIS
1	C	186	GLN
1	B	478	GLN

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 78 ligands modelled in this entry, 23 are monoatomic - leaving 55 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	$\#\|Z\| > 2$
3	SIN	G	604	-	7,7,7	1.05	0	8,8,8	1.72	1 (12%)
2	ADP	F	601	4	24,29,29	1.12	2 (8%)	29,45,45	1.28	3 (10%)
6	ALA	H	605	-	5,5,5	1.08	0	6,6,6	1.66	2 (33%)
7	GOL	C	1010	-	5,5,5	1.11	0	5,5,5	0.88	0
7	GOL	C	1012	-	5,5,5	0.66	0	5,5,5	1.43	1 (20%)
3	SIN	C	1006	-	7,7,7	1.25	0	8,8,8	1.73	3 (37%)
7	GOL	G	606	-	5,5,5	1.12	0	5,5,5	0.88	0
7	GOL	H	607	-	5,5,5	1.69	2 (40%)	5,5,5	0.79	0
6	ALA	F	607	-	5,5,5	0.96	0	6,6,6	1.25	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	ALA	G	605	-	5,5,5	1.17	1 (20%)	6,6,6	1.45	2 (33%)
7	GOL	F	609	-	5,5,5	0.79	0	5,5,5	1.39	0
7	GOL	A	911	-	5,5,5	1.30	0	5,5,5	0.80	0
7	GOL	G	607	-	5,5,5	1.13	1 (20%)	5,5,5	1.09	0
7	GOL	A	908	-	5,5,5	0.90	0	5,5,5	0.97	0
8	GZ3	G	601	4,5	8,9,9	3.45	3 (37%)	9,13,13	2.05	3 (33%)
7	GOL	C	1008	-	5,5,5	0.78	0	5,5,5	1.22	1 (20%)
8	GZ3	H	601	4	8,9,9	3.41	3 (37%)	9,13,13	1.68	2 (22%)
6	ALA	D	1007	-	5,5,5	1.29	1 (20%)	6,6,6	1.48	2 (33%)
3	SIN	A	902	4	7,7,7	1.18	0	8,8,8	1.80	3 (37%)
2	ADP	A	901	4	24,29,29	0.92	1 (4%)	29,45,45	1.25	4 (13%)
7	GOL	F	612	-	5,5,5	0.91	0	5,5,5	0.69	0
7	GOL	F	610	-	5,5,5	0.63	0	5,5,5	1.40	1 (20%)
6	ALA	E	606	-	5,5,5	1.13	0	6,6,6	1.16	1 (16%)
3	SIN	F	606	-	7,7,7	1.15	0	8,8,8	1.61	4 (50%)
7	GOL	F	608	-	5,5,5	1.43	1 (20%)	5,5,5	0.45	0
7	GOL	E	608	-	5,5,5	0.98	0	5,5,5	1.10	0
7	GOL	F	611	-	5,5,5	1.07	0	5,5,5	0.99	0
6	ALA	C	1007	-	5,5,5	1.23	1 (20%)	6,6,6	1.28	1 (16%)
8	GZ3	F	602	4,5	8,9,9	3.62	4 (50%)	9,13,13	1.75	1 (11%)
7	GOL	E	610	-	5,5,5	0.86	0	5,5,5	1.00	0
7	GOL	D	1008	-	5,5,5	0.87	0	5,5,5	0.84	0
8	GZ3	E	601	4	8,9,9	2.84	4 (50%)	9,13,13	2.60	5 (55%)
3	SIN	D	1006	-	7,7,7	0.99	0	8,8,8	1.38	0
3	SIN	B	1002	4	7,7,7	1.19	0	8,8,8	2.07	3 (37%)
6	ALA	B	1007	-	5,5,5	1.29	1 (20%)	6,6,6	0.80	0
2	ADP	C	1001	4	24,29,29	1.22	3 (12%)	29,45,45	1.11	2 (6%)
7	GOL	C	1011	-	5,5,5	1.07	0	5,5,5	0.92	0
7	GOL	C	1009	-	5,5,5	1.36	0	5,5,5	0.91	0
6	ALA	A	907	-	5,5,5	1.53	2 (40%)	6,6,6	1.24	1 (16%)
3	SIN	D	1002	4	7,7,7	1.18	0	8,8,8	2.06	2 (25%)
7	GOL	B	1009	-	5,5,5	0.86	0	5,5,5	1.04	0
7	GOL	H	606	-	5,5,5	1.29	0	5,5,5	0.81	0
7	GOL	B	1010	-	5,5,5	1.08	0	5,5,5	1.66	1 (20%)
3	SIN	E	605	-	7,7,7	1.18	0	8,8,8	1.48	2 (25%)
3	SIN	B	1006	-	7,7,7	1.33	0	8,8,8	1.62	2 (25%)
7	GOL	A	909	-	5,5,5	0.89	0	5,5,5	0.87	0
7	GOL	A	910	-	5,5,5	0.82	0	5,5,5	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GOL	B	1008	-	5,5,5	0.60	0	5,5,5	1.55	1 (20%)
7	GOL	E	607	-	5,5,5	0.55	0	5,5,5	1.59	1 (20%)
3	SIN	C	1002	4	7,7,7	1.14	1 (14%)	8,8,8	1.68	2 (25%)
3	SIN	H	604	-	7,7,7	1.21	0	8,8,8	1.72	3 (37%)
2	ADP	B	1001	4	24,29,29	0.96	2 (8%)	29,45,45	1.14	1 (3%)
2	ADP	D	1001	4	24,29,29	1.28	3 (12%)	29,45,45	1.23	2 (6%)
7	GOL	E	609	-	5,5,5	1.58	1 (20%)	5,5,5	0.77	0
3	SIN	A	906	-	7,7,7	1.12	0	8,8,8	1.95	4 (50%)

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	SIN	G	604	-	-	3/5/5/5	-
2	ADP	F	601	4	-	0/12/32/32	0/3/3/3
6	ALA	H	605	-	-	2/4/4/4	-
7	GOL	C	1010	-	-	2/4/4/4	-
7	GOL	C	1012	-	-	0/4/4/4	-
3	SIN	C	1006	-	-	3/5/5/5	-
7	GOL	G	606	-	-	1/4/4/4	-
7	GOL	H	607	-	-	0/4/4/4	-
6	ALA	F	607	-	-	0/4/4/4	-
6	ALA	G	605	-	-	0/4/4/4	-
7	GOL	F	609	-	-	2/4/4/4	-
7	GOL	A	911	-	-	3/4/4/4	-
7	GOL	G	607	-	-	2/4/4/4	-
7	GOL	A	908	-	-	4/4/4/4	-
8	GZ3	G	601	4,5	-	2/6/9/9	-
7	GOL	C	1008	-	-	0/4/4/4	-
8	GZ3	H	601	4	-	5/6/9/9	-
6	ALA	D	1007	-	-	0/4/4/4	-
3	SIN	A	902	4	-	4/5/5/5	-
2	ADP	A	901	4	-	0/12/32/32	0/3/3/3
7	GOL	F	612	-	-	2/4/4/4	-
7	GOL	F	610	-	-	4/4/4/4	-
6	ALA	E	606	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SIN	F	606	-	-	3/5/5/5	-
7	GOL	F	608	-	-	2/4/4/4	-
7	GOL	E	608	-	-	2/4/4/4	-
7	GOL	F	611	-	-	1/4/4/4	-
6	ALA	C	1007	-	-	3/4/4/4	-
8	GZ3	F	602	4,5	-	5/6/9/9	-
7	GOL	E	610	-	-	3/4/4/4	-
7	GOL	D	1008	-	-	3/4/4/4	-
8	GZ3	E	601	4	-	2/6/9/9	-
3	SIN	D	1006	-	-	1/5/5/5	-
3	SIN	B	1002	4	-	4/5/5/5	-
6	ALA	B	1007	-	-	3/4/4/4	-
2	ADP	C	1001	4	-	2/12/32/32	0/3/3/3
7	GOL	C	1011	-	-	2/4/4/4	-
7	GOL	C	1009	-	-	0/4/4/4	-
6	ALA	A	907	-	-	1/4/4/4	-
3	SIN	D	1002	4	-	4/5/5/5	-
7	GOL	B	1009	-	-	2/4/4/4	-
7	GOL	H	606	-	-	0/4/4/4	-
7	GOL	B	1010	-	-	2/4/4/4	-
3	SIN	E	605	-	-	3/5/5/5	-
3	SIN	B	1006	-	-	2/5/5/5	-
7	GOL	A	909	-	-	4/4/4/4	-
7	GOL	A	910	-	-	2/4/4/4	-
7	GOL	B	1008	-	-	0/4/4/4	-
7	GOL	E	607	-	-	3/4/4/4	-
3	SIN	C	1002	4	-	4/5/5/5	-
3	SIN	H	604	-	-	4/5/5/5	-
2	ADP	B	1001	4	-	0/12/32/32	0/3/3/3
2	ADP	D	1001	4	-	0/12/32/32	0/3/3/3
7	GOL	E	609	-	-	2/4/4/4	-
3	SIN	A	906	-	-	3/5/5/5	-

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	601	GZ3	CAA-CAH	-7.54	1.32	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	601	GZ3	CAA-CAH	-7.01	1.33	1.50
8	F	602	GZ3	CAA-CAH	-6.82	1.33	1.50
8	E	601	GZ3	CAA-CAH	-6.44	1.34	1.50
8	F	602	GZ3	PAJ-CAG	6.23	1.85	1.76

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	601	GZ3	CAA-CAH-CAI	4.58	122.81	115.69
8	F	602	GZ3	OAC-PAJ-CAG	-4.47	102.51	115.24
3	D	1002	SIN	C2-C3-C4	-4.26	104.44	113.60
8	E	601	GZ3	OAC-PAJ-CAG	-4.10	103.58	115.24
8	H	601	GZ3	OAC-PAJ-CAG	-3.98	103.93	115.24

There are no chirality outliers.

5 of 111 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1006	SIN	C1-C2-C3-C4
7	A	908	GOL	O1-C1-C2-C3
7	A	909	GOL	O1-C1-C2-O2
7	A	909	GOL	O1-C1-C2-C3
7	A	909	GOL	C1-C2-C3-O3

There are no ring outliers.

29 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	604	SIN	1	0
6	H	605	ALA	1	0
7	C	1012	GOL	2	0
7	H	607	GOL	1	0
6	F	607	ALA	1	0
6	G	605	ALA	1	0
7	F	609	GOL	2	0
7	G	607	GOL	1	0
8	G	601	GZ3	4	0
8	H	601	GZ3	1	0
6	D	1007	ALA	1	0
3	A	902	SIN	1	0
2	A	901	ADP	1	0

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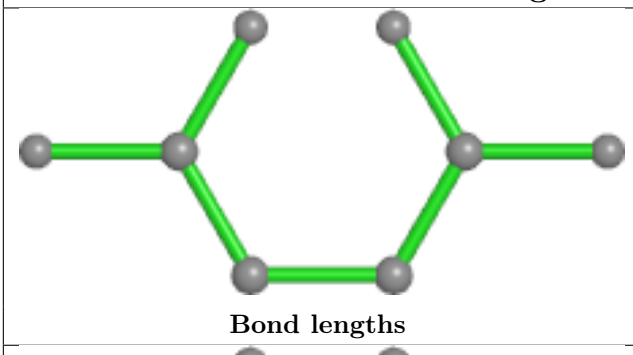
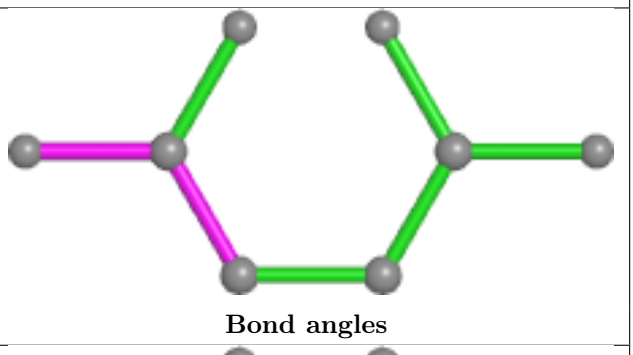
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	612	GOL	2	0
7	F	610	GOL	1	0
7	E	608	GOL	2	0
6	C	1007	ALA	1	0
8	F	602	GZ3	1	0
3	B	1002	SIN	2	0
6	B	1007	ALA	1	0
7	C	1011	GOL	1	0
7	C	1009	GOL	3	0
6	A	907	ALA	1	0
3	D	1002	SIN	2	0
7	B	1009	GOL	1	0
7	A	909	GOL	2	0
7	A	910	GOL	2	0
3	C	1002	SIN	1	0
3	H	604	SIN	1	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.

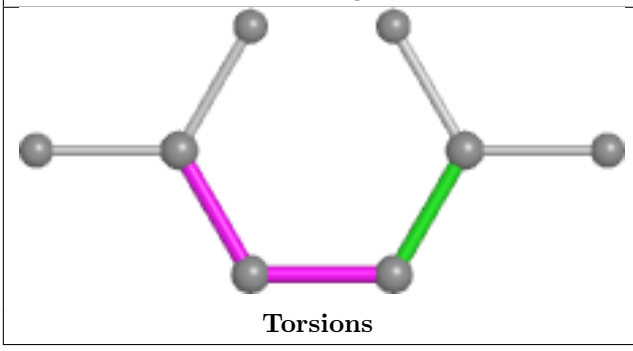
Ligand SIN G 604



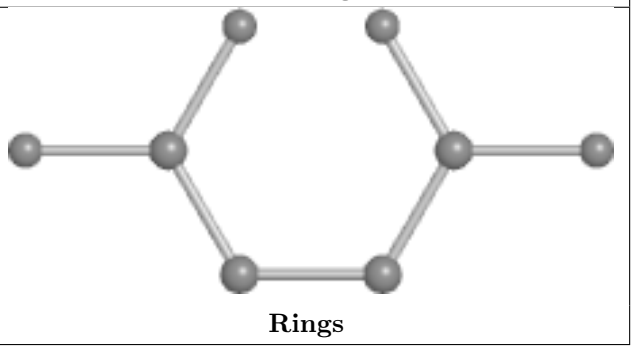
Bond lengths



Bond angles

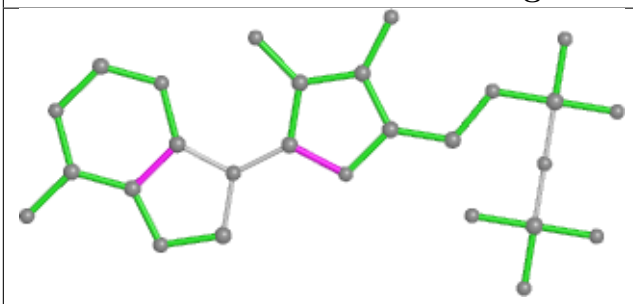


Torsions

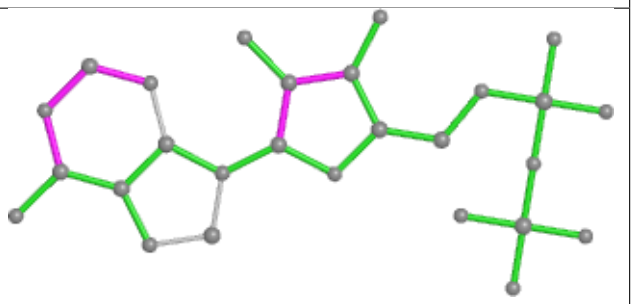


Rings

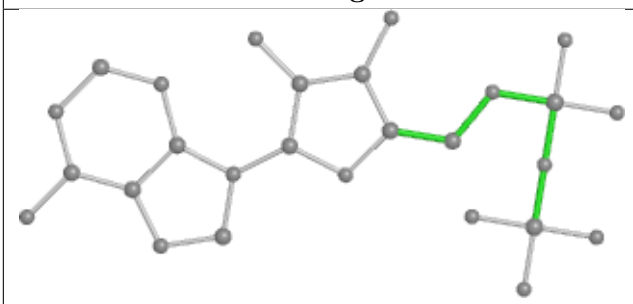
Ligand ADP F 601



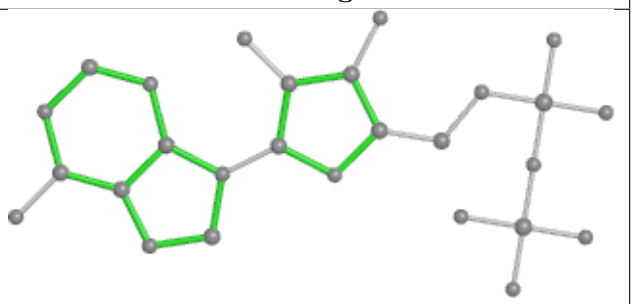
Bond lengths



Bond angles

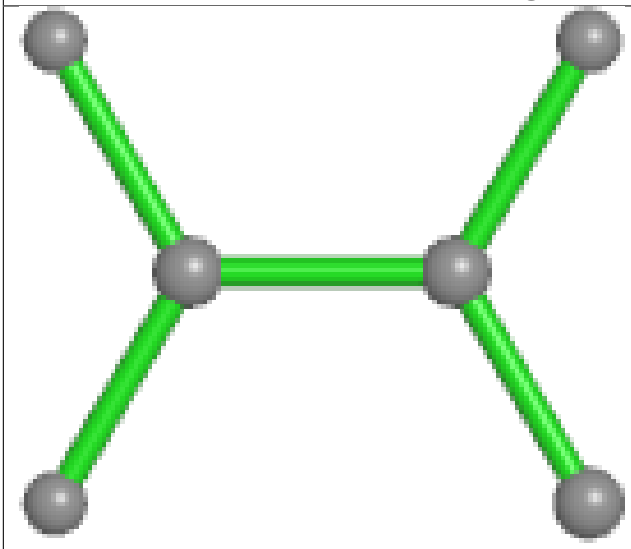


Torsions



Rings

Ligand ALA H 605



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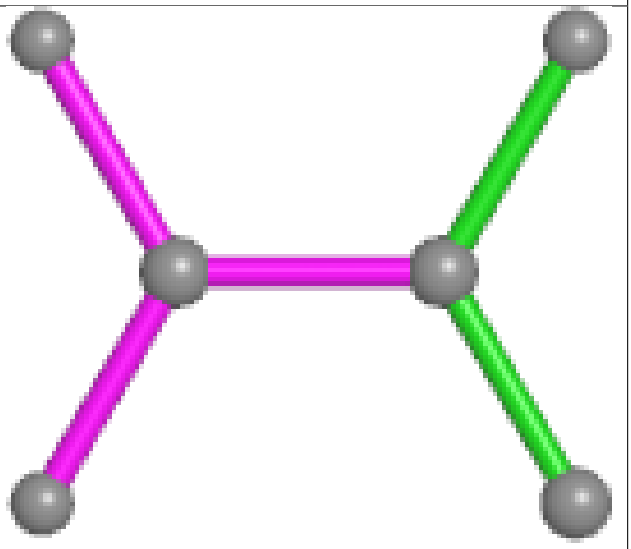
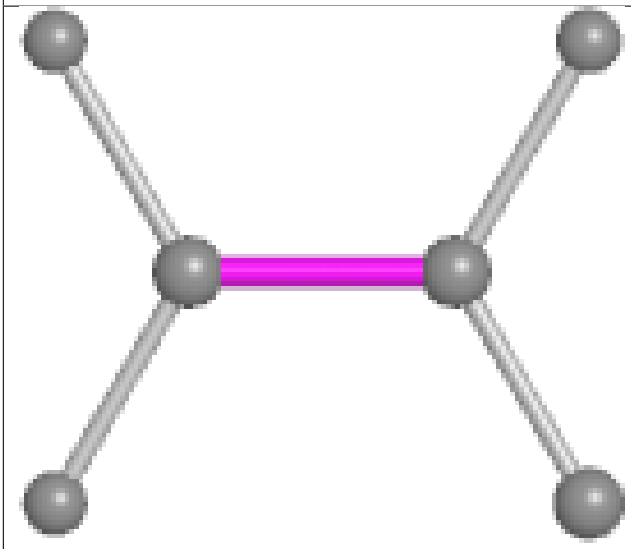
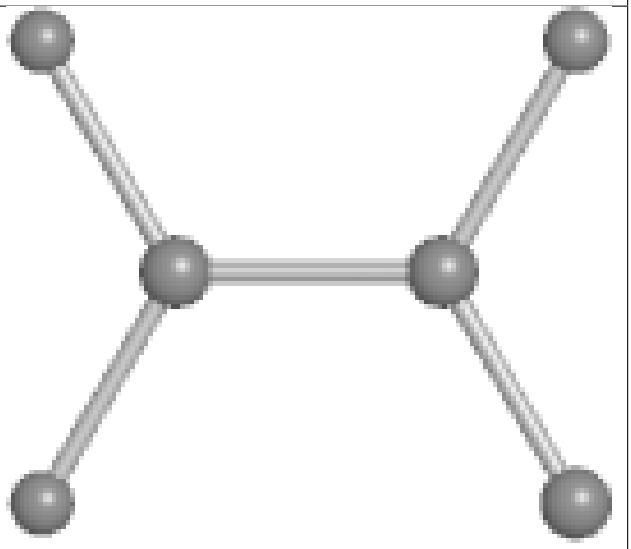


Bond angles

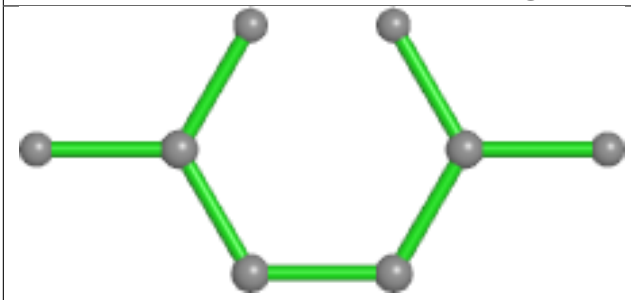


Torsions

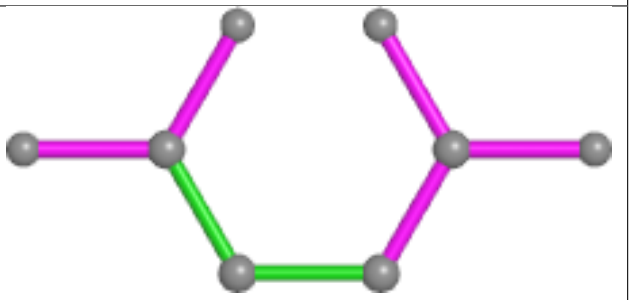


Rings

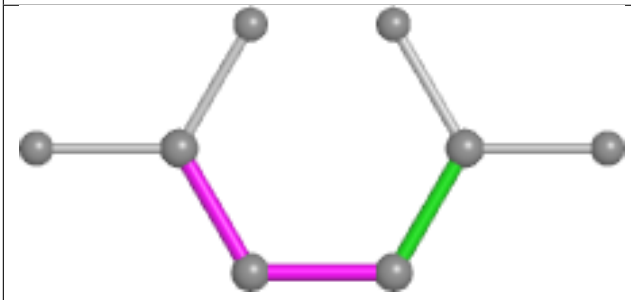
Ligand SIN C 1006



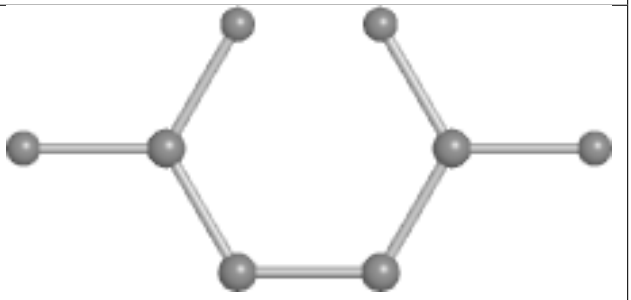
Bond lengths



Bond angles

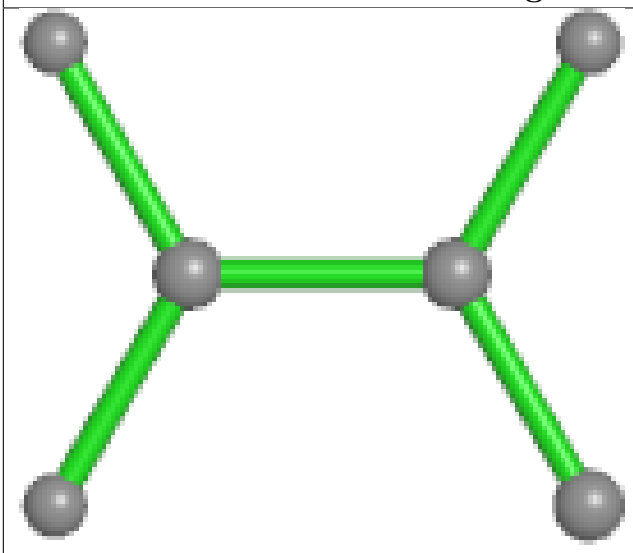


Torsions



Rings

Ligand ALA F 607



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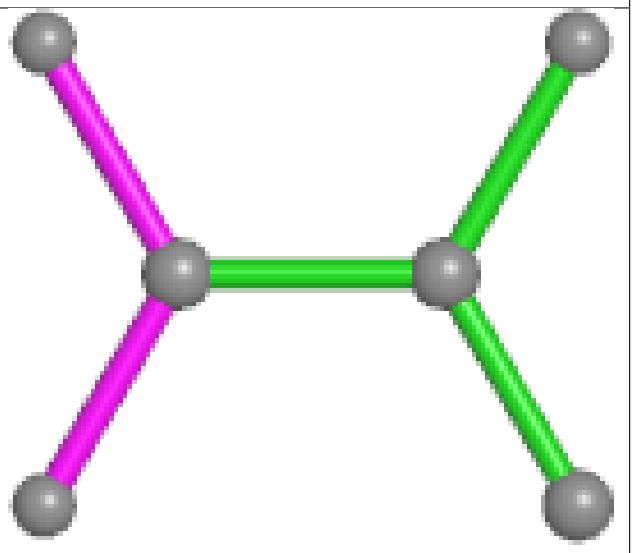
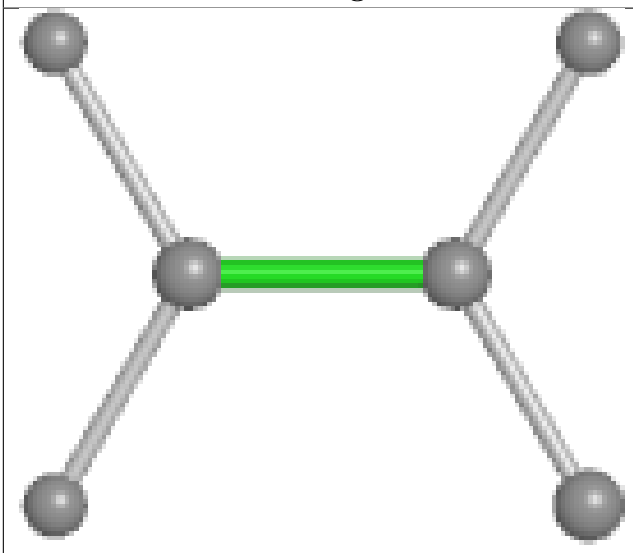
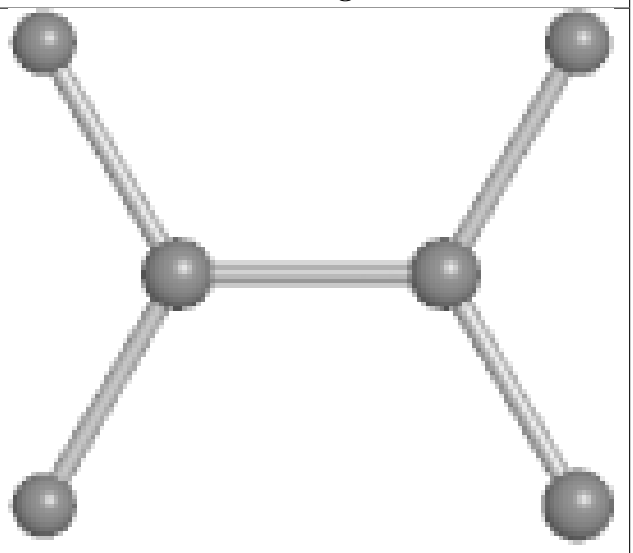


Bond angles

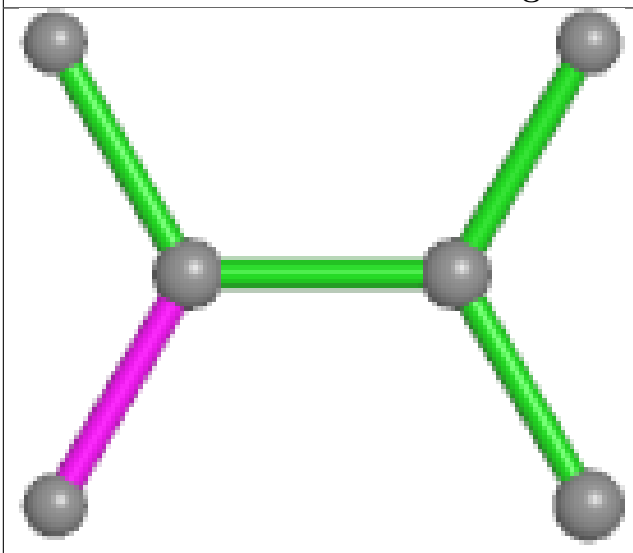


Torsions

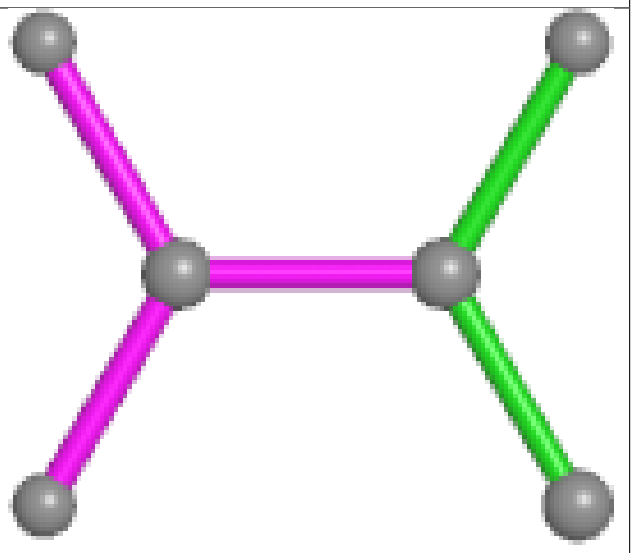


Rings

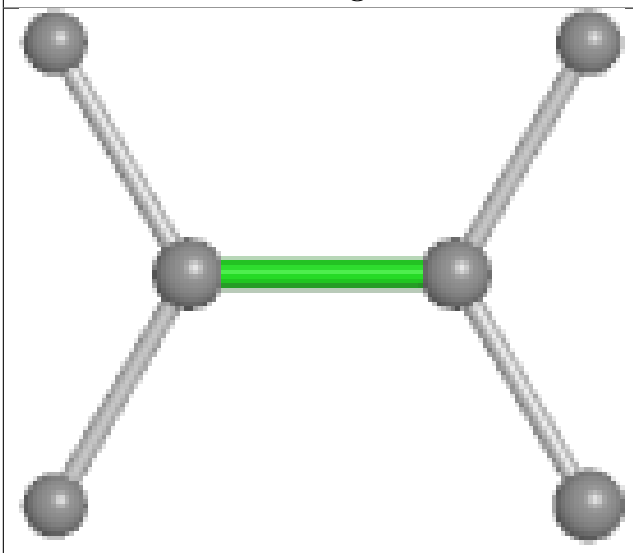
Ligand ALA G 605



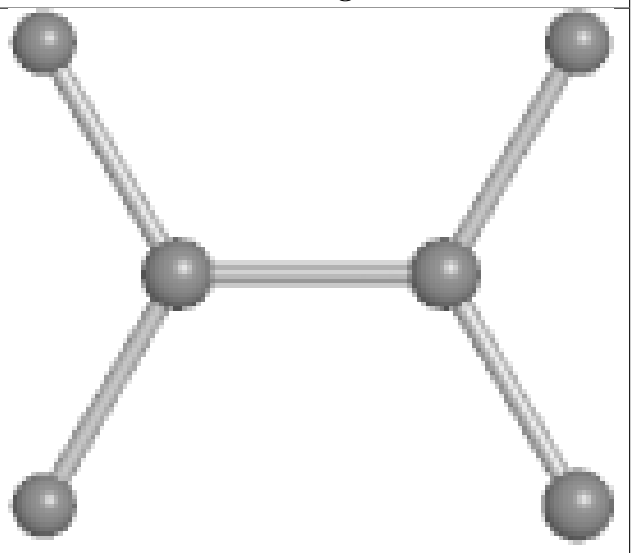
Bond lengths



Bond angles

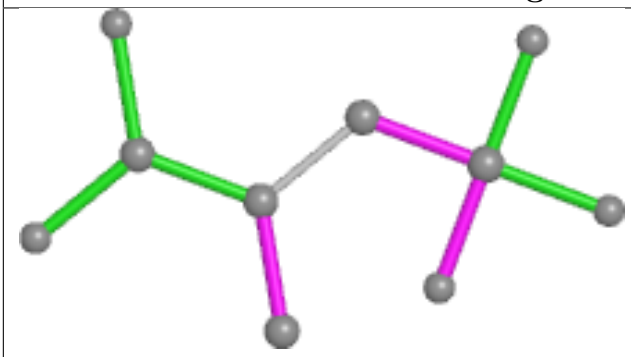


Torsions



Rings

Ligand GZ3 G 601



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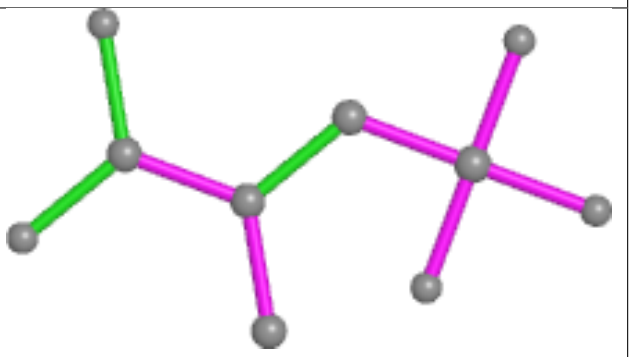
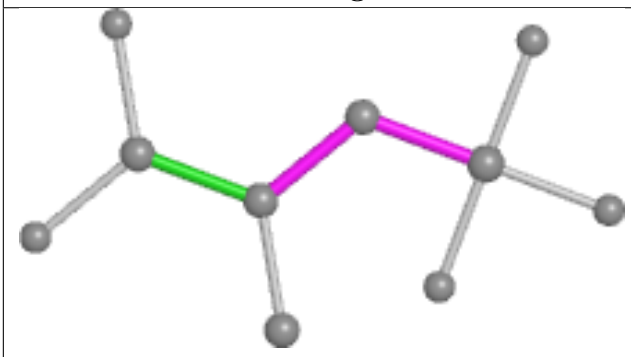
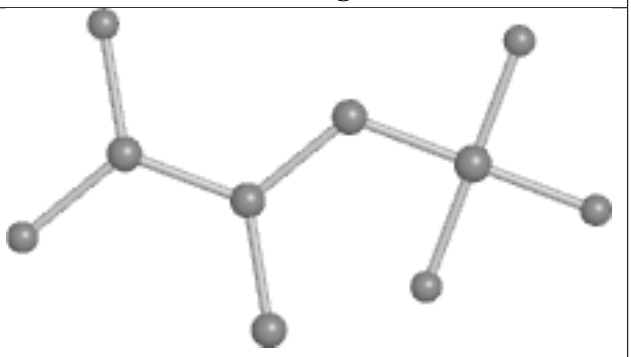


Bond angles

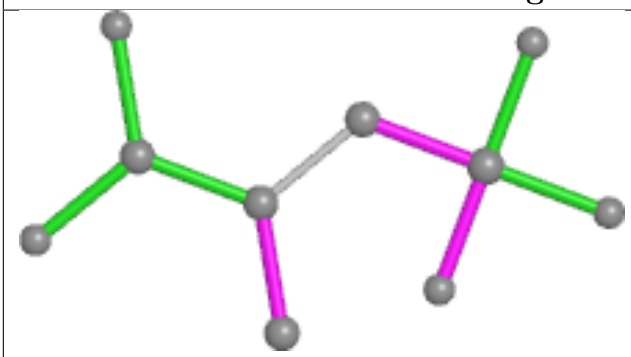


Torsions

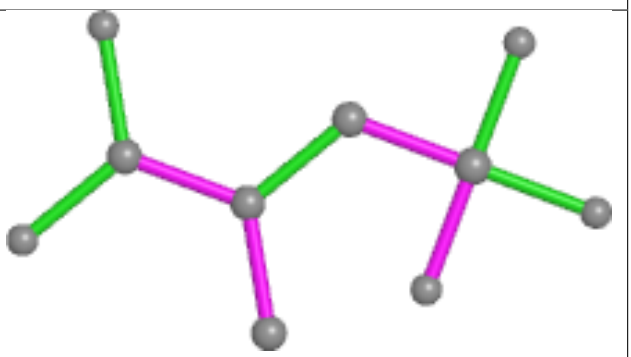


Rings

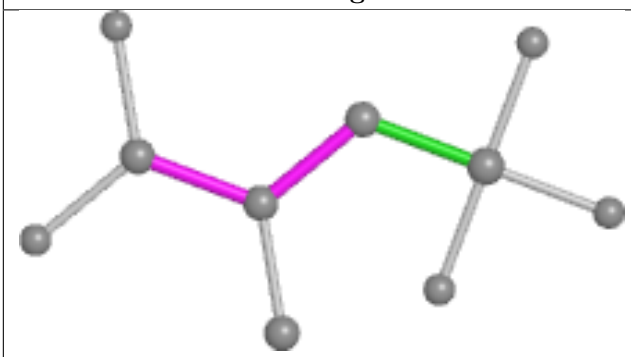
Ligand GZ3 H 601



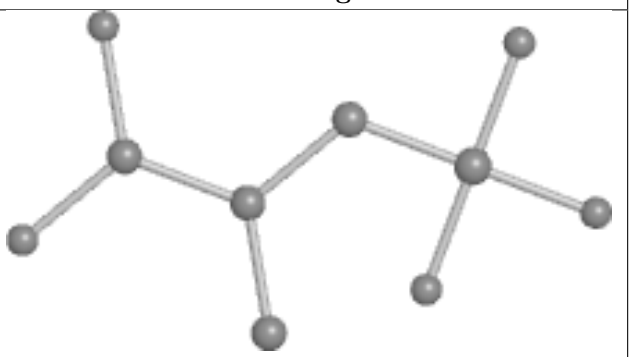
Bond lengths



Bond angles

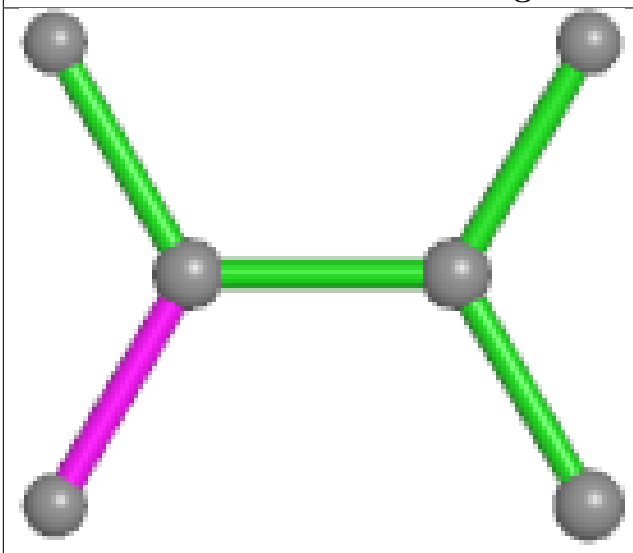


Torsions



Rings

Ligand ALA D 1007



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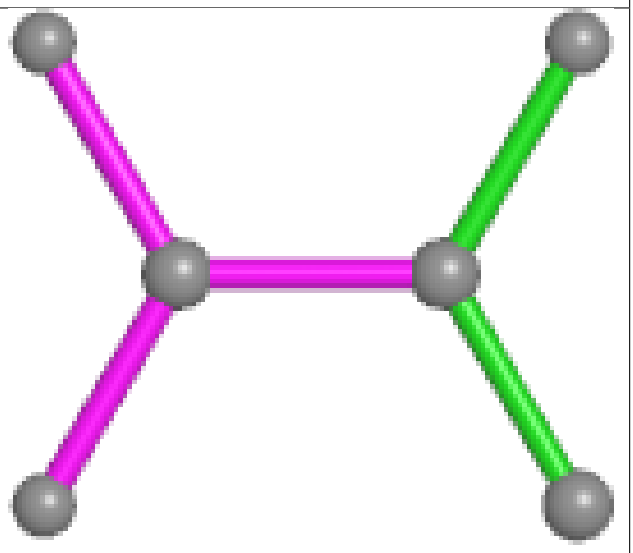
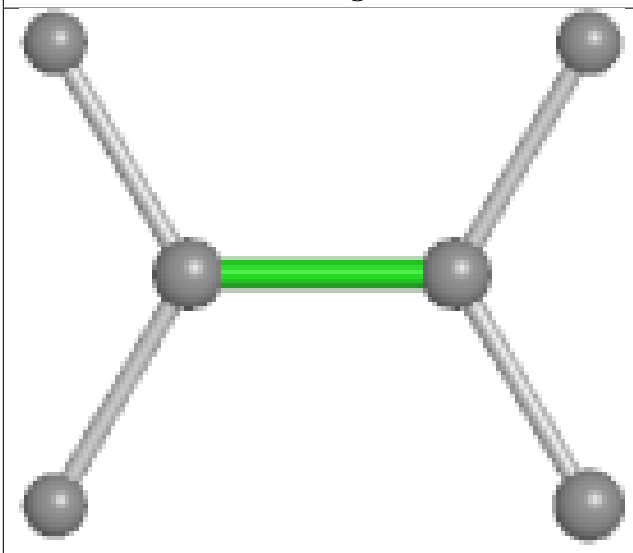
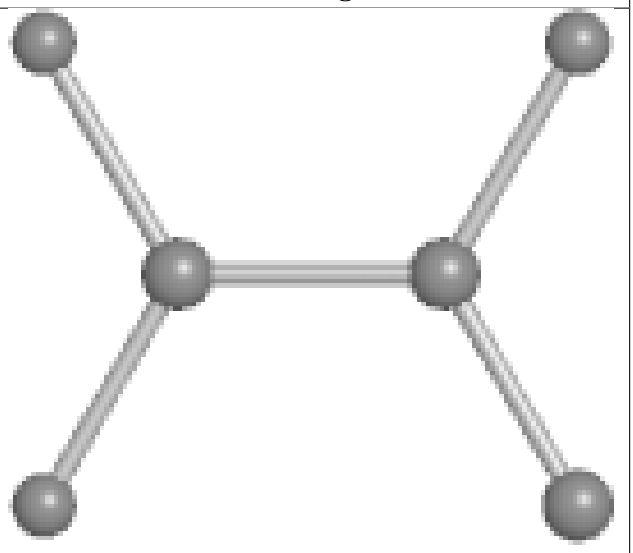


Bond angles

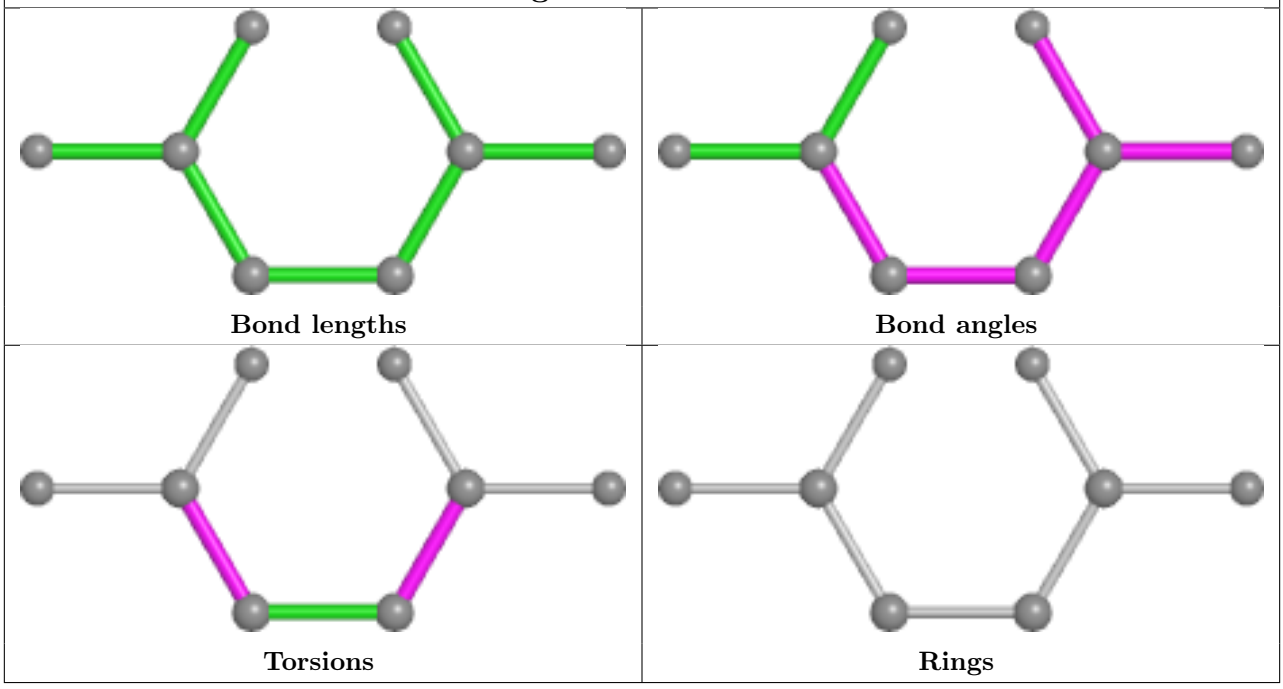


Torsions

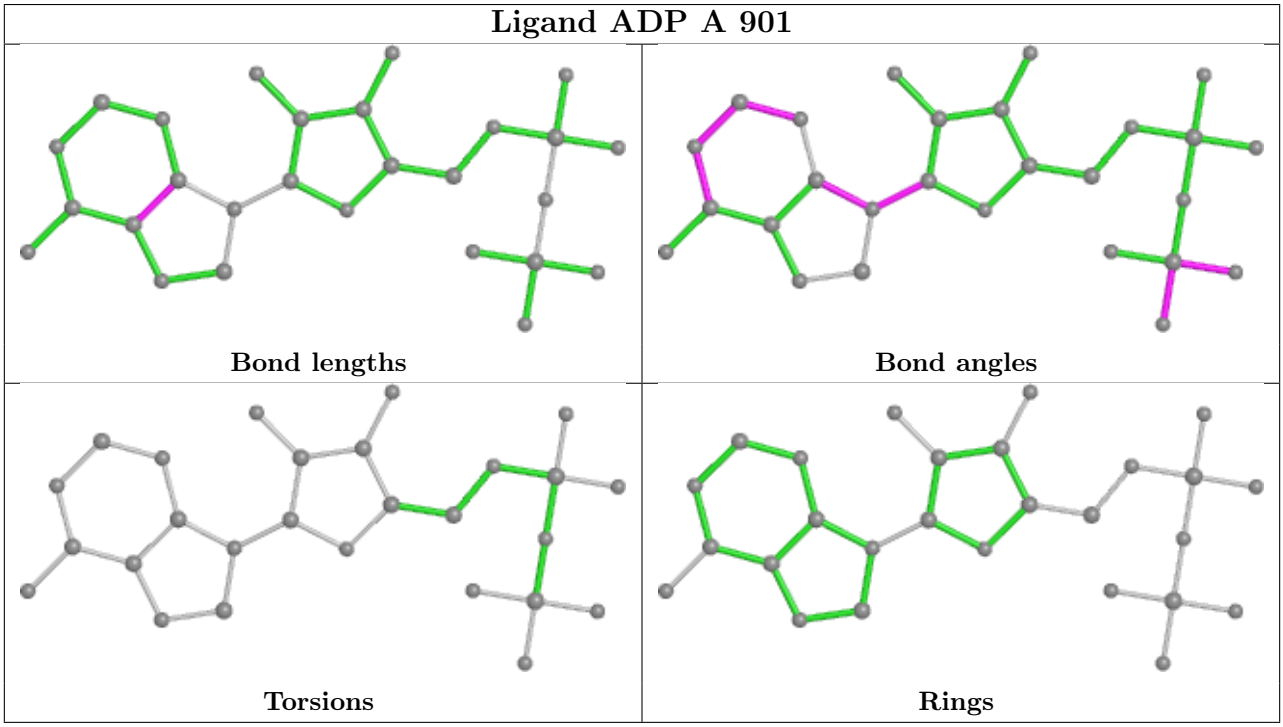


Rings

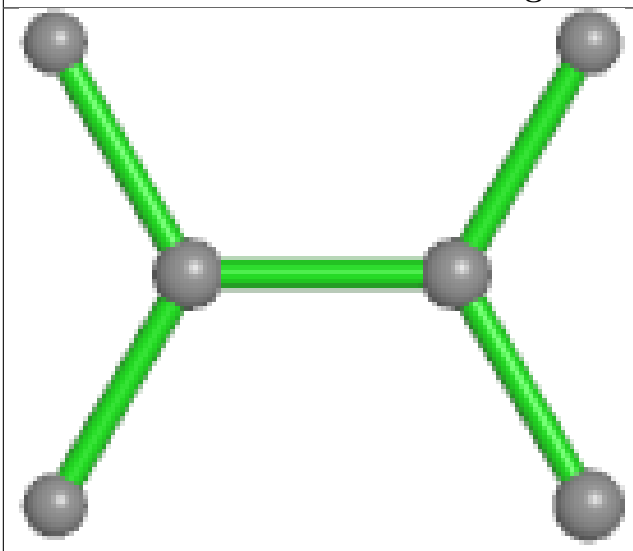
Ligand SIN A 902



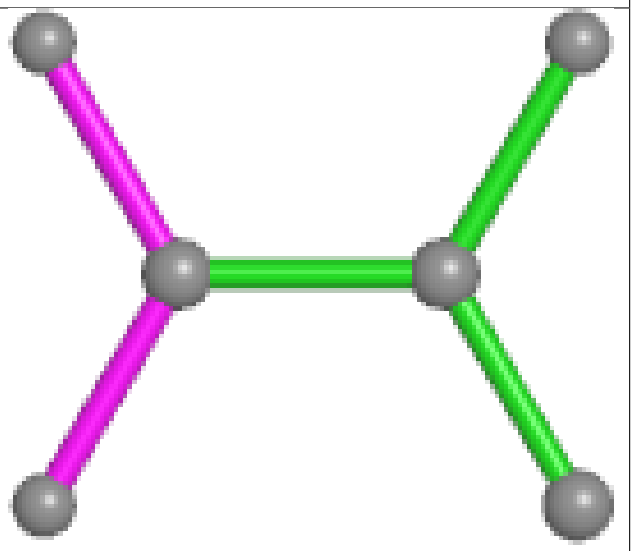
Ligand ADP A 901



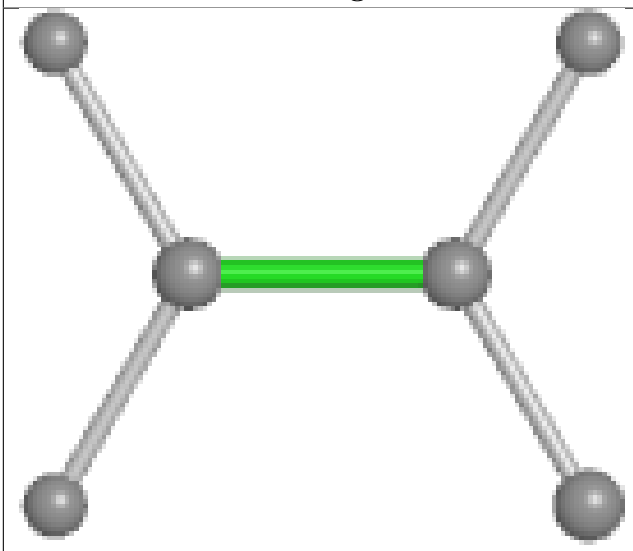
Ligand ALA E 606



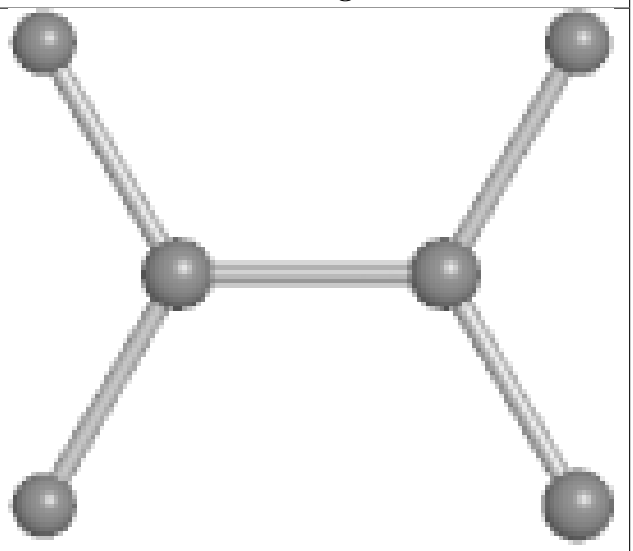
Bond lengths



Bond angles

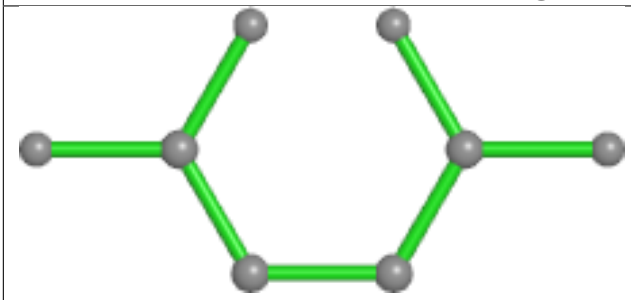


Torsions

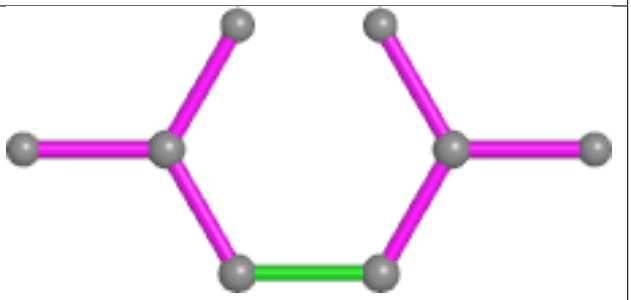


Rings

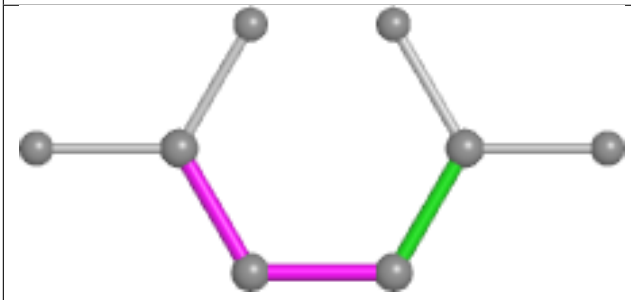
Ligand SIN F 606



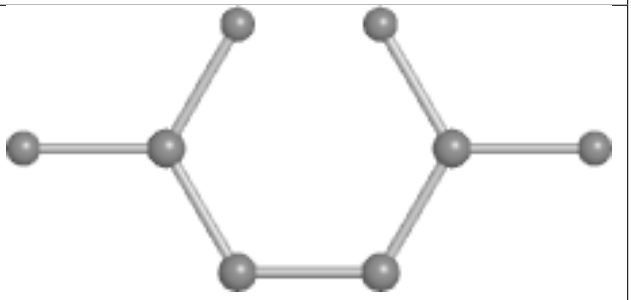
Bond lengths



Bond angles

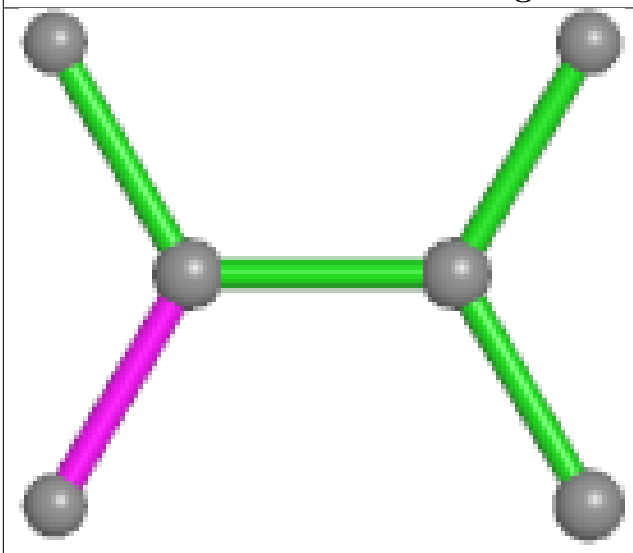


Torsions



Rings

Ligand ALA C 1007



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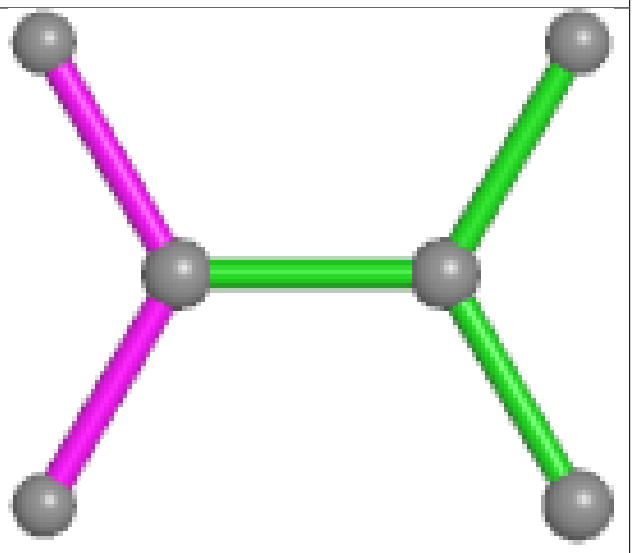
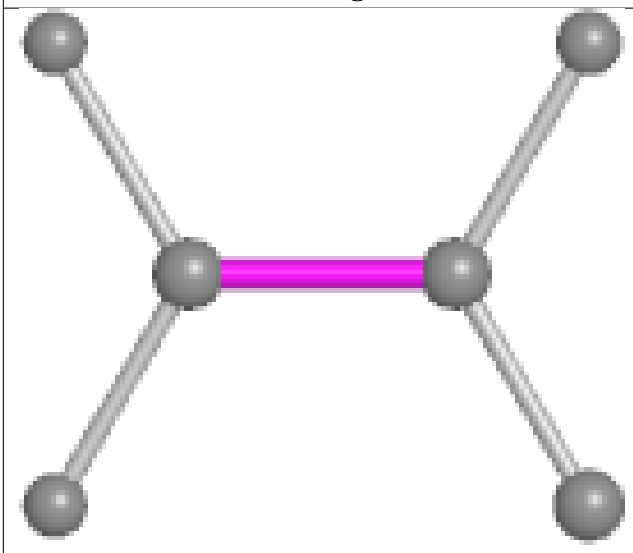
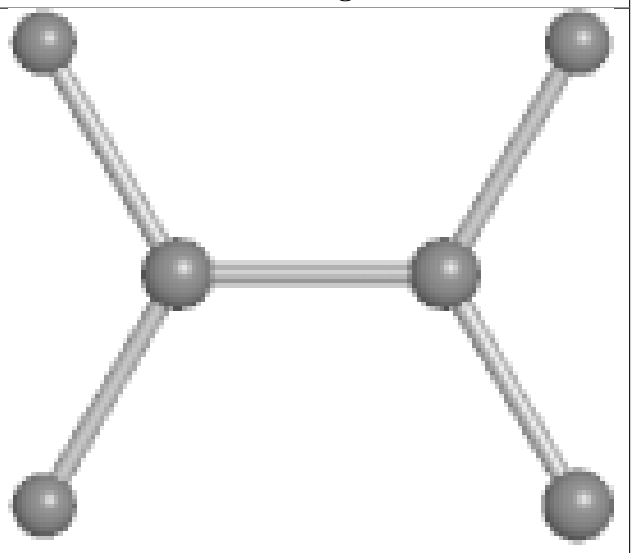


Bond angles

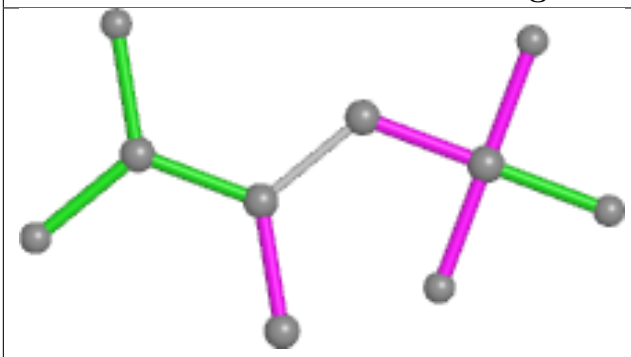


Torsions

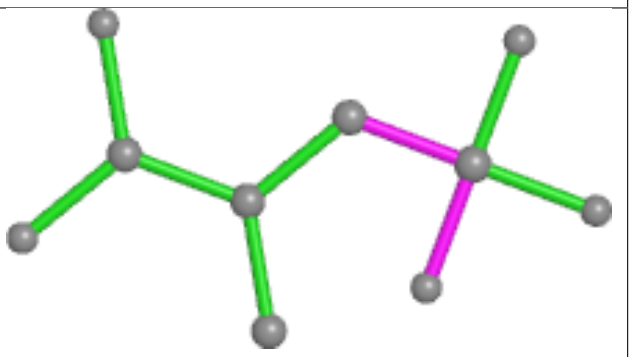


Rings

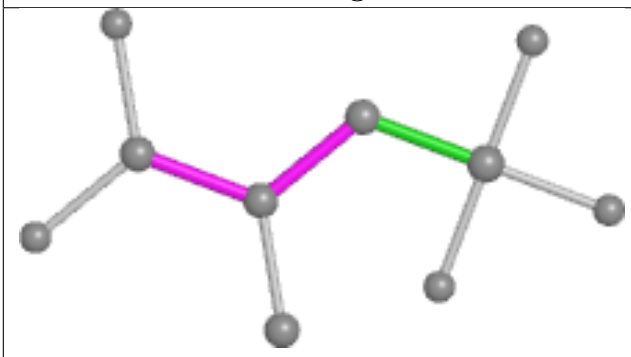
Ligand GZ3 F 602



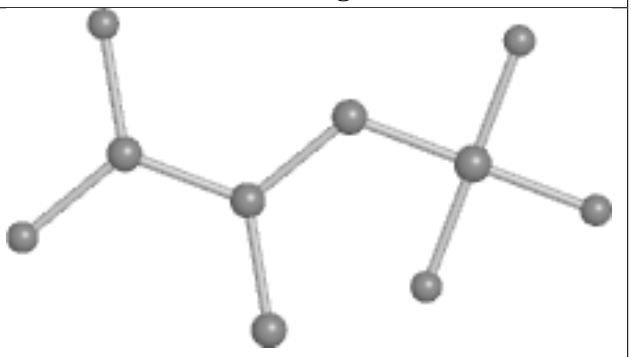
Bond lengths



Bond angles

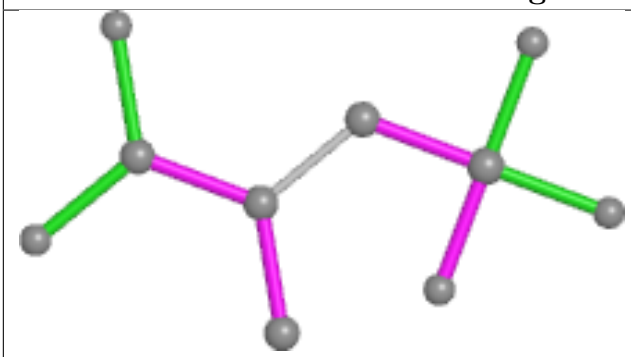


Torsions

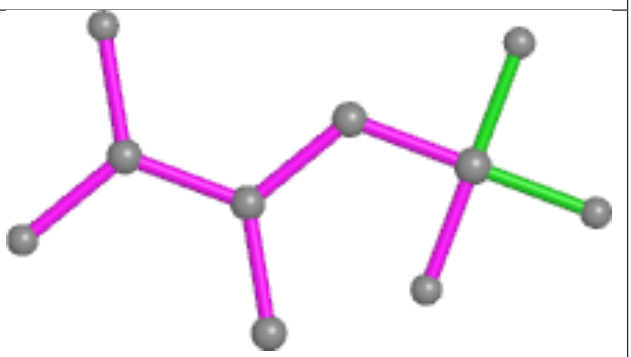


Rings

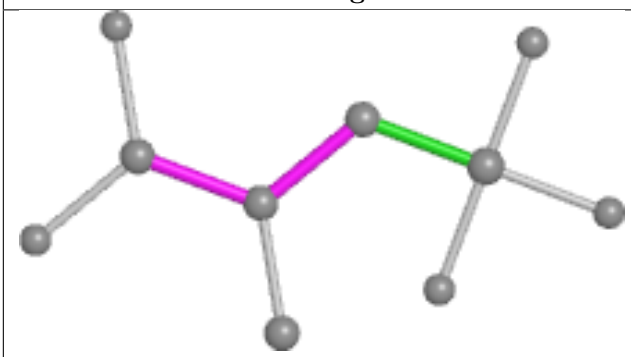
Ligand GZ3 E 601



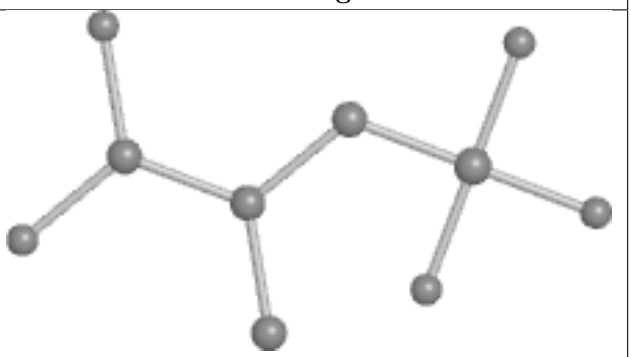
Bond lengths



Bond angles

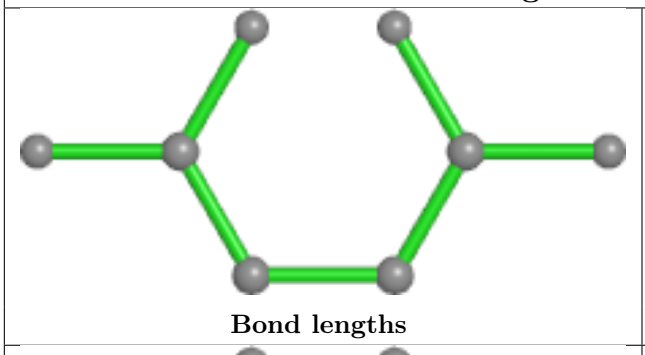


Torsions

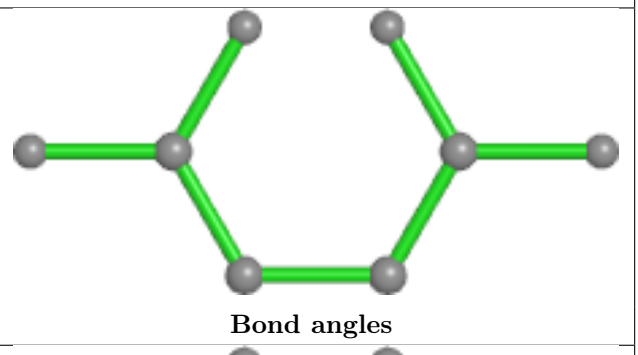


Rings

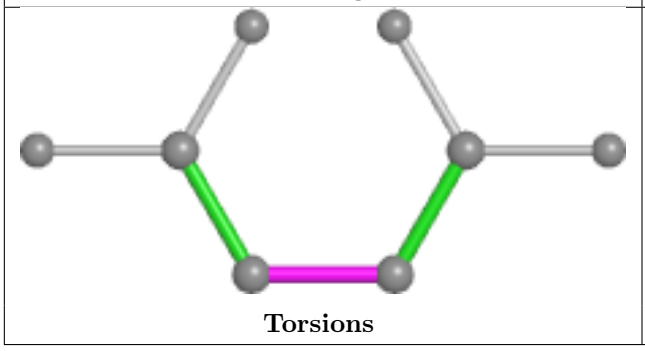
Ligand SIN D 1006



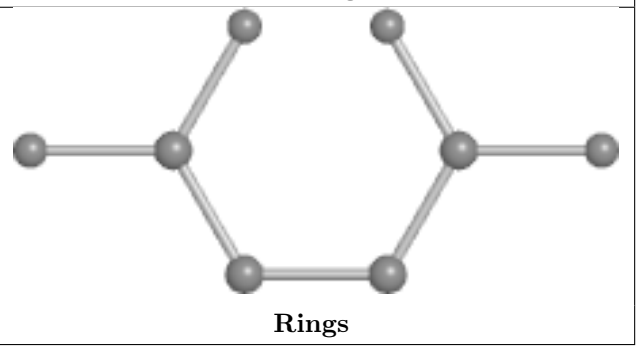
Bond lengths



Bond angles

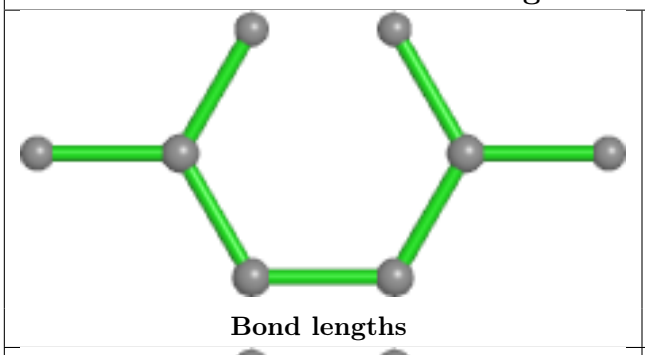


Torsions

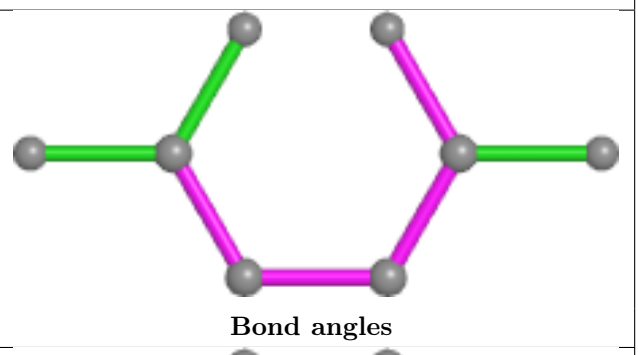


Rings

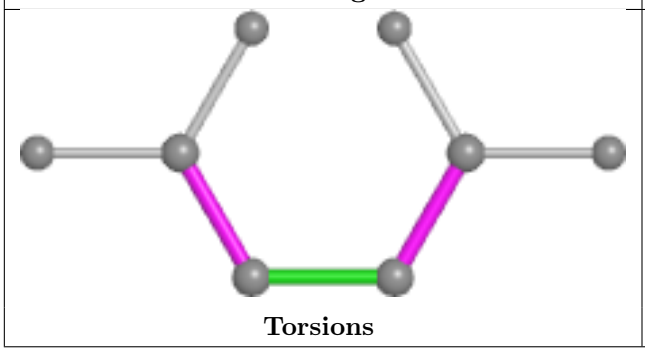
Ligand SIN B 1002



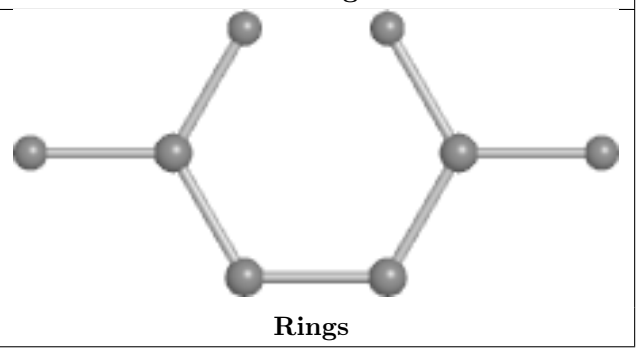
Bond lengths



Bond angles

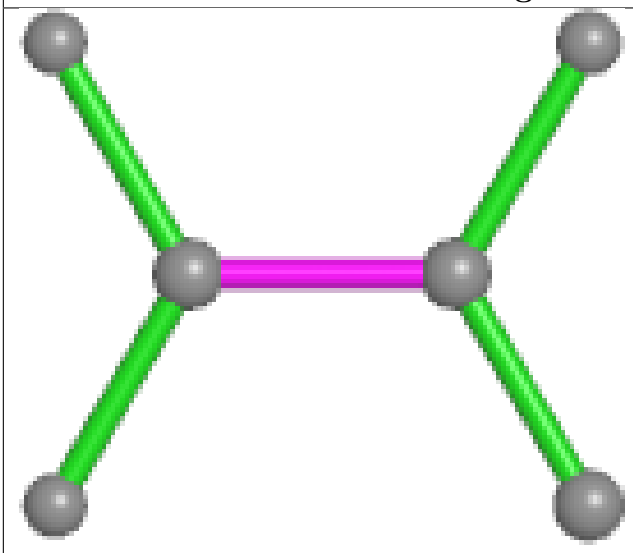


Torsions

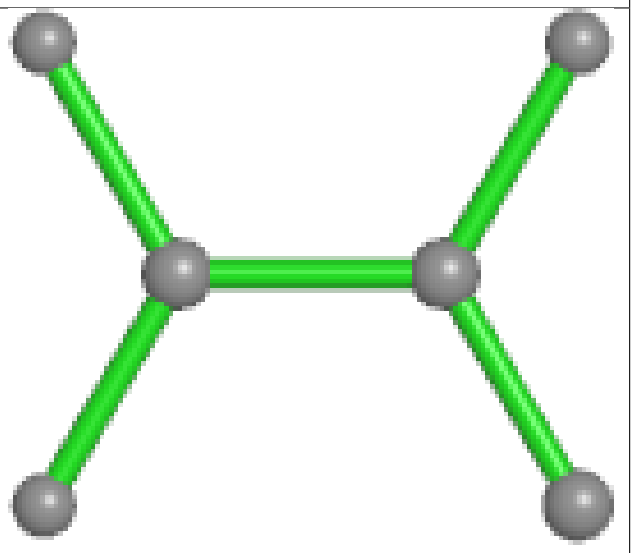


Rings

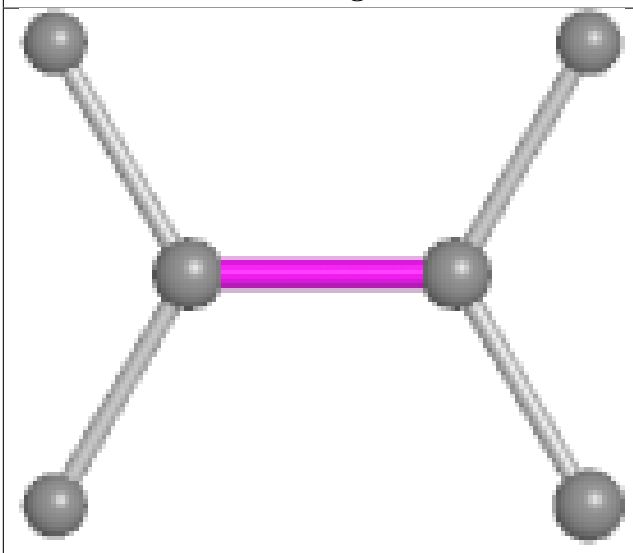
Ligand ALA B 1007



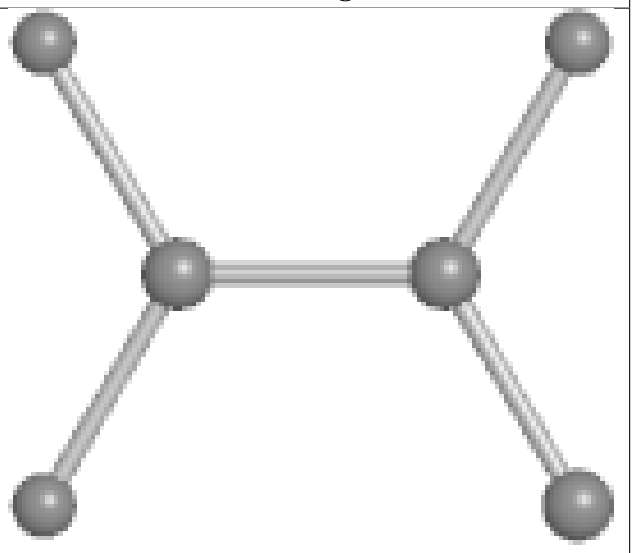
Bond lengths



Bond angles

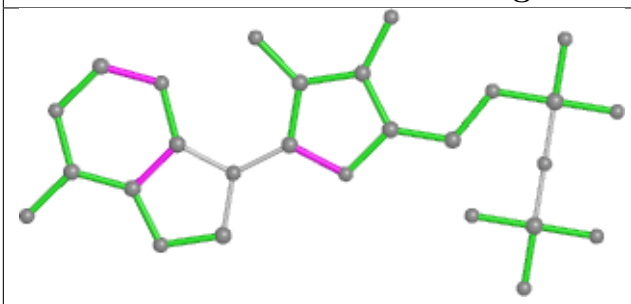


Torsions

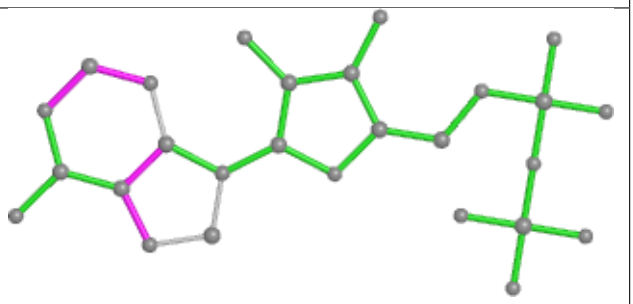


Rings

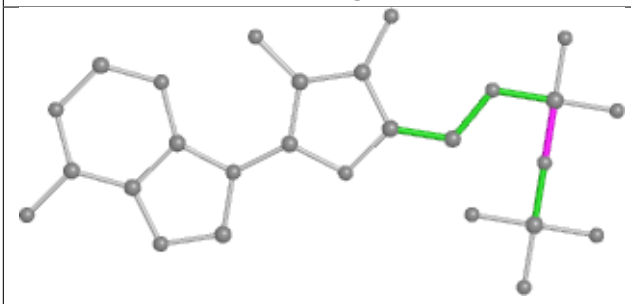
Ligand ADP C 1001



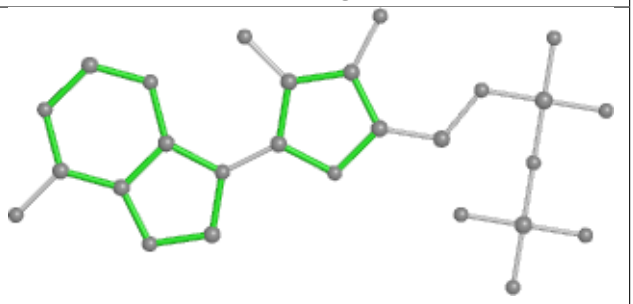
Bond lengths



Bond angles

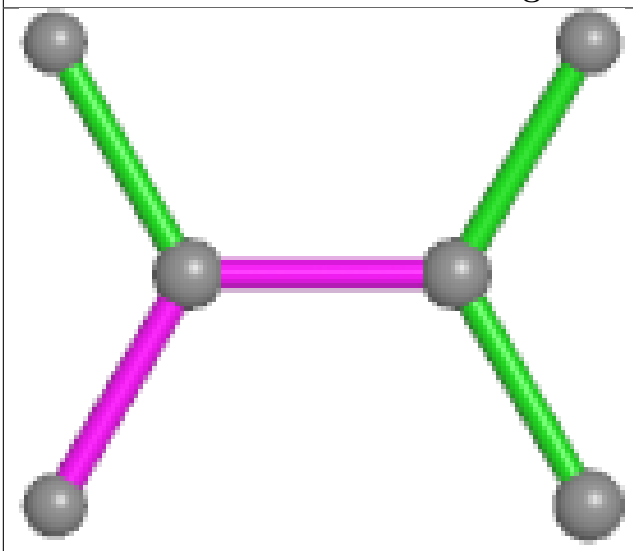


Torsions

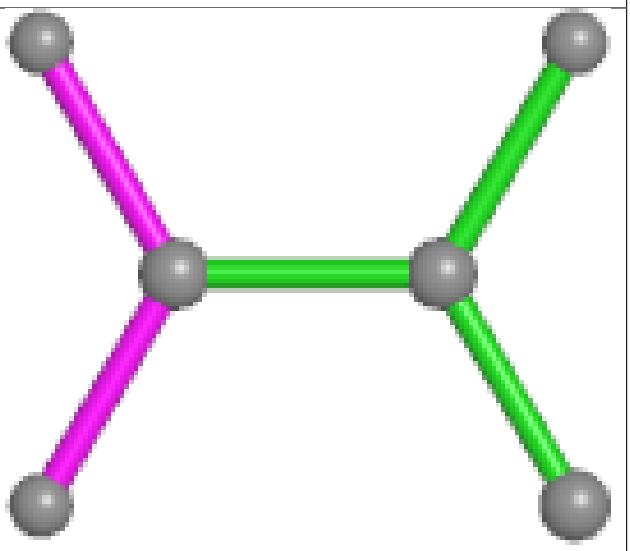


Rings

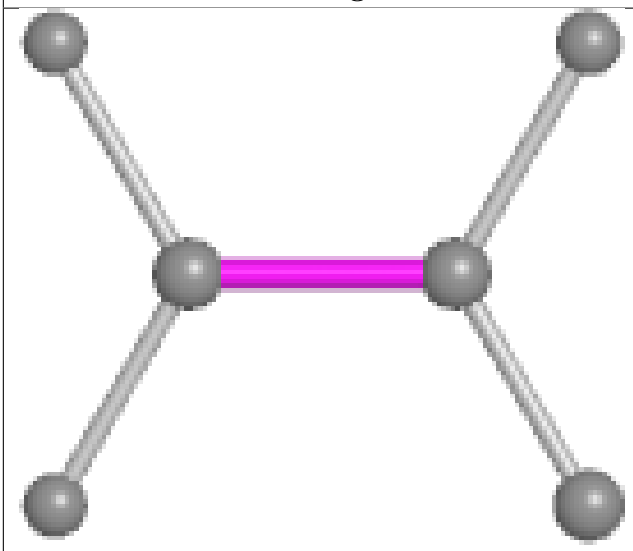
Ligand ALA A 907



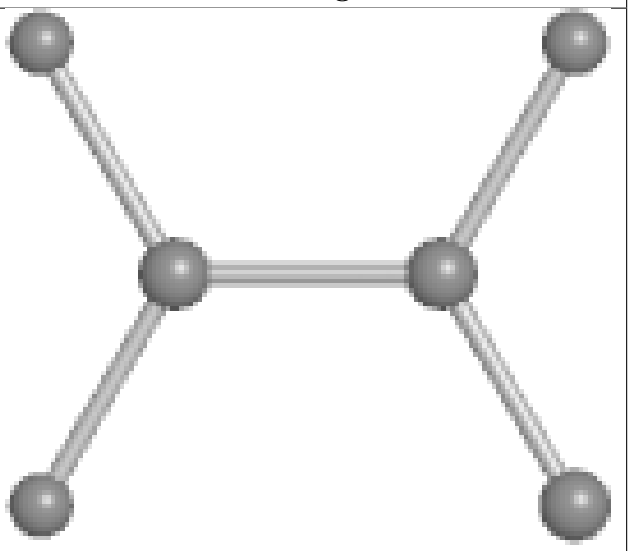
Bond lengths



Bond angles

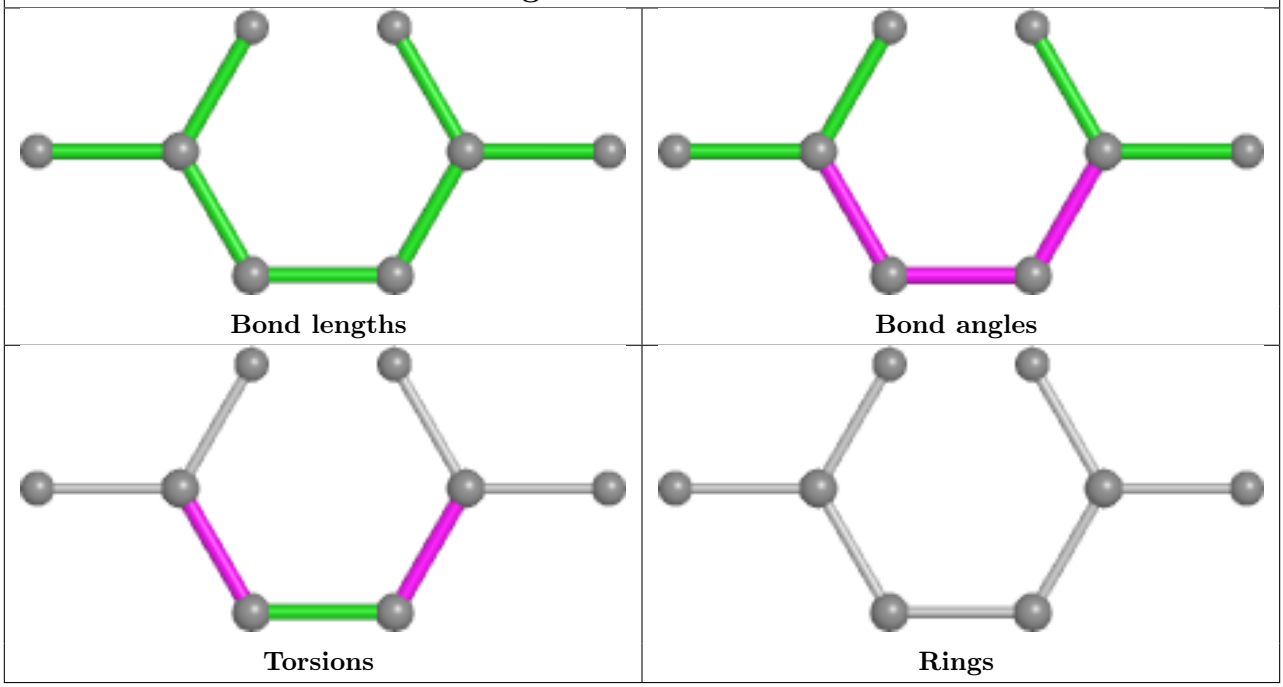


Torsions

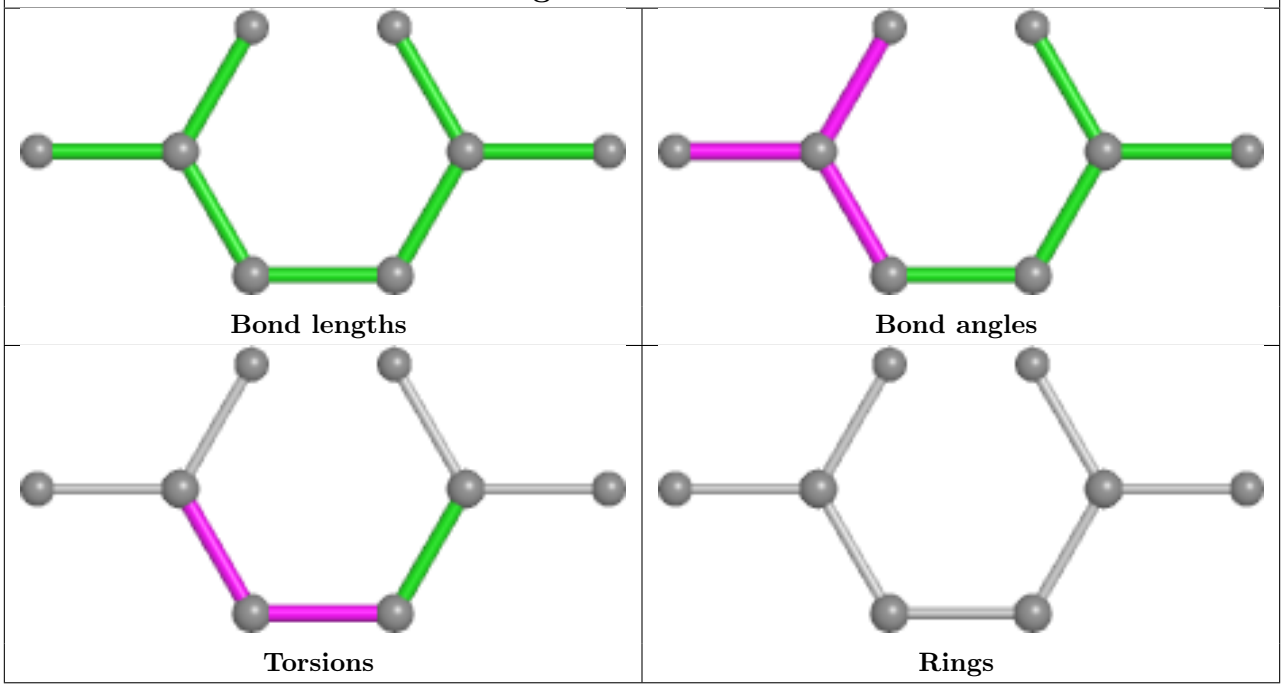


Rings

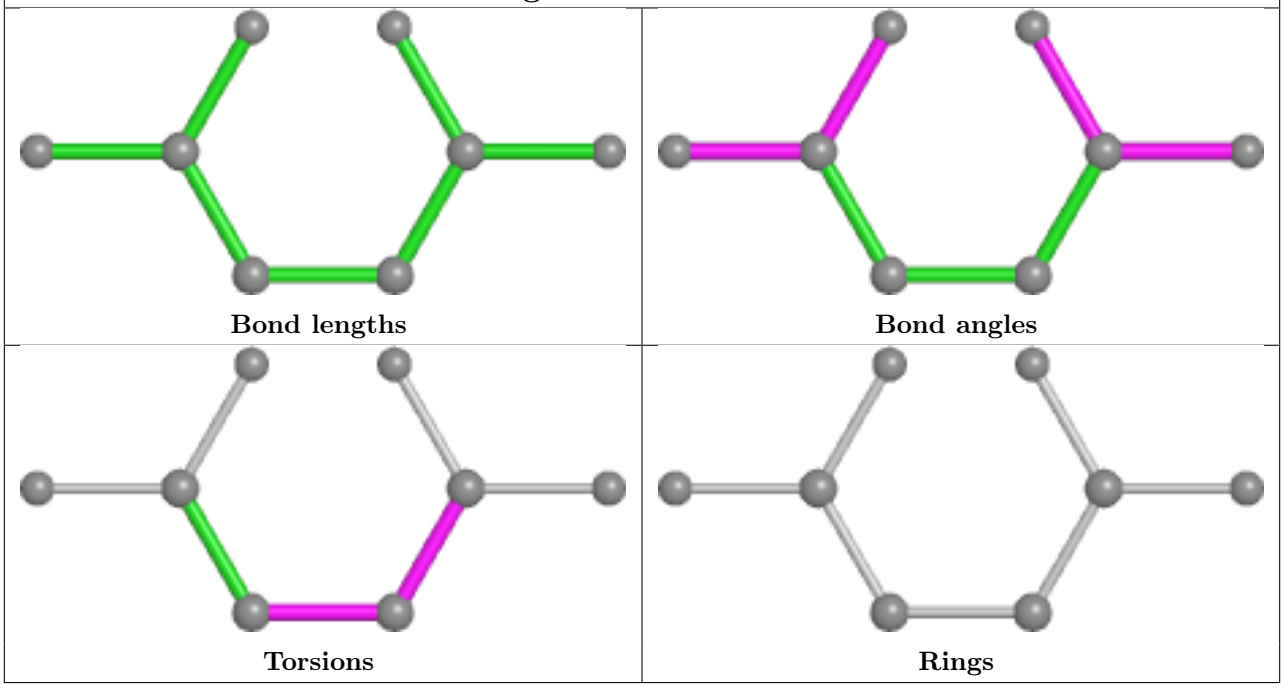
Ligand SIN D 1002



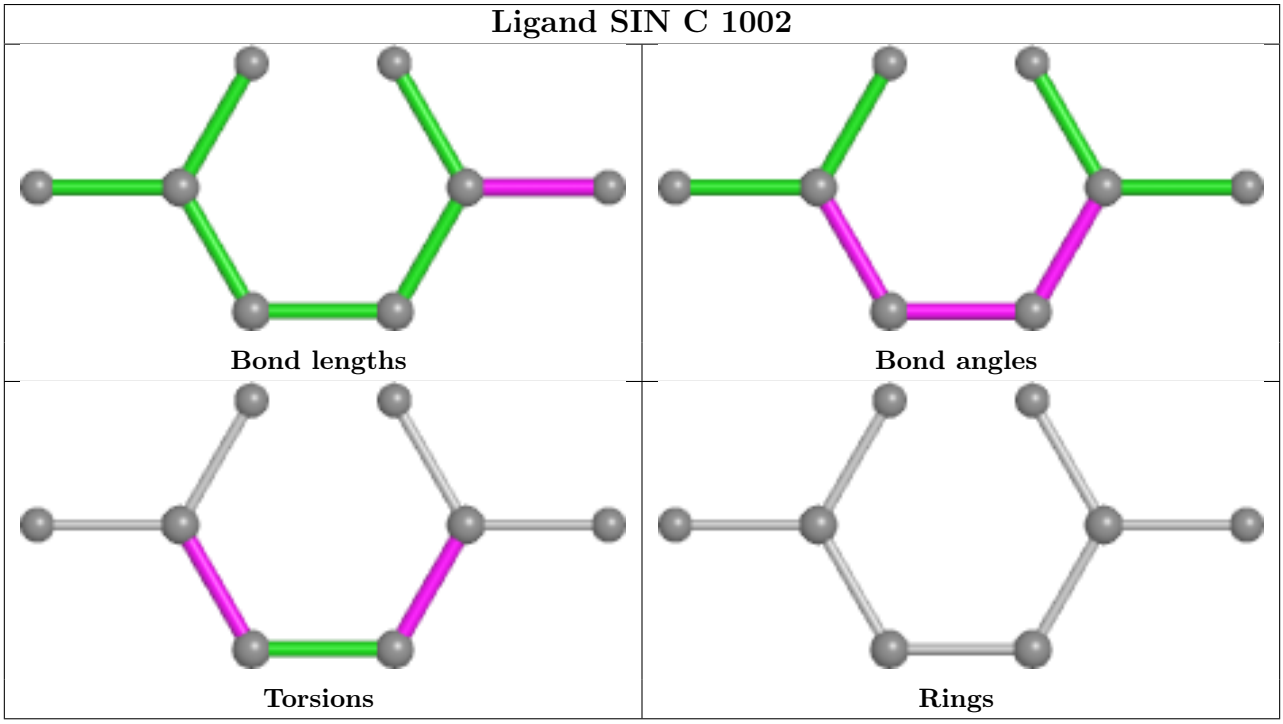
Ligand SIN E 605



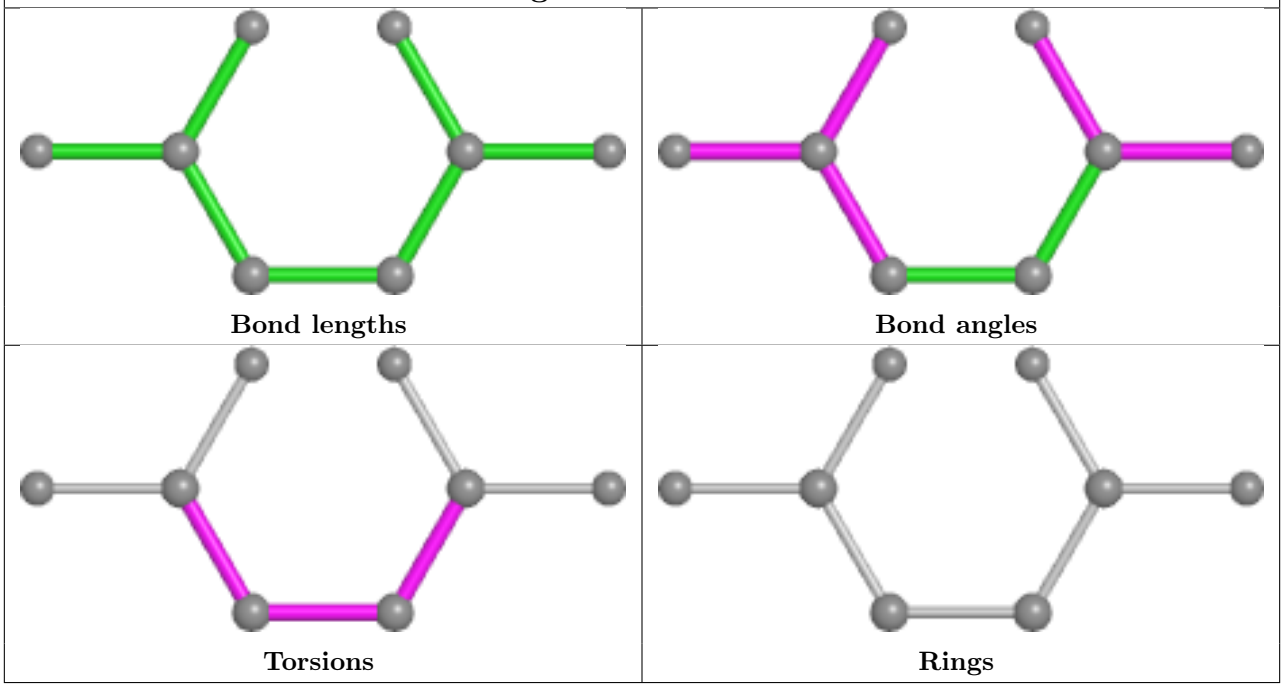
Ligand SIN B 1006



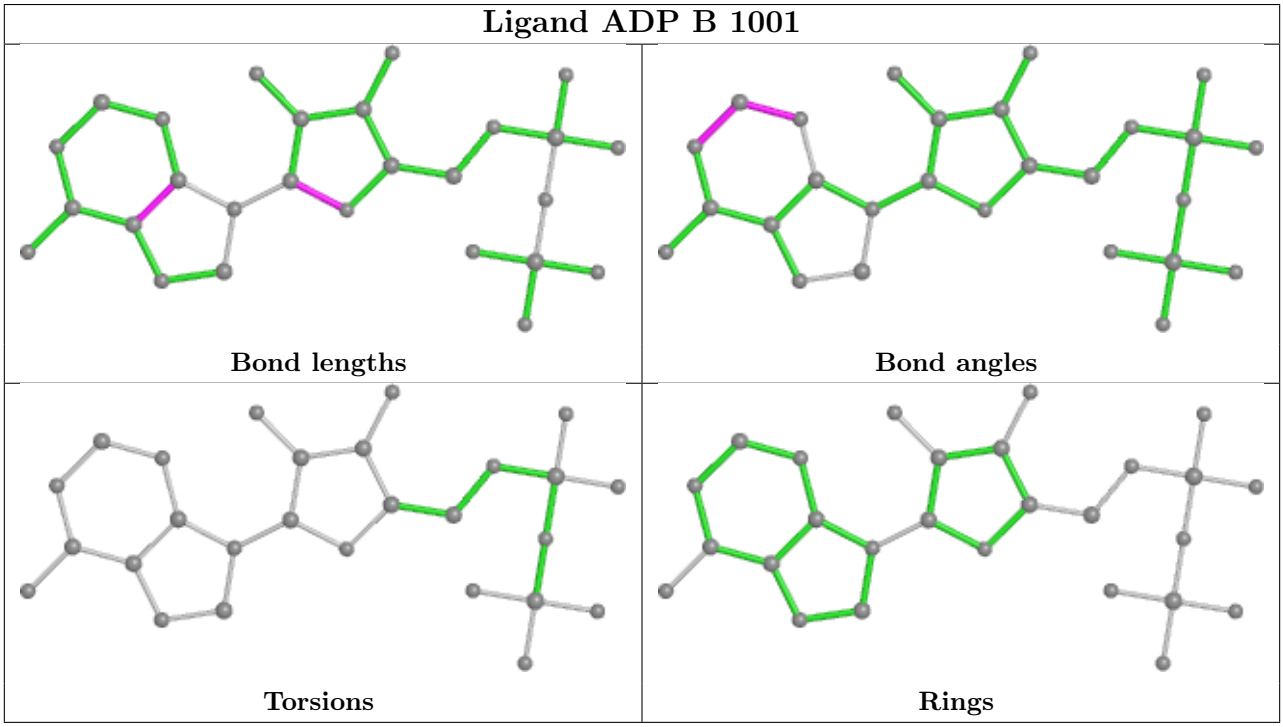
Ligand SIN C 1002



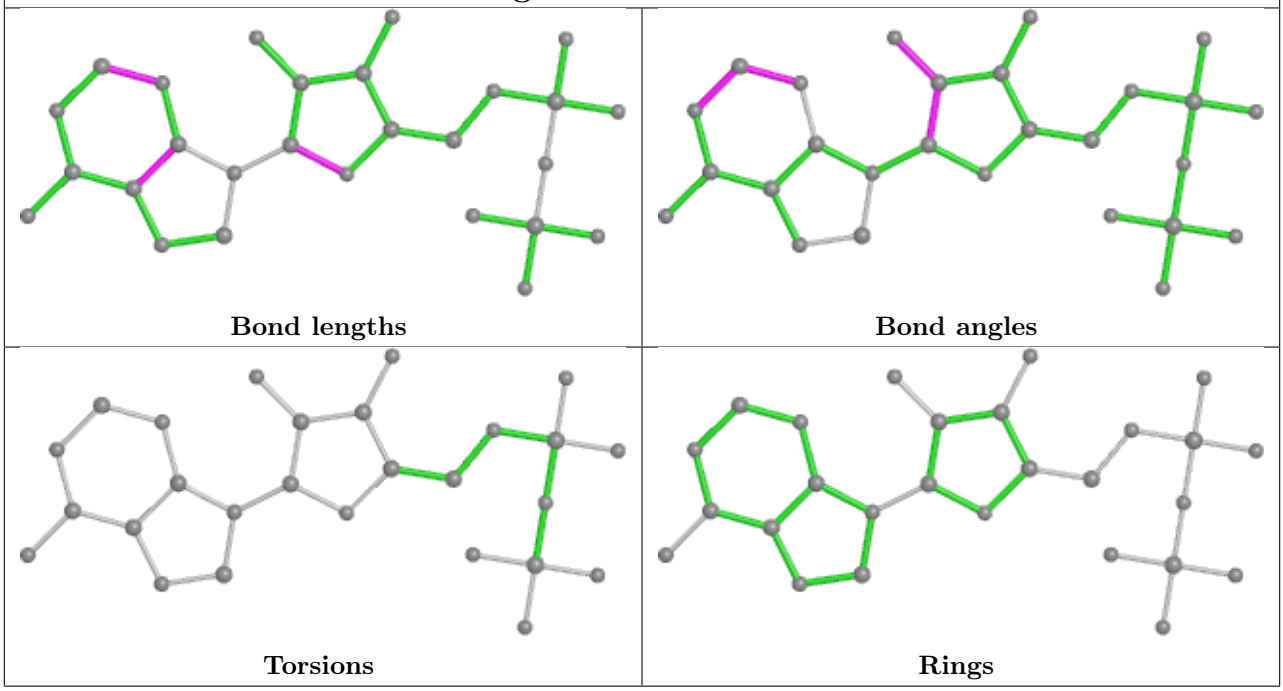
Ligand SIN H 604



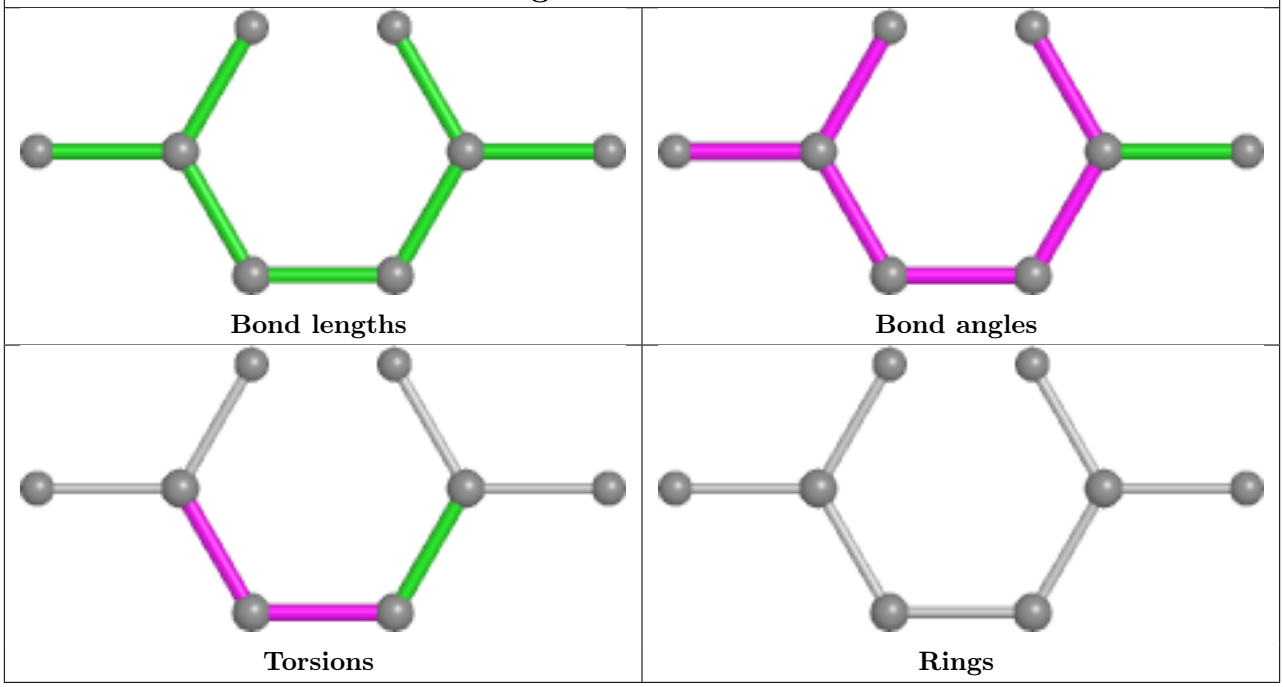
Ligand ADP B 1001



Ligand ADP D 1001



Ligand SIN A 906



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	519/531 (97%)	-0.37	5 (0%) 82 86	15, 21, 36, 54	0
1	B	519/531 (97%)	-0.48	2 (0%) 92 94	14, 21, 38, 58	0
1	C	519/531 (97%)	-0.10	28 (5%) 25 34	15, 27, 53, 82	0
1	D	522/531 (98%)	-0.39	4 (0%) 86 89	16, 26, 42, 60	0
1	E	519/531 (97%)	-0.62	1 (0%) 95 96	14, 19, 34, 61	0
1	F	515/531 (96%)	-0.33	6 (1%) 79 83	15, 23, 45, 65	0
1	G	506/531 (95%)	0.11	60 (11%) 4 6	15, 23, 76, 98	0
1	H	522/531 (98%)	-0.45	2 (0%) 92 94	15, 20, 37, 59	0
All	All	4141/4248 (97%)	-0.33	108 (2%) 56 64	14, 22, 46, 98	0

The worst 5 of 108 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	202	LEU	9.3
1	G	139	LEU	9.0
1	G	201	PHE	7.1
1	G	151	CYS	5.8
1	G	214	ALA	5.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (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
7	GOL	E	607	6/6	0.88	0.18	30,35,42,44	0
8	GZ3	G	601	10/10	0.89	0.14	24,29,48,82	0
3	SIN	C	1006	8/8	0.90	0.16	21,43,51,60	0
7	GOL	E	609	6/6	0.90	0.13	21,27,31,33	0
7	GOL	F	612	6/6	0.90	0.17	25,36,44,47	0
7	GOL	C	1011	6/6	0.90	0.12	33,45,55,55	0
7	GOL	F	610	6/6	0.91	0.12	31,33,35,43	0
3	SIN	D	1006	8/8	0.91	0.14	25,47,57,61	0
8	GZ3	F	602	10/10	0.91	0.13	20,28,38,48	0
7	GOL	C	1012	6/6	0.91	0.14	38,46,53,64	0
7	GOL	C	1010	6/6	0.92	0.12	35,41,45,45	0
7	GOL	F	609	6/6	0.92	0.17	30,35,36,38	0
3	SIN	A	906	8/8	0.93	0.12	19,36,41,46	0
3	SIN	B	1006	8/8	0.93	0.10	18,34,43,43	0
3	SIN	E	605	8/8	0.93	0.13	20,31,52,53	0
3	SIN	F	606	8/8	0.93	0.12	23,44,59,62	0
3	SIN	G	604	8/8	0.93	0.12	22,43,53,53	0
3	SIN	H	604	8/8	0.94	0.10	21,32,46,49	0
7	GOL	A	910	6/6	0.94	0.10	35,39,40,47	0
7	GOL	F	611	6/6	0.94	0.11	29,32,34,35	0
7	GOL	A	911	6/6	0.94	0.10	30,34,35,36	0
7	GOL	G	606	6/6	0.94	0.10	27,32,39,40	0
7	GOL	E	608	6/6	0.94	0.12	27,30,39,40	0
3	SIN	C	1002	8/8	0.94	0.09	29,34,40,44	0
7	GOL	E	610	6/6	0.95	0.20	25,28,33,40	0
7	GOL	B	1009	6/6	0.95	0.17	28,34,37,37	0
7	GOL	G	607	6/6	0.95	0.16	25,35,40,43	0
7	GOL	B	1010	6/6	0.95	0.12	30,39,49,49	0
7	GOL	C	1008	6/6	0.95	0.09	30,33,43,47	0
8	GZ3	H	601	10/10	0.95	0.12	24,27,40,45	0
7	GOL	F	608	6/6	0.96	0.07	25,27,32,35	0
7	GOL	C	1009	6/6	0.96	0.15	28,36,39,42	0
7	GOL	A	908	6/6	0.96	0.13	22,27,29,33	0
7	GOL	A	909	6/6	0.96	0.07	30,36,40,40	0
3	SIN	B	1002	8/8	0.96	0.12	18,20,25,25	0
7	GOL	D	1008	6/6	0.96	0.14	26,28,39,43	0
2	ADP	F	601	27/27	0.96	0.18	30,41,47,54	0

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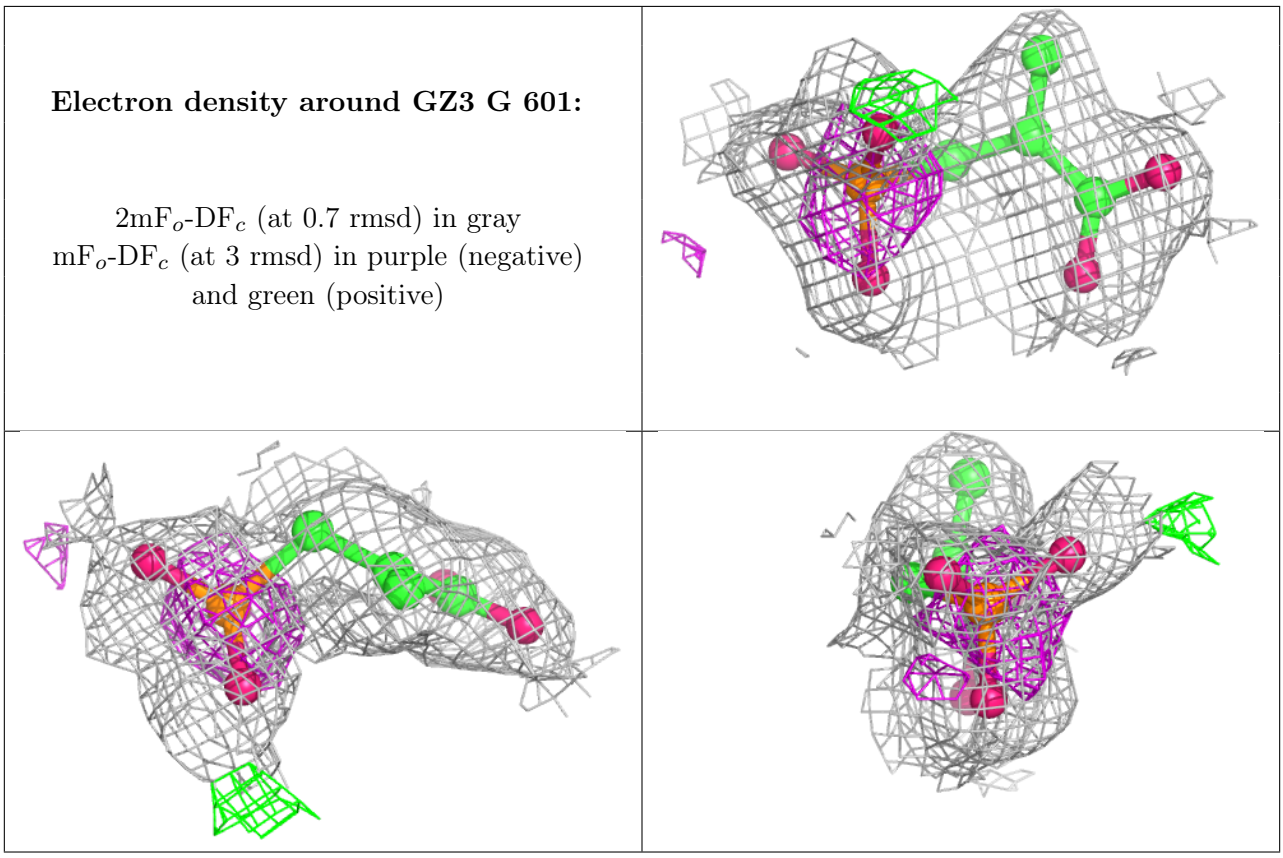
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GZ3	E	601	10/10	0.96	0.08	16,25,34,36	0
3	SIN	A	902	8/8	0.96	0.11	18,22,29,29	0
2	ADP	C	1001	27/27	0.96	0.08	26,36,44,46	0
3	SIN	D	1002	8/8	0.96	0.10	22,28,31,31	0
6	ALA	B	1007	6/6	0.97	0.09	17,20,21,22	0
7	GOL	H	606	6/6	0.97	0.09	21,29,31,33	0
7	GOL	H	607	6/6	0.97	0.11	25,29,37,40	0
6	ALA	F	607	6/6	0.97	0.10	16,18,20,20	0
6	ALA	G	605	6/6	0.97	0.10	17,19,22,23	0
4	MN	H	608	1/1	0.97	0.10	59,59,59,59	0
6	ALA	A	907	6/6	0.97	0.12	16,17,20,21	0
6	ALA	D	1007	6/6	0.98	0.06	19,21,22,22	0
6	ALA	E	606	6/6	0.98	0.10	14,15,17,19	0
2	ADP	D	1001	27/27	0.98	0.07	21,26,31,31	0
6	ALA	C	1007	6/6	0.98	0.10	19,21,21,22	0
7	GOL	B	1008	6/6	0.98	0.09	19,23,24,30	0
4	MN	G	602	1/1	0.99	0.05	30,30,30,30	0
4	MN	H	602	1/1	0.99	0.06	25,25,25,25	0
2	ADP	B	1001	27/27	0.99	0.09	15,17,20,23	0
5	K	A	905	1/1	0.99	0.09	18,18,18,18	0
5	K	B	1004	1/1	0.99	0.08	18,18,18,18	0
5	K	C	1005	1/1	0.99	0.08	30,30,30,30	0
5	K	D	1005	1/1	0.99	0.08	26,26,26,26	0
2	ADP	A	901	27/27	0.99	0.10	16,19,22,25	0
4	MN	A	904	1/1	0.99	0.07	21,21,21,21	0
4	MN	B	1005	1/1	0.99	0.08	20,20,20,20	0
4	MN	D	1003	1/1	0.99	0.09	27,27,27,27	0
4	MN	E	603	1/1	0.99	0.03	47,47,47,47	0
4	MN	F	603	1/1	0.99	0.05	53,53,53,53	0
4	MN	F	604	1/1	0.99	0.07	22,22,22,22	0
6	ALA	H	605	6/6	0.99	0.07	15,17,18,19	0
5	K	G	603	1/1	1.00	0.05	22,22,22,22	0
5	K	H	603	1/1	1.00	0.05	22,22,22,22	0
4	MN	D	1004	1/1	1.00	0.07	22,22,22,22	0
4	MN	E	602	1/1	1.00	0.05	25,25,25,25	0
4	MN	A	903	1/1	1.00	0.10	21,21,21,21	0
4	MN	C	1003	1/1	1.00	0.04	33,33,33,33	0
4	MN	C	1004	1/1	1.00	0.07	30,30,30,30	0
4	MN	B	1003	1/1	1.00	0.08	21,21,21,21	0
5	K	E	604	1/1	1.00	0.05	24,24,24,24	0
5	K	F	605	1/1	1.00	0.05	23,23,23,23	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.

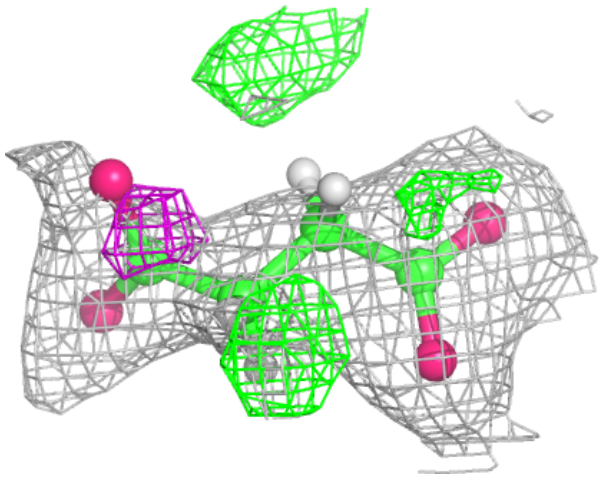
Electron density around GZ3 G 601:

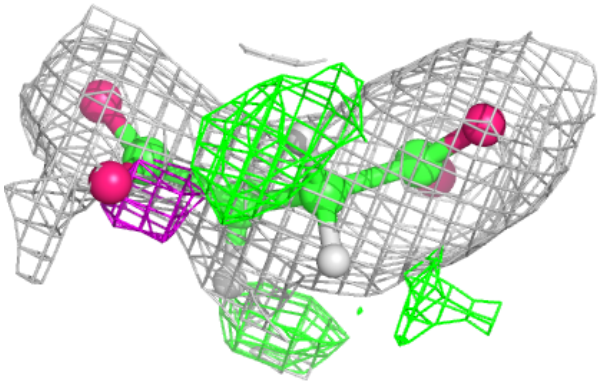
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

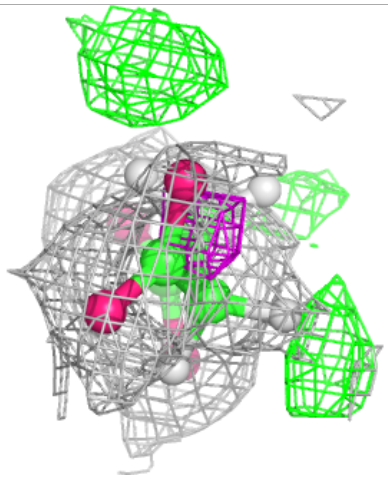


Electron density around SIN C 1006:

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

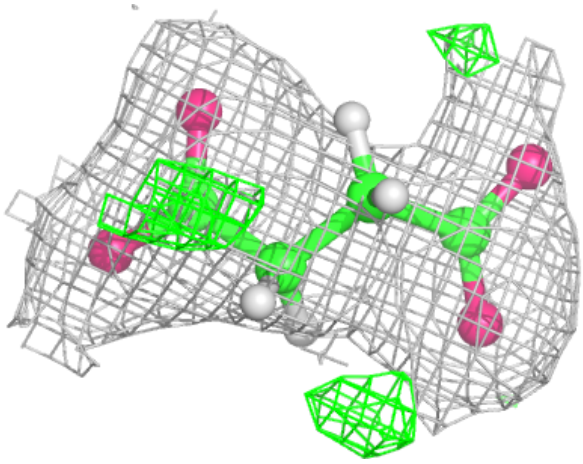


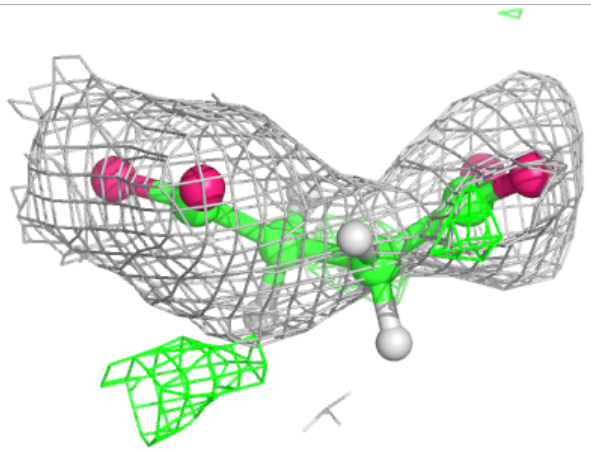


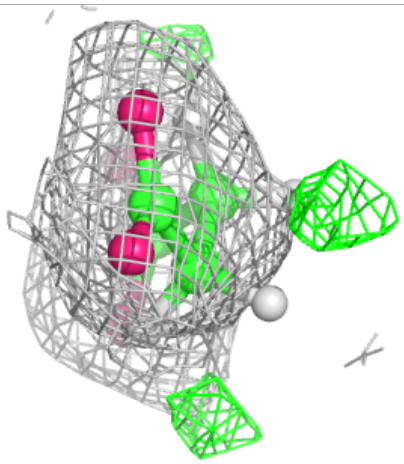


Electron density around SIN D 1006:

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

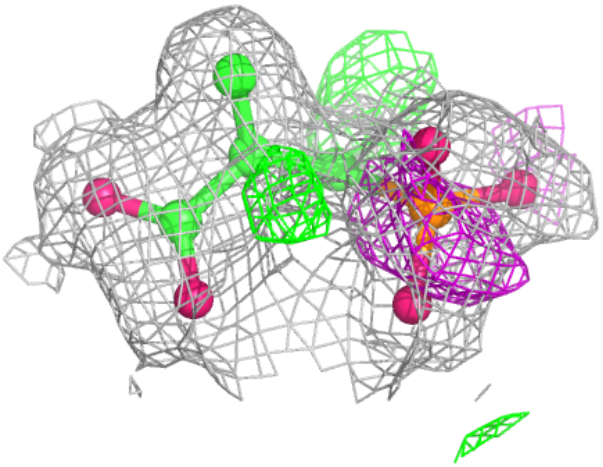


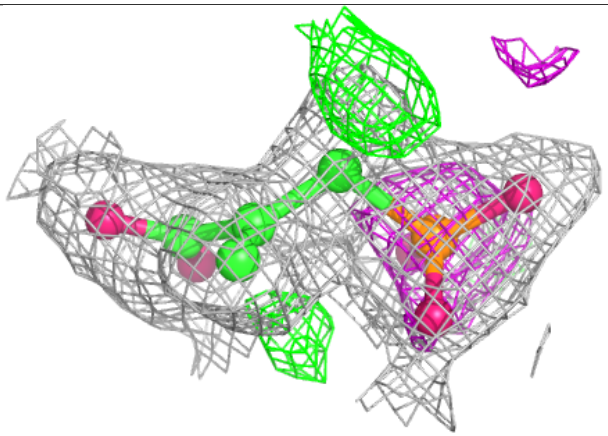


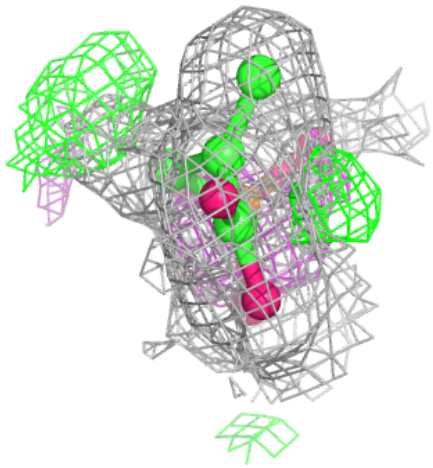


Electron density around GZ3 F 602:

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

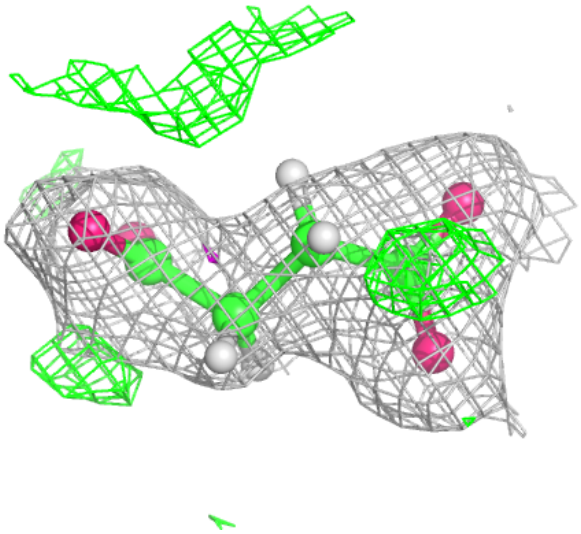


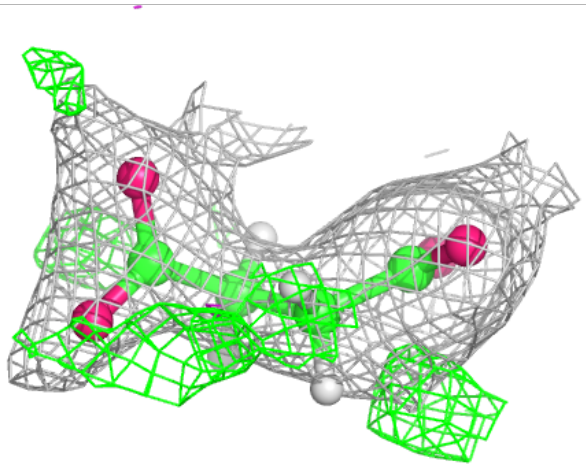


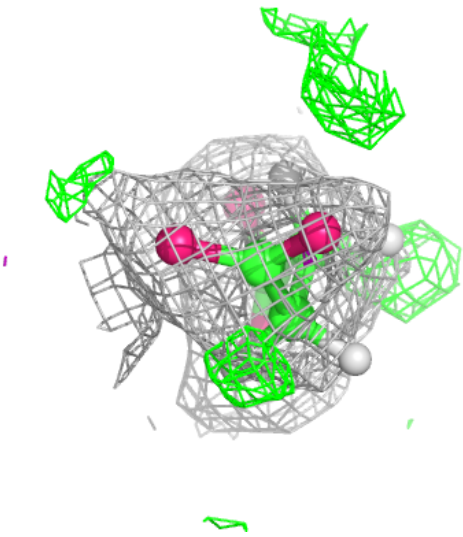


Electron density around SIN A 906:

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

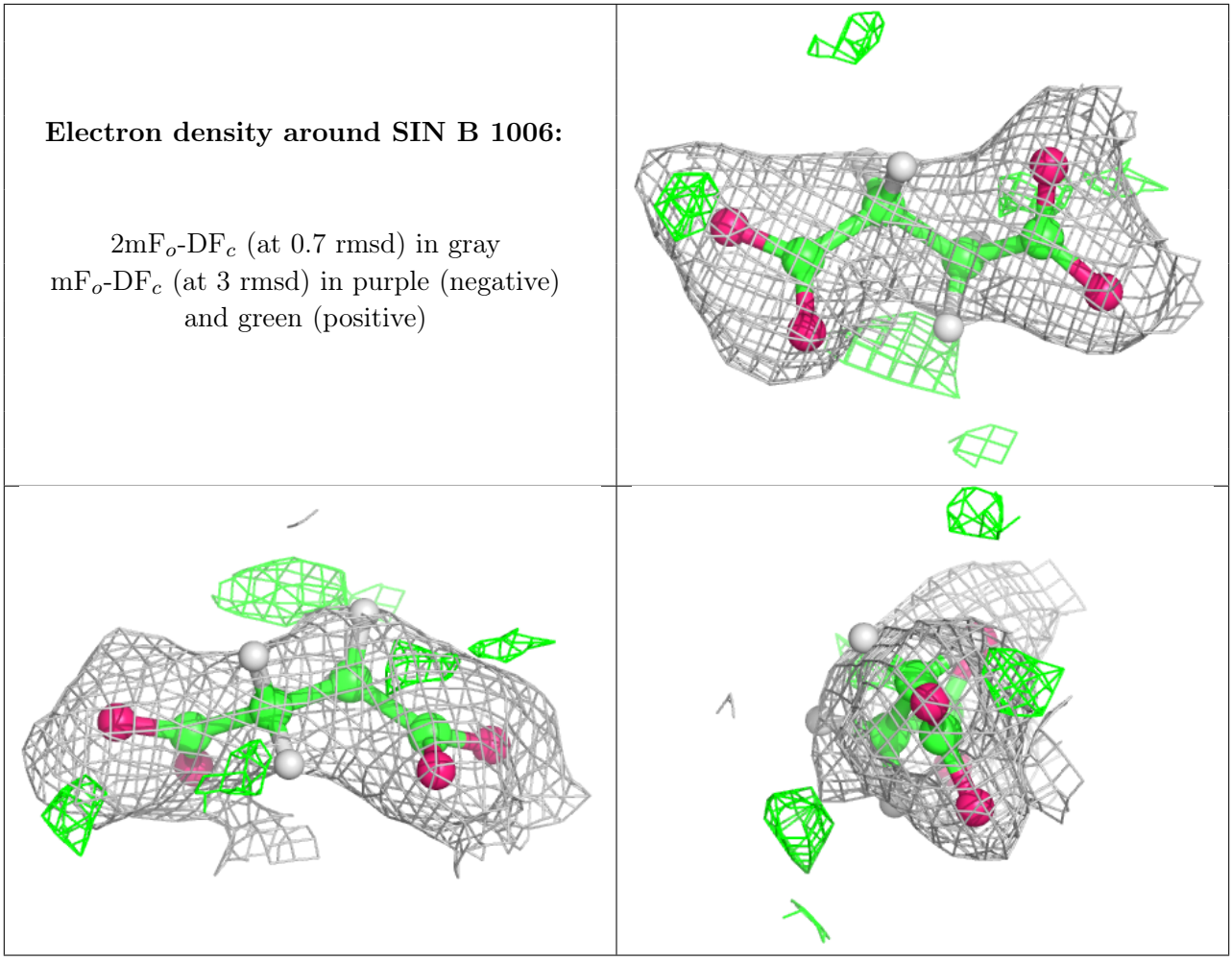






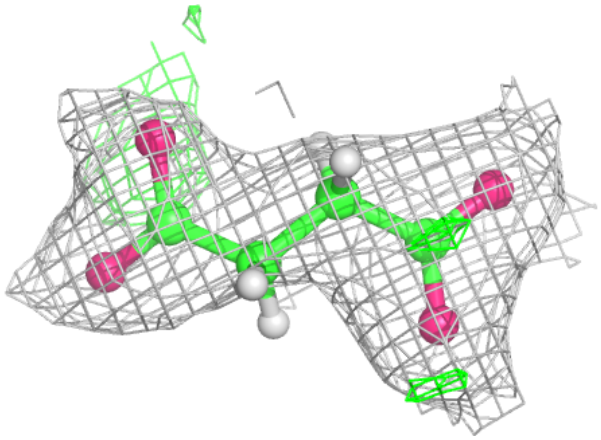
Electron density around SIN B 1006:

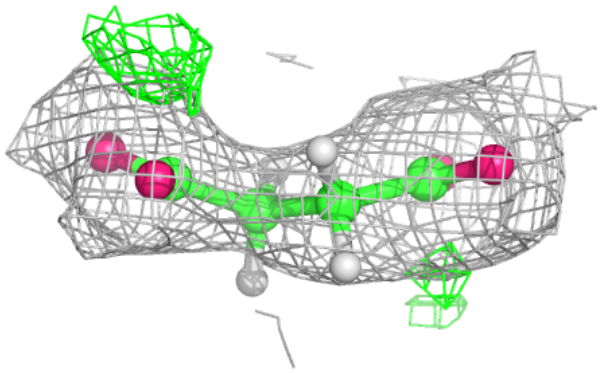
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

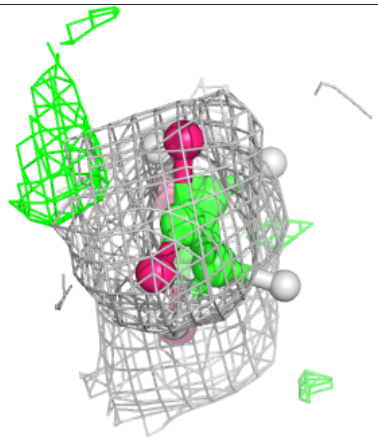


Electron density around SIN E 605:

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

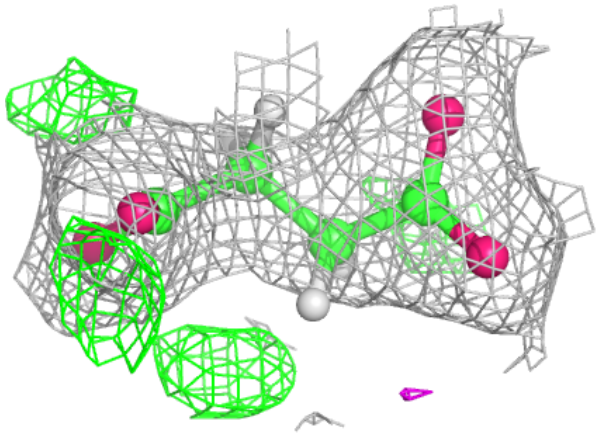


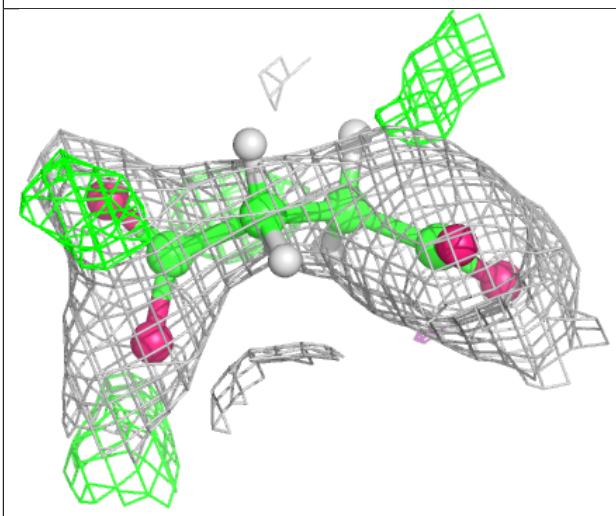


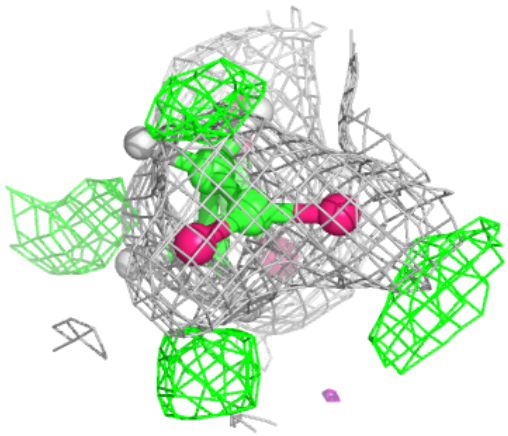


Electron density around SIN F 606:

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

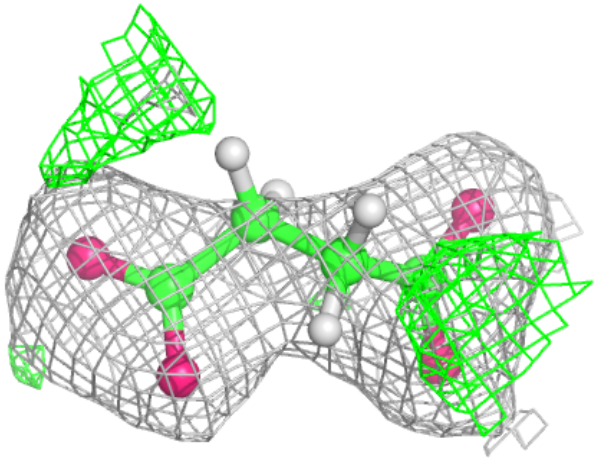


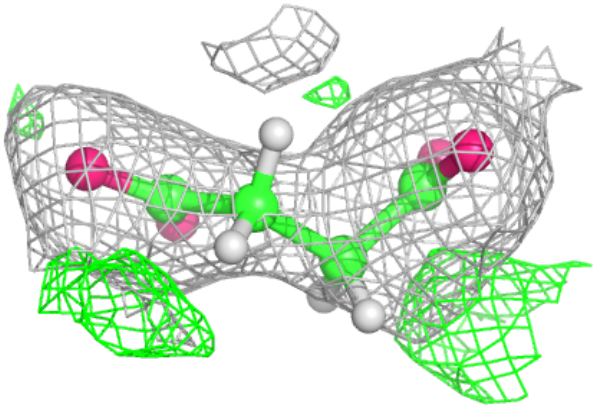


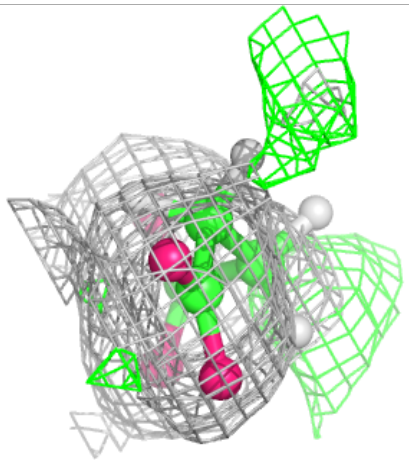


Electron density around SIN G 604:

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

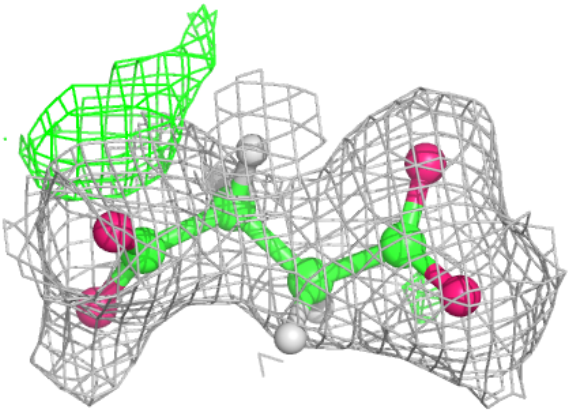


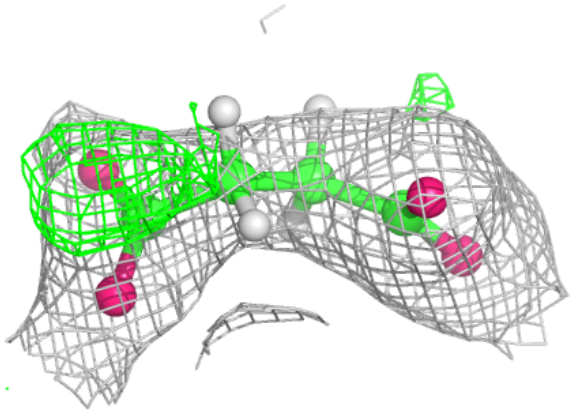


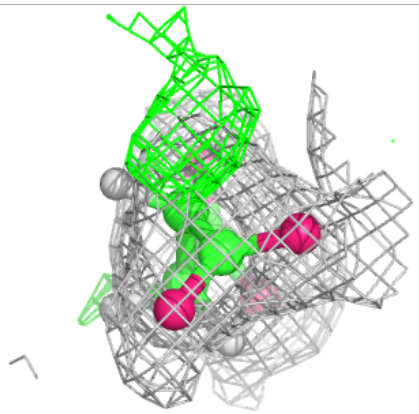


Electron density around SIN H 604:

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

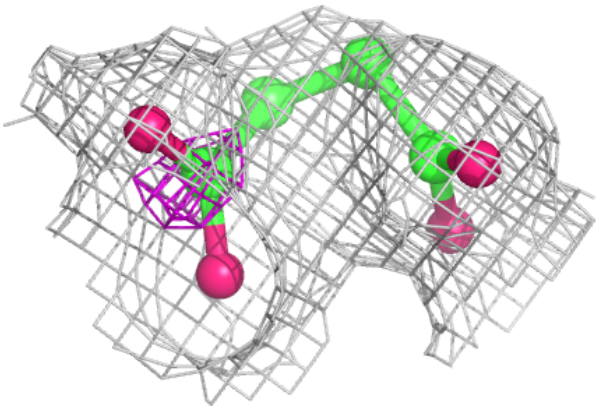


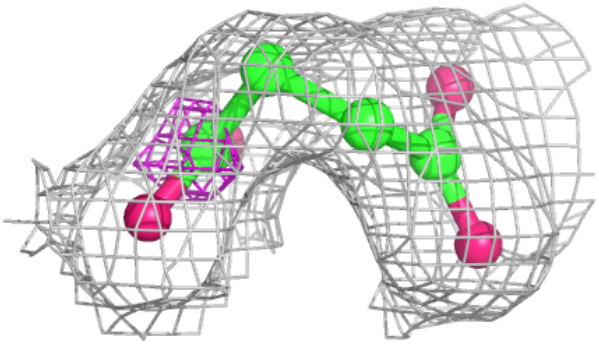


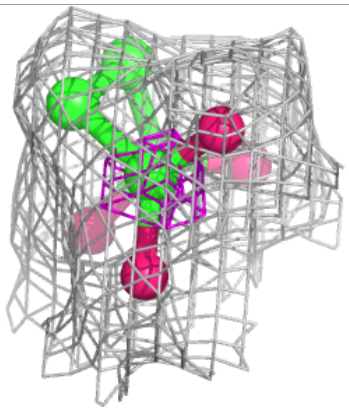


Electron density around SIN C 1002:

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

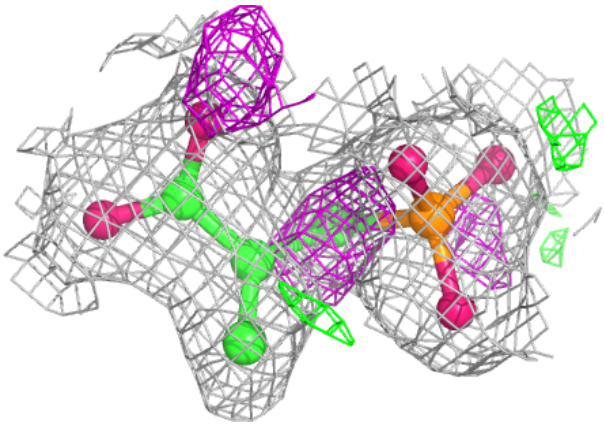


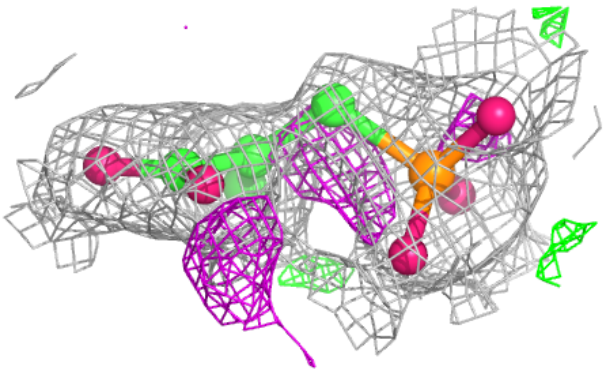


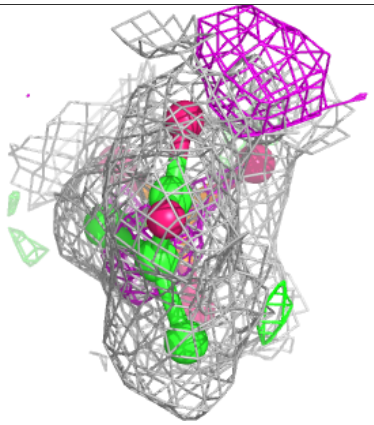


Electron density around GZ3 H 601:

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

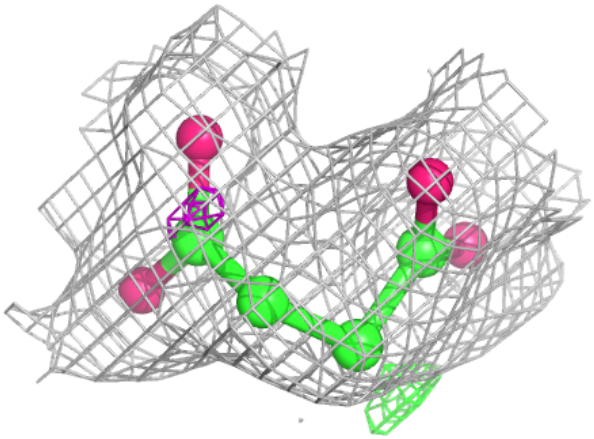


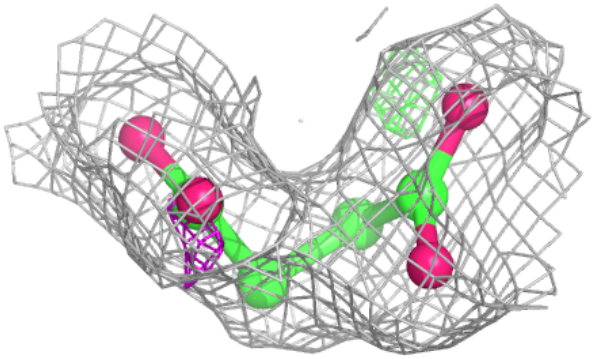


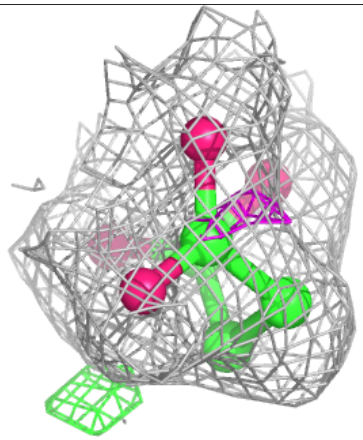


Electron density around SIN B 1002:

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

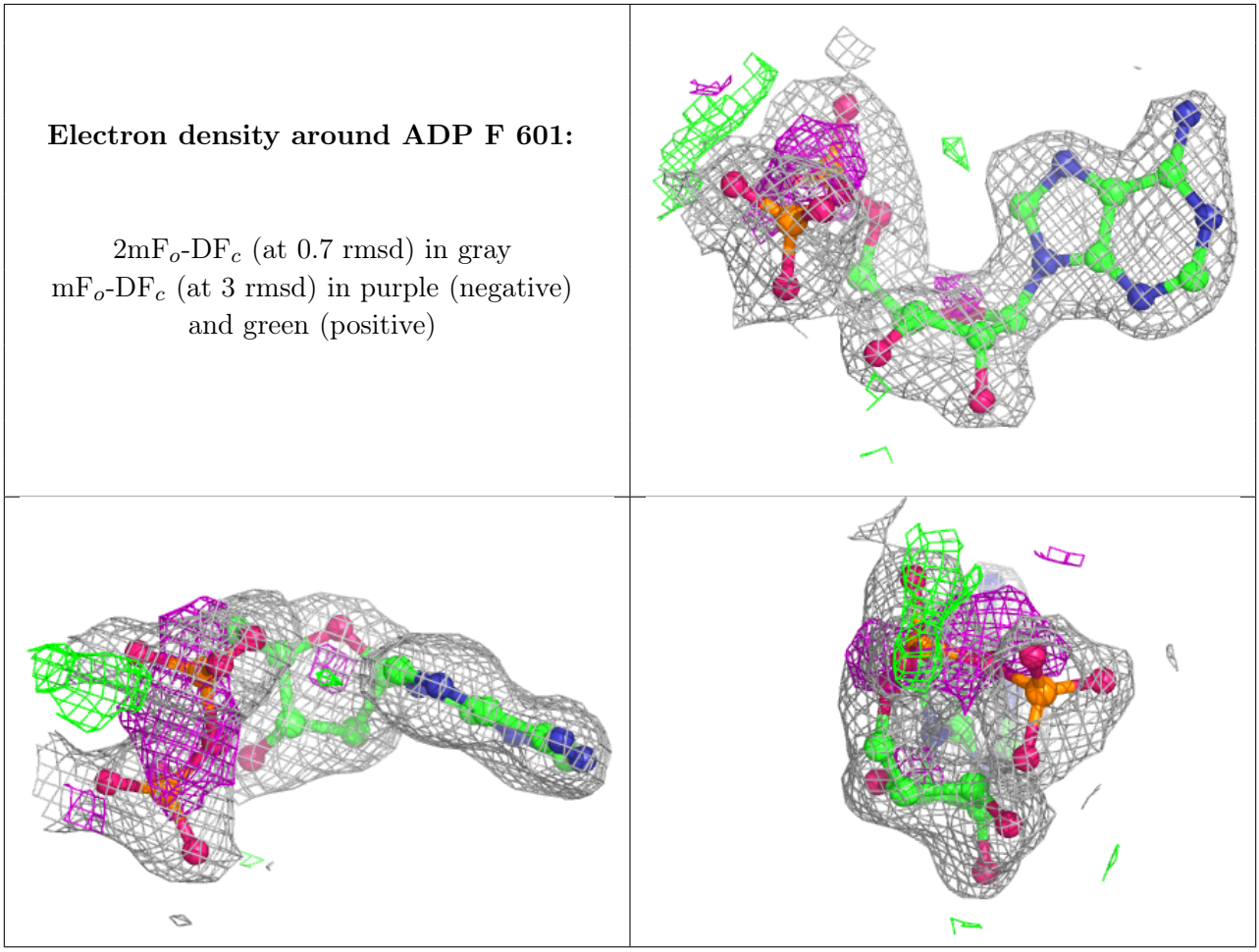






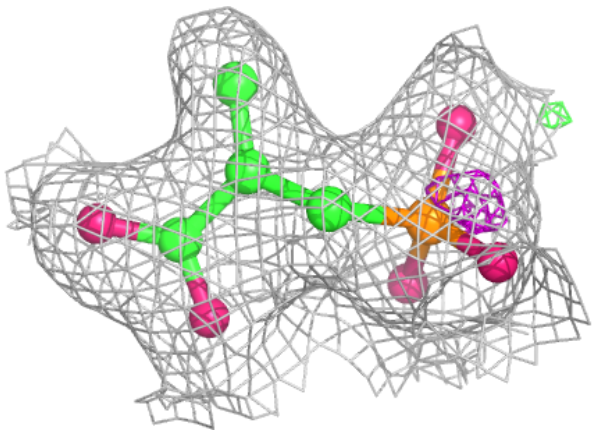
Electron density around ADP F 601:

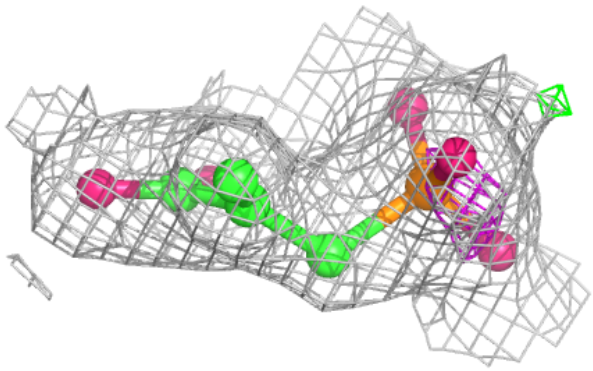
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

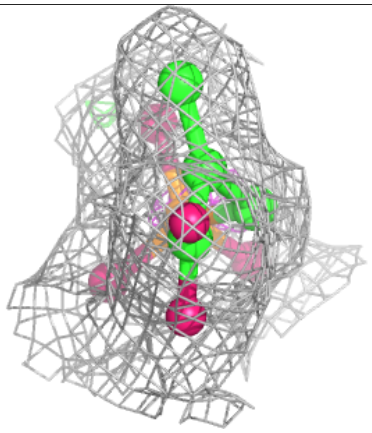


Electron density around GZ3 E 601:

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

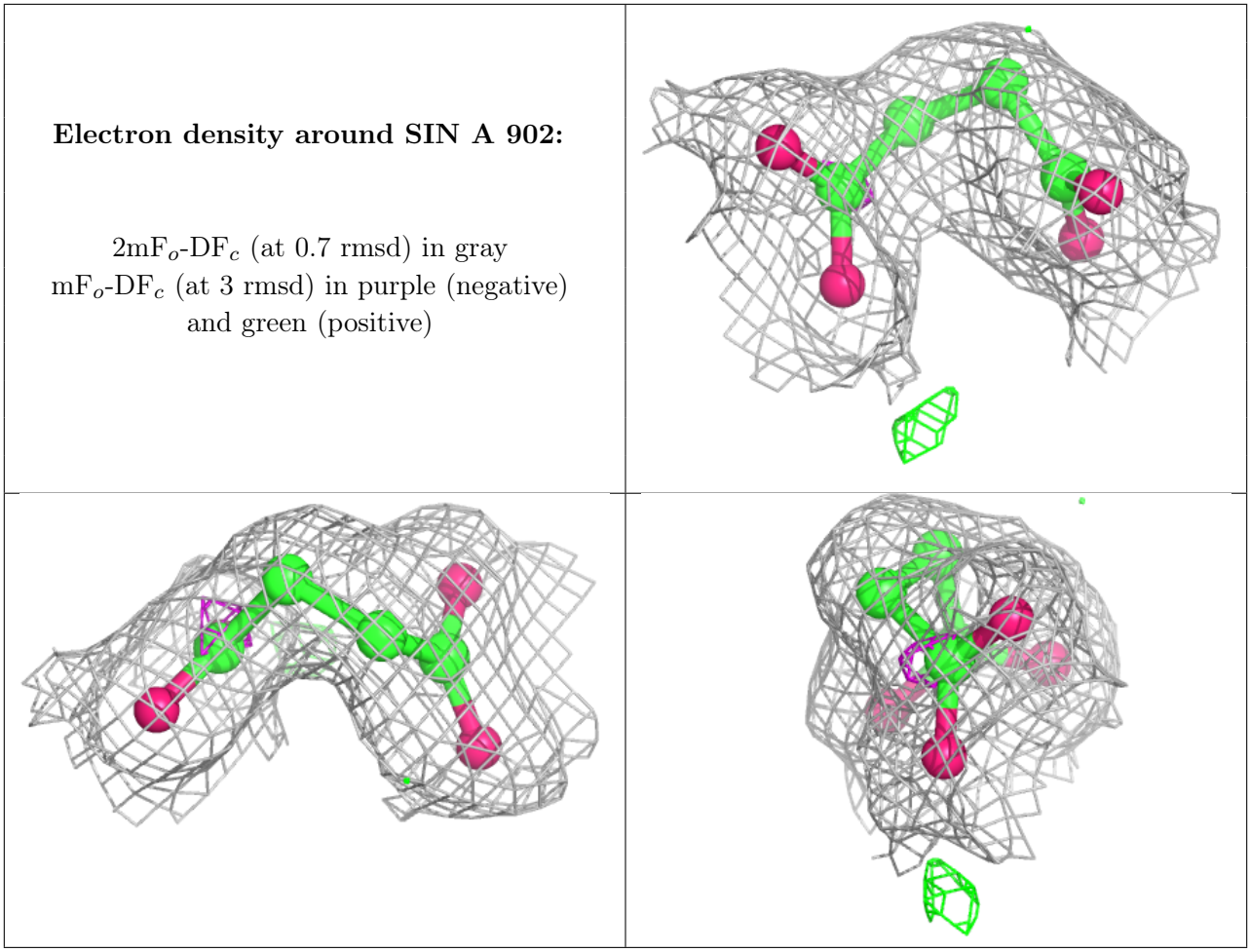






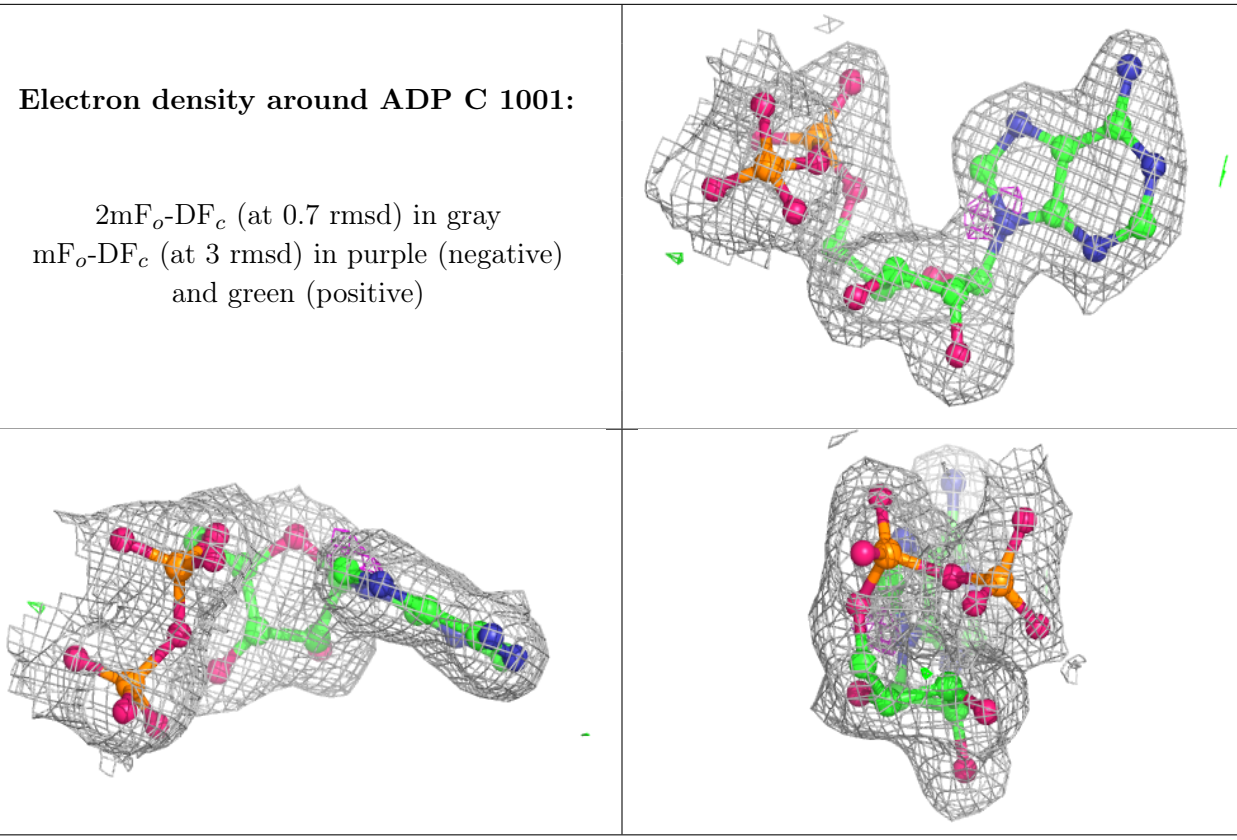
Electron density around SIN A 902:

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



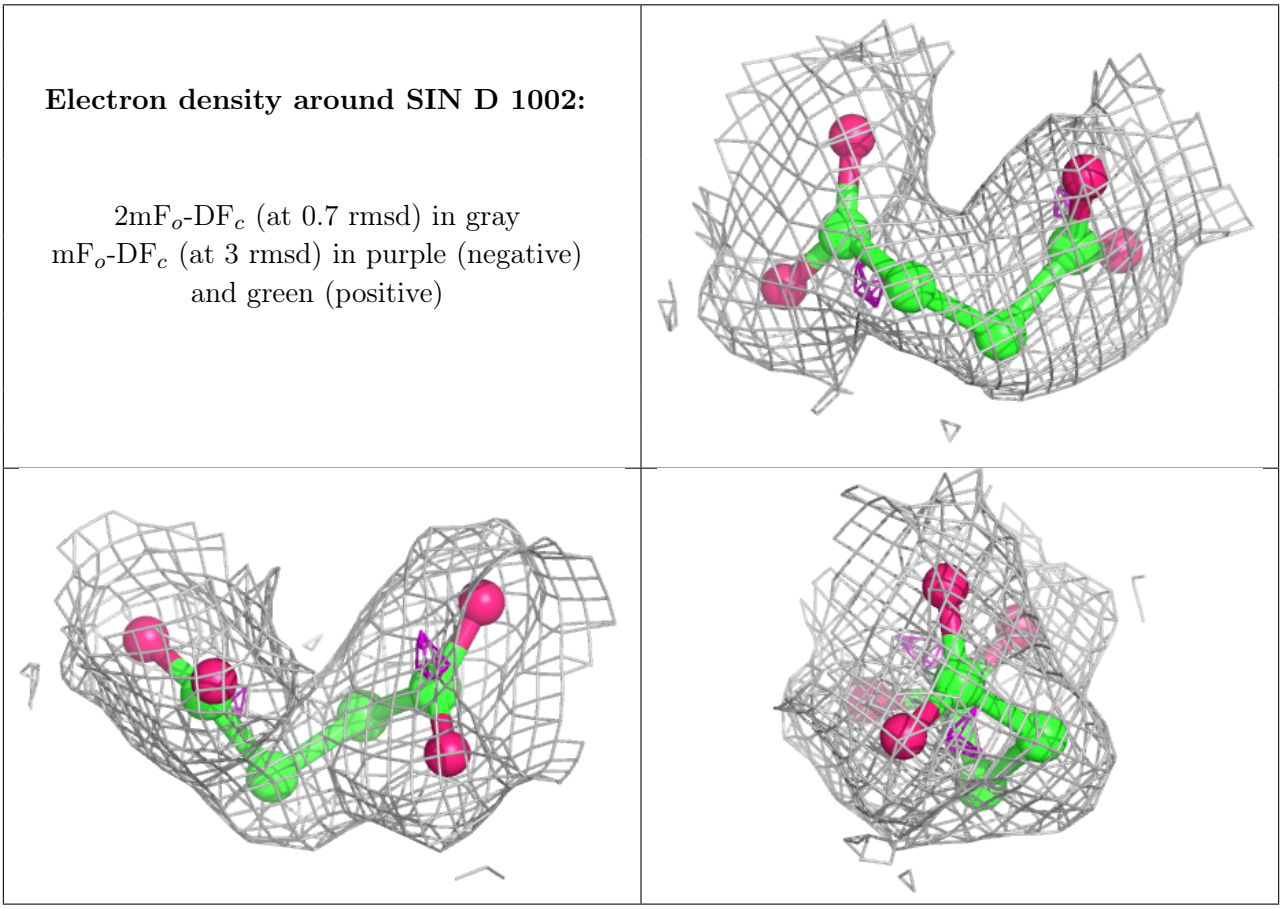
Electron density around ADP C 1001:

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



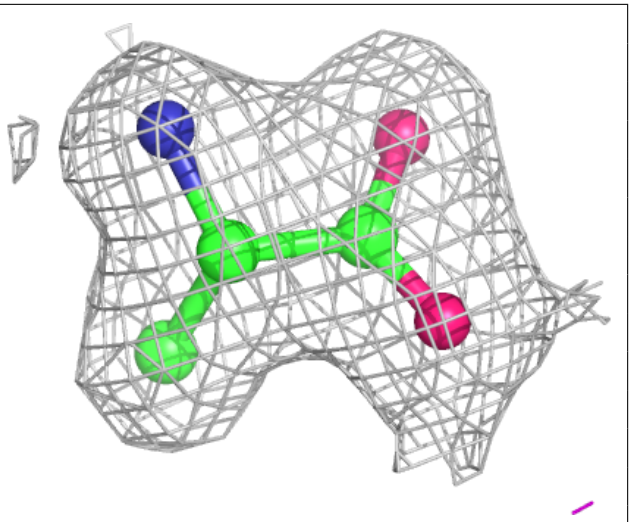
Electron density around SIN D 1002:

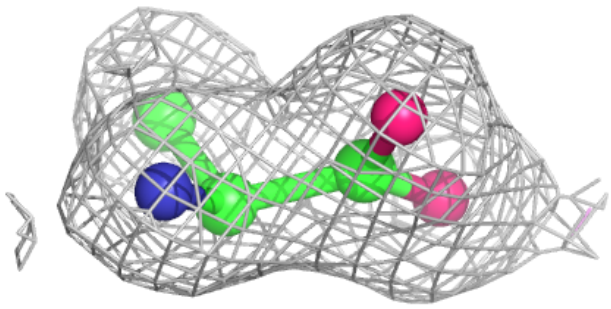
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

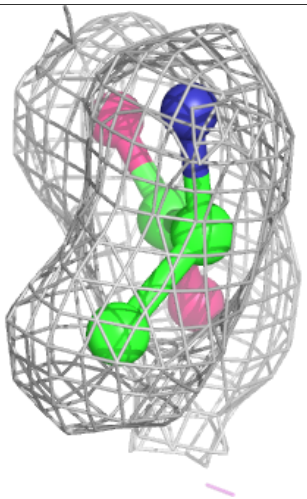


Electron density around ALA B 1007:

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

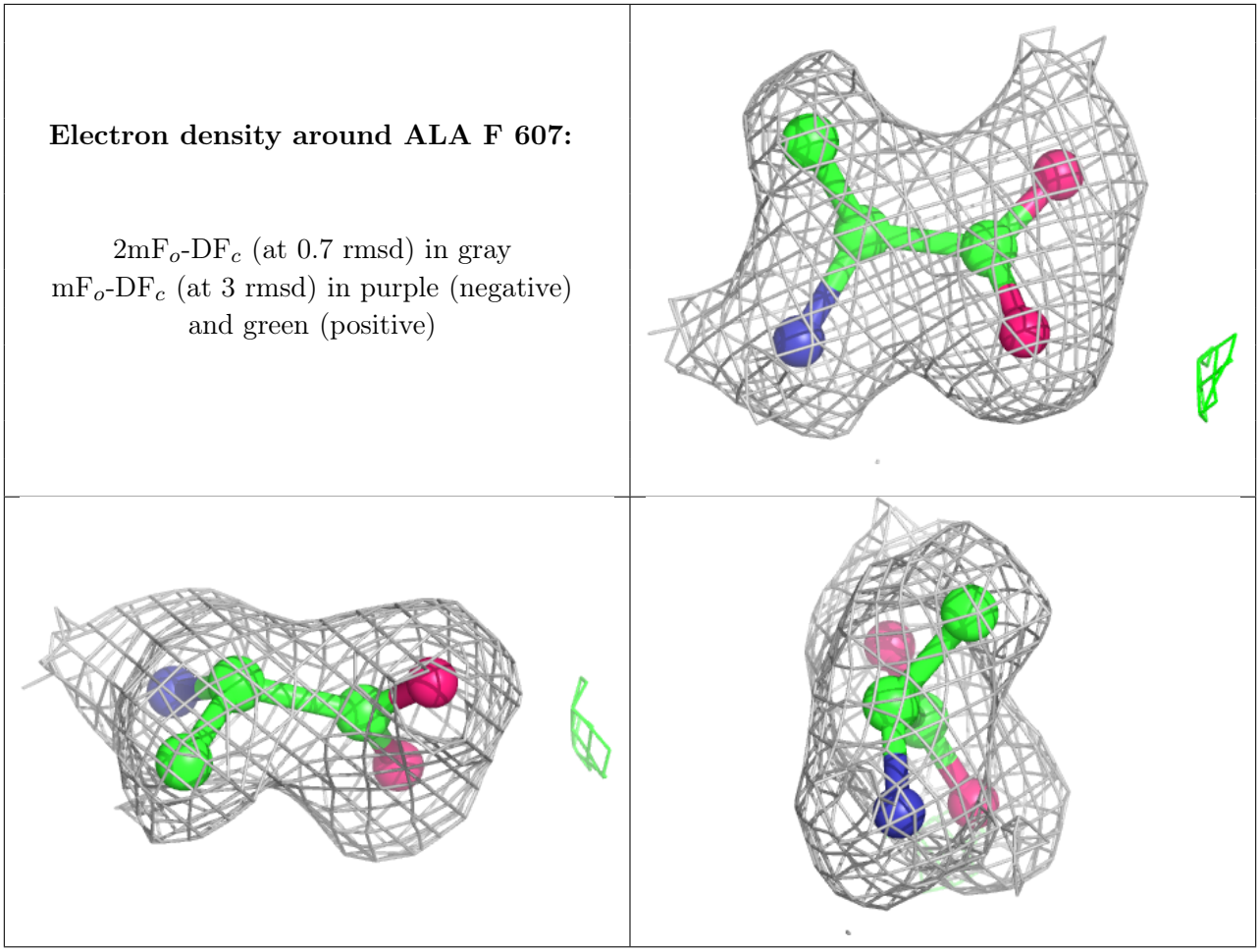






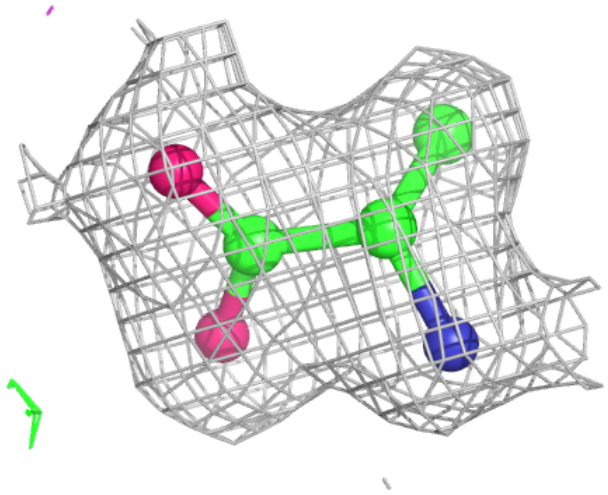
Electron density around ALA F 607:

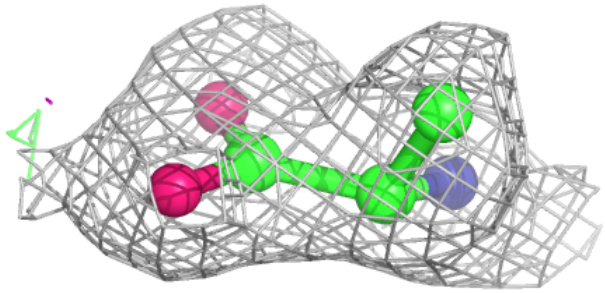
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

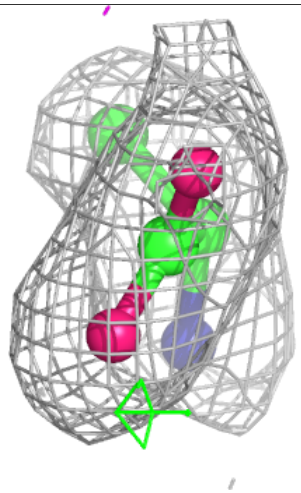


Electron density around ALA G 605:

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

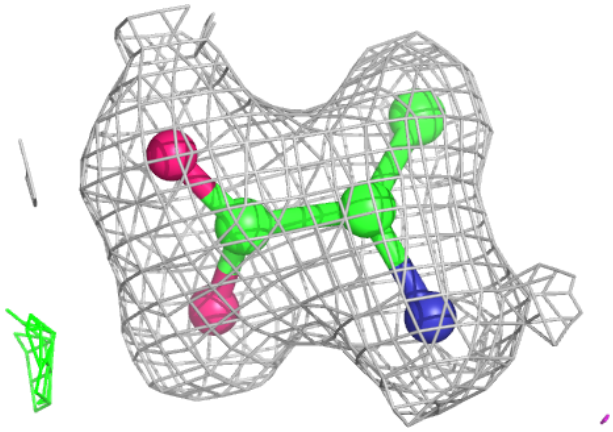


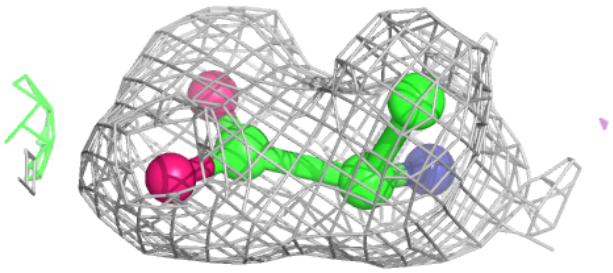


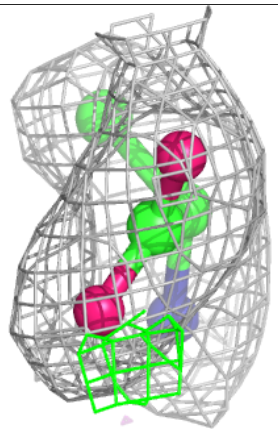


Electron density around ALA A 907:

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

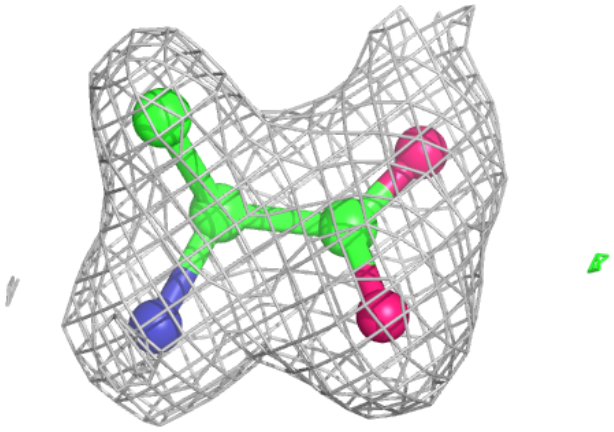


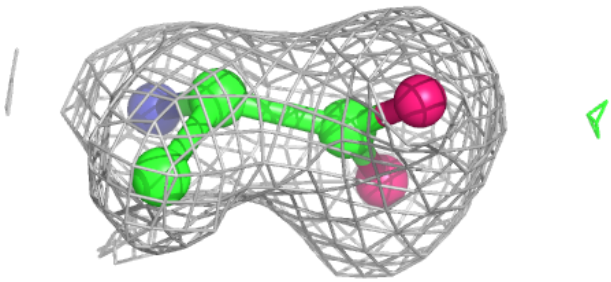


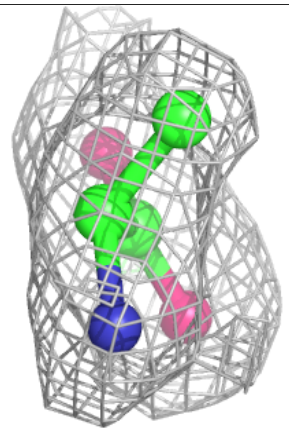


Electron density around ALA D 1007:

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

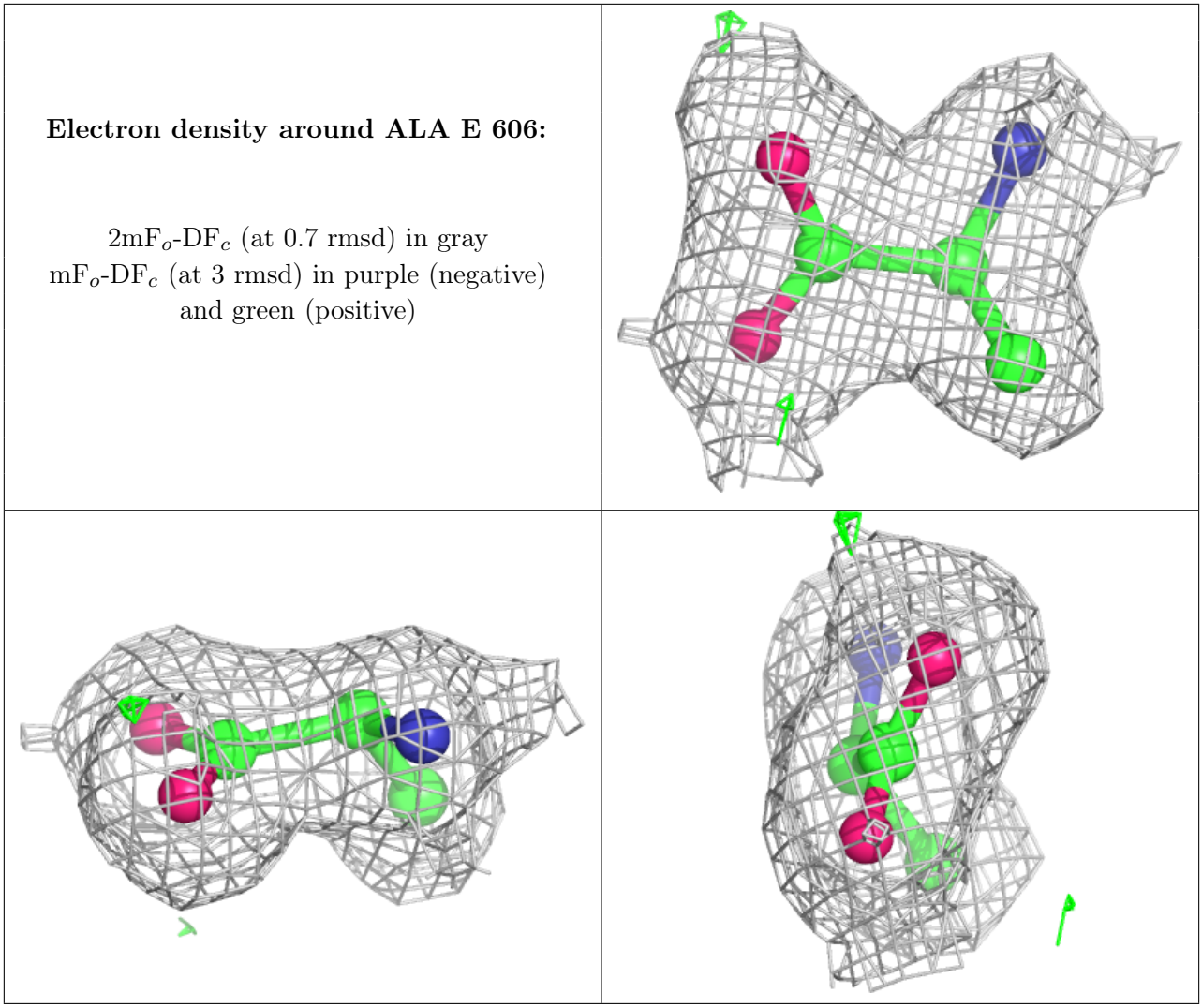






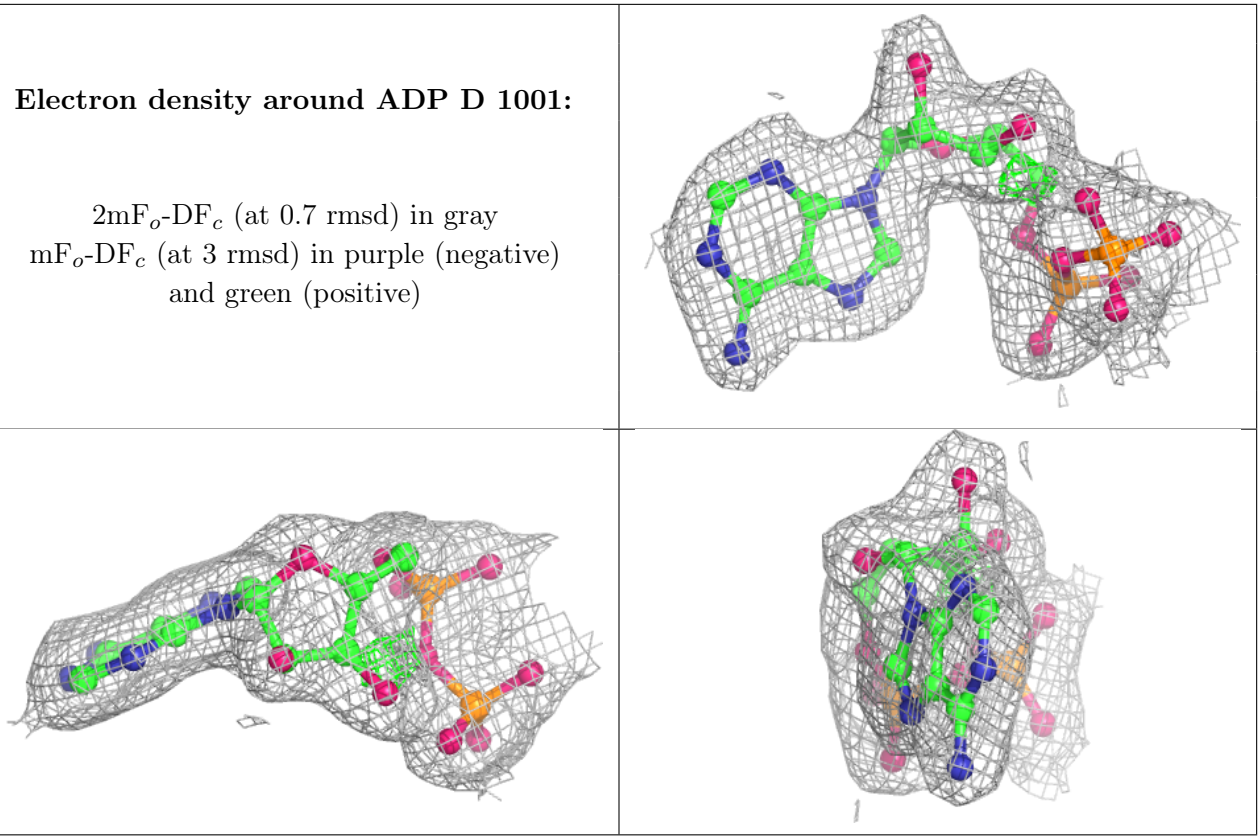
Electron density around ALA E 606:

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



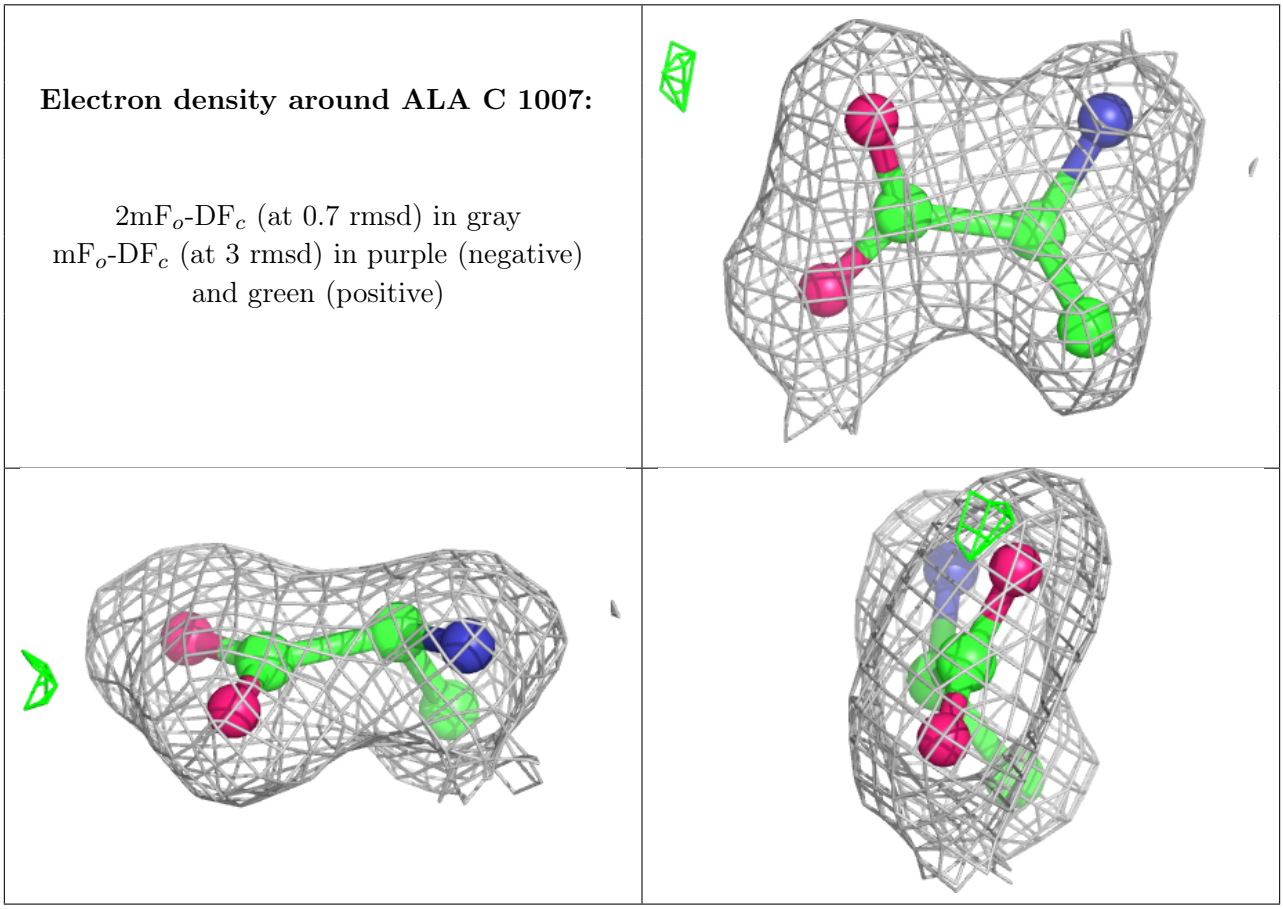
Electron density around ADP D 1001:

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



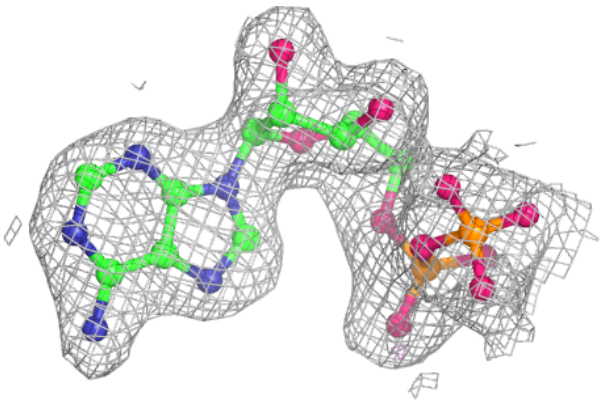
Electron density around ALA C 1007:

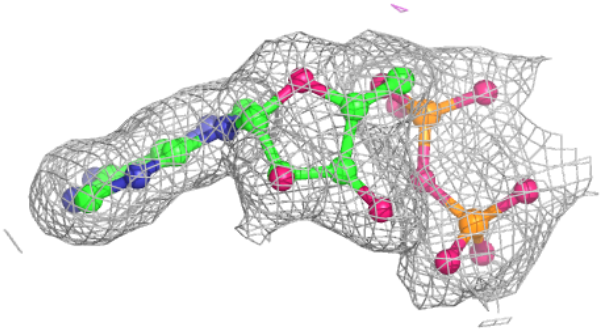
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

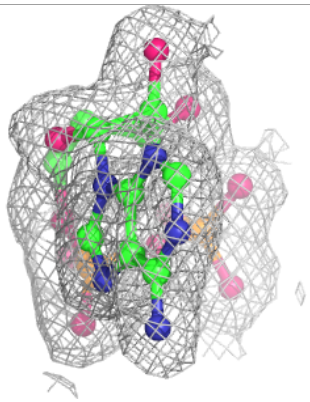


Electron density around ADP B 1001:

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

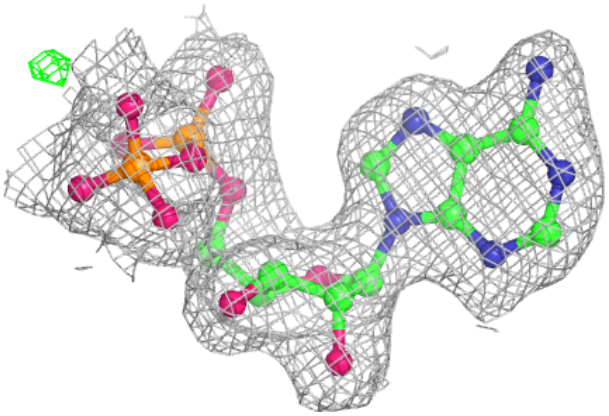


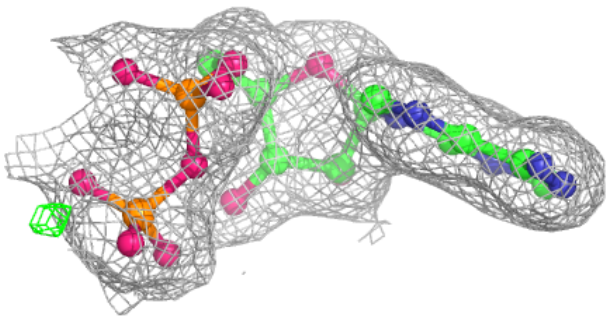


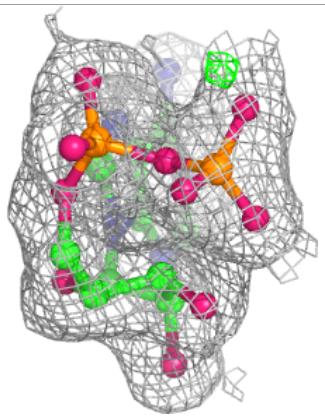


Electron density around ADP A 901:

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

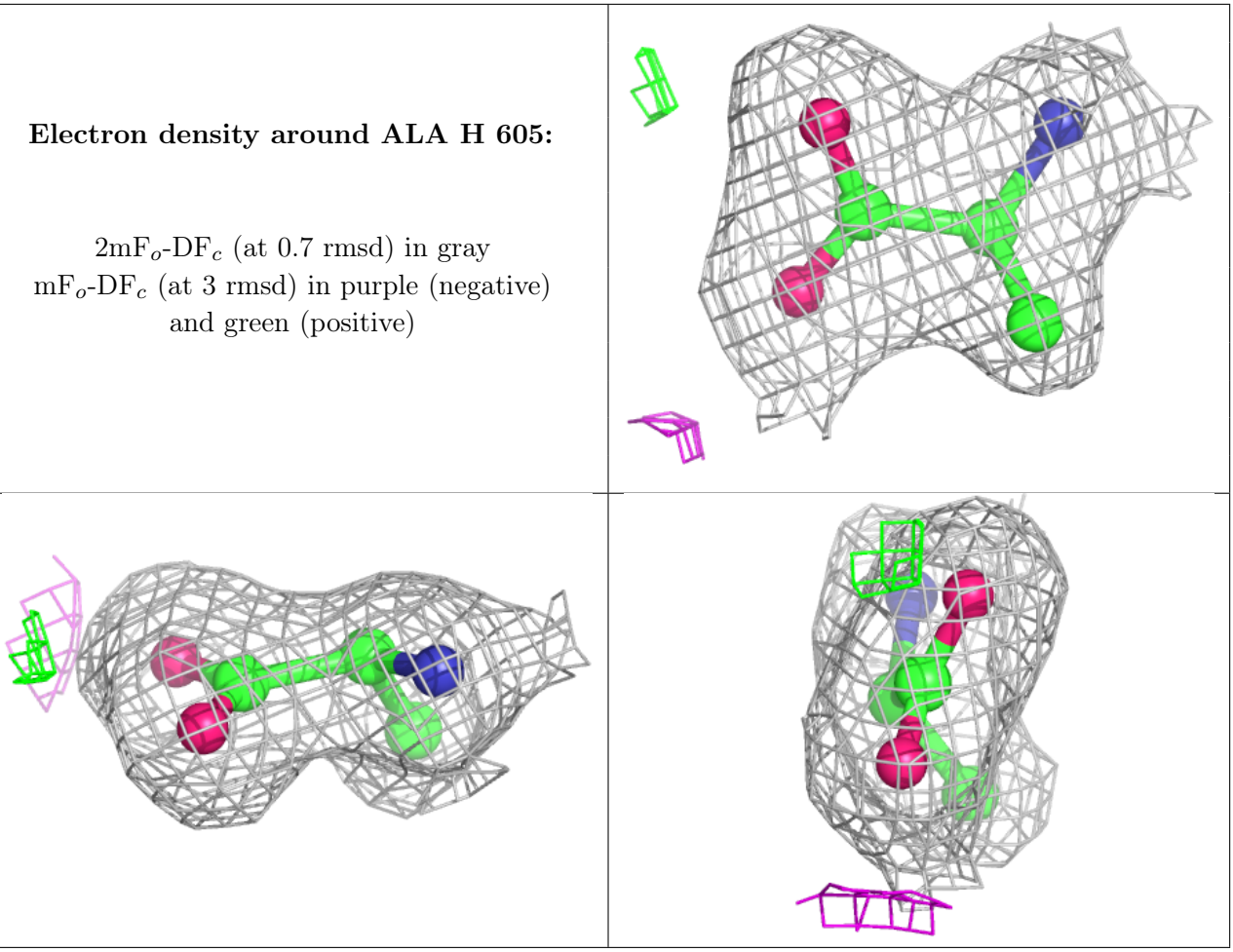






Electron density around ALA H 605:

$2mF_o$-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.